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Julien Sabin

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UNIVERSITÉ DE CERGY-PONTOISE

# Stabilité, dispersion et création de paires pour certains systèmes quantiques infinis

THÈSE DE DOCTORAT EN MATHÉMATIQUES

*présentée par*

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## Résumé

Cette thèse est consacrée à l'étude mathématique des propriétés de stabilité de systèmes quantiques infinis, décrits par des modèles non linéaires. Dans les chapitres 1 et 2, on étudie l'instabilité du vide relativiste menant au phénomène de création de paires électron-positron. Dans le chapitre 3, on considère la dynamique de ce même vide relativiste couplé à un champ scalaire. Les chapitres 4 et 5 sont consacrés au caractère dispersif de la dynamique non linéaire de Hartree pour des perturbations de la mer de Fermi, et en particulier à sa stabilité orbitale et asymptotique. Enfin, le chapitre 6 introduit une notion générale d'entropie relative entre deux états comportant une infinité de particules.

## Abstract

This thesis is devoted to the mathematical study of stability properties of infinite quantum systems described by nonlinear models. In chapters 1 and 2, we study the instability of the relativistic vacuum leading to the phenomenon of electron-positron pair production. In chapter 3, we consider the dynamics of this same relativistic vacuum coupled to a scalar field. Chapters 4 and 5 are devoted to the dispersive behaviour of the nonlinear Hartree dynamics for perturbations of the Fermi sea, and in particular to its orbital and asymptotic stability. Finally, chapter 6 introduces a general notion of relative entropy between states having infinitely many particles.



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# Introduction

Cette thèse a pour but l'étude de modèles non linéaires décrivant des systèmes quantiques avec un nombre infini de particules. Nous modélisons de tels systèmes par un opérateur borné  $\gamma$  de rang infini sur  $L^2(\mathbb{R}^d)$ . Nous utilisons des modèles relativistes, basés sur l'opérateur de Dirac dans  $\mathbb{R}^3$ , et non-relativistes, basés sur le Laplacien dans  $\mathbb{R}^d$ . Nous étudions la stabilité de certains états de référence  $\gamma_{\text{ref}}$ , à la fois d'un point de vue variationnel et d'un point de vue dynamique. Dans le cas des modèles relativistes, l'opérateur de référence est appelé *mer de Dirac*, alors que dans le cas non-relativiste il est appelé *mer de Fermi*. Les Chapitres 1 et 2 sont consacrés à l'étude variationnelle du phénomène de création de paires électron-positron en mécanique quantique relativiste, reflétant l'*instabilité* de la mer de Dirac. Le Chapitre 3 a pour objet la dynamique couplée de la mer de Dirac avec une équation des ondes, et à l'existence de solutions globales en temps pour ce système d'équations. Le Chapitre 4 traite de l'existence globale de solutions dans l'espace d'énergie pour la dynamique non linéaire de Hartree engendrée par une perturbation de la mer de Fermi, et le Chapitre 5 de la *dispersion* en temps long de ces perturbations, montrant ainsi la *stabilité* de la mer de Fermi. Enfin, le Chapitre 6 introduit une nouvelle notion d'entropie relative entre des opérateurs de rang infini.

Les techniques utilisées sont celles de l'analyse non linéaire des opérateurs de rang infini, comprenant entre autres des méthodes variationnelles, de la théorie spectrale, ainsi que des équations aux dérivées partielles d'évolution. Cette introduction a pour but d'expliquer les concepts physiques et les objets mathématiques mis en jeu, ainsi que de résumer les résultats obtenus dans la thèse.

## 1. Motivation physique et cadre mathématique

Afin d'expliquer le formalisme mathématique que nous utilisons pour modéliser un nombre infini de particules quantiques, décrivons d'abord la situation de systèmes finis. Une présentation plus détaillée peut être trouvée dans les livres de Lieb et Seiringer [LS10] ou de Cancès, Le Bris, et Maday [CLM06].

**1.1. Une particule.** Une particule quantique se déplaçant dans l'espace euclidien à  $d$  dimensions et possédant  $q$  degrés internes de liberté<sup>1</sup> est représentée par une

---

<sup>1</sup>Dans les Chapitres 1, 2 et 3, nous considérons le cas  $d = 3$ ,  $q = 4$ . À partir du Chapitre 4, nous traitons le cas d'une dimension  $d$  quelconque, avec  $q = 1$ .

fonction d'onde normalisée  $\Psi \in L^2(\mathbb{R}^d, \mathbb{C}^q) \simeq L^2(\mathbb{R}^d \times \{1, \dots, q\}, \mathbb{C})$ . La quantité

$$\rho_\Psi(x) := \sum_{\sigma=1}^q |\Psi(x, \sigma)|^2 \quad (1)$$

s'interprète alors comme la densité de probabilité de présence de la particule dans l'espace. Sa transformée de Fourier<sup>2</sup>  $\widehat{\Psi}$  est également normalisée dans  $L^2(\mathbb{R}^d, \mathbb{C}^q)$  et  $\sum_{\sigma=1}^q |\widehat{\Psi}(\cdot, \sigma)|^2$  représente la densité de moment cinétique. L'énergie d'une telle particule ainsi que son évolution temporelle sont décrites par le même objet appelé *Hamiltonien* du système quantique étudié. C'est un opérateur auto-adjoint  $H$  sur l'espace de Hilbert sous-jacent, ici  $L^2(\mathbb{R}^d, \mathbb{C}^q)$ . De manière générale, l'énergie  $\mathcal{E}(\Psi)$  de la particule dans l'état  $\Psi$  vaut

$$\mathcal{E}(\Psi) = \langle \Psi, H\Psi \rangle,$$

où  $\langle \cdot, \cdot \rangle$  désigne le produit scalaire dans  $L^2(\mathbb{R}^d, \mathbb{C}^q)$ . Si la particule se trouve dans l'état  $\Psi_0$  à un temps  $t_0 \in \mathbb{R}$ , alors l'état  $\Psi(t)$  de la particule en fonction du temps  $t \in \mathbb{R}$  est l'unique solution du problème de Cauchy

$$\begin{cases} i\partial_t \Psi = H\Psi, \\ \Psi|_{t=t_0} = \Psi_0, \end{cases}$$

qui n'est autre que

$$\Psi(t) = e^{-itH}\Psi_0, \quad \forall t \in \mathbb{R}.$$

Lorsque la particule subit l'influence d'un potentiel  $V$ , on peut décomposer le Hamiltonien selon

$$H = T + V(x), \quad (2)$$

où  $T$  est l'opérateur d'énergie cinétique. Ce dernier est un opérateur de multiplication en variables de Fourier, c'est-à-dire que pour tout  $f \in L^2(\mathbb{R}^d, \mathbb{C}^q)$  on a la relation

$$\widehat{Tf}(k, \sigma) = \sum_{\sigma'=1}^q T(k)_{\sigma\sigma'} \widehat{f}(k, \sigma'), \quad \forall (k, \sigma) \in \mathbb{R}^d \times \{1, \dots, q\}.$$

Cela signifie qu'on associe à chaque moment  $k \in \mathbb{R}^d$  un poids  $T(k)$  qui est une matrice hermitienne sur  $\mathbb{C}^q$ . En mécanique quantique non-relativiste et en absence de toute champ magnétique (cas des Chapitres 4 et 5), ce poids est identique au poids classique

$$T_{\text{nr}}(k) = \frac{|k|^2}{2m} \text{Id}_{\mathbb{C}^q},$$

---

<sup>2</sup>Notre convention sera toujours

$$\widehat{f}(k, \sigma) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} f(x, \sigma) e^{-ik \cdot x} dx, \quad \forall k \in \mathbb{R}^d,$$

pour toute fonction  $f \in L^1(\mathbb{R}^d, \mathbb{C}^q)$ , afin d'obtenir une isométrie sur  $L^2(\mathbb{R}^d, \mathbb{C}^q)$ .

où  $m$  désigne la masse de la particule considérée. En particulier, son action sur la fonction d'onde  $\Psi$  est donnée par le Laplacien,

$$T_{\text{nr}}\Psi = \frac{1}{2m}(-\Delta\Psi),$$

au sens des distributions. En mécanique quantique relativiste (cas des Chapitres 1 à 3), avec  $d = 3$  et  $q = 4$  on choisit plutôt l'opérateur de Dirac [**Tha92**],

$$T_{\text{r}}(k) = \begin{pmatrix} m & 0 & k_3 & k_1 - ik_2 \\ 0 & m & k_1 + ik_2 & -k_3 \\ k_3 & k_1 - ik_2 & -m & 0 \\ k_1 + ik_2 & -k_3 & 0 & -m \end{pmatrix}. \quad (3)$$

Dans la décomposition (2) de  $H$ , le potentiel  $V$  est quant à lui vu comme un opérateur de multiplication en variables d'espace : pour tout  $f \in L^2(\mathbb{R}^d, \mathbb{C}^q)$ , on a

$$(Vf)(x, \sigma) := \sum_{\sigma'=1}^q V(x)_{\sigma\sigma'} f(x, \sigma'), \quad \forall (x, \sigma) \in \mathbb{R}^d \times \{1, \dots, q\}.$$

Dans le cas particulier où  $V(x)_{\sigma\sigma'} = V(x)\delta(\sigma - \sigma')$ , remarquons que l'énergie potentielle du système dans l'état  $\Psi$  vaut

$$\langle \Psi, V\Psi \rangle = \sum_{\sigma=1}^q \int_{\mathbb{R}^d} V(x) |\Psi(x, \sigma)|^2 dx = \int_{\mathbb{R}^d} V(x) \rho_{\Psi}(x) dx,$$

où  $\rho_{\Psi}$  a été définie en (1). On constate alors qu'elle coïncide avec l'énergie d'interaction classique entre la densité de particules  $\rho_{\Psi}$  et le potentiel  $V$ . Remarquons enfin qu'à tout état  $\Psi$  on peut associer un opérateur de rang 1 sur  $L^2(\mathbb{R}^d, \mathbb{C}^q)$ , le projecteur orthogonal sur la droite engendrée par  $\Psi$ . En notation de Dirac, cet opérateur s'écrit

$$\gamma_{\Psi} := |\Psi\rangle\langle\Psi|.$$

Réciproquement, tout projecteur orthogonal de rang 1 sur  $L^2(\mathbb{R}^d, \mathbb{C}^q)$  peut s'écrire de cette manière. Il existe plusieurs avantages à écrire les états quantiques sous cette forme. Premièrement, remarquons que pour tout opérateur  $A$  sur  $L^2(\mathbb{R}^d, \mathbb{C}^q)$ , la quantité  $\langle \Psi, A\Psi \rangle$  est invariante si l'on change  $\Psi$  en  $e^{i\theta}\Psi$ , où  $e^{i\theta}$  est un facteur de phase quelconque. Cela signifie que les fonctions d'onde  $\Psi$  et  $e^{i\theta}\Psi$  représentent le même état quantique. L'opérateur  $\gamma_{\Psi}$  tient compte de cette invariance : on a bien sûr  $\gamma_{\Psi} = \gamma_{e^{i\theta}\Psi}$ . De plus, l'énergie de l'état  $\Psi$  peut s'écrire trivialement sous la forme

$$\mathcal{E}(\Psi) = \text{Tr}(H\gamma_{\Psi}),$$

où la trace est prise sur l'espace de Hilbert  $L^2(\mathbb{R}^d, \mathbb{C}^q)$ . L'évolution d'une fonction d'onde  $\Psi_0$  à partir d'un temps  $t_0$  est décrite de manière équivalente par la solution

du problème de Cauchy, appelé *équation de von Neumann*,

$$\begin{cases} i\partial_t \gamma = [H, \gamma], \\ \gamma|_{t=t_0} = |\Psi_0\rangle\langle\Psi_0|, \end{cases}$$

où  $[H, \gamma]$  désigne le commutateur entre  $H$  et  $\gamma$ . Enfin, le noyau intégral de l'opérateur  $\gamma_\Psi$ , défini par la relation

$$(\gamma_\Psi f)(x, \sigma) = \sum_{\sigma'=1}^q \int_{\mathbb{R}^d} \gamma_\Psi(x, y)_{\sigma\sigma'} f(y, \sigma') dy, \quad \forall (x, \sigma) \in \mathbb{R}^d \times \{1, \dots, q\},$$

pour tout  $f \in L^2(\mathbb{R}^d, \mathbb{C}^q)$ , est donné par la formule

$$\gamma_\Psi(x, y)_{\sigma\sigma'} = \Psi(x, \sigma) \overline{\Psi(y, \sigma')}, \quad \forall (x, y, \sigma, \sigma') \in \mathbb{R}^{2d} \times \{1, \dots, q\}^2.$$

En particulier, on constate que la densité  $\rho_\Psi$  définie par (1) peut s'exprimer comme

$$\rho_\Psi(x) = \text{Tr}_{\mathbb{C}^q} \gamma_\Psi(x, x), \quad \forall x \in \mathbb{R}^d,$$

ce qui permet d'écrire l'énergie d'un projecteur orthogonal  $\gamma$  de rang 1 quelconque

$$\mathcal{E}(\gamma) = \text{Tr}(T\gamma) + \int_{\mathbb{R}^d} V(x) \rho_\gamma(x) dx,$$

où  $\rho_\gamma(x) = \text{Tr}_{\mathbb{C}^q} \gamma(x, x)$ . Cette formulation de l'énergie se révélera utile par la suite.

**1.2. Plusieurs particules.** Un système de  $N$  particules quantiques identiques est également décrit par une fonction d'onde normalisée  $\Psi$ , mais qui appartient cette fois-ci à l'espace

$$L^2(\mathbb{R}^d, \mathbb{C}^q)^{\otimes N} \simeq L^2((\mathbb{R}^d)^N, (\mathbb{C}^q)^{\otimes N}) \simeq L^2((\mathbb{R}^d \times \{1, \dots, q\})^N, \mathbb{C}).$$

Si ces  $N$  particules quantiques sont de plus indiscernables (ce que nous allons supposer à partir de maintenant, afin de simplifier certaines définitions), alors leur fonction d'onde doit satisfaire une hypothèse de symétrie supplémentaire correspondant à différents types de particules. La statistique de Fermi s'applique aux particules appelées fermions, et impose que pour toute permutation  $\tau$  de l'ensemble  $\{1, \dots, N\}$ , on doit avoir la relation

$$\Psi\left((x_{\tau(1)}, \sigma_{\tau(1)}), \dots, (x_{\tau(N)}, \sigma_{\tau(N)})\right) = \varepsilon(\tau) \Psi\left((x_1, \sigma_1), \dots, (x_N, \sigma_N)\right),$$

où  $\varepsilon(\tau)$  désigne la signature de la permutation  $\tau$ . L'autre statistique qui nous intéresse est la statistique de Bose, s'appliquant aux bosons, et qui est définie par la relation

$$\Psi\left((x_{\tau(1)}, \sigma_{\tau(1)}), \dots, (x_{\tau(N)}, \sigma_{\tau(N)})\right) = \Psi\left((x_1, \sigma_1), \dots, (x_N, \sigma_N)\right).$$

De manière générale, ces relations signifient que la densité  $|\Psi|^2$  est invariante si l'on permute l'indexation des particules. D'autres statistiques existent en dimension  $d = 2$ ,

mais nous ne les aborderons pas. La densité associée aux fonctions d'onde pour des particules indiscernables est définie par

$$\rho_{\Psi}(x) = N \sum_{\sigma_1, \dots, \sigma_N=1}^q \int_{(\mathbb{R}^d)^{N-1}} \left| \Psi\left((x, \sigma_1), (x_2, \sigma_2), \dots, (x_N, \sigma_N)\right) \right|^2 dx_2 \cdots dx_N,$$

pour tout  $x \in \mathbb{R}^d$ . Elle vérifie  $\int_{\mathbb{R}^d} \rho_{\Psi}(x) dx = N$  et représente la densité spatiale de particules. De la même manière qu'avec une seule particule, on peut définir à partir de  $\Psi$  un opérateur  $\gamma_{\Psi}^{(1)}$  sur  $L^2(\mathbb{R}^d, \mathbb{C}^q)$  par son noyau :

$$\begin{aligned} \gamma_{\Psi}^{(1)}(x, y)_{\sigma\sigma'} &= N \sum_{\sigma_2, \dots, \sigma_N=1}^q \int_{(\mathbb{R}^d)^{N-1}} \Psi\left((x, \sigma), (x_2, \sigma_2), \dots, (x_N, \sigma_N)\right) \times \\ &\quad \times \overline{\Psi\left((y, \sigma'), (x_2, \sigma_2), \dots, (x_N, \sigma_N)\right)} dx_2 \cdots dx_N. \end{aligned}$$

L'opérateur  $\gamma_{\Psi}^{(1)}$  est auto-adjoint sur  $L^2(\mathbb{R}^d, \mathbb{C}^q)$ , positif, à trace, et vérifie  $\text{Tr} \gamma_{\Psi}^{(1)} = N$ . Dans le cas fermionique, on a de plus  $\gamma_{\Psi}^{(1)} \leq 1$ , qui n'est autre que le principe de Pauli : deux fermions ne peuvent occuper le même état quantique. On a toujours la relation

$$\rho_{\Psi}(x) = \text{Tr}_{\mathbb{C}^q} \gamma_{\Psi}^{(1)}(x, x), \quad \forall x \in \mathbb{R}^d.$$

Nous avons ajouté un exposant dans la notation  $\gamma_{\Psi}^{(1)}$  par rapport à la notation  $\gamma_{\Psi}$  introduite pour une particule, car dans le cas de  $N$  particules, on peut définir de manière analogue  $N$  opérateurs indexés par  $k \in \{1, \dots, N\}$ , appelés *matrices densités à  $k$  corps*, agissant sur  $L^2(\mathbb{R}^d, \mathbb{C}^q)^{\otimes k}$ . Par exemple, définissons la matrice densité à deux corps  $\gamma_{\Psi}^{(2)}$ , par son noyau intégral

$$\begin{aligned} \gamma_{\Psi}^{(2)}(x_1, \sigma_1, x_2, \sigma_2; y_1, \sigma'_1, y_2, \sigma'_2) &:= \frac{N(N-1)}{2} \sum_{\sigma_3, \dots, \sigma_N=1}^q \int_{(\mathbb{R}^d)^{N-2}} \times \\ &\quad \times \Psi\left((x_1, \sigma_1), (x_2, \sigma_2), (x_3, \sigma_3), \dots, (x_N, \sigma_N)\right) \times \\ &\quad \times \overline{\Psi\left((y_1, \sigma'_1), (y_2, \sigma'_2), (x_3, \sigma_3), \dots, (x_N, \sigma_N)\right)} dx_3 \cdots dx_N. \end{aligned}$$

Notons que la matrice densité à  $k$  corps peut se déduire de la matrice densité à  $k+1$  corps en prenant une trace partielle. La matrice densité à  $N$  corps associée à  $\Psi$  n'est autre que le projecteur orthogonal de rang 1 sur  $L^2(\mathbb{R}^d, \mathbb{C}^q)^{\otimes N}$ ,

$$\gamma_{\Psi}^{(N)} := |\Psi\rangle\langle\Psi|,$$

de telle sorte qu'un état quantique est uniquement déterminé par l'ensemble de ses matrices densités à  $k$  corps. Nous verrons que ces opérateurs sont particulièrement utiles pour écrire l'énergie d'un système à  $N$  particules.

En plus des termes d'énergie cinétique et d'énergie potentielle liés à l'influence du potentiel  $V$  sur chacune des particules, le Hamiltonien  $H$  du système peut décrire les

interactions entre les particules du système, à travers un potentiel d'interaction  $W$ . Supposons pour simplifier que celui-ci ne dépend pas des degrés internes de libertés des particules, qu'il ne modélise que l'interaction entre deux particules, et enfin que cette interaction ne dépend que de la position relative de ces deux particules. On peut alors écrire le Hamiltonien  $H_N$  du système à  $N$  particules comme

$$H_N = \sum_{j=1}^N (T_j + V(x_j)) + \sum_{1 \leq k < \ell \leq N} W(x_k - x_\ell).$$

Ici la notation  $T_j + V(x_j)$  indique que l'on fait agir l'opérateur à un corps  $T + V$  uniquement sur la variable  $x_j$ , et  $\sum_{1 \leq k < \ell \leq N} W(x_k - x_\ell)$  est un opérateur de multiplication sur  $L^2(\mathbb{R}^d, \mathbb{C}^q)^{\otimes N}$ , où  $W : \mathbb{R}^d \rightarrow \mathbb{R}$  est une fonction paire fixe. Notons que l'opérateur  $H_N$  stabilise le sous-espace des fonctions d'onde fermioniques et bosoniques. En utilisant le formalisme des matrices densités, on peut écrire l'énergie de l'état  $\Psi$  comme

$$\langle \Psi, H_N \Psi \rangle = \text{Tr}_{L^2} \left( (T + V) \gamma_\Psi^{(1)} \right) + \text{Tr}_{L^2 \otimes L^2} \left( W \gamma_\Psi^{(2)} \right).$$

L'avantage de cette formulation est que le nombre  $N$  de particules apparaît uniquement à travers  $\gamma_\Psi^{(1)}$  et  $\gamma_\Psi^{(2)}$ , et ainsi est plus adaptée pour traiter le cas  $N = +\infty$ . Nous introduisons maintenant une classe d'états qui sont décrits uniquement par leur matrice densité à un corps  $\gamma_\Psi^{(1)}$ .

**1.3. Approximation de Hartree-Fock.** Il existe un exemple très simple de fonction d'onde fermionique à  $N$  corps qui est uniquement déterminée par sa matrice densité à un corps. Si  $(\varphi_j)_{1 \leq j \leq N}$  est une famille orthonormée dans  $L^2(\mathbb{R}^d, \mathbb{C}^q)$ , alors

$$\begin{aligned} \Psi \left( (x_1, \sigma_1), \dots, (x_N, \sigma_N) \right) &:= \frac{1}{\sqrt{N!}} \det(\varphi_j(x_i, \sigma_i))_{1 \leq i, j \leq N} \\ &=: \varphi_1 \wedge \dots \wedge \varphi_N(x_1, \sigma_1, \dots, x_N, \sigma_N) \end{aligned}$$

définit une fonction d'onde fermionique à  $N$  corps. Un tel état est appelé état de Hartree-Fock (ou déterminant de Slater), et représente des fermions dont les fonctions d'onde sont respectivement  $\varphi_1, \dots, \varphi_N$ . Sa matrice densité à un corps vaut

$$\gamma_\Psi^{(1)} = \sum_{j=1}^N |\varphi_j\rangle \langle \varphi_j|,$$

et est donc un projecteur orthogonal de rang  $N$ . Comme tout projecteur orthogonal de rang  $N$  fournit une telle famille  $(\varphi_j)_{1 \leq j \leq N}$  comme base orthonormée de son image, on en déduit qu'il existe une correspondance bijective explicite entre les déterminants de Slater et les projecteurs orthogonaux de rang  $N$  sur  $L^2(\mathbb{R}^d, \mathbb{C}^q)$ . Autrement dit, ces états quantiques particuliers sont uniquement déterminés par leurs matrices densités

à un corps  $\gamma_\Psi^{(1)}$ , et on peut écrire explicitement leur énergie en fonction de  $\gamma_\Psi^{(1)}$ . Un calcul montre que

$$\begin{aligned} \langle \Psi, H_N \Psi \rangle &=: \mathcal{E}_{\text{HF}}^V \left( \gamma_\Psi^{(1)} \right) \\ &= \text{Tr} \left( (T + V) \gamma_\Psi^{(1)} \right) + \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} W(x - y) \left[ \rho_\Psi(x) \rho_\Psi(y) - |\gamma_\Psi^{(1)}(x, y)|^2 \right] dx dy, \end{aligned}$$

où  $\mathcal{E}_{\text{HF}}^V$  désigne la fonctionnelle de Hartree-Fock. Le terme de l'énergie faisant intervenir  $\rho_\Psi(x) \rho_\Psi(y)$  est appelé *terme direct*, et celui faisant intervenir  $|\gamma(x, y)|^2$  *terme d'échange*. Lorsque le terme d'échange est négligé, on parle de l'énergie de Hartree-Fock *réduite*, définie par

$$\mathcal{E}_{\text{rHF}}^V \left( \gamma_\Psi^{(1)} \right) = \text{Tr} \left( (T + V) \gamma_\Psi^{(1)} \right) + \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} W(x - y) \rho_\Psi(x) \rho_\Psi(y) dx dy.$$

On voit donc qu'il existe une notion d'état quantique et d'énergie associés à tout projecteur orthogonal  $\gamma$  de rang  $N$  sur l'espace à un corps  $L^2(\mathbb{R}^d, \mathbb{C}^q)$ . Cette énergie est d'ailleurs *non linéaire* en la variable  $\gamma_\Psi^{(1)}$ , contrairement au cas où la variable est une fonction d'onde pour lequel l'énergie est linéaire en  $|\Psi\rangle\langle\Psi|$ . Cette restriction aux projecteurs orthogonaux de rang  $N$  a donc l'avantage de fournir un formalisme où la contrainte du nombre de particules est très simple, le prix à payer étant que la variable n'est plus une fonction d'onde mais un opérateur, et que l'énergie n'est plus linéaire. L'approximation de Hartree-Fock pour les systèmes à  $N$  corps a été le sujet de beaucoup de travaux mathématiques, par exemple les articles pionniers de Lieb et Simon [LS77a] ou de Bach [Bac92].

**1.4. Systèmes quantiques infinis.** Formellement, un état quantique avec une infinité de particules devrait être représenté par une fonction d'onde dépendant d'une "infinité de variables". De manière équivalente, il pourrait être décrit par une hiérarchie infinie de matrices densité à  $k$  corps, ce qui est plus adéquat pour écrire son énergie comme nous venons de le voir. Cependant, cette hiérarchie serait composée d'une infinité d'opérateurs agissant tous sur des espaces différents, et serait ainsi peu aisée à manipuler. Nous nous restreignons donc aux états de Hartree-Fock, qui sont uniquement déterminés par le premier élément de cette hiérarchie : leur matrice densité à un corps qui est un projecteur orthogonal, de rang  $N$  pour les systèmes à  $N$  corps. La généralisation à un nombre infini de particules est alors claire : il suffit de considérer des *projecteurs orthogonaux de rang infini*. Si  $(\varphi_j)_{j \geq 1}$  est une base hilbertienne de l'image d'un tel projecteur  $\gamma$ , alors la fonction d'onde associée est formellement un déterminant de Slater infini

$$\varphi_1 \wedge \cdots \wedge \varphi_N \wedge \cdots .$$



Dans la prochaine section, nous expliquons que l'on peut associer à de tels opérateurs une notion d'état quantique, de la même manière que l'on associe un déterminant de Slater à un projecteur orthogonal de rang fini.

**1.5. États quasi-libres.** Si  $\gamma$  est un projecteur orthogonal de rang infini, il existe un unique état quantique abstrait sur une  $C^*$ -algèbre, que l'on appelle *état quasi-libre*, de matrice densité à un corps  $\gamma$  [BR87]. Une présentation plus détaillée de ce concept est donnée dans l'Appendice C du Chapitre 1. Nous ne l'explicitons pas davantage dans cette introduction pour simplifier l'exposé. Cette relation entre matrices densités à un corps et états quasi-libres est un des principaux thèmes du Chapitre 1. En particulier, il est parfois plus facile de définir certaines quantités physiques avec la notion d'état plutôt qu'avec la notion de matrice densité, et vice versa. Nous avons déjà vu que l'énergie d'un état quasi-libre s'exprimait de manière simple à partir de la matrice densité. Cependant, nous verrons dans le Chapitre 1 que d'autres quantités, comme par exemple la *probabilité de créer une paire électron-positron*, se définit naturellement à partir de l'état quasi-libre, et pas de la matrice densité. C'est pourquoi il est important de comprendre la relation entre ces deux objets.

L'énergie d'un tel état, définie formellement par  $\mathcal{E}_{\text{HF}}(\gamma)$ , doit bien sûr être infinie. Nous allons voir qu'il est cependant possible de donner un sens aux *différences* d'énergies de tels états. Par la suite, nous considérerons des opérateurs  $\gamma$  qui ne sont pas des projecteurs orthogonaux, mais qui satisfont seulement la contrainte  $0 \leq \gamma \leq 1$ . Dans cette thèse, ils décriront tous un système quantique infini, dans le sens où le nombre moyen de particules de l'état  $\gamma$ , qui n'est autre que  $\text{Tr } \gamma$ , est infini. Chaque opérateur  $0 \leq \gamma \leq 1$  correspond aussi à un unique état abstrait, voir l'Appendice C du Chapitre 1.

Nous décrivons à présent deux approches des systèmes quantiques infinis. La première est l'approche *variationnelle*, et consiste à définir une fonctionnelle d'énergie (relative) pour de tels systèmes, à prouver l'existence de minimiseurs pour cette fonctionnelle, et à étudier leurs propriétés. La seconde est l'approche *dynamique*, dans laquelle on considère l'évolution temporelle de systèmes infinis, son caractère bien posé, et son comportement en temps long, dans un voisinage d'un état de référence.

**1.6. Énergie relative et problème de minimisation.** Comme il a été dit plus haut, nous étudions des perturbations d'états quantiques de référence, qui eux-même décrivent un nombre infini de particules. Afin d'expliquer la notion d'énergie relative,

prenons l'exemple où l'état de référence est un projecteur orthogonal de la forme<sup>3</sup>

$$\gamma_{\text{ref}} = \mathbb{1}(T \leq \mu),$$

où l'on rappelle que  $T$  est l'opérateur d'énergie cinétique sur  $L^2(\mathbb{R}^d, \mathbb{C}^q)$  et  $\mu \in \mathbb{R}$  est appelé *niveau de Fermi*. La notation  $\mathbb{1}(T \leq \mu)$  est comprise au sens du calcul fonctionnel pour l'opérateur autoadjoint  $T : \mathbb{1}(T \leq \mu) = f(T)$  où  $f$  est la fonction bornée  $f(x) = \mathbb{1}(x \leq \mu)$ . Comme  $T$  est un opérateur de multiplication dans le domaine de Fourier,  $\gamma_{\text{ref}}$  est toujours de rang infini (s'il est non-nul). Il représente donc bien un système quantique avec un nombre infini de particules. De plus, il possède une énergie infinie puisque l'opérateur  $T\gamma_{\text{ref}}$  n'est jamais compact, et donc en particulier n'est pas à trace. On peut même rigoureusement écrire, au sens de la trace des opérateurs négatifs,

$$\text{Tr}(T - \mu)\gamma_{\text{ref}} = -\infty.$$

Il est maintenant crucial de remarquer que cette énergie est formellement la plus basse que l'on puisse atteindre (au-delà du fait qu'elle vaille  $-\infty$ !). En effet, si l'on prend l'exemple d'une matrice hermitienne  $A$  en dimension finie, il n'est pas difficile de voir que

$$\mathbb{1}(A \leq 0) = \text{argmin} \{ \text{Tr}(A\gamma), 0 \leq \gamma \leq 1 \}.$$

Cette propriété persiste en dimension infinie, dans le sens suivant : si  $0 \leq \gamma \leq 1$  est un opérateur tel que  $\gamma - \gamma_{\text{ref}}$  est de rang fini (et d'image incluse dans le domaine de  $T$ ), et si  $\gamma_{\text{ref}}^\perp := 1 - \gamma_{\text{ref}}$ , alors on a

$$\begin{aligned} \text{Tr}(T - \mu)(\gamma - \gamma_{\text{ref}}) &= \text{Tr}(\gamma_{\text{ref}}^\perp + \gamma_{\text{ref}})(T - \mu)(\gamma - \gamma_{\text{ref}}) \\ &= \text{Tr} |T - \mu| (\gamma_{\text{ref}}^\perp (\gamma - \gamma_{\text{ref}}) \gamma_{\text{ref}}^\perp - \gamma_{\text{ref}} (\gamma - \gamma_{\text{ref}}) \gamma_{\text{ref}}) \\ &= \text{Tr} |T - \mu| [\gamma_{\text{ref}}^\perp \gamma \gamma_{\text{ref}}^\perp + \gamma_{\text{ref}} (1 - \gamma) \gamma_{\text{ref}}] \\ &\geq 0. \end{aligned}$$

Notons que les deux derniers opérateurs dont on prend la trace sont positifs : on a

$$\gamma_{\text{ref}}^\perp (\gamma - \gamma_{\text{ref}}) \gamma_{\text{ref}}^\perp = \gamma_{\text{ref}}^\perp \gamma \gamma_{\text{ref}}^\perp \geq 0, \quad \gamma_{\text{ref}} (\gamma - \gamma_{\text{ref}}) \gamma_{\text{ref}} = -\gamma_{\text{ref}} (1 - \gamma) \gamma_{\text{ref}} \leq 0.$$

Ainsi, on a bien formellement

$$\text{Tr}(T - \mu)\gamma \geq \text{Tr}(T - \mu)\gamma_{\text{ref}},$$

même si les termes de cette inégalité sont infinis. Seule l'inégalité  $\text{Tr}(T - \mu)(\gamma - \gamma_{\text{ref}}) \geq 0$  est rigoureusement vérifiée, puisque l'opérateur  $(T - \mu)(\gamma - \gamma_{\text{ref}})$  est à trace.

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<sup>3</sup>A partir du Chapitre 4, nous considérons des états plus généraux que ceux-ci (notamment pour inclure les effets liés à la température), et la notion d'énergie relative doit alors comprendre l'entropie du système, voir le Chapitre 6.

On définit alors l'énergie cinétique relative de  $\gamma$  par rapport à  $\gamma_{\text{ref}}$ ,  $\mathcal{E}_{\text{kin}}(\gamma, \gamma_{\text{ref}})$ , en généralisant la formule précédente, c'est-à-dire

$$\mathcal{E}_{\text{kin}}(\gamma, \gamma_{\text{ref}}) := \text{Tr} |T - \mu|^{1/2} (\gamma_{\text{ref}}^\perp (\gamma - \gamma_{\text{ref}}) \gamma_{\text{ref}}^\perp - \gamma_{\text{ref}} (\gamma - \gamma_{\text{ref}}) \gamma_{\text{ref}}) |T - \mu|^{1/2}. \quad (4)$$

Elle est bien définie pour tout  $0 \leq \gamma \leq 1$  tel que les opérateurs positifs

$$|T - \mu|^{1/2} \gamma_{\text{ref}}^\perp (\gamma - \gamma_{\text{ref}}) \gamma_{\text{ref}}^\perp |T - \mu|^{1/2}, -|T - \mu|^{1/2} \gamma_{\text{ref}} (\gamma - \gamma_{\text{ref}}) \gamma_{\text{ref}} |T - \mu|^{1/2}$$

soient à trace. Le fait que l'énergie cinétique relative est une quantité positive joue un rôle prépondérant lorsque l'on veut définir la densité  $\rho_\gamma$  d'un état d'énergie cinétique relative finie par rapport à  $\gamma_{\text{ref}}$ , voir le Chapitre 4. Cette notion d'énergie relative entre deux opérateurs de rang infini a été introduite pour la première fois par Hainzl, Lewin, et Séré dans [HLS05a].

A partir de l'énergie cinétique relative, on peut construire différentes notions d'énergie relative d'un état  $\gamma$  par rapport à  $\gamma_{\text{ref}}$ , notamment en introduisant l'énergie potentielle due à un potentiel extérieur  $V$  ou l'énergie d'interaction via un potentiel d'interaction  $W$ , comme pour la fonctionnelle de Hartree-Fock. Comme ces énergies relatives seront différentes selon le modèle que nous étudions, nous n'en ferons pas de description générale et nous détaillerons chacune d'entre elles lors du résumé des résultats de chaque Chapitre de cette thèse. On peut ensuite étudier l'existence de minimiseurs pour ces énergies. La difficulté est que ces énergies sont toutes non linéaires, que la variable est un opérateur non compact sur un espace de dimension infinie, que ces fonctionnelles sont parfois non convexes et présentent souvent des défauts de compacité. Ces problèmes n'ont été considérés que très récemment, et le premier résultat concernant la minimisation de telles fonctionnelles a été montré par Hainzl, Lewin, et Séré [HLS05b] concernant l'opérateur de Dirac. D'autres problèmes de minimisation ont ensuite été traités dans [HLS07, HLS09a], ainsi que dans [CDL08a, CDL08b, CL10] pour des travaux similaires concernant les cristaux quantiques.

**1.7. Dynamique des systèmes quantiques infinis.** Les états de Hartree-Fock apparaissent naturellement comme une sous-classe des états quantiques, paramétrés par un opérateur  $\gamma$ , et leur énergie peut donc être vue comme une fonctionnelle de cet opérateur. Ces concepts se généralisent aux opérateurs  $\gamma$  de rang infini, permettant de décrire des systèmes quantiques infinis. Leur évolution temporelle est un peu plus subtile. En effet, si l'on considère l'équation de Schrödinger

$$\begin{cases} i\partial_t \Psi = H_N \Psi, \\ \Psi|_{t=t_0} = \varphi_1 \wedge \cdots \wedge \varphi_N, \end{cases}$$

il est en général faux que  $\Psi(t)$  est aussi un état de Hartree-Fock pour  $t \neq t_0$ . C'est par contre le cas si les particules du système n'interagissent pas entre elles, c'est-à-dire

si  $W = 0$ . Dans ce cas, chacune des fonctions d'onde constituant le déterminant de Slater évolue indépendamment, et on peut écrire

$$\Psi(t) = \varphi_1(t) \wedge \cdots \wedge \varphi_N(t),$$

où chaque  $\varphi_j(t)$  est l'unique solution du problème de Cauchy

$$\begin{cases} i\partial_t \varphi_j = (T + V)\varphi_j, \\ \varphi_j(t)|_{t=t_0} = \varphi_j. \end{cases}$$

De manière équivalente, la matrice densité à un corps de  $\Psi(t)$ ,  $\gamma_{\Psi(t)}^{(1)}$ , est l'unique solution de l'équation

$$\begin{cases} i\partial_t \gamma_{\Psi}^{(1)} = [T + V, \gamma_{\Psi}^{(1)}], \\ \gamma_{\Psi}^{(1)}(t)|_{t=t_0} = \sum_{j=1}^N |\varphi_j\rangle\langle\varphi_j|. \end{cases}$$

Si  $W \neq 0$ , on ne peut plus faire cette réduction, et les évolutions des matrices densité à  $k$  corps de  $\Psi$  sont toutes couplées entre elles, menant à un système d'équations que l'on appelle *hiérarchie BBGKY*. Dans l'optique d'étudier la dynamique des systèmes quantiques infinis, nous cherchons une équation portant uniquement sur la matrice densité à un corps  $\gamma$ , et qui tient aussi compte des interactions entre les particules. Nous considérons donc l'équation de *Hartree*, qui prend la forme

$$\begin{cases} i\partial_t \gamma = [T + W * \rho_{\gamma}, \gamma], \\ \gamma|_{t=t_0} = \gamma_0. \end{cases}$$

Ici, nous avons noté  $\rho_{\gamma}$  la densité de l'opérateur  $\gamma$ , et  $W * \rho_{\gamma}$  désigne l'opérateur de multiplication par la fonction

$$W * \rho_{\gamma}(x) := \int_{\mathbb{R}^d} W(x - y)\rho_{\gamma}(y) dy, \quad \forall x \in \mathbb{R}^d,$$

qu'on appelle potentiel de Hartree engendré par  $\rho_{\gamma}$ . Nous avons également imposé  $V = 0$ , car nous n'étudions pas l'influence d'un potentiel extérieur dans cette thèse. L'équation de Hartree peut être obtenue à partir de l'évolution à  $N$  corps, à la limite  $N \rightarrow \infty$  avec un potentiel  $W$  dépendant de  $N$ , par exemple avec  $W_N := N^{-1}W$  [BGGM03, EESY04, BPS13]. L'équation de Hartree est également non linéaire, puisque le potentiel  $W * \rho_{\gamma}$  dépend de la solution  $\gamma$ .

La généralisation aux systèmes quantiques infinis est alors claire : il suffit de considérer une donnée initiale  $0 \leq \gamma_0 \leq 1$  de trace infinie. Notons que sous certaines hypothèses sur le potentiel  $W * \rho_{\gamma}$ , l'opérateur  $\gamma(t)$  est unitairement conjugué à  $\gamma_0$ . En particulier, le rang et la trace de  $\gamma_0$  sont préservés, et  $\gamma(t)$  décrit aussi un système quantique infini. Remarquons également que la densité  $\rho_{\gamma}$  d'un opérateur  $\gamma \geq 0$  tel que  $\text{Tr } \gamma = +\infty$  n'est en général pas bien définie, ce qui constitue une difficulté majeure.

Le premier résultat concernant de telles équations a été obtenu par Hainl, Lewin, et Sparber [HLS05c], toujours dans le cadre de l'opérateur de Dirac. Une équation similaire a été étudiée par Cancès et Stoltz [CS12] dans le cas de cristaux quantiques. Le Chapitre 4 est consacré à l'étude de solutions globales pour l'équation de Hartree dans le cas où  $T = -\Delta$ , qui possède la différence fondamentale avec les travaux cités de ne pas présenter de *trou spectral*. Nous considérons de plus une classe générale de données initiales. Dans le Chapitre 5, nous étudions le comportement en temps long de cette équation, et notamment ses propriétés *dispersives*. L'étude de la dispersion pour les systèmes quantiques infinis est un sujet qui n'a jamais été abordé à notre connaissance, et cette thèse présente les premiers travaux dans cette direction.

Pour résumer, nous avons vu que le formalisme des matrices densité à un corps apparaissait naturellement en mécanique quantique des systèmes finis, et qu'il se généralise au cas des systèmes infinis. Même si ces systèmes infinis possèdent une énergie infinie, on peut définir rigoureusement une notion d'énergie relative. On peut également définir la dynamique de tels systèmes en interaction, dont la justification est cependant moins immédiate. Enfin, nous insistons sur le fait que ce formalisme est intrinsèquement non linéaire. Ceci clot notre discussion générale sur la description mathématique des systèmes quantiques infinis. Nous présentons maintenant les résultats obtenus dans cette thèse.

## 2. Résultats des Chapitres 1, 2, et 3 : modèles relativistes

Les Chapitres 1, 2, et 3 traitent tous d'un modèle non linéaire de mécanique quantique relativiste appelé modèle de Bogoliubov-Dirac-Fock. Les Chapitres 1 et 2 sont plus particulièrement consacrés au phénomène de création de paires électron-positron. Nous introduisons brièvement ces concepts avant de présenter les résultats de ces trois chapitres.

**2.1. Paires électron-positron en mécanique quantique relativiste.** La mécanique quantique relativiste repose sur l'introduction d'un opérateur d'énergie cinétique différent du cas non-relativiste : l'opérateur de Dirac (3). Il a été introduit par Dirac à partir de la fin des années 1920 [Dir28, Dir30, Dir33, Dir34a, Dir34b] dans le but d'inclure certains effets relativistes dans le formalisme de la mécanique quantique. Il décrit l'énergie cinétique d'un électron dont la vitesse est comparable à celle de la lumière, ce qui est par exemple le cas des électrons de coeur d'un noyau lourd. C'est un opérateur auto-adjoint sur l'espace de Hilbert  $L^2(\mathbb{R}^3, \mathbb{C}^4)$  de domaine  $H^1(\mathbb{R}^3, \mathbb{C}^4)$ , de la forme

$$D_m := \boldsymbol{\alpha} \cdot (-i\nabla) + \beta m = \sum_{j=1}^3 \alpha_j (-i\partial_{x_j}) + \beta m,$$

où  $\alpha_1, \alpha_2, \alpha_3, \beta$  sont des matrices  $4 \times 4$  définies par

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}, \quad j = 1, 2, 3, \quad \beta = \begin{pmatrix} \text{Id}_{\mathbb{C}^2} & 0 \\ 0 & -\text{Id}_{\mathbb{C}^2} \end{pmatrix},$$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Ici,  $m$  désigne la masse d'un électron, et on a choisi un système d'unités tel que la vitesse de la lumière ainsi que la constante de Planck réduite valent 1 :

$$c = 1 = \hbar.$$

L'opérateur de Dirac vérifie la relation fondamentale

$$D_m^2 = -\Delta + m^2,$$

qui provient de la quantification de l'énergie relativiste classique  $E$  d'une particule de masse  $m$  et de moment cinétique  $k$  :

$$E^2 = k^2 + m^2.$$

Le spectre de l'opérateur de Dirac est

$$\sigma(D_m) = (-\infty, -m^2] \cup [m^2, +\infty),$$

et est donc en particulier non borné inférieurement. Les états d'énergie cinétique négative posent *a priori* un problème puisqu'aucun électron d'énergie cinétique négative n'a jamais été observé. Dirac postule ainsi que le vide relativiste est constitué d'une infinité de particules virtuelles d'énergie cinétique négative. Par le principe de Pauli, un électron réel ne peut occuper un état d'énergie cinétique négative puisque ces états sont déjà occupés et que les électrons sont des fermions. Avec cette interprétation, un électron réel a effectivement une énergie cinétique positive. Le vide relativiste s'identifie donc à une "mer" d'électrons virtuels, la mer de Dirac, dont la distribution est uniforme dans l'espace et ainsi inobservable. Dans le formalisme de la section précédente, on peut dire que la matrice densité à un corps du vide relativiste est donc

$$\gamma_{\text{ref}} = \mathbb{1}(D_m \leq 0).$$

L'une des conséquences d'un tel postulat est qu'une source d'énergie suffisamment forte peut exciter l'un de ces électrons virtuels pour que son énergie cinétique devienne positive. Ce faisant, cet électron excité laisse un "trou" dans la mer de Dirac, qui lui même s'interprète comme une particule d'énergie cinétique positive. Ainsi, un tel processus produit une paire de particules possédant chacune une énergie cinétique positive. Cette paire est constituée d'un électron et de son anti-particule. Cette conséquence de l'interprétation de Dirac était d'abord uniquement théorique, car une telle anti-particule de l'électron n'avait jamais été observée. Dirac pensa d'ailleurs dans un premier temps que cette anti-particule n'était autre que le proton, ce qui se

révéla impossible du fait de sa masse trop importante. Il la baptisa *positron*, et elle fut observée en 1933 par Anderson [And33]. Ce phénomène est donc appelé *création de paire électron-positron*. L'un des objectifs de cette thèse est d'étudier ce phénomène d'un point de vue mathématique. Remarquons que l'existence d'un tel mécanisme change drastiquement l'approche physique du vide. Des particules peuvent apparaître ou disparaître spontanément, et ce en nombre arbitraire. C'est pourquoi les physiciens utilisent désormais le concept de champ plutôt que celui de mer de Dirac. La théorie de Dirac n'est en fait que l'une des bases de la *théorie quantique des champs*, dont les prévisions coïncident de manière spectaculaire avec les expériences. Nous allons voir que le point de vue de la mer de Dirac permet tout de même de capturer certains effets physiques importants tels que la polarisation du vide ou la renormalisation de charge en électrodynamique quantique.

Il existe différentes sources de production de paires électron-positron, comme l'interaction entre un noyau et un photon d'énergie suffisamment grande par exemple. Nous considérons le cas où une paire est produite lorsqu'un champ électrique extérieur et *classique* est appliqué au vide. Heisenberg, Euler [HE36] et Schwinger [Sch51] ont prédit théoriquement qu'un champ de ce type (qui de plus est constant en temps et uniforme en espace) pouvait créer des paires électron-positron dans le vide. On appelle donc ce phénomène *l'effet Schwinger*. Il n'a cependant pas encore été observé expérimentalement, du fait de l'intensité extrêmement importante des champs électriques qu'il faut produire pour pouvoir le distinguer des autres sources de création de paires [Dun09, Taj09, BMN<sup>+</sup>10]. Notre but est également d'étudier la création de paires par un champ électrique classique de forte intensité. Comme les électrons virtuels de la mer de Dirac sont des particules chargées, leur distribution est modifiée par la présence d'un champ électrique : on dit que le vide se *polarise*, et ce phénomène est donc appelé *polarisation du vide*. D'un point de vue mathématique, on peut se demander quelle est la nouvelle matrice densité à un corps qui décrit le vide en présence de ce champ extérieur. Pour répondre à cette question, nous utilisons le formalisme du modèle de *Bogoliubov-Dirac-Fock*.

**2.2. Le modèle de Bogoliubov-Dirac-Fock.** Il a été introduit en 1989 par Chaix, Iracane, et Lions [CI89, CIL89] afin d'étudier la stabilité du vide libre  $\gamma_{\text{ref}}$  lorsqu'on le perturbe par un champ électrique extérieur. Ce modèle a été repris et développé par Gravejat, Hainzl, Lewin, Séré, et Solovej dans une série d'articles sur laquelle nous nous basons [HLSS07]. En utilisant le formalisme des matrices densités à un corps, il permet de définir une notion d'énergie relative d'un état quelconque par rapport à la mer de Dirac libre, en présence d'un champ extérieur. Cette énergie, que l'on appelle énergie de Bogoliubov-Dirac-Fock (BDF), repose sur l'énergie de Hartree-Fock introduite dans la section précédente. Afin de simplifier la présentation, nous ne considérons ici que le modèle réduit, c'est-à-dire le modèle de Hartree-Fock sans terme

d'échange. Considérons ainsi un potentiel extérieur  $V$ , et le potentiel d'interaction  $W$  de Coulomb :

$$W(x) = \frac{1}{|x|}, \quad \forall x \in \mathbb{R}^3.$$

L'énergie BDF réduite, notée  $\mathcal{E}_{\text{rBDF}}^V$ , est la différence formelle entre l'énergie de Hartree-Fock réduite d'un état quelconque  $0 \leq \gamma \leq 1$  et celle de la mer de Dirac libre  $\gamma_{\text{ref}} = \mathbf{1}(D_m \leq 0)$  :

$$\mathcal{E}_{\text{rBDF}}^V(\gamma) := \mathcal{E}_{\text{rHF}}^V(\gamma - 1/2) - \mathcal{E}_{\text{rHF}}^0(\gamma_{\text{ref}} - 1/2).$$

L'exposant  $V$  dans l'énergie de Hartree-Fock réduite  $\mathcal{E}_{\text{rHF}}^V$  désigne l'énergie en présence du potentiel extérieur  $V$ . La variable de l'énergie de Hartree-Fock est ici  $\gamma - 1/2$  au lieu de  $\gamma$ , pour des raisons d'invariance par conjugaison de charge [**Sch51**, **HLS07**]. Comme indiqué dans notre discussion sur les systèmes infinis, chacune des énergies de cette différence est formellement infinie. Cependant, on peut lui donner un sens en restreignant le système dans un cube de taille  $L$ , auquel cas ces deux énergies sont bien définies, puis en passant à la *limite thermodynamique*  $L \rightarrow \infty$  [**HLS07**]. On arrive ainsi à l'expression

$$\mathcal{E}_{\text{rBDF}}^V(\gamma) = \text{Tr } D_m(\gamma - \gamma_{\text{ref}}) + \int_{\mathbb{R}^3} V(x) \rho_{\gamma - \gamma_{\text{ref}}}(x) dx + \frac{1}{2} \iint_{\mathbb{R}^6} \frac{\rho_{\gamma - \gamma_{\text{ref}}}(x) \rho_{\gamma - \gamma_{\text{ref}}}(y)}{|x - y|} dx dy.$$

Ici, la trace  $\text{Tr } D_m(\gamma - \gamma_{\text{ref}})$  est interprétée au sens de l'énergie cinétique relative (4) introduite dans la section 1.6. En particulier, elle est toujours positive et cela implique que  $\gamma = \gamma_{\text{ref}}$  est l'unique minimiseur de cette énergie lorsque  $V = 0$  : la mer de Dirac libre est bien l'état de plus basse énergie en l'absence de champ extérieur. Ici, on a utilisé le fait que

$$\iint_{\mathbb{R}^6} \frac{\rho_{\gamma - \gamma_{\text{ref}}}(x) \rho_{\gamma - \gamma_{\text{ref}}}(y)}{|x - y|} dx dy = 4\pi \int_{\mathbb{R}^3} \frac{|\widehat{\rho_{\gamma - \gamma_{\text{ref}}}}(k)|^2}{|k|^2} \geq 0$$

pour tout  $\gamma$ , même si la densité  $\rho_{\gamma - \gamma_{\text{ref}}}$  n'a pas de signe a priori. Le vide polarisé est alors défini comme l'état de plus basse énergie, lorsque  $V \neq 0$ . A partir de maintenant, on choisira  $V$  comme étant le potentiel Coulombien engendré par une densité de charge  $\nu : \mathbb{R}^3 \rightarrow \mathbb{R}$  :

$$V(x) = -(\nu * |\cdot|^{-1})(x) = - \int_{\mathbb{R}^3} \frac{\nu(y)}{|x - y|} dy, \quad \forall x \in \mathbb{R}^3.$$

Cela permet en particulier d'associer l'énergie potentielle associée à  $V$  avec l'énergie d'interaction, pour avoir l'inégalité

$$\int_{\mathbb{R}^3} V(x) \rho_{\gamma - \gamma_{\text{ref}}}(x) dx + \frac{1}{2} \iint_{\mathbb{R}^6} \frac{\rho_{\gamma - \gamma_{\text{ref}}}(x) \rho_{\gamma - \gamma_{\text{ref}}}(y)}{|x - y|} dx dy \geq -\frac{1}{2} \iint_{\mathbb{R}^6} \frac{\nu(x) \nu(y)}{|x - y|} dx dy,$$

et ainsi constater que l'énergie  $\mathcal{E}_{\text{rBDF}}^V$  est bornée inférieurement. Dans [**HLS05b**], il est prouvé que l'énergie  $\mathcal{E}_{\text{rBDF}}^V$  (même lorsque le terme d'échange est inclus) ne possède aucun minimiseur parmi l'ensemble des  $\gamma$  pour lesquels elle est bien définie. Ceci est



dû à une *divergence ultraviolette* bien connue en électrodynamique quantique. Pour trouver des minimiseurs, il faut régulariser cette divergence. Dans cette thèse, on suit [HLS05a, HLS05b] en introduisant un paramètre de cut-off ultraviolet  $\Lambda > 0$ . L'espace de Hilbert  $L^2(\mathbb{R}^3, \mathbb{C}^4)$  est alors remplacé par l'espace

$$\mathfrak{H}_\Lambda := \{f \in L^2(\mathbb{R}^3, \mathbb{C}^4), \text{supp } \widehat{f} \subset B(0, \Lambda)\},$$

qui consiste à couper les hautes fréquences. Remarquons que l'opérateur de Dirac, qui est un opérateur de multiplication en Fourier, est borné sur  $\mathfrak{H}_\Lambda$ . Ainsi, l'espace  $\mathcal{K}_\Lambda$  des opérateurs pour lesquels  $\text{Tr } D_m(\gamma - \gamma_{\text{ref}})$  est finie est exactement

$$\mathcal{K}_\Lambda := \{0 \leq \gamma \leq 1, \quad \gamma_{\text{ref}}(\gamma - \gamma_{\text{ref}})\gamma_{\text{ref}}, \quad \gamma_{\text{ref}}^\perp(\gamma - \gamma_{\text{ref}})\gamma_{\text{ref}}^\perp \in \mathfrak{S}^1(\mathfrak{H}_\Lambda)\},$$

où  $\gamma_{\text{ref}}^\perp = 1 - \gamma_{\text{ref}}$  et  $\mathfrak{S}^1(\mathfrak{H}_\Lambda)$  désigne l'espace des opérateurs à trace sur  $\mathfrak{H}_\Lambda$ . On peut montrer que  $\mathcal{E}_{\text{rBDF}}^V$  est bien définie sur  $\mathcal{K}_\Lambda$ , et qu'elle admet cette fois-ci un minimiseur  $\gamma_V$  sur  $\mathfrak{H}_\Lambda$ , que l'on interprète comme la matrice densité à un corps du vide polarisé par  $V$  [HLS05b]. En tant que solution d'un problème de minimisation sous contrainte,  $\gamma_V$  satisfait une équation d'Euler-Lagrange de la forme

$$\gamma_V = \mathbf{1} (\Pi_\Lambda [D_m + (\rho_{\gamma_V - \gamma_{\text{ref}}} - \nu) * |\cdot|^{-1}] \Pi_\Lambda < 0) + \delta, \quad (5)$$

où  $0 \leq \delta = \delta^* \leq \mathbf{1}(\Pi_\Lambda [D_m + (\rho_{\gamma_V - \gamma_{\text{ref}}} - \nu) * |\cdot|^{-1}] \Pi_\Lambda = 0)$  et  $\Pi_\Lambda$  est l'opérateur de multiplication en Fourier par l'indicatrice de  $B(0, \Lambda)$ . Si l'on néglige l'opérateur  $\delta$ , alors on interprète  $\gamma_V$  comme le projecteur spectral négatif d'un opérateur de Dirac en présence d'un potentiel qui dépend lui-même de  $\gamma_V$  : les particules du vide se réarrangent afin d'obtenir l'énergie la plus basse possible.

On peut retirer le paramètre de régularisation en étudiant la limite  $\Lambda \rightarrow \infty$  de l'opérateur  $\gamma_V$ . Il se trouve que la *réponse linéaire* en  $V$  de cet opérateur est logarithmiquement divergente en  $\Lambda$  [HLS05a]. Cette divergence a une conséquence physique importante que l'on appelle *renormalisation de charge*, et qui a été étudiée mathématiquement par Gravejat, Lewin, et Séré [GLS09, GLS11] dans le cas du modèle BDF réduit. La divergence logarithmique à la limite  $\Lambda \rightarrow \infty$  doit être contrôlée si l'on veut enlever le paramètre de régularisation. Dans le Chapitre 2, la méthode que nous employons consiste à introduire la constante de structure fine  $\alpha > 0$  dans le modèle en modifiant l'énergie de la façon suivante :

$$\mathcal{E}_{\text{rBDF}}^V(\gamma) = \text{Tr } D_m(\gamma - \gamma_{\text{ref}}) - \alpha \int_{\mathbb{R}^6} \frac{\nu(y)\rho_{\gamma - \gamma_{\text{ref}}}(x)}{|x - y|} dx dy + \frac{\alpha}{2} \int_{\mathbb{R}^6} \frac{\rho_{\gamma - \gamma_{\text{ref}}}(x)\rho_{\gamma - \gamma_{\text{ref}}}(y)}{|x - y|} dx dy.$$

Nous pouvons alors étudier la limite  $\Lambda \rightarrow \infty$  en fixant  $\alpha \log \Lambda$ . On montre dans le Chapitre 2 que cette condition suffit à contrôler la divergence, et permet d'obtenir un résultat non trivial à la limite.

Enfin, mentionnons qu'il existe plusieurs types d'énergies BDF. Celle que nous avons considéré dans la discussion précédente ne contenait pas le terme d'échange de

l'énergie de Hartree-Fock, c'est pourquoi on l'appelle énergie BDF réduite, ou énergie rBDF. On peut aussi inclure le terme d'échange, ce qui mène à l'énergie suivante

$$\mathcal{E}_{\text{BDF}}^V(Q) = \text{Tr } D_m Q - \alpha \int_{\mathbb{R}^6} \frac{\nu(y)\rho_Q(x)}{|x-y|} dx dy + \frac{\alpha}{2} \int_{\mathbb{R}^6} \frac{\rho_Q(x)\rho_Q(y) - |Q(x,y)|^2}{|x-y|} dx dy,$$

où nous avons noté  $Q = \gamma - \gamma_{\text{ref}}$ . L'existence de minimiseurs pour cette énergie est prouvée dans [HLS05b], et est significativement plus difficile que pour l'énergie réduite puisque le terme d'échange rend la fonctionnelle non convexe. Il est également montré que  $\mathcal{E}_{\text{BDF}}^V$  admet des minimiseurs qui sont des projecteurs orthogonaux, c'est-à-dire que l'opérateur  $\delta$  est absent de la formulation (5). On verra que cela sera utile dans le Chapitre 1. Le désavantage de la fonctionnelle  $\mathcal{E}_{\text{BDF}}^V$  est qu'elle ne peut pas se dériver comme différence d'énergie de Hartree-Fock dans une limite thermodynamique. Si l'on veut effectuer cette procédure avec le terme d'échange, la fonctionnelle limite possède une forme légèrement différente :

$$\tilde{\mathcal{E}}_{\text{BDF}}(Q) = \text{Tr } \mathcal{D}_m Q - \alpha \int_{\mathbb{R}^6} \frac{\nu(y)\rho_Q(x)}{|x-y|} dx dy + \frac{\alpha}{2} \int_{\mathbb{R}^6} \frac{\rho_Q(x)\rho_Q(y) - |Q(x,y)|^2}{|x-y|} dx dy,$$

où  $\mathcal{D}_m$  est un opérateur de Dirac effectif, lui-même solution d'une équation non linéaire, et  $Q = \gamma - \mathcal{P}_-^0$  avec  $\mathcal{P}_-^0 := \mathbf{1}(\mathcal{D}_m \leq 0)$ . Cette fonctionnelle a été dérivée dans [HLS07], et paraît plus pertinente d'un point de vue physique et variationnel. Nous l'aborderons également dans les Chapitres 1 et 2.

**2.3. Création de paires statique ou dynamique.** Il existe deux approches dans la description mathématique du phénomène de création de paires électron-positron. La première, que l'on appelle *dynamique*, consiste à étudier l'évolution temporelle de la mer de Dirac libre lorsque l'on allume un potentiel extérieur fort que l'on éteint progressivement. La question est alors de savoir si pour un temps assez grand, une fois que le potentiel extérieur est éteint, des paires sont apparues. Cette approche a été proposée par Nenciu [Nen80, Nen87], puis étudiée par Pickl et Dürr [PD08] pour montrer que certains potentiels évoluant adiabatiquement pouvaient produire des paires électron-positron. Ils considèrent l'équation de Dirac dépendant du temps

$$\begin{cases} i\partial_t \Psi = (D_m + V(t))\Psi, \\ \Psi|_{t=0} = \Psi_0, \end{cases}$$

où  $V(t)$  est un potentiel à support compact en espace-temps. Sous certaines hypothèses sur  $V$ , Pickl et Dürr montrent l'existence de données initiales  $\Psi_0$  telles que  $\mathbf{1}(D_m \leq 0)\Psi_0 = \Psi_0$ , c'est-à-dire possédant une énergie cinétique négative, telles que  $\lim_{t \rightarrow +\infty} \|\mathbf{1}(D_m \leq 0)\Psi(t)\| = 0$ , ce qui signifie que la fonction d'onde a une énergie cinétique positive pour un temps assez grand, ce qui correspond à l'image de la création de paire électron-trou. Dans leur travail, la limite  $t \rightarrow +\infty$  est couplée à une limite adiabatique, signifiant que l'échelle de temps est également dilatée.

Nous adoptons une autre approche, qui est celle de la création de paires *statique*. Nous considérons le vide polarisé défini comme minimiseur de l'énergie BDF dans un potentiel extérieur. Nous nous intéressons alors au nombre de particules réelles que décrit ce nouvel état quantique : est-il plus avantageux énergétiquement d'avoir des électrons ou positrons réels dans le vide polarisé, et, si oui, combien ? D'un point de vue électrostatique, on s'attend effectivement à ce que ce nombre de particules soit très grand si le champ est très fort. En effet, si l'on place un noyau de charge positive très élevée dans le vide, il est favorable de placer le plus d'électrons possibles au voisinage de ce noyau, afin de faire baisser l'énergie. On ne peut cependant pas en placer un trop grand nombre en vertu du principe de Pauli et de la répulsion mutuelle de ces électrons. De la même manière, il n'est pas favorable énergétiquement de placer des positrons dans cet état quantique, qui coûteraient à la fois de l'énergie électrostatique et cinétique. Ainsi, on peut raisonnablement imaginer que l'état de plus basse énergie ne comporte que des électrons, dans cette configuration. On parle tout de même de création de paires électron-positron, car le processus qui mène à cette configuration peut être compris comme une paire qui se crée au voisinage du noyau avec un positron qui s'échappe à l'infini et un électron qui reste attiré par le noyau. Notre approche est néanmoins stationnaire et ne dépend pas d'un processus dynamique. Elle est moins pertinente d'un point de vue physique, mais a l'avantage d'inclure une large classe de potentiels extérieurs, comme nous allons le voir dans les Chapitres 1 et 2. Enfin, nous pouvons traiter le cas de particules en interaction, contrairement à l'approche de Pickl et Dürr qui suppose que les particules de la mer de Dirac n'interagissent pas entre elles, et donc que leur dynamique est décrite par l'équation de Dirac à un corps.

La création de paires dynamique pour des particules en interaction est un problème extrêmement intéressant, mais suppose une connaissance de la dynamique non linéaire des perturbations de systèmes quantiques infinis, qui est l'objet des Chapitres 3, 4, et 5.

La création de paires statique pour des particules qui n'interagissent pas a été traitée par Klaus et Scharf [KS77b] et par Hainzl [Hai04]. Dans ce cas, la matrice densité à un corps du vide polarisé par un potentiel  $V$  est explicite : il s'agit juste de

$$\gamma_V = \mathbf{1} (D_m + V \leq 0),$$

puisque l'état de plus basse énergie pour ce système est obtenu en remplissant tous les états d'énergie négative de l'opérateur  $D_m + V$ . Sous certaines hypothèses sur  $V$ , Klaus et Scharf prouvent que cet état quantique possède des particules réelles si et seulement si il existe une valeur propre  $\lambda(t)$  de l'opérateur  $D_m + tV$  qui change de signe lorsque  $t$  varie de 0 à 1 : on allume progressivement le potentiel  $V$  et on suit le parcours de ses valeurs propres. Si par exemple une valeur propre  $\lambda(t)$  est positive pour  $t < t_0$  et négative pour  $t > t_0$ , alors la fonction propre associée  $\varphi(t)$  possède une énergie positive pour  $t < t_0$  et négative pour  $t > t_0$  : il est donc plus

avantageux énergétiquement de laisser cet état quantique inoccupé lorsque  $t < t_0$ , puis de l'occuper lorsque  $t > t_0$ . Klaus et Scharf montrent que cette transition résulte alors en la production d'une particule réelle. Dans le Chapitre 2, nous examinerons ce qu'il advient de ce résultat pour le modèle non linéaire incluant les interactions entre les particules du vide.

**2.4. Résultats du Chapitre 1 : estimation de la probabilité de créer une paire.** Le premier chapitre de cette thèse a fait l'objet d'une publication dans les *Annales Henri Poincaré*. Nous étudions la production de paires électron-positron dans le vide relativiste soumis à un champ extrêmement fort. Nous prouvons une estimée explicite sur la probabilité qu'une ou plusieurs paires se forment spontanément, en fonction de la force du champ électrique appliqué au vide. L'état quantique de référence est la mer de Dirac libre tronquée dans les hautes fréquences,

$$\gamma_{\text{ref}} = \mathbb{1}(D \leq 0),$$

où  $D := D_1$  est l'opérateur de Dirac d'une particule de masse  $m = 1$ , agissant sur  $\mathfrak{H}_\Lambda$  où  $\Lambda > 0$  est le paramètre de troncature. Durant tout ce chapitre, ce paramètre  $\Lambda > 0$  restera fixé, et nous n'étudierons pas le comportement de nos résultats lorsque  $\Lambda \rightarrow +\infty$ . Nous perturbons la mer de Dirac libre en introduisant un potentiel électrique extérieur  $V$  engendré par une densité de charge  $Z\nu$  :

$$V(x) = V_Z(x) = - \left( Z\nu * \frac{1}{|\cdot|} \right) (x) = -Z \int_{\mathbb{R}^3} \frac{\nu(y)}{|x-y|} dy.$$

Ici,  $\nu$  est une densité de charge fixe que l'on suppose non-nulle. Elle représente par exemple un profil de charge déterminé par un noyau "étendu" que l'on place dans le vide. Le paramètre  $Z$  mesure alors la charge totale de ce noyau, que l'on suppose très importante :  $Z \gg 1$ . A cause de l'invariance par conjugaison de charge du modèle, on ne fait aucune hypothèse de signe sur  $V_Z$  : un potentiel arbitrairement positif ou négatif peut produire des paires, à partir du moment où il est assez fort. La théorie de Bogoliubov-Dirac-Fock affirme alors qu'il existe un projecteur orthogonal  $\gamma_Z$  sur  $\mathfrak{H}_\Lambda$  qui représente le vide polarisé par  $V_Z$ . Il est construit comme minimiseur de la fonctionnelle de Bogoliubov-Dirac-Fock introduite dans la section précédente, et est ainsi l'état quantique de plus basse énergie en présence de  $V_Z$ . Ici, on peut considérer n'importe laquelle des différentes énergies BDF présentées précédemment (avec ou sans terme d'échange, avec  $D_m$  ou  $\mathcal{D}_m$ ). Notre résultat principal est le suivant, qui montre que si  $Z$  est suffisamment grand, alors une paire est créée dans le vide avec une forte probabilité.

**Théorème 1** (Théorème 1.1, Chapitre 1). *La probabilité  $p_Z$  que l'opérateur  $\gamma_Z$  possède au moins une paire électron-positron satisfait l'estimée*

$$p_Z \geq 1 - e^{-cZ^{2/3}},$$

où  $c > 0$  ne dépend que de la densité  $\nu$ .

La principale problématique de ce premier chapitre est donc d'évaluer le nombre de particules réelles que décrit cet état quantique  $\gamma_Z$ . On traite en fait la question plus générale : comment lit-on le nombre de particules que comporte un état quantique sur sa matrice densité à un corps ?

Pour répondre à cette question, prenons l'exemple d'un opérateur  $0 \leq \gamma \leq 1$  tel que  $\text{Tr } \gamma < +\infty$ , qui représente la matrice densité à un corps d'un système quantique à plusieurs particules. Si  $\gamma$  est un projecteur, alors  $\text{Tr } \gamma = N$  est un entier et on connaît l'unique état (quasi-libre, voir le Chapitre 1) de matrice densité  $\gamma$  : c'est le déterminant de Slater

$$\varphi_1 \wedge \cdots \wedge \varphi_N,$$

où  $(\varphi_j)_{1 \leq j \leq N}$  est une base orthonormale de l'image de  $\gamma$ . Ainsi, on sait que  $\gamma$  représente exactement  $N$  particules. Si  $\gamma$  n'est plus un projecteur orthogonal, alors l'état quantique que représente  $\gamma$  n'est plus une fonction d'onde mais un *état mixte* : une combinaison statistique d'états à plusieurs particules. La question est donc de connaître la *probabilité* que l'état possède  $N$  particules, en fonction de sa matrice densité à un corps. Comme nous l'avons expliqué dans la section 1.5, cette quantité est plus facilement définie à partir de l'état quasi-libre associé (voir le Chapitre 1). On souhaite cependant l'exprimer en fonction de la matrice densité à un corps, puisque c'est l'objet que l'on construit via la théorie BDF. Si l'on note par  $p_N$  la probabilité que l'état quantique que représente  $\gamma$  possède  $N$  particules, alors on montre que

$$p_N = \sum_{\substack{I \subset \mathbb{N} \\ \#I=N}} \prod_{i \in I} \lambda_i \prod_{j \notin I} (1 - \lambda_j),$$

où  $(\lambda_i)_{i \geq 0}$  sont les valeurs propres de  $\gamma$ . Notons que l'on a bien

$$\sum_{N \geq 0} p_N = \prod_{i \geq 0} (\lambda_i + 1 - \lambda_i) = 1.$$

En particulier, la probabilité que l'état quasi-libre de matrice densité à un corps  $\gamma$  possède *au moins une particule* est  $1 - p_0$ , et vérifie

$$1 - p_0 = 1 - \prod_{i \geq 0} (1 - \lambda_i) \geq 1 - e^{-\text{Tr } \gamma}.$$

Ceci fournit un critère simple pour que cette probabilité vale 1 : que  $\gamma$  possède la valeur propre 1. Si ce n'est pas le cas, on constate que cette probabilité est très proche de 1 si  $\text{Tr } \gamma$  est très grand. On voit ainsi que l'on peut lire de cette manière le nombre de particules qu'un état quasi-libre possède, en fonction de sa matrice densité à un corps. Nous avons cependant présenté une situation très simplifiée, et en général il n'existe pas de relation aussi explicite. Une partie significative du Chapitre 1 est consacrée à l'étude de telles relations, dans un cadre plus général. On discute notamment les

états quantiques non seulement décrits par une matrice densité à un corps, mais en plus par une matrice de *pairing*, bien connue en théorie de la supraconductivité.

La situation est plus compliquée pour notre cas de perturbation de la mer de Dirac par un champ extérieur puisque les états que l'on décrit possèdent évidemment une infinité de particules. La bonne quantité à évaluer est plutôt le nombre de particules d'un état *relativement à la mer de Dirac libre*. C'est ce que nous expliquons dans le Chapitre 1, via une procédure qui est un cas particulier de la représentation de Araki-Wyss [AW64]. On peut alors montrer une inégalité similaire :

$$p_Z \geq 1 - e^{-c \operatorname{Tr}(\gamma_{\text{ref}}^\perp Q_Z \gamma_{\text{ref}}^\perp - \gamma_{\text{ref}} Q_Z \gamma_{\text{ref}})},$$

où  $p_Z$  désigne la probabilité de posséder au moins une particule de plus que le vide libre,  $Q_Z := \gamma_Z - \gamma_{\text{ref}}$ , et  $\gamma_{\text{ref}}^\perp := 1 - \gamma_{\text{ref}}$ . Nous sommes donc intéressés par le comportement de

$$\operatorname{Tr}(\gamma_{\text{ref}}^\perp Q_Z \gamma_{\text{ref}}^\perp - \gamma_{\text{ref}} Q_Z \gamma_{\text{ref}})$$

pour  $Z$  grand. Une étude de la fonctionnelle BDF montre que

$$\operatorname{Tr}(\gamma_{\text{ref}}^\perp Q_Z \gamma_{\text{ref}}^\perp - \gamma_{\text{ref}} Q_Z \gamma_{\text{ref}}) \gtrsim Z^{-1} |\mathcal{E}_{\text{BDF}}^{V_Z}(Q_Z)|,$$

et nous voulons donc connaître l'asymptotique de l'énergie  $\mathcal{E}_{\text{BDF}}^{V_Z}(Q_Z)$  du vide polarisé par un noyau de charge  $Z$  quand  $Z$  est grand. On peut obtenir la borne inférieure

$$\mathcal{E}_{\text{BDF}}^{V_Z}(Q) \geq -\frac{Z^2}{2} \int_{\mathbb{R}^6} \frac{\nu(x)\nu(y)}{|x-y|} dx dy, \quad \forall Q \in \mathcal{K}_\Lambda,$$

qui suggère que  $\mathcal{E}_{\text{BDF}}^{V_Z}(Q_Z) \sim -cZ^2$  pour  $Z$  grand. Cependant, cette borne serait atteinte si  $\rho_{Q_Z} \simeq Z\nu$ , c'est-à-dire si la densité du vide polarisé compense celle du potentiel extérieur. Un tel phénomène est proscrit par la présence du cut-off  $\Lambda$  : en effet, on peut montrer qu'il existe une constante  $C_\Lambda > 0$  telle que pour tout  $Q \in \mathcal{K}_\Lambda$ , on ait

$$\|\rho_Q\|_{L^\infty} \leq C_\Lambda.$$

En particulier, la densité du vide polarisé ne peut être arbitrairement grande à cause de la présence du cut-off, et donc ne peut compenser la densité extérieure. On peut même obtenir une borne inférieure qui corrobore cette intuition :

$$\mathcal{E}_{\text{BDF}}^{V_Z}(Q_Z) \geq \inf \left\{ -Z \int_{\mathbb{R}^6} \frac{\nu(y)\rho(x)}{|x-y|} dx dy + \frac{1}{2} \int_{\mathbb{R}^6} \frac{\rho(x)\rho(y)}{|x-y|} dx dy, \|\rho\|_{L^\infty} \leq C_\Lambda \right\}.$$

Le terme de droite de cette inégalité est d'ordre  $-cZ^{5/3}$ , qui est bien strictement plus grand que  $-cZ^2$ . On peut en fait montrer que cette borne est optimale en construisant des états test pour le problème de minimisation. Ainsi, on prouve que

$$\mathcal{E}_{\text{BDF}}^{V_Z}(Q_Z) \sim -cZ^{5/3},$$

cette puissance de  $Z$  étant purement dûe à la présence du cut-off. On arrive donc au résultat suivant,

$$p_Z \geq 1 - e^{-cZ^{2/3}},$$

qui montre bien que pour un champ extérieur extrêmement fort, la probabilité de produire au moins une paire est très proche de 1. Dans le cas de l'énergie BDF (c'est-à-dire avec le terme d'échange), on peut même obtenir une estimée sur la probabilité de produire au moins  $N$  paires, pour tout entier fixe  $N$ .

**2.5. Résultats du Chapitre 2 : étude perturbative de la création de paires.** Le Chapitre 2 est tiré d'un article publié dans *SIAM Journal of Mathematical Analysis*. Son objet est l'étude du vide polarisé par un champ extérieur d'intensité  $Z \gg 1$ , dans la limite  $\alpha \rightarrow 0$  et  $\Lambda \rightarrow \infty$ , où l'on rappelle que  $\alpha$  désigne la constante de structure fine et  $\Lambda$  est le paramètre de cut-off en hautes fréquences. Plus précisément, on considère la limite  $\alpha \rightarrow 0$  avec  $\alpha Z = \kappa$  et  $\alpha \log \Lambda$  fixés. On a déjà vu que la limite où  $\alpha \log \Lambda$  est fixé se justifie par la divergence logarithmique de la réponse linéaire de la mer de Dirac. La limite où  $\alpha Z$  est fixé et  $\alpha \rightarrow 0$  s'interprète de la façon suivante. L'équation d'Euler-Lagrange satisfaite par un projecteur qui minimise l'énergie BDF dans un potentiel extérieur  $ZV$  est la suivante :

$$Q = \mathbf{1} \left( \Pi_\Lambda \left[ D + \alpha ZV + \alpha \left( \rho_Q * |\cdot|^{-1} - \frac{Q(x, y)}{|x - y|} \right) \right] \Pi_\Lambda \leq 0 \right) - P_-^0.$$

Ainsi, on constate que fixer  $\alpha Z = \kappa$  revient à fixer l'opérateur  $D + \kappa V$ , afin qu'uniquement les termes non linéaires de cette équation possèdent un facteur  $\alpha \ll 1$ . Cela permet d'étudier le vide polarisé lorsque la non linéarité est faible, ou, de manière équivalente, lorsque les interactions entre les particules sont faibles. Ce choix de paramètres nous permet d'étudier la création de paires lorsque les interactions sont faibles, et ainsi de la comparer au résultat de Klaus et Scharf traitant du cas où les interactions sont absentes ( $\alpha = 0$ ). En particulier, ils montrent qu'une particule est créée dès qu'une valeur propre de l'opérateur  $D + \kappa V$  change de signe en variant le paramètre  $\kappa$ . Qu'arrive-t-il à ce résultat lorsque les interactions sont présentes, c'est-à-dire lorsque  $\alpha > 0$  ?

Nous définissons d'abord un critère déterminant si une particule est créée dans le cas où les interactions sont présentes, en s'appuyant sur le cas où elles ne le sont pas. Pour cela, on suppose que l'opérateur  $D + \kappa V$  possède une unique valeur propre  $\lambda(\kappa)$  dans un intervalle fixe  $[\mu_-, \mu_+]$  autour de 0 :  $\mu_- < 0 < \mu_+$ . Cette valeur propre change de signe lorsque  $\kappa$  passe une valeur critique  $\kappa_c$ , et on suppose que

$$\lambda(\kappa) \in [\mu_-, \mu_+], \forall \kappa \in [\kappa_c - \varepsilon, \kappa_c + \varepsilon],$$

pour un certain  $\varepsilon > 0$ . Sans perte de généralité, on suppose que  $\lambda(\kappa) > 0$  pour  $\kappa < \kappa_c$ , et que  $\lambda(\kappa) < 0$  pour  $\kappa > \kappa_c$ . Cela implique que le vide polarisé lorsque  $\alpha = 0$ , qui

est simplement  $\gamma_{\kappa V} = \mathbb{1}(D + \kappa V \leq 0)$ , satisfait la relation

$$\gamma_{\kappa V} = \begin{cases} \mathbb{1}(D + \kappa V \leq \mu_-) & \text{si } \kappa < \kappa_c, \\ \mathbb{1}(D + \kappa V \leq \mu_+) & \text{si } \kappa > \kappa_c. \end{cases}$$

Cette écriture met en évidence la discontinuité dans le vide polarisé  $\gamma_{\kappa V}$  lorsqu'une valeur propre change de signe. Lorsque  $\alpha > 0$ , on peut considérer l'analogie non linéaire de ces équations

$$Q_{\pm} = \mathbb{1} \left( \Pi_{\Lambda} \left[ D + \kappa V + \alpha \left( \rho_{Q_{\pm}} * |\cdot|^{-1} - \frac{Q_{\pm}(x, y)}{|x - y|} \right) \right] \Pi_{\Lambda} \leq \mu_{\pm} \right) - P_{-}^0.$$

On peut montrer que les opérateurs  $Q_{\pm}$  sont en fait des minimiseurs de l'énergie BDF dans des domaines de *charge fixée*, si  $\alpha$  est assez petit. On peut également montrer que la différence de charge entre ces deux opérateurs est exactement 1 : l'opérateur  $Q_{+}$  possède un électron de plus que l'opérateur  $Q_{-}$ , toujours si  $\alpha > 0$  est assez petit. Ce résultat s'appuie bien sûr sur le fait que l'opérateur  $D + \kappa V$  possède une valeur propre unique dans l'intervalle  $[\mu_{-}, \mu_{+}]$ . Ainsi,  $Q_{+}$  et  $Q_{-}$  représentent tous deux des vides polarisés, dans des domaines de charges différents. On pose alors la question de savoir lequel possède l'énergie la plus basse et si, lorsque l'on fait varier le paramètre  $\kappa$ , il y a une transition dans celui qui possède l'énergie la plus basse. Si une telle transition se produit, on l'interprète comme la production d'une particule dans le vide : il devient alors plus avantageux d'ajouter ou de retirer une particule du vide. Nous posons également la question du paramètre critique  $\kappa_c(\alpha)$  pour lequel la transition arrive : est-il plus grand ou plus petit que  $\kappa_c$  ? Autrement dit, a-t-on besoin d'un champ extérieur plus fort pour créer une paire avec  $\alpha > 0$  que lorsque  $\alpha = 0$  ?

La première étape consiste à montrer que les opérateurs  $Q_{\pm}$  existent. En effet, ils satisfont une équation non linéaire avec un potentiel extérieur  $\kappa V$  qui n'est pas petit. L'existence de solutions à une telle équation ne rentre donc pas dans le cadre des hypothèses de [HLS05a], où il est supposé que le potentiel extérieur est suffisamment petit. Nous prouvons l'existence des opérateurs  $Q_{\pm}$  pour  $\alpha$  assez petit et  $\Lambda$  assez grand, tels que  $\alpha \log \Lambda$  reste borné.

**Théorème 2** (Théorème 2.1, Chapitre 2). *Soit  $\mu$  qui n'appartient pas au spectre de l'opérateur  $D + \kappa V$ . Alors pour tout  $\alpha > 0$  assez petit et pour tout  $\Lambda$  assez grand tels que  $\alpha \log \Lambda$  soit fixé, il existe une unique solution à l'équation*

$$Q = \mathbb{1} \left( \Pi_{\Lambda} \left[ D + \kappa V + \alpha \left( \rho_Q * |\cdot|^{-1} - \frac{Q(x, y)}{|x - y|} \right) \right] \Pi_{\Lambda} \leq \mu \right) - P_{-}^0.$$

Lorsque  $\alpha \rightarrow 0$  avec  $\alpha \log \Lambda$  fixé, on a de plus la limite

$$Q \longrightarrow \mathbb{1} \left( D + \frac{\kappa}{1 + \frac{2}{3\pi} \alpha \log \Lambda} V \leq \mu \right) - P_{-}^0, \quad (6)$$

pour la topologie des opérateurs Hilbert-Schmidt.



Ce résultat est obtenu par une méthode de point fixe similaire à [HLS05a]. La limite (6) montre une discontinuité en  $\alpha = 0$  qui n'est autre qu'une formulation de la renormalisation de charge, analogue aux résultats de [GLS09], qui ne traitent que le modèle réduit. Une conséquence de notre travail est donc une preuve de la renormalisation de charge lorsque le terme d'échange est inclus, dans la limite  $\alpha \rightarrow 0$ ,  $\alpha \log \Lambda$  fixe.

La seconde étape consiste à comparer l'énergie de  $Q_+$  et  $Q_-$  afin de déterminer lequel possède la plus basse énergie, en variant le paramètre  $\kappa$ . Pour cela, on introduit la fonction

$$F(\kappa, \alpha) = \mathcal{E}_{\text{BDF}}^{\kappa V}(Q_+) - \mathcal{E}_{\text{BDF}}^{\kappa V}(Q_-),$$

dont on étudie la limite  $\alpha \rightarrow 0$ , toujours avec  $\alpha \log \Lambda$  fixé. Si  $F(\kappa, \alpha)$  change de signe lorsque  $\kappa$  augmente, alors une particule est créée (si on passe de positif à négatif) ou annihilée (si on passe de négatif à positif). On obtient le développement suivant :

**Théorème 3** (Théorème 2.2, Chapitre 2). *Dans la limite où  $\alpha \rightarrow 0$  avec  $\alpha \log \Lambda$  fixé, on a*

$$F(\kappa, \alpha) = \lambda \left( \frac{\kappa}{1 + \frac{2}{3\pi} \alpha \log \Lambda} \right) + O_{\alpha \rightarrow 0}(\alpha),$$

où le  $O(\alpha)$  est uniforme en  $\kappa \in [\kappa_c - \varepsilon, \kappa_c + \varepsilon]$ .

En particulier, on voit que  $F$  change de signe pour

$$\kappa_c(\alpha) = \left( 1 + \frac{2}{3\pi} \alpha \log \Lambda \right) \kappa_c + O(\alpha) > \kappa_c$$

pour  $\alpha > 0$  assez petit. On en déduit qu'il faut un champ extérieur plus fort lorsque les interactions entre les particules sont présentes pour produire une paire. Ceci est dû à l'effet d'écrantage de la renormalisation de charge qui rend le potentiel effectif plus faible que le potentiel imposé. Dans l'Appendice B du Chapitre 2, nous fournissons un calcul du second terme dans le développement de  $F$ ,

$$F(\kappa, \alpha) = \lambda \left( \frac{\kappa}{1 + \frac{2}{3\pi} \alpha \log \Lambda} \right) + c\alpha + O_{\alpha \rightarrow 0}(\alpha^{3/2}),$$

qui prend la forme

$$c = \langle \varphi, H(\kappa)\varphi \rangle,$$

où  $\varphi$  est le vecteur propre associé à la valeur propre  $\lambda \left( \frac{\kappa}{1 + \frac{2}{3\pi} \alpha \log \Lambda} \right)$ . Il serait particulièrement intéressant de connaître le signe de  $c$ , pour savoir si l'ordre suivant diminue ou augmente  $\kappa_c(\alpha)$ . De plus, c'est à cet ordre que le terme d'échange intervient dans l'énergie. Cependant, l'expression de  $H(\kappa)$  que nous obtenons ne nous permet pas de déduire le signe de  $c$ .

**2.6. Résultats du Chapitre 3 : existence globale pour une équation de Dirac couplée à une équation des ondes.** Le Chapitre 3 est un premier pas dans l'étude de la dynamique de la mer de Dirac

$$\gamma_{\text{ref}} = \mathbb{1}(D \leq 0)$$

soumise à des champs extérieurs. Nous étudions la couplage entre le vide de Dirac et un champ scalaire, ce dernier évoluant selon une équation des ondes ou de Klein-Gordon. Le but est d'étudier les effets de *retard* dans l'interaction entre la mer de Dirac et un champ. L'équation type que l'on étudie est

$$\begin{cases} i\partial_t \gamma = [\Pi_\Lambda(D + V)\Pi_\Lambda, \gamma], \\ (\partial_t^2 - \Delta)V = 4\pi\rho_{\gamma-1/2}. \end{cases} \quad (7)$$

Dans cette formulation, la mer de Dirac est perturbée par le potentiel  $V$ , qui lui-même satisfait une équation des ondes dont le terme source est la densité de la mer de Dirac. Ainsi,  $V$  est interprété comme un potentiel retardé, engendré par la distribution de charge de la mer de Dirac. On peut aussi penser que cette équation modélise l'évolution d'un champ scalaire dans un milieu inhomogène : la mer de Dirac polarisée par ce même champ.

**Théorème 4** (Théorème 3.2, Chapitre 3). *Pour tout  $\Lambda > 0$  et pour toute donnée initiale*

$$(\gamma_0, V_0, (\partial_t V)|_{t=0}) \in (\gamma_{\text{ref}} + \mathfrak{S}^2(\mathfrak{H}_\Lambda)) \times H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3),$$

où  $\mathfrak{S}^2(\mathfrak{H}_\Lambda)$  désigne l'ensemble des opérateurs Hilbert-Schmidt sur  $\mathfrak{H}_\Lambda$ , il existe une unique solution globale  $(\gamma, V) \in C^0(\mathbb{R}, (\gamma_{\text{ref}} + \mathfrak{S}^2) \times H^1)$  à (7).

On prouve ce résultat par une méthode de point fixe associée à un argument de type conservation de l'énergie. Le point crucial est la présence du cut-off  $\Lambda$  en hautes fréquences, qui facilite grandement les estimées. En particulier, on peut se poser la question du comportement de cette équation lorsque  $\Lambda \rightarrow \infty$ . Dans le même esprit que le cas stationnaire, la première quantité à étudier est la réponse linéaire  $B_\Lambda(t)$ . On montre que, contrairement au cas stationnaire, cette réponse linéaire est *bornée* en  $\Lambda$  dès que  $t \neq 0$ . On a même l'estimée

$$|B_\Lambda(t)| \leq C(1 + \log |t|),$$

pour tout  $t \neq 0$ . Ainsi, on voit que les effets de retard améliorent le comportement de la réponse linéaire. Il est alors naturel d'essayer de passer à la limite  $\Lambda \rightarrow \infty$  dans cette équation, et d'obtenir une formule de *renormalisation de charge dépendante du temps*. Dans le Chapitre 3, nous expliquons la stratégie qu'il faut adopter pour accomplir cette tâche. En particulier, une compréhension des propriétés dispersives du propagateur  $e^{-itD}$  agissant sur les opérateurs est nécessaire. Pour les fonctions, ces propriétés sont notamment données par les inégalités de Strichartz. On peut

généraliser ces inégalités au cas des opérateurs à trace via des inégalités triangulaires. Cependant, les opérateurs apparaissant dans notre équation ne sont justement pas à trace en général : par exemple, le terme  $[V, \gamma_{\text{ref}}]$  ne l'est pas en général. Il est donc nécessaire de mieux comprendre les propriétés dispersives de  $e^{-itD}$  lorsqu'il agit sur des opérateurs qui ne sont typiquement pas à trace. Avant de traiter le cas de l'opérateur de Dirac, il est naturel d'étudier cette question dans le cas du Laplacien. C'est la motivation principale des Chapitres 4 à 6.

### 3. Résultats des Chapitres 4, 5, et 6 : dynamique non linéaire de Hartree

#### 3.1. Résultats du Chapitre 4 : existence globale dans l'espace d'énergie.

Le Chapitre 4 est consacré à l'existence de solutions globales pour l'équation non linéaire de Hartree

$$\begin{cases} i\partial_t \gamma = [-\Delta + w * \rho_\gamma, \gamma], \\ \gamma|_{t=0} = \gamma_0, \end{cases} \quad (8)$$

où  $\gamma$  est un opérateur autoadjoint borné sur  $L^2(\mathbb{R}^d)$  et  $w$  est un potentiel d'interaction très lisse et à courte portée. Contrairement au cas de l'équation de Dirac, la dimension d'espace  $d$  est maintenant quelconque. On suppose également qu'il n'y a qu'un seul degré de liberté interne :  $q = 1$ . Cette équation est une généralisation de l'équation de Hartree pour des fonctions

$$\begin{cases} i\partial_t u = (-\Delta + w * |u|^2)u, \\ u|_{t=0} = u_0. \end{cases} \quad (9)$$

La première différence entre (8) et (9) est qu'il existe beaucoup d'états stationnaires pour (8) : tout opérateur de la forme

$$\gamma_{\text{ref}} = \gamma_f = f(-\Delta)$$

est une solution stationnaire de (8) si  $f : \mathbb{R}_+ \rightarrow \mathbb{R}$  est telle que  $\int_{\mathbb{R}^d} |f(k^2)| dk < +\infty$ . Ces états sont aussi stationnaires pour l'équation de Schrödinger libre (c'est-à-dire (8) avec  $w = 0$ ), alors que (9) avec  $w = 0$  ne possède aucun état stationnaire dans  $L^2(\mathbb{R}^d)$ . On a déjà vu en section 1.6 un exemple d'un tel opérateur :

$$\gamma_f = \mathbf{1}(-\Delta \leq \mu),$$

avec  $\mu > 0$ , ce qui correspond au cas de la *température nulle*. D'autres exemples physiques existent à *température positive*  $T > 0$  :

$$\gamma_f = \frac{1}{1 + e^{\frac{-\Delta - \mu}{T}}}, \quad \gamma_f = \frac{1}{e^{\frac{-\Delta - \mu}{T}} - 1}, \quad \gamma_f = e^{\frac{\Delta + \mu}{T}}, \quad (10)$$

qui sont respectivement les distributions de Fermi-Dirac, de Bose-Einstein, et de Boltzmann. On s'intéresse aux perturbations de ces états stationnaires et à leur stabilité en temps long. Dans le Chapitre 4, la donnée initiale  $\gamma_0$  est ainsi supposée d'énergie

relative finie par rapport à un opérateur  $\gamma_f$ . On s'intéresse donc à la variable réduite

$$Q = \gamma - \gamma_f,$$

qui satisfait l'équation

$$\begin{cases} i\partial_t Q = [-\Delta + w * \rho_Q, \gamma_f + Q], \\ Q|_{t=0} = Q_0. \end{cases} \quad (11)$$

Notons que le fait de travailler avec des opérateurs offre une nouvelle échelle d'espaces de Banach qui n'existe pas dans les cas des fonctions : les espaces de Schatten  $\mathfrak{S}^p$ , définis comme l'ensemble des opérateurs  $A$  sur  $L^2(\mathbb{R}^d)$  tels que  $\text{Tr}|A|^p < +\infty$ . Ils sont un outil fondamental dans l'ensemble de cette thèse.

La seconde différence avec l'équation (9) est le contrôle de la densité  $\rho_Q$ . Alors que pour des fonctions, les propriétés de  $|u|^2$  (intégrabilité, dérivabilité) sont directement liées à celles de  $u$ , la relation entre  $\rho_Q$  et  $Q$  est moins explicite. C'est pourquoi nous commençons par prouver l'existence locale de solutions pour  $Q$  dans des espaces  $X$  tels qu'on ait une estimée du type

$$\|\rho_Q\|_{L^q(\mathbb{R}^d)} \leq C \|Q\|_X, \quad \forall Q \in X,$$

pour un certain exposant  $q \geq 1$ . Les espaces  $X$  sont des espaces de Schatten avec un poids de type Sobolev, qui peuvent être vus comme des généralisations des espaces de Sobolev  $H^s(\mathbb{R}^d)$ . De la même manière qu'il est généralement aisé de montrer l'existence locale de solutions pour des équations de Schrödinger non linéaires dans  $H^s(\mathbb{R}^d)$  avec  $s > d/2$ , on montre que l'équation de Hartree est localement bien posée lorsque  $s$  est assez grand :

**Théorème 5** (Théorème 4.3, Chapitre 4). *Soit  $d \geq 1$ ,  $1 \leq p < \infty$  et  $s > d(p-1)/p$  ou  $s \geq 0$  si  $p = 1$ . Soient  $w$  et  $f$  des fonctions assez régulières. Alors, pour tout opérateur  $Q_0$  borné sur  $L^2(\mathbb{R}^d)$  tel que  $(1 - \Delta)^{s/2} Q_0 \in \mathfrak{S}^p$ , il existe une unique solution  $Q(t)$  de (11) locale en temps telle que  $(1 - \Delta)^{s/2} Q(t) \in \mathfrak{S}^p$  pour tout temps d'existence  $t$ .*

Notons qu'il faut contrôler également des termes absents lorsque l'on étudie (9) : ceux qui font intervenir l'état stationnaire  $\gamma_f$ . Il faut en effet estimer des termes comme  $[w * \rho_Q, \gamma_f]$ . Pour cela, on exploite leur structure en tant que produit d'un opérateur de multiplication en espace  $w * \rho_Q$  par un opérateur de multiplication en Fourier  $\gamma_f$ . Ainsi, on constate encore l'importance de l'invariance par translation de l'état de référence  $\gamma_f$ .

Les solutions sont globalisées par une méthode de conservation de l'énergie. Là encore, une difficulté nouvelle apparaît puisque l'énergie n'est définie que relativement à l'opérateur  $\gamma_f$ . Lorsque  $\gamma_f$  est de la forme

$$\gamma_f = \mathbf{1}(-\Delta \leq \mu) = \Pi_\mu^-$$

pour un certain  $\mu > 0$ , cet espace d'énergie a été introduit par Frank, Lewin, Lieb et Seiringer dans [FLLS12]. En utilisant les propriétés spécifiques de cet espace d'énergie, on montre alors la conservation de l'énergie relative par rapport à  $\gamma_f$ ,

$$\mathcal{E}(Q) := \text{Tr}(-\Delta - \mu)Q + \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y)\rho_Q(x)\rho_Q(y) dx dy,$$

le long du flot de l'équation de Hartree. Cette énergie est positive sous l'hypothèse *défocalisante* que  $\widehat{w} \geq 0$ . En effet, en écrivant l'énergie d'interaction en variables de Fourier, on obtient

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y)\rho_Q(x)\rho_Q(y) dx dy = (2\pi)^{d/2} \int_{\mathbb{R}^d} \widehat{w}(k)|\widehat{\rho}_Q(k)|^2 dk.$$

On en déduit l'existence *globale* de solutions par une *inégalité de Lieb-Thirring*, qui montre exactement que l'énergie relative contrôle certaines normes de la densité  $\rho_Q$  de la solution. Ces inégalités de Lieb-Thirring dans le cas de perturbations de la mer de Fermi  $\gamma_f$  ont été montrées dans [FLLS12], et ne sont valables que pour  $d \geq 2$ .

**Théorème 6** (Théorème 4.4, Chapitre 4). *Soit  $d \geq 2$  et  $w$  une fonction assez régulière, défocalisante. Alors, pour toute donnée initiale  $\gamma_0$  d'énergie relative finie par rapport à  $\Pi_\mu^-$ , c'est-à-dire telle que*

$$\text{Tr}(-\Delta - \mu)(\gamma_0 - \Pi_\mu^-) < +\infty,$$

*il existe une unique solution  $\gamma(t)$  à (8) globale en temps, telle que pour tout  $t$ ,  $\gamma(t)$  est d'énergie relative finie par rapport à  $\Pi_\mu^-$ . De plus, l'énergie relative est conservée le long du flot,*

$$\mathcal{E}(\gamma(t) - \Pi_\mu^-) = \mathcal{E}(\gamma_0 - \Pi_\mu^-),$$

*pour tout  $t$ .*

Si  $\gamma_f$  n'est plus la forme  $\mathbb{1}(-\Delta \leq \mu)$ , ce qui est le cas des distributions définies par (10), on doit introduire une nouvelle notion d'énergie relative : l'énergie *libre* relative. Cette nouvelle énergie fait intervenir des *entropies*. L'énergie libre est définie par la formule

$$\mathcal{F}(\gamma) = \text{Tr}(-\Delta - \mu)\gamma - T \text{Tr} S(\gamma),$$

où  $S$  est une entropie spécifique à chacune des distributions  $\gamma_f$  considérées. Par exemple, la distribution de Fermi-Dirac est le minimiseur (toujours formel puisque son énergie est infinie) de l'énergie libre pour l'entropie

$$S(\gamma) = -\gamma \log \gamma - (1 - \gamma) \log(1 - \gamma).$$

On définit alors formellement l'*entropie relative* par la relation

$$\mathcal{H}(\gamma, \gamma_f) = \mathcal{F}(\gamma) - \mathcal{F}(\gamma_f),$$

c'est une quantité positive puisque  $\gamma_f$  est le minimiseur de  $\mathcal{F}$ . Cette interprétation variationnelle implique une propriété cruciale de l'énergie libre : elle satisfait également

une inégalité de Lieb-Thirring. De la même manière qu'à température nulle, on exploitera ce fait pour montrer que les solutions de l'équation de Hartree d'entropie relative finie par rapport à  $\gamma_f$  sont globales.

La définition rigoureuse de l'entropie relative  $\mathcal{H}(\gamma, \gamma_f)$  est délicate puisque les opérateurs  $\gamma$  et  $\gamma_f$  sont de rang infini sur un espace de dimension infinie. Le Chapitre 6 est consacré à cette définition, en se basant sur la propriété fondamentale de *monotonie de l'entropie*. En particulier, nous pouvons définir une entropie relative non seulement pour les distributions de Fermi-Dirac, de Bose-Einstein, et de Boltzmann, mais aussi pour une classe générale de  $\gamma_f$ , que l'on appelle *états de Gibbs généralisés*. Toutes les entropies relatives associées satisfont une inégalité de Lieb-Thirring, ce qui permet encore de montrer que les solutions d'entropie relative finie par rapport à  $\gamma_f$  sont globales.

La difficulté de ces espaces d'énergie à température positive est qu'ils sont beaucoup moins explicites qu'à température nulle. En particulier, la meilleure information que l'on possède sur leur régularité en termes d'espaces de Schatten-Sobolev est donnée par l'inégalité de Klein

$$\mathcal{H}(\gamma, \gamma_f) \geq C \operatorname{Tr}(1 - \Delta)(\gamma - \gamma_f)^2.$$

Cette régularité est généralement plus faible que celles pour lesquelles on a déjà montré l'existence locale (de la même manière que l'espace d'énergie  $H^1(\mathbb{R}^d)$  n'est pas du type  $H^s(\mathbb{R}^d)$  pour  $s > d/2$  dès que  $d \geq 2$ ). A température positive, on doit donc montrer un résultat d'existence locale pour la régularité optimale donnée par l'inégalité de Klein. Dans le cadre des équations de Schrödinger non linéaires, un des outils pour obtenir l'existence locale de solutions avec régularité faible sont les inégalités de Strichartz. Dans le cas des opérateurs, ces inégalités ont été obtenues récemment dans [FLLS13]. En particulier, on donne un sens moyenné en temps à la densité  $\rho_Q$ , en montrant qu'elle appartient à des espaces de type  $L_t^p(I, L_x^q(\mathbb{R}^d))$  : la densité  $\rho_{Q(t)}$  ne peut être définie ponctuellement en  $t$  à cause de la régularité trop faible de l'opérateur  $Q(t)$ , mais elle peut l'être presque partout grâce aux inégalités de Strichartz. Cette faible régularité implique en particulier que nous ne pouvons traiter que les cas  $d \leq 3$ .

**Théorème 7** (Théorème 4.9, Chapitre 4). *Soit  $d = 1, 2, 3$ ,  $w$  une fonction assez régulière, défocalisante, et  $\gamma_f$  un état de Gibbs généralisé. Alors, pour tout  $\gamma_0$  d'entropie relative finie par rapport à  $\gamma_f$ , c'est-à-dire tel que*

$$\mathcal{H}(\gamma_0, \gamma_f) < +\infty,$$

*il existe une unique solution  $\gamma(t)$  à (8) globale en temps, telle que  $\gamma(t)$  est d'entropie relative finie par rapport à  $\gamma_f$  pour tout  $t$ . De plus, l'énergie libre relative est conservée*

le long du flot : pour tout  $t$ ,

$$\begin{aligned} \mathcal{H}(\gamma(t), \gamma_f) + \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y) \rho_{\gamma(t)-\gamma_f}(x) \rho_{\gamma(t)-\gamma_f}(y) dx dy \\ = \mathcal{H}(\gamma_0, \gamma_f) + \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y) \rho_{\gamma_0-\gamma_f}(x) \rho_{\gamma_0-\gamma_f}(y) dx dy. \end{aligned}$$

**3.2. Résultats du Chapitre 5 : dispersion en temps long.** Dans le Chapitre 5, nous continuons l'étude de l'équation non linéaire de Hartree pour les opérateurs, et nous nous intéressons plus particulièrement au comportement en temps long des petites solutions de cette équation. On montre la stabilité asymptotique de certains états stationnaires  $\gamma_f$ , dans le sens où

$$\gamma(t) \xrightarrow[t \rightarrow \pm\infty]{} \gamma_f,$$

faiblement dans l'espace des opérateurs bornés sur  $L^2$ , si la donnée initiale  $\gamma_0$  est assez proche de  $\gamma_f$ .

**Théorème 8** (Théorème 5.1, Chapitre 5). *Soient  $w$  et  $f$  des fonctions assez régulières, satisfaisant de plus la condition*

$$\|\check{g}\|_{L^1(\mathbb{R}^2)} \|\widehat{w}\|_{L^\infty(\mathbb{R}^2)} < 4\pi,$$

où  $g(k) := f(|k|^2)$  et  $\check{g}$  désigne la transformée de Fourier inverse de  $g$ . Alors, il existe  $\varepsilon_0 > 0$  tel que pour tout  $\gamma_0 \in \gamma_f + \mathfrak{S}^{4/3}$  avec

$$\|\gamma_0 - \gamma_f\|_{\mathfrak{S}^{4/3}} \leq \varepsilon_0,$$

il existe une unique solution  $\gamma \in \gamma_f + C^0 \mathfrak{S}^2$  de (8) globale en temps. De plus,  $\gamma(t)$  diffuse vers une solution de l'équation libre dans l'espace de Schatten  $\mathfrak{S}^4$  : il existe  $Q_\pm \in \mathfrak{S}^4$  tels que

$$\|\gamma(t) - \gamma_f - e^{it\Delta} Q_\pm e^{-it\Delta}\|_{\mathfrak{S}^4} \xrightarrow[t \rightarrow \pm\infty]{} 0.$$

La preuve de ce résultat repose sur le fait que la densité  $\rho_{\gamma(t)} - \rho_{\gamma_f}$  vérifie

$$\rho_\gamma - \rho_{\gamma_f} \in L_t^p(\mathbb{R}, L_x^q(\mathbb{R}^d)),$$

pour un certain couple d'exposants  $(p, q)$  avec  $p \neq \infty$ . La stratégie usuelle pour prouver ce genre d'estimée est d'écrire l'équation sous forme de Duhamel,

$$Q(t) = e^{it\Delta} Q_0 e^{-it\Delta} - i \int_0^t e^{i(t-s)\Delta} [w * \rho_{Q(s)}, \gamma_f + Q(s)] e^{i(s-t)\Delta} ds,$$

où  $Q(t) = \gamma(t) - \gamma_f$  et  $Q_0 = \gamma_0 - \gamma_f$ . Le fait que la densité du premier terme  $e^{it\Delta} Q_0 e^{-it\Delta}$  soit dans un  $L_t^p L_x^q$  est précisément l'objet des inégalités de Strichartz *homogènes*. Le second terme est d'habitude traité via des inégalités de Strichartz *inhomogènes*, qui dans le cas des équations de Schrödinger non linéaires suffisent souvent à conclure. Dans notre cas, ces inégalités ne permettent pas d'obtenir le résultat désiré, et on doit

en fait développer la solution  $Q(t)$  en une *série de Dyson* afin d'exploiter pleinement la structure de l'équation. Ce développement fait apparaître des commutateurs du type

$$[w * \rho_{Q(t_1)}, [w * \rho_{Q(t_2)}, [\dots, [w * \rho_{Q(t_n)}, \gamma_f] \dots]]]$$

comportant l'état stationnaire  $\gamma_f$ , d'ordres de plus en plus élevés en  $\rho_Q$ . Lorsque  $n = 1$ , ce terme est linéaire en  $\rho_Q$  et est donc la *réponse linéaire* dépendant du temps de la mer de Fermi. Cette réponse linéaire, bien connue en physique, est la source d'instabilités notamment à température nulle, qui nous empêchent de traiter ce cas. Elle est également responsable de la condition  $\|\check{g}\|_{L^1(\mathbb{R}^2)} \|\widehat{w}\|_{L^\infty(\mathbb{R}^2)} < 4\pi$ . Cette condition peut en fait être relâchée en étudiant précisément les propriétés de la réponse linéaire. De plus, on verra que l'on sait estimer les commutateurs d'ordre  $n$  lorsque  $n \geq d + 1$ . En particulier, plus la dimension  $d$  est grande, plus nous devons traiter de termes spécifiques. C'est pourquoi notre résultat ne concerne que la dimension 2, car nous ne sommes pour l'instant capables que de traiter les termes d'ordre 1 et 2.

**3.3. Résultats du Chapitre 6 : définition de l'entropie relative.** Le Chapitre 6 est consacré à la notion d'entropie relative que nous avons évoquée dans notre présentation du Chapitre 4. Nous définissons une entropie relative (ou énergie libre relative) de la forme

$$\mathcal{H}(A, B) = \text{Tr}(S(A) - S(B) - S'(B)(A - B)),$$

où  $S : [0, 1] \rightarrow \mathbb{R}$  est une fonction convexe dérivable sur  $]0, 1[$  et  $0 \leq A, B \leq 1$  sont des matrices hermitiennes sur un espace vectoriel de dimension finie quelconque. L'objectif est de pouvoir étendre cette définition au cas de la dimension infinie, via une limite

$$\lim_{k \rightarrow \infty} \mathcal{H}(P_k A P_k, P_k B P_k),$$

où  $(P_k)$  est une suite croissante de projecteurs orthogonaux de rangs finis sur un espace de Hilbert  $\mathfrak{H}$ , tels que  $P_k \rightarrow 1$  fortement sur  $\mathfrak{H}$ . C'est la procédure habituelle en mécanique statistique pour définir des objets en dimension infinie à partir de leur définition en dimension finie. Nous montrons qu'une condition suffisante pour que cette limite existe et soit indépendante du choix de la suite  $(P_k)$  est que l'entropie relative  $\mathcal{H}$  soit *monotone*, c'est-à-dire que pour toutes matrices  $A, B$  et pour tout projecteur orthogonal  $P$ , on a la relation

$$\mathcal{H}(PAP, PBP) \leq \mathcal{H}(A, B).$$

On montre que cette condition est équivalente au fait que la fonction  $S'$  soit *monotone au sens des opérateurs*, ce qui veut dire que si  $A \leq B$  au sens des matrices hermitiennes, alors  $S'(A) \leq S'(B)$ . Notons que la monotonie de l'entropie relative implique une propriété fondamentale de l'entropie associée : sa *sous-additivité forte*. Ceci fait le lien avec une conjecture de Petz qui stipule qu'une entropie possède la propriété



de sous-additivité forte si et seulement si  $S'$  est monotone au sens des opérateurs [AHP10].

La monotonie de l'entropie relative nous permet ensuite de montrer des propriétés très utiles pour le Chapitre 4 comme l'inégalité de Klein ou des propriétés de continuité.

#### 4. Conclusions et Perspectives

Dans cette thèse, nous étudions plusieurs modèles non linéaires dans lesquels la variable est un opérateur de rang infini. Nous prouvons ainsi certaines propriétés de stabilité ou d'instabilité des mers de Dirac et de Fermi, sous des perturbations stationnaires (potentiel extérieur), ou dynamiques (évolution d'un état proche). Cela nécessite d'introduire de nouveaux outils de méthodes variationnelles ou d'équation aux dérivées partielles en dimension infinie.

L'étape suivante concernant la création de paires électron-positron est naturellement l'étude dynamique de ce phénomène, dans le cadre non linéaire que nous avons présenté. Comme nous l'avons vu, cela nécessite une meilleure compréhension des propriétés dispersives des systèmes infinis décrits par l'opérateur de Dirac. On a constaté que le cas du Laplacien contenait déjà un certain nombre de subtilités, qui suggèrent que le cas de l'opérateur de Dirac est significativement plus difficile. De manière générale, l'étude des équations de Schrödinger non linéaires dont la variable est un opérateur non compact est un sujet encore largement ouvert.

## CHAPTER 1

# Static electron-positron pair creation in strong fields for a nonlinear Dirac model

This chapter is an extended version of an article published in *Annales Henri Poincaré* [Sab13b]. Appendices B and C are not present in the published version. Appendix B provides a detailed explanation on how to include the exchange term in our study. Appendix C is a general introduction to quasi-free states and their properties, completing the results presented in the article.

### Abstract

We consider the Hartree-Fock approximation of Quantum Electrodynamics, with the exchange term neglected. We prove that the probability of static electron-positron pair creation for the Dirac vacuum polarized by an external field of strength  $Z$  behaves as  $1 - \exp(-\kappa Z^{2/3})$  for  $Z$  large enough. Our method involves two steps. First we estimate the vacuum expectation of general quasi-free states in terms of their total number of particles, which can be of general interest. Then we study the asymptotics of the Hartree-Fock energy when  $Z \rightarrow +\infty$  which gives the expected bounds.

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## 1. Introduction

In 1930, Dirac [Dir30] suggested the idea of identifying the vacuum with a sea of virtual electrons with negative kinetic energy. His theory implies that when a sufficiently strong source of energy is provided to the vacuum, some virtual electrons are excited into real electrons, leaving “holes” in the Dirac sea. These holes can be interpreted as positrons, the anti-particles of the electrons, which were experimentally observed in 1933 by Anderson [And33]. The extraction of an electron from the Dirac sea is usually called *electron-positron pair creation*. Sauter [Sau31], and Heisenberg-Euler [HE36] considered the possibility that an external electromagnetic field could excite the Dirac sea to create those pairs. Schwinger [Sch51] then computed the probability of dynamical pair creation by a constant, uniform, external electric field in the framework of Quantum Electrodynamics (QED). The specific phenomenon of pair production triggered by an external, non-quantized field is thus labeled the *Schwinger effect*. It is remarkable that this effect is different from the absorption of photons by the vacuum, which is another possible source for pair creation. The Schwinger effect is based on the fact that the vacuum acts as a polarizable medium which can decay into electron-positron pairs when excited by a sufficiently strong electric field. Although the modern formulation of QED no longer describes the vacuum as a sea of virtual particles, Dirac’s theory is still valid in the mean-field approximation [HLSS07].

Experimentally, pair creation in electric fields has not been observed yet because it is only non-negligible in a very strong field. However, recent progress in laser physics has permitted to create very strong fields, making the observation of the Schwinger effect possible in the near future [Dun09, Taj09, BMN<sup>+</sup>10].

One has to distinguish between *dynamical* and *static* pair creation. Dynamical pair creation consists in studying the time evolution of the vacuum state when an external field is progressively turned on, so that a pair consisting of a scattering electron and a corresponding hole in the Dirac sea is created. The external field is then progressively switched off, and one has to check if the pair still exists when the field is completely turned off. Static pair creation, on the other hand, consists in the study of the absolute ground state (the polarized vacuum) of the Hamiltonian in an external field. Therefore, it is a time-independent process. In this context, the vacuum with an additional particle is energetically more favorable than the vacuum without particle. Static pair creation is easier to study than dynamical pair creation, but it is also a bit less relevant from the physical point of view.

When the interactions between particles are neglected (the so-called *linear* case), *static* pair creation was mathematically studied by Klaus and Scharf [KS77b]. They proved that the probability of pair creation becomes 1 when the strength of the positive external field sufficiently increases such that an eigenvalue of the Hamiltonian

of the system crosses zero. In the linear case, *dynamical* pair creation is a very involved phenomenon, whose properties were mathematically understood very recently. Nenciu [Nen80, Nen87] proved that there is a discontinuity in the probability to create pairs as the strength of a specific external field increases, in the adiabatic limit. Later on, Pickl and Dürr [PD08, Pic05] proved that the probability of pair creation tends to 1 in the adiabatic limit, for general over-critical external fields, by carefully studying the resonances created by the eigenvalues diving into the essential spectrum of the Hamiltonian of the system.

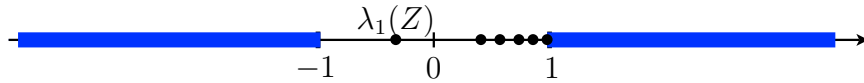
This article is devoted to the mathematical study of *static* pair creation in a *nonlinear* model describing the polarized vacuum, taking into account the interactions between particles. This model was first proposed by Chaix and Iracane [CI89] in 1989 and it has recently been given a solid mathematical ground in a series of papers by Gravejat, Hainzl, Lewin, Séré, and Solovej [HLS05a, HLS05b, HLS07, HLS09a, GLS09]. As in those papers, the main difficulty of our work is the nonlinearity of the model. The more involved study of dynamical pair creation for the same model will be the subject of future work.

In the considered model, the polarized vacuum in a potential generated by a density of charge  $Z\nu$  is described by an operator  $P_Z$  on  $L^2(\mathbb{R}^3, \mathbb{C}^4)$  (a density matrix). This operator is a solution to the nonlinear equation

$$\begin{cases} P_Z &= \chi_{(-\infty, \mu]}(D_Z) + \delta \\ D_Z &= D^0 + \alpha \left( \rho_{P_Z - \frac{1}{2}} - Z\nu \right) \star |\cdot|^{-1} \end{cases} ,$$

where  $D^0 := -i\boldsymbol{\alpha} \cdot \nabla + \beta$  is the (free) Dirac operator and  $\delta$  is any self-adjoint operator such that  $0 \leq \delta \leq 1$  with  $\text{range}(\delta) \subset \ker(D_Z)$ . Discarding the operator  $\delta$ , we see that  $P_Z$  is the ground state in the grand canonical ensemble of a dressed Dirac operator with density of charge  $Z\nu$  perturbed by the density  $\rho_{P_Z - \frac{1}{2}}$  of the vacuum. The polarized vacuum therefore interacts with itself.

We shall consider the operator  $P_Z$  in the limit  $Z \rightarrow +\infty$ . Of our particular interest is the probability that pairs are generated, which is a nonlinear function of  $P_Z$  (see Section 2.1 below). The usual picture [KS77b, SS82, Hai04] is that if the first eigenvalue  $\lambda_1(Z)$  of  $D_Z$  is negative, as showed in Figure 1, then the vacuum becomes charged and the probability of creating at least one pair is 1. In the linear case, Hainzl [Hai04] showed that the charge of the vacuum in the external density  $Z\nu$  is exactly the number of eigenvalues (counted with multiplicity) of the operator  $D^0 - tZ\nu \star |\cdot|^{-1}$  crossing 0 when we increase  $t$  from 0 to 1. Here, because of the nonlinearity of the model we study, detecting for which values of  $Z$  the first eigenvalue will cross 0 is very difficult. However, the probability of pair creation can be very close to 1 without any crossing, as we will explain in Section 2.1.

FIGURE 1. Spectrum of the mean-field one body Hamiltonian  $D_Z$ .

More precisely, we prove that the probability of static pair creation behaves as  $1 - \exp(-\kappa Z^{2/3})$  (see Theorem 1.1), where  $Z$  is the charge of a nucleus put in the vacuum, and  $\kappa$  is a constant depending on different parameters of the model such as the cut-off or the shape of the nucleus. The proof relies on the large- $Z$  asymptotics of the polarized vacuum energy, which is obtained by using an appropriate trial state. This asymptotics implies that the average number of particles of the polarized vacuum is of order  $Z^{2/3}$ . We then use general estimates showing that the probability to create pairs for a quasi-free quantum state is bigger than  $1 - \exp(-\kappa' N)$ , where  $N$  is the average number of particles of the quantum state and  $\kappa'$  is a universal constant. Since for the polarized vacuum  $N \simeq Z^{2/3}$ , the result follows.

The paper is organized as follows. In Section 1 we introduce the Bogoliubov-Dirac-Fock model and we state our main result. In Section 2, we prove the general estimates on quasi-free states on Fock space, which are of independent interest. In the end of Section 2 we come back to our particular setting. In Section 3, we study the large- $Z$  asymptotics of the polarized vacuum energy. Finally, in Section 4 we prove Theorem 1.1 using the tools developed in Section 2 and 3. In Appendix A, we recall some properties of product states, which are used in Section 2.

## 2. Estimate on the probability to create pairs

**2.1. Probability to create a pair.** The first quantity to define is the probability to create a pair. Let  $\mathfrak{H}_+, \mathfrak{H}_-$  be (separable) Hilbert spaces, representing the one particle (resp. anti-particle) space. The natural space to describe a system with an arbitrary number of particles/anti-particles is the Fock space

$$\mathcal{F}_0 := \mathcal{F}(\mathfrak{H}_+) \otimes \mathcal{F}(\mathfrak{H}_-),$$

with the usual notation  $\mathcal{F}(\mathfrak{H}) := \bigoplus_{N \geq 0} \wedge_1^N \mathfrak{H}$  for any Hilbert space  $\mathfrak{H}$  and with the convention  $\wedge_1^0 \mathfrak{H} := \mathbb{C}$ . We also define the *vacuum state*  $\Omega := \Omega_+ \otimes \Omega_- \in \mathcal{F}_0$  where  $\Omega_{\pm} := 1 \oplus 0 \oplus 0 \cdots \in \mathcal{F}(\mathfrak{H}_{\pm})$ . Recall that a state over  $\mathcal{F}_0$  can be defined<sup>1</sup> as a positive linear functional  $\omega : \mathcal{B}(\mathcal{F}_0) \rightarrow \mathbb{C}$  with  $\omega(\text{Id}_{\mathcal{F}_0}) = 1$ , where  $\mathcal{B}(\mathcal{F}_0)$  is the set of all bounded linear operators on  $\mathcal{F}_0$ . Notice that any normalized  $\psi \in \mathcal{F}_0$  defines a state  $\omega_{\psi}$  (called *pure state*) by the formula  $\omega_{\psi}(A) = \langle \psi, A\psi \rangle_{\mathcal{F}_0}$ , where  $\langle \cdot, \cdot \rangle_{\mathcal{F}_0}$  is the usual inner product on  $\mathcal{F}_0$ . Following [Pic05, Corollary 4.1], [Tha92, Eq. (10.154)],

<sup>1</sup>For convenience, we will later define a state as a linear form on the tensor product of CAR algebras  $\mathfrak{A}[\mathfrak{H}_+] \otimes \mathfrak{A}[\mathfrak{H}_-] \subset \mathcal{B}(\mathcal{F}_0)$ , which in our context does not change anything since all the states we consider are normal.

and [Nen87, Section 2], we define the probability  $p(\omega)$  for a state  $\omega$  to create a particle/anti-particle pair by

$$\boxed{p(\omega) := 1 - \omega(|\Omega\rangle\langle\Omega|)}, \quad (1.2.1)$$

where  $|\Omega\rangle\langle\Omega| \in \mathcal{B}(\mathcal{F}_0)$  is the orthogonal projection on  $\mathbb{C}\Omega$ . For a pure state  $\psi = \psi_{0,0} \oplus \psi_{0,1} \oplus \psi_{1,0} \oplus \cdots \in \mathcal{F}_0$ , we have  $p(\omega_\psi) = 1 - |\psi_{0,0}|^2$ . Therefore,  $p(\omega_\psi) = 0$  if and only if  $\psi = \Omega$  (the vacuum has probability zero to create pairs), while  $p(\omega_\psi) = 1$  if and only if  $\psi_{0,0} = 0$ . In the latter case, notice that  $\psi$  does not literally contain pairs, in the sense that its number of particles may not be equal to its number of anti-particles. This definition merely measures the probability that a state contains real particles/anti-particles.

Typically,  $\Omega$  represents the free (or bare) vacuum and we want to measure the probability of a perturbation  $\Omega'$  of  $\Omega$ , representing the polarized (or dressed) vacuum in the presence of an external electric field, to have pairs. Assuming that  $\Omega'$  is a pure quasi-free state, we have the well-known formula (see e.g. [Tha92, Theorem 10.6], [BLS94, Theorem 2.2], or [HLS09a, Theorem 5])

$$\Omega' = \prod_{i \geq 1} \frac{1}{\sqrt{1 + \lambda_i^2}} \prod_{n=1}^N a_0^*(f_n) \prod_{m=1}^M b_0^*(g_m) \prod_{i \geq 1} (1 + \lambda_i a_0^*(v_i) b_0^*(u_i)) \Omega, \quad (1.2.2)$$

where  $a_0^*$  (resp.  $b_0^*$ ) is the free particle (resp. anti-particle) creation operator,  $(f_n)_n \cup (v_i)_i$  (resp.  $(g_m)_m \cup (u_i)_i$ ) is an orthonormal set for  $\mathfrak{H}_+$  (resp.  $\mathfrak{H}_-$ ), and  $(\lambda_i)_i \in \ell^2(\mathbb{R}_+)$ .

From the formula (1.2.2), we see that  $p(\omega_{\Omega'}) = 1$  as soon as  $N > 0$  or  $M > 0$ . Moreover, in this case real particles in the states  $(f_n)_n$  and real anti-particles in the states  $(g_m)_m$  have been created. In the linear case, Klaus and Scharf [KS77b] proved that  $N, M \neq 0$  if the external field is strong enough. However, there can be a high probability to create pairs even when  $N = M = 0$ . Indeed, since in this case we have

$$|\langle \Omega', \Omega \rangle_{\mathcal{F}_0}|^2 = \prod_{i \geq 1} \frac{1}{1 + \lambda_i^2},$$

one sees that  $p(\omega_{\Omega'})$  is close to 1 when the  $\lambda_i$  are large enough. One simple condition is that  $\sum_i \lambda_i^2 (1 + \lambda_i^2)^{-1}$  is large enough, by the inequality

$$\prod_{i \geq 1} \frac{1}{1 + \lambda_i^2} \leq \exp \left[ - \sum_i \frac{\lambda_i^2}{1 + \lambda_i^2} \right].$$

Note that this is indeed (half) the average total number of particle of the state  $\Omega'$  (number of particle + number of anti-particle),

$$\omega_{\Omega'}(\mathcal{N}) = 2 \sum_i \frac{\lambda_i^2}{1 + \lambda_i^2},$$

where  $\mathcal{N}$  is the usual number operator on  $\mathcal{F}_0$  (see formula (1.3.22)). Hence  $p(\omega_{\Omega'})$  is close to 1 when  $\omega_{\Omega'}(\mathcal{N})$  is large enough. While the non-vanishing  $N, M$  case can be interpreted as the creation of real particles, this second explanation for an increasing  $p(\omega_{\Omega'})$  can be interpreted as a “virtual pair creation”. In this article, we study an analog of “virtual pair creation” for more general states than those given by formula (1.2.2).

**2.2. Static pair creation in the reduced BDF approximation.** For non-interacting electrons in an external field  $V$ , the polarized vacuum  $\Omega'$  is the unique Hartree-Fock state whose density matrix is [KS77b, Hai04]

$$P = \chi_{(-\infty, \mu]}(D^0 + V).$$

In this article, we will rather use the reduced Bogoliubov-Dirac-Fock approximation, a non-linear model enabling to describe an interacting vacuum in which  $V$  is a function of  $P$  itself. It was introduced by Hainzl, Lewin, Séré and Solovej in a series of articles [HLS05a, HLS05b, HLS07, HLS09a] after the pioneering work of Chaix, Iracane, and Lions [CI89, CIL89]. We will now briefly recall the model and the results needed for our study.

In units where  $m = c = \hbar = 1$ , the reduced Bogoliubov-Dirac-Fock (rBDF) energy functional is the (formal) difference between the energy of the state  $P$  and that of the free vacuum  $P_-^0 = \chi_{(-\infty, \mu]}(D^0)$ , with the exchange term dropped. It depends only on the variable  $Q = P - P_-^0$ ,

$$\mathcal{E}_\nu^{\text{rBDF}}(Q) := \text{Tr}_0(D^0 Q) - \alpha D(\rho_Q, \nu) + \frac{\alpha}{2} D(\rho_Q, \rho_Q). \quad (1.2.3)$$

Here,  $\alpha > 0$  is the coupling constant and  $\nu : \mathbb{R}^3 \rightarrow \mathbb{R}$  is the external charge density belonging to the Coulomb space

$$\mathcal{C} := \left\{ f \in \mathcal{S}'(\mathbb{R}^3) : \int_{\mathbb{R}^3} \frac{|\widehat{f}(k)|^2}{|k|^2} dk < +\infty \right\},$$

endowed with the inner product  $D(\rho_1, \rho_2) = \int |k|^{-2} \widehat{\rho}_1(k) \overline{\widehat{\rho}_2(k)}$  (the hat denotes the Fourier transform<sup>2</sup>). We also use the notation  $\|\rho\|_{\mathcal{C}} = D(\rho, \rho)^{1/2}$  for any  $\rho \in \mathcal{C}$ . In order to define the domain of the rBDF energy functional, let us fix a cut-off  $\Lambda > 0$  and define the one-particle Hilbert space

$$\mathfrak{H}_\Lambda := \left\{ f \in L^2(\mathbb{R}^3, \mathbb{C}^4), \quad \text{supp } \widehat{f} \subset B(0, \Lambda) \right\}.$$

The operator  $D^0 = -i\boldsymbol{\alpha} \cdot \nabla + \beta$  is the usual Dirac operator on  $L^2(\mathbb{R}^3, \mathbb{C}^4)$ , where  $\alpha_1, \alpha_2, \alpha_3, \beta$  are the Dirac matrices acting on  $\mathbb{C}^4$ ,

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad i = 1, 2, 3, \quad \beta = \begin{pmatrix} \text{Id}_{\mathbb{C}^2} & 0 \\ 0 & -\text{Id}_{\mathbb{C}^2} \end{pmatrix},$$

<sup>2</sup>Our convention is  $\widehat{f}(k) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} f(x) e^{-ik \cdot x} dx, \quad \forall k \in \mathbb{R}^3$ .



and  $(\sigma_i)_{i=1,2,3}$  are the Pauli matrices,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The operator  $D^0$  stabilizes  $\mathfrak{H}_\Lambda$ , and its restriction to  $\mathfrak{H}_\Lambda$  defines a bounded operator on  $\mathfrak{H}_\Lambda$ , which we still denote by  $D^0$ . For convenience we introduce  $P_+^0 := 1 - P_-^0$ . We denote by  $\mathfrak{S}_p(\mathfrak{H})$  the Schatten class of all bounded operators  $A$  on the Hilbert space  $\mathfrak{H}$  such that  $\text{Tr}(|A|^p) < \infty$ . For any operator  $Q$  on  $\mathfrak{H}_\Lambda$  and for any  $\varepsilon, \varepsilon' \in \{+, -\}$ , we let  $Q_{\varepsilon\varepsilon'} := P_\varepsilon^0 Q P_{\varepsilon'}^0$  and we define

$$\mathfrak{S}_{1,P_-^0}(\mathfrak{H}_\Lambda) := \{Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda), \quad Q_{++}, Q_{--} \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)\}.$$

It is a Banach space endowed with the norm

$$\|Q\|_{1,P_-^0} := \|Q_{++}\|_{\mathfrak{S}_1} + \|Q_{--}\|_{\mathfrak{S}_1} + \|Q_{+-}\|_{\mathfrak{S}_2} + \|Q_{-+}\|_{\mathfrak{S}_2}.$$

For any  $Q \in \mathfrak{S}_{1,P_-^0}(\mathfrak{H}_\Lambda)$ , we define its generalized trace by

$$\text{Tr}_0(Q) := \text{Tr}(Q_{++} + Q_{--}),$$

and its density  $\rho_Q$  by  $\rho_Q(x) := \text{Tr}_{\mathbb{C}^4}(Q(x, x))$  for all  $x \in \mathbb{R}^3$ , where  $Q(x, y)$  denotes the  $4 \times 4$  matrix kernel of  $Q$ . This density  $\rho_Q$  is well defined since  $\text{supp } \widehat{Q}(\cdot, \cdot) \subset B(0, \Lambda) \times B(0, \Lambda)$  implies that  $Q(\cdot, \cdot)$  is smooth. Furthermore, it is proved in [HLS09a, Lemma 1] that  $\rho_Q \in L^2(\mathbb{R}^3) \cap \mathcal{C}$  for any  $Q \in \mathfrak{S}_{1,P_-^0}(\mathfrak{H}_\Lambda)$ . We conclude that the rBDF energy functional is well-defined on the convex set

$$\mathcal{K} := \left\{ Q \in \mathfrak{S}_{1,P_-^0}(\mathfrak{H}_\Lambda), \quad Q = Q^*, \quad -P_-^0 \leq Q \leq 1 - P_-^0 \right\}. \quad (1.2.4)$$

Notice that the kinetic part of the rBDF energy is well defined since

$$\text{Tr}_0(D^0 Q) = \text{Tr}(|D^0|(Q_{++} - Q_{--})).$$

The variational set  $\mathcal{K}$  is the convex hull of  $\{P - P_-^0, P = P^2 = P^*, P - P_-^0 \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)\}$ , where  $P$  is the density matrix of a pure Hartree-Fock state, which is a Hilbert-Schmidt perturbation of the free vacuum  $P_-^0$ . The rigorous derivation of the rBDF energy functional and the motivation for this functional setting can be found in [HLS07, HLS05a].

For any  $Z > 0$  and  $\nu \in \mathcal{C}$ , the rBDF energy functional  $\mathcal{E}_{\text{rBDF}}^{Z\nu}$  admits global minimizers  $Q_Z$  on  $\mathcal{K}$ . Minimizers are not necessarily unique, but they always share the same density  $\rho_Z := \rho_{Q_Z}$ . Any minimizer  $Q_Z$  satisfies the self-consistent equation

$$\begin{cases} Q_Z &= \chi_{(-\infty, \mu]}(D_Z) - P_-^0 + \delta \\ D_Z &= D^0 + \alpha(\rho_Z - Z\nu) \star |\cdot|^{-1} \end{cases}, \quad (1.2.5)$$

where  $\delta$  is a self-adjoint operator such that  $0 \leq \delta \leq 1$  and  $\text{range}(\delta) \subset \ker(D_Z)$ . Hence, uniqueness holds if and only if  $\ker(D_Z) = \{0\}$ . Notice that since the density  $\rho_Z$  is unique, the operator  $D_Z$  is itself unique. Any minimizer of  $\mathcal{E}_{\text{rBDF}}^{Z\nu}$  on  $\mathcal{K}$  is interpreted as a generalized one-particle density matrix of a BDF state  $\omega_{\text{vac}}^{Z\nu}$  (see

Section 3.6) representing the *polarized vacuum* in the potential  $Z\nu \star |\cdot|^{-1}$ . When there is a unique minimizer  $Q_Z$ , it is a difference of two projectors and hence it is the generalized one-particle density matrix of a pure state. We emphasize that there is no charge constraint in this minimization problem: In fact, the polarized vacuum could (and should) be charged when  $Z$  is very large. In this case, one may think that an electron-positron pair is created, with the positron sent to infinity.

We want to estimate  $p(\omega_{\text{vac}}^{Z\nu})$  in terms of  $Z$ , and confirm the picture that the stronger the field, the more pairs are created. As a consequence, we will fix a non-zero density  $\nu$  (interpreted as the shape of the external charge density) and study  $p_Z := p(\omega_{\text{vac}}^{Z\nu})$  for  $Z > 0$  large. Our main result is the following.

**Theorem 1.1.** *Let  $\alpha > 0$  and  $\Lambda > 0$ . Let  $\nu \in \mathcal{C}$  such that  $\int_{\mathbb{R}^3} (1 + |x|)|\nu(x)| dx < \infty$  and  $q := \int_{\mathbb{R}^3} \nu \neq 0$ . Then, there exists a constant  $Z_1 > 0$  and a constant  $\kappa > 0$  such that for all  $Z > Z_1$  we have*

$$\boxed{p_Z \geq 1 - e^{-\kappa Z^{2/3}}.} \quad (1.2.6)$$

The constant  $Z_1$  is equal to  $\widetilde{Z}_1 / \int_{\mathbb{R}^3} |\nu|$  where  $\widetilde{Z}_1$  is defined in Equation (1.4.34) and  $\widetilde{Z}_1$  depends only on  $\Lambda$ ,  $\alpha$ ,  $|q|$ , and  $\int_{\mathbb{R}^3} |x||\nu|$ . The constant  $\kappa$  equals  $0.0941248 \dots \times C(\int_{\mathbb{R}^3} |\nu|)^{2/3}$ , where  $C$  is defined in Equation (1.4.35) below.

**Remark 1.1.** The assumption  $|x|\nu \in L^1(\mathbb{R}^3)$  allows us to have an explicit estimate. If we remove this assumption, we can still prove the weaker result that  $p_Z \rightarrow 1$  as  $Z \rightarrow \infty$ . In the sequel, by rescaling  $Z$  if needed, we will assume that

$$\boxed{\int_{\mathbb{R}^3} |\nu| = 1.}$$

If  $\int \nu = 0$ , we expect an asymptotics lower than  $Z^{2/3}$ , but we are unable to prove it.

**Remark 1.2.** We will see that  $Z_1 \sim \text{const.} \times \alpha^{-3/2}$  as  $\alpha \rightarrow 0$ .

Theorem 1.1 says that in a very strong field,  $Z \gg 1$ , the probability to create at least one electron-positron pair is very close to 1. It is reasonable to think that for some sufficiently large  $Z$ , the first eigenvalue of  $D_Z$  crosses 0 in which case  $p_Z = 1$ . However, determining the behaviour of the eigenvalue of  $D_Z$  as  $Z$  increases is difficult because of the nonlinearity of the model and because we are in a regime far from being perturbative. For all these reasons, the estimate (1.2.6) on  $p_Z$  is the best we have so far. For very large  $Z$ , one expects that many electron-positron pairs will be generated. We conjecture that we have indeed  $\omega_{\text{vac}}^{Z\nu}(\mathcal{P}_k) \rightarrow 0$  as  $Z \rightarrow +\infty$  for all  $k \in \mathbb{N}$ , where  $\mathcal{P}_k$  is the orthogonal projector on the  $k$ -particle space in Fock space (see Section 3). This would mean that for large  $Z$ , the probability to create at least  $k$ -pairs is very close to 1. Our method of proof only gives this result for  $k = 0$ . However, if we assume that  $\omega_{\text{vac}}^{Z\nu}$  is a *pure* quasi-free state for all  $Z$  large enough (which is the case if  $0 \notin \sigma(D_Z)$ ), then the conjecture follows from Proposition 1.3 below.

**Remark 1.3.** Our method can also be applied when the exchange term is included, leading to an estimate similar to (1.2.6). For the sake of simplicity, we shall only make remarks on how to deal with this more general model. With exchange term, the free vacuum has to be modified [HLS07]. It is described by an orthogonal projection  $\mathcal{P}_-$  on  $\mathfrak{H}_\Lambda$ , which is the negative spectral projection of an effective free Dirac operator  $\mathcal{D}^0$ . Then,  $P_-^0$  and  $D^0$  are replaced by  $\mathcal{P}_-$  and  $\mathcal{D}^0$  everywhere. The BDF energy now contains an exchange term:

$$\mathcal{E}_\nu^{\text{BDF}}(Q) := \text{Tr}_{\mathcal{P}_-}(\mathcal{D}^0 Q) - \alpha D(\nu, \rho_Q) + \frac{\alpha}{2} D(\rho_Q, \rho_Q) - \frac{\alpha}{2} \iint \frac{|Q(x, y)|^2}{|x - y|} dx dy.$$

By Lieb's variational principle, minimizers can always be chosen to be pure, which means that  $Q + \mathcal{P}_-$  is a projection. Using Proposition 1.3 below, we are able to provide an estimate on the probability to create at least  $k$ -pairs in this case. In Remarks 1.13 and 1.15, we will explain how to adapt our result to this setting.

**Remark 1.4.** From a physical point of view, fixing the cut-off  $\Lambda$  while taking  $Z \rightarrow +\infty$  might lead to an underestimation of  $p_Z$ . Without the cut-off, we expect the energy to be of order  $Z^2$  for large  $Z$  (see Remark 1.12). which would lead to replacing  $Z^{2/3}$  by  $Z$  in (1.2.6). With the cut-off, the particles of the vacuum cannot fully react to the huge energy brought by the external potential.

**2.3. Strategy of the proof.** The proof contains two parts. The first one consists in estimating the vacuum expectation  $\omega(|\Omega\rangle\langle\Omega|)$  for a quasi-free state  $\omega$ , in terms of its average number of particle  $\omega(\mathcal{N})$ . These estimates are of independent interest and therefore we also provide several other estimates for the distribution of quasi-free states in the  $k$ -particle spaces. These results are contained in Section 3.

In a second part, we prove an estimate on the energy of the polarized vacuum,

$$E(Z) := \mathcal{E}_{Z\nu}^{\text{rBDF}}(Q_{\text{vac}}^{Z\nu}) = \inf \{ \mathcal{E}_{Z\nu}^{\text{rBDF}}(Q), \quad Q \in \mathcal{K} \}, \quad (1.2.7)$$

from above by  $-cZ^{5/3}$ . We will also give a lower bound  $E(Z) \gtrsim -Z^{5/3}$  to show that the power  $5/3$  is optimal, although we only need the upper bound for the proof of Theorem 1.1. From this estimate, we then infer that the average number of particles (counted relatively to that of the free vacuum, see Section 3.6) in the polarized vacuum satisfies

$$\text{Tr}((Q_{\text{vac}}^{Z\nu})_{++} - (Q_{\text{vac}}^{Z\nu})_{--}) \gtrsim Z^{2/3}.$$

The precise statements of these results and their proofs can be found in Section 4. Finally, in Section 5, we combine the two parts and prove Theorem 1.1.

### 3. On the distribution of quasi-free states in the $k$ -particle spaces

In this section, we consider general quasi-free states. Only in Section 3.6 we come back to our particular situation of pair creation. We start by introducing the notation used throughout this section.

**3.1. Notation.** Let  $(\mathfrak{H}, \langle \cdot, \cdot \rangle)$  be a complex, separable Hilbert space whose inner product  $\langle \cdot, \cdot \rangle$  is linear in the second argument. We also need an anti-linear operator  $J : \mathfrak{H} \rightarrow \mathfrak{K}$  such that  $J^*J = \text{Id}_{\mathfrak{H}}$ , where  $(\mathfrak{K}, \langle \cdot, \cdot \rangle_{\mathfrak{K}})$  is another complex Hilbert space<sup>3</sup>. Let  $\mathcal{F} := \bigoplus_{N \geq 0} \mathfrak{H}^N$  be the associated Fock space with  $\mathfrak{H}^N := \wedge_1^N \mathfrak{H}$ . We still denote by  $\Omega = 1 \oplus 0 \oplus \cdots \in \mathcal{F}$  the vacuum vector. For  $k \in \mathbb{N}$ , we denote by  $\mathcal{P}_k \in \mathcal{B}(\mathcal{F})$  the orthogonal projection on  $\mathfrak{H}^k \subset \mathcal{F}$ . We recall from Section 2.1 that  $\mathcal{B}(\mathcal{F})$  is the space of all linear bounded operators on  $\mathcal{F}$ . Let  $\mathfrak{A}[\mathfrak{H}]$  be the CAR unital  $C^*$ -subalgebra of  $\mathcal{B}(\mathcal{F})$  generated by the usual creation (resp. annihilation operators)  $a^*(f)$  (resp.  $a(f)$ ), for  $f \in \mathfrak{H}$ . We denote by  $\mathcal{N}$  the particle number operator on  $\mathcal{F}$ ,

$$\mathcal{N} := \bigoplus_{k \geq 0} k \text{Id}_{\mathfrak{H}^k} = \sum_{i \geq 0} a^*(f_i) a(f_i)$$

for any orthonormal basis  $(f_i)_{i \geq 0}$  in  $\mathfrak{H}$ . Then  $\mathcal{P}_k = \mathbf{1}_{\{\mathcal{N}=k\}}$  for all  $k \in \mathbb{N}$ . A state on  $\mathfrak{A}[\mathfrak{H}]$  is a non-negative linear functional  $\omega : \mathfrak{A}[\mathfrak{H}] \rightarrow \mathbb{C}$  which is normalized:  $\omega(\text{Id}_{\mathcal{F}}) = 1$ . A state  $\omega$  is called *normal* if there exists a non-negative operator  $G$  on  $\mathcal{F}$  (sometimes called the density matrix of  $\omega$ ) such that  $\text{Tr}_{\mathcal{F}}(G) = 1$  and  $\omega(A) = \text{Tr}_{\mathcal{F}}(GA)$  for all  $A \in \mathfrak{A}[\mathfrak{H}]$ . Of particular interest are the *pure* states which are normal states with  $G = |\psi\rangle\langle\psi|$  for  $\psi \in \mathcal{F}$  with  $\|\psi\|_{\mathcal{F}} = 1$ . We define the average particle number of  $\omega$  as

$$\omega(\mathcal{N}) := \sum_{i \geq 0} \omega(a^*(f_i) a(f_i)) \in [0, +\infty].$$

The *one-particle density matrix* (1-pdm)  $\gamma$  of  $\omega$  is the operator defined by

$$\langle g, \gamma f \rangle := \omega(a^*(f) a(g)),$$

for all  $f, g \in \mathfrak{H}$ . It is a self-adjoint operator on  $\mathfrak{H}$ , satisfying  $0 \leq \gamma \leq 1$ . In the same fashion, we define its *pairing matrix*  $\alpha : \mathfrak{K} \rightarrow \mathfrak{H}$  which is a linear operator on  $\mathfrak{K}$  by

$$\langle \alpha J f, g \rangle := \omega(a^*(f) a^*(g)),$$

for all  $f, g \in \mathfrak{H}$ . It satisfies  $(\alpha J)^* = -\alpha J$ . Moreover, if we define the operator  $\Gamma(\gamma, \alpha)$  on  $\mathfrak{H} \oplus \mathfrak{K}$  by block

$$\Gamma(\gamma, \alpha) := \begin{pmatrix} \gamma & \alpha \\ \alpha^* & 1 - J\gamma J^* \end{pmatrix}, \quad (1.3.8)$$

then  $0 \leq \Gamma(\gamma, \alpha) \leq 1$ , see [BLS94, Lemma 2.1]. This last relation implies that

$$\gamma^2 + \alpha\alpha^* \leq \gamma, \quad (1.3.9)$$

---

<sup>3</sup>Recall that the adjoint  $J^*$  of an anti-linear operator is defined as  $\langle J^* f, g \rangle := \langle J g, f \rangle_{\mathfrak{K}}$  for all  $f \in \mathfrak{K}$  and  $g \in \mathfrak{H}$ . Typically, one chooses  $\mathfrak{K} = \mathfrak{H}$  and  $J$  the complex conjugation, or  $\mathfrak{K} = \mathfrak{H}^*$  and  $J(f) = \langle f, \cdot \rangle$  [Sol07]. Here we keep  $\mathfrak{K}$  abstract because this will be useful for the construction of BDF states in Section 3.6.

in the sense of quadratic forms on  $\mathfrak{H}$ . Notice also that  $\omega(\mathcal{N}) = \text{Tr}(\gamma)$ . A state  $\omega$  is called *quasi-free* if for any operators  $e_1, \dots, e_{2p}$  which are either a  $a^*(f)$  or a  $a(g)$  for any  $f, g \in \mathfrak{H}$ , then  $\omega(e_1 e_2 \dots e_{2p-1}) = 0$  for any  $p \geq 1$  and

$$\omega(e_1 e_2 \dots e_{2p}) = \sum_{\pi \in \widetilde{\mathcal{S}}_{2p}} (-1)^{\varepsilon(\pi)} \omega(e_{\pi(1)} e_{\pi(2)}) \dots \omega(e_{\pi(2p-1)} e_{\pi(2p)}), \quad (1.3.10)$$

where  $\widetilde{\mathcal{S}}_{2p}$  is the set of permutations of  $\{1, \dots, 2p\}$  which verify  $\pi(1) < \pi(3) < \dots < \pi(2p-1)$  and  $\pi(2j-1) < \pi(2j)$  for all  $1 \leq j \leq p$ , and  $\varepsilon(\pi)$  is the parity of the permutation  $\pi$ . The relation (1.3.10) is called the Wick formula. From this definition, we see that a quasi-free state is completely determined by its density matrices  $(\gamma, \alpha)$ . We recall [BLS94, Theorem 2.3]

**Proposition 1.1.** *For any  $(\gamma, \alpha)$  such that  $0 \leq \Gamma(\gamma, \alpha) \leq 1$  with additionally  $\text{Tr}(\gamma) < +\infty$ , there exists a unique quasi-free state  $\omega$  on  $\mathfrak{A}[\mathfrak{H}]$  with finite number of particles such that  $\gamma$  is its 1-particle density matrix and  $\alpha$  its pairing matrix. Furthermore,  $\omega$  is normal: there exists  $G : \mathcal{F} \rightarrow \mathcal{F}$  with  $0 \leq G \leq 1$  and  $\text{Tr}_{\mathcal{F}}(G) = 1$  such that  $\omega(A) = \text{Tr}_{\mathcal{F}}(GA)$  for all  $A \in \mathfrak{A}[\mathfrak{H}]$ .*

Now, we need some terminology, which is not universal in the literature. We call *Hartree-Fock* (HF) states the quasi-free states with  $\text{Tr}(\gamma) < +\infty$  and  $\alpha = 0$ , because when such states are pure, they are usual Slater determinants. Quasi-free states with  $\text{Tr}(\gamma) < +\infty$  and  $\alpha \neq 0$ , are called *Hartree-Fock-Bogoliubov* (HFB) states. Pure HFB states are particularly simple since they are Bogoliubov rotations of the vacuum  $\Omega$ . The aim of this section is to study the distribution of quasi-free states in the particle subspaces  $\mathfrak{H}^k$ , in terms of  $\text{Tr}(\gamma)$ . Our results are different for HF or HFB, pure or mixed states.

**3.2. Motivation.** Quasi-free states are also called *Gaussian* states, in particular because they can be written as (limits of) Gibbs states of quadratic Hamiltonians (i.e. normal states with density matrices  $e^{-\beta\mathbb{H}}/\text{Tr}(e^{-\beta\mathbb{H}})$ , where  $\mathbb{H}$  is a quadratic Hamiltonian). The Gaussian character of quasi-free states is however deeper. In this section we will show that the distribution of a quasi-free state  $\omega$  over the different  $\mathfrak{H}^k$ , that is  $(\omega(\mathcal{P}_k))_{k \geq 0}$ , also has some Gaussian characteristics. More precisely, we will provide estimates of the form

$$\omega(\mathcal{P}_k) \leq c_k e^{-c' \omega(\mathcal{N})}.$$

This estimate means that a quasi-free state which has a large average number of particles  $\omega(\mathcal{N}) \gg 1$  necessarily has an exponentially small vacuum expectation

$$\omega(|\Omega\rangle\langle\Omega|) \leq c_0 e^{-c' \omega(\mathcal{N})}.$$

Let us explain the picture in a commutative setting. Let  $f(x) = \pi^{-1/2} e^{-|x-a|^2}$  for  $a \in \mathbb{R}_+$  be a Gaussian function such that  $\int_{\mathbb{R}} f = 1$ . Then  $a = \int_{\mathbb{R}} x f(x) dx$

is the average position of  $f$ , as described in Figure 2. Now if  $a$  goes to  $+\infty$ , the whole function moves to infinity and in particular  $f(0)$  becomes smaller and smaller:  $f(0) = \pi^{-1/2}e^{-a^2}$ . In other words, as the average position of  $f$  goes to infinity,  $f(0)$  goes to zero (and this is true for any  $f(x_0)$  with  $x_0$  fixed). We will prove a similar fact for quasi-free states. Indeed, for any quasi-free state  $\omega$  we have  $1 = \omega(\text{Id}_{\mathcal{F}}) = \sum_{k \geq 0} \omega(\mathcal{P}_k)$ , which is the analog of  $\int_{\mathbb{R}} f(x) dx = 1$ . We also know that  $\omega(\mathcal{N}) = \sum_{k \geq 0} k\omega(\mathcal{P}_k)$  is the average number of particle of  $\omega$ ; it is the analog of  $\int_{\mathbb{R}} xf(x) dx$ . We want to prove that when  $\omega(\mathcal{N})$  is large, then the main part of  $\omega$  lives in the high- $k$  particle spaces, that is  $\omega$  “follows” its average number of particles, as shown in Figure 2. The analog of  $f(0)$  in this case is  $\omega(|\Omega\rangle\langle\Omega|)$  and we thus want to prove that  $\omega(|\Omega\rangle\langle\Omega|)$  goes to zero as  $\omega(\mathcal{N})$  goes to  $+\infty$ , for any quasi-free state  $\omega$ . A natural extension of this result would be that  $\omega(\mathcal{P}_{k_0})$  also goes to zero for any fixed  $k_0$ .

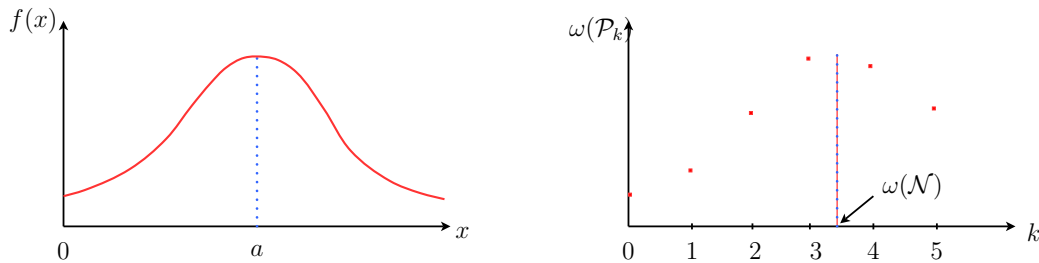


FIGURE 2. Analogy between a Gaussian function and a quasi-free state

We will provide explicit estimates depending on the properties of the quasi-free state (pure, mixed, HF or HFB). In the most general case of mixed HFB states, we only derive a bound on the vacuum expectation. The following table tells us where each case is treated.

	Pure	Mixed
HF ( $\alpha = 0$ )	Section 3.3	
HFB ( $\alpha \neq 0$ )	Section 3.4	Section 3.5

In spite of their usefulness, we have not found the following estimates in the literature. One main reason is probably that  $e^{-\beta\mathcal{N}}$  does *not* belong to the CAR algebra, hence  $\omega(e^{-\beta\mathcal{N}})$  only makes sense for normal states.

**Remark 1.5.** A useful tool for the proofs of the following results is the notion of *product state*. A product state  $\otimes_i \omega_i$  is a state on  $\mathcal{F}(\oplus_i \mathfrak{H}_i) \simeq \otimes_i \mathcal{F}(\mathfrak{H}_i)$  when each  $\omega_i$  is a state on  $\mathcal{F}(\mathfrak{H}_i)$ . While this notion is intuitive, we recall how it is precisely defined in Appendix A.

### 3.3. Hartree-Fock case.

**Proposition 1.2** (HF case). *Let  $\omega$  be a quasi-free state with  $\text{Tr}(\gamma) < +\infty$  and  $\alpha = 0$ . Then for any  $\beta \geq 0$  we have*

$$\boxed{\omega(e^{-\beta\mathcal{N}}) = \text{Det}_{\mathfrak{H}}(1 + (e^{-\beta} - 1)\gamma)}. \quad (1.3.11)$$

We also have the following estimate

$$\boxed{\omega(\mathcal{P}_k) \leq \frac{(e \text{Tr}(\gamma))^k}{k!} e^{-\text{Tr}(\gamma)},} \quad (1.3.12)$$

for all  $k \geq k_0$  while  $\omega(\mathcal{P}_k) = 0$  if  $k < k_0$ , where  $k_0 := \dim \ker(\gamma - 1)$ .

**Remark 1.6.** This estimate implies that for any fixed  $k \in \mathbb{N}$ ,  $\omega(\mathcal{P}_k) \rightarrow 0$  as  $\text{Tr}(\gamma) \rightarrow +\infty$ , which is the expected behaviour.

**Remark 1.7.** A more theoretical corollary of (1.3.11) is that for any fixed  $f : \mathbb{N} \rightarrow \mathbb{C}$  vanishing at infinity,  $\omega(f(\mathcal{N}))$  goes to zero as  $\text{Tr}(\gamma)$  goes to  $+\infty$ . This uses the fact that the algebra of these  $f$ s is generated by the  $(e^{-\beta})_{\beta \geq 0}$ . In the same fashion, one can also prove that  $\omega(K) \rightarrow 0$  as  $\text{Tr}(\gamma) \rightarrow +\infty$ , for any fixed compact operator  $K$ .

**PROOF.** Since  $\gamma$  is trace-class it can be diagonalized in an orthonormal basis  $(f_i)_{i \in \mathbb{N}}$ ,  $\gamma = \sum_{i \geq 0} \lambda_i |f_i\rangle\langle f_i|$ . For all  $i$ , let  $\omega_i$  be the unique quasi-free state on  $\mathcal{F}(\mathbb{C}f_i)$  having  $\lambda_i \text{Id}_{\mathbb{C}f_i}$  as 1-pdm and  $0_{\mathbb{C}f_i}$  as its pairing matrix. Then by Proposition 1.9 in Appendix A, one has  $\omega = \otimes_i \omega_i$ . Moreover, since

$$Te^{-\beta\mathcal{N}}T^* = \bigotimes_{i \in \mathbb{N}} (1 + (e^{-\beta} - 1)a^*(f_i)a(f_i)),$$

where  $T$  is the isometry between  $\mathcal{F}(\oplus_i \mathfrak{H}_i)$  and  $\otimes_i \mathcal{F}(\mathfrak{H}_i)$  defined in Appendix A, we have

$$\begin{aligned} \omega(e^{-\beta\mathcal{N}}) &= \prod_{i \in \mathbb{N}} \omega_i(1 + (e^{-\beta} - 1)a^*(f_i)a(f_i)) = \prod_{i \in \mathbb{N}} (1 + (e^{-\beta} - 1)\lambda_i) \\ &= \text{Det}_{\mathfrak{H}}(1 + (e^{-\beta} - 1)\gamma). \end{aligned}$$

To prove (1.3.12), we notice that for all  $\beta \geq 0$ ,  $\omega(e^{-\beta\mathcal{N}}) = \sum_{k \geq 0} e^{-\beta k} \omega(\mathcal{P}_k)$ , and we identify the coefficients of  $e^{-\beta k}$  in  $\prod_{i \in \mathbb{N}} (1 + (e^{-\beta} - 1)\lambda_i)$ . This yields

$$\begin{aligned} \omega(\mathcal{P}_k) &= \sum_{\substack{I \subset \mathbb{N} \\ \#I=k}} \prod_{i \in I} \lambda_i \prod_{j \notin I} (1 - \lambda_j) \\ &\leq \sum_{\substack{I \subset \mathbb{N} \\ \#I=k}} \left( \prod_{i \in I} \lambda_i \right) e^{-\sum_{j \notin I} \lambda_j} \\ &\leq e^{-\text{Tr}(\gamma)} \sum_{\substack{I \subset \mathbb{N} \\ \#I=k}} \prod_{i \in I} \lambda_i e^{\lambda_i} \\ &\leq \frac{e^k}{k!} e^{-\text{Tr}(\gamma)} \sum_{i_1, \dots, i_k \in \mathbb{N}} \lambda_{i_1} \cdots \lambda_{i_k} = \frac{(e \text{Tr}(\gamma))^k}{k!} e^{-\text{Tr}(\gamma)}, \end{aligned}$$

where we used that  $0 \leq \lambda_i \leq 1$  for all  $i$ . Notice from the first equality that  $\omega(\mathcal{P}_k) = 0$  if  $k < \dim \ker(\gamma - 1)$ .  $\square$

### 3.4. Pure Hartree-Fock-Bogoliubov case.

**Proposition 1.3** (Pure HFB case). *Let  $\omega$  a quasi-free pure state with  $\text{Tr}(\gamma) < +\infty$ . Then for any  $\beta \geq 0$  we have*

$$\omega(e^{-\beta\mathcal{N}}) = \text{Det}_{\mathfrak{H}} \sqrt{1 + (e^{-2\beta} - 1)\gamma}. \quad (1.3.13)$$

We also have the following estimate for all  $k = k_0 + 2\ell$  with  $k_0 := \dim \ker(\gamma - 1)$  and  $\ell \geq 0$

$$\omega(\mathcal{P}_k) \leq \frac{e^{k/2}}{\ell!} \left( \frac{\text{Tr}(\gamma)}{2} \right)^\ell e^{-\frac{\text{Tr}(\gamma)}{2}}, \quad (1.3.14)$$

while  $\omega(\mathcal{P}_k) = 0$  if  $k < k_0$  or  $k = k_0 + 2\ell + 1$ .

**PROOF.** It is well-known [BLS94, Theorem 2.6] that  $\omega$  is pure if and only if  $\Gamma(\gamma, \alpha)^2 = \Gamma(\gamma, \alpha)$ , which is equivalent to  $\gamma^2 + \alpha\alpha^* = \gamma$  and  $[\gamma, \alpha J] = 0$ . The operator  $\gamma$  is trace-class and  $\alpha J$  is anti-hermitian and Hilbert-Schmidt, hence both  $\gamma$  and  $\alpha J$  are diagonalizable. Since they commute, they are simultaneously diagonalizable. Remember that any anti-hermitian can be diagonalized in  $1 \times 1$  blocks corresponding to its kernel and  $2 \times 2$  blocks. Hence there exists a decomposition  $\mathfrak{H} = \bigoplus_{i \geq 0} \mathfrak{H}_i$ , with  $\dim(\mathfrak{H}_i) \leq 2$  such that

- For all  $i$ ,  $\gamma$  and  $\alpha J$  stabilize  $\mathfrak{H}_i$ ;
- If  $\dim(\mathfrak{H}_i) = 1$  then  $\gamma|_{\mathfrak{H}_i} = \lambda_i \text{Id}_{\mathfrak{H}_i}$ ,  $\alpha J|_{\mathfrak{H}_i} = 0$ ;
- If  $\dim(\mathfrak{H}_i) = 2$  then  $\gamma|_{\mathfrak{H}_i} = \begin{pmatrix} \lambda_i & 0 \\ 0 & \lambda_i \end{pmatrix}$ ,  $\alpha J|_{\mathfrak{H}_i} = \begin{pmatrix} 0 & \alpha_i \\ -\alpha_i & 0 \end{pmatrix}$  with  $\alpha_i \in \mathbb{R}$  and  $\alpha_i^2 = \lambda_i - \lambda_i^2$ .



In particular,  $\omega = \otimes_{i \geq 0} \omega_i$  where  $\omega_i$  is the quasi-free state on  $\mathcal{F}(\mathfrak{H}_i)$  with 1-pdm  $\gamma|_{\mathfrak{H}_i} =: \gamma_i$  and pairing matrix  $\alpha J|_{\mathfrak{H}_i}$ . Let us now prove that for all  $i$

$$\omega_i(e^{-\beta \mathcal{N}_i}) = \text{Det}_{\mathfrak{H}_i} \sqrt{1 + (e^{-2\beta} - 1)\gamma_i}, \quad (1.3.15)$$

where  $\mathcal{N}_i$  is the number operator on  $\mathcal{F}(\mathfrak{H}_i)$ . First we consider the case  $\dim(\mathfrak{H}_i) = 1$ , and let  $f_i \in \mathfrak{H}_i$  be a normalized vector. Then  $\mathcal{F}(\mathfrak{H}_i) = \mathbb{C} \oplus \mathbb{C}f_i$  and  $\mathcal{N}_i = a^*(f_i)a(f_i)$  so that  $e^{-\beta \mathcal{N}_i} = 1 + (e^{-\beta} - 1)a^*(f_i)a(f_i)$ . Therefore

$$\omega_i(e^{-\beta \mathcal{N}_i}) = 1 + (e^{-\beta} - 1)\lambda_i.$$

Since  $\gamma^2 + \alpha\alpha^* = \gamma$ , we have  $\alpha_i = 0$  if  $\dim(\mathfrak{H}_i) = 1$  hence  $\lambda_i = 0$  or  $\lambda_i = 1$ . In both cases we have

$$\omega_i(e^{-\beta \mathcal{N}_i}) = \text{Det}_{\mathfrak{H}_i} \sqrt{1 + (e^{-2\beta} - 1)\gamma_i}.$$

Now suppose  $\dim(\mathfrak{H}_i) = 2$  and let  $(f_i, g_i)$  be an orthonormal basis of  $\mathfrak{H}_i$  such that in this basis  $\gamma|_{\mathfrak{H}_i}$  and  $\alpha J|_{\mathfrak{H}_i}$  have the form given above. Then  $\mathcal{F}(\mathfrak{H}_i) = \mathbb{C} \oplus \mathbb{C}f_i \oplus \mathbb{C}g_i \oplus \mathbb{C}f_i \wedge g_i$  and  $\mathcal{N}_i = a^*(f_i)a(f_i) + a^*(g_i)a(g_i)$ , so that

$$e^{-\beta \mathcal{N}_i} = (1 + (e^{-\beta} - 1)a^*(f_i)a(f_i))(1 + (e^{-\beta} - 1)a^*(g_i)a(g_i)).$$

We deduce that

$$\begin{aligned} \omega_i(e^{-\beta \mathcal{N}_i}) &= 1 + (e^{-\beta} - 1)\omega_i(\mathcal{N}_i) + (e^{-\beta} - 1)^2\omega_i(a^*(f_i)a(f_i)a^*(g_i)a(g_i)) \\ &= 1 + (e^{-\beta} - 1)\omega_i(\mathcal{N}_i) + (e^{-\beta} - 1)^2[\omega_i(a^*(f_i)a(f_i))\omega_i(a^*(g_i)a(g_i)) \\ &\quad - \omega_i(a^*(f_i)a^*(g_i))\omega_i(a(f_i)a(g_i)) + \omega_i(a^*(f_i)a(g_i))\omega_i(a(f_i)a^*(g_i))] \\ &= 1 + 2(e^{-\beta} - 1)\lambda_i + (e^{-\beta} - 1)^2(\lambda_i^2 + \alpha_i^2) \\ &= 1 + 2(e^{-\beta} - 1)\lambda_i + (e^{-\beta} - 1)^2\lambda_i \\ &= 1 + (e^{-2\beta} - 1)\lambda_i = \text{Det}_{\mathfrak{H}_i} \sqrt{1 + (e^{-2\beta} - 1)\gamma_i}, \end{aligned}$$

where in the second equality we used Wick's relation for  $\omega_i$ . The equality (1.3.13) then follows by taking the product of the relations (1.3.15). Putting aside the indices  $i$  such that  $\lambda_i = 1$ , we obtain

$$\omega(e^{-\beta \mathcal{N}}) = e^{-\beta k_0} \prod_{i \in \mathbb{N}} (1 + (e^{-2\beta} - 1)\lambda_i),$$

where  $k_0 := \dim \ker(\gamma - 1)$ . Identifying the coefficient of  $e^{-\beta k}$  in both sides, as in the proof of Proposition 1.2, we find that  $\omega(\mathcal{P}_k) = 0$  for all  $k < k_0$ , and that

$$\begin{aligned} \omega(\mathcal{P}_k) &= \sum_{\substack{I \subset \mathbb{N} \\ \#I = \ell}} \prod_{i \in I} \lambda_i \prod_{j \notin I} (1 - \lambda_j) \\ &\leq \frac{e^\ell}{\ell!} \left( \frac{\text{Tr}(\gamma) - k_0}{2} \right)^\ell e^{-\frac{\text{Tr}(\gamma) - k_0}{2}} \leq \frac{e^{k/2}}{\ell!} \left( \frac{\text{Tr}(\gamma)}{2} \right)^\ell e^{-\frac{\text{Tr}(\gamma)}{2}}, \end{aligned}$$

for  $k = k_0 + 2\ell$  with  $\ell \geq 0$ . This concludes the proof of Proposition 1.3.  $\square$

**3.5. Mixed Hartree-Fock-Bogoliubov case.** In the most general case of a mixed HFB state, we cannot apply the same strategy as in the previous cases, i.e. identify  $\omega$  as a product of states living on smaller dimensional spaces. Indeed,  $\gamma$  and  $\alpha J$  can have no common stable finite-dimensional subspaces. However, we can still prove an estimate on the vacuum expectation.

**Proposition 1.4** (Vacuum Expectation of a Mixed HFB State). *Let  $\omega$  a quasi-free state with  $\text{Tr}(\gamma) < +\infty$ . Then we have the following estimate*

$$\boxed{\omega(|\Omega\rangle\langle\Omega|) \leq e^{-a \text{Tr}(\gamma)}} \quad (1.3.16)$$

where  $a = \max_{\beta \geq 0} \frac{3(e^\beta - 1)}{4e^{3\beta} + 7e^\beta - 8} = 0.0941248 \dots$

**Remark 1.8.** We believe that for any sequence of quasi-free state  $(\omega_n)_n$  with finite number of particles, we have  $\omega_n(e^{-\beta \mathcal{N}}) \rightarrow 0$  as  $\omega_n(\mathcal{N}) \rightarrow +\infty$  for all  $\beta > 0$ , as it was the case in the previous sections. However, our method does not provide this result.

PROOF. Let  $\omega$  be a quasi-free state with  $\text{Tr}(\gamma) < +\infty$ . According to [BLS94, Eq. (2b.26)], there exists a Bogoliubov map  $\mathcal{V} : \mathfrak{H} \oplus \mathfrak{K} \rightarrow \mathfrak{H} \oplus \mathfrak{K}$ , i.e. a unitary operator of the form

$$\mathcal{V} = \begin{pmatrix} U & J^* V J^* \\ V & J U J^* \end{pmatrix}. \quad (1.3.17)$$

with  $\text{Tr}(V^* V) < +\infty$ , such that

$$\mathcal{V} \Gamma(\gamma, \alpha) \mathcal{V}^* = \Gamma(D, 0) \quad (1.3.18)$$

with  $D = \text{diag}(\lambda_i)_{i \geq 0}$ ,  $\sum_i \lambda_i < +\infty$ , and  $0 \leq \lambda_i \leq 1/2$  for all  $i$ . Let  $\omega'$  be the unique HF state associated with  $\Gamma(D, 0)$  given by Proposition 1.1. Let us also denote by  $\mathbb{U}$  the unitary operator on  $\mathcal{F}$  lifting  $\mathcal{V}$  [Sol07, Theorem 9.5]. Then

$$\omega(|\Omega\rangle\langle\Omega|) = \omega'(\mathbb{U}|\Omega\rangle\langle\Omega|\mathbb{U}^*) = \omega'(|\Omega_{\mathbb{U}}\rangle\langle\Omega_{\mathbb{U}}|),$$

with  $|\Omega_{\mathbb{U}}\rangle = \mathbb{U}|\Omega\rangle$ . We now estimate  $|\Omega_{\mathbb{U}}\rangle\langle\Omega_{\mathbb{U}}|$  by  $e^{-\beta \mathcal{N}}$  for any  $\beta \geq 0$ . Thus, let us fix  $\beta \geq 0$ . At the end, we will optimize over  $\beta$ . By [Sol07, Eq. (67)] we can write

$$|\Omega_{\mathbb{U}}\rangle = \prod_{i=-K}^{-1} a^*(\eta_i) \prod_{i \geq 0} (\alpha_i - \beta_i a^*(\eta_{2i}) a^*(\eta_{2i+1})) |\Omega\rangle,$$

where  $(\eta_i)_{i \in \mathbb{Z}}$  is an orthonormal basis in  $\mathfrak{H}$ ,  $(\eta_i)_{-K \leq i \leq -1}$  are eigenvectors of  $V^* V$  for the eigenvalue 1,  $\alpha_i^2 + \beta_i^2 = 1$  for all  $i \geq 0$ , and  $(\beta_i^2)_{i \geq 0}$  are the eigenvalues of  $V^* V$  strictly between 0 and 1, which are all of multiplicity 2. We interpret this equality by saying that

$$|\Omega_{\mathbb{U}}\rangle = T^*(\otimes_i |\psi_i\rangle) \in T^*(\otimes_i \mathcal{F}(\mathfrak{H}_i)) = \mathcal{F},$$

where  $\mathfrak{H}_i = \mathbb{C}\eta_i$ ,  $|\psi_i\rangle = \eta_i$  for  $-K \leq i \leq -1$ ,  $\mathfrak{H}_i = \mathbb{C}\eta_{2i+1} \oplus \mathbb{C}\eta_{2i}$ ,  $|\psi_i\rangle = \alpha_i - \beta_i \eta_{2i} \wedge \eta_{2i+1}$  for  $i \geq 0$ , and  $\mathfrak{H}_i = \mathbb{C}\eta_i$ ,  $|\psi_i\rangle = \Omega_i$  (the vacuum in  $\mathcal{F}(\mathfrak{H}_i)$ ) if  $i < -K$ . Recall that the operator  $T$  is the unitary transformation between  $\mathcal{F}(\oplus_i \mathfrak{H}_i)$  and  $\otimes_i \mathcal{F}(\mathfrak{H}_i)$  defined

in Appendix A . If  $-K \leq i \leq -1$ , then  $\mathcal{F}(\mathfrak{H}_i) = \mathbb{C} \oplus \mathbb{C}\eta_i$  and the matrix of  $|\psi_i\rangle\langle\psi_i|$  in the basis  $(1, \eta_i)$  can be dominated by

$$|\psi_i\rangle\langle\psi_i| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \leq e^\beta \begin{pmatrix} 1 & 0 \\ 0 & e^{-\beta} \end{pmatrix} = e^{\beta - \beta\mathcal{N}_i} \leq e^{\frac{e^{2\beta}-1}{2} - \beta\mathcal{N}_i},$$

where as usual  $\mathcal{N}_i$  is the number operator on  $\mathcal{F}(\mathfrak{H}_i)$ . If  $i < -K$  then  $\mathcal{F}(\mathfrak{H}_i) = \mathbb{C} \oplus \mathbb{C}\eta_i$  and we have

$$|\psi_i\rangle\langle\psi_i| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \leq \begin{pmatrix} 1 & 0 \\ 0 & e^{-\beta} \end{pmatrix} = e^{-\beta\mathcal{N}_i}.$$

Now if  $i \geq 0$  then  $\mathcal{F}(\mathfrak{H}_i) = \mathbb{C} \oplus \mathbb{C}\eta_{2i} \oplus \mathbb{C}\eta_{2i+1} \oplus \mathbb{C}\eta_{2i} \wedge \eta_{2i+1}$ . In the basis  $(1, \eta_{2i}, \eta_{2i+1}, \eta_{2i} \wedge \eta_{2i+1})$  the matrix of  $|\psi_i\rangle\langle\psi_i|$  can be dominated by

$$\begin{aligned} |\psi_i\rangle\langle\psi_i| &= \begin{pmatrix} \alpha_i^2 & 0 & 0 & -\alpha_i\beta_i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -\alpha_i\beta_i & 0 & 0 & \beta_i^2 \end{pmatrix} \leq e^{(e^{2\beta}-1)\beta_i^2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{-\beta} & 0 & 0 \\ 0 & 0 & e^{-\beta} & 0 \\ 0 & 0 & 0 & e^{-2\beta} \end{pmatrix} \\ &= e^{(e^{2\beta}-1)\beta_i^2 - \beta\mathcal{N}_i}, \end{aligned}$$

since with

$$A = \begin{pmatrix} \alpha_i^2 & -\alpha_i\beta_i \\ -\alpha_i\beta_i & \beta_i^2 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 0 \\ 0 & e^{-2\beta} \end{pmatrix}$$

we have  $B^{-1/2}AB^{-1/2} \leq (1 + (e^{2\beta} - 1)\beta_i^2)\text{Id}_{\mathbb{C}^2} \leq e^{(e^{2\beta}-1)\beta_i^2}\text{Id}_{\mathbb{C}^2}$ . We know that

$$\text{Tr}(V^*V) = \sum_{i=-K}^{-1} 1 + \sum_{i \geq 0} 2\beta_i^2,$$

so that

$$\begin{aligned} |\Omega_U\rangle\langle\Omega_U| &= T^* \left[ \bigotimes_{i \in \mathbb{Z}} |\psi_i\rangle\langle\psi_i| \right] T \\ &\leq T^* \left[ \bigotimes_{i=-K}^{-1} e^{\frac{e^{2\beta}-1}{2} - \beta\mathcal{N}_i} \otimes \bigotimes_{i \geq 0} e^{\frac{e^{2\beta}-1}{2} 2\beta_i^2 - \beta\mathcal{N}_i} \otimes \bigotimes_{i < -K} e^{-\beta\mathcal{N}_i} \right] T \\ &= \exp \left( \frac{e^{2\beta} - 1}{2} \left( \sum_{i=-K}^{-1} 1 + \sum_{i \geq 0} 2\beta_i^2 \right) - \beta \sum_i \mathcal{N}_i \right) \\ &= e^{\frac{e^{2\beta}-1}{2} \text{Tr}(V^*V) - \beta\mathcal{N}}. \end{aligned}$$

Here we have used that for any operators  $A, B, C, D$ , such that  $0 \leq A \leq B$  and  $0 \leq C \leq D$  it holds  $0 \leq A \otimes C \leq B \otimes D$ . We obtain the estimate

$$\omega(|\Omega\rangle\langle\Omega|) \leq e^{\frac{e^{2\beta}-1}{2} \text{Tr}(V^*V)} \omega'(e^{-\beta\mathcal{N}}) \leq e^{\frac{e^{2\beta}-1}{2} \text{Tr}(V^*V) + (e^{-\beta} - 1) \text{Tr}(D)}, \quad (1.3.19)$$

where we have used that  $\omega'(e^{-\beta\mathcal{N}}) \leq e^{(e^{-\beta}-1)\omega'(\mathcal{N})}$ , which is a consequence of the equality (1.3.11) applied to the HF state  $\omega'$ . Unfortunately, the estimate (1.3.19) is not good enough because the constant  $(e^{2\beta} - 1)/2$  in front of  $\text{Tr}(V^*V)$  is positive, while  $\text{Tr}(V^*V)$  represents the number of particles of  $|\Omega_{\mathbb{U}}\rangle$ . We will thus get another estimate by exchanging the roles of  $\omega'$  and  $|\Omega_{\mathbb{U}}\rangle$ . The idea is to see  $|\Omega_{\mathbb{U}}\rangle$  as the state and  $\omega'$  as the observable. Since  $\ker(D - 1) = \{0\}$ , it is well-known that  $\omega'$  is a normal state with density matrix  $G = Z^{-1}\Upsilon(M)$  where  $M = \frac{D}{1-D}$ ,  $Z = \text{Tr}_{\mathcal{F}}(\Upsilon(M))$ , and

$$\Upsilon(M) := \bigoplus_{N \geq 0} M^{\otimes N} : \mathcal{F} \rightarrow \mathcal{F} \quad (1.3.20)$$

(see for instance [JOPP11, Proposition 6.6 (1)]). Hence we can write

$$\omega(|\Omega\rangle\langle\Omega|) = \omega'(|\Omega_{\mathbb{U}}\rangle\langle\Omega_{\mathbb{U}}|) = \text{Tr}(Z^{-1}\Upsilon(M)|\Omega_{\mathbb{U}}\rangle\langle\Omega_{\mathbb{U}}|) = \omega_{\mathbb{U}}(Z^{-1}\Upsilon(M)),$$

where  $\omega_{\mathbb{U}}$  is the pure state associated with the vector  $|\Omega_{\mathbb{U}}\rangle$ . We know that  $\omega_{\mathbb{U}}(\mathcal{N}) = \text{Tr}(V^*V)$ . Hence if we can dominate  $Z^{-1}\Upsilon(M)$  by  $e^{-\beta'\mathcal{N}}$  for a certain  $\beta' \geq 0$ , we will get another estimate on  $\omega(|\Omega\rangle\langle\Omega|)$  by applying equality (1.3.13) to the pure state  $\omega_{\mathbb{U}}$ . Let  $(\mu_i)_i$  the eigenvalues of  $M$ ,  $\mu_i = \frac{\lambda_i}{1-\lambda_i}$ . The spectrum of  $\Upsilon(M)$  on  $\mathfrak{H}^k$  is

$$\sigma(\Upsilon(M)|_{\mathfrak{H}^k}) = \left\{ \prod_{i \in I} \mu_i, \quad I \subset \mathbb{N}, \quad \#I = k \right\},$$

so that for  $I \subset \mathbb{N}$  of cardinal  $k$  we have

$$Z^{-1} \prod_{i \in I} \mu_i = \prod_{i \geq 0} \frac{1}{1 + \mu_i} \prod_{i \in I} \mu_i = \prod_{i \geq 0} (1 - \lambda_i) \prod_{i \in I} \frac{\lambda_i}{1 - \lambda_i} = \prod_{i \notin I} (1 - \lambda_i) \prod_{i \in I} \lambda_i.$$

Using  $0 \leq \lambda_i \leq 1/2$  for all  $i$ , we finally get  $Z^{-1}\Upsilon(M)|_{\mathfrak{H}^k} \leq 1/2^k$  so that

$$Z^{-1}\Upsilon(M) \leq e^{-(\ln 2)\mathcal{N}}.$$

Equality (1.3.13) now implies that  $\omega_{\mathbb{U}}(e^{-\beta'\mathcal{N}}) \leq e^{\frac{e^{-2\beta'}-1}{2}\omega_{\mathbb{U}}(\mathcal{N})}$  for all  $\beta' \geq 0$ . Choosing  $\beta' = \ln 2$ , one gets

$$\omega(|\Omega\rangle\langle\Omega|) \leq \omega_{\mathbb{U}}(e^{-(\ln 2)\mathcal{N}}) \leq e^{-\frac{3}{8}\text{Tr}(V^*V)}. \quad (1.3.21)$$

Interpolating the inequalities (1.3.19) and (1.3.21) we get

$$\omega(|\Omega\rangle\langle\Omega|) \leq e^{\theta(e^{-\beta}-1)\text{Tr}(D) + \left[\theta\frac{e^{2\beta}-1}{2} - (1-\theta)\frac{3}{8}\right]\text{Tr}(V^*V)},$$

for all  $\beta \geq 0$  and  $0 \leq \theta \leq 1$ . We choose  $\theta$  such that the coefficients before  $\text{Tr}(D)$  and  $\text{Tr}(V^*V)$  are equal since we have  $\text{Tr}(V^*V) + \text{Tr}(D) \geq \text{Tr}(U^*DU) + \text{Tr}(V^*(1-D)V) = \text{Tr}(\gamma)$  by (1.3.18), using  $UU^* \leq 1$  and  $1 - D \leq 1$ . We thus choose

$$\theta = \frac{3}{7 - 8e^{-\beta} + 4e^{2\beta}},$$

and we obtain

$$\omega(|\Omega\rangle\langle\Omega|) \leq e^{\frac{3(e^{\beta}-1)}{8-7e^{\beta}-4e^{3\beta}}\text{Tr}(\gamma)},$$

for all  $\beta \geq 0$ . Optimizing the coefficient before  $\text{Tr}(\gamma)$ , we get the desired estimate with  $\beta \simeq 0.36443$  and  $\theta \simeq 0.308194$ .  $\square$

**3.6. Bogoliubov-Dirac-Fock case.** In this section we introduce the correct setup for studying electron-positron pair creation. Let  $\mathfrak{H}$  be a Hilbert space and  $\Pi$  be an orthogonal projection on  $\mathfrak{H}$ . We also need an anti-unitary operator  $J$  as in Section 3.1, with the additional assumptions that  $\mathfrak{K} = \mathfrak{H}$  (i.e.  $J$  maps  $\mathfrak{H}$  to  $\mathfrak{H}$ ) and that  $J\Pi J^* = \Pi$  or  $J\Pi J^* = 1 - \Pi$ . The particle/anti-particle spaces are given by  $\mathfrak{H}_+ = (1 - \Pi)\mathfrak{H}$  and  $\mathfrak{H}_- = J\Pi\mathfrak{H}$ . Notice that  $\mathfrak{H}_- = \Pi\mathfrak{H}$  or  $\mathfrak{H}_- = (1 - \Pi)\mathfrak{H}$ . In the context given by Section 2.2, we have  $\mathfrak{H} = \mathfrak{H}_\Lambda$ ,  $\Pi = P_-^0$  and  $J = i\beta\alpha_2\mathcal{C}$  the charge conjugation operator on  $\mathfrak{H}_\Lambda$  (i.e. such that  $J(D^0 + V)J^* = -(D^0 - V)$  for any scalar potential  $V$ ), with  $\mathcal{C}$  the complex conjugation on  $\mathfrak{H}_\Lambda$ . With this choice, vectors of  $\mathfrak{H}_-$  are interpreted as states with a positive energy relatively to the Hamiltonian with an opposite charge. Hence, they represent positronic states. Notice that this specific  $J$  verifies  $J P_-^0 J^* = P_+^0 = 1 - P_-^0$ . In the sequel, we will keep a triplet  $(\mathfrak{H}, \Pi, J)$  satisfying the assumptions given above.

The mathematical description of Bogoliubov-Dirac-Fock states is a special case of the well known Araki-Wyss representation [AW64] (see [JOPP11, Section 6.4] for a review). Let  $\mathcal{F}_0 = \mathcal{F}(\mathfrak{H}_+) \otimes \mathcal{F}(\mathfrak{H}_-)$ . For  $f \in \mathfrak{H}_+$  and  $g \in \mathfrak{H}_-$  we denote by  $a_+^*(f)$  and  $a_-^*(g)$  the usual creation operators on  $\mathcal{F}(\mathfrak{H}_+)$  and  $\mathcal{F}(\mathfrak{H}_-)$ , respectively. We now define the ‘‘creation operator’’ on  $\mathcal{F}_0$  for all  $f \in \mathfrak{H}$  by

$$\psi^*(f) := a_+^*((1 - \Pi)f) \otimes \text{Id}_{\mathcal{F}(\mathfrak{H}_-)} + \Upsilon(-\text{Id}_{\mathcal{F}(\mathfrak{H}_+)}) \otimes a_-(J\Pi f),$$

where  $\Upsilon$  is the operation defined by Equation (1.3.20). The operators  $(\psi^*(f))_f$  are not exactly the usual creation operators in the full Fock space since they create a particle in the state  $(1 - \Pi)f$ , and at the same time they annihilate a anti-particle in the state  $J\Pi f$ , according to the ‘‘particle-hole’’ picture of Dirac’s theory. However, they still satisfy the CAR thanks to the ‘‘twist’’  $\Upsilon(-\text{Id}_{\mathcal{F}(\mathfrak{H}_+)})$  on the second term. A *Bogoliubov-Dirac-Fock* (BDF) state is, by definition, a quasi-free state  $\omega$  on the  $C^*$ -algebra  $\mathfrak{A}_0 \subset \mathcal{B}(\mathcal{F}_0)$  generated by the  $(\psi(f))_{f \in \mathfrak{H}}$ . We define the normal ordering  $:\psi^*(f)\psi(g):$  of the operator  $\psi^*(f)\psi(g)$  by

$$\begin{aligned} :\psi^*(f)\psi(g): &= a_+^*(f_+)a_+(g_+) \otimes \text{Id}_{\mathcal{F}(\mathfrak{H}_-)} + a_+^*(f_+)\Upsilon(-\text{Id}_{\mathcal{F}(\mathfrak{H}_+)}) \otimes a_-^*(Jg_-) \\ &\quad + \Upsilon(-\text{Id}_{\mathcal{F}(\mathfrak{H}_+)}) a_+(g_+) \otimes a_-(Jf_-) - \text{Id}_{\mathcal{F}(\mathfrak{H}_+)} \otimes a_-^*(Jg_-)a_-(Jf_-), \end{aligned}$$

where  $h_+ = (1 - \Pi)h$  and  $h_- = \Pi h$  for all  $h$ . It corresponds to moving all the creation operators  $a^*$  to the left of annihilation operators  $a$ . For any BDF state  $\omega$ , we define its renormalized one-particle density matrix  $Q : \mathfrak{H} \rightarrow \mathfrak{H}$  by

$$\langle g, Qf \rangle = \omega(:\psi^*(f)\psi(g):).$$

and its pairing matrix  $p : \mathfrak{H} \rightarrow \mathfrak{H}$  by the usual formula

$$\langle pJf, g \rangle = \omega(\psi^*(f)\psi^*(g)).$$

Recall that we have already defined the 1-pdm  $\gamma$  by  $\langle g, \gamma f \rangle = \omega(\psi^*(f)\psi(g))$ . Therefore, we have the relation  $\gamma = \Pi + Q$ . If  $\mathcal{N}$  is the number operator on  $\mathcal{F}_0$ ,

$$\mathcal{N} = \sum_i a_+^*(\varphi_{i,+})a_+(\varphi_{i,+}) \otimes \text{Id}_{\mathcal{F}(\mathfrak{H}_-)} + \text{Id}_{\mathcal{F}(\mathfrak{H}_+)} \otimes a_-^*(\varphi_{i,-})a_-(\varphi_{i,-}), \quad (1.3.22)$$

where  $(\varphi_{i,+})_i, (\varphi_{i,-})_i$  are orthonormal basis for, respectively,  $\mathfrak{H}_+$  and  $\mathfrak{H}_-$ , then

$$\omega(\mathcal{N}) = \text{Tr}(Q_{++} - Q_{--}),$$

where  $Q_{++} := (1 - \Pi)Q(1 - \Pi)$  and  $Q_{--} = \Pi Q \Pi$ . Hence,  $\omega(\mathcal{N}) < +\infty$  is equivalent to having  $Q \in \mathfrak{S}_{1,\Pi}(\mathfrak{H}) := \{Q \in \mathfrak{S}_2(\mathfrak{H}), Q_{++}, Q_{--} \in \mathfrak{S}_1(\mathfrak{H})\}$ . Notice also that as in the HFB case we have  $pp^* \leq \gamma - \gamma^2 = Q_{++} - Q_{--} - Q^2$ , thus  $p \in \mathfrak{S}_2(\mathfrak{H})$  as soon as  $\omega(\mathcal{N}) < +\infty$ .

**Remark 1.9.** The other natural number operator  $\sum_i \psi^*(f_i)\psi(f_i)$  gives the total number of particles in the system, that is also those of the vacuum  $\Pi$ . If  $\dim(\mathfrak{H}_-) = +\infty$ , this number is just  $+\infty$ . However, we only want to count the number of particles relative to the vacuum  $\Pi$ . That is why the operator  $\mathcal{N}$  is chosen here: It counts the number of “real” electrons  $\varphi_{i,+}$  and the number of “holes”  $\varphi_{i,-}$  in the vacuum.

The following proposition is an easy adaptation of the arguments given in [BBHS99, pp. 449–450]. We give the complete proof here to clarify the link between BDF states and HFB states.

**Proposition 1.5** (Link between HFB and BDF States). *Let  $(Q, p) \in \mathfrak{S}_{1,\Pi}(\mathfrak{H}) \times \mathfrak{S}_2(\mathfrak{H})$  such that*

$$0 \leq \Gamma(\Pi + Q, p) = \begin{pmatrix} \Pi + Q & p \\ p^* & 1 - J(\Pi + Q)J^* \end{pmatrix} \leq 1$$

*as an operator on  $\mathfrak{H} \oplus \mathfrak{H}$ . Then there exists a unique, normal, BDF state on  $\mathcal{F}_0$  having  $Q$  as renormalized 1-pdm and  $p$  as pairing matrix.*

**PROOF.** We are going to construct an HFB state on  $\mathfrak{A}[\mathfrak{H}_+ \oplus \mathfrak{H}_-]$  using Proposition 1.1, and then transform it into a BDF state having the desired property via the unitary transformation (which is a particular case of the one introduced in Appendix A)

$$T : \mathcal{F}(\mathfrak{H}_+ \oplus \mathfrak{H}_-) \rightarrow \mathcal{F}_0 = \mathcal{F}(\mathfrak{H}_+) \otimes \mathcal{F}(\mathfrak{H}_-),$$

defined linearly by its action on each  $N$ -particle space

$$\begin{aligned} T\varphi_{i_1,+} \wedge \cdots \wedge \varphi_{i_k,+} \wedge \varphi_{j_1,-} \wedge \cdots \wedge \varphi_{j_{N-k},-} = \\ (\varphi_{i_1,+} \wedge \cdots \wedge \varphi_{i_k,+}) \otimes (\varphi_{j_1,-} \wedge \cdots \wedge \varphi_{j_{N-k},-}), \end{aligned}$$

with the convention  $T\Omega = \Omega_+ \otimes \Omega_-$ . Since  $T$  leaves the scalar product invariant and maps an orthonormal basis for  $\mathcal{F}(\mathfrak{H}_+ \oplus \mathfrak{H}_-)$  onto an orthonormal basis for  $\mathcal{F}_0$ , it naturally extends to a unique unitary operator on  $\mathcal{F}(\mathfrak{H}_+ \oplus \mathfrak{H}_-)$ . It induces the following transformation of the CAR:

$$\begin{cases} Ta(f)T^* &= \psi(f_+) + \psi^*(f_-), \\ T^*\psi(f)T &= a(f_+) + a^*(f_-). \end{cases} \quad (1.3.23)$$

Define  $p_{++} = (1 - \Pi)p(1 - \Pi)$ ,  $p_{+-} = (1 - \Pi)p\Pi$ , etc. Suppose also that we are in the case where  $J\Pi J^* = 1 - \Pi$ , and write  $\mathfrak{H}_+^0 = (1 - \Pi)\mathfrak{H} = \mathfrak{H}_+$ ,  $\mathfrak{H}_-^0 = \Pi\mathfrak{H}$ . We now introduce

$$\gamma_0 := \begin{pmatrix} Q_{++} & p_{++} \\ p_{++}^* & -JQ_{--}J^* \end{pmatrix}, \quad \alpha_0 := \begin{pmatrix} p_{+-} & Q_{+-} \\ -JQ_{-+}J^* & p_{-+}^* \end{pmatrix},$$

where  $\gamma_0 : \mathfrak{H}_+^0 \oplus \mathfrak{H}_+^0 \rightarrow \mathfrak{H}_+^0 \oplus \mathfrak{H}_+^0$  and  $\alpha_0 : \mathfrak{H}_-^0 \oplus \mathfrak{H}_-^0 \rightarrow \mathfrak{H}_+^0 \oplus \mathfrak{H}_+^0$ . Let us define  $\mathcal{J} : \mathfrak{H}_+^0 \oplus \mathfrak{H}_+^0 \rightarrow \mathfrak{H}_-^0 \oplus \mathfrak{H}_-^0$  by

$$\mathcal{J} = \begin{pmatrix} J & 0 \\ 0 & J^* \end{pmatrix},$$

and the operator  $\Gamma_0$  on  $(\mathfrak{H}_+^0 \oplus \mathfrak{H}_+^0) \oplus (\mathfrak{H}_-^0 \oplus \mathfrak{H}_-^0)$  by

$$\Gamma_0 = \Gamma(\gamma_0, \alpha_0) = \begin{pmatrix} \gamma_0 & \alpha_0 \\ \alpha_0^* & 1 - \mathcal{J}^*\gamma_0\mathcal{J} \end{pmatrix}.$$

We now show that there exists a HFB state  $\omega_0$  on  $\mathfrak{A}[\mathfrak{H}_+^0 \oplus \mathfrak{H}_+^0]$  having  $\Gamma_0$  as density matrix. Hence we prove that  $0 \leq \Gamma_0 \leq 1$ . Let us first write the block decomposition of  $\Gamma(\Pi + Q, p)$  as an operator on  $\mathfrak{H}_+^0 \oplus \mathfrak{H}_-^0 \oplus \mathfrak{H}_+^0 \oplus \mathfrak{H}_-^0 = \mathfrak{H} \oplus \mathfrak{H}$

$$\Gamma(\Pi + Q, p) = \begin{pmatrix} Q_{++} & Q_{+-} & p_{++} & p_{+-} \\ Q_{-+} & 1 + Q_{--} & p_{-+} & p_{--} \\ p_{++}^* & p_{-+}^* & -JQ_{--}J^* & -JQ_{-+}J^* \\ p_{++}^* & p_{-+}^* & -JQ_{+-}J^* & 1 - JQ_{++}J^* \end{pmatrix},$$

where we have used that  $J\mathfrak{H}_\pm^0 = \mathfrak{H}_\mp^0$  to write the lower right block. Let us consider the unitary operator  $W : \mathfrak{H}_+^0 \oplus \mathfrak{H}_+^0 \oplus \mathfrak{H}_-^0 \oplus \mathfrak{H}_-^0 \rightarrow \mathfrak{H}_+^0 \oplus \mathfrak{H}_-^0 \oplus \mathfrak{H}_+^0 \oplus \mathfrak{H}_-^0$  whose matrix is

$$W = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix}.$$

Then, as it was noticed in [BBHS99], we have the relation

$$\Gamma_0 = W^*\Gamma(\Pi + Q, p)W.$$

By assumption, we have  $0 \leq \Gamma(\Pi + Q, p) \leq 1$ , so that  $0 \leq \Gamma_0 \leq 1$  as well. Now we have  $\text{Tr}(\gamma_0) = \text{Tr}(Q_{++} - Q_{--}) < \infty$  hence by Proposition 1.1 with  $\mathfrak{H} = \mathfrak{H}_+^0 \oplus \mathfrak{H}_+^0 = \mathfrak{H}_+ \oplus \mathfrak{H}_-$  and  $\mathfrak{K} = \mathfrak{H}_-^0 \oplus \mathfrak{H}_-^0$ , there exists a unique, normal, HFB state  $\omega_0$  on  $\mathcal{F}(\mathfrak{H}_+ \oplus \mathfrak{H}_-)$  with

finite number of particles having  $\Gamma_0$  as density matrix. We define a state on  $\mathcal{F}_0$  via the unitary operator  $T$  by

$$\omega(A) = \omega_0(T^*AT), \quad \forall A \in \mathcal{B}(\mathcal{F}_0).$$

By (1.3.23),  $\omega$  is the quasi-free state with renormalized 1-pdm  $Q$  and pairing matrix  $p$ . Furthermore,  $\omega$  is obviously normal since  $\omega_0$  is normal. This concludes the proof of Proposition 1.5, in the case where  $J\Pi J^* = 1 - \Pi$ . If  $J\Pi J^* = \Pi$ , the proof is the same with  $W : \mathfrak{H}_+^0 \oplus \mathfrak{H}_-^0 \oplus \mathfrak{H}_+^0 \oplus \mathfrak{H}_-^0 \rightarrow \mathfrak{H}_+^0 \oplus \mathfrak{H}_-^0 \oplus \mathfrak{H}_+^0 \oplus \mathfrak{H}_-^0$  whose matrix is

$$W = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$

which is the same as in [BBHS99] where  $J$  was the complex conjugation. With this choice of  $W$ ,  $W^*\Gamma(\Pi + Q, p)W$  is the density matrix of a HFB state with  $\mathfrak{H} = \mathfrak{H}_+^0 \oplus \mathfrak{H}_-^0 = \mathfrak{K}$ .  $\square$

**Corollary 1.1** (Vacuum Expectation of a BDF State). *Let  $\omega$  be a BDF state with renormalized one-particle density matrix  $Q$  such that  $\text{Tr}(Q_{++} - Q_{--}) < +\infty$ . Then we have the estimate*

$$\omega(|\Omega_0\rangle\langle\Omega_0|) \leq e^{-a\text{Tr}(Q_{++}-Q_{--})}, \quad (1.3.24)$$

where  $a$  is the same constant as in Proposition 1.4 and  $\Omega_0$  is the vacuum in  $\mathcal{F}_0$ .

**PROOF.** Use Proposition 1.4 to the HFB mixed state  $\omega_0$  constructed in the proof of Proposition 1.5.  $\square$

**Remark 1.10.** In [HLS07], the rBDF energy (1.2.3) is derived by evaluating the QED Hamiltonian on BDF states. As usual in mean-field theories, this energy only depends on  $(Q, p)$ . However, since the interaction between the particles is repulsive, any minimizer of the rBDF energy has  $p = 0$ . This explains why we can take  $p = 0$  for the polarized vacuum in the proof of Theorem 1.1.

#### 4. Asymptotics of the polarized vacuum energy in strong external fields

**4.1. Main results.** In this section, we study the asymptotics of the reduced BDF ground state energy  $E(Z)$  for large  $Z$ , where we recall that  $E(Z) = \inf\{\mathcal{E}_{Z\nu}^{\text{rBDF}}(Q), Q \in \mathcal{K}\}$ , with  $\mathcal{K}$  defined by Equation (1.2.4).

**Proposition 1.6** (Upper Bound). *Let  $\alpha > 0$  and  $\Lambda > 0$ . Let  $\nu \in \mathcal{C} \cap L^1(\mathbb{R}^3, \mathbb{R})$  be such that  $\int |\nu| = 1$  and  $q = \int \nu \neq 0$ . Then*

$$\limsup_{Z \rightarrow +\infty} \frac{E(Z)}{Z^{5/3}} \leq -c_1 \alpha \Lambda |q|^{5/3}, \quad (1.4.25)$$

where  $c_1 = 2^{-23/3} 3^{1/3} \pi^{-4/3} = 0.001543\dots$



To estimate the convergence rate of  $E(Z)Z^{-5/3}$ , we need a further assumption on the decay of  $\nu$  at infinity.

**Proposition 1.7** (Convergence Rate). *Let  $\alpha > 0$  and  $\Lambda > 0$ . Let  $\nu \in \mathcal{C} \cap L^1(\mathbb{R}^3, \mathbb{R})$  be such that  $\int |x||\nu(x)| dx < +\infty$ ,  $\int |\nu| = 1$  and  $q = \int \nu \neq 0$ . Then there exists a constant  $\widetilde{Z}_1 = \widetilde{Z}_1(\Lambda, \alpha, |q|, \|\nu\|_1) > 0$  such that*

$$\forall Z > \widetilde{Z}_1, \quad E(Z) \leq -\frac{c_1}{2} \alpha \Lambda |q|^{5/3} Z^{5/3}, \quad (1.4.26)$$

where  $c_1$  is defined in Proposition 1.6.

**Remark 1.11.** The constant  $\widetilde{Z}_1$  behaves as  $\Lambda^3$  when  $\Lambda \rightarrow \infty$ , as  $\alpha^{-3/2}$  when  $\alpha \rightarrow 0$  and as  $|q|^{-4}$  when  $q \rightarrow 0$ . It is probably not optimal.

We also give a lower bound for  $E(Z)$ , proving that the power  $Z^{5/3}$  is optimal.

**Proposition 1.8** (Lower Bound). *Let  $\alpha > 0$ ,  $\Lambda > 0$ , and  $\nu \in \mathcal{C} \cap L^1(\mathbb{R}^3, \mathbb{R})$  with  $\int |\nu| = 1$ . Then for all  $Z > 0$  we have*

$$\boxed{E(Z) \geq -c_2 \alpha \Lambda Z^{5/3}}, \quad (1.4.27)$$

where  $c_2 := 2^{-4/3} 3^{2/3} \pi^{-1/3} = 0.563626\dots$

From the asymptotics of  $E(Z)$  in Proposition 1.7 we can now derive a lower bound on the total number of particles and anti-particles in the polarized vacuum.

**Corollary 1.2** (Average Particle Number of the Polarized Vacuum). *Let  $\alpha > 0$ ,  $\Lambda > 0$ . Let  $\nu \in \mathcal{C} \cap L^1(\mathbb{R}^3, \mathbb{R})$  with  $\int |\nu| = 1$ ,  $\int |x||\nu(x)| dx < +\infty$ , and  $q = \int \nu \neq 0$ . Then for any minimizer  $Q$  for  $E(Z)$  and for all  $Z > \widetilde{Z}_1$ , we have*

$$\text{Tr}(Q_{++} - Q_{--}) \geq CZ^{2/3}, \quad (1.4.28)$$

where  $\widetilde{Z}_1$  is the same as in Proposition 1.7 and  $C$  is a constant independent of  $Z$ , given in Equation (1.4.35) below.

**4.2. Proof of the lower bound.** We first give the proof of the lower bound in Proposition 1.8, which is easier than the upper bound.

**Lemma 1.1.** *For any  $Q \in \mathcal{K}$ ,  $\rho_Q \in L^\infty(\mathbb{R}^3)$  and  $\|\rho_Q\|_{L^\infty} \leq \frac{\Lambda^3}{6\pi^2}$ .*

PROOF. The proof will only use the fact that any  $Q \in \mathcal{K}$  is a bounded operator on  $\mathfrak{H}_\Lambda$ . Hence, let  $Q \in \mathcal{K}$  and  $V \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ . Since  $\rho_Q \in L^2(\mathbb{R}^3)$  we know that

$$\int \rho_Q V = \text{Tr}_0(QV),$$

where in the trace  $V$  is seen as a multiplication operator on  $L^2(\mathbb{R}^3, \mathbb{C}^4)$ . Let us denote by  $\Pi_\Lambda$  the multiplication operator by  $\mathbf{1}_{B(0,\Lambda)}$  in Fourier space. Since  $Q$  is an operator

on  $\mathfrak{H}_\Lambda$ , we have  $\Pi_\Lambda Q \Pi_\Lambda = Q$ . Now assume that  $V \geq 0$ . Then

$$\left| \int \rho_Q V \right| = |\text{Tr}_0(Q \Pi_\Lambda V \Pi_\Lambda)| \leq \|\Pi_\Lambda V \Pi_\Lambda\|_{\mathfrak{S}_1} = \|\sqrt{V} \Pi_\Lambda\|_{\mathfrak{S}_2}^2 \leq (2\pi)^{-3} \int V \times \frac{4}{3} \pi \Lambda^3,$$

where we used  $\|Q\| \leq 1$  and the Kato-Seiler-Simon inequality:

$$\forall p \geq 2, \quad \|f(x)g(p)\|_{\mathfrak{S}_p} \leq (2\pi)^{-3/p} \|f\|_{L^p} \|g\|_{L^p}.$$

Now if  $V$  is not necessarily non-negative, we split  $V = V_+ - V_-$  with  $V_+ = \max(V, 0)$  and  $V_- = \max(-V, 0)$ . Then we apply the previous bound twice to obtain

$$\left| \int \rho_Q V \right| \leq \left| \int \rho_Q V_+ \right| + \left| \int \rho_Q V_- \right| \leq \frac{\Lambda^3}{6\pi^2} \left( \int V_+ + \int V_- \right) = \frac{\Lambda^3}{6\pi^2} \|V\|_{L^1}.$$

By the density of  $L^1 \cap L^2$  in  $L^1$  and by the fact that  $(L^1)' \simeq L^\infty$ , we get the result.  $\square$

**Remark 1.12.** Lemma 1.1 is crucial to understand the  $Z^{5/3}$  behaviour of  $E(Z)$ . Indeed, an easy lower bound to  $\mathcal{E}_{\text{rBDF}}^{Z\nu}$  is  $\mathcal{E}_{\text{rBDF}}^{Z\nu}(Q) \geq -\alpha Z^2 D(\nu, \nu)/2$  for all  $Q$ , using the positivity of the kinetic energy and completing the square in the other terms. One may think that this lower bound would be attained by a  $Q$  such that  $\rho_Q \simeq Z\nu$ , i.e. by a state the charge density of which compensates the external field. However, Lemma 1.1 implies that such a state cannot exist in  $\mathcal{K}$ , precisely because of the cut-off  $\Lambda$ . In other words, the vacuum cannot “follow” the external field when the field is too strong.

PROOF OF PROPOSITION 1.8. . Let  $Q \in \mathcal{K}$ , then

$$\mathcal{E}_{Z\nu}^{\text{rBDF}}(Q) \geq \tilde{\mathcal{E}}^{Z\nu}(\rho_Q) := -\alpha D(\rho_Q, Z\nu) + \frac{\alpha}{2} D(\rho_Q, \rho_Q).$$

We also know that for all  $Q \in \mathcal{K}$ , one has  $\|\rho_Q\|_{L^\infty} \leq \frac{\Lambda^3}{6\pi^2} =: \delta$ , so that

$$E(Z) \geq \tilde{E}(Z, \delta) := \inf \left\{ \tilde{\mathcal{E}}^{Z\nu}(\rho), \rho \in \mathcal{C} \cap L^\infty(\mathbb{R}^3), \|\rho\|_{L^\infty} \leq \delta \right\}.$$

The variational problem  $\tilde{E}(Z, \delta)$  has the scaling property  $\tilde{E}(Z, \delta) = Z^2 \tilde{E}(1, \delta/Z)$ . Define  $\varepsilon = \delta/Z$ . We will now show that

$$\tilde{E}(1, \varepsilon) \geq -\frac{3}{4} (8\pi\varepsilon)^{1/3},$$

which then implies Proposition 1.8. Let  $\rho$  be a trial state for  $\tilde{E}(1, \varepsilon)$ . Let  $R > 0$  and write  $|\cdot|^{-1} = V_1 + V_\infty$  with  $V_1 := \mathbf{1}_{|x| \leq R} |\cdot|^{-1} \in L^1(\mathbb{R}^3)$  and  $V_\infty := \mathbf{1}_{|x| \geq R} |\cdot|^{-1} \in L^\infty(\mathbb{R}^3)$ . On the one hand

$$\left| \int_{\mathbb{R}^3} \rho(\nu \star V_1) \right| \leq \varepsilon \|\nu \star V_1\|_{L^1} \leq \varepsilon \|\nu\|_{L^1} \|V_1\|_{L^1} = 2\pi\varepsilon R^2,$$

where in the last inequality we used Young's inequality and  $\int |\nu| = 1$ . On the other hand,

$$\int_{\mathbb{R}^3} \rho(\nu \star V_\infty) = \int_{\mathbb{R}^3} \rho(x) \left( \int_{|y| \geq R} \frac{\nu(x-y)}{|y|} dy \right) dx = \int_{|y| \geq R} \frac{\tilde{\rho}(y)}{|y|} dy,$$

where  $\tilde{\rho} := \tilde{\nu} \star \rho$  and  $\tilde{\nu}(x) = \nu(-x)$  for all  $x \in \mathbb{R}^3$ . Since  $\int_{|y| \geq R} \frac{\tilde{\rho}(y)}{|y|} = D(\tilde{\rho}, f)$  with  $f = (4\pi)^{-1} \delta_{|x|=R}$ , as in [LS77b, Proof of Theorem II.3], we have

$$- \int_{|y| \geq R} \frac{\tilde{\rho}(y)}{|y|} dy + \frac{1}{2} D(\tilde{\rho}, \tilde{\rho}) \geq -\frac{1}{2} D(f, f) = -\frac{1}{2R}.$$

Notice that

$$D(\tilde{\rho}, \tilde{\rho}) = 4\pi(2\pi)^3 \int_{\mathbb{R}^3} \frac{|\widehat{\rho}(k)|^2 |\widehat{\nu}(k)|^2}{|k|^2} dk \leq D(\rho, \rho),$$

since  $|\widehat{\nu}(k)| \leq (2\pi)^{-3/2} \|\nu\|_{L^1} = (2\pi)^{-3/2}$  for all  $k$ . Hence,

$$\tilde{E}(1, \varepsilon) \geq -2\pi\alpha\varepsilon R^2 - \frac{\alpha}{2R}.$$

Optimizing over  $R$ , one gets the result. This finishes the proof of Proposition 1.8.  $\square$

**Remark 1.13.** When the exchange term is included, the minimization set  $\mathcal{K}$  is different, but Lemma 1.1 remains valid. If  $0 \leq \alpha < 4/\pi$ , the proof of Proposition 1.8 applies, using that

$$\mathrm{Tr}_{\mathcal{P}_-^0}(\mathcal{D}^0 Q) - \frac{\alpha}{2} \iint \frac{|Q(x, y)|^2}{|x - y|} dx dy \geq 0,$$

for all  $Q$ , by Kato's inequality.

**4.3. Proof of the upper bound.** Both Propositions 1.6 and 1.7 are proved via appropriate trial states. Before turning to the estimates, we start by explaining our choice of the trial states. In the sequel, we will assume that  $\int \nu > 0$ . The case  $\int \nu < 0$  is treated in the same fashion, except for the choice of the trial state (see Remark 1.14). We define the operator  $Q$  on  $\mathfrak{H}_\Lambda$  by its kernel in Fourier space. For all  $p, q \in \mathbb{R}^3$ , let

$$\widehat{Q}(p, q) = \widehat{\gamma}(p, q) X(p) X(q)^*,$$

with

$$\widehat{\gamma}(p, q) = (2\pi)^{-3/2} \int_{B(0, \Lambda/2)} d\ell g_r(p - \ell) \widehat{F}_r(p - q) g_r(q - \ell)$$

and

$$X(p) = U(p) [(1 \ 0 \ 0 \ 0)^t]$$

with

$$U(p) = a_+(p) + a_-(p) \beta \frac{\boldsymbol{\alpha} \cdot p}{|p|}, \quad a_\pm(p) = \frac{1}{\sqrt{2}} \sqrt{1 \pm \frac{1}{\sqrt{1 + |p|^2}}}. \quad (1.4.29)$$

The operator  $U(p)$  is unitary on  $\mathbb{C}^4$  for all  $p$  and it diagonalizes  $D^0(p) := \boldsymbol{\alpha} \cdot p + \beta$  as  $U(p)D^0(p)U(p)^* = \sqrt{1 + |p|^2}\beta$ . In the definition of  $\widehat{\gamma}$ , we choose  $0 < r < \Lambda/2$  (a small number which will eventually tend to zero),  $g_r = r^{-3/2}g(\cdot/r)$  with  $g \in L^2(\mathbb{R}^3, \mathbb{R})$ ,  $\int g^2 = 1$  and  $\text{supp}(g) \subset B(0, 1)$ . We also choose  $F_r = F(r \cdot)$  with  $F \in L^1(\mathbb{R}^3, \mathbb{R})$  such that  $0 \leq F(x) \leq 1$  for all  $x$ .

**Lemma 1.2.** *The operator  $Q$  belongs to the variational set  $\mathcal{K}$ .*

PROOF. First, notice that  $Q$  defines a Hilbert-Schmidt operator on  $L^2(\mathbb{R}^3, \mathbb{C}^4)$  since

$$\begin{aligned} \|Q(\cdot, \cdot)\|_{L^2(\mathbb{R}^3, \mathbb{C}^4)}^2 &\leq (2\pi)^{-3} \|g_r\|_{L^2}^2 \int_{B(0, \Lambda/2)} d\ell \int_{\mathbb{R}^3} dp \left( |\widehat{F}_r|^2 \star |\tau_\ell g_r|^2 \right) (p) \\ &\leq (2\pi)^{-3} \|g_r\|_{L^2}^2 \int_{B(0, \Lambda/2)} d\ell \left\| |\widehat{F}_r|^2 \star |\tau_\ell g_r|^2 \right\|_{L^1} \\ &\leq \frac{\text{vol}(B(0, \Lambda/2))}{(2\pi)^3} \|g_r\|_{L^2}^4 \|F_r\|_{L^1}^2 < \infty \end{aligned}$$

by Young's inequality. It is self-adjoint because  $\widehat{Q}(p, q) = \overline{\widehat{Q}(q, p)}$  for all  $p, q$ , and we have  $\text{supp } \widehat{Q}(\cdot, \cdot) \subset (B(0, \Lambda/2) + \text{supp } g_r)^2 \subset B(0, \Lambda)^2$  hence  $Q$  is an operator with range in  $\mathfrak{H}_\Lambda$ . Since for all  $\varphi \in \mathfrak{H}_\Lambda$  we have

$$\widehat{Q}\varphi(p) = \left( \int_{\mathbb{R}^3} \widehat{\gamma}(p, q) \langle X(q), \widehat{\varphi}(q) \rangle_{\mathbb{C}^4} dq \right) X(p),$$

we conclude  $Q_{--} = Q_{+-} = Q_{-+} = 0$  so that  $Q = Q_{++}$ . Let  $\varphi \in \mathfrak{H}_+^0$ . Then

$$\begin{aligned} \langle Q\varphi, \varphi \rangle_{L^2(\mathbb{R}^3, \mathbb{C}^4)} &= (2\pi)^{-3/2} \int_{B(0, \Lambda/2)} d\ell \left\langle (\tau_\ell g) X \widehat{\varphi}, \widehat{F} \star ((\tau_\ell g) X \widehat{\varphi}) \right\rangle_{L^2(\mathbb{R}^3, \mathbb{C}^4)} \\ &= \int_{B(0, \Lambda/2)} d\ell \int_{\mathbb{R}^3} dx F(x) \left\| \mathcal{F}^{-1}((\tau_\ell g) X \widehat{\varphi})(x) \right\|_{\mathbb{C}^4}^2 \\ &\leq \int_{B(0, \Lambda/2)} d\ell \int_{\mathbb{R}^3} dp \|g(p - \ell) X(p) \widehat{\varphi}(p)\|_{\mathbb{C}^4}^2 \leq \|\varphi\|_{L^2(\mathbb{R}^3, \mathbb{C}^4)}^2, \end{aligned}$$

where we have denoted by  $\mathcal{F}^{-1}$  the inverse Fourier transform. Hence  $-P_-^0 \leq Q \leq 1 - P_-^0$ . Finally,  $\text{Tr}(Q) = \int_{\mathbb{R}^3} \widehat{\gamma}(p, p) \|X(p)\|_{\mathbb{C}^4}^2 dp \leq (2\pi)^{-3} \int F < +\infty$ , so that  $Q \in \mathfrak{S}_1(\mathfrak{H}_\Lambda) \subset \mathfrak{S}_{1, P_-^0}(\mathfrak{H}_\Lambda)$ .  $\square$

Since for any  $R \in \mathcal{K}$  we have the formula

$$\widehat{\rho}_R(k) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \text{Tr}_{\mathbb{C}^4}(\widehat{R}(p + k, p)) dp, \quad \forall k \in \mathbb{R}^3,$$

the density of  $Q$  can be written as  $\rho_Q = \rho_1 + \rho_2$  where for all  $k$ ,

$$\widehat{\rho}_1(k) = (2\pi)^{-3} V_\Lambda \widehat{F}_r(k) g_r \star \widetilde{g}_r(-k)$$

and

$$\widehat{\rho}_2(k) = (2\pi)^{-3} V_\Lambda \widehat{F}_r(k) \int_{\mathbb{R}^3} g_r(p) g_r(p+k) \langle X(p), (X(p+k) - X(p)) \rangle_{\mathbb{C}^4} dp$$

with  $V_\Lambda := \text{vol}(B(0, \Lambda/2))$  and  $\widetilde{g} := g(-\cdot)$ .

**PROOF OF PROPOSITION 1.6.** We start by estimating the terms giving the  $Z^{5/3}$  behaviour. We have

$$D(\rho_1, Z\nu) = 4\pi Z \frac{V_\Lambda}{(2\pi)^3} r^{-2} \int_{B(0, 2\Lambda)} \widehat{F}(k) \frac{g \star \widetilde{g}(-k) \overline{\widehat{\nu}(rk)}}{|k|^2} dk$$

and

$$D(\rho_1, \rho_1) = 4\pi \left( \frac{V_\Lambda}{(2\pi)^3} \right)^2 r^{-5} \int_{B(0, 2\Lambda)} |\widehat{F}(k)|^2 \frac{|g \star \widetilde{g}(-k)|^2}{|k|^2} dk.$$

We choose  $r$  such that  $(2\pi)^{-3/2} qZ \frac{V_\Lambda}{(2\pi)^3} r^{-2} = \left( \frac{V_\Lambda}{(2\pi)^3} \right)^2 r^{-5}$ , ie  $r = \frac{1}{\sqrt{2\pi}} \left( \frac{qZ}{V_\Lambda} \right)^{-1/3}$ . The constraint  $r < \Lambda/2$  is equivalent to  $qZ > \frac{1}{(2\pi)^{3/2}} \frac{4\pi}{3}$ , which is automatically satisfied in the limit  $Z \rightarrow +\infty$ . We will come back to it in the proof of Proposition 1.7. We thus get by the dominated convergence theorem

$$\begin{aligned} \lim_{Z \rightarrow +\infty} Z^{-5/3} \left( -\alpha D(\rho_1, Z\nu) + \frac{\alpha}{2} D(\rho_1, \rho_1) \right) &= 2^{-11/6} 3^{-1/3} \pi^{-13/6} \alpha \Lambda q^{5/3} \times \\ &\left( - \int_{B(0, 2\Lambda)} \frac{\widehat{F}(k) g \star \widetilde{g}(-k)}{|k|^2} dk + \frac{1}{2} \int_{B(0, 2\Lambda)} \frac{|\widehat{F}(k) g \star \widetilde{g}(-k)|^2}{|k|^2} dk \right). \end{aligned} \quad (1.4.30)$$

We now want to optimize the right side with respect to  $g$  and  $F$ . We choose  $F = \mathbf{1}_{B(0, a)}$  and  $g = (3(4\pi)^{-1} b^{-3})^{1/2} \mathbf{1}_{B(0, b)}$  with  $a > 0$  and  $b \in (0, 1)$ , and we optimize over  $a$  and  $b$ . Since  $g \star \widetilde{g}(k) = (\text{vol}(B(0, b)))^{-1} \text{vol}(B(0, b) \cap B(-k, b))$  for all  $k$  and since  $B(-k/2, b - |k|/2) \subset B(0, b) \cap B(-k, b)$  for all  $|k| \leq 2b$ , we have

$$g \star \widetilde{g}(k) \geq \mathbf{1}_{B(0, 2b)}(k) \left( 1 - \frac{|k|}{2b} \right)^3.$$

For all  $|k| \leq 2b$ , we also have

$$\widehat{F}(k) \geq \widehat{F}(0) - \frac{\int |x| F}{(2\pi)^{3/2}} 2b = \frac{a^3}{\sqrt{2\pi}} \left( \frac{2}{3} - ab \right).$$

Therefore,

$$\begin{aligned} \int_{B(0, 2\Lambda)} \frac{\widehat{F}(k) g \star \widetilde{g}(-k)}{|k|^2} dk &\geq \frac{a^3}{\sqrt{2\pi}} \left( \frac{2}{3} - ab \right) \int_{B(0, 2b)} \left( 1 - \frac{|k|}{2b} \right)^3 \frac{dk}{|k|^2} \\ &= \sqrt{2\pi} a^3 b \left( \frac{2}{3} - ab \right). \end{aligned}$$

Then, using  $|\widehat{F}(k)| \leq 4\pi a^3/(3(2\pi)^{3/2})$  and  $|g \star \widetilde{g}(k)| \leq 1$  for all  $k$ , we obtain

$$\int_{B(0,2\Lambda)} \frac{|\widehat{F}(k)g \star \widetilde{g}(-k)|^2}{|k|^2} \leq \frac{16}{9}a^6b. \quad (1.4.31)$$

Hence for the  $Z^{5/3}$  term we find that

$$\lim_{Z \rightarrow +\infty} Z^{-5/3} \left( -\alpha D(\rho_1, Z\nu) + \frac{\alpha}{2} D(\rho_1, \rho_1) \right) \leq 2^{-11/6} 3^{-1/3} \pi^{-13/6} \alpha \Lambda q^{5/3} \times \\ a^3 b \left( \sqrt{2\pi} \left( ab - \frac{2}{3} \right) + \frac{8}{9} a^3 \right).$$

Optimizing the right side over all  $a > 0$  and  $b \in (0, 1)$  we get the result. It now remains to prove that the other terms in  $\mathcal{E}_{Z\nu}^{\text{rBDF}}(Q)$  are of lower order than  $Z^{5/3}$ . We begin with the kinetic energy,

$$\text{Tr}_0(D^0Q) \leq \sqrt{1 + \Lambda^2} \text{Tr}(Q) = (2\pi)^{-3} r^{-3} \int F = (2\pi)^{-3/2} \frac{\sqrt{1 + \Lambda^2}}{\Lambda^3} a^3 q Z.$$

For the terms involving  $\rho_2$ , we first use that for all  $p, k$ ,

$$\|X(p+k) - X(p)\| \leq \|U(p+k) - U(p)\| \leq \frac{7}{\sqrt{2}} |k|. \quad (1.4.32)$$

Consequently, for all  $k$ ,

$$\widehat{\rho}_2(k) \leq \frac{7V_\Lambda}{\sqrt{2}(2\pi)^3} r^{-3} |\widehat{F}(k/r)| |g \star \widetilde{g}(-k/r)| |k|.$$

Using this bound together with the estimates leading to (1.4.31), one finds that

$$\begin{cases} |D(\rho_2, Z\nu)| & \leq \beta_1 \Lambda^2 q^{1/3} Z^{4/3} \\ |D(\rho_1, \rho_2)| & \leq \beta_2 \Lambda^2 q^{4/3} Z^{4/3} \\ |D(\rho_2, \rho_2)| & \leq \beta_3 \Lambda^3 q Z, \end{cases} \quad \text{with} \quad \begin{cases} \beta_1 = 2^{19/3} 3^{-2/3} 7\pi^{23/6} a^3 b^2 \\ \beta_2 = 2^{11/6} 3^{-8/3} 7\pi^{-7/3} a^6 b^2 \\ \beta_3 = 2^{-3/2} 3^{-4} 7^2 \pi^{-5/2} a^6 b^3. \end{cases}$$

We conclude that

$$\limsup_{Z \rightarrow +\infty} \frac{E(Z)}{Z^{5/3}} \leq \lim_{Z \rightarrow +\infty} \frac{\mathcal{E}_{Z\nu}^{\text{rBDF}}(Q)}{Z^{5/3}} = -c_1 \alpha \Lambda q^{5/3}.$$

□

**Remark 1.14.** The proof is the same when  $\int \nu < 0$ , using  $X(p) = U(p) (0 \ 0 \ 0 \ 1)^t$  and  $\widehat{Q}(p, q) = -\widehat{\gamma}(p, q) X(p) X(q)^*$ . The trial state  $Q$  now satisfies  $Q = Q_{--}$ , so that  $\widehat{\rho}_Q$  is negative around 0.

To estimate the convergence rate of  $E(Z)$  towards  $-c_1 \alpha \Lambda |q|^{5/3} Z^{5/3}$ , we will use the first moment  $\int |x| |\nu|$  to control the convergence of  $\widehat{\nu}(k)$  to  $\widehat{\nu}(0)$ .

PROOF OF PROPOSITION 1.7. We assume  $q > 0$  (the case  $q < 0$  follows from obvious modifications). We split the term  $D(\rho_1, Z\nu)$  into

$$D(\rho_1, Z\nu) = \frac{4\pi|q|Z}{(2\pi)^{3/2}} \int_{B(0,2\Lambda)} \frac{\widehat{\rho}_1(k)}{|k|^2} dk + R_1,$$

with

$$R_1 = 4\pi Z \int_{B(0,2\Lambda)} \frac{\widehat{\rho}_1(k)\overline{\widehat{\nu}(k)} - \widehat{\nu}(0)}{|k|^2} dk.$$

We use that  $|\widehat{\nu}(k) - \widehat{\nu}(0)| \leq (2\pi)^{-3/2} \|x|\nu\|_1 |k|$  for all  $k$  to estimate

$$|R_1| \leq 2^{5/3} 3^{-5/3} \pi^{-11/6} a^3 b^2 \|x|\nu\|_1 \Lambda^2 |q|^{1/3} Z^{4/3}.$$

Hence we have for all  $|q|Z > \frac{1}{(2\pi)^{3/2}} \frac{4\pi}{3}$ ,

$$E(Z) \leq \mathcal{E}_{Z\nu}^{\text{rBDF}}(Q) \leq -c_1 \alpha \Lambda |q|^{5/3} Z^{5/3} (1 - B_1 Z^{-1/3} - B_2 Z^{-2/3}), \quad (1.4.33)$$

with

$$B_1 = 2^{28/3} 3^{-2} \pi^{-1/2} a^3 b^2 \|x|\nu\|_1 \Lambda |q|^{-4/3} + 2^{4/3} 3^{-1} 7\pi^{31/6} a^3 b^2 \Lambda |q|^{-4/3} \\ + 2^{51/6} 3^{-3} 7\pi^{-1} a^6 b^2 \Lambda |q|^{-1/3}$$

and

$$B_2 = 2^{37/6} 3^{-1/3} \pi^{4/3} a^3 \frac{\sqrt{1+\Lambda^2}}{\Lambda^4} \alpha^{-1} |q|^{-2/3} + 2^{31/6} 3^{-11/3} 7^2 \pi^{-7/6} a^6 b^3 \Lambda^2 |q|^{-2/3}.$$

We furthermore have  $1 - B_1 X - B_2 X^2 \geq 1/2$  for  $0 \leq X \leq X_0$  with

$$X_0 = \frac{B_1}{2B_2} \left( \sqrt{1 + \frac{2B_2}{B_1^2}} - 1 \right),$$

therefore Proposition 1.7 holds with

$$\widetilde{Z}_1 := \max \left( X_0^{-3}, \frac{1}{(2\pi)^{3/2}} \frac{4\pi}{3|q|} \right). \quad (1.4.34)$$

□

PROOF OF COROLLARY 1.2. For any  $Q \in \mathcal{K}$ , we have  $D(\rho_Q, \rho_Q)^{1/2} \leq C_\Lambda \|Q\|_{1, P_-^0}$ , by [HLS09a, Lemma 1]. The constraint  $-P_-^0 \leq Q \leq 1 - P_-^0$  can be rewritten as  $Q_{++} - Q_{--} \geq Q^2$ . Defining  $X := [\text{Tr}(Q_{++} - Q_{--})]^{1/2}$  we get

$$2\|Q_{+-}\|_{\mathfrak{S}_2}^2 = 2\|Q_{-+}\|_{\mathfrak{S}_2}^2 = \|Q_{++}\|_{\mathfrak{S}_2}^2 + \|Q_{--}\|_{\mathfrak{S}_2}^2 \leq \|Q\|_{\mathfrak{S}_2}^2 \leq X^2,$$

and thus  $\|Q\|_{1, P_-^0} \leq X^2 + \sqrt{2}X$ . Using the Cauchy-Schwarz inequality for the Coulomb scalar product we also get that  $D(\rho_Q, Z\nu) \leq C_\Lambda Z \|\nu\|_{\mathcal{C}} (X^2 + \sqrt{2}X)$  for all  $Q \in \mathcal{K}$ .

From this estimate and the inequality (1.4.26), we can see that for all  $Z > \widetilde{Z}_1$  and for all minimizer  $Q^{\text{vac}}$  for  $E(Z)$ ,

$$-\alpha C_\Lambda Z \|\nu\|_c (X^2 + \sqrt{2}X) \leq \mathcal{E}_{Z\nu}^{\text{rBDF}}(Q^{\text{vac}}) = E(Z) \leq -\frac{c_1}{2} \alpha \Lambda |q|^{5/3} Z^{5/3}.$$

Hence  $X \geq (\sqrt{1+2a}-1)/\sqrt{2}$  with  $a = \frac{c_1 \Lambda |q|^{5/3}}{2C_\Lambda \|\nu\|_c} Z^{2/3}$ . We get

$$\text{Tr}(Q_{++}^{\text{vac}} - Q_{--}^{\text{vac}}) = X^2 \geq \frac{1}{2} \left( \sqrt{1+2a} - 1 \right)^2 \geq CZ^{2/3},$$

where

$$C = \left( \sqrt{1 + \frac{c_1 \Lambda |q|^{5/3}}{C_\Lambda \|\nu\|_c} \widetilde{Z}_1^{2/3} - 1} \right)^2 \widetilde{Z}_1^{-2/3}. \quad (1.4.35)$$

□

**Remark 1.15.** When the exchange term is included, the bound of Proposition 1.7 remains valid, with different constants. In this case, the function  $a_\pm(p)$  becomes

$$a_\pm(p) = \frac{1}{\sqrt{2}} \sqrt{1 \pm \frac{g_0(|p|)}{\sqrt{g_0(|p|)^2 + g_1(|p|)^2}}},$$

using the notation of [HLS07]. The BDF energy can be estimated from above by a reduced BDF energy involving  $\mathcal{P}_-^0$  and  $\mathcal{D}^0$ , which is treated in the same way using that  $\nabla U \in L^\infty(B(0, \Lambda))$  (which is used in (1.4.32)).

## 5. Proof of Theorem 1.1

**PROOF OF THEOREM 1.1.** Let  $Q$  be any minimizer for  $E(Z)$ , and let  $\omega$  be the unique BDF state on  $\mathcal{F}(\mathfrak{H}_+) \oplus \mathcal{F}(\mathfrak{H}_-)$  having  $Q$  as its generalized 1-pdm and  $p = 0$  as its pairing matrix, defined by Proposition 1.5. Then by Corollary 1.1, we have

$$p_Z = 1 - \omega(|\Omega\rangle\langle\Omega|) \geq 1 - e^{-a \text{Tr}(Q_{++} - Q_{--})}.$$

Now by Corollary 1.2, we know that  $\text{Tr}(Q_{++} - Q_{--}) \geq CZ^{2/3}$  for all  $Z > \widetilde{Z}_1$ , thus  $p_Z \geq 1 - e^{-\kappa Z^{2/3}}$  with  $\kappa := aC$ . □

## A. Product states

Given a (at most) countable family of separable Hilbert spaces  $(\mathfrak{H}_i)_{i \in \mathbb{N}}$  and a family  $(\omega_i)_{i \in \mathbb{N}}$  of quasi-free states such that  $\omega_i$  is a state on  $\mathcal{F}(\mathfrak{H}_i)$  for all  $i \in \mathbb{N}$ , we want to give a meaning to the product state  $\otimes_{i \in \mathbb{N}} \omega_i$  as a quasi-free state on  $\mathcal{F}(\oplus_{i \in \mathbb{N}} \mathfrak{H}_i)$ . We first consider the unitary transformation

$$\begin{aligned} T : \quad & \mathcal{F}\left(\bigoplus_{i \in \mathbb{N}} \mathfrak{H}_i\right) & \longrightarrow & \bigotimes_{i \in \mathbb{N}} \mathcal{F}(\mathfrak{H}_i) \\ & \bigwedge_{j \in J_{i_1}} \varphi_{j, i_1} \wedge \cdots \wedge \bigwedge_{j \in J_{i_k}} \varphi_{j, i_k} & \longmapsto & \bigwedge_{j \in J_{i_1}} \varphi_{j, i_1} \otimes \cdots \otimes \bigwedge_{j \in J_{i_k}} \varphi_{j, i_k}, \end{aligned}$$



where  $i_1 < \dots < i_k$  are elements of  $\mathbb{N}$  and for each  $1 \leq \ell \leq k$ ,  $(\varphi_{j,i_\ell})_{j \in \mathbb{N}}$  is an orthonormal basis for  $\mathfrak{H}_{i_\ell}$  and  $J_{i_\ell} \subset \mathbb{N}$  is finite. We recall the definition of a product state on a tensor product of  $C^*$ -algebras [Gui66, Proposition 2.9].

**Theorem 1.2.** *Let  $(\mathfrak{A}_i)_{i \in \mathbb{N}}$  be a collection of (unital)  $C^*$ -algebras and let  $\omega_i$  be a state on  $\mathfrak{A}_i$  for all  $i$ . There exists a unique state on  $\otimes_i \mathfrak{A}_i$ , denoted by  $\otimes_i \omega_i$  such that for any  $(A_{i_1}, \dots, A_{i_\ell}) \in \mathfrak{A}_{i_1} \times \dots \times \mathfrak{A}_{i_\ell}$  with any indices  $i_1 < \dots < i_\ell$ , we have  $\otimes_i \omega_i(A_{i_1} \otimes \dots \otimes A_{i_\ell}) = \prod_{k=1}^{\ell} \omega_{i_k}(A_{i_k})$ .*

**Remark 1.16.** Recall that the tensor product  $\otimes_i \mathfrak{A}_i$  is defined as the inductive limit of the  $C^*$ -algebras  $\otimes_{i \in J} \mathfrak{A}_i$  with  $J$  finite, or equivalently as the completion (for a certain  $*$ -norm) of  $\otimes_i \mathfrak{A}_i$  seen as a tensor product of unital algebras [Gui66].

In the particular case where  $\mathfrak{A}_i = \mathfrak{A}[\mathfrak{H}_i]$  for all  $i \in \mathbb{N}$ , the tensor product  $\otimes_i \mathfrak{A}_i$  is also a CAR algebra generated by the operators

$$\widehat{a}(f_j) := \Upsilon(-\text{Id}_{\mathfrak{H}_0}) \otimes \dots \otimes \Upsilon(-\text{Id}_{\mathfrak{H}_{j-1}}) \otimes a_j(f_j),$$

where  $j \in \mathbb{N}$ ,  $f_j \in \mathfrak{H}_j$  and  $a_j$  is the annihilation operator on  $\mathcal{F}(\mathfrak{H}_j)$  for all  $j$ . Notice the “twisting” operator  $\Upsilon(-\text{Id})$  on the left, defined in (1.3.20), used to ensure that the  $(\widehat{a}(f_j))_{f_j, j}$  satisfy the CAR. Notice also that we have the relation  $\widehat{a}(f_j) = T a(f_j) T^*$ , where  $a(f_j)$  is the usual annihilation operator on  $\mathcal{F}(\oplus_i \mathfrak{H}_i)$ .

**Proposition 1.9.** *Let  $(\omega_i)_{i \in \mathbb{N}}$  be a collection of quasi-free states such that  $\omega_i$  is defined on  $\mathfrak{A}[\mathfrak{H}_i]$  for all  $i$ . Let  $(\gamma_i, \alpha_i)_i$  be the collection of their density matrices, and assume that  $\sum_i \text{Tr}_{\mathfrak{H}_i}(\gamma_i) < +\infty$ . Let  $\omega$  be the unique quasi-free state on  $\mathfrak{A}[\oplus_i \mathfrak{H}_i]$  having  $\gamma := \oplus_i \gamma_i$  as 1-pdm and  $\alpha := \oplus_i \alpha_i$  as pairing matrix. Then we have*

$$\forall A \in \mathfrak{A}[\oplus_i \mathfrak{H}_i], \quad \omega(A) = \otimes_i \omega_i(T A T^*).$$

As a consequence, the product state  $\otimes_i \omega_i$  can be considered as a state on  $\mathfrak{A}[\oplus_i \mathfrak{H}_i]$ .

**Remark 1.17.** The state  $\omega$  is well-defined by Proposition 1.1, since  $\text{Tr}(\gamma) = \sum_i \text{Tr}_{\mathfrak{H}_i}(\gamma_i)$  is finite.

**PROOF.** We will show that the state  $\otimes_i \omega_i$  is quasi-free on the CAR generated by the  $(\widehat{a}(f_j))_{f_j, j}$ . This proves the result because the state  $\otimes_i \omega_i(T \cdot T^*)$  is then quasi-free and one easily shows that it has  $\oplus_i \gamma_i$  as 1-pdm and  $\oplus_i \alpha_i$  as pairing matrix. Since the density matrices determine uniquely the quasi-free state, we must have  $\otimes_i \omega_i(T \cdot T^*) = \omega$ . Therefore we only have to show the Wick relation for the state  $\otimes_i \omega_i$ . Let us first notice that it is enough to prove it for products of the form

$$X := \widehat{a}^\# \left( f_1^{(i_1)} \right) \dots \widehat{a}^\# \left( f_{2k_1}^{(i_1)} \right) \dots \widehat{a}^\# \left( f_1^{(i_N)} \right) \dots \widehat{a}^\# \left( f_{2k_N}^{(i_N)} \right),$$

with  $i_1 < \dots < i_N$ ,  $k_\ell \in \mathbb{N}$ ,  $f_p^{(i_\ell)} \in \mathfrak{H}_{i_\ell}$  for all  $1 \leq p \leq 2k_\ell$ ,  $1 \leq \ell \leq N$ , and where  $\#$  means star or no star. This means two things:

- (1) We can restrict to ordered products with respect to the decomposition  $\bigoplus_{i \in \mathbb{N}} \mathfrak{H}_i$ : The  $2k_1$  first creation/annihilation operators  $\widehat{a}^\# \left( f_p^{(i_1)} \right)$  with  $1 \leq p \leq 2k_1$  all create/annihilate particles belonging to  $\mathfrak{H}_{i_1}$ , then the following  $2k_2$  creation/annihilation  $\widehat{a}^\# \left( f_p^{(i_2)} \right)$  with  $1 \leq p \leq 2k_2$  create/annihilate particles belonging to  $\mathfrak{H}_{i_2}$ , etc. We can always order in this way any product of  $a^\#$ s because Wick's formula does not depend on the choice of an ordering.
- (2) We can restrict to products where there is an even number of particles created/annihilated in each space  $\mathfrak{H}_{i_\ell}$ . If not the case, both sides of Wick relation can easily be shown to vanish.

This being said, let us compute  $\omega(X)$  as follows

$$\begin{aligned}
\omega(X) &= \otimes_i \omega_i \left[ \Upsilon(-\text{Id}_{\mathfrak{H}_0})^{\sum_{\ell=1}^N 2k_\ell} \otimes \dots \otimes \Upsilon(-\text{Id}_{\mathfrak{H}_{i_1-1}})^{\sum_{\ell=1}^N 2k_\ell} \otimes \right. \\
&\quad \left. a^\# \left( f_1^{(i_1)} \right) \dots a^\# \left( f_{2k_1}^{(i_1)} \right) \Upsilon(-\text{Id}_{\mathfrak{H}_{i_1}})^{\sum_{\ell=2}^N 2k_\ell} \otimes \dots \otimes a^\# \left( f_1^{(i_N)} \right) \dots a^\# \left( f_{2k_N}^{(i_N)} \right) \right] \\
&= \prod_{\ell=1}^N \omega_{i_\ell} \left[ a^\# \left( f_1^{(i_\ell)} \right) \dots a^\# \left( f_{2k_\ell}^{(i_\ell)} \right) \right] \\
&= \prod_{\ell=1}^N \sum_{\pi_\ell \in \widetilde{\mathcal{S}}_{2k_\ell}} (-1)^{\varepsilon(\pi_\ell)} \omega_{i_\ell} \left[ a^\# \left( f_{\pi_\ell(1)}^{(i_\ell)} \right) a^\# \left( f_{\pi_\ell(2)}^{(i_\ell)} \right) \right] \times \dots \\
&\quad \dots \times \omega_{i_\ell} \left[ a^\# \left( f_{\pi_\ell(2k_\ell-1)}^{(i_\ell)} \right) a^\# \left( f_{\pi_\ell(2k_\ell)}^{(i_\ell)} \right) \right].
\end{aligned}$$

Let us rewrite  $X$  as follows

$$X = \widehat{a}^\#(f_1) \dots \widehat{a}^\#(f_{2k_1}) \widehat{a}^\#(f_{2k_1+1}) \dots \widehat{a}^\#(f_{2(k_1+\dots+k_N)}).$$

The right side of Wick's formula reads

$$Y = \sum_{\pi \in \widetilde{\mathcal{S}}_{2K}} (-1)^{\varepsilon(\pi)} (\otimes_i \omega_i) \left[ \widehat{a}^\#(f_{\pi(1)}) \widehat{a}^\#(f_{\pi(2)}) \right] \dots (\otimes_i \omega_i) \left[ \widehat{a}^\#(f_{\pi(2K-1)}) \widehat{a}^\#(f_{\pi(2K)}) \right],$$

with  $K := k_1 + \dots + k_N$ . We claim that this sum only contains terms with  $\pi$  leaving invariant each interval of the form  $[2k_\ell + 1, 2k_{\ell+1}]$ . This claim is proved by induction on  $K$ : We introduce

$$W_\rho^K(e_1 \dots e_{2K}) := \sum_{\pi \in \widetilde{\mathcal{S}}_{2K}} (-1)^{\varepsilon(\pi)} \rho(e_{\pi(1)} e_{\pi(2)}) \dots \rho(e_{\pi(2K-1)} e_{\pi(2K)}).$$

For  $\pi \in \widetilde{\mathcal{S}}_{2K}$ , we have  $\pi(1) = 1$ , hence we have the induction formula

$$W_\rho^K(e_1 \dots e_{2K}) = \sum_{i=2}^{2K} (-1)^i \rho(e_1 e_i) W_\rho^{K-1}(e_2 \dots \widehat{e}_i \dots e_{2K}).$$

In our case where  $e_j = \widehat{a}^\#(f_j)$  and  $\rho = \otimes_i \omega_i$ , we see that  $\rho(e_1 e_i) \neq 0$  if and only if  $i \leq 2k_1$ . Hence, by induction on  $K$ , the only permutations  $\pi \in \widetilde{\mathcal{S}}_{2K}$  giving rise to a non-zero term in  $Y$  are those which leave invariant the intervals  $[2k_\ell + 1, 2k_{\ell+1}]$  with  $1 \leq \ell \leq N$ . We can thus write

$$\begin{aligned} Y &= \prod_{\ell=1}^N \sum_{\pi_\ell \in \widetilde{\mathcal{S}}_{2k_\ell}} (-1)^{\varepsilon(\pi_\ell)} (\otimes_i \omega_i) \left[ \widehat{a}^\# \left( f_{\pi_\ell(2k_\ell-1)}^{(i_\ell)} \right) \widehat{a}^\# \left( f_{\pi_\ell(2k_\ell)}^{(i_\ell)} \right) \right] \times \cdots \\ &\quad \cdots \times (\otimes_i \omega_i) \left[ \widehat{a}^\# \left( f_{\pi_\ell(1)}^{(i_\ell)} \right) \widehat{a}^\# \left( f_{\pi_\ell(2)}^{(i_\ell)} \right) \right] \\ &= \prod_{\ell=1}^N \sum_{\pi_\ell \in \widetilde{\mathcal{S}}_{2k_\ell}} (-1)^{\varepsilon(\pi_\ell)} \omega_{i_\ell} \left[ a^\# \left( f_{\pi_\ell(2k_\ell-1)}^{(i_\ell)} \right) a^\# \left( f_{\pi_\ell(2k_\ell)}^{(i_\ell)} \right) \right] \times \cdots \\ &\quad \cdots \times \omega_{i_\ell} \left[ a^\# \left( f_{\pi_\ell(1)}^{(i_\ell)} \right) a^\# \left( f_{\pi_\ell(2)}^{(i_\ell)} \right) \right] = \omega(X). \end{aligned}$$

This proves that the state  $\otimes_i \omega_i$  is quasi-free, which concludes the proof.  $\square$

## B. Including the exchange term

When we take into account the exchange term, the free vacuum  $\mathcal{P}_-^0$  is an orthogonal projection on  $\mathfrak{H}_\Lambda$  solving the equation

$$\begin{cases} \mathcal{P}_-^0 &= \chi_{(-\infty, 0]}(\mathcal{D}^0), \\ \mathcal{D}^0 &= D^0 - \alpha \frac{(\mathcal{P}_-^0 - 1/2)(x, y)}{|x-y|}, \end{cases}$$

The operator  $\gamma^0 = \mathcal{P}_-^0 - 1/2$  is constructed in [HLS07] for  $0 \leq \alpha < 4/\pi$  as the unique minimizer of the energy

$$\mathcal{T}(f) := \frac{1}{(2\pi)^3} \int_{B(0, \Lambda)} \text{Tr}_{\mathbb{C}^4}(D^0(p)f(p)) dp - \frac{\alpha}{(2\pi)^5} \iint_{B(0, \Lambda)^2} \frac{\text{Tr}_{\mathbb{C}^4}(f(p)f(q))}{|p-q|^2} dp dq$$

over all translation-invariant  $f = f(-i\nabla)$  with  $f \in L^\infty(B(0, \Lambda), \mathcal{S}_4(\mathbb{C}))$  ( $\mathcal{S}_4(\mathbb{C})$  denoting the vector space of all  $4 \times 4$  self-adjoint complex matrices) satisfying  $-\text{Id}_{\mathbb{C}^4}/2 \leq f \leq \text{Id}_{\mathbb{C}^4}/2$ . It can be shown [HLS07] that the self consistent operator  $\mathcal{D}^0$  is a multiplication operator in Fourier space, taking the form

$$\mathcal{D}^0(p) = \frac{g_1(|p|)}{|p|} \alpha \cdot p + g_0(|p|)\beta,$$

where  $g_0, g_1 \in L^\infty([0, \Lambda], \mathbb{R})$  satisfy

$$g_1(x) \geq x, \quad g_0(x) \geq 1, \quad g_1(x) \leq g_0(x)x.$$

The BDF energy with exchange term reads for any  $Q \in \mathcal{K}$ ,

$$\mathcal{E}_\nu^{\text{BDF}}(Q) := \text{Tr}_0(\mathcal{D}^0 Q) - \alpha D(\nu, \rho_Q) + \frac{\alpha}{2} D(\rho_Q, \rho_Q) - \frac{\alpha}{2} \iint \frac{|Q(x, y)|^2}{|x-y|} dx dy.$$

The variational set becomes

$$\mathcal{K} := \{Q \in \mathfrak{S}_{1, \mathcal{P}_-^0}, \quad Q = Q^*, \quad -\mathcal{P}_-^0 \leq Q \leq 1 - \mathcal{P}_-^0\}.$$

Define

$$E(Z) := \inf\{\mathcal{E}_{Z\nu}^{\text{BDF}}(Q), Q \in \mathcal{K}\},$$

which is well-defined for  $0 \leq \alpha < 4/\pi$  by [HLS05b].

To adapt the previous results to the case with exchange term, one first needs to study the asymptotics of  $E(Z)$  as  $Z \rightarrow +\infty$ . Notice that the lower bound is the same since by the Kato inequality, for  $0 \leq \alpha < 4/\pi$ ,

$$\text{Tr}_0(\mathcal{D}^0 Q) - \frac{\alpha}{2} \iint \frac{|Q(x, y)|^2}{|x - y|} dx dy \geq 0,$$

so that

$$E(Z) \geq \inf \left\{ -\alpha D(Z\nu, \rho) + \frac{\alpha}{2} D(\rho, \rho), \rho \in \mathcal{C}, \|\rho\|_{L^\infty} \leq \frac{\Lambda^3}{6\pi^2} \right\} \geq cZ^{5/3}.$$

We can obtain the upper bound by the same method as in the proofs of Propositions 1.6 and 1.7, majoring the BDF energy by the rBDF one. One has to modify the definition of  $a_\pm(p)$  in (1.4.29) by

$$a_\pm(p) = \frac{1}{\sqrt{2}} \sqrt{1 \pm \frac{g_0(|p|)}{\sqrt{g_0(|p|)^2 + g_1(|p|)^2}}}.$$

The operator  $U(p)$  on  $\mathbb{C}^4$  defined by

$$U(p) = a_+(p)\text{Id}_{\mathbb{C}^4} + a_-(p)\beta \frac{\boldsymbol{\alpha} \cdot p}{|p|}$$

is unitary and diagonalizes  $\mathcal{D}^0(p)$ :

$$U(p)\mathcal{D}^0(p)U(p)^* = \sqrt{g_0(|p|)^2 + g_1(|p|)^2}\beta.$$

From the proof of the upper bound, we see that the only additional information we have to provide is an estimation of  $\|\nabla U\|_{L^\infty}$  which, by definition of  $U$ , amounts to estimate  $\|\nabla a_\pm\|_{L^\infty}$  and  $\|a_-(p)/|p|\|_{L^\infty}$ . Let us pose  $g(p) = g_1(|p|)^2/g_0(|p|)^2 \geq 0$ . Then,  $|a_-(p)| \leq \sqrt{g(p)}/2 \leq |p|/2$ , and hence  $a_-(p)/|p| \in L^\infty(B(0, \Lambda))$ . Moreover, since  $p \mapsto g_0(|p|) \in C^\infty(\overline{B(0, \Lambda)})$  is positive and  $p \mapsto g_0(|p|)^2 + g_1(|p|)^2 \in C^\infty(\overline{B(0, \Lambda)})$  is positive, we see that  $p \mapsto a_+(p) \in C^\infty(\overline{B(0, \Lambda)})$ . The same reasoning can be applied to  $a_-(p)$  on  $\overline{B(0, \Lambda)} \setminus \{0\}$ , the only thing to verify being that  $\nabla a_-(p)$  stays bounded as  $p \rightarrow 0$ . We see that it is the case because we have

$$|\sqrt{g_0(|p|)^2 + g_1(|p|)^2} - g_0(|p|)| \leq C|p|^2,$$

implying that  $|\nabla(\sqrt{g_0(|p|)^2 + g_1(|p|)^2} - g_0(|p|))| \leq C|p|$  on a neighborhood of 0. We moreover have that for all  $|p| \leq \Lambda$ ,

$$|\sqrt{g_0(|p|)^2 + g_1(|p|)^2} - g_0(|p|)| \geq \frac{\sqrt{\|g_0\|_{L^\infty}^2 + \Lambda^2} - \|g_0\|_{L^\infty}}{\Lambda} |p|^2,$$

which implies that

$$|\nabla \sqrt{g_0(|p|)^2 + g_1(|p|)^2} - g_0(|p|)| = \frac{1}{2} \frac{|\nabla(\sqrt{g_0(|p|)^2 + g_1(|p|)^2} - g_0(|p|))|}{\sqrt{g_0(|p|)^2 + g_1(|p|)^2} - g_0(|p|)} \leq C,$$

for  $p$  in some neighborhood of 0. This shows that  $\nabla a_-(p)$  remains bounded as  $p \rightarrow 0$ . Hence, Propositions 1.6, 1.7, 1.8, and Corollary 1.2 still hold with the exchange term, using  $\nabla U \in L^\infty(B(0, \Lambda))$ .

**Theorem 1.3** (Probability to produce at least a pair for the full BDF model). *Let  $\alpha > 0$  and  $\Lambda > 0$ . Let  $\nu \in \mathcal{C}$  such that  $\int_{\mathbb{R}^3} (1 + |x|)|\nu(x)| dx < \infty$ ,  $\int_{\mathbb{R}^3} \nu \neq 0$  and  $\int_{\mathbb{R}^3} |\nu| = 1$ . Then, there exists a constant  $Z_1 = Z_1(\alpha, \Lambda, \nu) > 0$  and a constant  $\kappa = \kappa(\alpha, \Lambda, \nu) > 0$  such that for all  $Z > Z_1$  we have, for the full BDF model,*

$$\boxed{p_Z \geq 1 - e^{-\kappa Z^{2/3}}.} \quad (1.B.36)$$

For the full BDF model, we furthermore know that the minimizer is a projection and hence is associated to a pure state in the Fock space. We thus can use Proposition 1.3 to estimate the probability to produce at least  $N$  pairs. This probability is defined for any state  $\omega$  on  $\mathcal{F}(\mathfrak{H}_+) \otimes \mathcal{F}(\mathfrak{H}_-)$  by the formula

$$p_N(\omega) := 1 - \sum_{k=0}^N \sum_{\ell=0}^k \omega(\mathcal{P}_{\ell,+} \otimes \mathcal{P}_{k-\ell,-}),$$

where  $\mathcal{P}_{j,\pm}$  denotes the orthogonal projection on the  $j$ -particle sector in  $\mathcal{F}(\mathfrak{H}_\pm)$ .

**Theorem 1.4** (Probability to produce at least  $N$  pairs for the full BDF model). *Let  $N \in \mathbb{N}$ ,  $\alpha > 0$  and  $\Lambda > 0$ . Let  $\nu \in \mathcal{C}$  such that  $\int_{\mathbb{R}^3} (1 + |x|)|\nu(x)| dx < \infty$ ,  $\int_{\mathbb{R}^3} \nu \neq 0$  and  $\int_{\mathbb{R}^3} |\nu| = 1$ . Then, there exists a constant  $Z_1 = Z_1(N, \alpha, \Lambda, \nu) > 0$  and constants  $\kappa_1 = \kappa_1(\alpha, \Lambda, \nu) > 0$ ,  $\kappa_2 = \kappa_2(\alpha, \Lambda, \nu) > 0$  such that for all  $Z > Z_1$  we have, for the full BDF model,*

$$\boxed{p_{N,Z} \geq 1 - \left( \sum_{k=0}^N \frac{(\kappa_2 Z)^k}{[k/2]!} \right) e^{-\kappa_1 Z^{2/3}},} \quad (1.B.37)$$

**Remark 1.18.** Fixing  $N$  and taking  $Z \rightarrow +\infty$  leads to  $p_{N,Z} \rightarrow 1$ . This shows that an infinite number of particles is produced when  $Z \rightarrow +\infty$ .

PROOF. If  $T$  denotes the isometry used in Proposition 1.5, we see that we have

$$T^* \left( \sum_{\ell=0}^k \mathcal{P}_{\ell,+} \otimes \mathcal{P}_{k-\ell,-} \right) T = \mathcal{P}_k,$$

where  $\mathcal{P}_k$  is the orthogonal projection on the  $k$ -particle sector in  $\mathcal{F}(\mathfrak{H}_- \oplus \mathfrak{H}_+)$ . Hence,  $p_{N,Z} = 1 - \sum_{k=0}^N \omega_{0,Z}(\mathcal{P}_k)$  where  $\omega_{0,Z}$  is the HFB state constructed in the proof of Proposition 1.5, associated to renormalized density matrices  $(Q, p) = (Q_Z, 0)$ ,  $Q_Z$  being any minimizer of the full BDF energy. Using now Proposition 1.3, we obtain

$$\omega_{0,Z}(\mathcal{P}_k) \leq e^{k/2} \frac{\left( \frac{\text{Tr}(Q_{Z,++} - Q_{Z,--})}{2} \right)^\ell}{\ell!} e^{-\frac{\text{Tr}(Q_{Z,++} - Q_{Z,--})}{2}},$$

for  $k = k_0 + 2\ell$ ,  $\ell \geq 0$ ,  $k_0 := \dim \ker(Q_{Z,++} - Q_{Z,--} - 1)$ . If  $k$  is not of this form, we have  $\omega_{0,Z}(\mathcal{P}_k) = 0$ . The lower bound on  $\text{Tr}(Q_{Z,++} - Q_{Z,--})$  is

$$\text{Tr}(Q_{Z,++} - Q_{Z,--}) \geq cZ^{2/3},$$

while a trivial upper bound coming from  $\mathcal{E}_{\text{BDF}}^{Z\nu}(Q_Z) \leq 0$  is

$$\text{Tr}(Q_{Z,++} - Q_{Z,--}) \leq CZ^2.$$

We thus deduce that

$$\omega_{0,Z}(\mathcal{P}_k) \leq e^{k/2} \frac{(CZ^2)^\ell}{\ell!} e^{-cZ^{2/3}}.$$

We obtain an estimate depending only on  $N$ , using additional assumptions. Namely, using that  $\ell \leq \lfloor k/2 \rfloor$  and the fact that  $a^n/n! \leq a^{n+1}/(n+1)!$  if  $a \geq n+1$ , we deduce that if  $CZ^2 \geq \lfloor N/2 \rfloor$ , we have

$$\omega_{0,Z}(\mathcal{P}_k) \leq e^{k/2} \frac{(CZ^2)^{\lfloor k/2 \rfloor}}{\lfloor k/2 \rfloor!} e^{-cZ^{2/3}},$$

which thus holds for all  $k \leq N$ . □

### C. Quasi-free states

In this section, we precise some facts about quasi-free states that were not needed explicitly for the article, but which may be useful in another context.

**C.1. Fock space, creation and annihilation operators.** Here, we precise the objects introduced in Section 3.1. The Fock space  $\mathcal{F}$  over the Hilbert space  $\mathfrak{H}$  consists of all sequences  $\Psi = (\Psi_N)_{N \in \mathbb{N}}$ , where  $\Psi_N \in \mathfrak{H}^N$  for all  $N$ , such that  $\sum_{N \geq 0} \|\Psi_N\|_{\mathfrak{H}^N}^2 < +\infty$ . It is a Hilbert space when endowed with the inner product

$$\forall \Psi, \Phi \in \mathcal{F}, \langle \Psi, \Phi \rangle_{\mathcal{F}} := \sum_{N \geq 0} \langle \Psi_N, \Phi_N \rangle_{\mathfrak{H}^N}.$$

For any  $f \in \mathfrak{H}$ , the *creation operator*  $a^*(f) : \mathfrak{H}^N \rightarrow \mathfrak{H}^{N+1}$  is defined by  $a^*(f)\Omega := f \in \mathfrak{H}$  in the 0-particle sector and for all  $N \geq 1$ , by its action on the  $N$ -particle sector

on an orthonormal basis  $(\varphi_{i_1} \wedge \cdots \wedge \varphi_{i_N})_{0 \leq i_1 < \cdots < i_N}$ , where  $(\varphi_i)_{i \in \mathbb{N}}$  is an orthonormal basis of  $\mathfrak{H}$ :

$$a^*(f)\varphi_{i_1} \wedge \cdots \wedge \varphi_{i_N} := f \wedge \varphi_{i_1} \wedge \cdots \wedge \varphi_{i_N}.$$

Here, we have used the notation for any  $g_1, \dots, g_M \in \mathfrak{H}$ ,

$$g_1 \wedge \cdots \wedge g_M := \frac{1}{\sqrt{M!}} \sum_{\sigma \in \mathfrak{S}_M} \varepsilon(\sigma) g_{\sigma(1)} \otimes \cdots \otimes g_{\sigma(M)} \in \mathfrak{H}^M.$$

The operator  $a^*(f)$  is extended to all finite combinations of  $\varphi_I := \varphi_{i_1} \wedge \cdots \wedge \varphi_{i_N}$  by linearity, and to all of  $\mathfrak{H}^N$  by continuity thanks to the following estimates:

$$\left\| a^*(f) \left( \sum_{\text{finite}} a_I \varphi_I \right) \right\|_{\mathfrak{H}^{N+1}}^2 = \sum_{I, J} \overline{a_I} a_J \begin{vmatrix} \|f\|^2 & \langle \varphi_{i_1}, f \rangle & \cdots & \langle \varphi_{i_N}, f \rangle \\ \langle f, \varphi_{j_1} \rangle & \langle \varphi_{i_1}, \varphi_{j_1} \rangle & \cdots & \langle \varphi_{i_N}, \varphi_{j_1} \rangle \\ \vdots & & & \vdots \\ \langle f, \varphi_{j_N} \rangle & \langle \varphi_{i_1}, \varphi_{j_N} \rangle & \cdots & \langle \varphi_{i_N}, \varphi_{j_N} \rangle \end{vmatrix},$$

which implies after developing with respect to the first column and then to the first line that

$$\begin{aligned} \left\| a^*(f) \left( \sum_{\text{finite}} a_I \varphi_I \right) \right\|_{\mathfrak{H}^{N+1}}^2 &= \|f\|^2 \sum_I |a_I|^2 \\ &\quad - \left\| \sum_I a_I \sum_{\ell=1}^N (-1)^\ell \langle f, \varphi_{i_\ell} \rangle \varphi_{i_1} \wedge \cdots \wedge \widehat{\varphi_{i_\ell}} \wedge \cdots \wedge \varphi_{i_N} \right\|_{\mathfrak{H}^{N-1}}^2 \\ &\leq \|f\|^2 \left\| \sum_I a_I \varphi_I \right\|_{\mathfrak{H}^N}^2. \end{aligned}$$

In these computations we have used the fundamental formula

$$\langle g_1 \wedge \cdots \wedge g_M, h_1 \wedge \cdots \wedge h_M \rangle = \det(\langle g_i, h_j \rangle)_{1 \leq i, j \leq M}.$$

This defines  $a^*(f) : \mathfrak{H}^N \rightarrow \mathfrak{H}^{N+1}$  as a bounded operator. The same kind of computation leads to the definition of the adjoint  $a(f)$  of  $a^*(f)$ , called the *annihilation operator*, as  $a(f)\Omega = 0$  and

$$a(f)\varphi_{i_1} \wedge \cdots \wedge \varphi_{i_{N+1}} = \sum_{k=1}^{N+1} (-1)^{k+1} \langle f, \varphi_{i_k} \rangle \varphi_{i_1} \wedge \cdots \wedge \widehat{\varphi_{i_k}} \wedge \cdots \wedge \varphi_{i_{N+1}} \in \mathfrak{H}^N.$$

The operator  $a(f)$  can also be extended by linearity and continuity to the whole  $\mathfrak{H}^{N+1}$ . The operators  $a^*(f)$  and  $a(f)$  are finally defined on the entire Fock space  $\mathcal{F}$ , thanks to the equality previously derived: for any  $\psi \in \mathfrak{H}^N$ , we have

$$\|a^*(f)\psi\|_{\mathfrak{H}^{N+1}}^2 + \|a(f)\psi\|_{\mathfrak{H}^{N-1}}^2 = \|f\|^2 \|\psi\|_{\mathfrak{H}^N}^2.$$

This relation can be generalized to obtain the so-called *canonical anti-commutation relations* (CAR) satisfied by the creation and annihilation operators: for all  $f, g \in \mathfrak{H}$  we have

$$\begin{cases} a^*(f)a(g) + a(g)a^*(f) = \langle f, g \rangle \text{Id}_{\mathcal{F}}, \\ a^*(f)a^*(g) + a^*(g)a^*(f) = 0. \end{cases}$$

As in Section 3.1, we denote by  $\mathfrak{A}[\mathfrak{H}]$  the  $C^*$ -algebra generated by the family  $\{a(f), f \in \mathfrak{H}\}$ . We define on  $\mathcal{F}$  the number operator

$$\mathcal{N} := \bigoplus_{N \in \mathbb{N}} N \text{Id}_{\mathfrak{H}^N}.$$

It is an unbounded non-negative operator on  $\mathcal{F}$  with domain

$$\mathcal{D}(\mathcal{N}) = \left\{ (\Psi_N)_{N \in \mathbb{N}} \in \mathcal{F}, \sum_{N \in \mathbb{N}} N^2 \|\Psi_N\|_{\mathfrak{H}^N}^2 < +\infty \right\}.$$

If  $(\varphi_i)_{i \in \mathbb{N}}$  a complete orthonormal set in  $\mathfrak{H}$ , then we have the equivalent definition

$$\mathcal{N} = \sum_{i \in \mathbb{N}} a^*(\varphi_i)a(\varphi_i),$$

where the sum converges in the sense of quadratic forms on the domain  $\mathcal{D}(\mathcal{N})$ , which means that for all  $\Phi, \Psi \in \mathcal{D}(\mathcal{N})$ ,

$$\lim_{n \rightarrow \infty} \sum_{i=0}^n \langle a^*(\varphi_i)a(\varphi_i)\Psi, \Phi \rangle_{\mathcal{F}} = \langle \Psi, \mathcal{N}\Phi \rangle_{\mathcal{F}}.$$

Notice that the convergence actually holds on the form domain  $\mathcal{D}(\mathcal{N}^{1/2})$ , and that it does not depend on the choice of the basis  $(\varphi_i)$ . This can be easily seen since for any  $N \in \mathbb{N}$ ,  $\sum_i a^*(\varphi_i)a(\varphi_i)$  converges in  $\mathcal{B}(\mathfrak{H}^N)$  towards  $N \text{Id}_{\mathfrak{H}^N}$ : we have

$$\forall 1 \leq i_1 < \dots < i_N, a^*(\varphi_i)a(\varphi_i)\varphi_I = \begin{cases} 0 & \text{if } i \notin I \\ \varphi_I & \text{if } i \in I \end{cases} \quad (I := \{i_1, \dots, i_N\}),$$

which implies that

$$\begin{aligned} \left( N - \sum_{i=0}^n a^*(\varphi_i)a(\varphi_i) \right) \left( \sum_I a_I \varphi_I \right) &= N \sum_I a_I \varphi_I - \sum_{i=0}^n \sum_{I, i \in I} a_I \varphi_I \\ &= N \sum_I a_I \varphi_I - \sum_{k=1}^N k \sum_{I, \#(I \cap [0, n])=k} a_I \varphi_I \\ &= \sum_{k=0}^{N-1} (N-k) \sum_{I, \#(I \cap [0, n])=k} a_I \varphi_I \\ &= \sum_{\substack{I, \\ \#(I \cap [0, n]) \leq N-1}} (N - \#(I \cap [0, n])) a_I \varphi_I. \end{aligned}$$



As a consequence,

$$\left\| \left( N - \sum_{i=0}^n a^*(\varphi_i)a(\varphi_i) \right) \left( \sum_I a_I \varphi_I \right) \right\|_{\mathfrak{H}^N} \leq N \left( \sum_{I, \#(I \cap [0, n]) \leq N-1} |a_I|^2 \right)^{1/2},$$

the right side going to 0 as  $n \rightarrow +\infty$ , by the dominated convergence theorem. Hence, for any  $\Phi, \Psi \in \mathcal{D}(\mathcal{N}^{1/2})$  we have

$$\left\langle \left( \mathcal{N} - \sum_{i=0}^n a^*(\varphi_i)a(\varphi_i) \right) \Psi, \Phi \right\rangle_{\mathcal{F}} = \sum_{N \geq 0} \left\langle \left( N - \sum_{i=0}^n a^*(\varphi_i)a(\varphi_i) \right) \Psi_N, \Phi_N \right\rangle_{\mathfrak{H}^N}.$$

For any  $N \in \mathbb{N}$ , we have seen that

$$\left\langle \left( N - \sum_{i=0}^n a^*(\varphi_i)a(\varphi_i) \right) \Psi_N, \Phi_N \right\rangle_{\mathfrak{H}^N} \longrightarrow 0$$

as  $n \rightarrow +\infty$ , with the explicit estimate

$$\left| \left\langle \left( N - \sum_{i=0}^n a^*(\varphi_i)a(\varphi_i) \right) \Psi_N, \Phi_N \right\rangle_{\mathfrak{H}^N} \right| \leq N \|\Psi_N\|_{\mathfrak{H}^N} \|\Phi_N\|_{\mathfrak{H}^N}.$$

By the dominated convergence theorem, we conclude that for any  $\Phi, \Psi \in \mathcal{D}(\mathcal{N}^{1/2})$  we have

$$\lim_{n \rightarrow \infty} \sum_{i=0}^n \langle a^*(\varphi_i)a(\varphi_i)\Psi, \Phi \rangle_{\mathcal{F}} = \langle \Psi, \mathcal{N}\Phi \rangle_{\mathcal{F}}.$$

The number operator  $\mathcal{N}$  does *not* belong to the CAR algebra  $\mathfrak{A}[\mathfrak{H}]$ , simply because it is not bounded. Hence, for a state  $\omega$  on  $\mathfrak{A}[\mathfrak{H}]$  as defined in Section 3.1, we *define*  $\omega(\mathcal{N})$  to be the quantity

$$\omega(\mathcal{N}) := \sum_{i \geq 0} \omega(a^*(\varphi_i)a(\varphi_i)),$$

which is always a well-defined quantity in  $\mathbb{R}_+ \cup \{+\infty\}$ . For a state  $\omega$  on  $\mathcal{B}(\mathcal{F})$ , we have a priori another notion of average number of particles, namely

$$\sum_{N \geq 0} N \omega(\mathcal{P}_N) \in \mathbb{R}_+ \cup \{+\infty\}.$$

For a pure state  $\omega = |\Psi\rangle\langle\Psi|$  with  $\Psi \in \mathcal{D}(\mathcal{N}^{1/2})$ , we have seen that these two notions coincide. If  $\Psi \notin \mathcal{D}(\mathcal{N}^{1/2})$ , it is also easy to see that they also coincide, the two being  $+\infty$ . Knowing this for pure states, we deduce that they coincide for normal states. However, for non-normal states they may not coincide, and we will provide an example of such a state below.

We finish this section by precisizing the link between states defined on  $\mathfrak{A}[\mathfrak{H}]$  or on  $\mathcal{B}(\mathcal{F})$ . Since the commutant  $\mathfrak{A}[\mathfrak{H}]'$  of the algebra  $\mathfrak{A}[\mathfrak{H}]$  in  $\mathcal{B}(\mathcal{F})$  is equal to  $\mathbb{C}$  [PR94, Thm 2.4.2], by the von Neumann density theorem [BR87, Cor. 2.4.15]

the algebra  $\mathfrak{A}[\mathfrak{H}]$  is dense in  $\mathcal{B}(\mathcal{F})$  for the weak- $*$  topology of  $\mathcal{B}(\mathcal{F})$  induced by the duality  $(\mathfrak{S}_1(\mathcal{F}))^* = \mathcal{B}(\mathcal{F})$  where  $\mathfrak{S}_1(\mathcal{F})$  is the set of all trace-class operators on  $\mathcal{F}$ . Equivalently, for any  $B \in \mathcal{B}(\mathcal{F})$ , there exists a sequence  $(A_n) \subset \mathfrak{A}[\mathfrak{H}]$  such that for any  $G \in \mathfrak{S}_1(\mathcal{F})$  we have

$$\lim_{n \rightarrow \infty} \text{Tr}_{\mathcal{F}}(GA_n) = \text{Tr}_{\mathcal{F}}(GB).$$

As a consequence, a normal state on  $\mathfrak{A}[\mathfrak{H}]$  can be uniquely extended to the whole  $\mathcal{B}(\mathcal{F})$  because it is continuous with respect to the topology of  $\mathcal{B}(\mathcal{F})$  for which  $\mathfrak{A}[\mathfrak{H}]$  is dense. In general, a state  $\omega$  on  $\mathfrak{A}[\mathfrak{H}]$  can be extended to a continuous linear functional  $\tilde{\omega}$  on the whole  $\mathcal{B}(\mathcal{F})$ , with  $\|\omega\| = \|\tilde{\omega}\|$ , by the Hahn-Banach theorem. Positivity of  $\tilde{\omega}$  holds since  $\mathfrak{A}[\mathfrak{H}]$  is unital: we have  $\tilde{\omega}(\text{Id}_{\mathcal{F}}) = 1 = \|\tilde{\omega}\|$ , which is actually equivalent to the positivity of  $\tilde{\omega}$  [BR87, Prop. 2.3.11]. Hence, any state on  $\mathfrak{A}[\mathfrak{H}]$  can be extended to a state on  $\mathcal{B}(\mathcal{F})$ . However, uniqueness of these extensions is not guaranteed, and is actually equivalent to the fact that  $\mathfrak{A}[\mathfrak{H}]$  is a *hereditary*  $C^*$ -subalgebra of  $\mathcal{B}(\mathcal{F})$  [Kus90]. However, the only hereditary  $C^*$ -subalgebra of  $\mathcal{B}(\mathcal{F})$  containing  $\text{Id}_{\mathcal{F}}$  is  $\mathcal{B}(\mathcal{F})$  itself, so that uniqueness of extensions does not hold in general.

**C.2. Quasi-free states.** We are interested in a certain class of states on  $\mathfrak{A}[\mathfrak{H}]$  called *quasi-free* states, as defined in Section 3.1. To any state on  $\mathfrak{A}[\mathfrak{H}]$  is associated its *one-particle density matrix*  $\gamma$  and its *pairing matrix*  $\alpha$  which are such that the operator on  $\mathfrak{H} \oplus \mathfrak{K}$

$$\Gamma(\gamma, \alpha) := \begin{pmatrix} \gamma & \alpha \\ \alpha^* & 1 - J\gamma J^* \end{pmatrix},$$

satisfies  $0 \leq \Gamma(\gamma, \alpha) \leq \text{Id}_{\mathfrak{H} \oplus \mathfrak{K}}$ . This relation means that for all  $f, g \in \mathfrak{H}$ ,

$$0 \leq \langle \gamma f, f \rangle + \langle (1 - \gamma)g, g \rangle + 2 \text{Re} \langle \alpha Jg, f \rangle \leq \|f\|^2 + \|g\|^2.$$

It is equivalent to the relation

$$|\langle \alpha Jf, g \rangle|^2 \leq \langle \gamma f, f \rangle \langle (1 - \gamma)g, g \rangle, \quad \forall f, g \in \mathfrak{H},$$

which is the Cauchy-Schwarz inequality for states [BR87, Lemma 2.3.10]

$$|\omega(A^*B)|^2 \leq \omega(A^*A)\omega(B^*B), \quad \forall A, B \in \mathfrak{A}[\mathfrak{H}]$$

with  $A = a(f)$  and  $B = a^*(g)$ .

Quasi-free states are uniquely characterized by their associated operator  $\Gamma(\gamma, \alpha)$ . We defined them with the Wick formula (1.3.10), but there exist equivalent definitions of quasi-free states, for instance in terms of the so-called truncated functionals [BR97, p.42]. Quasi-free states with  $\alpha = 0$  can be also characterized by the relation

$$\omega(a^*(f_{i_1}) \cdots a^*(f_{i_n}) a(g_{j_1}) \cdots a(g_{j_m})) = \delta_{nm} \det \left( [\langle g_{j_k}, \gamma f_{i_\ell} \rangle]_{\substack{1 \leq k \leq m \\ 1 \leq \ell \leq n}} \right),$$

see for instance [JOPP11, Section 7.3]. Proposition 1.1 associates to any  $\Gamma(\gamma, \alpha)$  of the previous form such that  $0 \leq \Gamma(\gamma, \alpha) \leq \text{Id}_{\mathfrak{H} \oplus \mathfrak{K}}$  with  $\text{Tr} \gamma < +\infty$ , a quasi-free

state on  $\mathfrak{A}[\mathfrak{H}]$  having  $(\gamma, \alpha)$  as density matrices. This state is furthermore normal, and hence has a unique extension to  $\mathcal{B}(\mathcal{F})$ . In the following sections, we provide explicit constructions of a quasi-free state having a prescribed  $(\gamma, \alpha)$ , in two cases: the Hartree-Fock case and the pure Hartree-Fock-Bogoliubov case.

C.2.1. *Hartree-Fock states.* We begin with Hartree-Fock states, that is  $\text{Tr}(\gamma) < +\infty$  and  $\alpha = 0$ .

For any operator  $M$  on  $\mathfrak{H}$ , we recall the definition (1.3.20) of the (possibly unbounded) operator  $\Upsilon(M)$  on  $\mathcal{F}$  by its action on  $\mathfrak{H}^N$ :

$$\Upsilon(M)f_{i_1} \wedge \cdots \wedge f_{i_N} := Mf_{i_1} \wedge \cdots \wedge Mf_{i_N}.$$

It must not be confused with the usual second quantization of  $M$  defined by

$$d\Gamma(M)f_{i_1} \wedge \cdots \wedge f_{i_N} := \sum_{k=1}^N f_{i_1} \wedge \cdots \wedge Mf_{i_k} \wedge \cdots \wedge f_{i_N}.$$

By convention we choose  $\Upsilon(M)\Omega = \Omega$ ,  $d\Gamma(M)\Omega = \Omega$ . If  $M$  has only discrete spectrum  $\{\lambda_i\}$ , we have

$$\sigma(\Upsilon(M)) = \overline{\left\{ \prod_{i \in I} \lambda_i, \quad I \subset \mathbb{N}, \quad \#I < +\infty \right\}};$$

$$\sigma(d\Gamma(M)) = \overline{\left\{ \sum_{i \in I} \lambda_i, \quad I \subset \mathbb{N}, \quad \#I < +\infty \right\}}.$$

Hence,  $\Upsilon(M)$  is bounded if  $\|M\| < 1$  and  $d\Gamma(M)$  is bounded if  $M \in \mathfrak{S}_1(\mathfrak{H})$ . The operator  $\Upsilon(M)$  satisfies the obvious but crucial intertwining property with the creation operators:

$$\boxed{\Upsilon(M)a^*(f) = a^*(Mf)\Upsilon(M)}, \quad (1.C.38)$$

for all  $f \in \mathfrak{H}$ . The operators  $\Upsilon(M)$  and  $d\Gamma(M)$  are linked by the following identity when  $M$  is for instance compact and self-adjoint

$$\Upsilon(e^{-M}) = e^{-d\Gamma(M)}.$$

We also have the following lemma

**Lemma 1.3.** *Let  $M$  a non-negative, trace-class, self-adjoint operator on  $\mathfrak{H}$ . Then  $\Upsilon(M)$  is trace-class on  $\mathcal{F}$  and we have*

$$\text{Tr}_{\mathcal{F}}(\Upsilon(M)) = \text{Det}_{\mathfrak{H}}(1 + M). \quad (1.C.39)$$

PROOF. Assume that  $(f_i)$  is a complete set of eigenvectors for  $M$ , with associated eigenvalues  $(\lambda_i)$ . Then

$$\begin{aligned}
\mathrm{Tr}_{\mathcal{F}}(\Upsilon(M)) &= \sum_{N=0}^{\infty} \mathrm{Tr}_{\mathfrak{H}^N}(\Upsilon(M)) \\
&= 1 + \sum_{N=1}^{\infty} \sum_{1 \leq i_1 < \dots < i_N} \langle \Upsilon(M) f_{i_1} \wedge \dots \wedge f_{i_N}, f_{i_1} \wedge \dots \wedge f_{i_N} \rangle_{\mathfrak{H}^N} \\
&= 1 + \sum_{N=1}^{\infty} \sum_{1 \leq i_1 < \dots < i_N} \lambda_{i_1} \dots \lambda_{i_N} \\
&= \prod_{i=1}^{\infty} (1 + \lambda_i) \\
&= \mathrm{Det}_{\mathfrak{H}}(1 + M),
\end{aligned}$$

the product being convergent because  $\mathrm{Tr}_{\mathfrak{H}}(M) = \sum_i \lambda_i < +\infty$ .  $\square$

For a non-negative, trace-class, self-adjoint operator  $M$ , we can set  $Z = \mathrm{Tr}_{\mathcal{F}}(\Upsilon(M))$  and define the normal state  $\omega_G$  with density matrix  $G = Z^{-1}\Upsilon(M)$ .

**Proposition 1.10.** *Let  $\gamma$  a 1-particle density matrix, i.e.  $0 \leq \gamma \leq 1$ . Assume furthermore that  $\mathrm{Tr}(\gamma) < +\infty$  and that  $\ker(\gamma - 1) = \{0\}$ . Then the normal state  $\omega_G$  with  $G = Z^{-1}\Upsilon\left(\frac{\gamma}{1-\gamma}\right)$  and  $Z = \mathrm{Tr}_{\mathcal{F}}\left(\Upsilon\left(\frac{\gamma}{1-\gamma}\right)\right)$  is quasi-free and has  $\gamma$  as 1-particle density matrix and  $\alpha = 0$  as pairing matrix.*

PROOF. Let  $M = \frac{\gamma}{1-\gamma}$ , which is well-defined, non-negative and trace-class since  $0 \leq \gamma < 1$  and  $\gamma$  is trace-class hence compact so that  $(1-\gamma)^{-1}$  is bounded. The state  $\omega_G$  is quasi-free following the same proof as in [Gau60], for it relies on the relation (1.C.38). To see that the pairing vanishes we remark that for each  $N$ ,  $\Upsilon(M)$  maps  $\mathfrak{H}^N$  into itself and that  $a(f)a(g)|_{\mathfrak{H}^0 \oplus \mathfrak{H}^1} = 0$  so that

$$\begin{aligned}
\omega_G(a(f)a(g)) &= Z^{-1} \mathrm{Tr}_{\mathcal{F}}(\Upsilon(M)a(f)a(g)) \\
&= Z^{-1} \sum_{N \geq 2} \sum_{1 \leq i_1 < \dots < i_N} \underbrace{\langle \Upsilon(M)a(f)a(g) f_{i_1} \wedge \dots \wedge f_{i_N}, \rangle}_{\in \mathfrak{H}^{N-2}} \underbrace{f_{i_1} \wedge \dots \wedge f_{i_N}}_{\in \mathfrak{H}^N} \rangle_{\mathcal{F}} \\
&= 0,
\end{aligned}$$

for all  $f, g \in \mathfrak{H}$ . To show that the 1-particle density matrix of  $\omega_G$  is  $\gamma$ , we use the relation (1.C.38)

$$\begin{aligned}
\omega_G(a^*(f)a(g)) &= Z^{-1} \mathrm{Tr}_{\mathcal{F}}(\Upsilon(M)a^*(f)a(g)) \\
&= Z^{-1} \mathrm{Tr}_{\mathcal{F}}(\Upsilon(M)a(g)a^*(Mf)) \\
&= \langle g, Mf \rangle_{\mathfrak{H}} - \omega_G(a^*(Mf)a(g)),
\end{aligned}$$

so that

$$\omega_G(a^*((1+M)f)a(g)) = \langle g, Mf \rangle_{\mathfrak{H}}.$$

Hence the 1-particle density matrix of  $\omega_G$  is  $\frac{M}{1+M} = \gamma$ .  $\square$

We use this explicit construction of Hartree-Fock states to provide an alternative proof of Proposition 1.2, in the special case  $\ker(\gamma - 1) = \{0\}$ .

**Corollary 1.3.** *Let  $\gamma$  be a trace-class 1-particle density matrix with  $\ker(\gamma - 1) = \{0\}$  and let  $\omega$  be the state given by Proposition 1.10. Let  $k \in \mathbb{N}$ . We have the following estimate*

$$\omega(\mathcal{P}_{\mathfrak{H}^k}) \leq \frac{(e \operatorname{Tr}(\gamma))^k}{k!} e^{-\operatorname{Tr}(\gamma)}, \quad (1.C.40)$$

where  $\mathcal{P}_{\mathfrak{H}^k}$  is the orthogonal projector onto  $\mathfrak{H}^k \subset \mathcal{F}$ .

PROOF. Let  $(f_i)$  a complete orthonormal set of eigenvectors for  $\gamma$ ,  $(\lambda_i)$  the associated eigenvalues and  $\mu_i = \frac{\lambda_i}{1-\lambda_i}$ . Notice that

$$Z = \operatorname{Tr}_{\mathcal{F}} \left( \Upsilon \left( \frac{\gamma}{1-\gamma} \right) \right) = \operatorname{Det}_{\mathfrak{H}} \left( 1 + \frac{\gamma}{1-\gamma} \right) = \prod_{i \geq 1} \frac{1}{1-\lambda_i}.$$

We then compute

$$\begin{aligned} \omega(\mathcal{P}_{\mathfrak{H}^k}) &= Z^{-1} \operatorname{Tr}_{\mathfrak{H}^k}(\Upsilon(M)) \\ &= Z^{-1} \sum_{1 \leq i_1 < \dots < i_k} \langle \Upsilon(M) f_{i_1} \wedge \dots \wedge f_{i_k}, f_{i_1} \wedge \dots \wedge f_{i_k} \rangle_{\mathfrak{H}^k} \\ &= Z^{-1} \sum_{1 \leq i_1 < \dots < i_k} \mu_{i_1} \dots \mu_{i_k} \\ &= \prod_{i \geq 1} (1-\lambda_i) \sum_{1 < i_1 < \dots < i_k} \frac{\lambda_{i_1}}{1-\lambda_{i_1}} \dots \frac{\lambda_{i_k}}{1-\lambda_{i_k}} \\ &= \sum_{1 < i_1 < \dots < i_k} \lambda_{i_1} \dots \lambda_{i_k} \prod_{j \notin \{i_1, \dots, i_k\}} (1-\lambda_j), \end{aligned}$$

and we conclude as in the proof of Proposition 1.2.  $\square$

To remove the condition  $\ker(\gamma - 1) = \{0\}$ , we split the Hilbert space as  $\mathfrak{H} = \mathfrak{H}_0 \oplus \mathfrak{H}_1$  with  $\mathfrak{H}_1 = \ker(\gamma - 1)$  and  $\mathfrak{H}_0 = \mathfrak{H}_1^\perp$  and using Proposition 1.9 we deduce the

**Proposition 1.11.** *Let  $\gamma$  a trace-class 1-pdm, and let  $\mathfrak{H} = \mathfrak{H}_0 \oplus \mathfrak{H}_1$  the decomposition as above. Define  $\gamma_0 := \gamma|_{\mathfrak{H}_0}$  and  $(\varphi_1, \dots, \varphi_q)$  an orthonormal basis of the finite-dimensional space  $\mathfrak{H}_1$ . Let  $\omega_0$  the normal state on  $\mathcal{F}(\mathfrak{H}_0)$  with density matrix  $Z^{-1} \Upsilon \left( \frac{\gamma_0}{1-\gamma_0} \right)$  with  $Z := \operatorname{Tr}_{\mathcal{F}(\mathfrak{H}_0)} \left( \Upsilon \left( \frac{\gamma_0}{1-\gamma_0} \right) \right)$ , and  $\omega_1$  the pure state on  $\mathcal{F}(\mathfrak{H}_1)$  given by the Slater determinant  $\varphi_1 \wedge \dots \wedge \varphi_q$ . Then the quasi-free state  $\omega := \omega_0 \otimes \omega_1$  on  $\mathcal{F} = \mathcal{F}(\mathfrak{H}_0) \otimes \mathcal{F}(\mathfrak{H}_1)$  has  $\gamma$  as 1-pdm and  $\alpha = 0$  as pairing matrix.*

**Remark 1.19.** The state  $\omega$  is also a normal state with density matrix  $G_\omega$  given by, as an operator on  $\mathcal{F} = \mathcal{F}(\mathfrak{H}_0) \otimes \mathcal{F}(\mathfrak{H}_1)$ ,

$$G_\omega := Z^{-1} \Upsilon \left( \frac{\gamma_0}{1 - \gamma_0} \right) \otimes (|\varphi_1 \wedge \cdots \wedge \varphi_q\rangle \langle \varphi_1 \wedge \cdots \wedge \varphi_q|). \quad (1.C.41)$$

We can also deduce from this result an alternative proof of Proposition 1.2, even if  $\ker(\gamma - 1) = \{0\}$ .

**Corollary 1.4.** *Let  $\gamma$  a trace-class 1-particle density matrix. Let  $\omega$  be the state defined in the last Proposition. Then, if  $N < \dim \ker(\gamma - 1)$ ,  $\omega(\mathcal{P}_{\mathfrak{H}^N}) = 0$ . Else,*

$$\omega(\mathcal{P}_{\mathfrak{H}^N}) \leq \frac{(e \operatorname{Tr}(\gamma))^N}{N!} e^{-\operatorname{Tr}(\gamma)}.$$

PROOF. Let  $T : \mathcal{F}(\mathfrak{H}) \rightarrow \mathcal{F}(\mathfrak{H}_0) \otimes \mathcal{F}(\mathfrak{H}_1)$  be the isometry defined in Section A. Then,

$$\mathcal{P}_{\mathfrak{H}^N} = T^* \left( \sum_{k=0}^N \mathcal{P}_{\mathfrak{H}_0^k} \otimes \mathcal{P}_{\mathfrak{H}_1^{N-k}} \right) T^*.$$

Hence, we have

$$\omega(\mathcal{P}_{\mathfrak{H}^N}) = \sum_{k=0}^N \omega_0(\mathcal{P}_{\mathfrak{H}_0^{N-k}}) \omega_1(\mathcal{P}_{\mathfrak{H}_1^k}).$$

Notice that for all  $k$ ,  $\omega_1(\mathcal{P}_{\mathfrak{H}_1^k}) = \delta_{k,q}$ , where  $q := \dim \ker(\gamma - 1)$ . Denoting by  $(\lambda_i)_{i \geq 0}$  the eigenvalues of  $\gamma$  different from 1, we deduce from the proof of Corollary 1.3 that

$$\omega(\mathcal{P}_{\mathfrak{H}^N}) = \omega_0(\mathcal{P}_{\mathfrak{H}_0^{N-q}}) = \sum_{\substack{I \subset \mathbb{N} \\ \#I = N-q}} \prod_{i \in I} \lambda_i \prod_{j \notin I} (1 - \lambda_j).$$

If we new denote by  $\lambda_{-q} = 1, \dots, \lambda_{-1} = 1$  the other eigenvalues of  $\gamma$ , we have

$$\sum_{\substack{I \subset \mathbb{N} \\ \#I = N-q}} \prod_{i \in I} \lambda_i \prod_{j \notin I} (1 - \lambda_j) = \sum_{\substack{J \subset \mathbb{N} \cup \{-q, \dots, -1\} \\ \#J = N}} \prod_{i \in J} \lambda_i \prod_{j \notin J} (1 - \lambda_j),$$

and we conclude as before.  $\square$

As a corollary of these estimates, we precise what was announced in Remark 1.7.

**Corollary 1.5.** *Let  $(\gamma_n)_{n \in \mathbb{N}}$  a sequence of trace-class 1-pdm such that*

$$\lim_{n \rightarrow \infty} \operatorname{Tr}(\gamma_n) = +\infty.$$

*Let  $(\omega_n)_{n \in \mathbb{N}}$  the sequence of finite-number of particle, quasi-free normal states having  $\gamma_n$  as 1-pdm,  $\alpha_n = 0$  as pairing matrix and  $G_n$  as density matrix. Then for any compact operator  $K$  on  $\mathcal{F}$ , we have*

$$\lim_{n \rightarrow \infty} \omega_n(K) = 0.$$

*Equivalently,  $(G_n)$  converges to 0 for the weak- $\star$  topology of  $\mathfrak{S}_1(\mathcal{F})$ .*

PROOF. Let  $\varepsilon > 0$  and  $K$  a compact operator. Let  $K_\varepsilon$  a finite-rank operator such that  $\|K - K_\varepsilon\|_{\mathcal{B}(\mathcal{F})} \leq \varepsilon$ . Since  $\left(\sum_{j=0}^n \mathcal{P}_{\mathfrak{H}^j}\right)_{n \in \mathbb{N}}$  converges towards  $\text{Id}_{\mathcal{F}}$  for the strong operator topology, there exists a  $k_0(\varepsilon) \in \mathbb{N}$  such that for all  $k \geq k_0(\varepsilon)$ ,

$$\left\| \left( \sum_{j=0}^k \mathcal{P}_{\mathfrak{H}^j} \right) K_\varepsilon \left( \sum_{j=0}^k \mathcal{P}_{\mathfrak{H}^j} \right) - K_\varepsilon \right\|_{\mathcal{B}(\mathcal{F})} \leq \varepsilon.$$

Finally, we have

$$-\|K_\varepsilon\| \sum_{j=0}^k \mathcal{P}_{\mathfrak{H}^j} \leq \left( \sum_{j=0}^k \mathcal{P}_{\mathfrak{H}^j} \right) K_\varepsilon \left( \sum_{j=0}^k \mathcal{P}_{\mathfrak{H}^j} \right) \leq \|K_\varepsilon\| \sum_{j=0}^k \mathcal{P}_{\mathfrak{H}^j},$$

so that

$$|\omega_n(K)| \leq 2\varepsilon + \|K_\varepsilon\| \sum_{j=0}^k \omega_n(\mathcal{P}_{\mathfrak{H}^j}).$$

For all  $j$ ,  $\omega_n(\mathcal{P}_{\mathfrak{H}^j}) \rightarrow 0$  as  $n \rightarrow \infty$  by the estimate (1.C.40). For  $n$  large enough, we thus have

$$\|K_\varepsilon\| \sum_{j=0}^k \omega_n(\mathcal{P}_{\mathfrak{H}^j}) < \varepsilon,$$

so that

$$|\omega_n(K)| \leq 3\varepsilon.$$

□

**Corollary 1.6.** *Let  $f : \mathbb{R} \rightarrow \mathbb{R}$  a bounded function that vanishes at infinity, and  $(\gamma_n)_{n \in \mathbb{N}}$  a sequence of trace-class 1-pdm as in Corollary 1.5. Then*

$$\lim_{n \rightarrow \infty} \omega_n(f(\mathcal{N})) = 0.$$

PROOF. Let  $\varepsilon > 0$ . For any  $n$  we have with obvious notations

$$\begin{aligned} \omega_n(f(\mathcal{N})) &= Z_n^{-1} \text{Tr}_{\mathcal{F}}(\Upsilon(M_n)f(\mathcal{N})) = Z_n^{-1} \sum_{k \geq 0} \text{Tr}_{\mathfrak{H}^k}(\Upsilon(M_n)f(\mathcal{N})) \\ &= Z_n^{-1} \sum_{k \geq 0} f(k) \text{Tr}_{\mathfrak{H}^k}(\Upsilon(M_n)). \end{aligned}$$

Let  $k_0$  large enough such that  $|f(k)| \leq \varepsilon$  for  $k \geq k_0$ . Hence

$$\left| Z_n^{-1} \sum_{k \geq k_0} f(k) \text{Tr}_{\mathfrak{H}^k}(\Upsilon(M_n)) \right| \leq \varepsilon Z_n^{-1} \sum_{k \geq k_0} \text{Tr}_{\mathfrak{H}^k}(\Upsilon(M_n)) \leq \varepsilon Z_n^{-1} \sum_{k \geq 0} \text{Tr}_{\mathfrak{H}^k}(\Upsilon(M_n)) = \varepsilon.$$

Since for all  $k$ ,  $\omega_n(\mathcal{P}_{\mathfrak{H}^k})$  goes to 0 as  $n$  goes to infinity, we have for  $n$  large enough

$$\left| Z_n^{-1} \sum_{k < k_0} f(k) \text{Tr}_{\mathfrak{H}^k}(\Upsilon(M_n)) \right| \leq \|f\|_\infty Z_n^{-1} \sum_{k < k_0} \text{Tr}_{\mathfrak{H}^k}(\Upsilon(M_n)) = \|f\|_\infty \sum_{k < k_0} \omega_n(\mathcal{P}_{\mathfrak{H}^k}) \leq \varepsilon,$$

so that  $|\omega_n(f(\mathcal{N}))| \leq 2\varepsilon$  and the Corollary is proved.  $\square$

Let us finish this section with some remarks concerning these sequences of states. Hence, let  $(\gamma_n)$  be a sequence of trace-class operators on  $\mathfrak{H}$  such that  $0 \leq \gamma_n \leq 1$  for all  $n$ . Denote by  $\omega_n$  the unique quasi-free state on  $\mathcal{B}(\mathcal{F})$  having  $\gamma_n$  as 1-pdm and 0 as pairing matrix. Recall that it is equivalent to define  $\omega_n$  on  $\mathcal{B}(\mathcal{F})$  or on its  $C^*$ -subalgebra  $\mathfrak{A}[\mathfrak{H}]$  since  $\omega_n$  is a normal state. As a uniformly bounded sequence of linear forms on the *separable* normed vector space  $\mathfrak{A}[\mathfrak{H}]$ ,  $(\omega_n)$  admits a weak-\* (i.e. pointwise) convergent subsequence  $(\omega_{n_k})_k$ , converging towards a bounded linear form  $\omega$  on  $\mathfrak{A}[\mathfrak{H}]$ , by the Banach-Alaoglu Theorem. Notice that  $\omega$  is also a state, since the definition of state is stable by pointwise convergence. Likewise,  $\omega$  is also a quasi-free state. Its pairing matrix is also 0, while its 1-pdm  $\gamma$  is the weak-\* limit of  $(\gamma_n)$  seen a bounded sequence in  $\mathcal{B}(\mathfrak{H})$ . For the moment, we cannot say if  $\gamma$  is trace-class since the Fatou lemma only gives an upper bound on  $\text{Tr } \gamma$ :

$$\text{Tr } \gamma = \sum_{i \geq 0} \omega(a^*(f_i)a(f_i)) \leq \liminf_{k \rightarrow \infty} \sum_{i \geq 0} \omega_{n_k}(a^*(f_i)a(f_i)) = \lim_{k \rightarrow \infty} \text{Tr } \gamma_{n_k} = +\infty.$$

We will see in a few lines that we indeed have  $\text{Tr } \gamma = +\infty$ , and hence that  $\gamma \notin \mathfrak{S}_1(\mathfrak{H})$ .

We cannot extract a subsequence  $(\omega_{n_k})$  converging towards a state on the whole  $\mathcal{B}(\mathcal{F})$ , since  $\mathcal{B}(\mathcal{F})$  is not separable in general. However, we can extract a convergent *subnet* from  $(\omega_n)$  on  $\mathcal{B}(\mathcal{F})$ , that is there exists a directed set  $A$  (i.e. a non-empty set with a pre-order relation such that every pair of elements of  $A$  admits an upper bound), a monotone function  $h : A \rightarrow \mathbb{N}$  which is cofinal (i.e. for all  $n \in \mathbb{N}$ ,  $\exists \alpha \in A$ ,  $h(\alpha) \geq n$ ), such that the net  $(\omega_{h(\alpha)})_{\alpha \in A}$  converges towards a state  $\tilde{\omega}$  on  $\mathcal{B}(\mathcal{F})$ . Here, convergence of nets means that for any neighborhood  $\mathcal{V}$  of  $\tilde{\omega}$  in  $\mathcal{B}(\mathcal{F})$ , there exists  $\beta \in A$  such that for all  $\alpha \geq \beta$ ,  $\omega_{h(\alpha)} \in \mathcal{V}$ . Of course,  $\tilde{\omega}$  and  $\omega$  coincide on  $\mathfrak{A}[\mathfrak{H}]$  since every subnet of a converging net converges towards the same limit. In the following, we will not distinguish these two states. By definition, for any  $B \in \mathcal{B}(\mathcal{F})$  we have

$$\lim_{\alpha} \omega_{h(\alpha)}(B) = \omega(B).$$

Hence, if we apply this result to  $B = \mathcal{P}_N$  for any  $N \in \mathbb{N}$ , we see that  $\omega(\mathcal{P}_N) = 0$  for all  $N \in \mathbb{N}$ , by Corollary 1.4. Hence, the state  $\omega$  only lives “at infinity” on  $\mathcal{F}$ . Despite this property, let us recall that  $\omega$  is not zero since  $\omega(\text{Id}_{\mathcal{F}}) = 1$ . Similarly, by Corollaries 1.5 and 1.6, we have for any compact operator  $K$  on  $\mathcal{F}$  and any  $f : \mathbb{N} \rightarrow \mathbb{C}$  going to 0 at infinity,  $\omega(K) = 0$  and  $\omega(f(\mathcal{N})) = 0$ . From these properties, we deduce that  $\omega$  is *not* normal: indeed if it were, we would have

$$1 = \omega(\text{Id}_{\mathcal{F}}) = \lim_{M \rightarrow +\infty} \omega \left( \sum_{N=0}^M \mathcal{P}_N \right) = \lim_{M \rightarrow \infty} (0) = 0.$$



Since  $\omega$  is not normal, we must also have  $\text{Tr } \gamma = +\infty$  by Proposition 1.11. This shows in particular that

$$0 = \sum_{N=0}^{\infty} N\omega(\mathcal{P}_N) \neq \sum_{i \geq 0} \omega(a^*(f_i)a(f_i)) = \text{Tr } \gamma = +\infty.$$

Let us also mention that, as any state on  $\mathcal{B}(\mathcal{F})$ ,  $\omega$  can be restricted to the  $C^*$ -subalgebra  $\mathcal{K}(\mathcal{F})$  of  $\mathcal{B}(\mathcal{F})$ , consisting of all compact operators over  $\mathcal{F}$ . Then,  $\omega|_{\mathcal{K}(\mathcal{F})}$  is a bounded linear form on  $\mathcal{K}(\mathcal{F})$ , and since  $(\mathcal{K}(\mathcal{F}))^* \simeq \mathfrak{S}_1(\mathcal{F})$ , there exists  $G_\omega \in \mathfrak{S}_1(\mathcal{F})$  such that for all  $K \in \mathcal{K}(\mathcal{F})$ ,  $\omega(K) = \text{Tr}_{\mathcal{F}}(G_\omega K)$ . Then,  $\omega$  can be split as  $\omega = \omega_1 + \omega_2$  with  $\omega_1(A) = \text{Tr}_{\mathcal{F}}(G_\omega A)$  for all  $A \in \mathcal{B}(\mathcal{F})$  and  $\omega_2(K) = 0$  for all  $K \in \mathcal{K}(\mathcal{F})$ . Hence,  $\omega_1$  is called the *normal part* of  $\omega$ . Let us mention that  $\omega_1$  and  $\omega_2$  are not necessarily states since they need not to be normalized. Of course, here we have  $\omega_1 \equiv 0$ : the normal part of  $\omega$  is trivial.

C.2.2. *Pure states.* We now turn to the HFB Pure State case. In order to define those states, we first have to recall some facts about Bogoliubov maps.

**Definition 1.1.** A Bogoliubov map  $\mathbf{U}$  is a unitary operator on  $\mathfrak{H} \oplus \mathfrak{K}$  with the block decomposition

$$\mathbf{U} = \begin{pmatrix} U & J^*VJ^* \\ V & JUJ^* \end{pmatrix}. \quad (1.C.42)$$

The fact that  $\mathbf{U}$  is unitary is equivalent to the following relations on  $U, V$

$$\begin{cases} UU^* + J^*VV^*J = \text{Id}_{\mathfrak{H}}, \\ U^*U + V^*V = \text{Id}_{\mathfrak{H}}, \\ V^*JU + U^*J^*V = 0_{\mathfrak{H}}, \\ UV^* + J^*VU^* = 0_{\mathfrak{H}}. \end{cases}$$

The particular form (1.C.42) of  $\mathbf{U}$  ensures that if we define for  $f \in \mathfrak{H}$  the operator

$$b(f) := a(Uf) + a^*(J^*Vf),$$

then the  $(b(f))_{f \in \mathfrak{H}}$  satisfy the CAR. It also ensures that if  $\Gamma$  has the form (1.3.8), then  $\mathbf{U}\Gamma\mathbf{U}^*$  still has the form (1.3.8). By Theorem 1.1, if the corresponding  $\gamma_{\mathbf{U}}$  is trace-class, we can then associate a unique quasi-free state to  $\mathbf{U}\Gamma\mathbf{U}^*$ . The relation between this state and the state associated to  $\Gamma$  is given by the following theorem.

**Theorem 1.5.** [Sol07, Theorem 9.5] *If  $\mathbf{U}$  is a Bogoliubov map such that  $\text{Tr}(V^*V) < +\infty$ , then there exists a unitary operator  $\mathbb{U} : \mathcal{F} \rightarrow \mathcal{F}$  implementing  $\mathbf{U}$  in the sense that for all  $f \in \mathfrak{H}$ ,*

$$\mathbb{U}a(f)\mathbb{U}^* = a(Uf) + a^*(J^*Vf).$$

*The condition  $\text{Tr}(V^*V) < +\infty$  is also necessary for the existence of such a  $\mathbb{U}$ , and is referred as the Shale-Stinespring condition. Furthermore, if  $\Gamma$  is a density matrix of*

the form (1.3.8) with associated quasi-free state  $\omega$ , then the state  $\omega_{\mathbb{U}}$  defined by

$$\omega_{\mathbb{U}}(A) = \omega(\mathbb{U}A\mathbb{U}^*), \quad \forall A \in \mathcal{B}(\mathcal{F})$$

has  $\mathbf{U}^*\Gamma\mathbf{U}$  as density matrix. In other words, the following diagram is commutative

$$\begin{array}{ccc} \Upsilon & \xrightarrow{\text{Th. (1.1)}} & \omega \\ \downarrow & & \downarrow \\ \mathbf{U}^*\Upsilon\mathbf{U} & \xrightarrow{\text{Th. (1.1)}} & \omega_{\mathbb{U}} \end{array}$$

**Remark 1.20.** Under the Shale-Stinespring condition, one sees that the 1-pdm  $\gamma_{\mathbb{U}}$  associated to the density matrix  $\mathbf{U}^*\Gamma\mathbf{U}$  verifies  $\text{Tr}(\gamma_{\mathbb{U}}) < +\infty$  if  $\gamma$  does, since

$$\gamma_{\mathbb{U}} = U^*\gamma U + V^*\alpha^*U + U^*\alpha V + V^*J(1 - \gamma)J^*V,$$

so that we can apply Theorem 1.1 to  $\mathbf{U}^*\Gamma\mathbf{U}$ . The last assertion of Theorem (1.5) is then justified.

**Remark 1.21.** A byproduct of the proof of Theorem 1.5 in [Sol07] is the following form of the vacuum rotated by  $\mathbb{U}$ :

$$\mathbb{U}|\Omega\rangle = \prod_{i \in I''} a^*(\eta_i) \prod_{i \in I'} (\alpha_i - \beta_i a^*(\eta_{2i}) a^*(\eta_{2i-1})) |\Omega\rangle, \quad (1.C.43)$$

where  $(\eta_i)_{i \in \mathbb{N}}$  is a complete orthonormal set in  $\mathfrak{H}$ ,  $(\eta_i)_{i \in I''}$  are eigenvectors of  $V^*V$  for the eigenvalue 1,  $I'' \cap \{2i, 2i - 1; i \in I'\} = \emptyset$ ,  $\alpha_i^2 + \beta_i^2 = 1$ , and  $(\beta_i^2)_{i \in I'}$  are the eigenvalues of  $V^*V$  strictly between 0 and 1, which are all of multiplicity 2.

**Remark 1.22.** A byproduct of the proof of Theorem 2.3 in [BLS94] is the fact that density matrices of quasi-free states with finite number of particles are diagonalizable by Bogoliubov maps: for any density matrix  $\Gamma$  of the form (1.3.8) with  $\text{Tr}(\gamma) < +\infty$  there exists a Bogoliubov map  $\mathbf{U}$  satisfying the Shale-Stinespring condition such that

$$\mathbf{U}^*\Gamma\mathbf{U} = \begin{pmatrix} \lambda_1 & & & & & \\ & \lambda_2 & & & & \\ & & \ddots & & & \\ & & & 1 - \lambda_1 & & \\ & 0 & & & 1 - \lambda_2 & \\ & & & & & \ddots \end{pmatrix},$$

where the  $(\lambda_i)$  are the eigenvalues of  $\Gamma$  between 0 and 1/2. The corresponding state  $\omega_{\mathbb{U}}$  has  $\gamma_{\mathbb{U}} = \text{diag}(\lambda_i)$  as 1-pdm and  $\alpha_{\mathbb{U}} = 0$  as pairing matrix. Since  $\gamma$  is trace-class and  $\mathbf{U}$  satisfies the Shale-Stinespring condition, we have according Remark 1.20 that  $\sum_i \lambda_i = \text{Tr}(\gamma_{\mathbb{U}}) < +\infty$ .

We now detail properties of HFB pure states.

**Proposition 1.12.** [BLS94, Theorem 2.6] *A quasi-free state  $\omega$  with finite number of particle is pure if and only if its density matrix  $\Gamma$  is a projector:  $\Gamma^2 = \Gamma$ . Equivalently, there exists a Bogoliubov map  $\mathbf{U}$  satisfying the Shale-Stinepring condition such that  $\omega = \omega_{\mathbb{U}|\Omega}$ . Furthermore, the 1-pdm of  $\omega$  is  $\gamma = J^*VV^*J$  and its pairing matrix is  $\alpha = J^*VU^*J^*$ .*

**Remark 1.23.** This Theorem says that not all the  $\psi \in \mathcal{F}$  with finite number of particles define quasi-free states: only those who are Bogoliubov rotations of the vacuum  $|\Omega\rangle$  are quasi-free.

**Remark 1.24.** The second part of Theorem 1.12 is a direct corollary of Remark 1.22: since  $\Gamma$  is a projector its only eigenvalue between 0 and 1/2 is 0 so that there exists a Bogoliubov map  $\mathbf{U}$  such that

$$\Gamma = \mathbf{U} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \mathbf{U}^* = \mathbf{U}\Gamma_0\mathbf{U}^*.$$

Notice then that  $\Gamma_0$  is the density matrix of the pure state associated with the vacuum  $|\Omega\rangle$  so that  $\omega = \omega_{\mathbb{U}|\Omega}$  as announced.

An immediate consequence of the fact that  $\Gamma^2 = \Gamma$  for quasi-free pure states with finite number of particles is the following corollary, that we used in the proof of Proposition 1.3.

**Corollary 1.7.** *A quasi-free state with finite number of particles is pure if and only if we have the relations*

$$\begin{cases} \gamma = \gamma^2 + \alpha\alpha^*, \\ \gamma\alpha J = \alpha J\gamma. \end{cases} \quad (1.C.44)$$

## CHAPTER 2

# Charge renormalization and static electron/positron pair production for a nonlinear Dirac model with weak interactions

This chapter is an extended version of an article published in *SIAM Journal of Mathematical Analysis* [Sab13a]. Appendix B is not present in the published version, and provides the computation of the next order expansion of the function  $F$ .

### Abstract

The Hartree-Fock approximation of Quantum Electrodynamics provides a rigorous framework for the description of relativistic electrons in external fields. This nonlinear model takes into account the infinitely many virtual electrons of Dirac's vacuum as well as the Coulomb interactions between all the particles. The state of the system is an infinite-rank projection satisfying a nonlinear equation. In this paper, we construct solutions to this equation, in the regime of weak interactions (that is, small coupling constant  $\alpha$ ), and strong external fields (that is, large atomic charge  $Z$  such that  $\alpha Z := \kappa$  stays fixed). In this regime, we are able to remove the ultraviolet cut-off  $\Lambda$  as soon as  $\alpha \log \Lambda$  stays fixed. As an application of this result, we compare the critical strength  $\kappa_c(\alpha)$  of the external potential needed to produce an additional particle in the vacuum, when  $\alpha = 0$  or  $\alpha > 0$ . We prove that  $\lim_{\alpha \rightarrow 0} \kappa_c(\alpha)/\kappa_c(0) > 1$ , and we identify the limit exactly. Because of the dielectric behavior of Dirac's vacuum, static electron/positron pair production occurs in the interacting case for a stronger field than in the non-interacting case, which is a mere consequence of charge renormalization.

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## 1. Introduction

The relativistic kinetic energy of a quantum electron is described by the Dirac operator  $D^0 = -i\boldsymbol{\alpha} \cdot \nabla + \beta$  acting on  $L^2(\mathbb{R}^3, \mathbb{C}^4)$ , where  $\boldsymbol{\alpha} = (\alpha_j)_{j=1,2,3}$  and

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}, \quad \forall j = 1, 2, 3, \quad \beta = \begin{pmatrix} \text{Id}_{\mathbb{C}^2} & 0 \\ 0 & -\text{Id}_{\mathbb{C}^2} \end{pmatrix},$$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Here, the units are taken so that the reduced Planck's constant  $\hbar$ , the speed of light  $c$ , and the mass of an electron  $m_e$ , are all set to 1. The spectrum of the Dirac operator is  $\sigma(D^0) = (-\infty, -1] \cup [1, +\infty)$ . To explain why real electrons have a positive kinetic energy, Dirac suggested to postulate that, in nature, all the negative kinetic energy states of the Dirac operator are already occupied by virtual electrons. Thus, the relativistic vacuum is composed of infinitely many charged, virtual particles, usually called the *Dirac sea*.

In an external electromagnetic field, the distribution of charge of the Dirac sea changes. This phenomenon is called *vacuum polarization*. In the same spirit, a negative kinetic energy virtual electron can turn into a positive kinetic energy real electron when given enough energy. This transformation results in a ‘‘hole’’ in the Dirac sea, which itself has a positive energy with respect to the fully filled Dirac sea. This hole can thus be observed and is identified with the anti-particle of the electron, the positron. Hence, such a process is labeled *electron/positron pair production*. In this paper, we are interested in the case where this energy is brought to the vacuum by an external, classical electric field. This situation has been originally considered by Sauter[Sau31], Heisenberg-Euler [HE36], and Schwinger [Sch51]. Since it is non-negligible compared to the other sources of pair production only for huge electric fields, it has not yet been observed experimentally. However, the creation of such a strong field could be achieved in the near future, due to recent progress in laser physics [Dun09].

There exists two approaches to the problem of electron/positron pair production under an external electric potential  $V$ . The first one consists in studying the vacuum in its ground state, in the presence of  $V$ . One tries to determine if the vacuum then contains real particles or not, if  $V$  is strong enough. In other words, for large  $V$  one expects that it is energetically more favorable for the vacuum to contain real electrons or positrons, than to contain no real particle at all. If the vacuum contains real particles, we say that the external potential  $V$  produces pairs, or more precisely produces particles. Indeed, for this formulation of electron/positron pair production, called *static* pair production, it is not necessary that the number of electrons created is the same as the number of positrons created. We still refer to it as pair production

though, because one can think of it as a localized particle together with an anti-particle at infinity. The second approach consists in studying the time evolution of the vacuum with no electron and no positron (the *free* vacuum), when the external field is compactly supported in time. One wants to determine if, for large times, some pairs still exist. In this case, notice that it is necessarily pairs that are produced since the total charge of the system is conserved. The second approach is thus called *dynamical* pair production. While dynamical pair production may be more relevant from a physical point of view, it is also much harder to study mathematically.

Only a few mathematical results are known about electron/positron pair production. Indeed, one has to deal with infinitely many relativistic particles, interacting with an external field and possibly with each other. The correct theory to describe such systems is Quantum Electrodynamics, which has only been formulated in a perturbative fashion so far. Even the apparently simpler many-body theory of  $N$  relativistic electrons is not well-defined mathematically. For the time being, one has to make approximations to obtain results about such systems.

The case where the interactions between the particles are neglected is one of these approximations. In this setting, everything reduces to the spectral theory of the one-body operator  $D^0 + V$ , for which the issue of dealing with an infinite number of particles does not exist anymore. The problem of static pair production has been studied by Klaus and Scharf [KS77b]. The question of dynamical pair production has been tackled in the non-interacting case by Pickl and Dürr [PD08], who proved that pairs were created for a certain class of potentials adiabatically evolving in time. This relies on a subtle analysis of the dispersive properties of the essential spectrum of the Dirac operator.

When the interactions between the particles are taken into account, one can perform a mean-field approximation to again reduce the problem to the one-body space. The additional difficulty compared to the case without interactions is that the state of the system is not described by a wavefunction anymore, but rather by a *one-body density matrix*, an infinite-rank operator on the one-body space (usually an orthogonal projection). The idea of performing a mean-field approximation of Quantum Electrodynamics goes back to Chaix and Iracane [CI89]. The first rigorous models formulating these ideas were developed by Chaix, Iracane, and Lions [CIL89], and by Bach, Barbaroux, Helffer, and Siedentop [BBHS99], who proved the stability of the free vacuum. In [BBHS99], the authors included external fields but neglected the vacuum polarization effects. These effects were treated rigorously for the first time by Hainzl and Siedentop in [HS03]. Later on, another model, which described vacuum polarization in a fully consistent way, was introduced by Hainzl, Lewin, and Séré in 2005 [HLS05a]. A variational approach for this model was then developed [HLS05b]. The same model was afterwards precised by starting from an interacting free vacuum [HLS07]. It was finally extended in a series of articles by Gravejat,

Hainzl, Lewin, and Séré [**HLS09a**, **GLS09**, **GLS11**, **GHLS13**]. In the present article, we will use the latter, called the *Bogoliubov-Dirac-Fock* model. In particular, the polarized vacuum is constructed in a rigorous fashion as a ground state of a certain nonlinear energy functional. Static electron/positron pair production has already been studied by the author in this framework in a previous work [**Sab13b**].

In the case without interactions, the one-body density matrix of the vacuum polarized by a potential  $V$  is given by

$$P = \chi_{(-\infty, 0]}(D^0 + V).$$

If  $V$  is smooth enough, the eigenvalues of  $D^0 + \kappa V$  are continuous with respect to the parameter  $\kappa$ . Klaus and Scharf [**KS77b**] proved (in the case  $V \leq 0$ ) that a particle is created in the vacuum if one of these eigenvalues *crosses 0* when increasing  $\kappa$ . If it crosses from the right to the left, it corresponds to the creation of an electron, while if it crosses from the left to the right, it corresponds to the creation of a positron. By the min-max principle of [**DES00**], in the case  $V \leq 0$  eigenvalues can only decrease so only electrons are created. This picture was confirmed by Hainzl [**Hai04**], from the point of view of the charge density of the system. When interactions are turned on, the one-body density matrix of the polarized vacuum satisfies a nonlinear equation of the form

$$P = \chi_{(-\infty, 0]}(D^0 + V + \alpha X_P), \quad (2.1.1)$$

where  $X_P$  is an operator depending on  $P$  (see Equation (2.2.6) below) and  $\alpha > 0$  is a coupling constant controlling the size of the non-linearity (or, equivalently, the size of the interactions). The number  $\alpha$  can also be interpreted as the square of the charge of an electron,  $\alpha = e^2$ , in which case it should also appear in front of the electric potential  $V$ . Since we are interested in pair production in strong fields, it is also natural to consider a fixed potential  $V$  (interpreted as the shape of a nucleus, for instance), which strength is controlled by a parameter  $Z > 0$  (interpreted as the charge of the nucleus). The equation satisfied by  $P$  is then

$$P = \chi_{(-\infty, 0]}(D^0 + (\alpha Z)V + \alpha X_P), \quad (2.1.2)$$

As a consequence, studying (2.1.1) for  $V$  fixed and  $\alpha > 0$  small is the same as studying (2.1.2) for  $\alpha Z$  fixed and  $\alpha > 0$  small, which is a well-known regime in the physics literature [**MPS98**, **RGA71**, **GR77**, **Sha02**]. In the sequel, we will thus write  $\kappa = \alpha Z$ . The existence of a solution to (2.1.2) is non trivial. Actually, one can show that there is *no* projection on  $L^2(\mathbb{R}^3, \mathbb{C}^4)$  satisfying (2.1.2). One way to circumvent this problem is to impose an ultraviolet cut-off  $\Lambda > 0$ , and to solve instead

$$P = \chi_{(-\infty, 0]}(\Pi_\Lambda(D^0 + \kappa V + \alpha X_P)\Pi_\Lambda), \quad (2.1.3)$$

where  $\Pi_\Lambda$  is the multiplication operator in Fourier space by  $\mathbf{1}_{B(0, \Lambda)}$ . We will show (Theorem 2.1) that for a general class of  $V$ , Equation (2.1.3) has a unique solution



for  $\kappa$  fixed if  $\alpha$  is small enough,  $\Lambda$  is large enough, and  $\alpha \log \Lambda$  fixed. Furthermore, we will show that this projection  $P$  satisfies

$$P - \chi_{(-\infty, 0]} \left( D^0 + \frac{\kappa}{1 + \frac{2}{3\pi} \alpha \log \Lambda} V \right) \rightarrow 0$$

in the Hilbert-Schmidt topology, as  $\alpha \rightarrow 0$  with  $\alpha \log \Lambda$  and  $\kappa$  fixed. We interpret this result as a *first order charge renormalization* of our model, meaning that we can compute the screening induced by the polarized vacuum explicitly in terms of  $\alpha$  and  $\Lambda$ . The term “first order” refers here to the fact that this is valid only in the limit  $\alpha \rightarrow 0$ . Roughly speaking, if we put an external potential  $V$  in the vacuum, what we observe in return (in the limit  $\alpha \rightarrow 0$ ) is a screened potential  $V_{\text{scr}}$ , with

$$V_{\text{scr}} = \frac{1}{1 + \frac{2}{3\pi} \alpha \log \Lambda} V. \quad (2.1.4)$$

A similar formula was already obtained in [GLS09], and it was valid *for all*  $\alpha > 0$ . However, in [GLS09], the non-linearity  $X_P$  is simpler than the one we consider in this article (namely, it does not contain the so-called *exchange term*). Here, we obtain (2.1.4) only in the limit  $\alpha \rightarrow 0$ , but we manage to include the exchange term.

Finally, we study static pair production for this model with interactions. Because of the nonlinearity  $X_P$ , it is not clear if the picture provided by Klaus and Scharf is still valid, that is if an eigenvalue of  $D(\alpha, \kappa V) := \Pi_\Lambda(D^0 + \kappa V + \alpha X_P)\Pi_\Lambda$  crosses 0 when  $\kappa$  is increased, then a particle is created. Instead, we will compare two operators

$$P_+ = \chi_{(-\infty, \mu_+]} \left( \Pi_\Lambda(D^0 + \kappa V + \alpha X_{P_+})\Pi_\Lambda \right),$$

and

$$P_- = \chi_{(-\infty, \mu_-]} \left( \Pi_\Lambda(D^0 + \kappa V + \alpha X_{P_-})\Pi_\Lambda \right),$$

where  $-1 < \mu_- < 0 < \mu_+ < 1$ . If the operator  $D^0 + \kappa V$  has an eigenvalue  $\lambda(\kappa V) \in (\mu_-, \mu_+)$  and  $\alpha$  is small enough,  $P_-$  is interpreted as the polarized vacuum with a certain charge  $q$ , while  $P_+$  is the polarized vacuum with charge  $q + 1$ . We want to determine which one is the most advantageous energetically. To do so, we introduce the function

$$F(\kappa, \alpha) = \mathcal{E}(P_+) - \mathcal{E}(P_-),$$

where  $\mathcal{E}$  is the energy functional which will be defined in the next section. Our second result (Theorem 2.2) provides an explicit formula valid for  $\alpha$  small enough and  $\alpha \log \Lambda$  fixed

$$F(\kappa, \alpha) = \lambda(\kappa V_{\text{scr}}) + \mathcal{O}_{\alpha \rightarrow 0}(\alpha),$$

where  $V_{\text{scr}}$  is given by (2.1.4). In particular, if  $\lambda(\kappa V)$  is positive for  $\kappa < \kappa_c$  and negative for  $\kappa > \kappa_c$ , then the polarized vacuum has charge  $q$  for  $\kappa < \kappa_c(\alpha)$  and charge

$q+1$  for  $\kappa > \kappa_c(\alpha)$ : an electron is created; if  $\lambda(\kappa V)$  is negative for  $\kappa < \kappa_c$  and positive for  $\kappa > \kappa_c$ , then a positron is created. Furthermore, we have

$$\kappa_c(\alpha) \longrightarrow \left(1 + \frac{2}{3\pi}\alpha \log \Lambda\right) \kappa_c > \kappa_c$$

as  $\alpha \rightarrow 0$  with  $\alpha \log \Lambda$  fixed. Hence, due to the screening of the polarized vacuum, static pair production in the interacting case requires a stronger potential than in the non-interacting case.

In principle, we can expand explicitly the function  $F$  to any order. For instance, we can compute the next order of  $F$  in  $\alpha$ , that is  $\lim_{\alpha \rightarrow 0}(F(\kappa, \alpha) - \lambda(\kappa V_{\text{scr}}))/\alpha$ . We are interested in the sign of this quantity, which would determine the growth of  $F$  to the next order. Unfortunately, we were not able to determine its sign, due to the complicated form of this term. It remains an interesting open problem to compute this sign. Finally, let us mention [Sok], where the same regime  $\alpha \rightarrow 0$ ,  $\alpha \log \Lambda$  fixed is studied without external field and for the vacuum of charge 1, interpreted as an electron together with the Dirac sea.

The paper is organized as follows. In Section 1, we introduce the model and present our main results. The proofs are given in Section 2.

## 2. Main results

In this section, we first explain the setting of the Bogoliubov-Dirac-Fock (BDF) model, and we state our results later.

**2.1. The Bogoliubov-Dirac-Fock model.** The content of this section can be found in [HLS05a, HLS05b, HLS07, HLS09a, GLS09]. Let  $\mathfrak{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$ . For any  $\Lambda > 0$ , we define

$$\mathfrak{H}_\Lambda := \{f \in \mathfrak{H}, \quad \text{supp} \widehat{f} \subset B(0, \Lambda)\},$$

where the hat denotes the Fourier transform of  $f$ , defined for  $f$  integrable by

$$\widehat{f}(\xi) := \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} f(x) e^{-ix \cdot \xi} dx,$$

and  $B(0, \Lambda)$  denotes the ball of center 0 and radius  $\Lambda$  in  $\mathbb{C}^4$ . We call such a  $\Lambda$  a *cut-off* in Fourier space. Since the Dirac operator  $D^0$  is a multiplication operator by  $p \mapsto \boldsymbol{\alpha} \cdot p + \beta$  in Fourier space, it stabilizes  $\mathfrak{H}_\Lambda$  and its restriction to  $\mathfrak{H}_\Lambda$  as an operator is denoted by  $D_\Lambda^0$ . Notice that  $D_\Lambda^0$  is bounded and that  $\|D_\Lambda^0\|_{\mathfrak{H}_\Lambda \rightarrow \mathfrak{H}_\Lambda} = \sqrt{1 + \Lambda^2}$ . We use the notation  $P_{\Lambda,-}^0 = \chi_{(-\infty, 0]}(D_\Lambda^0)$  (resp.  $P_{\Lambda,+}^0 = \chi_{[0, +\infty)}(D_\Lambda^0)$ ) for the negative (resp. positive) spectral projection of the Dirac operator  $D_\Lambda^0$ . For any bounded operator  $A$  over  $\mathfrak{H}_\Lambda$  and any  $\varepsilon, \varepsilon' = +, -$ , we define the block matrices  $A_{\varepsilon\varepsilon'} := P_{\Lambda,\varepsilon}^0 A P_{\Lambda,\varepsilon'}^0$ . We also define the associated spectral subspaces  $\mathfrak{H}_{\Lambda,\pm} := P_{\Lambda,\pm}^0 \mathfrak{H}_\Lambda$ . For any separable Hilbert space  $\mathcal{H}$  and any  $p > 0$ , we denote by  $\mathfrak{S}_p(\mathcal{H})$  the Schatten class of all bounded

operators  $A$  over  $\mathcal{H}$  such that  $\|A\|_{\mathfrak{S}_p}^p := \text{Tr} |A|^p < +\infty$ , where  $|A| = A^*A$ . We then introduce the vector space

$$\mathfrak{S}_{1,P_{\Lambda,-}^0}(\mathfrak{H}_\Lambda) := \{Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda), \quad Q_{++}, Q_{--} \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)\}.$$

It is a Banach space endowed with the norm

$$\|Q\|_{1,P_{\Lambda,-}^0} := \|Q_{++}\|_{\mathfrak{S}_1} + \|Q_{--}\|_{\mathfrak{S}_1} + \|Q_{+-}\|_{\mathfrak{S}_2} + \|Q_{-+}\|_{\mathfrak{S}_2}.$$

For any  $Q \in \mathfrak{S}_{1,P_{\Lambda,-}^0}$ , we define its generalized trace, which was first defined in [HLS05a], by

$$\text{Tr}_0(Q) := \text{Tr}(Q_{++} + Q_{--}).$$

Any  $Q \in \mathfrak{S}_{1,P_{\Lambda,-}^0}$  has an integral kernel  $Q(\cdot, \cdot) \in L^2(\mathbb{R}^3 \times \mathbb{R}^3, \mathcal{M}_4(\mathbb{C}))$ , where  $\mathcal{M}_4(\mathbb{C})$  denotes the set of all  $4 \times 4$  complex matrices. Thanks to the cut-off in Fourier space, it has a unique smooth representative allowing to define the *density of charge*  $\rho_Q$  associated to  $Q$ , defined by  $\rho_Q(x) = \text{Tr}_{\mathbb{C}^4} Q(x, x)$  for all  $x \in \mathbb{R}^3$ . It satisfies  $\rho_Q \in L^2(\mathbb{R}^3) \cap \mathcal{C}$ , where  $\mathcal{C}$  denotes the *Coulomb space*,

$$\mathcal{C} := \left\{f, \quad \int_{\mathbb{R}^3} \frac{|\widehat{f}(p)|^2}{|p|^2} dp < +\infty\right\} = \dot{H}^{-1}(\mathbb{R}^3).$$

For any  $f, g \in \mathcal{C}$ , the Coulomb inner product between  $f$  and  $g$  is defined as

$$D(f, g) := 4\pi \int_{\mathbb{R}^3} \frac{\widehat{f}(p)\overline{\widehat{g}(p)}}{|p|^2} dp.$$

If  $f, g$  are smooth enough (e.g.  $L^{6/5} \cap \mathcal{C}$ ), then

$$D(f, g) = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{f(x)\overline{g(y)}}{|x-y|} dx dy.$$

In the BDF theory, a quantum state is described by a self-adjoint operator  $P$  on  $\mathfrak{H}_\Lambda$  such that  $0 \leq P \leq 1_{\mathfrak{H}_\Lambda}$  in the sense of operators. Such a  $P$  is called a *one-body density matrix*. For instance, the operator  $P_{\Lambda,-}^0$  represents the quantum state of the (free) Dirac sea. For any one-body density matrix  $P$ , we define its *renormalized one-body density matrix* by  $Q = P - P_{\Lambda,-}^0$ . The set of all admissible quantum states is then

$$\mathcal{K}_\Lambda := \{Q \in \mathfrak{S}_{1,P_{\Lambda,-}^0}, \quad Q = Q^*, \quad -P_{\Lambda,-}^0 \leq Q \leq 1 - P_{\Lambda,-}^0\}.$$

For any  $Q$  such that  $-P_{\Lambda,-}^0 \leq Q \leq 1 - P_{\Lambda,-}^0$ , we have  $Q_{++} \geq 0$ ,  $-Q_{--} \geq 0$  and the inequality

$$Q^2 \leq Q_{++} - Q_{--},$$

so that  $Q \in \mathfrak{S}_2$  if  $Q_{++}, Q_{--} \in \mathfrak{S}_1$ . The quantity  $\text{Tr}(Q_{++})$  (resp.  $\text{Tr}(Q_{--})$ ) represents the average number of electrons (resp. positrons) of the system. Hence, the convex set  $\mathcal{K}_\Lambda$  represents the set of all quantum state with a finite average number of electrons

and positrons. The BDF energy of any quantum state  $Q \in \mathcal{K}_\Lambda$ , which was introduced in [HLS05a], is

$$\mathcal{E}_V^{\text{BDF}}(Q) = \text{Tr}_0(D_\Lambda^0 Q) + \alpha \int_{\mathbb{R}^3} \rho_Q V + \frac{\alpha}{2} D(\rho_Q, \rho_Q) - \frac{\alpha}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|Q(x, y)|^2}{|x - y|} dx dy. \quad (2.2.5)$$

Here,  $V$  is the external electric potential and  $\alpha > 0$  is the coupling constant. The first term of this energy represents the kinetic energy of the system. The second term is the interaction energy between the external potential and the density of charge  $\rho_Q$  of the system. The third term, usually called *direct term*, is the Coulomb electrostatic energy of the density of charge  $\rho_Q$ . The last term, well-known in Hartree-Fock theory, is called the *exchange term*. It is well-defined for  $Q \in \mathcal{K}_\Lambda$  by the Hardy-Kato inequality

$$\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|Q(x, y)|^2}{|x - y|} dx dy \leq \frac{\pi}{2} \text{Tr}(|D_\Lambda^0| Q^2),$$

the right term being finite since  $D_\Lambda^0$  is bounded. Since  $P_{\Lambda, \pm}^0 D_\Lambda^0 = \pm |D_\Lambda^0| P_{\Lambda, \pm}^0$ , the kinetic energy can be rewritten as

$$\text{Tr}_0 D_\Lambda^0 Q = \text{Tr} |D_\Lambda^0| (Q_{++} - Q_{--}),$$

which is finite for  $Q \in \mathcal{K}_\Lambda$ . The direct term is also well-defined since  $\rho_Q \in \mathcal{C}$ . Finally, we assume that  $V$  is given by the Coulomb potential generated by a fixed external density of charge  $\nu \in \mathcal{C}$  of strength  $Z > 0$ :

$$V = -Z\nu \star \frac{1}{|\cdot|},$$

so that we can rewrite

$$\int_{\mathbb{R}^3} \rho_Q V = -D(\rho_Q, Z\nu).$$

With this choice of  $V$  and by the Hardy-Kato inequality, we find that  $\mathcal{E}_\nu^{\text{BDF}}(Q)$  is well-defined for any  $Q \in \mathcal{K}_\Lambda$ , and that it is bounded-below for  $0 \leq \alpha \leq 4/\pi$  since it satisfies

$$\mathcal{E}_\nu^{\text{BDF}}(Q) \geq -\frac{\alpha Z^2}{2} D(\nu, \nu), \quad \forall Q \in \mathcal{K}_\Lambda.$$

It was proved in [HLS05b] that for any  $\nu \in \mathcal{C}$ , for any  $Z > 0$ , and for any  $0 \leq \alpha < 4/\pi$ , the BDF energy has at least one minimizer on  $\mathcal{K}_\Lambda$ . If  $\nu \equiv 0$ , then  $Q = 0$  is the unique global minimizer of the BDF energy. If  $\nu \neq 0$ , uniqueness does not hold in general. However, there always exists one minimizer  $\bar{Q}$  such that  $\bar{Q} + P_{\Lambda, -}^0$  is an orthogonal projection. More precisely, this minimizer satisfies the following self-consistent equation

$$\begin{cases} \bar{Q} &= \chi_{(-\infty, 0]}(D_{\bar{Q}}) - P_{\Lambda, -}^0, \\ D_{\bar{Q}} &= \Pi_\Lambda(D^0 - \alpha Z V_\nu + \alpha(V_{\rho_{\bar{Q}}} - R_{\bar{Q}}))\Pi_\Lambda, \end{cases} \quad (2.2.6)$$

where  $\Pi_\Lambda$  is the multiplication by  $\mathbf{1}_{B(0,\Lambda)}$  in Fourier space,  $V_\rho := \rho \star |\cdot|^{-1}$  for any  $\rho$ , and  $R_Q := \frac{Q(x,y)}{|x-y|}$  for any  $Q$ . This minimizer is interpreted as the polarized vacuum in the presence of  $V_\nu$ .

**2.2. Static pair production.** We now present the setting we use to study pair production. As we said in the introduction, we consider the vacuum polarized by a density of charge  $Z\nu$ . Moreover, we consider the limit of weak interactions, ie  $\alpha \rightarrow 0$  and strong external field  $Z \rightarrow +\infty$ , with  $\alpha Z$  fixed. Hence, we define a new parameter,

$$\kappa := \alpha Z.$$

We make the following assumption on  $\nu \in L^2(\mathbb{R}^3) \cap \mathcal{C}$ . We assume that there exists an eigenvalue  $\lambda(\kappa\nu)$  of multiplicity 1 of the operator  $D^{\kappa\nu} := D^0 - \kappa V_\nu$  on  $\mathfrak{H}$  that *crosses* 0 at some value  $\kappa = \kappa_c \in \mathbb{R}$ . In mathematical terms, it means that there exists  $\kappa_c \in \mathbb{R}$  and  $\varepsilon > 0$  such that

- For all  $\kappa \in [\kappa_c - \varepsilon, \kappa_c + \varepsilon]$ , the operator  $D^{\kappa\nu}$  on  $\mathfrak{H}$  has only one eigenvalue in some fixed neighborhood  $\mathcal{V}$  of 0, of multiplicity 1. We denote this eigenvalue by  $\lambda(\kappa\nu)$ , that is

$$\{\lambda(\kappa\nu)\} := \sigma(D^{\kappa\nu}) \cap \mathcal{V}. \quad (2.2.7)$$

- For  $\kappa \in [\kappa_c - \varepsilon, \kappa_c)$ ,  $\lambda(\kappa\nu) > 0$ , and for  $\kappa \in (\kappa_c, \kappa_c + \varepsilon]$ ,  $\lambda(\kappa\nu) < 0$ .

The assumption of multiplicity 1 is made for simplification and it can be easily removed. For the sake of clarity, we will also absorb  $\kappa_c$  in  $\nu$  by assuming in the following that

$$\boxed{\kappa_c = 1.}$$

We could also assume that  $\lambda(\kappa\nu)$  changes sign the other way around, which only changes the physical interpretation: a positron is created instead of an electron. Of course, since  $\nu \in L^2(\mathbb{R}^3) \cap \mathcal{C}$ , the eigenvalue  $\lambda(\kappa\nu)$  is a continuous function of  $\kappa$ . Hence, there exist  $-1 < \mu_- < 0 < \mu_+ < 1$  such that for all  $\kappa \in [1 - \varepsilon, 1 + \varepsilon]$ ,  $\lambda(\kappa) \in (\mu_-, \mu_+)$  and  $\mu_\pm \notin \sigma(D^{\kappa\nu})$ .

The BDF vacuum polarized by  $Z\nu$  is a solution to the equation

$$\begin{cases} Q &= \chi_{(-\infty, 0]}(D_Q) - P_{\Lambda, -}^0, \\ D_Q &= \Pi_\Lambda(D^{\kappa\nu} + \alpha(V_{\rho_Q} - R_Q))\Pi_\Lambda. \end{cases} \quad (2.2.8)$$

Here, the operator  $D_Q$  is seen an operator on  $\mathfrak{H}_\Lambda$ . The non-interacting vacuum in presence of the density of charge  $Z\nu$  is given by

$$Q_{\text{lin}}(\kappa) = \chi_{(-\infty, 0]}(D^{\kappa\nu}) - P_-^0,$$

where  $P_-^0 = \chi_{(-\infty, 0]}(D^0)$  is the negative spectral projection of the Dirac operator in  $\mathfrak{H}$ . Notice that, with our notations, the non-interacting vacuum satisfies

$$\begin{cases} Q_{\text{lin}}(\kappa) &= Q_{\text{lin}, -}(\kappa) &= \chi_{(-\infty, \mu_-]}(D^{\kappa\nu}) - P_-^0 &\text{if } \kappa < 1; \\ Q_{\text{lin}}(\kappa) &= Q_{\text{lin}, +}(\kappa) &= \chi_{(-\infty, \mu_+]}(D^{\kappa\nu}) - P_-^0 &\text{if } \kappa > 1. \end{cases}$$

Consider the non-linear analogue of these equations, ie

$$Q_{\pm}(\kappa, \alpha) = \chi_{(-\infty, \mu_{\pm}]}(\Pi_{\Lambda}(D^{\kappa\nu} + \alpha(V_{\rho_Q} - R_Q))\Pi_{\Lambda}) - F_{\Lambda, -}^0. \quad (2.2.9)$$

Our first result shows the existence of solutions to this equation. By an easy adaptation of [HLS05a, Theorem 2], it can be shown that, for  $\alpha$  small enough,  $Q_{-}(\kappa, \alpha)$  (resp.  $Q_{+}(\kappa, \alpha)$ ) is a minimizer of the BDF energy in the domain of charge  $\text{Tr}_0(Q_{\text{lin}, -}(\kappa)) = q$  (resp.  $\text{Tr}_0(Q_{\text{lin}, +}(\kappa)) = q+1$ ). Hence,  $Q_{+}(\kappa, \alpha)$  has one electron more than  $Q_{-}(\kappa, \alpha)$ , as in the linear case. We want to know which one of these two has the lowest BDF energy. To answer this question, we introduce the function

$$F(\kappa, \alpha) = \mathcal{E}_{Z\nu}^{\text{BDF}}(Q_{+}(\kappa, \alpha)) - \mathcal{E}_{Z\nu}^{\text{BDF}}(Q_{-}(\kappa, \alpha)). \quad (2.2.10)$$

If  $F$  changes sign while increasing  $\kappa$ , it means that the vacuum gains one particle, as explained in the introduction. Our second result provides an expansion of  $F(\kappa, \alpha)$  as  $\alpha \rightarrow 0$  with  $\alpha \log \Lambda$  fixed.

**2.3. Statement of the results.** Our first result concerns the existence of solutions to the equation (2.2.9). In [HLS05a], it has been solved by a fixed-point argument when  $\mu = 0$ , for  $\alpha$  small enough, for  $\Lambda$  large enough, and for  $\nu \in L^2(\mathbb{R}^3) \cap \mathcal{C}$  such that  $\|\kappa\nu\|_{L^2 \cap \mathcal{C}}$  is small enough. Here, we need to solve it for  $\mu \notin \sigma(D^{\kappa\nu})$  and under no smallness assumption on the parameter  $\kappa$  (indeed, if  $\kappa$  is too small,  $D^{\kappa\nu}$  cannot have an eigenvalue near 0, which we assume in our application to pair production). Hence, we have to go beyond the method of [HLS05a]. A solution to (2.2.8) can be found by a minimization argument, as in [HLS05b]. With this technique, no assumption on the smallness of  $\|\kappa\nu\|_{L^2 \cap \mathcal{C}}$  and of  $\alpha$  (except  $\alpha < 4/\pi$ ) is needed. By the same arguments, one can solve (2.2.9) with general  $\mu$  by minimizing the BDF energy in sectors of charge  $N$ , given by  $\mathcal{K}_{\Lambda}(N) := \{Q \in \mathcal{K}_{\Lambda}, \text{Tr}_0(Q) = N\}$ . The existence of minimizers in these charge sectors has been proved in [HLS09a], under the assumption of a binding condition, well-known in many-body theories. However, we do not know if these binding conditions are satisfied in the regime of parameters we consider. Even if we could prove this binding condition, the range of  $\mu$ s for which we can solve (2.2.9), ie the range of the map  $N \mapsto \mu$ , is not known. This range has been studied carefully in [GLS09], as well as the verification of the binding condition, in the case where the exchange term is neglected in the BDF energy. In the setting of our study, nothing is known about this issue. For all these reasons, we solve (2.2.9) by a fixed-point argument, following the method of [HLS05a]. This approach has also the advantage of furnishing a priori estimates on the solution of (2.2.9) in adequate norms, which are useful in proving the renormalization formula (2.1.4) and also in the proof of Theorem 2.2.

Before stating our result, we have to introduce the Banach space where we will find solutions to (2.2.9), which was introduced in [HLS05a]. For any  $x \in \mathbb{R}^3$ , we use

the notation  $E(x) := \sqrt{1+x^2}$ . We define the space

$$\mathcal{X} := \mathcal{Q} \times (L^2(\mathbb{R}^3) \cap \mathcal{C}),$$

where

$$\mathcal{Q} := \{Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda), \|Q\|_{\mathcal{Q}}^2 := \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} E(p-q)^2 E(p+q) |\widehat{Q}(p,q)|^2 dp dq < +\infty\}.$$

The vector space  $\mathcal{X}$  is a Banach space, endowed with the canonical norm

$$\|(Q, \rho)\|_{\mathcal{X}} := \|Q\|_{\mathcal{Q}} + \|\rho\|_{L^2 \cap \mathcal{C}}.$$

We find solutions to (2.2.9) by applying a fixed-point argument to the couple  $(Q, \rho_Q)$ . That is why the Banach space  $\mathcal{X}$  contains both the one-body density matrices  $Q$  as well as the densities of charge  $\rho$ .

**Theorem 2.1.** *Let  $\nu \in L^2(\mathbb{R}^3) \cap \mathcal{C}$ ,  $\mu \in (-1, 1)$ , and  $\varepsilon \geq 0$  such that*

$$\forall \kappa \in [1 - \varepsilon, 1 + \varepsilon], \quad \mu \notin \sigma(D^{\kappa\nu}). \quad (2.2.11)$$

*Assume furthermore that*

$$\int_{\mathbb{R}^3} \log(2 + |k|)^2 |\widehat{\nu}(k)|^2 dk < +\infty.$$

*Then, there exists  $L_0 = L_0(\mu, \nu, \varepsilon) > 0$ ,  $\alpha_0 = \alpha_0(\mu, \nu, \varepsilon) > 0$ ,  $\Lambda_0 = \Lambda_0(\mu, \nu, \varepsilon) > 0$ , and  $R_0 = R_0(\mu, \nu, \varepsilon) > 0$  such that for all  $0 \leq \alpha \leq \alpha_0$  and  $\Lambda \geq \Lambda_0$  satisfying  $\alpha \log \Lambda \leq L_0(\mu, \nu, \varepsilon)$ , and for all  $\kappa \in [1 - \varepsilon, 1 + \varepsilon]$ , the equation*

$$Q = \chi_{(-\infty, \mu]}(\Pi_\Lambda(D^0 - \kappa V_\nu + \alpha(V_{\rho_Q} - R_Q))\Pi_\Lambda) - P_{\Lambda, -}^0 \quad (2.2.12)$$

*has a unique solution  $(Q, \rho_Q) \in \mathcal{X}$  such that*

$$\|(Q + G_{1,0}(\kappa\nu_{\text{ren}}), \rho_Q - B_\Lambda \kappa\nu_{\text{ren}})\|_{\mathcal{X}} \leq R_0. \quad (2.2.13)$$

*Here, we used the notations*

$$\nu_{\text{ren}} := \frac{1}{1 + \alpha B_\Lambda} \nu, \quad (2.2.14)$$

*and for any  $\rho \in L^2(\mathbb{R}^3) \cap \mathcal{C}$ ,  $G_{1,0}(\rho) \in \mathcal{Q}$  is defined by*

$$G_{1,0}(\rho) = \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D_\Lambda^0 + i\eta} \Pi_\Lambda V_\rho \Pi_\Lambda \frac{1}{D_\Lambda^0 + i\eta} d\eta. \quad (2.2.15)$$

*Finally, the function  $B_\Lambda$  is given by*

$$B_\Lambda = \frac{1}{\pi} \int_0^{\frac{\Lambda}{\sqrt{1+\Lambda^2}}} \frac{z^2 - z^4/3}{1 - z^2} dz = \frac{2}{3\pi} \log \Lambda - \frac{5}{9\pi} + \frac{2 \log 2}{3\pi} + \mathcal{O}_{\Lambda \rightarrow \infty}(\Lambda^{-2}). \quad (2.2.16)$$

**Remark 2.1.** The function  $B_\Lambda$  already appeared in the previous works [HLS05a, HLS05b, GLS09]. It is logarithmically divergent in the cut-off  $\Lambda$ . This kind of divergence is well-known in Quantum Electrodynamics, and has been noticed in the early days of this theory by Dirac. The reason why we study the regime where  $\alpha \log \Lambda$  is bounded is to control this divergence.

**Remark 2.2.** One can apply this theorem to  $\varepsilon = 0$ , in which case the condition on  $\mu, \nu$  is simply  $\mu \notin \sigma(D^\nu)$ . Here, we allow  $\varepsilon > 0$  since we need estimates uniform in  $\kappa$  for the proof of Theorem 2.2.

**Corollary 2.1** (First order charge renormalization). *Under the assumptions of Theorem 2.1, and if we denote by  $Q(\kappa\nu, \alpha)$  the solution of (2.2.12) given by Theorem 2.1, we have as  $\alpha \rightarrow 0$  with  $\alpha \log \Lambda \leq L_0$  fixed:*

$$\boxed{Q(\kappa\nu, \alpha) - Q_{\text{lin}}(\kappa\nu_{\text{ren}}) \longrightarrow 0}$$

in  $\mathcal{Q}$ , where

$$\boxed{Q_{\text{lin}}(\kappa\nu_{\text{ren}}) = \chi_{(-\infty, \mu]}(\Pi_\Lambda(D^0 - \kappa V_{\nu_{\text{ren}}})\Pi_\Lambda) - P_{\Lambda, -}^0.}$$

**Remark 2.3.** This corollary does not imply the convergence of  $Q(\kappa\nu, \alpha)$  as  $\alpha \rightarrow 0$  towards  $\chi_{(-\infty, \mu]}(D^{\kappa\nu_{\text{ren}}}) - P_-^0$  in  $\mathcal{Q}$ , merely because this last operator does *not* belong to  $\mathcal{Q}$ . However, it belongs to  $\mathfrak{S}_2$  by [KS77a]. Since convergence in  $\mathcal{Q}$  implies convergence in  $\mathfrak{S}_2$ , we deduce that

$$Q(\kappa\nu, \alpha) \longrightarrow \chi_{(-\infty, \mu]}(D^{\kappa\nu_{\text{ren}}}) - P_-^0$$

in  $\mathfrak{S}_2$ , as  $\alpha \rightarrow 0$  with  $\alpha \log \Lambda \leq L_0$  fixed.

**Remark 2.4.** By (2.2.16), in the limit  $\alpha \rightarrow 0$  with  $\alpha \log \Lambda$  fixed, we have

$$\nu_{\text{ren}} = \frac{1}{1 + \frac{2}{3\pi}\alpha \log \Lambda} \nu,$$

which was the form used in the introduction.

Thanks to Theorem 2.1, we can build a solution to (2.2.12) with  $\nu \in L^2(\mathbb{R}^3) \cap \mathcal{C}$  satisfying the assumptions of Section 2.2, for  $\mu = \mu_\pm$ , for any  $\kappa \in [1 - \varepsilon, 1 + \varepsilon]$ , and for any  $\alpha > 0$  small enough,  $\Lambda$  large enough such that  $\alpha \log \Lambda$  is small enough. Since the corresponding  $Q_\pm(\kappa\nu, \alpha)$  belongs to  $\mathcal{Q} \subset \mathfrak{S}_2(\mathfrak{H}_\Lambda)$  and is a difference of orthogonal projections, we can use the fact that

$$P = P^2 = P^* \Rightarrow (P - P_{\Lambda, -}^0)^2 = (P - P_{\Lambda, -}^0)_{++} - (P - P_{\Lambda, -}^0)_{--},$$

to infer that  $Q_\pm(\kappa, \alpha) \in \mathcal{K}_\Lambda$ , hence the function  $F$  given by (2.2.10) is well-defined. Our second result is the following:

**Theorem 2.2.** *Let  $\nu \in L^2(\mathbb{R}^3) \cap \mathcal{C}$  satisfying the assumptions of Section 2.2, with furthermore*

$$\int_{\mathbb{R}^3} \log(2 + |k|)^2 |\widehat{\nu}(k)|^2 dk < +\infty.$$

*Then, for  $\alpha$  small enough, for  $\Lambda$  large enough such that  $\alpha \log \Lambda$  is small enough, we have the following expansion for all  $\kappa \in [1 - \varepsilon, 1 + \varepsilon]$ :*

$$\boxed{F(\kappa, \alpha) = \lambda(\kappa\nu_{\text{ren}}) + \mathcal{O}_{\alpha \rightarrow 0}(\alpha),} \tag{2.2.17}$$



where  $\mathcal{O}_{\alpha \rightarrow 0}(\alpha)$  denotes a function which absolute value is  $\leq C\alpha$  for  $\alpha$  small, where  $C$  only depends on  $\mu$ ,  $\nu$ , and  $\varepsilon$ .

**Remark 2.5.** Theorem 2.2 shows that for  $\alpha$  small enough, the BDF vacuum for  $\kappa > \kappa_c(\alpha)$  has one electron more than the BDF vacuum for  $\kappa < \kappa_c(\alpha)$ , with  $\kappa_c(\alpha) \sim_{\alpha \rightarrow 0} 1 + \alpha B_\Lambda > 1 = \kappa_c$ . In words, charge renormalization hinders pair production.

**Remark 2.6.** One could look for the next order in the expansion (2.2.17), i.e. look for a number  $c$  such that

$$F(\kappa, \alpha) = \lambda(\kappa\nu_{\text{ren}}) + c\alpha + o_{\alpha \rightarrow 0}(\alpha).$$

Of particular importance would be the determination of the sign of  $c$ , since it would give the next order influence of the interactions on pair production. Indeed, the first term in the expansion of  $F$ ,  $\lambda(\kappa\nu_{\text{ren}})$  is purely an effect of charge renormalization, and not a direct consequence of the interactions between the particles (though charge renormalization is itself a consequence of the interactions). It can be shown that  $c = \langle \varphi, H(\kappa\nu_{\text{ren}})\varphi \rangle$ , where  $\varphi \in \mathfrak{H}$  is the eigenvector associated to  $\lambda(\kappa\nu_{\text{ren}})$ , and  $H(\kappa\nu_{\text{ren}})$  is a self-adjoint operator on  $\mathfrak{H}$ . However, we could not determine if  $H(\kappa\nu_{\text{ren}})$  had a sign, because of its very complicated form. For this reason, the next order expansion of  $F$  is provided in Appendix B. In principle, our method enables to compute the expansion of  $F$  to any order.

**Remark 2.7.** When the exchange term is included, the operators  $P_-^0$  and  $D^0$  should in principle be replaced by effective operators  $\mathcal{P}_-^0$  and  $\mathcal{D}^0$  on  $\mathfrak{H}_\Lambda$  satisfying a non-linear equation and which depend on both  $\alpha$  and  $\Lambda$ , see [HLS07]. Our strategy works the same with  $\mathcal{P}_-^0$  and  $\mathcal{D}^0$ , but the estimates are even more technical. In particular, in Corollary 2.1, the operator  $D^0 - \kappa V_{\nu_{\text{ren}}}$  becomes

$$D_{\text{eff}} = g_1'(0)\boldsymbol{\alpha} \cdot (-i\nabla) + g_0(0)\beta - \frac{\kappa}{1 + \alpha B_\Lambda} V_\nu, \quad (2.2.18)$$

where

$$g_1'(0) = 1 + \frac{2}{3\pi}\alpha \log \Lambda, \quad g_0(0) = \frac{g_1'(0)}{1 - \frac{1}{3\pi}\alpha \log \Lambda}, \quad B_\Lambda = \frac{2 \log \Lambda}{3\pi g_1'(0)}.$$

In terms of mass and charge renormalization, the interpretation of this operator is not completely clear to us (see [LS00] and [HLS07, Sect. 2.5] for a discussion).

The rest of the article is devoted to the proofs of Theorem 2.1 and Theorem 2.2.

### 3. Proofs

**3.1. Proof of Theorem 2.1.** The strategy for solving (2.2.12) in [HLS05a] was to see the operator

$$D_Q := D_\Lambda^0 + \alpha \Pi_\Lambda (V_{\rho_Q - Z\nu} - R_Q) \Pi_\Lambda$$

as a small perturbation of  $D_\Lambda^0$  if  $\alpha$  is small enough, and then use the resolvent formula to expand

$$\chi_{(-\infty, \mu]}(D_Q) - \chi_{(-\infty, \mu]}(D_\Lambda^0)$$

in powers of  $\alpha$ , to find a functional to which they apply the fixed-point theorem of Banach-Picard. Here, we obviously cannot follow this strategy since  $\alpha Z = \kappa$  is fixed and not small. Instead, we have to find a new reference operator  $D_{\text{ref}}$ , independent of  $Q$ , satisfying  $D_Q = D_{\text{ref}} + \mathcal{O}(\alpha)$ , in an adequate sense. We choose

$$D_{\text{ref}} := D_\Lambda^0 - \Pi_\Lambda V_{\kappa\nu_{\text{ren}}} \Pi_\Lambda + \alpha \Pi_\Lambda R_{1,0}(\kappa\nu_{\text{ren}}) \Pi_\Lambda, \quad (2.3.19)$$

where<sup>1</sup>  $R_{1,0}(\kappa\nu_{\text{ren}}) := R[G_{1,0}(\kappa\nu_{\text{ren}})]$  is the exchange term associated to  $G_{1,0}(\kappa\nu_{\text{ren}})$ , which was defined in (2.2.15), and  $\nu_{\text{ren}}$  was defined in (2.2.14).

**Remark 2.8.** A more obvious choice for  $D_{\text{ref}}$  would have been  $D_{\text{ref}} = D_\Lambda^0 - \Pi_\Lambda V_{\kappa\nu} \Pi_\Lambda$ . Unfortunately, for this choice we do not have  $D_Q - D_{\text{ref}} = \mathcal{O}(\alpha)$  since there remains diverging terms in the expression  $\Pi_\Lambda (V_{\rho_Q} - R_Q) \Pi_\Lambda$ . These terms diverge precisely as  $\log \Lambda$ , and extracting them leads to the expression (2.3.19).

With this new reference operator, Equation (2.2.12) is equivalent to

$$Q = \chi_{(-\infty, \mu]}(D_{\text{ref}} + \alpha \Pi_\Lambda [V_{\rho_Q + \rho_{\text{ref}}} - R_{Q+Q_{\text{ref}}}] \Pi_\Lambda) - P_{\text{ref}}, \quad (2.3.20)$$

where

$$P_{\text{ref}} := \chi_{(-\infty, \mu]}(D_{\text{ref}}), \quad Q_{\text{ref}} := P_{\text{ref}} - P_{\Lambda,-}^0 + G_{1,0}(\kappa\nu_{\text{ren}}), \quad \rho_{\text{ref}} := \rho_{P_{\text{ref}} - P_{\Lambda,-}^0} - B_\Lambda \kappa \nu_{\text{ren}}.$$

Under adequate conditions on  $\nu$ , we will show that  $\|(Q_{\text{ref}}, \rho_{\text{ref}})\|_{\mathcal{X}} = \mathcal{O}_{\alpha \rightarrow 0}(1)$ , so that we are able to solve (2.3.20) by a fixed-point argument. First, we need to derive some properties of the operator  $D_{\text{ref}}$ .

3.1.1. *Spectral properties of the operator  $D_{\text{ref}}$ .* We first recall the following general result, which was partly contained in [HLS05a].

**Lemma 2.1.** *Let  $\rho \in L^2(\mathbb{R}^3) \cap \mathcal{C}$  and  $Q \in \mathcal{Q}$ . Then, we have*

$$\|V_\rho\|_{L^\infty} \leq 2\sqrt{\pi} \|\rho\|_{L^2 \cap \mathcal{C}}, \quad (2.3.21)$$

and there exists  $C > 0$  such that for all  $\eta \in \mathbb{R}$ ,

$$\|V_\rho |D^0 + i\eta|^{-1}\|_{\mathfrak{S}_6} \leq \frac{C}{E(\eta)^{1/2}} \|\rho\|_{\mathcal{C}}. \quad (2.3.22)$$

For any  $\eta \in \mathbb{R}$ , we have

$$\|R_Q |D^0 + i\eta|^{-1}\|_{\mathfrak{S}_2} \leq \frac{C_0}{E(\eta)^{1/2}} \|Q\|_{\mathcal{Q}}, \quad (2.3.23)$$

<sup>1</sup>Here and in the sequel, for any operator  $Q$  with integral kernel  $Q(x, y)$ ,  $R[Q]$  (or  $R_Q$ ) is the operator which kernel is given by  $\frac{Q(x, y)}{|x-y|}$ , and for any density of charge  $\rho$ ,  $V[\rho]$  (or  $V_\rho$ ) is the Coulomb potential generated by  $\rho$ , i.e.  $V[\rho] := \rho \star |\cdot|^{-1}$ .

where

$$C_0 := \frac{\sqrt{2}}{\pi^2} \inf_{\tau \in (0,2)} \sup_{x \in \mathbb{R}^3} \left( E(2x)^\tau \int_{\mathbb{R}^3} \frac{du}{E(2u)^{1+\tau} |u-x|^2} \right). \quad (2.3.24)$$

Finally, we have the estimates,

$$\|R_Q |D^0|^{-1}\|_{L^2 \rightarrow L^2} = \|R_Q\|_{H^1 \rightarrow L^2} \leq 2\|Q\|_{\mathfrak{S}_2}, \quad (2.3.25)$$

$$\|R_Q |D^0|^{-1/2}\|_{L^2 \rightarrow L^2} = \|R_Q\|_{H^{1/2} \rightarrow L^2} \leq \frac{\pi}{2} \|Q\|_{\mathfrak{Q}}. \quad (2.3.26)$$

PROOF. Inequality (2.3.21) was proved in [HLS05a, Lemma 3]. Inequality (2.3.22) is a consequence of the Kato-Seiler-Simon inequality

$$\forall p \geq 2, \forall f, g \in L^p(\mathbb{R}^3), \quad \|f(x)g(-i\nabla)\|_{\mathfrak{S}_p} \leq (2\pi)^{-3/p} \|f\|_{L^p} \|g\|_{L^p}, \quad (2.3.27)$$

of the Sobolev inequality  $\|V_\rho\|_{L^6} \leq C\|\nabla V_\rho\|_{L^2} = C\|\rho\|_C$ , and of

$$\left\| \frac{1}{|\boldsymbol{\alpha} \cdot p + \beta + i\eta|} \right\|_{L^6}^6 = \int_{\mathbb{R}^3} \frac{dp}{(E(p)^2 + \eta^2)^3} = \frac{C}{E(\eta)^3}.$$

Finally, inequality (2.3.23) is proved using the fact that for all  $p, q \in \mathbb{R}^3$ ,

$$\frac{E(p+q)E(\eta)}{(E(p)^2 + \eta^2)E(p-q)} \leq 2,$$

hence

$$\begin{aligned} \|R_Q |D^0 + i\eta|^{-1}\|_{\mathfrak{S}_2}^2 &= \iint \frac{|\widehat{R}_Q(p, q)|^2}{E(p)^2 + \eta^2} dp dq \\ &\leq \frac{2}{E(\eta)} \iint \frac{E(p-q)^2}{E(p+q)} |\widehat{R}_Q(p, q)|^2 dp dq \leq \frac{C_0^2}{E(\eta)} \|Q\|_{\mathfrak{Q}}^2, \end{aligned}$$

where the second inequality was proved in [HLS05a, Lemma 8]. To prove (2.3.25), let  $\varphi \in H^1$ . Then, by the Hölder inequality we have for all  $x \in \mathbb{R}^3$ ,

$$|R_Q \varphi(x)|^2 \leq \int_{\mathbb{R}^3} |Q(x, y)|^2 dy \int_{\mathbb{R}^3} \frac{|\varphi(y)|^2}{|x-y|^2} dy.$$

By the Hardy inequality, one deduces

$$\|R_Q \varphi\|_{L^2}^2 \leq 4\|Q\|_{\mathfrak{S}_2}^2 \|\nabla \varphi\|_{L^2}^2 \leq 4\|Q\|_{\mathfrak{S}_2}^2 \| |D^0| \varphi \|_{L^2}^2.$$

The proof of (2.3.26) relies on the same computation for  $\varphi \in H^{1/2}$ :

$$|R_Q \varphi(x)|^2 \leq \int_{\mathbb{R}^3} \frac{|Q(x, y)|^2}{|x-y|} dy \int_{\mathbb{R}^3} \frac{|\varphi(y)|^2}{|x-y|} dy,$$

so that by the Hardy-Kato inequality applied to both terms,

$$\|R_Q \varphi\|_{L^2}^2 \leq \frac{\pi^2}{4} \text{Tr}(|D^0| Q^2) \langle |D^0| \varphi, \varphi \rangle_{L^2} \leq \frac{\pi^2}{4} \|Q\|_{\mathfrak{Q}}^2 \| |D^0|^{1/2} \varphi \|_{L^2}^2.$$

□

**Lemma 2.2** (Properties of  $G_{1,0}(\rho)$ ). *Let  $\rho \in L^2(\mathbb{R}^3) \cap \mathcal{C}$ . Then, for any  $\Lambda > 1$ , the operator  $G_{1,0}(\rho)$  defined by (2.2.15) satisfies for some  $C > 0$ :*

$$\|G_{1,0}(\rho)\|_{\mathcal{Q}} \leq C \sqrt{\log \Lambda} \|\rho\|_{L^2 \cap \mathcal{C}}, \quad (2.3.28)$$

$$\|G_{1,0}(\rho)\|_{\mathfrak{S}_2} \leq 4 \|\rho\|_{\mathcal{C}}. \quad (2.3.29)$$

PROOF. Inequality (2.3.28) was proved in [HLS05a, Lemma 11]. It relies of the explicit form of the integral kernel of  $G_{1,0}(\rho)$  in Fourier space, obtained by the residuum formula:

$$\forall p, q \in \mathbb{R}^3, \quad \widehat{G_{1,0}(\rho)}(p, q) = \frac{1}{2(2\pi)^{3/2}} \widehat{V}_\rho(p - q) M(p, q), \quad (2.3.30)$$

where the function  $M$  is defined by

$$M(p, q) = \frac{1}{E(p) + E(q)} \left( \frac{\alpha \cdot p + \beta}{E(p)} \frac{\alpha \cdot q + \beta}{E(q)} - 1 \right). \quad (2.3.31)$$

It was proved in [HLS05a, Lemma 12] that

$$|M(p, q)|^2 \leq 16 \frac{|p - q|^2}{E(p + q)^4}, \quad (2.3.32)$$

hence

$$\|G_{1,0}(\rho)\|_{\mathfrak{S}_2}^2 \leq \frac{64}{\pi} \int_{\mathbb{R}^3} |k|^2 |\widehat{V}_\rho(k)|^2 dk \int_{\mathbb{R}^3} \frac{d\ell}{E(\ell)^4} = 16 \|\rho\|_{\mathcal{C}}^2,$$

where we used that  $\int_{\mathbb{R}^3} E(\ell)^{-4} d\ell = \pi^2$ .  $\square$

Combining Lemmas 2.1 and 2.2, we infer that for any  $\alpha > 0$  and  $\Lambda > 1$ , the operator  $D_{\text{ref}}$  is bounded and self-adjoint on  $\mathfrak{H}_\Lambda$ . The following result ensures that  $D_{\text{ref}}$  has a gap around  $\mu$  for  $\alpha$  small enough and  $\Lambda$  large enough. For any  $\omega \in L^2(\mathbb{R}^3) \cap \mathcal{C}$ , we introduce the auxiliary operator on  $\mathfrak{H}_\Lambda$ ,

$$D_{\text{ref}}(\omega) := D_\Lambda^0 - \Pi_\Lambda V_\omega \Pi_\Lambda + \alpha \Pi_\Lambda R_{1,0}(\omega) \Pi_\Lambda, \quad (2.3.33)$$

so that  $D_{\text{ref}} = D_{\text{ref}}(\kappa \nu_{\text{ren}})$ .

**Lemma 2.3.** *Let  $\nu \in L^2(\mathbb{R}^3) \cap \mathcal{C}$  and  $\mu \in (-1, 1)$ . Let  $\varepsilon \geq 0$  such that for all  $s \in [1 - \varepsilon, 1 + \varepsilon]$ ,  $\mu \notin \sigma_{\mathfrak{H}}(D^{s\nu})$ . Then for all  $L > 0$ , there exists  $\alpha_0 = \alpha_0(\mu, \nu, \varepsilon, L) > 0$ ,  $\Lambda_0 = \Lambda_0(\mu, \nu, \varepsilon, L) > 1$  and  $\xi_0 = \xi_0(\mu, \nu, \varepsilon, L) > 0$  such that for all  $0 \leq \alpha \leq \alpha_0$ , for all  $\Lambda \geq \Lambda_0$  satisfying  $\alpha \sqrt{\log \Lambda} \leq L$ , and for all  $s \in [1 - \varepsilon, 1 + \varepsilon]$ , we have  $d(\mu, \sigma_{\mathfrak{H}_\Lambda}(D_{\text{ref}}(s\nu))) \geq \xi_0$ .*

PROOF. The proof is done by contradiction. Assume there exists  $\alpha_n \rightarrow 0$ ,  $\Lambda_n \rightarrow +\infty$  satisfying  $\alpha_n \sqrt{\log \Lambda_n} \leq L$ ,  $s_n \in [1 - \varepsilon, 1 + \varepsilon]$  such that  $d(\mu, \sigma_{\mathfrak{H}_{\Lambda_n}}(D_{\text{ref}}(s_n \nu))) \leq 1/n$ . Up to extracting a subsequence, we can assume  $s_n \rightarrow s \in [1 - \varepsilon, 1 + \varepsilon]$ . Since  $d(\mu, \sigma_{\mathfrak{H}_{\Lambda_n}}(D_{\text{ref}}(s_n \nu))) \leq 1/n$ , there exists  $\varphi_n \in \mathfrak{H}_{\Lambda_n} := \mathfrak{H}_{\Lambda_n}$  with  $\|\varphi_n\|_{L^2} = 1$  and  $\|(D_n - \mu)\varphi_n\|_{L^2} \leq 2/n$ , with  $D_n := D_{\text{ref}}(s_n \nu)$ . For any  $\eta \in \mathbb{R}$  and  $n \in \mathbb{N}$  we have

$$D_n \varphi_n = (1 + \Pi_n(\alpha_n R_n(s_n \nu) - V_{s_n \nu}))(D^0 + i\eta)^{-1}(D^0 + i\eta)\varphi_n - i\eta \varphi_n,$$

where we used the notations  $\Pi_n := \Pi_{\Lambda_n}$  and  $R_n(s_n\nu) := R_{1,0}(s_n\nu)$ . Now for  $\eta$  large enough, we have  $\|V_{s_n\nu}(D^0 + i\eta)^{-1}\| < 1$  by (2.3.22), and  $\|\alpha_n R_{1,0}^{(n)}(\omega)(D^0 + i\eta)^{-1}\| < 1$  by (2.3.23) and the fact that  $\alpha_n \sqrt{\log \Lambda_n} \leq L$ . Then, we have for such a  $\eta$ ,

$$(D^0 + i\eta)\varphi_n = \frac{1}{(1 + \Pi_n(\alpha_n R_n(s_n\nu) - V_{s_n\nu})(D^0 + i\eta)^{-1})} (D_n\varphi_n + i\eta\varphi_n),$$

showing that  $(\varphi_n)_n$  is bounded in  $H^1(\mathbb{R}^3)$ . Hence, up to a subsequence we can assume  $\varphi_n \rightharpoonup \varphi$  in  $H^1(\mathbb{R}^3)$ . This implies that  $D^0\varphi_n \rightharpoonup D^0\varphi$  and  $\mu\varphi_n \rightharpoonup \mu\varphi$  weakly in  $L^2(\mathbb{R}^3)$ . Since  $V_{s\nu}(D^0)^{-1}$  is a compact operator we also have  $V_{s_n\nu}\varphi_n \rightarrow V_{s\nu}\varphi$  strongly in  $L^2(\mathbb{R}^3)$  and hence  $\Pi_n V_{s_n\nu}\varphi_n \rightarrow V_{s\nu}\varphi$  strongly in  $L^2(\mathbb{R}^3)$ . Using (2.3.25) and (2.3.29), we infer that

$$\|\alpha_n R_n(s_n\nu)|D^0|^{-1}\|_{L^2 \rightarrow L^2} \leq 2\alpha_n \|G_{1,0}(s_n\nu)\|_{\mathfrak{S}_2} \leq 8\alpha_n(1 + \varepsilon)\|\nu\|_{\mathcal{C}} \rightarrow 0.$$

We thus have  $\Pi_n \alpha_n R_n(s_n\nu)\varphi_n$  converging strongly to 0 in  $L^2$ . Hence,  $D_n\varphi_n \rightharpoonup (D^0 - V_{s\nu})\varphi$  weakly in  $L^2$  and since  $\|(D_n - \mu)\varphi_n\|_{L^2} \leq 2/n$ , we have  $(D^0 - V_{s\nu})\varphi = \mu\varphi$ . But  $\mu \notin \sigma_{\mathfrak{S}}(D^{s\nu})$ , hence we must have  $\varphi = 0$ . This implies that  $\Pi_n V_{s_n\nu}\varphi_n \rightarrow 0$  strongly in  $L^2(\mathbb{R}^3)$ . We deduce  $(D^0 - \mu)\varphi_n \rightarrow 0$  strongly in  $L^2$ , which is a contradiction by the Weyl criterion for the essential spectrum since  $\|\varphi_n\|_{L^2} = 1$ ,  $\varphi_n \rightharpoonup 0$  weakly in  $L^2$  and  $\mu \in (-1, 1)$ .  $\square$

**Lemma 2.4.** *Let  $\omega \in L^2(\mathbb{R}^3) \cap \mathcal{C}$  and  $\mu \in (-1, 1)$  such that  $\mu \notin \sigma(D_{\text{ref}}(\omega))$ . Then for all  $\alpha \geq 0$  such that  $8\alpha\|\omega\|_{\mathcal{C}} < 1 - |\mu|$ , the operator  $|D^0|(D_{\text{ref}}(\omega) - \mu)^{-1}$  (extended by 0 on  $\mathfrak{H}_{\Lambda}^{\perp}$ ) is bounded on  $L^2(\mathbb{R}^3, \mathbb{C}^4)$ , and we have*

$$\left\| |D^0| \frac{1}{D_{\text{ref}}(\omega) - \mu} \right\|_{L^2 \rightarrow L^2} \leq \theta(\mu, \omega),$$

where

$$\theta(\mu, \omega) = \left(1 - \frac{8\alpha\|\omega\|_{\mathcal{C}}}{1 - |\mu|}\right)^{-1} \frac{1}{1 - |\mu|} \left(1 + \frac{2\sqrt{\pi}\|\omega\|_{\mathcal{C}}}{d(\mu, \sigma(D_{\text{ref}}(\omega)))}\right).$$

PROOF. By the resolvent identity, we have

$$\frac{1}{D_{\text{ref}}(\omega) - \mu} = \frac{1}{D_{\Lambda}^0 - \mu} + \frac{1}{D_{\Lambda}^0 - \mu} \Pi_{\Lambda}(V_{\omega} - \alpha R_{1,0}(\omega)) \Pi_{\Lambda} \frac{1}{D_{\text{ref}}(\omega) - \mu}.$$

Using  $\| |D^0|(D_{\Lambda}^0 - \mu)^{-1} \|_{L^2 \rightarrow L^2} \leq (1 - |\mu|)^{-1}$  and  $\|R_{1,0}(\omega)|D^0|^{-1}\|_{L^2 \rightarrow L^2} \leq 8\|\omega\|_{\mathcal{C}}$  by (2.3.25) and (2.3.29), we obtain

$$\left(1 - \frac{8\alpha\|\omega\|_{\mathcal{C}}}{1 - |\mu|}\right) \left\| |D^0| \frac{1}{D_{\text{ref}}(\omega) - \mu} \right\|_{L^2 \rightarrow L^2} \leq \frac{1}{1 - |\mu|} \left(1 + \frac{2\sqrt{\pi}\|\omega\|_{L^2 \cap \mathcal{C}}}{d(\mu, \sigma(D_{\text{ref}}(\omega)))}\right).$$

$\square$

Lemma 2.3 ensures that we can use Cauchy's formula to  $P_{\text{ref}}$  since  $D_{\text{ref}}$  has a gap around  $\mu$ . The next result is the analogue of [HLS05a, Lemma 9]. It ensures that

the operator  $D_Q$  also has a gap around  $\mu$ . For any  $Q \in \mathcal{Q}$  and  $\omega, \rho' \in L^2(\mathbb{R}^3) \cap \mathcal{C}$  we define the following operator on  $\mathfrak{H}_\Lambda$ :

$$D_{\omega, \rho', Q} = D_{\text{ref}}(\omega) + \alpha \Pi_\Lambda (V_{\rho'} - R_Q) \Pi_\Lambda. \quad (2.3.34)$$

With this notation, we have  $D_Q = D_{\kappa\nu_{\text{ren}}, \rho_Q + \rho_{\text{ref}}, Q + Q_{\text{ref}}}$ .

**Lemma 2.5.** *Let  $\omega \in L^2(\mathbb{R}^3) \cap \mathcal{C}$ ,  $\mu \in (-1, 1)$ ,  $\alpha \geq 0$ ,  $\Lambda > 0$ ,  $(Q, \rho') \in \mathcal{X}$  be such that the following conditions are satisfied:*

- (1)  $\mu \notin \sigma(D_{\text{ref}}(\omega))$ ;
- (2)  $8\alpha \|\omega\|_{\mathcal{C}} < 1 - |\mu|$ ;
- (3)  $\alpha b \|(Q, \rho')\|_{\mathcal{X}} < 1$ ,

where, using the notations of Lemma 2.4,

$$b := \frac{1}{d(\mu, \sigma(D_{\text{ref}}(\omega)))} + \theta(\mu, \omega).$$

Then, we have the operator inequality

$$|D_{\omega, \rho', Q} - \mu| \geq (1 - \alpha b \|(Q, \rho')\|_{\mathcal{X}}) |D_{\text{ref}}(\omega) - \mu|.$$

In particular,  $\mu \notin \sigma(D_{\omega, \rho', Q})$ .

**Remark 2.9.** The conditions listed in the above lemma give a non trivial relation between  $\alpha$  and  $\mu$  (recall that  $D_{\text{ref}}(\omega)$  depends on  $\alpha$ ). Fortunately, these conditions are satisfied if  $\mu \in (-1, 1)$ ,  $\mu \notin \sigma(D^0 - V_\omega)$  and  $\alpha$  is small enough by Lemma 2.3.

**PROOF.** We adapt the proof of [HLS05a, Lemma 9] to our case. First of all, since  $\sigma_{\text{ess}}(D_{\text{ref}}(\omega)) = [-E(\Lambda), -1] \cup [1, E(\Lambda)]$  and  $\mu \in (-1, 1)$ ,  $\mu \notin \sigma(D_{\text{ref}}(\omega))$ , we have  $d(\mu, \sigma(D_{\text{ref}}(\omega))) > 0$ . Let  $u \in \mathfrak{H}_\Lambda$ . By Lemma 2.1, we have

$$\|\Pi_\Lambda V_{\rho'} u\|_{L^2} \leq \|V_{\rho'}\|_{L^\infty} \|u\|_{L^2} \leq \frac{2\sqrt{\pi} \|\rho'\|_{L^2 \cap \mathcal{C}}}{d(\mu, \sigma(D_{\text{ref}}(\omega)))} \| |D_{\text{ref}}(\omega) - \mu| u \|_{L^2},$$

where we used the operator inequality  $|D_{\text{ref}}(\omega) - \mu| \geq d(\mu, \sigma(D_{\text{ref}}(\omega)))$ . For the exchange term, we write

$$\|\Pi_\Lambda R_Q u\|_{L^2} \leq \|R_Q |D^0|^{-1}\|_{\mathfrak{S}_2} \left\| |D^0| \frac{1}{|D_{\text{ref}}(\omega) - \mu|} \right\|_{L^2 \rightarrow L^2} \| |D_{\text{ref}}(\omega) - \mu| u \|_{L^2}.$$

By Lemma 2.4, this implies

$$\|\Pi_\Lambda R_Q u\|_{L^2} \leq C_0 \|Q\|_{\mathcal{Q}} \theta(\mu, \omega) \| |D_{\text{ref}}(\omega) - \mu| u \|_{L^2},$$

showing that

$$|\Pi_\Lambda (V_{\rho'} - R_Q) \Pi_\Lambda| \leq \left( \frac{1}{d(\mu, \sigma(D_{\text{ref}}(\omega)))} + \theta(\mu, \omega) \right) \|(Q, \rho')\|_{\mathcal{X}} |D_{\text{ref}}(\omega) - \mu|.$$

□

3.1.2. *Resolvent expansion.* Now that we know sufficient conditions on our parameters to prove that both  $D_{\text{ref}}$  and  $D_Q$  have a gap around  $\mu$ , we can use Cauchy formula, and then resolvent expansion (at least formally for the moment), to see that (2.3.20) is equivalent to

$$Q = \frac{1}{2\pi} \int_{\mathbb{R}} \left( \frac{1}{D_{\text{ref}} - \mu + i\eta} - \frac{1}{D_Q - \mu + i\eta} \right) d\eta,$$

which leads to

$$Q = \sum_{n \geq 1} \frac{(-1)^{n+1} \alpha^n}{2\pi} \int_{\mathbb{R}} \frac{1}{D_{\text{ref}} - \mu + i\eta} \times \\ \times \left( \Pi_{\Lambda}(V_{\rho_Q + \rho_{\text{ref}}} - R_{Q+Q_{\text{ref}}}) \Pi_{\Lambda} \frac{1}{D_{\text{ref}} - \mu + i\eta} \right)^n d\eta.$$

We write it as

$$Q = \sum_{n \geq 1} \alpha^n G_n^{\kappa\nu\text{ren}}(Q + Q_{\text{ref}}, \rho_Q + \rho_{\text{ref}}), \quad (2.3.35)$$

where for any  $Q \in \mathcal{Q}$ ,  $\omega, \rho' \in L^2(\mathbb{R}^3) \cap \mathcal{C}$ ,

$$G_n^{\omega}(Q, \rho') = \frac{(-1)^{n+1}}{2\pi} \int_{\mathbb{R}} \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta} \left( \Pi_{\Lambda}(V_{\rho'} - R_Q) \Pi_{\Lambda} \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta} \right)^n d\eta. \quad (2.3.36)$$

We will prove in particular that (2.3.35) makes sense by showing that the series converges in  $\mathcal{Q}$ , for  $\alpha$  small enough. Equation (2.3.35) implies that

$$\rho_Q = \sum_{n \geq 1} \alpha^n \rho[G_n^{\kappa\nu\text{ren}}(Q + Q_{\text{ref}}, \rho_Q + \rho_{\text{ref}})]. \quad (2.3.37)$$

We use the same trick as in [HLS05a], by writing

$$\rho[G_1^{\omega}(Q, \rho')] = \rho[G_{1,0}(\rho')] + J_1^{\omega}(Q, \rho'),$$

where we recall that  $G_{1,0}(\rho')$  was defined in (2.2.15). It was proved in [HLS05a] that

$$\forall k \in \mathbb{R}^3, \quad \mathcal{F}[\rho[G_{1,0}(\rho')]](k) = -B_{\Lambda}(k) \widehat{\rho}'(k),$$

where  $\mathcal{F}[f] := \widehat{f}$ . The function  $B_{\Lambda}(k)$  is computed in [GLS09, Eq.(88)]. It satisfies  $B_{\Lambda}(k) = 0$  for  $|k| > 2\Lambda$  while for  $|k| \leq 2\Lambda$  we have the formula

$$B_{\Lambda}(k) = \frac{1}{\pi} \int_0^{Z_{\Lambda}(|k|)} \frac{z^2 - z^4/3}{(1 - z^2)(1 + |k|^2(1 - z^2)/4)} dz \\ + \frac{|k|}{2\pi} \int_0^{Z_{\Lambda}(|k|)} \frac{z - z^3/3}{\sqrt{1 + \Lambda^2 - |k|z/2}} dz,$$

with

$$Z_{\Lambda}(r) = \frac{\sqrt{1 + \Lambda^2} - \sqrt{1 + (\Lambda - r)^2}}{r}, \quad \forall r \geq 0.$$

Notice that  $B_\Lambda = B_\Lambda(0)$ . Defining  $J_n^\omega(Q, \rho') := \rho[G_n^\omega(Q, \rho')]$  for  $n \geq 2$ , we see that (2.3.37) is equivalent to

$$\begin{aligned} \forall k \in \mathbb{R}^3, \quad \mathcal{F}[\rho_Q + \rho_{\text{ref}}](k) &= \frac{1}{1 + \alpha B_\Lambda(k)} \widehat{\rho_{\text{ref}}}(k) \\ &\quad + \sum_{n \geq 1} \frac{\alpha^n}{1 + \alpha B_\Lambda(k)} \mathcal{F}[J_n^{\nu_{\text{ren}}}(Q + Q_{\text{ref}}, \rho_Q + \rho_{\text{ref}})](k). \end{aligned}$$

Hence, the couple  $(Q, \rho_Q + \rho_{\text{ref}})$  satisfies

$$(Q, \rho_Q + \rho_{\text{ref}}) = \Phi(Q, \rho_Q + \rho_{\text{ref}}) = (\Phi_1^{\kappa_{\nu_{\text{ren}}}}(Q + Q_{\text{ref}}, \rho_Q + \rho_{\text{ref}}), \Phi_2^{\kappa_{\nu_{\text{ren}}}}(Q + Q_{\text{ref}}, \rho_Q + \rho_{\text{ref}})),$$

where

$$\Phi_1^\omega(Q, \rho') = \sum_{n \geq 1} \alpha^n G_n^\omega(Q, \rho'),$$

$$\forall k \in \mathbb{R}^3, \quad \mathcal{F}[\Phi_2^\omega(Q, \rho')](k) = \frac{1}{1 + \alpha B_\Lambda(k)} \widehat{\rho_{\text{ref}}}(k) + \sum_{n \geq 1} \frac{\alpha^n}{1 + \alpha B_\Lambda(k)} \mathcal{F}[J_n^\omega(Q, \rho')](k).$$

We prove that  $\Phi$  stabilizes a certain ball in  $\mathcal{X}$  and that it is contractant on this ball. By the Banach-Picard theorem, it proves Theorem 2.1. To do so, we need estimates on the function  $\Phi$ .

3.1.3. *Estimates on  $\Phi$ .* We begin by a useful result about commutators.

**Lemma 2.6.** *Let  $\rho \in L^2(\mathbb{R}^3) \cap \mathcal{C}$  and  $Q \in \mathcal{Q}$ . Then we have the following estimates:*

$$\forall 0 < \zeta < 1, \quad \forall t > \zeta + \frac{1}{2}, \quad \|[|D^0|^\zeta, V_\rho] |D^0|^{-t}\|_{\mathfrak{S}_2} \leq C \|\rho\|_{\mathcal{C}}, \quad (2.3.38)$$

$$\forall 0 < \zeta < 1, \quad \forall t > \zeta, \quad \|[|D^0|^\zeta, R_Q] |D^0|^{-t}\|_{\mathfrak{S}_2} \leq C \|Q\|_{\mathcal{Q}}. \quad (2.3.39)$$

PROOF. We begin by noticing that, if  $T$  is a self-adjoint operator, we have

$$\|[|D^0|^\zeta, T] |D^0|^{-t}\|_{\mathfrak{S}_2} \leq \sqrt{2} \|[|D^0|^\zeta, T^>] |D^0|^{-t}\|_{\mathfrak{S}_2},$$

where  $\widehat{T^>}(p, q) = T(p, q) \chi_{|p| > |q|}$  for all  $p, q \in \mathbb{R}^3$ . Indeed,

$$\begin{aligned} \|[|D^0|^\zeta, T] |D^0|^{-t}\|_{\mathfrak{S}_2}^2 &= \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|E(p)^\zeta - E(q)^\zeta|^2}{E(q)^{2t}} |\widehat{T}(p, q)|^2 dp dq \\ &= \iint_{|p| > |q|} \dots + \iint_{|p| < |q|} \dots, \end{aligned}$$

and using  $|\widehat{T}(p, q)| = |\widehat{T}(q, p)|$  we find

$$\begin{aligned} \iint_{|p| < |q|} \frac{|E(p)^\zeta - E(q)^\zeta|^2}{E(q)^{2t}} |\widehat{T}(p, q)|^2 dp dq &\leq \iint_{|p| < |q|} \frac{|E(p)^\zeta - E(q)^\zeta|^2}{E(p)^{2t}} |\widehat{T}(p, q)|^2 dp dq \\ &= \iint_{|p| > |q|} \frac{|E(p)^\zeta - E(q)^\zeta|^2}{E(q)^{2t}} |\widehat{T}(p, q)|^2 dp dq. \end{aligned}$$



Hence, to estimate  $\| [|D^0|^\zeta, T] |D^0|^{-t} \|_{\mathfrak{S}_2}$ , it is sufficient to estimate  $\| [|D^0|^\zeta, T^>] |D^0|^{-t} \|_{\mathfrak{S}_2}$  or  $\| [|D^0|^\zeta, T^<] |D^0|^{-t} \|_{\mathfrak{S}_2}$ . Now let  $A = [|D^0|^\zeta, V_\rho^>] |D^0|^{-t}$ . For any  $|p| > |q|$ , we have by the mean value theorem

$$|E(p)^\zeta - E(q)^\zeta| \leq \zeta E(q)^{\zeta-1} |E(p) - E(q)| \leq \frac{\zeta}{2} E(q)^{\zeta-1} |p - q|.$$

Hence,

$$\|A\|_{\mathfrak{S}_2}^2 \leq \zeta \iint_{\mathbb{R}^3 \times \mathbb{R}^3} |p - q|^2 |\widehat{V}_\rho(p - q)|^2 \frac{dp dq}{E(q)^{2(t-\zeta+1)}} \leq C \|\rho\|_{\mathcal{C}}^2,$$

since  $2(t - \zeta + 1) > 3$ . To prove (2.3.39), the same strategy only works in the case  $t \geq 1/2 \geq \zeta$  (notice here that the equality  $t = \zeta = 1/2$  is authorized). In the general case, first assume  $0 < \zeta < 1/2$ . Then, using the formula

$$\forall 0 < \zeta < 1, \forall x > 0, \quad x^\zeta = \frac{\sin(\pi\zeta)}{\pi} \int_0^\infty \left(1 - \frac{s}{x+s}\right) \frac{ds}{s^{1-\zeta}},$$

we find

$$[|D^0|^\zeta, R_Q] = \frac{\sin(\pi\zeta)}{\pi} \int_0^\infty \frac{1}{|D^0|+s} [|D^0|, R_Q] \frac{1}{|D^0|+s} s^\zeta ds.$$

We then estimate

$$\begin{aligned} \| [|D^0|^\zeta, R_Q] |D^0|^{-t} \|_{\mathfrak{S}_2} &\leq \frac{\sin(\pi\zeta)}{\pi} \int_0^\infty \left\| \frac{|D^0|^{\frac{1}{2}}}{|D^0|+s} \right\|_{L^2 \rightarrow L^2} \times \\ &\quad \times \| |D^0|^{-\frac{1}{2}} [|D^0|, R_Q] |D^0|^{-\frac{1}{2}} \|_{\mathfrak{S}_2} \left\| \frac{|D^0|^{\frac{1}{2}-t}}{|D^0|+s} \right\|_{L^2 \rightarrow L^2} s^\zeta ds. \end{aligned} \quad (2.3.40)$$

Setting  $B = |D^0|^{-\frac{1}{2}} [|D^0|, R_Q] |D^0|^{-\frac{1}{2}}$ , one has

$$\begin{aligned} \|B\|_{\mathfrak{S}_2}^2 &= \iint_{\mathbb{R}^3 \times \mathbb{R}^3} |\widehat{R}_Q(p - q)|^2 \frac{(E(p) - E(q))^2}{E(p)E(q)} dp dq \\ &\leq C \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{E(p - q)^2}{E(p + q)} |\widehat{R}_Q(p - q)|^2 dp dq \\ &\leq C \|Q\|_{\mathcal{Q}}^2, \end{aligned}$$

where the last inequality was proved in [HLS05a, Lemma 8]. Now assuming  $t > \zeta > 0$  we have  $\tau := \frac{1}{2} - t \leq 1$ , hence using

$$\forall \tau \leq 1, \forall s \geq 0 \quad \sup_{x \geq 1} \frac{x^\tau}{x+s} \leq \frac{1}{(1+s)^{1-\max(\tau, 0)}}, \quad (2.3.41)$$

we deduce

$$\| [|D^0|^\zeta, R_Q] |D^0|^{-t} \|_{\mathfrak{S}_2} \leq C \int_0^\infty \frac{s^\zeta ds}{(1+s)^{\min(t+1, 3/2)}} \|Q\|_{\mathcal{Q}},$$

the right side being finite since  $t > \zeta$  and  $\zeta < 1/2$ . If  $1/2 \leq \zeta < 1$ , we write  $|D^0|^\zeta = |D^0|^{\zeta'} |D^0|^{1/2}$  with  $0 \leq \zeta' < 1/2$  to infer

$$|D^0|^\zeta = \frac{\sin(\pi\zeta')}{\pi} \int_0^\infty \frac{|D^0|^{3/2}}{|D^0| + s} \frac{ds}{s^{1-\zeta'}}.$$

Now for all  $s \geq 0$  we have

$$\left[ \frac{|D^0|^{3/2}}{|D^0| + s}, R_Q^\zeta \right] = \frac{1}{|D^0| + s} (s[|D^0|^{3/2}, R_Q^\zeta] + [|D^0|^{1/2}, |D^0| R_Q^\zeta |D^0|]) \frac{1}{|D^0| + s},$$

If  $B_1 = |D^0|^{-1/2} [|D^0|^{3/2}, R_Q^\zeta] |D^0|^{-1}$ , then

$$\begin{aligned} \|B_1\|_{\mathfrak{E}_2}^2 &= \iint_{|p| < |q|} \frac{|E(p)^{3/2} - E(q)^{3/2}|^2}{E(p)E(q)^2} |\widehat{R}_Q(p, q)|^2 dp dq \\ &\leq C \iint_{|p| < |q|} \frac{E(p-q)^2}{E(p+q)} |\widehat{R}_Q(p, q)|^2 dp dq \leq C \|Q\|_{\mathcal{Q}}^2. \end{aligned}$$

If  $B_2 = |D^0|^{-1} [|D^0|^{1/2}, |D^0| R_Q^\zeta |D^0|] |D^0|^{-3/2}$ , then

$$\begin{aligned} \|B_2\|_{\mathfrak{E}_2}^2 &= \iint_{|p| < |q|} \frac{|E(p)^{1/2} - E(q)^{1/2}|^2 E(p)^2 E(q)^2}{E(p)^2 E(q)^3} |\widehat{R}_Q(p, q)|^2 dp dq \\ &\leq C \iint_{|p| > |q|} \frac{E(p-q)^2}{E(p+q)} |\widehat{R}_Q(p, q)|^2 dp dq \leq C \|Q\|_{\mathcal{Q}}^2. \end{aligned}$$

We deduce that if  $B_3 = [|D^0|^\zeta, R_Q^\zeta] |D^0|^{-t}$ , we have, using (2.3.41) again

$$\begin{aligned} \|B_3\|_{\mathfrak{E}_2} &\leq C \|Q\|_{\mathcal{Q}} \int_0^\infty \left( s \left\| \frac{|D^0|^{1/2}}{|D^0| + s} \right\| \left\| \frac{|D^0|^{1-t}}{|D^0| + s} \right\| + \left\| \frac{|D^0|}{|D^0| + s} \right\| \left\| \frac{|D^0|^{3/2-t}}{|D^0| + s} \right\| \right) \frac{ds}{s^{1-\zeta'}} \\ &\leq C \|Q\|_{\mathcal{Q}} \int_0^\infty \left( \frac{s^{\zeta'}}{(1+s)^{\min(t+1/2, 3/2)}} + \frac{s^{\zeta'-1}}{(1+s)^{\min(t-1/2, 1)}} \right) ds, \end{aligned}$$

the right side being finite since  $t > \zeta' + 1/2 = \zeta$  and  $3/2 - \zeta' > 1$ .  $\square$

The next proposition is the analogue of [HLS05a, Proposition 10]. It is the main tool to prove the contractivity of the map  $\Phi$ .

**Proposition 2.1.** *Let  $\omega \in L^2(\mathbb{R}^3) \cap \mathcal{C}$ ,  $\mu \in (-1, 1)$ ,  $\alpha \geq 0$ ,  $\Lambda > 1$ ,  $(Q, \rho') \in \mathcal{X}$  be such that the following conditions are satisfied:*

- (1)  $\mu \notin \sigma(D_{\text{ref}}(\omega))$ ;
- (2)  $\mu \notin \sigma(D_{\omega, \rho', Q})$ ;
- (3)  $8\alpha \|\omega\|_{\mathcal{C}} < 1 - |\mu|$ .

Then, we have the following estimates:

$$\begin{aligned} \|(\Phi_1^\omega(Q, \rho'), \Phi_2^\omega(Q, \rho'))\|_{\mathcal{X}} &\leq 2\sqrt{\pi} \|\rho_{\text{ref}}\|_{L^2 \cap \mathcal{C}} + \alpha\sqrt{\log \Lambda} \Xi \|(Q, \rho')\|_{\mathcal{X}} \\ &\quad + \sum_{n \geq 2} \left( \alpha \Xi \|(Q, \rho')\|_{\mathcal{X}} \right)^n, \\ \|((\Phi_1^\omega)'(Q, \rho'), (\Phi_2^\omega)'(Q, \rho'))\| &\leq \alpha\sqrt{\log \Lambda} \Xi + \alpha \sum_{n \geq 2} n \left( \alpha \Xi \|(Q, \rho')\|_{\mathcal{X}} \right)^{n-1}, \end{aligned} \quad (2.3.42)$$

with

$$\Xi := C(\mu)(1 + \alpha\sqrt{\log \Lambda})^{14} (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^{14}) \theta(\mu, \omega)^6, \quad (2.3.43)$$

where  $C(\mu) > 0$  is some constant only depending on  $\mu$ , and  $\theta(\mu, \omega)$  is defined in Lemma 2.4.

PROOF. We start by estimating  $\Phi_1^\omega = \sum_{n \geq 1} \alpha^n G_n^\omega$  in norm  $\|\cdot\|_{\mathcal{Q}}$ . The difficulty relies in the fact that the definition of the norm  $\|\cdot\|_{\mathcal{Q}}$  uses the Fourier representation of the kernel of the operator considered. In [HLS05a], it was not an issue since all the studied operators, for instance the resolvent  $(D_\Lambda^0 + i\eta)^{-1}$ , have an explicit kernel in Fourier space. This is not the case in our setting: the kernel in Fourier space of the resolvent  $(D_{\text{ref}}(\omega) - \mu + i\eta)^{-1}$  is not explicit. It is thus harder to estimate the  $\mathcal{Q}$ -norms of these operators. To circumvent this difficulty, we will expand the resolvent  $(D_{\text{ref}}(\omega) - \mu + i\eta)^{-1}$  in terms of the resolvent  $(D_\Lambda^0 - \mu + i\eta)^{-1}$  and of  $\omega$ , in each  $G_n^\omega$  separately. The terms only containing resolvents of the form  $(D_\Lambda^0 - \mu + i\eta)^{-1}$  can be estimated via the results of [HLS05a], while the terms still containing resolvents of the form  $(D_{\text{ref}}(\omega) - \mu + i\eta)^{-1}$  decay faster and can be estimated using inequalities of the form  $\|Q\|_{\mathcal{Q}} \lesssim \| |D^0|^{\frac{3}{2}} Q \|_{\mathfrak{S}_2}$ . Indeed, the norm  $\| |D^0|^{\frac{3}{2}} \cdot \|_{\mathfrak{S}_2}$  is a rough upper bound for the  $\mathcal{Q}$ -norm, but has the advantage of being computable without using the kernel in Fourier space of the operator. We thus expand the resolvent as

$$\forall \eta \in \mathbb{R}, \quad \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta} = A_0(\eta) + A_1(\eta),$$

with

$$\begin{aligned} A_0(\eta) &= \frac{1}{D_\Lambda^0 - \mu + i\eta} \sum_{k=0}^4 \left( Y(\omega, \alpha) \frac{1}{D_\Lambda^0 - \mu + i\eta} \right)^k, \\ A_1(\eta) &= \left( \frac{1}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) \right)^5 \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta}, \end{aligned} \quad (2.3.44)$$

$$Y(\omega, \alpha) := \Pi_\Lambda (V_\omega - \alpha R_{1,0}(\omega)) \Pi_\Lambda.$$

Let  $n \geq 1$  and write

$$\begin{aligned} G_n^\omega(Q, \rho') &= \frac{(-1)^{n+1}}{2\pi} \sum_{x \in \{0,1\}^{n+1}} \int_{\mathbb{R}} A_{x_0}(\eta) \prod_{j=1}^n (X A_{x_j}(\eta)) \, d\eta \\ &= \frac{(-1)^{n+1}}{2\pi} \sum_{x \in \{0,1\}^{n+1}} G_{n,x}, \end{aligned}$$

where we used the notation

$$X := V_{\rho'} - R_Q. \quad (2.3.45)$$

The term  $G_{n,(0,\dots,0)}$  was already estimated in [HLS05a, Proposition 10],

$$\|G_{n,(0,\dots,0)}\|_{\mathcal{Q}} \leq \kappa_n (1 + (\alpha\sqrt{\log \Lambda})^4)^{n+1} (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^4)^{n+1} \|(Q, \rho')\|^n, \quad (2.3.46)$$

where  $\kappa_n = C(\mu)^n$  for  $n \geq 2$  and  $\kappa_1 = C(\mu)\sqrt{\log \Lambda}$ , for some number  $C(\mu)$  only depending on  $\mu$ . Actually, the estimate (2.3.46) was obtained for  $\mu = 0$  in [HLS05a]. The way to obtain it for any  $\mu$  is to replace Equation (58) in [HLS05a] by

$$\frac{1}{\sqrt{(E(p) - \mu)^2 + \eta^2}} \frac{1}{\sqrt{(E(q) - \mu)^2 + \eta^2}} \leq \frac{2C'(\mu)}{E(p+q)E(\eta)}, \quad \forall p, q \in \mathbb{R}^3, \forall \eta \in \mathbb{R}, \quad (2.3.47)$$

for some  $C'(\mu)$ . It remains to treat  $G_{n,x}$  with  $x \neq (0, \dots, 0)$ . Using that for any  $p, q \in \mathbb{R}^3$  one has

$$E(p-q)^2 E(p+q) \leq E(p)^3 + 2E(p)^2 E(q) + 2E(p)E(q)^2 + E(q)^3,$$

we deduce that

$$\|Q\|_{\mathcal{Q}}^2 \leq \| |D^0|^{\frac{3}{2}} Q \|_{\mathfrak{S}_2}^2 + 2 \| |D^0| Q |D^0|^{\frac{1}{2}} \|_{\mathfrak{S}_2}^2 + 2 \| |D^0|^{\frac{1}{2}} Q |D^0| \|_{\mathfrak{S}_2}^2 + \| Q |D^0|^{\frac{3}{2}} \|_{\mathfrak{S}_2}^2, \quad (2.3.48)$$

for any  $Q \in \mathcal{Q}$  such that the right side is well defined. To estimate  $\|G_{n,x}\|_{\mathcal{Q}}$ , we will estimate the right side of (2.3.48) with  $Q = G_{n,x}$ .

**Lemma 2.7** (Estimates on  $A_0(\eta)$ ,  $A_1(\eta)$ ). *Let  $\eta \in \mathbb{R}$ . We have the following estimates.*

$$\begin{cases} \|A_0(\eta)\| + \| |D^0| A_0(\eta) \| \leq C(\mu) (1 + (\alpha\sqrt{\log \Lambda})^4) (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^4), \\ \|A_1(\eta)\| + \| |D^0| A_1(\eta) \| \leq C(\mu) (1 + (\alpha\sqrt{\log \Lambda})^5) \|\omega\|_{L^2 \cap \mathcal{C}}^5 \theta(\mu, \omega). \end{cases} \quad (2.3.49)$$

For all  $0 \leq \sigma < \frac{1}{2}$ , we have

$$\left\| |D^0|^{\frac{3}{2} + \sigma} A_1(\eta) \right\|_{\mathfrak{S}_2} \leq \frac{C(\mu) (1 + \alpha\sqrt{\log \Lambda})^5 \|\omega\|_{L^2 \cap \mathcal{C}}^5 \theta(\mu, \omega)}{E(\eta)^{3/2}}, \quad (2.3.50)$$

and for any  $B \in \mathfrak{S}_2$  such that  $|D^0|^{\frac{3}{2} + \sigma} B \in \mathfrak{S}_2$ , we have

$$\left\| |D^0|^{\frac{3}{2} + \sigma} A_0(\eta) X B \right\|_{\mathfrak{S}_2} \leq C(\mu) (1 + \alpha\sqrt{\log \Lambda})^4 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^4) \|(Q, \rho')\|_{\mathcal{X}} \left\| |D^0|^{\frac{3}{2} + \sigma} B \right\|_{\mathfrak{S}_2}. \quad (2.3.51)$$

We also have

$$\left\| |A_1(\eta)| |D^0|^{\frac{3}{2}} \right\|_{\mathfrak{S}_2} \leq \frac{C(\mu)(1 + \alpha\sqrt{\log \Lambda})^7 \|\omega\|_{L^2 \cap \mathcal{C}}^7 \theta(\mu, \omega)^3}{E(\eta)^{3/2}}, \quad (2.3.52)$$

and for any  $B \in \mathfrak{S}_2$  such that  $B|D^0|^{\frac{3}{2}} \in \mathfrak{S}_2$ , we have

$$\left\| |BXA_0(\eta)| |D^0|^{\frac{3}{2}} \right\|_{\mathfrak{S}_2} \leq C(\mu)(1 + \alpha\sqrt{\log \Lambda})^4 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^4) \|(Q, \rho')\|_X \left\| B|D^0|^{\frac{3}{2}} \right\|_{\mathfrak{S}_2}. \quad (2.3.53)$$

Finally, we have

$$\left\| |D^0| |A_1(\eta)| \right\|_{\mathfrak{S}_{6/5}} \leq \frac{C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 \|\omega\|_{L^2 \cap \mathcal{C}}^5 \theta(\mu, \omega)}{E(\eta)^{5/2}}, \quad (2.3.54)$$

and for any  $B$  such that  $|D^0|B \in \mathfrak{S}_{6/5}$ , we have

$$\left\| |D^0| |A_0(\eta)XB| \right\|_{\mathfrak{S}_{6/5}} \leq C(\mu)(1 + \alpha\sqrt{\log \Lambda})^4 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^4) \|(Q, \rho')\|_X \left\| |D^0|B \right\|_{\mathfrak{S}_{6/5}}, \quad (2.3.55)$$

**PROOF OF LEMMA 2.7.** To prove (2.3.49), just use  $\| |D^0| (D_\Lambda^0 - \mu + i\eta)^{-1} \|_{L^2 \rightarrow L^2} \leq C(\mu)$ ,  $\| Y(\omega, \alpha) |D^0|^{-1/2} \|_{L^2 \rightarrow L^2} \leq C(1 + \alpha\sqrt{\log \Lambda}) \|\omega\|_{L^2 \cap \mathcal{C}}$  and  $\| |D^0| (D_{\text{ref}}(\omega) - \mu + i\eta)^{-1} \|_{L^2 \rightarrow L^2} \leq \theta(\mu, \omega)$ . To prove (2.3.50), we write  $|D^0|^{\frac{3}{2} + \sigma} A_1(\eta) = B_1(\eta) + B_2(\eta)$  with

$$\begin{aligned} B_1(\eta) &:= \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) \frac{|D^0|^{\frac{1}{2} + \sigma}}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) \times \\ &\quad \times \left( \frac{1}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) \right)^3 \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta}, \\ B_2(\eta) &:= \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} \left[ |D^0|^{\frac{1}{2} + \sigma}, Y(\omega, \alpha) \right] \left( \frac{1}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) \right)^4 \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta}. \end{aligned}$$

Now  $B_1(\eta) = B_{11}(\eta) + B_{12}(\eta)$  with

$$\begin{aligned} B_{11}(\eta) &= \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) |D^0|^{-\frac{1}{2}} \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) |D^0|^{-\frac{1}{2}} \frac{|D^0|^{\frac{1}{2} + \sigma}}{D_\Lambda^0 - \mu + i\eta} \times \\ &\quad \times \left( Y(\omega, \alpha) \frac{1}{D_\Lambda^0 - \mu + i\eta} \right)^3 (D_\Lambda^0 - \mu + i\eta) \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta}, \end{aligned}$$

$$\begin{aligned} B_{12}(\eta) &= \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) |D^0|^{-\frac{1}{2}} \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} \left[ |D^0|^\sigma, Y(\omega, \alpha) \right] |D^0|^{-t} \times \\ &\quad \times \frac{|D^0|^t}{D_\Lambda^0 - \mu + i\eta} \left( Y(\omega, \alpha) \frac{1}{D_\Lambda^0 - \mu + i\eta} \right)^3 (D_\Lambda^0 - \mu + i\eta) \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta}, \end{aligned}$$

for some  $\frac{1}{2} + \sigma < t < 1$ . Using  $|D^0| |D^0 - \mu + i\eta|^{-1} \leq C(\mu)$ ,  $\|Y(\omega, \alpha) |D^0|^{-\frac{1}{2}}\|_{L^2 \rightarrow L^2} \leq C(\mu)(1 + \alpha\sqrt{\log \Lambda})\|\omega\|_{L^2 \cap \mathcal{C}}$  by (2.3.21) and (2.3.26),  $\|(D_\Lambda^0 - \mu + i\eta)(D_{\text{ref}}(\omega) - \mu + i\eta)^{-1}\|_{L^2 \rightarrow L^2} \leq C(\mu)\theta(\mu, \omega)$ ,  $\frac{1}{2} + \sigma < 1$ , and the two inequalities

$$\left\| V_\omega \frac{1}{D^0 - \mu + i\eta} \right\|_{\mathfrak{S}_6} \leq \frac{C(\mu)\|\omega\|_{\mathcal{C}}}{E(\eta)^{1/2}}, \quad (2.3.56)$$

obtained by (2.3.22),

$$\left\| R_{1,0}(\omega) \frac{1}{D^0 - \mu + i\eta} \right\|_{\mathfrak{S}_2} \leq \frac{C(\mu)\sqrt{\log \Lambda}\|\omega\|_{L^2 \cap \mathcal{C}}}{E(\eta)^{1/2}}, \quad (2.3.57)$$

obtained by (2.3.23) and (2.3.28), we get

$$\left\| Y(\omega, \alpha) \frac{1}{D^0 - \mu + i\eta} \right\|_{\mathfrak{S}_6} \leq \frac{C(\mu)(1 + \alpha\sqrt{\log \Lambda})\|\omega\|_{L^2 \cap \mathcal{C}}}{E(\eta)^{1/2}}, \quad (2.3.58)$$

hence

$$\|B_{11}(\eta)\|_{\mathfrak{S}_2} \leq \frac{C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 \|\omega\|_{L^2 \cap \mathcal{C}}^5 \theta(\mu, \omega)}{E(\eta)^{3/2}}.$$

The term  $B_{12}(\eta)$  is treated the same way, except that we use the commutator estimates of Lemma 2.6, to get

$$\| [|D^0|^\sigma, Y(\omega, \alpha)] |D^0|^{-t} \|_{\mathfrak{S}_2} \leq C(\mu)(1 + \alpha\sqrt{\log \Lambda})\|\omega\|_{L^2 \cap \mathcal{C}}.$$

We thus find

$$\|B_{12}(\eta)\|_{\mathfrak{S}_2} \leq \frac{C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 \|\omega\|_{L^2 \cap \mathcal{C}}^5 \theta(\mu, \omega)}{E(\eta)^{3/2}}.$$

We next set  $B_2(\eta) = B_{21}(\eta) + B_{22}(\eta)$  with

$$\begin{aligned} B_{21}(\eta) &= \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} \left[ |D^0|^{\frac{1}{2} + \sigma}, Y(\omega, \alpha) \right] |D^0|^{-s} \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) \frac{|D^0|^{s-1}}{D_\Lambda^0 - \mu + i\eta} \times \\ &\quad \times \left( Y(\omega, \alpha) \frac{1}{D_\Lambda^0 - \mu + i\eta} \right)^3 (D_\Lambda^0 - \mu + i\eta) \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta} \end{aligned}$$

and

$$\begin{aligned} B_{22}(\eta) &= \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} \left[ |D^0|^{\frac{1}{2} + \sigma}, Y(\omega, \alpha) \right] |D^0|^{-s} \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} [|D^0|^{s-1}, Y(\omega, \alpha)] \times \\ &\quad \times |D^0|^{-u} \frac{|D^0|^u}{D_\Lambda^0 - \mu + i\eta} \left( Y(\omega, \alpha) \frac{1}{D_\Lambda^0 - \mu + i\eta} \right)^3 (D_\Lambda^0 - \mu + i\eta) \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta}, \end{aligned}$$

for some  $1 + \sigma < s < \frac{3}{2}$  and  $s - \frac{1}{2} < u < 1$ . Such a couple  $(s, u)$  exists since  $\sigma < \frac{1}{2}$ . Using the estimates as before, we obtain

$$\|B_2(\eta)\|_{\mathfrak{S}_2} \leq \frac{C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 \|\omega\|_{L^2 \cap \mathcal{C}}^5 \theta(\mu, \omega)}{E(\eta)^{3/2}}.$$

We thus have proved (2.3.50). Let us now prove (2.3.51). Hence, let  $B \in \mathfrak{S}_2$  such that  $|D^0|^{\frac{3}{2}+\sigma}B \in \mathfrak{S}_2$ . Recall that  $A_0(\eta)$  is the sum of five terms. We will treat the first two independently. We thus write

$$|D^0|^{\frac{3}{2}+\sigma}A_0(\eta)XB = H_1 + H_2 + H_3.$$

The first term to estimate is

$$H_1 := \frac{|D^0|^{\frac{3}{2}+\sigma}}{D_\Lambda^0 - \mu + i\eta}XB = \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta}X|D^0|^{\frac{1}{2}+\sigma}B + \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} \left[ |D^0|^{\frac{1}{2}+\sigma}, X \right] B.$$

By Lemma 2.6, we know that

$$\begin{aligned} \|X|D^0|^{-1}\|_{L^2 \rightarrow L^2} &\leq C\|(Q, \rho')\|_{\mathcal{X}}, \\ \left\| \left[ |D^0|^{\frac{1}{2}+\sigma}, X \right] |D^0|^{-\frac{3}{2}-\sigma} \right\|_{L^2 \rightarrow L^2} &\leq C\|(Q, \rho')\|_{\mathcal{X}}. \end{aligned} \quad (2.3.59)$$

Hence,

$$\|H_1\|_{\mathfrak{S}_2} \leq C(\mu)\|(Q, \rho')\|_{\mathcal{X}} \left\| |D^0|^{\frac{3}{2}+\sigma}B \right\|_{\mathfrak{S}_2}.$$

Next, we treat

$$\begin{aligned} H_2 &:= \frac{|D^0|^{\frac{3}{2}+\sigma}}{D_\Lambda^0 - \mu + i\eta}Y(\omega, \alpha)\frac{1}{D_\Lambda^0 - \mu + i\eta}XB \\ &= \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta}Y(\omega, \alpha)\frac{|D^0|^{\frac{1}{2}+\sigma}}{D_\Lambda^0 - \mu + i\eta}XB \\ &\quad + \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} \left[ |D^0|^{\frac{1}{2}+\sigma}, Y(\omega, \alpha) \right] \frac{1}{D_\Lambda^0 - \mu + i\eta}XB \\ &= H_{21} + H_{22}. \end{aligned}$$

The first term is easily estimated by

$$\begin{aligned} \|H_{21}\|_{\mathfrak{S}_2} &\leq C(\mu)\|Y(\omega, \alpha)|D^0|^{-1}\|_{L^2 \rightarrow L^2}\|H_1\|_{\mathfrak{S}_2} \\ &\leq C(\mu)(1 + \alpha\sqrt{\log \Lambda})\|\omega\|_{L^2 \cap \mathcal{C}}\|(Q, \rho')\|_{\mathcal{X}} \left\| |D^0|^{\frac{3}{2}+\sigma}B \right\|_{\mathfrak{S}_2}, \end{aligned}$$

while we notice that the second term can be estimated by

$$\begin{aligned} \|H_{22}\|_{\mathfrak{S}_2} &\leq C(\mu) \left\| \left[ |D^0|^{\frac{1}{2}+\sigma}, Y(\omega, \alpha) \right] |D^0|^{-\frac{3}{2}+\sigma} \right\|_{L^2 \rightarrow L^2} \|H_1\|_{\mathfrak{S}_2} \\ &\leq C(\mu)(1 + \alpha\sqrt{\log \Lambda})\|\omega\|_{L^2 \cap \mathcal{C}}\|(Q, \rho')\|_{\mathcal{X}} \left\| |D^0|^{\frac{3}{2}+\sigma}B \right\|_{\mathfrak{S}_2}. \end{aligned}$$

We conclude that

$$\|H_2\|_{\mathfrak{S}_2} \leq C(\mu)(1 + \alpha\sqrt{\log \Lambda})\|\omega\|_{L^2 \cap \mathcal{C}}\|(Q, \rho')\|_{\mathcal{X}} \left\| |D^0|^{\frac{3}{2}+\sigma}B \right\|_{\mathfrak{S}_2}.$$

The last term to control is

$$H_3 := \frac{|D^0|^{\frac{3}{2}+\sigma}}{D_\Lambda^0 - \mu + i\eta} \left( Y(\omega, \alpha)\frac{1}{D_\Lambda^0 - \mu + i\eta} \right)^2 \sum_{k=0}^2 \left( Y(\omega, \alpha)\frac{1}{D_\Lambda^0 - \mu + i\eta} \right)^k XB.$$

We use that  $\|H_3\|_{\mathfrak{S}_2} \leq \|H_{31}\|_{L^2 \rightarrow L^2} \|H_{32}\|_{\mathfrak{S}_2}$ , with

$$H_{31} := \frac{|D^0|^{\frac{3}{2}+\sigma}}{D_\Lambda^0 - \mu + i\eta} \left( Y(\omega, \alpha) \frac{1}{D_\Lambda^0 - \mu + i\eta} \right)^2,$$

$$H_{32} := \sum_{k=0}^2 \left( Y(\omega, \alpha) \frac{1}{D_\Lambda^0 - \mu + i\eta} \right)^k XB.$$

On the one hand we have

$$\|H_{32}\|_{\mathfrak{S}_2} \leq C(\mu)(1 + \alpha\sqrt{\log \Lambda})^2 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^2) \|(Q, \rho')\|_{\mathcal{X}} \left\| |D^0|^{\frac{3}{2}+\sigma} B \right\|_{\mathfrak{S}_2},$$

while on the other hand

$$\begin{aligned} H_{31} &= \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) \frac{|D^0|^{\frac{1}{2}+\sigma}}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) \frac{1}{D_\Lambda^0 - \mu + i\eta} \\ &+ \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} \left[ |D^0|^{\frac{1}{2}+\sigma}, Y(\omega, \alpha) \right] |D^0|^{-t} \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) |D^0|^{-\frac{1}{2}} \frac{|D^0|^{t-\frac{1}{2}}}{D_\Lambda^0 - \mu + i\eta} \\ &\quad + \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} \left[ |D^0|^{\frac{1}{2}+\sigma}, Y(\omega, \alpha) \right] |D^0|^{-t} \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} \times \\ &\quad \quad \quad \times \left[ |D^0|^{t-1}, Y(\omega, \alpha) \right] |D^0|^{-s} \frac{|D^0|^s}{D_\Lambda^0 - \mu + i\eta}, \end{aligned}$$

for some  $1 + \sigma < t < \frac{3}{2}$  and  $t - \frac{1}{2} < s < 1$ , so that writing

$$\begin{aligned} &\frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) \frac{|D^0|^{\frac{1}{2}+\sigma}}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) \frac{1}{D_\Lambda^0 - \mu + i\eta} \\ &= \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) |D^0|^{-\frac{1}{2}} \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) |D^0|^{-\frac{1}{2}} \frac{|D^0|^{\frac{1}{2}+\sigma}}{D_\Lambda^0 - \mu + i\eta} \\ &+ \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) |D^0|^{-\frac{1}{2}} \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} \left[ |D^0|^\sigma, Y(\omega, \alpha) \right] |D^0|^{-u} \frac{|D^0|^u}{D_\Lambda^0 - \mu + i\eta}, \end{aligned}$$

for some  $\frac{1}{2} + \sigma < u < 1$ , one has

$$\|H_{31}\|_{L^2 \rightarrow L^2} \leq C(\mu)(1 + \alpha\sqrt{\log \Lambda})^2 \|\omega\|_{L^2 \cap \mathcal{C}}^2.$$

Hence,

$$\|H_3\|_{\mathfrak{S}_2} \leq C(\mu)(1 + \alpha\sqrt{\log \Lambda})^4 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^4) \|(Q, \rho')\|_{\mathcal{X}} \left\| |D^0|^{\frac{3}{2}+\sigma} B \right\|_{\mathfrak{S}_2},$$

which finishes the proof of (2.3.51). Let us thus pass to (2.3.52). The proof is the same as (2.3.50), with a additional commutator between  $|D^0|^{\frac{1}{2}}$  and  $(D_{\text{ref}}(\omega) - \mu + i\eta)^{-1}$ .



Indeed, we have

$$\begin{aligned} A_1(\eta)|D^0|^{\frac{3}{2}} &= \left( \frac{1}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) \right)^5 |D^0|^{\frac{1}{2}} \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta} |D^0| \\ &\quad + \left( \frac{1}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) \right)^5 \left[ \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta}, |D^0|^{\frac{1}{2}} \right] |D^0| = T_1 + T_2. \end{aligned}$$

We have by the same method as before

$$\|T_1\|_{\mathfrak{S}_2} \leq \frac{C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 \|\omega\|_{L^2 \cap \mathcal{C}}^5 \theta(\mu, \omega)}{E(\eta)^{3/2}}.$$

Now notice that for any  $\zeta \in \mathbb{R}$ ,

$$\left[ \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta}, |D^0|^\zeta \right] = \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta} [ |D^0|^\zeta, Y(\omega, \alpha) ] \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta},$$

so that  $T_2 = T_{21} + T_{22}$  with

$$\begin{aligned} T_{21} &= \left( \frac{1}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) \right)^5 |D^0|^{t-1} \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta} |D^0| \times \\ &\quad \times |D^0|^{-t} \left[ |D^0|^{\frac{1}{2}}, Y(\omega, \alpha) \right] \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta} |D^0|, \end{aligned}$$

$$\begin{aligned} T_{22} &= \left( \frac{1}{D_\Lambda^0 - \mu + i\eta} Y(\omega, \alpha) \right)^5 \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta} [ |D^0|^{t-1}, Y(\omega, \alpha) ] \times \\ &\quad \times \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta} |D^0| |D^0|^{-t} \left[ |D^0|^{\frac{1}{2}}, Y(\omega, \alpha) \right] \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta} |D^0|, \end{aligned}$$

for some  $1 < t < \frac{3}{2}$ . Hence by the methods introduced before, we deduce that

$$\|T_2\|_{\mathfrak{S}_2} \leq \frac{C(\mu)(1 + \alpha\sqrt{\log \Lambda})^7 \|\omega\|_{L^2 \cap \mathcal{C}}^7 \theta(\mu, \omega)^3}{E(\eta)^{3/2}},$$

leading to (2.3.52). The proof of (2.3.53) is the same as the proof of (2.3.51). Next, we prove (2.3.54). It is because of this term that we have to expand  $(D_{\text{ref}}(\omega) - \mu + i\eta)^{-1}$  to the 5th order, as we can see from the following estimate:

$$\begin{aligned} \||D^0|A_1(\eta)\|_{\mathfrak{S}_{6/5}} &\leq \left\| \frac{|D^0|}{D_\Lambda^0 - \mu + i\eta} \right\|_{L^2 \rightarrow L^2} \left\| Y(\omega, \alpha) \frac{1}{D_\Lambda^0 - \mu + i\eta} \right\|_{\mathfrak{S}_6}^5 \times \\ &\quad \times \left\| (D_\Lambda^0 - \mu + i\eta) \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta} \right\|_{L^2 \rightarrow L^2} \\ &\leq \frac{C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 \|\omega\|_{L^2 \cap \mathcal{C}}^5 \theta(\mu, \omega)}{E(\eta)^{5/2}}, \end{aligned}$$

which is exactly (2.3.54). Finally, to prove (2.3.55), we simply notice that

$$\begin{aligned} \left\| |D^0| A_0(\eta) X B \right\|_{\mathfrak{S}_{6/5}} &\leq \left\| |D^0| A_0(\eta) \right\| \left\| |X| |D^0|^{-1} \right\| \left\| |D^0| B \right\|_{\mathfrak{S}_{6/5}} \\ &\leq C(\mu) (1 + \alpha \sqrt{\log \Lambda})^4 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^4) \|(Q, \rho')\|_{\mathcal{X}} \left\| |D^0| B \right\|_{\mathfrak{S}_{6/5}}, \end{aligned}$$

by inequalities (2.3.49) and (2.3.59). This ends the proof of Lemma 2.7.  $\square$

Let us now estimate  $\left\| |D^0|^{\frac{3}{2}} G_{n,x} \right\|_{\mathfrak{S}_2}$ . First, assume that  $x_0 = 1$ . We have

$$\left\| |D^0|^{\frac{3}{2}} G_{n,x} \right\|_{\mathfrak{S}_2} \leq \int_{\mathbb{R}} \left\| |D^0|^{\frac{3}{2}} A_1(\eta) \right\|_{\mathfrak{S}_2} \prod_{j=1}^n \|X A_{x_j}(\eta)\|_{L^2 \rightarrow L^2} d\eta. \quad (2.3.60)$$

We deduce from (2.3.49) that for all  $1 \leq j \leq n$ ,

$$\begin{aligned} \|X A_{x_j}(\eta)\|_{L^2 \rightarrow L^2} &\leq \|V_{\rho'} A_{x_j}(\eta)\|_{L^2 \rightarrow L^2} + \|R_Q A_{x_j}(\eta)\|_{L^2 \rightarrow L^2} \\ &\leq \|V_{\rho'}\|_{L^2 \rightarrow L^2} \|A_{x_j}(\eta)\|_{L^2 \rightarrow L^2} + \|R_Q |D^0|^{-1}\|_{\mathfrak{S}_2} \left\| |D^0| A_{x_j}(\eta) \right\|_{L^2 \rightarrow L^2} \\ &\leq C(\mu) (1 + \alpha \sqrt{\log \Lambda})^5 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^5) \theta(\mu, \omega) \|(Q, \rho')\|_{\mathcal{X}}. \end{aligned}$$

Hence, for all  $\eta \in \mathbb{R}$ ,

$$\prod_{j=1}^n \|X A_{x_j}(\eta)\|_{L^2 \rightarrow L^2} \leq \left( C(\mu) (1 + \alpha \sqrt{\log \Lambda})^5 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^5) \theta(\mu, \omega) \right)^n \|(Q, \rho')\|_{\mathcal{X}}^n. \quad (2.3.61)$$

Now by (2.3.50) applied with  $\sigma = 0$ , we have

$$\int_{\mathbb{R}} \left\| |D^0|^{\frac{3}{2}} A_1(\eta) \right\|_{\mathfrak{S}_2} d\eta \leq C(\mu) (1 + \alpha \sqrt{\log \Lambda})^5 \|\omega\|_{L^2 \cap \mathcal{C}}^5 \theta(\mu, \omega).$$

Hence, for all  $n \geq 1$  and for all  $x \in \{0, 1\}^{n+1}$  such that  $x_0 = 1$ , we have

$$\left\| |D^0|^{\frac{3}{2}} G_{n,x} \right\|_{\mathfrak{S}_2} \leq \left( C(\mu) (1 + \alpha \sqrt{\log \Lambda})^5 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^5) \theta(\mu, \omega) \right)^{n+1} \|(Q, \rho')\|_{\mathcal{X}}^n. \quad (2.3.62)$$

It remains to treat the case  $x \neq (0, \dots, 0)$  with  $x_0 \neq 1$ . Let  $n \geq 1$ ,  $x \in \{0, 1\}^{n+1}$  such that  $x \neq (0, \dots, 0)$  and  $x_0 = 0$ . Then there exists a smallest index  $j_0 \geq 1$  such that  $x_{j_0} = 1$ . We can thus write

$$G_{n,x} = \int_{\mathbb{R}} (A_0(\eta) X)^{j_0} A_1(\eta) \prod_{j=j_0+1}^n (X A_{x_j}(\eta)) d\eta.$$

Using (2.3.51)  $j_0$  times with  $\sigma = 0$  we get

$$\begin{aligned} \left\| |D^0|^{\frac{3}{2}} G_{n,x} \right\|_{\mathfrak{S}_2} &\leq \left( C(\mu) (1 + \alpha \sqrt{\log \Lambda})^4 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^4) \right)^{j_0} \|(Q, \rho')\|_{\mathcal{X}}^{j_0} \times \\ &\quad \times \int_{\mathbb{R}} \left\| |D^0|^{\frac{3}{2}} A_1(\eta) \prod_{j=j_0+1}^n (X A_{x_j}(\eta)) \right\|_{\mathfrak{S}_2} d\eta. \end{aligned}$$

We estimate the right side using the estimate (2.3.62) in the case  $x_0 = 1$ , and we obtain

$$\begin{aligned} \left\| |D^0|^{\frac{3}{2}} G_{n,x} \right\|_{\mathfrak{S}_2} &\leq \left( C(\mu)(1 + \alpha\sqrt{\log \Lambda})^4 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^4) \right)^{j_0} \|(Q, \rho')\|_{\mathcal{X}}^{j_0} \times \\ &\quad \times \left( C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^5) \theta(\mu, \omega) \right)^{n+1-j_0} \|(Q, \rho')\|_{\mathcal{X}}^{n-j_0}. \end{aligned}$$

Summing up, we have for all  $n \geq 1$  and all  $x$ ,

$$\left\| |D^0|^{\frac{3}{2}} G_{n,x} \right\|_{\mathfrak{S}_2} \leq \left( C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^5) \theta(\mu, \omega) \right)^{n+1} \|(Q, \rho')\|_{\mathcal{X}}^n. \quad (2.3.63)$$

We now estimate  $\left\| |D^0| G_{n,x} |D^0|^{\frac{1}{2}} \right\|_{\mathfrak{S}_2}$  and  $\left\| |D^0|^{\frac{1}{2}} G_{n,x} |D^0| \right\|_{\mathfrak{S}_2}$  for all  $n \geq 1$  and  $x \neq (0, \dots, 0)$ . We treat both cases at the same time by estimating

$$\left\| |D^0|^s G_{n,x} |D^0|^t \right\|_{\mathfrak{S}_2},$$

for any  $s, t \in [0, 1]$ . For  $x \neq (0, \dots, 0)$ , there exists a smallest index  $0 \leq j_0 \leq n$  such that  $x_{j_0} = 1$ . We distinguish three cases:  $j_0 = 0$ ,  $j_0 = n$ , and  $1 \leq j_0 \leq n-1$ . First, if  $j_0 = 0$ , then

$$\begin{aligned} \left\| |D^0|^s G_{n,x} |D^0|^t \right\|_{\mathfrak{S}_2} &\leq \int_{\mathbb{R}} \left\| |D^0|^s A_1(\eta) X \right\|_{\mathfrak{S}_2} \prod_{j=1}^{n-1} \left\| A_{x_j}(\eta) X \right\|_{L^2 \rightarrow L^2} \left\| A_{x_n}(\eta) |D^0|^t \right\|_{L^2 \rightarrow L^2} d\eta. \end{aligned}$$

Writing

$$\begin{aligned} |D^0|^s A_1(\eta) X &= \frac{|D^0|^s}{D_{\Lambda}^0 - \mu + i\eta} Y(\omega, \alpha) |D^0|^{-\frac{1}{2}} \frac{|D^0|}{D_{\Lambda}^0 - \mu + i\eta} |D^0|^{-\frac{1}{2}} Y(\omega, \alpha) \times \\ &\quad \times \left( \frac{1}{D_{\Lambda}^0 - \mu + i\eta} Y(\omega, \alpha) \right)^3 \frac{1}{D_{\text{ref}}(\omega) - \mu + i\eta} |D^0| |D^0|^{-1} X, \quad (2.3.64) \end{aligned}$$

We obtain from the estimates above that

$$\left\| |D^0|^s A_1(\eta) X \right\|_{\mathfrak{S}_2} \leq \frac{C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 \|\omega\|_{L^2 \cap \mathcal{C}}^5 \theta(\mu, \omega)}{E(\eta)^{3/2}} \|(Q, \rho')\|_{\mathcal{X}},$$

and one concludes that

$$\left\| |D^0|^s G_{n,x} |D^0|^t \right\|_{\mathfrak{S}_2} \leq \left( C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^5) \theta(\mu, \omega) \right)^{n+1} \|(Q, \rho')\|_{\mathcal{X}}^n.$$

Then, if  $j_0 = n$ , one has

$$\left\| |D^0|^s G_{n,x} |D^0|^t \right\|_{\mathfrak{S}_2} \leq \int_{\mathbb{R}} \left\| |D^0|^s A_0(\eta) \right\|_{L^2 \rightarrow L^2} \left\| X A_0(\eta) \right\|_{L^2 \rightarrow L^2}^{n-1} \left\| X A_1(\eta) |D^0|^t \right\|_{\mathfrak{S}_2} d\eta.$$

As before we have

$$\|XA_1(\eta)|D^0|^t\|_{\mathfrak{S}_2} \leq \frac{C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 \|\omega\|_{L^2 \cap \mathcal{C}}^5 \theta(\mu, \omega)}{E(\eta)^{3/2}} \|(Q, \rho')\|_{\mathcal{X}},$$

so that

$$\| |D^0|^s G_{n,x} |D^0|^t \|_{\mathfrak{S}_2} \leq \left( C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^5) \theta(\mu, \omega) \right)^{n+1} \|(Q, \rho')\|_{\mathcal{X}}^n.$$

Finally, if  $1 \leq j_0 \leq n-1$ , then we write

$$\begin{aligned} \| |D^0|^s G_{n,x} |D^0|^t \|_{\mathfrak{S}_2} &\leq \int_{\mathbb{R}} \| |D^0|^s A_0(\eta) \|_{L^2 \rightarrow L^2} \|XA_0(\eta)\|_{L^2 \rightarrow L^2}^{j_0-1} \|XA_1(\eta)X\|_{\mathfrak{S}_2} \times \\ &\quad \times \prod_{j=j_0+1}^{n-1} \|A_{x_j}(\eta)X\|_{L^2 \rightarrow L^2} \|A_{x_n}(\eta)|D^0|^t\|_{L^2 \rightarrow L^2} d\eta, \end{aligned}$$

and using that

$$\|XA_1(\eta)X\|_{\mathfrak{S}_2} \leq \frac{C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 \|\omega\|_{L^2 \cap \mathcal{C}}^5 \theta(\mu, \omega)}{E(\eta)^{3/2}} \|(Q, \rho')\|_{\mathcal{X}}^2,$$

obtained by the same decomposition as in (2.3.64), we find

$$\| |D^0|^s G_{n,x} |D^0|^t \|_{\mathfrak{S}_2} \leq \left( C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^5) \theta(\mu, \omega) \right)^{n+1} \|(Q, \rho')\|_{\mathcal{X}}^n.$$

Hence, for all  $s, t \in [0, 1]$ , for all  $x \neq (0, \dots, 0)$  and all  $n \geq 1$  we have

$$\| |D^0|^s G_{n,x} |D^0|^t \|_{\mathfrak{S}_2} \leq \left( C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^5) \theta(\mu, \omega) \right)^{n+1} \|(Q, \rho')\|_{\mathcal{X}}^n.$$

It remains to estimate  $\| |G_{n,x}|D^0|^{\frac{3}{2}} \|_{\mathfrak{S}_2}$ . The strategy is the same as the one for the estimation of  $\| |D^0|^{\frac{3}{2}} G_{n,x} \|_{\mathfrak{S}_2}$ , except that we first consider the case  $x_n = 1$ . For any  $x \in \{0, 1\}^{n+1}$  such that  $x_n = 1$ , we have

$$\| |G_{n,x}|D^0|^{\frac{3}{2}} \|_{\mathfrak{S}_2} \leq \int_{\mathbb{R}} \left( \prod_{j=0}^{n-1} \|A_{x_j}(\eta)X\|_{L^2 \rightarrow L^2} \right) \| |A_1(\eta)|D^0|^{\frac{3}{2}} \|_{\mathfrak{S}_2} d\eta. \quad (2.3.65)$$

In a similar fashion as the inequality (2.3.61), we have

$$\prod_{j=0}^{n-1} \|A_{x_j}(\eta)X\|_{L^2 \rightarrow L^2} \leq \left( C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^5) \theta(\mu, \omega)^2 \right)^n \|(Q, \rho')\|_{\mathcal{X}}^n,$$

with now the factor  $\theta(\mu, \omega)^2$  instead of  $\theta(\mu, \omega)$  as in (2.3.61) because of the term  $\|(D_{\text{ref}}(\omega) - \mu + i\eta)^{-1}|D^0\|_{L^2 \rightarrow L^2}$ . Using additionally (2.3.52), we get

$$\| |G_{n,x}|D^0|^{\frac{3}{2}} \|_{\mathfrak{S}_2} \leq \left( C(\mu)(1 + \alpha\sqrt{\log \Lambda})^7 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^7) \theta(\mu, \omega)^3 \right)^{n+1} \|(Q, \rho')\|_{\mathcal{X}}^n,$$

for all  $x \neq (0, \dots, 0)$  such that  $x_n = 1$ . We treat the general case  $x \neq (0, \dots, 0)$  in the same fashion as the estimate of  $\| |D^0|^{\frac{3}{2}} G_{n,x} \|_{\mathfrak{S}_2}$ , using (2.3.53), and we get the same

estimate as the  $x_n = 1$  case. Finally, by (2.3.48) we conclude that for any  $n \geq 1$  and any  $x \neq (0, \dots, 0)$ ,

$$\|G_{n,x}\|_{\mathcal{Q}} \leq \left( C(\mu)(1 + \alpha\sqrt{\log \Lambda})^7 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^7) \theta(\mu, \omega)^3 \right)^{n+1} \|(Q, \rho')\|_{\mathcal{X}}^n. \quad (2.3.66)$$

Combining this with (2.3.46), we can write

$$\forall n \geq 2, \quad \|G_n^\omega(Q, \rho')\|_{\mathcal{Q}} \leq \left( C(\mu)(1 + \alpha\sqrt{\log \Lambda})^7 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^7) \theta(\mu, \omega)^3 \right)^{n+1} \|(Q, \rho')\|_{\mathcal{X}}^n, \quad (2.3.67)$$

while

$$\|G_1^\omega(Q, \rho')\|_{\mathcal{Q}} \leq \left( C(\mu)(1 + \alpha\sqrt{\log \Lambda})^7 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^7) \theta(\mu, \omega)^3 \right)^2 \sqrt{\log \Lambda} \|(Q, \rho')\|_{\mathcal{X}}. \quad (2.3.68)$$

We sum it up as

$$\|\Phi_1^\omega(Q, \rho')\| \leq \alpha\sqrt{\log \Lambda} \Xi \|(Q, \rho')\|_{\mathcal{X}} + \sum_{n \geq 2} \left( \alpha \Xi \|(Q, \rho')\|_{\mathcal{X}} \right)^n, \quad (2.3.69)$$

with

$$\Xi := C(\mu) \left( (1 + \alpha\sqrt{\log \Lambda})^7 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^7) \theta(\mu, \omega)^3 \right)^2.$$

This is of course a rough estimate, but it has a simple form. We now turn to the estimates for the density terms, that is  $\Phi_2^\omega$ . We start by estimating  $J_n^\omega = \rho_{G_n^\omega}$  for  $n \geq 2$ . As for  $G_n^\omega$ , we write

$$J_n^\omega = \frac{(-1)^{n+1}}{2\pi} \sum_{x \in \{0,1\}^{n+1}} J_{n,x},$$

with  $J_{n,x} := \rho_{G_{n,x}}$ . It was proved in [HLS05a, Proposition 10] that

$$\forall n \geq 2, \quad \|J_{n,(0,\dots,0)}\|_{L^2 \cap \mathcal{C}} \leq \left( C(\mu)(1 + \alpha\sqrt{\log \Lambda})^4 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^4) \right)^{n+1} \|(Q, \rho')\|_{\mathcal{X}}^n, \quad (2.3.70)$$

To estimate  $\|J_{n,x}\|_{L^2 \cap \mathcal{C}}$  for  $x \neq (0, \dots, 0)$ , we use the following lemma.

**Lemma 2.8.** *For any operator  $Q$  on  $\mathfrak{H}_\Lambda$  such that  $|D^0|^{\frac{3}{2}+\sigma}Q \in \mathfrak{S}_2$  for some  $\sigma > 0$  and such that  $|D^0|Q \in \mathfrak{S}_{6/5}$ , then  $\rho_Q \in L^2 \cap \mathcal{C}$  and there exists a universal constant  $C$  such that*

$$\|\rho_Q\|_{L^2 \cap \mathcal{C}} \leq C \left( \| |D^0|^{\frac{3}{2}+\sigma}Q \|_{\mathfrak{S}_2} + \| |D^0|Q \|_{\mathfrak{S}_{6/5}} \right). \quad (2.3.71)$$

**PROOF.** We prove it by duality. Let  $V \in \mathfrak{H}_\Lambda$  be a smooth function. Then, for any  $Q$  as in the statement of the lemma, we have  $QV \in \mathfrak{S}_1$  with two different estimates on  $\|QV\|_{\mathfrak{S}_1}$ . First, we have

$$\|QV\|_{\mathfrak{S}_1} \leq \| |D^0|^{\frac{3}{2}+\sigma}Q \|_{\mathfrak{S}_2} \| |D^0|^{-\frac{3}{2}-\sigma}V \|_{\mathfrak{S}_2} \leq C \| |D^0|^{\frac{3}{2}+\sigma}Q \|_{\mathfrak{S}_2} \|V\|_{L^2},$$

by the Kato-Seiler-Simon inequality. This proves that  $\rho_Q \in L^2$  and that

$$\|\rho_Q\|_{L^2} \leq C \| |D^0|^{\frac{3}{2}+\sigma} Q \|_{\mathfrak{S}_2}.$$

Secondly, we have

$$\begin{aligned} \|QV\|_{\mathfrak{S}_1} &\leq \| |D^0| Q \|_{\mathfrak{S}_{6/5}} \| |D^0|^{-1} V \|_{\mathfrak{S}_6} \\ &\leq C \| |D^0| Q \|_{\mathfrak{S}_{6/5}} \|V\|_{L^6} \leq C \| |D^0| Q \|_{\mathfrak{S}_{6/5}} \|\nabla V\|_{L^2}, \end{aligned}$$

again by the Kato-Seiler-Simon inequality and the Sobolev inequality. This proves that  $\rho_Q \in \mathcal{C}$  and that

$$\|\rho_Q\|_{\mathcal{C}} \leq C \| |D^0| Q \|_{\mathfrak{S}_{6/5}}.$$

□

Let us first treat the case  $x_0 = 1$ . Let  $n \geq 1$  and  $x \neq (0, \dots, 0)$  with  $x_0 = 1$ . From inequalities (2.3.60), (2.3.50) with any  $0 < \sigma < \frac{1}{2}$ , and (2.3.54), we find

$$\begin{aligned} \left\| |D^0|^{\frac{3}{2}+\sigma} G_{n,x} \right\|_{\mathfrak{S}_2} &\leq \left( C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^5) \theta(\mu, \omega) \right)^{n+1} \|(Q, \rho')\|_{\mathcal{X}}^n, \\ \left\| |D^0| G_{n,x} \right\|_{\mathfrak{S}_{6/5}} &\leq \left( C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^5) \theta(\mu, \omega) \right)^{n+1} \|(Q, \rho')\|_{\mathcal{X}}^n. \end{aligned}$$

To deduce the general  $x$  case from the  $x_0 = 1$  case we use as usual (2.3.51) and (2.3.55). We thus have for all  $n \geq 2$ ,

$$\|J_n^\omega(Q, \rho')\|_{L^2 \cap \mathcal{C}} \leq \left( C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^5) \theta(\mu, \omega) \right)^{n+1} \|(Q, \rho')\|_{\mathcal{X}}^n.$$

It remains to estimate  $\|J_1^\omega(Q, \rho')\|_{L^2 \cap \mathcal{C}}$ . We have proved that for  $x \neq (0, 0)$ ,

$$\|J_{1,x}(Q, \rho')\|_{L^2 \cap \mathcal{C}} \leq C(\mu) \left( (1 + \alpha\sqrt{\log \Lambda})^5 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^5) \theta(\mu, \omega) \right)^2 \|(Q, \rho')\|_{\mathcal{X}}.$$

Let us write

$$A_0(\eta) = \frac{1}{D_\Lambda^0 - \mu + i\eta} + A_{01}(\eta),$$

so that

$$\begin{aligned} J_1^\omega(Q, \rho') &= -\rho \left[ \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D_\Lambda^0 - \mu + i\eta} R_Q \frac{1}{D_\Lambda^0 - \mu + i\eta} d\eta \right] \\ &\quad + \rho \left[ \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D_\Lambda^0 - \mu + i\eta} X A_{01}(\eta) d\eta \right] + \rho \left[ \frac{1}{2\pi} \int_{\mathbb{R}} A_{01}(\eta) X \frac{1}{D_\Lambda^0 - \mu + i\eta} d\eta \right] \\ &\quad + \rho \left[ \frac{1}{2\pi} \int_{\mathbb{R}} A_{01}(\eta) X A_{01}(\eta) d\eta \right] + \frac{1}{2\pi} \sum_{\substack{x \in \{0,1\}^2 \\ x \neq (0,0)}} J_{1,x}. \end{aligned}$$

By [HLS05a, Proposition 10], we deduce that

$$\|J_1^\omega(Q, \rho')\|_{L^2 \cap \mathcal{C}} \leq \left( C(\mu)(1 + \alpha\sqrt{\log \Lambda})^5 (1 + \|\omega\|_{L^2 \cap \mathcal{C}}^5) \theta(\mu, \omega) \right)^2 \sqrt{\log \Lambda} \|(Q, \rho')\|_{\mathcal{X}}.$$

This ends the proof of Proposition 2.1.  $\square$

**Proposition 2.2.** *Let  $\nu \in L^2(\mathbb{R}^3) \cap \mathcal{C}$  and  $\mu \in (-1, 1)$ . Let  $\varepsilon \geq 0$  such that for all  $s \in [1 - \varepsilon, 1 + \varepsilon]$ ,  $\mu \notin \sigma_{\mathfrak{H}}(D^{s\nu})$ . Assume furthermore that*

$$\int_{\mathbb{R}^3} \log(2 + |k|)^2 |\widehat{\nu}(k)|^2 dk < +\infty. \quad (2.3.72)$$

*There exists  $\alpha_1 = \alpha_1(\mu, \nu, \varepsilon) > 0$ ,  $\Lambda_1 = \Lambda_1(\mu, \nu, \varepsilon) \geq 1$ , and  $L_1 = L_1(\mu, \nu, \varepsilon) > 0$  such that for any  $0 \leq \alpha \leq \alpha_1$ , for any  $\Lambda \geq \Lambda_1$  satisfying  $\alpha \log \Lambda \leq L_1$ , and for any  $\kappa \in [1 - \varepsilon, 1 + \varepsilon]$  we have*

$$\|(Q_{\text{ref}}, \rho_{\text{ref}})\|_{\mathcal{X}} \leq C(\mu, \nu, \varepsilon). \quad (2.3.73)$$

PROOF. We split  $Q_{\text{ref}}$  into two terms,  $Q_{\text{ref}} = I + II$ , where

$$\begin{aligned} I &= \chi_{(-\infty, \mu]}(D_{\Lambda}^{\kappa\nu_{\text{ren}}}) - P_{\Lambda, -}^0 + G_{1,0}(\kappa\nu_{\text{ren}}), \\ II &= \chi_{(-\infty, \mu]}(D_{\text{ref}}) - \chi_{(-\infty, \mu]}(D_{\Lambda}^{\kappa\nu_{\text{ren}}}). \end{aligned}$$

Since  $\nu \in L^2(\mathbb{R}^3) \cap \mathcal{C}$ , we have  $V_{\nu} \in L^{\infty}$  and the eigenvalues of  $D^{s\nu}$  are continuous with respect to  $s$ . Thus, there exists  $\varepsilon' = \varepsilon'(\mu, \nu, \varepsilon) > \varepsilon$  such that  $\mu \notin \sigma_{\mathfrak{H}}(D^{s\nu})$  for all  $s \in [1 - \varepsilon', 1 + \varepsilon']$ . Hence, there exists  $L_0 = L_0(\mu, \nu, \varepsilon) > 0$  such that for all  $\kappa \in [1 - \varepsilon, 1 + \varepsilon]$ , for all  $\alpha \geq 0$  and for all  $\Lambda \geq 1$  satisfying  $\alpha \log \Lambda \leq L_0$  we have

$$\frac{\kappa}{1 + \alpha B_{\Lambda}} \in [1 - \varepsilon', 1 + \varepsilon'].$$

Using Lemma 2.3, this implies  $d(\mu, \sigma_{\mathfrak{H}_{\Lambda}}(D^{\kappa\nu_{\text{ren}}})) \geq \xi_0(\mu, \nu, \varepsilon, L_0(\mu, \nu, \varepsilon)) > 0$ , for all  $\kappa \in [1 - \varepsilon, 1 + \varepsilon]$ , for all  $\Lambda \geq \Lambda_0(\mu, \nu, \varepsilon, L_0(\mu, \nu, \varepsilon))$ , and for all  $\alpha \geq 0$  such that  $\alpha \log \Lambda \leq L_0$ . In particular,  $\mu \notin \sigma_{\mathfrak{H}_{\Lambda}}(D^{\kappa\nu_{\text{ren}}})$  and we can write

$$I = \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D_{\Lambda}^0 - \mu + i\eta} \Pi_{\Lambda} V_{\kappa\nu_{\text{ren}}} \Pi_{\Lambda} \frac{1}{D_{\Lambda}^0 - \mu + i\eta} \Pi_{\Lambda} V_{\kappa\nu_{\text{ren}}} \Pi_{\Lambda} \frac{1}{D_{\Lambda}^{\kappa\nu_{\text{ren}}} - \mu + i\eta} d\eta.$$

As in the proof of Proposition 2.1, we estimate this term by decomposing it into  $I = I_1 + I_2$ , with

$$\begin{aligned} I_1 &= \frac{1}{2\pi} \int_{\mathbb{R}} \left( \frac{1}{D_{\Lambda}^0 - \mu + i\eta} \Pi_{\Lambda} V_{\kappa\nu_{\text{ren}}} \Pi_{\Lambda} \right)^2 \times \\ &\quad \times \sum_{j=0}^2 \frac{1}{D_{\Lambda}^0 - \mu + i\eta} \left( \Pi_{\Lambda} V_{\kappa\nu_{\text{ren}}} \Pi_{\Lambda} \frac{1}{D_{\Lambda}^0 - \mu + i\eta} \right)^j d\eta, \end{aligned}$$

$$I_2 = \frac{1}{2\pi} \int_{\mathbb{R}} \left( \frac{1}{D_{\Lambda}^0 - \mu + i\eta} \Pi_{\Lambda} V_{\kappa\nu_{\text{ren}}} \Pi_{\Lambda} \right)^5 \frac{1}{D_{\Lambda}^{\kappa\nu_{\text{ren}}} - \mu + i\eta} d\eta.$$

By [HLS05a, Lemma 13, Lemma 15], we have

$$\|I_1\|_{\mathcal{Q}} \leq C(1 + \|\kappa\nu_{\text{ren}}\|_{L^2 \cap \mathcal{C}}^4).$$

Notice that

$$I_2 = \frac{1}{2\pi} \int_{\mathbb{R}} A_1(\eta)|_{\alpha=0, \omega=\kappa\nu_{\text{ren}}} d\eta,$$

where  $A_1(\eta)$  was defined in (2.3.44). By (2.3.48), (2.3.50), (2.3.52), and the trivial bound

$$\begin{aligned} 2\| |D^0| A_1(\eta)|_{\alpha=0, \omega=\kappa\nu_{\text{ren}}} |D^0|^{1/2} \|_{\mathfrak{S}_2} + 2\| |D^0|^{1/2} A_1(\eta)|_{\alpha=0, \omega=\kappa\nu_{\text{ren}}} |D^0| \|_{\mathfrak{S}_2} \\ \leq \frac{C(\mu) \|\kappa\nu_{\text{ren}}\|_{L^2 \cap \mathcal{C}}^5 \theta(\mu, \kappa\nu_{\text{ren}})|_{\alpha=0}}{E(\eta)^{3/2}}, \end{aligned}$$

we infer that

$$\|I_2\|_{\mathcal{Q}} \leq C(\mu) \|\kappa\nu_{\text{ren}}\|_{L^2 \cap \mathcal{C}}^7 \theta(\mu, \nu)|_{\alpha=0}^3.$$

Hence, for any  $\kappa \in [1 - \varepsilon, 1 + \varepsilon]$ ,

$$\|I\|_{\mathcal{Q}} \leq C(\mu) (1 + (1 + \varepsilon)^7 \|\nu\|_{L^2 \cap \mathcal{C}}^7) \theta(\mu, \kappa\nu_{\text{ren}})|_{\alpha=0}^3.$$

Since  $d(\mu, \sigma_{\mathfrak{S}_\Lambda}(D^{\kappa\nu_{\text{ren}}})) \geq \xi_0$ , we have  $\theta(\mu, \kappa\nu_{\text{ren}})|_{\alpha=0} \leq C(\mu, \nu, \varepsilon)$ , uniformly in  $\alpha \geq 0$  (the dependence on  $\alpha$  only being in  $\nu_{\text{ren}}$ , which is not obvious from the notation),  $\Lambda \geq \Lambda_0$  satisfying  $\alpha \log \Lambda \leq L_0$ . This leads to

$$\|I\|_{\mathcal{Q}} \leq C(\mu, \nu, \varepsilon).$$

By (2.3.28), this implies in particular that for  $\Lambda \geq 3$  so that  $\log \Lambda \geq 1$ ,

$$\|\chi_{(-\infty, \mu]}(D_{\Lambda}^{\kappa\nu_{\text{ren}}}) - P_{\Lambda, -}^0\|_{\mathcal{Q}} \leq C(\mu, \nu, \varepsilon) \sqrt{\log \Lambda}. \quad (2.3.74)$$

Using again Lemma 2.3, we know that for all  $0 \leq \alpha \leq \alpha_0$  and for all  $\Lambda \geq \Lambda_0$  satisfying  $\alpha \log \Lambda \leq L_0$ , we have  $d(\mu, \sigma_{\mathfrak{S}_\Lambda}(D_{\text{ref}})) \geq \xi_0$  for all  $\kappa \in [1 - \varepsilon, 1 + \varepsilon]$ . Hence, we can expand  $II$  by Kato's formula, as for  $I$ . To estimate this expansion by the same method as in the proof of Proposition 2.1, we need the additional condition

$$8\alpha \|\kappa\nu_{\text{ren}}\|_{\mathcal{C}} < 1 - |\mu|,$$

which ensures the finiteness of  $\theta(\mu, \kappa\nu_{\text{ren}})$ , as seen by Lemma 2.4. This condition is satisfied for all  $0 \leq \alpha \leq \alpha_1$ , for all  $\Lambda \geq \Lambda_0$  satisfying  $\alpha \log \Lambda \leq L_0$ , and for all  $\kappa \in [1 - \varepsilon, 1 + \varepsilon]$ , for a certain  $0 \leq \alpha_1 = \alpha_1(\mu, \nu, \varepsilon) \leq \alpha_0(\mu, \nu, \varepsilon)$ . Using the same method used to estimate  $\|I\|_{\mathcal{Q}}$  and the proof of Proposition 2.1, we find

$$\|II\|_{\mathcal{Q}} \leq C(\mu) \alpha \sqrt{\log \Lambda} (1 + \alpha \sqrt{\log \Lambda})^7 (1 + (1 + \varepsilon)^7 \|\nu\|_{L^2 \cap \mathcal{C}}^7) \theta(\mu, \kappa\nu_{\text{ren}})^3. \quad (2.3.75)$$

We still have  $\theta(\mu, \kappa\nu_{\text{ren}}) \leq C(\mu, \nu, \varepsilon)$  for all  $\kappa \in [1 - \varepsilon, 1 + \varepsilon]$ , and we also have  $\alpha \sqrt{\log \Lambda} \leq \alpha \log \Lambda \leq L_0$  if  $\Lambda \geq 3$ . Hence,

$$\|II\|_{\mathcal{Q}} \leq C(\mu, \nu, \varepsilon)$$

for all  $0 \leq \alpha \leq \alpha_1$ , for all  $\Lambda \geq \max(3, \Lambda_0)$  with  $\alpha \log \Lambda \leq L_0$  and for all  $\kappa \in [1 - \varepsilon, 1 + \varepsilon]$ . The estimate on  $\rho_{\text{ref}}$  is more subtle. We decompose it as

$$\rho_{\text{ref}} = -\mathcal{U}_\Lambda \kappa\nu_{\text{ren}} + \rho[I] + \rho[II].$$



The operator  $\mathcal{U}_\Lambda$  is the multiplication operator in Fourier space by the function  $U_\Lambda(|k|) := B_\Lambda - B_\Lambda(k)$ . It has been defined and studied in [GLS11]. In fact, combining [GLS11, Equation (3.3)] and [GLS11, Equation (A.3)], one gets the estimate

$$\forall \Lambda \geq 1, \forall r \geq 0, \quad 0 \leq U_\Lambda(r) \leq \kappa_1 \left( 1 + \frac{1}{3\pi} \log(1 + r^2) \right), \quad (2.3.76)$$

with  $\kappa_1 = 258/\pi$ . We deduce

$$\begin{aligned} \|\mathcal{U}_\Lambda \kappa \nu_{\text{ren}}\|_{\mathcal{C}} &\leq C(1 + \varepsilon) \|\nu\|_{L^2 \cap \mathcal{C}}, \\ \|\mathcal{U}_\Lambda \kappa \nu_{\text{ren}}\|_{L^2}^2 &\leq C(1 + \varepsilon)^2 \int_{\mathbb{R}^3} \log(2 + |k|)^2 |\widehat{\nu}(k)|^2 dk. \end{aligned}$$

Next, using the same ideas as before, one gets

$$\|\rho[I]\|_{L^2 \cap \mathcal{C}} \leq C(\mu)(1 + (1 + \varepsilon)^7 \|\nu\|_{L^2 \cap \mathcal{C}}^7) \theta(\mu, \kappa \nu_{\text{ren}})|_{\alpha=0}^3 \leq C(\mu, \nu, \varepsilon),$$

$$\|\rho[II]\|_{L^2 \cap \mathcal{C}} \leq C(\mu) \alpha \log \Lambda (1 + \alpha \sqrt{\log \Lambda})^7 (1 + (1 + \varepsilon)^7 \|\nu\|_{L^2 \cap \mathcal{C}}^7) \theta(\mu, \kappa \nu_{\text{ren}})^3 \leq C(\mu, \nu, \varepsilon),$$

which ends the proof.  $\square$

3.1.4. *End of the proof of Theorem 1.* We apply the fixed point theorem of Banach-Picard to the function  $\Phi$  defined earlier by

$$\Phi(Q, \rho') = (\Phi_1^{\kappa \nu_{\text{ren}}}(Q + Q_{\text{ref}}, \rho'), \Phi_2^{\kappa \nu_{\text{ren}}}(Q + Q_{\text{ref}}, \rho')),$$

for any  $(Q, \rho') \in B_{\mathcal{X}}(R) \subset \mathcal{X}$ , where

$$B_{\mathcal{X}}(R) = \{(Q, \rho') \in \mathcal{X}, \quad \|(Q + Q_{\text{ref}}, \rho')\|_{\mathcal{X}} \leq R\},$$

for a  $R > 0$  to be determined later on. For  $\Phi(Q, \rho')$  to be correctly defined, we have to check the assumptions of Proposition 2.1. First, as in the proof of Proposition 2.2, using Lemma 2.3, there exists  $L_0 = L_0(\mu, \nu, \varepsilon) > 0$  such that for all  $0 \leq \alpha \leq \alpha_0(\mu, \nu, \varepsilon, L_0)$ , for all  $\Lambda \geq \Lambda_0(\mu, \nu, \varepsilon, L_0)$  with  $\alpha \log \Lambda \leq L_0$ , we have  $\mu \notin \sigma_{\mathfrak{H}_\Lambda}(D_{\text{ref}})$  for all  $\kappa \in [1 - \varepsilon, 1 + \varepsilon]$ . Next, we assume additionally that

$$8\alpha \|\kappa \nu_{\text{ren}}\|_{\mathcal{C}} < 1 - |\mu|, \quad \alpha b \|(Q + Q_{\text{ref}}, \rho')\|_{\mathcal{X}} < 1.$$

This condition is verified if we assume furthermore that  $0 \leq \alpha \leq \alpha_2$  for a certain  $\alpha_2 = \alpha_2(\mu, \nu, \varepsilon, R) > 0$ . Using Lemma 2.5, it implies that  $\mu \notin \sigma_{\mathfrak{H}_\Lambda}(D_Q)$ , where we recall that

$$D_Q = \chi_{(-\infty, \mu]}(D_{\text{ref}} + \alpha \Pi_\Lambda (V_{\rho'} - R_{Q+Q_{\text{ref}}}) \Pi_\Lambda).$$

We can now use Proposition 2.1 to infer that for all  $(Q, \rho') \in B_{\mathcal{X}}(R)$ ,

$$\|\Phi'(Q, \rho')\|_{\mathcal{X} \rightarrow \mathcal{X}} \leq \alpha \sqrt{\log \Lambda} \Xi + \alpha \sum_{n \geq 0} n(\alpha \Xi R)^{n-1}. \quad (2.3.77)$$

Assuming  $\Lambda \geq 3$ , we have  $\alpha \sqrt{\log \Lambda} \leq \alpha \log \Lambda \leq L_0$ . Moreover, as in the proof of Proposition 2.2, we can show, using Lemma 2.3, that there exists  $C = C(\mu, \nu, \varepsilon) > 0$  such that for all  $0 \leq \alpha \leq \alpha_0$ , for all  $\Lambda \geq \Lambda_0$  with  $\alpha \log \Lambda \leq L_0$ , and for all  $\kappa \in$

$[1 - \varepsilon, 1 + \varepsilon]$  we have  $\Xi \leq C$ . As a consequence, the right side of (2.3.77) is finite as soon as  $\alpha \leq (CR)^{-1}/2 = \alpha_3 = \alpha_3(\mu, \nu, \varepsilon, R)$ . It thus satisfies

$$\forall (Q, \rho') \in B_{\mathcal{X}}(R), \quad \|\Phi'(Q, \rho')\|_{\mathcal{X}} \leq C_1 \sqrt{\alpha},$$

for some  $C_1 = C_1(\mu, \nu, \varepsilon, R) > 0$ . Hence,  $\Phi$  is a contraction on  $B_{\mathcal{X}}(R)$  if  $\alpha \leq (4C_1)^{-2} = \alpha_4 = \alpha_4(\mu, \nu, \varepsilon, R) > 0$ . It remains to prove that  $B_{\mathcal{X}}(R)$  is invariant under  $\Phi$ . For any  $(Q, \rho') \in B_{\mathcal{X}}(R)$ , we have

$$\begin{aligned} \|\Phi(Q, \rho') + (Q_{\text{ref}}, 0)\|_{\mathcal{X}} &\leq \|\Phi(Q, \rho') - \Phi(-Q_{\text{ref}}, 0)\|_{\mathcal{X}} + \|\Phi(-Q_{\text{ref}}, 0) + (Q_{\text{ref}}, 0)\|_{\mathcal{X}} \\ &\leq C_1 \sqrt{\alpha} R + \|(Q_{\text{ref}}, \rho_{\text{ref}})\|_{\mathcal{X}}. \end{aligned}$$

By Proposition 2.2, if  $0 \leq \alpha \leq \alpha_1$ ,  $\Lambda \geq \Lambda_1$ , and  $\alpha \log \Lambda \leq L_1$ , we have

$$\|(Q_{\text{ref}}, \rho_{\text{ref}})\|_{\mathcal{X}} \leq C = C(\mu, \nu, \varepsilon).$$

Since we have chosen  $\alpha$  such that  $C_1 \sqrt{\alpha} \leq 1/2$ ,  $\Phi$  stabilizes  $B_{\mathcal{X}}(R)$  if

$$R = 2C.$$

To recap, if  $0 \leq \alpha \leq \min(\alpha_0, \alpha_1, \alpha_2, \alpha_3, \alpha_4)$ ,  $\Lambda \geq \max(3, \Lambda_0, \Lambda_1)$  with  $\alpha \log \Lambda \leq \min(L_0, L_1)$ , then for any  $\kappa \in [1 - \varepsilon, 1 + \varepsilon]$ ,  $\Phi$  is a contraction on  $B_{\mathcal{X}}(R)$ , with  $R = R(\mu, \nu, \varepsilon) > 0$ . Hence, there exists a unique  $Q \in \mathcal{X}$  satisfying

$$\begin{aligned} Q &= \chi_{(-\infty, \mu]} \left( D_{\text{ref}} + \alpha \Pi_{\Lambda} \left[ V_{\rho_Q + \rho_{\text{ref}}} - R_{Q+Q_{\text{ref}}} \right] \Pi_{\Lambda} \right) - P_{\text{ref}}, \\ \|(Q + Q_{\text{ref}}, \rho_Q + \rho_{\text{ref}})\|_{\mathcal{X}} &\leq R. \end{aligned}$$

Defining  $\tilde{Q} := Q + Q_{\text{ref}} - G_{1,0}(\kappa \nu_{\text{ren}})$ , we have  $\rho_Q + \rho_{\text{ref}} = \rho_{\tilde{Q}} - B_{\Lambda} \kappa \nu_{\text{ren}}$  and we have proved that there is a unique solution to

$$\begin{aligned} \tilde{Q} &= \chi_{(-\infty, \mu]} \left( D_{\Lambda}^{\kappa \nu} + \alpha \Pi_{\Lambda} \left[ V_{\rho_{\tilde{Q}}} - R_{\tilde{Q}} \right] \Pi_{\Lambda} \right) - P_{\Lambda, -}^0, \\ \|(\tilde{Q} + G_{1,0}(\kappa \nu_{\text{ren}}), \rho_{\tilde{Q}} - B_{\Lambda} \kappa \nu_{\text{ren}})\|_{\mathcal{X}} &\leq R, \end{aligned}$$

which ends the proof of Theorem 2.1.

**3.2. Proof of Theorem 2.2.** Let  $\nu \in L^2(\mathbb{R}^3) \cap \mathcal{C}$ ,  $\mu_{\pm} \in (-1, 1)$ , and  $\varepsilon > 0$  satisfying the assumptions given in Section 2.2. Since the eigenvalues of  $D^{s\nu}$  are continuous with respect to  $s$ , there exists  $\varepsilon' > \varepsilon$  such that  $(\mu_{\pm}, \nu, \varepsilon')$  also satisfy the assumptions given in Section 2.2. By the same method as in the proofs of Lemma 2.3 and Proposition 2.2, there exists  $\alpha' = \alpha'(\mu, \nu, \varepsilon) > 0$ ,  $\Lambda' = \Lambda'(\mu, \nu, \varepsilon) \geq 1$ ,  $L' = L'(\mu, \nu, \varepsilon) > 0$  and  $\xi' = \xi'(\mu, \nu, \varepsilon) > 0$  such that for all  $0 \leq \alpha \leq \alpha'$ , for all  $\Lambda \geq \Lambda'$  satisfying  $\alpha \log \Lambda \leq L'$ , and for all  $\kappa \in [1 - \varepsilon, 1 + \varepsilon]$ , we have  $\kappa/(1 + \alpha B_{\Lambda}) \in [1 - \varepsilon', 1 + \varepsilon']$  and  $d(\mu_{\pm}, \sigma_{\mathfrak{H}}(D_{\Lambda}^{\kappa \nu_{\text{ren}}})) \geq \xi'$ . The following result ensures that the operator  $D_{\Lambda}^{\kappa \nu_{\text{ren}}}$  also has an eigenvalue in  $(\mu_-, \mu_+)$ , for  $\Lambda$  large enough.

**Lemma 2.9.** *Let  $\nu \in L^2 \cap \mathcal{C}$ ,  $\mu_{\pm} \in (-1, 1)$ , and  $\varepsilon > 0$  satisfying the assumptions given in Section 2.2. Then, there exists  $\Lambda'' = \Lambda''(\mu_{\pm}, \nu, \varepsilon) \geq \Lambda'$  and  $C = C(\mu_{\pm}, \nu, \varepsilon) > 0$  such that for any  $\Lambda \geq \Lambda''$ , for any  $0 \leq \alpha \leq \alpha'$  with  $\alpha \log \Lambda \leq L'$ , and for any  $\kappa \in [1 - \varepsilon, 1 + \varepsilon]$ , the operator  $D_{\Lambda}^{\kappa\nu_{\text{ren}}}$  on  $\mathfrak{H}_{\Lambda}$  possesses a simple eigenvalue  $\lambda(\kappa\nu_{\text{ren}}, \Lambda)$  in  $(\mu_-, \mu_+)$ , which verifies the estimate*

$$|\lambda(\kappa\nu_{\text{ren}}) - \lambda(\kappa\nu_{\text{ren}}, \Lambda)| \leq CE(\Lambda)^{-1}. \quad (2.3.78)$$

Furthermore, if we denote by  $\varphi(\kappa\nu_{\text{ren}}, \Lambda)$  the unique normalized eigenvector of  $D_{\Lambda}^{\kappa\nu_{\text{ren}}}$  for the eigenvalue  $\lambda(\kappa\nu_{\text{ren}}, \Lambda)$  such that  $\langle \varphi(\kappa\nu_{\text{ren}}), \varphi(\kappa\nu_{\text{ren}}, \Lambda) \rangle_{L^2} > 0$ , then we have

$$\|\varphi(\kappa\nu_{\text{ren}}) - \varphi(\kappa\nu_{\text{ren}}, \Lambda)\|_{H^1} \leq CE(\Lambda)^{-1}, \quad (2.3.79)$$

**Remark 2.10.** Since  $\kappa/(1 + \alpha B_{\Lambda}) \in [1 - \varepsilon', 1 + \varepsilon']$ , and  $(\mu_{\pm}, \nu, \varepsilon')$  satisfy the assumptions of Section 2.2,  $\lambda(\kappa\nu_{\text{ren}}) = \lambda(\kappa/(1 + \alpha B_{\Lambda})\nu)$  is well-defined.

PROOF. In order to compare  $D^{\kappa\nu_{\text{ren}}}$  with  $D_{\Lambda}^{\kappa\nu_{\text{ren}}}$ , we identify  $D_{\Lambda}^{\kappa\nu_{\text{ren}}}$  with the operator on  $\mathfrak{H}$  which is  $D_{\Lambda}^{\kappa\nu_{\text{ren}}}$  on  $\mathfrak{H}_{\Lambda}$  and 0 on  $(1 - \Pi_{\Lambda})\mathfrak{H}_{\Lambda}$ . Let  $\mathcal{C}$  be a complex, compact contour around  $(\mu_-, \mu_+)$ , of index 1, crossing  $\mathbb{R}$  only through  $\mu_-$  and  $\mu_+$ . This way  $\mathcal{C}$  remains uniformly far from  $\sigma_{\mathfrak{H}}(D^{\kappa\nu_{\text{ren}}})$  and  $\sigma_{\mathfrak{H}}(D_{\Lambda}^{\kappa\nu_{\text{ren}}})$ , for  $\Lambda \geq \Lambda'$ . We then have

$$\begin{aligned} \chi_{(\mu_-, \mu_+)}(D^{\kappa\nu_{\text{ren}}}) - \Pi_{\Lambda} \chi_{(\mu_-, \mu_+)}(D_{\Lambda}^{\kappa\nu_{\text{ren}}}) \Pi_{\Lambda} = \\ - \frac{1}{2i\pi} \int_{\mathcal{C}} \Pi_{\Lambda} \left( \frac{1}{D^{\kappa\nu_{\text{ren}}} - z} - \frac{1}{D_{\Lambda}^{\kappa\nu_{\text{ren}}} - z} \right) \Pi_{\Lambda} dz \\ - \frac{1}{2i\pi} \int_{\mathcal{C}} \left( (1 - \Pi_{\Lambda}) \frac{1}{D^{\kappa\nu_{\text{ren}}} - z} \Pi_{\Lambda} + \Pi_{\Lambda} \frac{1}{D^{\kappa\nu_{\text{ren}}} - z} (1 - \Pi_{\Lambda}) \right. \\ \left. + (1 - \Pi_{\Lambda}) \frac{1}{D^{\kappa\nu_{\text{ren}}} - z} (1 - \Pi_{\Lambda}) \right) dz = I + II, \end{aligned}$$

where  $I$  is only the term in the second line. For the second term, we write

$$\begin{aligned} \|II\|_{L^2 \rightarrow L^2} &\leq 3 \|(1 - \Pi_{\Lambda})|D^0|^{-1}\|_{L^2 \rightarrow L^2} \sup_{z \in \mathcal{C}} \left\| \frac{|D^0|}{D^{\kappa\nu_{\text{ren}}} - z} \right\|_{L^2 \rightarrow L^2} \\ &\leq C(\mu_{\pm}, \nu, \varepsilon) E(\Lambda)^{-1}. \end{aligned}$$

The first term is computed by the resolvent formula

$$I = \frac{1}{2i\pi} \int_{\mathcal{C}} \Pi_{\Lambda} \frac{1}{D^{\kappa\nu_{\text{ren}}} - z} (1 - \Pi_{\Lambda}) V_{\kappa\nu_{\text{ren}}} \Pi_{\Lambda} \frac{1}{D_{\Lambda}^{\kappa\nu_{\text{ren}}} - z} dz,$$

so that we have the estimation

$$\begin{aligned} \|I\|_{L^2 \rightarrow L^2} &\leq \sup_{z \in \mathcal{C}} \left\| \frac{|D^0|}{D^{\kappa\nu_{\text{ren}}} - z} \right\|_{L^2 \rightarrow L^2} \| |D^0|^{-1} (1 - \Pi_{\Lambda}) \|_{L^2 \rightarrow L^2} \sup_{z \in \mathcal{C}} \left\| \frac{1}{D_{\Lambda}^{\kappa\nu_{\text{ren}}} - z} \right\|_{\mathfrak{H}_{\Lambda} \rightarrow \mathfrak{H}_{\Lambda}} \\ &\leq C(\mu_{\pm}, \nu, \varepsilon) E(\Lambda)^{-1}. \end{aligned}$$

As a consequence, for  $\Lambda$  large enough such that for instance

$$\|\chi_{(\mu_-, \mu_+)}(D^{\kappa\nu_{\text{ren}}}) - \Pi_\Lambda \chi_{(\mu_-, \mu_+)}(D_\Lambda^{\kappa\nu_{\text{ren}}}) \Pi_\Lambda\|_{L^2 \rightarrow L^2} < 1,$$

the operator  $D_\Lambda^{\kappa\nu_{\text{ren}}}$  on  $\mathfrak{H}_\Lambda$  has a simple eigenvalue  $\lambda(\kappa\nu_{\text{ren}}, \Lambda) \in (\mu_-, \mu_+)$ . To estimate the difference between these eigenvalues, notice that we have proved that for any  $z \in [\mu_\pm - \delta_0, \mu_\pm + \delta_0]$ , for some  $\delta_0 = \delta_0(\mu_\pm, \nu, \varepsilon) > 0$  small enough

$$\left\| \frac{1}{D^{\kappa\nu_{\text{ren}}} - z} - \Pi_\Lambda \frac{1}{D_\Lambda^{\kappa\nu_{\text{ren}}} - z} \Pi_\Lambda \right\|_{L^2 \rightarrow L^2} \leq C(\mu_\pm, \nu, \varepsilon) E(\Lambda)^{-1}.$$

It implies that, for  $\Lambda$  large enough,

$$\left| \frac{1}{\lambda(\kappa\nu_{\text{ren}}) - z} - \frac{1}{\lambda(\kappa\nu_{\text{ren}}, \Lambda) - z} \right| \leq C(\mu_\pm, \nu, \varepsilon) E(\Lambda)^{-1}$$

and hence

$$|\lambda(\kappa\nu_{\text{ren}}) - \lambda(\kappa\nu_{\text{ren}}, \Lambda)| \leq C(\mu_\pm, \nu, \varepsilon) E(\Lambda)^{-1}.$$

Let us now consider the unique eigenvector  $\varphi(\kappa\nu_{\text{ren}}, \Lambda)$  as in the statement of the lemma. It is well-defined for  $\Lambda$  large enough since the operator

$$A := |\varphi(\kappa\nu_{\text{ren}})\rangle\langle\varphi(\kappa\nu_{\text{ren}})| - |\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle\langle\varphi(\kappa\nu_{\text{ren}}, \Lambda)|.$$

verifies

$$\begin{aligned} 0 &\leq \langle A\varphi(\kappa\nu_{\text{ren}}), \varphi(\kappa\nu_{\text{ren}}) \rangle_{L^2} = 1 - \langle \varphi(\kappa\nu_{\text{ren}}, \Lambda), \varphi(\kappa\nu_{\text{ren}}) \rangle_{L^2}^2 \\ &\leq \|A\|_{L^2 \rightarrow L^2} \leq C(\mu_\pm, \nu, \varepsilon) E(\Lambda)^{-1} < 1. \end{aligned}$$

Hence,  $\langle \varphi(\kappa\nu_{\text{ren}}, \Lambda), \varphi(\kappa\nu_{\text{ren}}) \rangle_{L^2} \neq 0$  and

$$\begin{aligned} \|\varphi(\kappa\nu_{\text{ren}}) - \varphi(\kappa\nu_{\text{ren}}, \Lambda)\|_{L^2}^2 &= 2(1 - \langle \varphi(\kappa\nu_{\text{ren}}), \varphi(\kappa\nu_{\text{ren}}, \Lambda) \rangle) \\ &\leq 2(1 - \langle \varphi(\kappa\nu_{\text{ren}}), \varphi(\kappa\nu_{\text{ren}}, \Lambda) \rangle^2) \leq C(\mu_\pm, \nu, \varepsilon) E(\Lambda)^{-1}. \end{aligned}$$

To obtain a control in  $H^1$ , we use the eigenvalue equation, which implies

$$\begin{aligned} D^0(\varphi(\kappa\nu_{\text{ren}}) - \varphi(\kappa\nu_{\text{ren}}, \Lambda)) &= \lambda(\kappa\nu_{\text{ren}})(\varphi(\kappa\nu_{\text{ren}}) - \varphi(\kappa\nu_{\text{ren}}, \Lambda)) \\ &\quad + (\lambda(\kappa\nu_{\text{ren}}) - \lambda(\kappa\nu_{\text{ren}}, \Lambda))\varphi(\kappa\nu_{\text{ren}}, \Lambda) \\ &\quad + V_{\kappa\nu_{\text{ren}}}(\varphi(\kappa\nu_{\text{ren}}) - \varphi(\kappa\nu_{\text{ren}}, \Lambda)) + (1 - \Pi_\Lambda)V_{\kappa\nu_{\text{ren}}}\varphi(\kappa\nu_{\text{ren}}, \Lambda). \end{aligned}$$

Using the fact that  $V_{\kappa\nu_{\text{ren}}}\varphi(\kappa\nu_{\text{ren}}, \Lambda)$  is bounded in  $H^1$  uniformly in  $\Lambda$ , we get the estimate in  $H^1$ .  $\square$

We now begin the proof of Theorem 2.2. Since we work with  $\kappa$  fixed we will omit the dependence on  $\kappa$  in our notations, meaning that we write  $Q_\pm(\alpha)$  instead of  $Q_\pm(\kappa, \alpha)$ . We assume  $0 \leq \alpha \leq \min(\alpha_0, \alpha')$ ,  $\Lambda \geq \max(\Lambda_0, \Lambda'')$  and  $\alpha \log \Lambda \leq \min(L_0, L')$ , where  $(\alpha_0, \Lambda_0, L_0)$  is given by Theorem 2.1 and  $(\alpha', \Lambda'', L')$  were given just above. In the sequel, we will use notations such as  $\mathcal{O}_{\alpha \rightarrow 0}(\alpha)$  (resp.  $\mathcal{O}_{\alpha \rightarrow 0}^X(\alpha)$ ) to denote a function of  $\alpha$  which is bounded in absolute value (resp. in norm  $\|\cdot\|_X$ )

for some space  $X$ ) by  $C\alpha$ , where  $C$  only depends on  $\mu_{\pm}, \nu, \varepsilon$ . In our regime of parameters, notice that we have for instance  $\mathcal{O}_{\Lambda \rightarrow \infty}(\sqrt{\log \Lambda}) = \mathcal{O}_{\alpha \rightarrow 0}(\sqrt{\alpha})$ . Likewise, in the following we will use the notation  $C$  for a constant only depending on  $\mu_{\pm}, \nu$  and  $\varepsilon$ , whose value may change from line to line.

We use the a priori bound (2.2.13) given by Theorem 2.1

$$\|(Q_{\pm}(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}}), \rho_{\pm}(\alpha) - B_{\Lambda}\kappa\nu_{\text{ren}})\|_{\mathcal{X}} = \mathcal{O}_{\alpha \rightarrow 0}(1), \quad (2.3.80)$$

where we used the shortcut notation  $\rho_{\pm}(\alpha) := \rho_{Q_{\pm}(\alpha)}$ . The self consistent equation for  $Q_{\pm}(\alpha)$  is

$$\begin{aligned} Q_{\pm}(\alpha) &= \chi_{(-\infty, \mu_{\pm}]} \left( \Pi_{\Lambda} \left( D_{\Lambda}^{\kappa\nu} + \alpha \left( V_{\rho_{\pm}(\alpha)} - R_{Q_{\pm}(\alpha)} \right) \right) \Pi_{\Lambda} \right) - P_{\Lambda, -}^0 \\ &= \chi_{(-\infty, \mu_{\pm}]} \left( D_{\text{ref}} + \alpha \Pi_{\Lambda} \left( V_{\rho_{\pm}(\alpha) - B_{\Lambda}\kappa\nu_{\text{ren}}} - R_{Q_{\pm}(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}})} \right) \Pi_{\Lambda} \right) - P_{\Lambda, -}^0 \\ &= \sum_{n \geq 1} \alpha^n G_{n, \pm} \left( Q_{\pm}(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}}), \rho_{\pm}(\alpha) - B_{\Lambda}\kappa\nu_{\text{ren}} \right) + Q_{\text{ref}, \pm}, \end{aligned}$$

where we used a notation similar to Section 3.1 (with a slight modification of the definition of  $Q_{\text{ref}, \pm}$ ):

$$\begin{aligned} Q_{\text{ref}, \pm} &:= \chi_{(-\infty, \mu_{\pm}]} \left( D_{\text{ref}} \right) - P_{\Lambda, -}^0, \\ D_{\text{ref}} &:= \Pi_{\Lambda} \left( D^{\kappa\nu_{\text{ren}}} + \alpha R_{1,0}(\kappa\nu_{\text{ren}}) \right) \Pi_{\Lambda}, \\ G_{n, \pm}(Q, \rho) &:= \frac{(-1)^{n+1}}{2\pi} \int_{\mathbb{R}} \frac{1}{D_{\text{ref}} - \mu_{\pm} + i\eta} \left( (V_{\rho} - R_Q) \frac{1}{D_{\text{ref}} - \mu_{\pm} + i\eta} \right)^n d\eta. \end{aligned}$$

Notice that  $G_{1,0}(\kappa\nu_{\text{ren}})$  is independent of the index  $\pm$ . By (2.3.67), we have for all  $n \geq 2$ ,

$$\|G_{n, \pm}(Q, \rho)\|_{\mathcal{Q}} \leq C \|(Q, \rho)\|^n,$$

so that

$$\|G_{n, \pm}(Q_{\pm}(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}}), \rho_{\pm}(\alpha) - B_{\Lambda}\kappa\nu_{\text{ren}})\|_{\mathcal{Q}} \leq C^n.$$

On the other hand,

$$G_{1, \pm}(Q, \rho) = G_{1,0, \pm}(\rho) - G_{0,1, \pm}(Q),$$

with

$$\begin{aligned} G_{1,0, \pm}(\rho) &:= \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D_{\text{ref}} - \mu_{\pm} + i\eta} \Pi_{\Lambda} V_{\rho} \Pi_{\Lambda} \frac{1}{D_{\text{ref}} - \mu_{\pm} + i\eta} d\eta, \\ G_{0,1, \pm}(Q) &:= \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D_{\text{ref}} - \mu_{\pm} + i\eta} \Pi_{\Lambda} R_Q \Pi_{\Lambda} \frac{1}{D_{\text{ref}} - \mu_{\pm} + i\eta} d\eta. \end{aligned}$$

Combining (2.3.66) and [HLS05a, Lemma 11], we get

$$\|G_{0,1, \pm}(Q)\|_{\mathcal{Q}} \leq C \|Q\|_{\mathcal{Q}}, \quad \|G_{1,0, \pm}(\rho)\|_{\mathcal{Q}} \leq C \sqrt{\log \Lambda} \|\rho\|_{L^2 \cap \mathcal{C}}.$$

Hence, using (2.2.13) we get

$$\|Q_{\pm}(\alpha) - Q_{\text{ref}, \pm}\|_{\mathcal{Q}} = \mathcal{O}_{\alpha \rightarrow 0}(\sqrt{\alpha}).$$

Now using (2.3.75), we deduce

$$\|Q_{\pm}(\alpha) - Q_{\text{lin}, \pm}(\kappa\nu_{\text{ren}})\|_{\mathcal{Q}} = \mathcal{O}_{\alpha \rightarrow 0}(\sqrt{\alpha}), \quad (2.3.81)$$

where

$$Q_{\text{lin},\pm}(\omega) = \chi_{(-\infty, \mu_{\pm}]}(D_{\Lambda}^{\omega}) - P_{\Lambda,-}^0,$$

which in particular implies Corollary 2.1. The self-consistent equation satisfied by  $\rho_{\pm}(\alpha)$  is

$$\begin{aligned} \rho_{\pm}(\alpha) &= \rho_{\text{ref},\pm} - \alpha B_{\Lambda}(\rho_{\pm}(\alpha) - B_{\Lambda}\kappa\nu_{\text{ren}}) + \alpha \mathcal{U}_{\Lambda}(\rho_{\pm}(\alpha) - B_{\Lambda}\kappa\nu_{\text{ren}}) \\ &\quad + \alpha \rho_{1,0,\pm,r}(\rho_{\pm}(\alpha) - B_{\Lambda}\kappa\nu_{\text{ren}}) - \alpha \rho_{0,1,\pm}(Q_{\pm}(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}})) \\ &\quad + \sum_{n \geq 2} \alpha^n \rho_{n,\pm}(Q_{\pm}(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}}), \rho_{\pm}(\alpha) - B_{\Lambda}\kappa\nu_{\text{ren}}), \end{aligned}$$

where  $\rho_{n,\pm}(Q, \rho) := \rho_{G_{n,\pm}(Q, \rho)}$  for all  $n \geq 2$ ,  $\rho_{\text{ref},\pm} := \rho_{Q_{\text{ref},\pm}}$  and for any  $\rho, Q$ ,

$$\begin{aligned} \rho_{1,0,\pm,r}(\rho) &:= \rho \left[ \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D_{\text{ref}} - \mu_{\pm} + i\eta} \Pi_{\Lambda} V_{\rho} \Pi_{\Lambda} \frac{1}{D_{\text{ref}} - \mu_{\pm} + i\eta} d\eta \right. \\ &\quad \left. - \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D^0 + i\eta} \Pi_{\Lambda} V_{\rho} \Pi_{\Lambda} \frac{1}{D^0 + i\eta} d\eta \right], \\ \rho_{0,1,\pm}(Q) &= \rho \left[ \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D_{\text{ref}} - \mu_{\pm} + i\eta} \Pi_{\Lambda} R_Q \Pi_{\Lambda} \frac{1}{D_{\text{ref}} - \mu_{\pm} + i\eta} d\eta \right]. \end{aligned}$$

We rewrite the self-consistent equation for  $\rho_{\pm}(\alpha)$  as

$$\begin{aligned} \rho_{\pm}(\alpha) - B_{\Lambda}\kappa\nu_{\text{ren}} &= \frac{1}{1 + \alpha B_{\Lambda}}(\rho_{\text{ref},\pm} - B_{\Lambda}\kappa\nu_{\text{ren}}) + \frac{\alpha}{1 + \alpha B_{\Lambda}} \mathcal{U}_{\Lambda}(\rho_{\pm}(\alpha) - B_{\Lambda}\kappa\nu_{\text{ren}}) \\ &\quad + \frac{\alpha}{1 + \alpha B_{\Lambda}} \rho_{1,0,\pm,r}(\rho_{\pm}(\alpha) - B_{\Lambda}\kappa\nu_{\text{ren}}) - \frac{\alpha}{1 + \alpha B_{\Lambda}} \rho_{0,1,\pm}(Q_{\pm}(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}})) \\ &\quad + \frac{1}{1 + \alpha B_{\Lambda}} \sum_{n \geq 2} \alpha^n \rho_{n,\pm}(Q_{\pm}(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}}), \rho_{\pm}(\alpha) - B_{\Lambda}\kappa\nu_{\text{ren}}). \end{aligned} \quad (2.3.82)$$

We now have the necessary estimates to compute the limit of  $F(\kappa, \alpha)$  as  $\alpha \rightarrow 0$ .

3.2.1. *Kinetic energy terms.* By (2.3.81), we have

$$Q_{+}(\alpha) = Q_{-}(\alpha) + |\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle\langle\varphi(\kappa\nu_{\text{ren}}, \Lambda)| + \mathcal{O}_{\alpha \rightarrow 0}^{\mathcal{Q}}(\sqrt{\alpha}). \quad (2.3.83)$$

For any projector  $P$  such that  $Q = P - P^0 \in \mathcal{K}_{\Lambda}$  we have

$$\text{Tr}_0(D^0 Q) = \||D^0|^{\frac{1}{2}} Q\|_{\mathfrak{S}_2}^2 \leq \|Q\|_{\mathcal{Q}}^2. \quad (2.3.84)$$

The subtlety of this estimate is that it only controls the kinetic energy by the  $\mathcal{Q}$ -norm only for  $Q$ 's that are of the form  $P - P^0$ . Indeed, it would be wrong to deduce from (2.3.83) that

$$\text{Tr}_0(D^0 Q_{+}(\alpha)) - \text{Tr}_0(D^0 Q_{-}(\alpha)) = \langle\varphi(\kappa\nu_{\text{ren}}, \Lambda), D^0 \varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle + \mathcal{O}_{\alpha \rightarrow 0}(\sqrt{\alpha})$$

since the operator  $Q_+(\alpha) - Q_-(\alpha) - |\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle\langle\varphi(\kappa\nu_{\text{ren}}, \Lambda)|$  is not of the form  $P - P^0$  for some projector  $P$ . Instead, one should see  $\text{Tr}_0(D^0 Q_\pm(\alpha))$  as a quadratic term by the first equality in (2.3.84). Writing  $Q_\pm(\alpha) = Q_{\text{lin},\pm}(\kappa\nu_{\text{ren}}) + Q_{\pm,r}(\alpha)$ , we thus have

$$\begin{aligned} \text{Tr}(|D^0|Q_\pm(\alpha)^2) &= \text{Tr}(|D^0|Q_{\text{lin},\pm}(\kappa\nu_{\text{ren}})^2) + \text{Tr}(|D^0|Q_{\pm,r}(\alpha)^2) \\ &\quad + \text{Tr}(|D^0|\{Q_{\text{lin},\pm}(\kappa\nu_{\text{ren}}), Q_{\pm,r}(\alpha)\}), \end{aligned} \quad (2.3.85)$$

where  $\{A, B\} := AB + BA$ . The first term has a good behaviour since  $Q_{\text{lin},\pm}(\kappa\nu_{\text{ren}})$  is of the form  $P - P^0$ , hence the first term is linear in  $Q_{\text{lin},\pm}(\kappa\nu_{\text{ren}})$  and we have

$$\begin{aligned} \text{Tr}(|D^0|Q_{\text{lin},+}(\kappa\nu_{\text{ren}})^2) - \text{Tr}(|D^0|Q_{\text{lin},-}(\kappa\nu_{\text{ren}})^2) \\ = \text{Tr}_0(D^0(Q_{\text{lin},+}(\kappa\nu_{\text{ren}}) - Q_{\text{lin},-}(\kappa\nu_{\text{ren}}))) \\ = \langle\varphi(\kappa\nu_{\text{ren}}, \Lambda), D^0\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle. \end{aligned} \quad (2.3.86)$$

The second term in (2.3.85) is controlled using that  $\|Q_{\pm,r}(\alpha)\|_{\mathcal{Q}} = \mathcal{O}_{\alpha \rightarrow 0}(\sqrt{\alpha})$ , hence  $\text{Tr}(|D^0|Q_{\pm,r}(\alpha)^2) \leq \|Q_{\pm,r}(\alpha)\|_{\mathcal{Q}}^2 = \mathcal{O}_{\alpha \rightarrow 0}(\alpha)$ . Finally, the term with the Poisson bracket in (2.3.85) cannot be shown to go to zero as  $\alpha \rightarrow 0$ . Indeed, it is just a  $\mathcal{O}_{\alpha \rightarrow 0}(1)$  since  $\|Q_{\text{lin},\pm}(\kappa\nu_{\text{ren}})\|_{\mathcal{Q}} = \mathcal{O}_{\Lambda \rightarrow \infty}(\sqrt{\log \Lambda})$  by (2.3.74) and  $\|Q_{\pm,r}(\alpha)\|_{\mathcal{Q}} = \mathcal{O}_{\alpha \rightarrow 0}(\sqrt{\alpha})$ . We will compute explicitly the non-vanishing term in this expression. We have

$$\begin{aligned} \text{Tr}_0(D^0 Q_+(\alpha)) - \text{Tr}_0(D^0 Q_-(\alpha)) &= \langle\varphi(\kappa\nu_{\text{ren}}, \Lambda), D^0\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle \\ &\quad + \text{Tr}(|D^0|\{Q_{\text{lin},+}(\kappa\nu_{\text{ren}}), (Q_{+,r}(\alpha) - Q_{-,r}(\alpha))\}) \\ &\quad + \langle\varphi(\kappa\nu_{\text{ren}}, \Lambda), \{|D^0|, Q_{-,r}(\alpha)\}\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle + \mathcal{O}_{\alpha \rightarrow 0}(\alpha). \end{aligned} \quad (2.3.87)$$

The computations are lengthy and done in Appendix A. We obtain:

$$\begin{aligned} \text{Tr}_0(D^0 Q_+(\alpha)) - \text{Tr}_0(D^0 Q_-(\alpha)) &= \langle\varphi(\kappa\nu_{\text{ren}}, \Lambda), D^0\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle \\ &\quad - \frac{\alpha B_\Lambda}{1 + \alpha B_\Lambda} \langle\varphi(\kappa\nu_{\text{ren}}, \Lambda), V_{\kappa\nu_{\text{ren}}}\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle + \mathcal{O}_{\alpha \rightarrow 0}(\alpha). \end{aligned} \quad (2.3.88)$$

In particular, notice that

$$\lim_{\alpha \rightarrow 0} \text{Tr}_0(D^0 Q_+(\alpha)) - \text{Tr}_0(D^0 Q_-(\alpha)) \neq \langle\varphi(\kappa\nu_{\text{ren}}), D^0\varphi(\kappa\nu_{\text{ren}})\rangle,$$

meaning that the difference of kinetic energy of the BDF vacuums does *not* converge to the difference of kinetic energy of the non-interacting vacuum. This shows the subtlety of the limit  $\alpha \rightarrow 0$ . Fortunately, the extra term in (2.3.88) will be compensated by another one coming from the direct term.

**3.2.2. Potential energy term.** The second term to compute in  $F$  is the only ‘‘true’’ linear term: that is  $-D(\kappa\nu, \cdot)$ . By (2.A.93), we have

$$\rho_+(\alpha) - \rho_-(\alpha) = \frac{1}{1 + \alpha B_\Lambda} |\varphi(\kappa\nu_{\text{ren}}, \Lambda)|^2 + \mathcal{O}_{\alpha \rightarrow 0}^{L^2 \cap \mathcal{C}}(\alpha), \quad (2.3.89)$$

which implies that

$$\begin{aligned} -D(\kappa\nu, \rho_+(\alpha) - \rho_-(\alpha)) &= -\frac{1}{1 + \alpha B_\Lambda} D(\kappa\nu, |\varphi(\kappa\nu_{\text{ren}}, \Lambda)|^2) + \mathcal{O}_{\alpha \rightarrow 0}(\alpha) \\ &= -\langle \varphi(\kappa\nu_{\text{ren}}, \Lambda), V_{\kappa\nu_{\text{ren}}} \varphi(\kappa\nu_{\text{ren}}, \Lambda) \rangle + \mathcal{O}_{\alpha \rightarrow 0}(\alpha) \end{aligned} \quad (2.3.90)$$

3.2.3. *Direct term.* The next term we have to treat is

$$\frac{\alpha}{2} \left( D(\rho_+(\alpha)) - D(\rho_-(\alpha)) \right) = \frac{\alpha}{2} \left( D(\rho_+(\alpha) - \rho_-(\alpha)) + 2D(\rho_+(\alpha) - \rho_-(\alpha), \rho_-(\alpha)) \right),$$

where  $D(\rho)$  is a shortcut notation for  $D(\rho, \rho)$ . By (2.A.93) and (2.2.13), we have

$$\alpha D(\rho_+(\alpha) - \rho_-(\alpha)) = \mathcal{O}_{\alpha \rightarrow 0}(\alpha),$$

$$\alpha D(\rho_+(\alpha) - \rho_-(\alpha), \rho_-(\alpha)) = \frac{\alpha B_\Lambda}{1 + \alpha B_\Lambda} \langle \varphi(\kappa\nu_{\text{ren}}, \Lambda), V_{\kappa\nu_{\text{ren}}} \varphi(\kappa\nu_{\text{ren}}, \Lambda) \rangle + \mathcal{O}_{\alpha \rightarrow 0}(\alpha).$$

Hence,

$$\frac{\alpha}{2} \left( D(\rho_+(\alpha)) - D(\rho_-(\alpha)) \right) = \frac{\alpha B_\Lambda}{1 + \alpha B_\Lambda} \langle \varphi(\kappa\nu_{\text{ren}}, \Lambda), V_{\kappa\nu_{\text{ren}}} \varphi(\kappa\nu_{\text{ren}}, \Lambda) \rangle + \mathcal{O}_{\alpha \rightarrow 0}(\alpha), \quad (2.3.91)$$

which exactly compensates the spurious term in (2.3.88).

3.2.4. *Exchange term.* Finally, we treat the last term of the energy, the exchange term. For any operator  $Q$ , we have

$$\begin{aligned} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|Q(x, y)|^2}{|x - y|} dx dy &= \int_{\mathbb{R}^3 \times \mathbb{R}^3} \text{Tr}_{\mathbb{C}^4} \left( E(p + q)^{\frac{1}{2}} \widehat{Q}(p, q)^* \frac{\widehat{R}_Q(p, q)}{E(p + q)^{\frac{1}{2}}} \right) dp dq \\ &\leq \|Q\|_{\mathcal{Q}} \left( \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{E(p - q)^2}{E(p + q)} |\widehat{R}_Q(p, q)|^2 dp dq \right)^{\frac{1}{2}} \\ &\leq C \|Q\|_{\mathcal{Q}}^2, \end{aligned}$$

where in the last inequality we used [HLS05a, Lemma 8]. The term we have to estimate is

$$\begin{aligned} &\frac{\alpha}{2} \left( \int_{\mathbb{R}^6} \frac{|[Q_+(\alpha)](x, y)|^2}{|x - y|} dx dy - \int_{\mathbb{R}^6} \frac{|[Q_-(\alpha)](x, y)|^2}{|x - y|} dx dy \right) \\ &= \frac{\alpha}{2} \int_{\mathbb{R}^6} \frac{|[Q_+(\alpha) - Q_-(\alpha)](x, y)|^2}{|x - y|} dx dy \\ &\quad + \alpha \int_{\mathbb{R}^6} \frac{\text{Tr}_{\mathbb{C}^4} ([Q_+(\alpha) - Q_-(\alpha)](x, y) [Q_-(\alpha)](x, y)^*)}{|x - y|} dx dy. \end{aligned}$$

By (2.3.83) together with  $\|Q_-(\alpha)\|_{\mathcal{Q}} = \mathcal{O}(\sqrt{\log \Lambda})$ , we have

$$\frac{\alpha}{2} \int_{\mathbb{R}^6} \frac{|[Q_+(\alpha) - Q_-(\alpha)](x, y)|^2}{|x - y|} dx dy = \mathcal{O}_{\alpha \rightarrow 0}(\alpha),$$



$$\begin{aligned} \alpha \int_{\mathbb{R}^6} \frac{\text{Tr}_{\mathbb{C}^4} ([Q_+(\alpha) - Q_-(\alpha)](x, y)[Q_-(\alpha)](x, y)^*)}{|x - y|} dx dy \\ = \alpha \langle \varphi(\kappa\nu_{\text{ren}}, \Lambda), R_{Q_-(\alpha)} \varphi(\kappa\nu_{\text{ren}}, \Lambda) \rangle + \mathcal{O}_{\alpha \rightarrow 0}(\alpha). \end{aligned} \quad (2.3.92)$$

Using that

$$|\langle \varphi(\kappa\nu_{\text{ren}}, \Lambda), R_{Q_-(\alpha)} \varphi(\kappa\nu_{\text{ren}}, \Lambda) \rangle| \leq \|R_{Q_-(\alpha)}\|_{H^1 \rightarrow L^2} \|\varphi(\kappa\nu_{\text{ren}}, \Lambda)\|_{H^1}^2,$$

and the fact that  $\|R_{Q_-(\alpha)}\|_{H^1 \rightarrow L^2} = \|R_{Q_-(\alpha)}|D^0|^{-1}\|_{L^2 \rightarrow L^2} \leq C\|Q_-(\alpha)\|_{\mathfrak{S}_2} = \mathcal{O}_{\alpha \rightarrow 0}(1)$ , we obtain

$$\frac{\alpha}{2} \left( \int_{\mathbb{R}^6} \frac{|[Q_+(\alpha)](x, y)|^2}{|x - y|} dx dy - \int_{\mathbb{R}^6} \frac{|[Q_-(\alpha)](x, y)|^2}{|x - y|} dx dy \right) = \mathcal{O}_{\alpha \rightarrow 0}(\alpha).$$

Regrouping (2.3.88), (2.3.90), (2.3.91), and (2.3.92) together, we get

$$F(\kappa, \alpha) = \lambda(\kappa\nu_{\text{ren}}, \Lambda) + \mathcal{O}_{\alpha \rightarrow 0}(\alpha).$$

Since  $\lambda(\kappa\nu_{\text{ren}}) = \lambda(\kappa\nu_{\text{ren}}, \Lambda) + \mathcal{O}(E(\Lambda)^{-1}) = \lambda(\kappa\nu_{\text{ren}}, \Lambda) + \mathcal{O}(e^{-\frac{1}{\alpha}}) = \lambda(\kappa\nu_{\text{ren}}, \Lambda) + \mathcal{O}(\alpha)$ , we deduce the theorem.  $\square$

### A. Kinetic energy estimates

We expand  $Q_{+,r}(\alpha) - Q_{-,r}(\alpha)$  up to  $\mathcal{O}_{\alpha \rightarrow 0}(\alpha^{3/2})$ . Recall that we have

$$\begin{aligned} Q_{\pm}(\alpha) &= Q_{\text{ref},\pm} + \alpha G_{1,0,\pm}(\rho_{\pm}(\alpha) - B_{\Lambda} \kappa\nu_{\text{ren}}) \\ &\quad - \alpha G_{0,1,\pm}(Q_{\pm}(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}})) + \mathcal{O}_{\alpha \rightarrow 0}^{\mathcal{Q}}(\alpha^2). \end{aligned}$$

Then, using similar methods as in the proof of Propositions 2.1 and 2.2, we obtain

$$G_{1,0,\pm}(\rho_{\pm}(\alpha) - B_{\Lambda} \kappa\nu_{\text{ren}}) = G_{1,0,\pm}^{(\kappa)}(\rho_{\pm}(\alpha) - B_{\Lambda} \kappa\nu_{\text{ren}}) + \mathcal{O}_{\alpha \rightarrow 0}^{\mathcal{Q}}(\sqrt{\alpha}),$$

$$G_{0,1,\pm}(Q_{\pm}(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}})) = G_{0,1,\pm}^{(\kappa)}(Q_{\pm}(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}})) + \mathcal{O}_{\alpha \rightarrow 0}^{\mathcal{Q}}(\sqrt{\alpha}),$$

with the notation

$$G_{1,0,\pm}^{(\kappa)}(\rho) := \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D_{\Lambda}^{\kappa\nu_{\text{ren}}} - \mu_{\pm} + i\eta} \Pi_{\Lambda} V_{\rho} \Pi_{\Lambda} \frac{1}{D_{\Lambda}^{\kappa\nu_{\text{ren}}} - \mu_{\pm} + i\eta} d\eta,$$

$$G_{0,1,\pm}^{(\kappa)}(Q) := \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D_{\Lambda}^{\kappa\nu_{\text{ren}}} - \mu_{\pm} + i\eta} \Pi_{\Lambda} R_Q \Pi_{\Lambda} \frac{1}{D_{\Lambda}^{\kappa\nu_{\text{ren}}} - \mu_{\pm} + i\eta} d\eta.$$

Hence,

$$\begin{aligned} Q_{\pm}(\alpha) &= Q_{\text{ref},\pm} + \alpha G_{1,0,\pm}^{(\kappa)}(\rho_{\pm}(\alpha) - B_{\Lambda} \kappa\nu_{\text{ren}}) \\ &\quad - \alpha G_{0,1,\pm}^{(\kappa)}(Q_{\pm}(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}})) + \mathcal{O}_{\alpha \rightarrow 0}^{\mathcal{Q}}(\alpha^{3/2}). \end{aligned}$$

This leads to the decomposition

$$Q_{+,r}(\alpha) - Q_{-,r}(\alpha) = Q_1 + \alpha Q_2 - \alpha Q_3 + \mathcal{O}_{\alpha \rightarrow 0}^{\mathcal{Q}}(\alpha^{3/2}),$$

with

$$Q_1 := Q_{\text{ref},+} - Q_{\text{lin},+}(\kappa\nu_{\text{ren}}) - (Q_{\text{ref},-} - Q_{\text{lin},-}(\kappa\nu_{\text{ren}})),$$

$$Q_2 := G_{1,0,+}^{(\kappa)}(\rho_+(\alpha) - B_\Lambda \kappa \nu_{\text{ren}}) - G_{1,0,-}^{(\kappa)}(\rho_-(\alpha) - B_\Lambda \kappa \nu_{\text{ren}}),$$

$$Q_3 := G_{0,1,+}^{(\kappa)}(Q_+(\alpha) + G_{1,0}(\kappa \nu_{\text{ren}})) - G_{0,1,-}^{(\kappa)}(Q_-(\alpha) + G_{1,0}(\kappa \nu_{\text{ren}})).$$

We will treat each of these three terms separately.

**A.1. Estimate on  $Q_1$ .** To expand  $Q_1$ , we write

$$Q_{\text{ref},\pm} - Q_{\text{lin},\pm}(\kappa \nu_{\text{ren}}) = \alpha G_{0,1,\pm}^{(\kappa)}(G_{1,0}(\kappa \nu_{\text{ren}})) - \alpha^2 G_{0,2,\pm}^{(\kappa)}(G_{1,0}(\kappa \nu_{\text{ren}})) + \mathcal{O}_{\alpha \rightarrow 0}^{\mathcal{Q}}(\alpha^{3/2}),$$

where for any  $Q$  we have

$$G_{0,2,\pm}^{(\kappa)}(Q) := \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D_\Lambda^{\kappa \nu_{\text{ren}}} - \mu_\pm + i\eta} \left( \Pi_\Lambda R_Q \Pi_\Lambda \frac{1}{D_\Lambda^{\kappa \nu_{\text{ren}}} - \mu_\pm + i\eta} \right)^2 d\eta.$$

Hence,

$$Q_1 = \alpha(G_{0,1,+}^{(\kappa)} - G_{0,1,-}^{(\kappa)})(G_{1,0}(\kappa \nu_{\text{ren}})) - \alpha^2(G_{0,2,+}^{(\kappa)} - G_{0,2,-}^{(\kappa)})(G_{1,0}(\kappa \nu_{\text{ren}})) + \mathcal{O}_{\alpha \rightarrow 0}^{\mathcal{Q}}(\alpha^{3/2}).$$

For  $p = 1, 2$  and  $Q \in \mathcal{Q}$ , we notice that

$$(G_{0,p,+}^{(\kappa)} - G_{0,p,-}^{(\kappa)})(Q) = \frac{1}{2i\pi} \oint_{\mathcal{C}} \frac{1}{D_\Lambda^{\kappa \nu_{\text{ren}}} - z} \left( \Pi_\Lambda R_Q \Pi_\Lambda \frac{1}{D_\Lambda^{\kappa \nu_{\text{ren}}} - z} \right)^p dz,$$

where  $\mathcal{C}$  is a contour around 0 in the complex plane which intersects the real axis only at  $\mu_-$  and  $\mu_+$ . By the residuum formula, one computes that

$$(G_{0,1,+}^{(\kappa)} - G_{0,1,-}^{(\kappa)})(G_{1,0}(\kappa \nu_{\text{ren}})) = |\varphi(\kappa \nu_{\text{ren}}, \Lambda)\rangle \langle S(\kappa \nu_{\text{ren}}) \varphi(\kappa \nu_{\text{ren}}, \Lambda)| + c.c.,$$

$$(G_{0,2,+}^{(\kappa)} - G_{0,2,-}^{(\kappa)})(G_{1,0}(\kappa \nu_{\text{ren}})) = |\varphi(\kappa \nu_{\text{ren}}, \Lambda)\rangle \langle S(\kappa \nu_{\text{ren}})^2 \varphi(\kappa \nu_{\text{ren}}, \Lambda)| + c.c.$$

$$+ |S(\kappa \nu_{\text{ren}}) \varphi(\kappa \nu_{\text{ren}}, \Lambda)\rangle \langle S(\kappa \nu_{\text{ren}}) \varphi(\kappa \nu_{\text{ren}}, \Lambda)|,$$

where  $c.c.$  denotes the adjoint of the preceding operator and

$$S(\kappa \nu_{\text{ren}}) := \frac{P_\varphi^\perp}{D_\Lambda^{\kappa \nu_{\text{ren}}} - \lambda(\kappa \nu_{\text{ren}}, \Lambda)} R_{1,0}(\kappa \nu_{\text{ren}}),$$

the operator  $P_\varphi^\perp$  being the projection on the orthogonal to  $\varphi(\kappa \nu_{\text{ren}}, \Lambda)$  in  $\mathfrak{H}_\Lambda$ . By (2.3.25), we have

$$\|S(\kappa \nu_{\text{ren}})\|_{H^1 \rightarrow H^1} = \mathcal{O}_{\alpha \rightarrow 0}(1).$$

Since the we have to estimate the kinetic energy of these quantities, we introduce a new norm corresponding exactly to the kinetic energy, for which the rank one terms above are easier to estimate. For any  $Q$  such that the following expression is well-defined, we set  $\|Q\|_{\text{kin}} := \| |D^0|^{1/2} Q \|_{\mathfrak{S}_2}$ . We thus see that for any  $\psi, \zeta \in H^1$ ,  $\| |\psi\rangle \langle \zeta \|_{\text{kin}} \leq \| \psi \|_{H^1} \| \zeta \|_{H^1}$ . For this norm, we can write

$$Q_1 = \alpha(|\varphi(\kappa \nu_{\text{ren}}, \Lambda)\rangle \langle S(\kappa \nu_{\text{ren}}) \varphi(\kappa \nu_{\text{ren}}, \Lambda)| + |S(\kappa \nu_{\text{ren}}) \varphi(\kappa \nu_{\text{ren}}, \Lambda)\rangle \langle \varphi(\kappa \nu_{\text{ren}}, \Lambda)|)$$

$$+ \mathcal{O}_{\alpha \rightarrow 0}^{\text{kin}}(\alpha^{3/2}) = \mathcal{O}_{\alpha \rightarrow 0}^{\text{kin}}(\alpha).$$

Using now that  $Q_{\text{lin},+}(\kappa\nu_{\text{ren}}) = -G_{1,0}(\kappa\nu_{\text{ren}}) + \mathcal{O}_{\alpha \rightarrow 0}^{\mathcal{Q}}(1)$ , we deduce

$$\begin{aligned} & \text{Tr}(|D^0|\{Q_{\text{lin},+}(\kappa\nu_{\text{ren}}), Q_1\}) \\ &= -2\alpha \text{Re}\langle \varphi(\kappa\nu_{\text{ren}}, \Lambda), \{|D^0|, G_{1,0}(\kappa\nu_{\text{ren}})\}S(\kappa\nu_{\text{ren}})\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle + \mathcal{O}_{\alpha \rightarrow 0}(\alpha). \end{aligned}$$

Next, we have

$$\begin{aligned} & |\langle \varphi(\kappa\nu_{\text{ren}}, \Lambda), \{|D^0|, G_{1,0}(\kappa\nu_{\text{ren}})\}S(\kappa\nu_{\text{ren}})\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle| \\ & \leq 2\|G_{1,0}(\kappa\nu_{\text{ren}})\|_{\mathfrak{S}_2}\|S(\kappa\nu_{\text{ren}})\|_{H^1 \rightarrow L^2}\|\varphi(\kappa\nu_{\text{ren}}, \Lambda)\|_{H^1}^2 = \mathcal{O}_{\alpha \rightarrow 0}(1), \end{aligned}$$

so that

$$\text{Tr}(|D^0|\{Q_{\text{lin},+}(\kappa\nu_{\text{ren}}), Q_1\}) = \mathcal{O}_{\alpha \rightarrow 0}(\alpha).$$

**A.2. Estimate on  $Q_2$ .** We split  $Q_2$  as

$$Q_2 = (G_{1,0,+}^{(\kappa)} - G_{1,0,-}^{(\kappa)})(\rho_+(\alpha) - B_\Lambda \kappa\nu_{\text{ren}}) + G_{1,0,-}^{(\kappa)}(\rho_+(\alpha) - \rho_-(\alpha)).$$

In the same fashion as before, the residuum formula leads to

$$\begin{aligned} & (G_{1,0,+}^{(\kappa)} - G_{1,0,-}^{(\kappa)})(\rho_+(\alpha) - B_\Lambda \kappa\nu_{\text{ren}}) = \\ & |\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle\langle S(V_+)\varphi(\kappa\nu_{\text{ren}}, \Lambda)| + |S(V_+)\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle\langle \varphi(\kappa\nu_{\text{ren}}, \Lambda)|, \end{aligned}$$

with  $V_+ := V_{\rho_+(\alpha) - B_\Lambda \kappa\nu_{\text{ren}}}$  and

$$S(V_+) := \frac{P_\varphi^\perp}{D_\Lambda^{\kappa\nu_{\text{ren}}} - \lambda(\kappa\nu_{\text{ren}}, \Lambda)}V_+.$$

Notice that we have  $\|S(V_+)\|_{L^2 \rightarrow H^1} = \mathcal{O}_{\alpha \rightarrow 0}(1)$ . The second term in the expansion of  $Q_2$  requires to develop  $\rho_+(\alpha) - \rho_-(\alpha)$  up to  $\mathcal{O}(\alpha)$ . Combining (2.3.82) with the estimates valid for any  $\rho \in L^2 \cap \mathcal{C}$ , any  $Q \in \mathcal{Q}$ , and any  $n \geq 2$ ,

$$\|\rho_{n,\pm}(Q, \rho)\|_{L^2 \cap \mathcal{C}} \leq C\|(Q, \rho)\|, \quad \|\rho_{1,0,\pm,r}(\rho)\|_{L^2 \cap \mathcal{C}} \leq C\|\rho\|_{L^2 \cap \mathcal{C}},$$

$$\rho_{0,1,\pm}(Q_\pm(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}})) = \rho_{0,1}(Q_\pm(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}})) + \mathcal{O}_{\alpha \rightarrow 0}^{L^2 \cap \mathcal{C}}(1),$$

where  $\rho_{0,1}(Q) := \rho[G_{0,1}(Q)]$ , we deduce that

$$\begin{aligned} \rho_+(\alpha) - \rho_-(\alpha) &= \frac{1}{1 + \alpha B_\Lambda}(\rho_{\text{ref},+} - \rho_{\text{ref},-}) + \frac{\alpha}{1 + \alpha B_\Lambda}\mathcal{U}_\Lambda(\rho_+(\alpha) - \rho_-(\alpha)) \\ &\quad - \frac{\alpha}{1 + \alpha B_\Lambda}\rho_{0,1}(Q_+(\alpha) - Q_-(\alpha)) + \mathcal{O}_{\alpha \rightarrow 0}^{L^2 \cap \mathcal{C}}(\alpha). \end{aligned}$$

Since  $\rho_{\text{ref},+} - \rho_{\text{ref},-} = |\varphi(\kappa\nu_{\text{ren}}, \Lambda)|^2 + \rho_{Q_1}$  and

$$\rho_{Q_1} = 2\alpha \text{Re} \left( \varphi(\kappa\nu_{\text{ren}}, \Lambda) \overline{S(\kappa\nu_{\text{ren}})\varphi(\kappa\nu_{\text{ren}}, \Lambda)} \right) + \mathcal{O}_{\alpha \rightarrow 0}^{L^2 \cap \mathcal{C}}(\alpha),$$

it remains to estimate  $\|\operatorname{Re}(\psi\bar{\zeta})\|_{L^2\cap\mathcal{C}}$  for any  $\psi, \zeta \in H^1$ . First, by the Sobolev imbedding  $H^1 \hookrightarrow L^6$ , we have  $\|\operatorname{Re}(\psi\bar{\zeta})\|_{L^2} \leq \|\psi\|_{L^4}\|\zeta\|_{L^4} \lesssim \|\psi\|_{H^1}\|\zeta\|_{H^1}$ . Secondly, by the Hardy-Littlewood-Sobolev inequality, we have

$$\|\operatorname{Re}(\psi\bar{\zeta})\|_{\mathcal{C}}^2 \lesssim \|\psi\|_{L^{6/5}}^2 \|\zeta\|_{L^{6/5}}^2 \lesssim \|\psi\|_{H^1}^2 \|\zeta\|_{H^1}^2.$$

Hence,

$$\left\| \operatorname{Re} \left( \varphi(\kappa\nu_{\text{ren}}, \Lambda) \overline{S(\kappa\nu_{\text{ren}})\varphi(\kappa\nu_{\text{ren}}, \Lambda)} \right) \right\|_{L^2\cap\mathcal{C}} = \mathcal{O}_{\alpha \rightarrow 0}(1),$$

and thus  $\rho_{\text{ref},+} - \rho_{\text{ref},-} = |\varphi(\kappa\nu_{\text{ren}}, \Lambda)|^2 + \mathcal{O}_{\alpha \rightarrow 0}^{L^2\cap\mathcal{C}}(\alpha)$ . For the third term in the expansion of  $\rho_+(\alpha) - \rho_-(\alpha)$ , we use  $Q_+(\alpha) - Q_-(\alpha) = |\varphi\rangle\langle\varphi| + \mathcal{O}^{\mathcal{Q}}(\sqrt{\alpha})$  and the estimate  $\|\rho_{0,1}(Q)\|_{L^2\cap\mathcal{C}} \leq C\sqrt{\log\Lambda}\|Q\|_{\mathcal{Q}}$  to infer

$$\rho_{0,1}(Q_+(\alpha) - Q_-(\alpha)) = \rho_{0,1}(|\varphi\rangle\langle\varphi|) + \mathcal{O}_{\alpha \rightarrow 0}^{L^2\cap\mathcal{C}}(1).$$

**Lemma 2.10.** *We have the estimate*

$$\|\rho_{0,1}(|\varphi\rangle\langle\varphi|)\|_{L^2\cap\mathcal{C}} = \mathcal{O}_{\alpha \rightarrow 0}(1).$$

**PROOF OF LEMMA 2.10.** We estimate the Coulomb norm by duality: for  $\zeta \in \mathcal{C}'$  a smooth function, we have

$$|\operatorname{Tr}(G_{0,1}(|\varphi\rangle\langle\varphi|)\zeta)| = |\operatorname{Tr}(R_{|\varphi\rangle\langle\varphi|}G_{1,0}(\zeta))| \leq \|R_{|\varphi\rangle\langle\varphi|}\|_{\mathfrak{S}_2} \|G_{1,0}(\zeta)\|_{\mathfrak{S}_2} \leq C\|\varphi\|_{H^1}^2 \|\zeta\|_{\mathcal{C}'}$$

Hence,  $\|\rho_{0,1}(|\varphi\rangle\langle\varphi|)\|_{\mathcal{C}} = \mathcal{O}_{\alpha \rightarrow 0}(1)$ . We cannot use the same method to estimate the  $L^2$ -norm, for which we have to be more precise. Let us use momentarily the shortcut notation  $\rho_{0,1} := \rho_{0,1}(|\varphi\rangle\langle\varphi|)$  and recall that for any  $k \in \mathbb{R}^3$  we have

$$\begin{aligned} |\widehat{\rho_{0,1}}(k)|^2 &= \left| \int_{\substack{|\ell-k/2| \leq \Lambda \\ |\ell+k/2| \leq \Lambda}} \operatorname{Tr}_{\mathbb{C}^4} \left( \widehat{R_{|\varphi\rangle\langle\varphi|}}(\ell-k/2, \ell+k/2) M(\ell-k/2, \ell+k/2) \right) d\ell \right|^2 \\ &\leq \int_{\mathbb{R}^3} \left| \widehat{R_{|\varphi\rangle\langle\varphi|}}(\ell-k/2, \ell+k/2) \right|^2 d\ell \int_{\mathbb{R}^3} |M(\ell-k/2, \ell+k/2)|^2 d\ell \\ &\leq C|k|^2 \int_{\mathbb{R}^3} \left| \widehat{R_{|\varphi\rangle\langle\varphi|}}(\ell-k/2, \ell+k/2) \right|^2 d\ell, \end{aligned}$$

where we used the estimate  $|M(p, q)|^2 \leq C|p-q|^2 E(p+q)^{-4}$  (recall that  $M(p, q)$  was defined in (2.3.31)). As a consequence, we have

$$\|\rho_{0,1}\|_{L^2}^2 \leq C \int_{\mathbb{R}^3} |p-q|^2 \left| \widehat{R_{|\varphi\rangle\langle\varphi|}}(p, q) \right|^2 dp dq = C \|[-i\nabla, R_{|\varphi\rangle\langle\varphi|}]\|_{(\mathfrak{S}_2)^3}^2.$$

But since  $[-i\nabla, R_{|\varphi\rangle\langle\varphi|}](x, y) = \frac{\nabla\varphi(x)\varphi(y)^* + \varphi(x)\nabla\varphi(y)^*}{|x-y|}$ , we infer from the Hardy inequality that  $\|\rho_{0,1}\|_{L^2} \leq C\|\varphi\|_{H^1}^2$ , so that  $\|\rho_{0,1}\|_{L^2} = \mathcal{O}_{\alpha \rightarrow 0}(1)$ .  $\square$

The last term to estimate in  $\rho_+(\alpha) - \rho_-(\alpha)$  is  $\mathcal{U}_\Lambda(\rho_+(\alpha) - \rho_-(\alpha))$ . Using (2.3.82), we have for all  $k \in \mathbb{R}^3$ ,

$$\begin{aligned} U_\Lambda(|k|)\mathcal{F}[\rho_\pm(\alpha) - B_\Lambda\kappa\nu_{\text{ren}}](k) &= \frac{U_\Lambda(|k|)}{1 + \alpha B_\Lambda(k)}\mathcal{F}[\rho_{\text{ref},\pm} - B_\Lambda\kappa\nu_{\text{ren}}](k) \\ &\quad + \frac{\alpha U_\Lambda(|k|)}{1 + \alpha B_\Lambda(k)}\mathcal{F}[\rho_{1,0,\pm,r}(\rho_\pm(\alpha) - B_\Lambda\kappa\nu_{\text{ren}})](k) \\ &\quad - \frac{\alpha U_\Lambda(|k|)}{1 + \alpha B_\Lambda(k)}\mathcal{F}[\rho_{0,1,\pm}(Q_\pm(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}}))](k) \\ &\quad + \frac{\alpha U_\Lambda(|k|)}{1 + \alpha B_\Lambda(k)}\sum_{n \geq 2} \alpha^{n-1}\mathcal{F}[\rho_{n,\pm}(Q_\pm(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}}), \rho_\pm(\alpha) - B_\Lambda\kappa\nu_{\text{ren}})](k). \end{aligned}$$

Since

$$\left| \frac{\alpha U_\Lambda(|k|)}{1 + \alpha B_\Lambda(k)} \right| \leq \alpha B_\Lambda + \left| \frac{\alpha B_\Lambda(k)}{1 + \alpha B_\Lambda(k)} \right| \leq C,$$

we have

$$\mathcal{U}_\Lambda(\rho_\pm(\alpha) - B_\Lambda\kappa\nu_{\text{ren}}) = \mathcal{V}_\Lambda(\rho_{\text{ref},\pm} - B_\Lambda\kappa\nu_{\text{ren}}) - \alpha \mathcal{V}_\Lambda \rho_{0,1}(Q_\pm(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}})) + \mathcal{O}_{\alpha \rightarrow 0}^{L^2 \cap \mathcal{C}}(1),$$

where  $\mathcal{V}_\Lambda$  is the Fourier multiplier by  $k \mapsto \frac{U_\Lambda(|k|)}{1 + \alpha B_\Lambda(k)}$ . Hence, for the difference of densities we obtain

$$\mathcal{U}_\Lambda(\rho_+(\alpha) - \rho_-(\alpha)) = \mathcal{V}_\Lambda(\rho_{\text{ref},+} - \rho_{\text{ref},-}) - \alpha \mathcal{V}_\Lambda \rho_{0,1}(Q_+(\alpha) - Q_-(\alpha)) + \mathcal{O}_{\alpha \rightarrow 0}^{L^2 \cap \mathcal{C}}(1).$$

We have already seen that  $\rho_{0,1}(Q_+(\alpha) - Q_-(\alpha)) = \mathcal{O}_{\alpha \rightarrow 0}^{L^2 \cap \mathcal{C}}(1)$ , and that  $\rho_{\text{ref},+} - \rho_{\text{ref},-} = |\varphi(\kappa\nu_{\text{ren}}, \Lambda)|^2 + \mathcal{O}_{\alpha \rightarrow 0}^{L^2 \cap \mathcal{C}}(\alpha)$ , which implies

$$\mathcal{U}_\Lambda(\rho_+(\alpha) - \rho_-(\alpha)) = \mathcal{V}_\Lambda |\varphi(\kappa\nu_{\text{ren}}, \Lambda)|^2 + \mathcal{O}_{\alpha \rightarrow 0}^{L^2 \cap \mathcal{C}}(1).$$

By (2.3.76) and the estimate  $(1 + \alpha B_\Lambda(k))^{-1} \leq 1$  following from  $B_\Lambda(k) \geq 0$ , it is enough to know that  $|\varphi|^2$  is bounded in  $H^1$  to prove that  $\mathcal{U}_\Lambda(\rho_+(\alpha) - \rho_-(\alpha)) = \mathcal{O}_{\alpha \rightarrow 0}^{L^2 \cap \mathcal{C}}(1)$ . Since  $\| |\varphi|^2 \|_{H^1} \leq C \| \varphi \|_{H^2}^2$  and  $\varphi$  is an eigenvector of  $D_\Lambda^{\kappa\nu_{\text{ren}}}$ , it is sufficient to control  $\| \nabla(V_{\kappa\nu_{\text{ren}}}\varphi) \|_{L^2}$ . By the Hardy-Littlewood-Sobolev together with  $|\nabla V_\nu| \leq C|\nu| \star |\cdot|^{-2}$ ,  $\nu \in L^2$  implies that  $\nabla V_\nu \in L^6$ , and  $\varphi \in H^1 \hookrightarrow L^3$  implies that  $\varphi \nabla V_{\kappa\nu_{\text{ren}}} \in L^2$ . Hence,  $\varphi = \mathcal{O}_{\alpha \rightarrow 0}^{H^2}(1)$  and  $\mathcal{U}_\Lambda(\rho_+(\alpha) - \rho_-(\alpha)) = \mathcal{O}_{\alpha \rightarrow 0}^{L^2 \cap \mathcal{C}}(1)$ . After these painful estimates, we obtain

$$\rho_+(\alpha) - \rho_-(\alpha) = \frac{1}{1 + \alpha B_\Lambda} |\varphi(\kappa\nu_{\text{ren}}, \Lambda)|^2 + \mathcal{O}_{\alpha \rightarrow 0}^{L^2 \cap \mathcal{C}}(\alpha), \quad (2.A.93)$$

which in turn implies

$$\begin{aligned} Q_2 &= |\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle \langle S(V_+)\varphi(\kappa\nu_{\text{ren}}, \Lambda)| + |S(V_+)\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle \langle \varphi(\kappa\nu_{\text{ren}}, \Lambda)| \\ &\quad + \frac{1}{1 + \alpha B_\Lambda} G_{1,0,-}^{(\kappa)}(|\varphi(\kappa\nu_{\text{ren}}, \Lambda)|^2) + \mathcal{O}_{\alpha \rightarrow 0}^{\mathcal{Q}}(\sqrt{\alpha}). \end{aligned}$$

This leads to the expansion

$$\begin{aligned} \text{Tr}(|D^0|\{Q_{\text{lin},+}(\kappa\nu_{\text{ren}}), \alpha Q_2\}) \\ = -2\alpha \text{Re}\langle \varphi(\kappa\nu_{\text{ren}}, \Lambda), \{|D^0|, G_{1,0}(\kappa\nu_{\text{ren}})\}S(V_+)\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle \\ + \frac{\alpha}{1 + \alpha B_\Lambda} \text{Tr}(|D^0|\{Q_{\text{lin},+}(\kappa\nu_{\text{ren}}), G_{1,0,-}^{(\kappa)}(|\varphi(\kappa\nu_{\text{ren}}, \Lambda)|^2)\}) + \mathcal{O}_{\alpha \rightarrow 0}(\alpha) \end{aligned}$$

As before we have

$$|\langle \varphi(\kappa\nu_{\text{ren}}, \Lambda), \{|D^0|, G_{1,0}(\kappa\nu_{\text{ren}})\}S(V_+)\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle| = \mathcal{O}_{\alpha \rightarrow 0}(1).$$

Furthermore, we write  $Q_{\text{lin},+}(\kappa\nu_{\text{ren}}) = -G_{1,0}(\kappa\nu_{\text{ren}}) + Q_{\text{lin},+,r}(\kappa\nu_{\text{ren}})$  and  $G_{1,0,-}^{(\kappa)}(|\varphi|^2) = G_{1,0}(|\varphi|^2) + G_{1,0,-,r}^{(\kappa)}(|\varphi|^2)$ , so that

$$\begin{aligned} \text{Tr}(|D^0|\{Q_{\text{lin},+}(\kappa\nu_{\text{ren}}), G_{1,0,-}^{(\kappa)}(|\varphi|^2)\}) &= -\text{Tr}(|D^0|\{G_{1,0}(\kappa\nu_{\text{ren}}), G_{1,0}(|\varphi|^2)\}) \\ &\quad - \text{Tr}(|D^0|\{G_{1,0}(\kappa\nu_{\text{ren}}), G_{1,0,-,r}^{(\kappa)}(|\varphi|^2)\}) + \text{Tr}(|D^0|\{Q_{\text{lin},+,r}(\kappa\nu_{\text{ren}}), G_{1,0}(|\varphi|^2)\}) \\ &\quad + \text{Tr}(|D^0|\{Q_{\text{lin},+,r}(\kappa\nu_{\text{ren}}), G_{1,0,-,r}^{(\kappa)}(|\varphi|^2)\}). \end{aligned}$$

We know that  $\|G_{1,0,-,r}^{(\kappa)}(|\varphi|^2)\|_{\mathcal{Q}} \leq C\|\varphi\|_{L^2 \cap \mathcal{C}} \leq C\|\varphi\|_{H^1}^2 = \mathcal{O}_{\alpha \rightarrow 0}(1)$ , and furthermore  $\|Q_{\text{lin},+,r}(\kappa\nu_{\text{ren}})\|_{\mathcal{Q}} = \mathcal{O}_{\alpha \rightarrow 0}(1)$ . Hence,

$$\text{Tr}(|D^0|\{Q_{\text{lin},+,r}(\kappa\nu_{\text{ren}}), G_{1,0,-,r}^{(\kappa)}(|\varphi|^2)\}) = \mathcal{O}_{\alpha \rightarrow 0}(1).$$

By [GLS09, Lemma 6] and the estimates of the first part of the paper, we have for any  $0 \leq \tau < 1/2$  and for any  $\rho \in L^2 \cap \mathcal{C}$ ,

$$\||D^0|^\tau G_{1,0}(\rho)\|_{\mathfrak{S}_2} \leq C\|\rho\|_{\mathcal{C}},$$

$$\||D^0|^{\tau+1/2} Q_{\text{lin},+,r}(\rho)\|_{\mathfrak{S}_2} \leq C\|\rho\|_{L^2 \cap \mathcal{C}},$$

$$\||D^0|^{\tau+1/2} G_{1,0,-,r}^{(\kappa)}(\rho)\|_{\mathfrak{S}_2} \leq C\|\rho\|_{L^2 \cap \mathcal{C}}.$$

Splitting  $|D^0| = |D^0|^\tau |D^0|^{1-\tau}$  for some  $0 < \tau < 1/2$ , we thus get

$$-\text{Tr}(|D^0|\{G_{1,0}(\kappa\nu_{\text{ren}}), G_{1,0,-,r}^{(\kappa)}(|\varphi|^2)\}) + \text{Tr}(|D^0|\{Q_{\text{lin},+,r}(\kappa\nu_{\text{ren}}), G_{1,0}(|\varphi|^2)\}) = \mathcal{O}_{\alpha \rightarrow 0}(1).$$

Finally,

$$\text{Tr}(|D^0|\{Q_{\text{lin},+}(\kappa\nu_{\text{ren}}), \alpha Q_2\}) = -\frac{\alpha}{1 + \alpha B_\Lambda} \text{Tr}(|D^0|\{G_{1,0}(\kappa\nu_{\text{ren}}), G_{1,0}(|\varphi|^2)\}) + \mathcal{O}_{\alpha \rightarrow 0}(\alpha).$$

We simplify the last expression in a general fashion. Let  $\rho_1, \rho_2 \in L^2 \cap \mathcal{C}$  and  $T(\rho_1, \rho_2) := \text{Tr}(|D^0| \{G_{1,0}(\rho_1), G_{1,0}(\rho_2)\})$ . Then,

$$\begin{aligned}
& T(\rho_1, \rho_2) \\
&= \frac{1}{32\pi^3} \int_{B(0,\Lambda)^2} (E(p) + E(q)) \widehat{V}_{\rho_1}(p-q) \overline{\widehat{V}_{\rho_2}(p-q)} \text{Tr}_{\mathbb{C}^4}(M(p,q)M(q,p)) \, dp \, dq \\
&= \frac{1}{4\pi^3} \int_{B(0,\Lambda)^2} \widehat{V}_{\rho_1}(p-q) \overline{\widehat{V}_{\rho_2}(p-q)} \frac{1}{E(p) + E(q)} \left(1 - \frac{1+p \cdot q}{E(p)E(q)}\right) \, dp \, dq \\
&= \frac{1}{4\pi} \int_{B(0,2\Lambda)} \widehat{V}_{\rho_1}(k) \overline{\widehat{V}_{\rho_2}(k)} |k|^2 B_\Lambda(k) \, dk \\
&= 4\pi \int_{B(0,2\Lambda)} B_\Lambda(k) \frac{\widehat{\rho}_1(k) \overline{\widehat{\rho}_2(k)}}{|k|^2} \, dk \\
&= B_\Lambda D(\rho_1, \rho_2) - 4\pi \int_{B(0,2\Lambda)} U_\Lambda(|k|) \frac{\widehat{\rho}_1(k) \overline{\widehat{\rho}_2(k)}}{|k|^2} \, dk.
\end{aligned}$$

where we recall that

$$\begin{aligned}
B_\Lambda(k) &= \frac{1}{\pi^2 |k|^2} \times \\
&\times \int_{\substack{|\ell+k/2| \leq \Lambda \\ |\ell-k/2| \leq \Lambda}} \frac{1}{E(\ell+k/2) + E(\ell-k/2)} \left(1 - \frac{1 + (\ell+k/2) \cdot (\ell-k/2)}{E(\ell+k/2)E(\ell-k/2)}\right) \, d\ell.
\end{aligned}$$

In our case  $\rho_1 = \kappa\nu_{\text{ren}}$  and  $\rho_2 = |\varphi|^2$ , since  $\mathcal{U}_\Lambda \nu \in \mathcal{C}$  because  $\nu \in L^2 \cap \mathcal{C}$ , we deduce

$$\begin{aligned}
\text{Tr}(|D^0| \{G_{1,0}(\kappa\nu_{\text{ren}}), G_{1,0}(|\varphi|^2)\}) &= B_\Lambda D(\kappa\nu_{\text{ren}}, |\varphi|^2) + \mathcal{O}_{\alpha \rightarrow 0}(1) \\
&= B_\Lambda \langle \varphi(\kappa\nu_{\text{ren}}, \Lambda), V_{\kappa\nu_{\text{ren}}} \varphi(\kappa\nu_{\text{ren}}, \Lambda) \rangle + \mathcal{O}_{\alpha \rightarrow 0}(1),
\end{aligned}$$

thus

$$\text{Tr}(|D^0| \{Q_{\text{lin},+}(\kappa\nu_{\text{ren}}), \alpha Q_2\}) = -\frac{\alpha B_\Lambda}{1 + \alpha B_\Lambda} \langle \varphi(\kappa\nu_{\text{ren}}, \Lambda), V_{\kappa\nu_{\text{ren}}} \varphi(\kappa\nu_{\text{ren}}, \Lambda) \rangle + \mathcal{O}_{\alpha \rightarrow 0}(\alpha).$$

**A.3. Estimate on  $Q_3$ .** As for  $Q_2$ , we first write

$$Q_3 = (G_{0,1,+}^{(\kappa)} - G_{0,1,-}^{(\kappa)})(Q_+(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}})) + G_{0,1,-}^{(\kappa)}(Q_+(\alpha) - Q_-(\alpha)).$$

By the residuum formula,

$$\begin{aligned}
& (G_{0,1,+}^{(\kappa)} - G_{0,1,-}^{(\kappa)})(Q_+(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}})) \\
&= |\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle \langle S(R_+) \varphi(\kappa\nu_{\text{ren}}, \Lambda) | + |S(R_+) \varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle \langle \varphi(\kappa\nu_{\text{ren}}, \Lambda) |,
\end{aligned}$$

where

$$S(R_+) := \frac{P_\varphi^\perp}{D_\Lambda^{\kappa\nu_{\text{ren}}} - \lambda(\kappa\nu_{\text{ren}}, \Lambda)} R(Q_+(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}})),$$

so that  $\|S(R_+)\|_{H^1 \rightarrow H^1} \leq C\|Q_+(\alpha) + G_{1,0}(\kappa\nu_{\text{ren}})\|_{\mathcal{Q}} = \mathcal{O}_{\alpha \rightarrow 0}(1)$ . Since  $\|G_{0,1,-}^{(\kappa)}(Q)\|_{\mathcal{Q}} \leq C\|Q\|_{\mathcal{Q}}$  and  $Q_+(\alpha) - Q_-(\alpha) = |\varphi\rangle\langle\varphi| + \mathcal{O}_{\alpha \rightarrow 0}^{\mathcal{Q}}(\sqrt{\alpha})$ , we have

$$G_{0,1,-}^{(\kappa)}(Q_+(\alpha) - Q_-(\alpha)) = G_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|) + \mathcal{O}_{\alpha \rightarrow 0}^{\mathcal{Q}}(\sqrt{\alpha}).$$

This leads to the expression

$$\begin{aligned} & \text{Tr}(|D^0|\{Q_{\text{lin},+}(\kappa\nu_{\text{ren}}), \alpha Q_3\}) \\ &= 2\alpha \text{Re}\langle\varphi(\kappa\nu_{\text{ren}}, \Lambda), \{|D^0|, Q_{\text{lin},+}(\kappa\nu_{\text{ren}})\}S(R_+)\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle \\ & \quad + \alpha \text{Tr}(|D^0|\{Q_{\text{lin},+}(\kappa\nu_{\text{ren}}), G_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\}) + \mathcal{O}_{\alpha \rightarrow 0}(\alpha). \end{aligned}$$

Again we have

$$|\langle\varphi(\kappa\nu_{\text{ren}}, \Lambda), \{|D^0|, Q_{\text{lin},+}(\kappa\nu_{\text{ren}})\}S(R_+)\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle| = \mathcal{O}_{\alpha \rightarrow 0}(1),$$

and

$$\begin{aligned} & \text{Tr}(|D^0|\{Q_{\text{lin},+}(\kappa\nu_{\text{ren}}), G_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\}) = -\text{Tr}(|D^0|\{G_{1,0}(\kappa\nu_{\text{ren}}), G_{0,1}(|\varphi\rangle\langle\varphi|)\}) \\ & - \text{Tr}(|D^0|\{G_{1,0}(\kappa\nu_{\text{ren}}), G_{0,1,-,r}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\}) + \text{Tr}(|D^0|\{Q_{\text{lin},+,r}(\kappa\nu_{\text{ren}}), G_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\}) \\ & \quad + \text{Tr}(|D^0|\{Q_{\text{lin},+,r}(\kappa\nu_{\text{ren}}), G_{0,1,-,r}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\}). \end{aligned}$$

Since  $\|Q_{\text{lin},+,r}(\kappa\nu_{\text{ren}})\|_{\mathcal{Q}} = \mathcal{O}_{\alpha \rightarrow 0}(1)$ ,  $\|G_{0,1,-,r}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\|_{\mathcal{Q}} = \mathcal{O}_{\alpha \rightarrow 0}(1)$ ,  $\|G_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\|_{\mathcal{Q}} = \mathcal{O}_{\alpha \rightarrow 0}(1)$ ,  $\|G_{1,0}(\kappa\nu_{\text{ren}})\|_{\mathfrak{S}_2} = \mathcal{O}_{\alpha \rightarrow 0}(1)$ , and  $\| |D^0| G_{0,1,-,r}^{(\kappa)}(|\varphi\rangle\langle\varphi|) \|_{\mathfrak{S}_2} = \mathcal{O}_{\alpha \rightarrow 0}(1)$ , we have

$$\begin{aligned} & -\text{Tr}(|D^0|\{G_{1,0}(\kappa\nu_{\text{ren}}), G_{0,1,-,r}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\}) + \text{Tr}(|D^0|\{Q_{\text{lin},+,r}(\kappa\nu_{\text{ren}}), G_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\}) \\ & \quad + \text{Tr}(|D^0|\{Q_{\text{lin},+,r}(\kappa\nu_{\text{ren}}), G_{0,1,-,r}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\}) = \mathcal{O}_{\alpha \rightarrow 0}(1). \end{aligned}$$

A short computation shows that

$$\text{Tr}(|D^0|\{G_{1,0}(\kappa\nu_{\text{ren}}), G_{0,1}(|\varphi\rangle\langle\varphi|)\}) = -\text{Tr}(G_{1,0}(\kappa\nu_{\text{ren}})R_{|\varphi\rangle\langle\varphi|}),$$

which implies

$$\begin{aligned} & |\text{Tr}(|D^0|\{G_{1,0}(\kappa\nu_{\text{ren}}), G_{0,1}(|\varphi\rangle\langle\varphi|)\})| \leq \|G_{1,0}(\kappa\nu_{\text{ren}})\|_{\mathfrak{S}_2} \|R_{|\varphi\rangle\langle\varphi|}\|_{\mathfrak{S}_2} \\ & \leq C\|\kappa\nu_{\text{ren}}\|_c \|\varphi\|_{H^1}^2 = \mathcal{O}_{\alpha \rightarrow 0}(1). \end{aligned}$$

Finally,

$$\text{Tr}(|D^0|\{Q_{\text{lin},+}(\kappa\nu_{\text{ren}}), \alpha Q_3\}) = \mathcal{O}_{\alpha \rightarrow 0}(\alpha).$$

The last term to estimate in (2.3.87) is thus  $\langle\varphi(\kappa\nu_{\text{ren}}, \Lambda), \{|D^0|, Q_{-,r}(\alpha)\}\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle$ .

We do so by writing

$$|\langle\varphi(\kappa\nu_{\text{ren}}, \Lambda), \{|D^0|, Q_{-,r}(\alpha)\}\varphi(\kappa\nu_{\text{ren}}, \Lambda)\rangle| \leq 2\|Q_{-,r}(\alpha)\|_{H^1 \rightarrow L^2} \|\varphi(\kappa\nu_{\text{ren}}, \Lambda)\|_{H^1}^2,$$



and it remains to estimate  $\|Q_{-,r}(\alpha)|D^0|^{-1}\|_{L^2 \rightarrow L^2}$ . Recall that  $Q_{-,r}(\alpha) = Q_-(\alpha) - Q_{\text{lin},-}(\kappa\nu_{\text{ren}})$ , which we develop up to  $\mathcal{O}(\alpha)$ . We have

$$Q_{-,r}(\alpha) = \alpha G_{0,1,-}^{(\kappa)}(G_{1,0}(\kappa\nu_{\text{ren}})) + \alpha G_{1,0}(\rho_-(\alpha) - B_\Lambda \kappa\nu_{\text{ren}}) + \mathcal{O}_{\alpha \rightarrow 0}^{\mathcal{Q}}(\alpha),$$

and writing for any  $Q$  that

$$\begin{aligned} G_{0,1,-}^{(\kappa)}(Q)|D^0|^{-1} &= \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D_\Lambda^{\kappa\nu_{\text{ren}}} - \mu_- + i\eta} \Pi_\Lambda R_Q |D^0|^{-1} \Pi_\Lambda \frac{1}{D_\Lambda^0 - \mu_- + i\eta} d\eta \\ &+ \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D_\Lambda^{\kappa\nu_{\text{ren}}} - \mu_- + i\eta} \Pi_\Lambda R_Q \Pi_\Lambda \frac{1}{D_\Lambda^0 - \mu_- + i\eta} \Pi_\Lambda V_{\kappa\nu_{\text{ren}}} \Pi_\Lambda \frac{1}{D_\Lambda^{\kappa\nu_{\text{ren}}} - \mu_- + i\eta} |D^0|^{-1} d\eta, \end{aligned}$$

one obtains

$$\|G_{0,1,-}^{(\kappa)}(Q)|D^0|^{-1}\|_{L^2 \rightarrow L^2} \leq C \|R_Q |D^0|^{-1}\|_{L^2 \rightarrow L^2} = \|R_Q\|_{H^1 \rightarrow L^2} \leq 2\|Q\|_{\mathfrak{S}_2}$$

by the Hardy inequality. Together with  $\|G_{1,0}(\kappa\nu_{\text{ren}})\|_{\mathfrak{S}_2} = \mathcal{O}_{\alpha \rightarrow 0}(1)$ , this implies

$$\|G_{0,1,-}^{(\kappa)}(G_{1,0}(\kappa\nu_{\text{ren}}))|D^0|^{-1}\|_{L^2 \rightarrow L^2} = \mathcal{O}_{\alpha \rightarrow 0}(1).$$

We also have  $\|G_{1,0}(\rho)\|_{L^2 \rightarrow L^2} \leq \|G_{1,0}(\rho)\|_{\mathfrak{S}_2} \leq C\|\rho\|_C$  for any  $\rho$ , and thus

$$\begin{aligned} \|G_{1,0}(\rho_-(\alpha) - B_\Lambda \kappa\nu_{\text{ren}})|D^0|^{-1}\|_{L^2 \rightarrow L^2} &\leq \|G_{1,0}(\rho_-(\alpha) - B_\Lambda \kappa\nu_{\text{ren}})\|_{L^2 \rightarrow L^2} \\ &\leq C\|\rho_-(\alpha) - B_\Lambda \kappa\nu_{\text{ren}}\|_C = \mathcal{O}_{\alpha \rightarrow 0}(1). \end{aligned}$$

As a consequence,

$$|\langle \varphi(\kappa\nu_{\text{ren}}, \Lambda), \{|D^0|, Q_{-,r}(\alpha)\} \varphi(\kappa\nu_{\text{ren}}, \Lambda) \rangle| = \mathcal{O}_{\alpha \rightarrow 0}(\alpha),$$

and hence

$$\begin{aligned} \text{Tr}_0(D^0 Q_+(\alpha)) - \text{Tr}_0(D^0 Q_-(\alpha)) &= \langle \varphi(\kappa\nu_{\text{ren}}, \Lambda), D^0 \varphi(\kappa\nu_{\text{ren}}, \Lambda) \rangle \\ &- \frac{\alpha B_\Lambda}{1 + \alpha B_\Lambda} \langle \varphi(\kappa\nu_{\text{ren}}, \Lambda), V_{\kappa\nu_{\text{ren}}} \varphi(\kappa\nu_{\text{ren}}, \Lambda) \rangle + \mathcal{O}_{\alpha \rightarrow 0}(\alpha). \end{aligned} \quad (2.A.94)$$

## B. Next order expansion of $F$

We want to identify the  $\alpha$ -term in the expansion of  $F(\kappa, \alpha)$ . In other words, we want to develop  $F(\kappa, \alpha)$  up to  $\mathcal{O}(\alpha^{3/2})$ . First, we write

$$Q_\pm(\alpha) = Q_\pm(\kappa\bar{\nu}) + Q_{\pm, \frac{1}{2}}(\alpha) + Q_{\pm, r}(\alpha),$$

$$\begin{aligned} Q_{\pm, \frac{1}{2}}(\alpha) &:= \alpha G_{0,1,\pm}^{(\kappa)}(G_{1,0}(\kappa\bar{\nu})) + \frac{\alpha}{1 + \alpha B_\Lambda} G_{1,0}(\rho_\pm(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu}) \\ &+ \alpha G_{1,0} \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right). \end{aligned}$$

We have  $Q_{\pm, \frac{1}{2}}(\alpha) = \mathcal{O}^{\mathcal{Q}}(\sqrt{\alpha})$  and  $Q_{\pm, r}(\alpha) = \mathcal{O}^{\mathcal{Q}}(\alpha)$ . Hence, for the kinetic energy we can write

$$\begin{aligned} \text{Tr}(|D^0|Q_+(\alpha)^2) - \text{Tr}(|D^0|Q_-(\alpha)^2) &= \langle \varphi(\kappa, \Lambda), D^0\varphi(\kappa, \Lambda) \rangle \\ &\quad + \text{Tr}(|D^0|Q_{+, \frac{1}{2}}(\alpha)^2) - \text{Tr}(|D^0|Q_{-, \frac{1}{2}}(\alpha)^2) \\ &\quad + \text{Tr}(|D^0|\{Q_+(\kappa\bar{\nu}), Q_{+, \frac{1}{2}}(\alpha)\}) - \text{Tr}(|D^0|\{Q_-(\kappa\bar{\nu}), Q_{-, \frac{1}{2}}(\alpha)\}) \\ &\quad + \text{Tr}(|D^0|\{Q_+(\kappa\bar{\nu}), Q_{+, r}(\alpha)\}) - \text{Tr}(|D^0|\{Q_-(\kappa\bar{\nu}), Q_{-, r}(\alpha)\}) + \mathcal{O}(\alpha^{3/2}). \end{aligned}$$

We decompose

$$\begin{aligned} \text{Tr}(|D^0|Q_{+, \frac{1}{2}}(\alpha)^2) - \text{Tr}(|D^0|Q_{-, \frac{1}{2}}(\alpha)^2) &= \text{Tr}(|D^0|(Q_{+, \frac{1}{2}}(\alpha) - Q_{-, \frac{1}{2}}(\alpha))Q_{+, \frac{1}{2}}(\alpha)) \\ &\quad + \text{Tr}(|D^0|Q_{-, \frac{1}{2}}(\alpha)(Q_{+, \frac{1}{2}}(\alpha) - Q_{-, \frac{1}{2}}(\alpha))). \end{aligned}$$

Using the notation  $S(Q) := S(R_Q)$  and  $S(\rho) := S(V_\rho)$  for any  $Q, \rho$ , we have

$$Q_{+, \frac{1}{2}}(\alpha) - Q_{-, \frac{1}{2}}(\alpha) = \alpha(|S(G_{1,0}(\kappa\bar{\nu}))\varphi\rangle\langle\varphi| + h.c.) + \frac{\alpha}{1 + \alpha B_\Lambda} G_{1,0}(|\varphi|^2).$$

Hence,

$$\begin{aligned} \text{Tr}(|D^0|(Q_{+, \frac{1}{2}}(\alpha) - Q_{-, \frac{1}{2}}(\alpha))Q_{+, \frac{1}{2}}(\alpha)) &= \alpha\langle Q_{+, \frac{1}{2}}(\alpha)\varphi, |D^0|S(G_{1,0}(\kappa\bar{\nu}))\varphi \rangle \\ &\quad + \alpha\langle Q_{+, \frac{1}{2}}(\alpha)S(G_{1,0}(\kappa\bar{\nu}))\varphi, |D^0|\varphi \rangle + \frac{\alpha}{1 + \alpha B_\Lambda} \text{Tr}(|D^0|G_{1,0}(|\varphi|^2)Q_{+, \frac{1}{2}}(\alpha)). \end{aligned}$$

Inserting the definition of  $Q_{+, \frac{1}{2}}(\alpha)$ , we get

$$\begin{aligned} \text{Tr}(|D^0|(Q_{+, \frac{1}{2}}(\alpha) - Q_{-, \frac{1}{2}}(\alpha))Q_{+, \frac{1}{2}}(\alpha)) &= \alpha^2\langle G_{0,1,+}^{(\kappa)}(G_{1,0}(\kappa\bar{\nu}))\varphi, |D^0|S(G_{1,0}(\kappa\bar{\nu}))\varphi \rangle \\ &\quad + \frac{\alpha^2}{1 + \alpha B_\Lambda} \langle G_{1,0}(\rho_\pm(\kappa\bar{\nu}) - B_\Lambda\kappa\bar{\nu})\varphi, |D^0|S(G_{1,0}(\kappa\bar{\nu}))\varphi \rangle \\ &\quad + \alpha^2\langle G_{1,0} \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi, |D^0|S(G_{1,0}(\kappa\bar{\nu}))\varphi \rangle \\ &\quad + \alpha^2\langle G_{0,1,+}^{(\kappa)}(G_{1,0}(\kappa\bar{\nu}))S(G_{1,0}(\kappa\bar{\nu}))\varphi, |D^0|\varphi \rangle \\ &\quad + \frac{\alpha^2}{1 + \alpha B_\Lambda} \langle G_{1,0}(\rho_+(\kappa\bar{\nu}) - B_\Lambda\kappa\bar{\nu})S(G_{1,0}(\kappa\bar{\nu}))\varphi, |D^0|\varphi \rangle \\ &\quad + \alpha^2\langle G_{1,0} \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) S(G_{1,0}(\kappa\bar{\nu}))\varphi, |D^0|\varphi \rangle \\ &\quad + \frac{\alpha^2}{1 + \alpha B_\Lambda} \text{Tr}(|D^0|G_{1,0}(|\varphi|^2)G_{0,1,+}^{(\kappa)}(G_{1,0}(\kappa\bar{\nu}))) \\ &\quad + \frac{\alpha^2}{(1 + \alpha B_\Lambda)^2} \text{Tr}(|D^0|G_{1,0}(|\varphi|^2)G_{1,0}(\rho_+(\kappa\bar{\nu}) - B_\Lambda\kappa\bar{\nu})) \\ &\quad + \frac{\alpha^2}{1 + \alpha B_\Lambda} \text{Tr} \left( |D^0|G_{1,0}(|\varphi|^2)G_{1,0} \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \right). \end{aligned}$$

All the inner product terms are  $\mathcal{O}(\alpha^2)$  since  $\|G_{1,0}(\rho)\|_{L^2 \rightarrow L^2} \lesssim \|\rho\|_c$  with furthermore  $\|G_{0,1}(Q)\|_{H^1 \rightarrow L^2} \lesssim \|Q\|_{\mathfrak{S}_2}$ . Hence,

$$\begin{aligned} \text{Tr}(|D^0|(Q_{+, \frac{1}{2}}(\alpha) - Q_{-, \frac{1}{2}}(\alpha))Q_{+, \frac{1}{2}}(\alpha)) &= \frac{\alpha^2}{1 + \alpha B_\Lambda} \text{Tr}(|D^0|G_{1,0}(|\varphi|^2)G_{0,1}(G_{1,0}(\kappa\bar{\nu}))) \\ &\quad + \frac{\alpha^2}{(1 + \alpha B_\Lambda)^2} \text{Tr}(|D^0|G_{1,0}(|\varphi|^2)G_{1,0}(\rho_+(\kappa\bar{\nu}) - B_\Lambda\kappa\bar{\nu})) \\ &\quad + \frac{\alpha^2}{1 + \alpha B_\Lambda} \text{Tr}\left(|D^0|G_{1,0}(|\varphi|^2)G_{1,0}\left(\frac{\alpha}{1 + \alpha B_\Lambda(k)}\rho_{0,1}(G_{1,0}(\kappa\bar{\nu}))\right)\right) + \mathcal{O}(\alpha^2). \end{aligned}$$

By the same reasoning, we find

$$\begin{aligned} \text{Tr}(|D^0|Q_{-, \frac{1}{2}}(\alpha)(Q_{+, \frac{1}{2}}(\alpha) - Q_{-, \frac{1}{2}}(\alpha))) &= \frac{\alpha^2}{1 + \alpha B_\Lambda} \text{Tr}(|D^0|G_{0,1}(G_{1,0}(\kappa\bar{\nu}))G_{1,0}(|\varphi|^2)) \\ &\quad + \frac{\alpha^2}{(1 + \alpha B_\Lambda)^2} \text{Tr}(|D^0|G_{1,0}(\rho_-(\kappa\bar{\nu}) - B_\Lambda\kappa\bar{\nu})G_{1,0}(|\varphi|^2)) \\ &\quad + \frac{\alpha^2}{1 + \alpha B_\Lambda} \text{Tr}\left(|D^0|G_{1,0}\left(\frac{\alpha}{1 + \alpha B_\Lambda(k)}\rho_{0,1}(G_{1,0}(\kappa\bar{\nu}))\right)G_{1,0}(|\varphi|^2)\right) + \mathcal{O}(\alpha^2). \end{aligned}$$

Hence,

$$\begin{aligned} \text{Tr}(|D^0|Q_{+, \frac{1}{2}}(\alpha)^2) - \text{Tr}(|D^0|Q_{-, \frac{1}{2}}(\alpha)^2) &= \frac{\alpha^2}{1 + \alpha B_\Lambda} \text{Tr}(|D^0|\{G_{1,0}(|\varphi|^2), G_{0,1}(G_{1,0}(\kappa\bar{\nu}))\}) \\ &+ \frac{\alpha^2}{(1 + \alpha B_\Lambda)^2} \text{Tr}(|D^0|\{G_{1,0}(|\varphi|^2)G_{1,0}(\rho_-(\kappa\bar{\nu}) - B_\Lambda\kappa\bar{\nu})\}) + \frac{\alpha^2}{(1 + \alpha B_\Lambda)^2} \text{Tr}(|D^0|G_{1,0}(|\varphi|^2)^2) \\ &\quad + \frac{\alpha^2}{1 + \alpha B_\Lambda} \text{Tr}\left(|D^0|\left\{G_{1,0}(|\varphi|^2), G_{1,0}\left(\frac{\alpha}{1 + \alpha B_\Lambda(k)}\rho_{0,1}(G_{1,0}(\kappa\bar{\nu}))\right)\right\}\right) + \mathcal{O}(\alpha^2). \end{aligned}$$

By the computations of the previous section,

$$\begin{aligned} \text{Tr}(|D^0|Q_{+, \frac{1}{2}}(\alpha)^2) - \text{Tr}(|D^0|Q_{-, \frac{1}{2}}(\alpha)^2) &= -\frac{\alpha^2}{1 + \alpha B_\Lambda} \text{Tr}(G_{1,0}(|\varphi|^2)R[G_{1,0}(\kappa\bar{\nu})]) + \frac{\alpha^2 B_\Lambda}{(1 + \alpha B_\Lambda)^2} \langle \varphi, V(\rho_-(\kappa\bar{\nu}) - B_\Lambda\kappa\bar{\nu})\varphi \rangle \\ &\quad + \frac{\alpha^2 B_\Lambda}{2(1 + \alpha B_\Lambda)^2} D(|\varphi|^2, |\varphi|^2) \\ &\quad + \frac{\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} \left\langle \varphi, V\left(\frac{\alpha}{1 + \alpha B_\Lambda(k)}\rho_{0,1}(G_{1,0}(\kappa\bar{\nu}))\right)\varphi \right\rangle + \mathcal{O}(\alpha^2). \end{aligned}$$

We treat the next term in the kinetic energy by writing

$$\begin{aligned} \text{Tr}(|D^0|\{Q_+(\kappa\bar{\nu}), Q_{+, \frac{1}{2}}(\alpha)\}) - \text{Tr}(|D^0|\{Q_-(\kappa\bar{\nu}), Q_{-, \frac{1}{2}}(\alpha)\}) \\ = \text{Tr}(|D^0|\{Q_+(\kappa\bar{\nu}), Q_{+, \frac{1}{2}}(\alpha) - Q_{-, \frac{1}{2}}(\alpha)\}) + \langle \varphi, \{|D^0|, Q_{-, \frac{1}{2}}(\alpha)\}\varphi \rangle. \end{aligned}$$

There is nothing to do about the second term,

$$\begin{aligned} \langle \varphi, \{|D^0|, Q_{-, \frac{1}{2}}(\alpha)\} \varphi \rangle &= 2\alpha \operatorname{Re} \langle |D^0| \varphi, G_{0,1,-}^{(\kappa)}(G_{1,0}(\kappa\bar{\nu})) \varphi \rangle \\ &\quad + \frac{2\alpha}{1 + \alpha B_\Lambda} \operatorname{Re} \langle |D^0| \varphi, G_{1,0}(\rho_-(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu}) \varphi \rangle \\ &\quad + 2\alpha \operatorname{Re} \left\langle |D^0| \varphi, G_{1,0} \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi \right\rangle. \end{aligned}$$

For the first term we write

$$\begin{aligned} \operatorname{Tr}(|D^0| \{Q_+(\kappa\bar{\nu}), Q_{+, \frac{1}{2}}(\alpha) - Q_{-, \frac{1}{2}}(\alpha)\}) &= 2\alpha \operatorname{Re} \langle S(G_{1,0}(\kappa\bar{\nu})) \varphi, \{|D^0|, Q_+(\kappa\bar{\nu})\} \varphi \rangle \\ &\quad + \frac{\alpha}{1 + \alpha B_\Lambda} \operatorname{Tr}(|D^0| \{Q_+(\kappa\bar{\nu}), G_{1,0}(|\varphi|^2)\}). \end{aligned}$$

Hence, writing  $Q_+(\kappa\bar{\nu}) = -G_{1,0}(\kappa\bar{\nu}) + Q_{+,r}(\kappa\bar{\nu})$ ,

$$\begin{aligned} \operatorname{Tr}(|D^0| \{Q_+(\kappa\bar{\nu}), Q_{+, \frac{1}{2}}(\alpha)\}) - \operatorname{Tr}(|D^0| \{Q_-(\kappa\bar{\nu}), Q_{-, \frac{1}{2}}(\alpha)\}) &= \\ 2\alpha \operatorname{Re} \langle S(G_{1,0}(\kappa\bar{\nu})) \varphi, \{|D^0|, Q_+(\kappa\bar{\nu})\} \varphi \rangle + \frac{\alpha}{1 + \alpha B_\Lambda} \operatorname{Tr}(|D^0| \{Q_+(\kappa\bar{\nu}), G_{1,0}(|\varphi|^2)\}) & \\ + 2\alpha \operatorname{Re} \langle |D^0| \varphi, G_{0,1,-}^{(\kappa)}(G_{1,0}(\kappa\bar{\nu})) \varphi \rangle + \frac{2\alpha}{1 + \alpha B_\Lambda} \operatorname{Re} \langle |D^0| \varphi, G_{1,0}(\rho_-(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu}) \varphi \rangle & \\ + 2\alpha \operatorname{Re} \left\langle |D^0| \varphi, G_{1,0} \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi \right\rangle. & \end{aligned}$$

The last term in the kinetic energy is the most painful to compute. As usual, we first write

$$\begin{aligned} \operatorname{Tr}(|D^0| \{Q_+(\kappa\bar{\nu}), Q_{+,r}(\alpha)\}) - \operatorname{Tr}(|D^0| \{Q_-(\kappa\bar{\nu}), Q_{-,r}(\alpha)\}) & \\ = \operatorname{Tr}(|D^0| \{Q_+(\kappa\bar{\nu}), Q_{+,r}(\alpha) - Q_{-,r}(\alpha)\}) + \langle \varphi, \{|D^0|, Q_{-,r}(\alpha)\} \varphi \rangle. & \end{aligned}$$

The advantage of this formulation is that it is enough to go to  $\mathcal{O}(\alpha^{3/2})$  for  $Q_{-,r}(\alpha)$  in the second term, while we have to go to the order  $\mathcal{O}(\alpha^2)$  only for the *difference*  $Q_{+,r}(\alpha) - Q_{-,r}(\alpha)$ . We have

$$\begin{aligned} Q_{\pm,r}(\alpha) &= -\alpha^2 G_{0,2,\pm}^{(\kappa)}(G_{1,0}(\kappa\bar{\nu})) + \frac{\alpha}{1 + \alpha B_\Lambda} (G_{1,0,\pm}^{(\kappa)} - G_{1,0})(\rho_{\pm}(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu}) \\ &\quad + \alpha (G_{1,0,\pm}^{(\kappa)} - G_{1,0}) \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \\ &\quad + \alpha G_{1,0} \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} (\rho_{0,1,\pm}^{(\kappa)} - \rho_{0,1})(G_{1,0}(\kappa\bar{\nu})) \right) \\ -\alpha G_{1,0} \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(Q_{\pm}(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu})) \right) &- \alpha G_{0,1,\pm}^{(\kappa)}(Q_{\pm}(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu})) + \mathcal{O}^{\mathcal{Q}}(\alpha^{3/2}). \end{aligned}$$

This leads to

$$\begin{aligned} \langle \varphi, \{|D^0|, Q_{-,r}(\alpha)\} \varphi \rangle &= \frac{2\alpha}{1 + \alpha B_\Lambda} \text{Re} \langle (G_{1,0,-}^{(\kappa)} - G_{1,0})(\rho_-(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu}) \varphi, |D^0| \varphi \rangle \\ &+ 2\alpha \text{Re} \left\langle (G_{1,0,-}^{(\kappa)} - G_{1,0}) \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi, |D^0| \varphi \right\rangle \\ &- 2\alpha \text{Re} \langle G_{0,1,-}^{(\kappa)} (Q_-(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu})) \varphi, |D^0| \varphi \rangle + \mathcal{O}(\alpha^{3/2}). \end{aligned}$$

We now write the monstrous expansion of  $Q_{+,r}(\alpha) - Q_{-,r}(\alpha)$  up to  $\mathcal{O}^2(\alpha^2)$ . We split it into two terms,

$$Q_{+,r}(\alpha) - Q_{-,r}(\alpha) = \textcircled{1} + \textcircled{2} + \mathcal{O}^{\text{kin}}(\alpha^2),$$

where  $\textcircled{1}$  collects the rank-one terms and  $\textcircled{2}$  collects the other messy terms. Here we go:

$$\begin{aligned} \textcircled{1} &= \frac{\alpha}{1 + \alpha B_\Lambda} (|S(\rho_+(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu}) \varphi\rangle \langle \varphi| + h.c.) - \alpha (|S(Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu})) \varphi\rangle \langle \varphi| + h.c.) \\ &+ \alpha \left( \left| S \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1,+}^{(\kappa)}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi \right\rangle \left\langle \varphi \right| + h.c. \right) \\ &- \alpha^2 \left( \left| S \left( G_{1,0} \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \right) \varphi \right\rangle \left\langle \varphi \right| + h.c. \right) \\ &- \alpha \left( \left| S \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu})) \right) \varphi \right\rangle \left\langle \varphi \right| + h.c. \right) \\ &- \alpha^2 (|S(G_{0,1,+}^{(\kappa)}(G_{1,0}(\kappa\bar{\nu}))) \varphi\rangle \langle \varphi| + h.c.), \end{aligned}$$

the last three terms being  $\mathcal{O}^{\text{kin}}(\alpha^{3/2})$ , and

$$\begin{aligned} \textcircled{2} &= \frac{\alpha}{1 + \alpha B_\Lambda} (G_{1,0,-}^{(\kappa)} - G_{1,0})(|\varphi|^2) - \frac{\alpha^2}{1 + \alpha B_\Lambda} G_{1,1,-}^{(\kappa)}(|\varphi|^2, G_{1,0}(\kappa\bar{\nu})) \\ &+ \alpha^2 G_{0,2,-}^{(\kappa)}(|\varphi\rangle \langle \varphi|, G_{1,0}(\kappa\bar{\nu})) - \alpha G_{0,1,-}^{(\kappa)}(|\varphi\rangle \langle \varphi|) - \frac{\alpha^2}{1 + \alpha B_\Lambda} G_{0,1,-}^{(\kappa)}(G_{1,0}(|\varphi|^2)) \\ &+ \frac{\alpha^2}{1 + \alpha B_\Lambda} G_{1,0} \left( \frac{U_\Lambda(|k|)}{1 + \alpha B_\Lambda(k)} |\varphi|^2 \right) + 2\alpha^2 G_{1,0} \left( \frac{1}{1 + \alpha B_\Lambda(k)} \text{Re}(S(G_{1,0}(\kappa\bar{\nu})) \varphi \bar{\varphi}) \right) \\ &+ \frac{\alpha^2}{1 + \alpha B_\Lambda} G_{1,0} \left( \frac{1}{1 + \alpha B_\Lambda(k)} \left( 2\text{Re}(S(\rho_+(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu}) \varphi \bar{\varphi}) + \rho_{1,0,-,r}^{(\kappa)}(|\varphi|^2) \right) \right) \\ &+ 2\alpha^2 G_{1,0} \left( \frac{1}{1 + \alpha B_\Lambda(k)} \text{Re} \left( S \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi \bar{\varphi} \right) \right) \\ &- 2\alpha^2 G_{1,0} \left( \frac{1}{1 + \alpha B_\Lambda(k)} \text{Re}(S(Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu})) \varphi \bar{\varphi}) \right) \end{aligned}$$

$$-\alpha^2 G_{1,0} \left( \frac{1}{1 + \alpha B_\Lambda(k)} \rho_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|) \right) - \frac{\alpha^2}{1 + \alpha B_\Lambda} G_{1,0} \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(|\varphi|^2)) \right),$$

where only the first term is  $\mathcal{O}^{\mathcal{Q}}(\alpha)$  and the other are  $\mathcal{O}^{\mathcal{Q}}(\alpha^{3/2})$ . As a consequence,

$$\begin{aligned} \text{Tr}(|D^0|\{Q_+(\kappa\bar{\nu}), \textcircled{1}\}) &= \frac{2\alpha}{1 + \alpha B_\Lambda} \text{Re}\langle S(\rho_+(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu})\varphi, \{|D^0|, Q_+(\kappa\bar{\nu})\}\varphi \rangle \\ &\quad - 2\alpha \text{Re}\langle S(Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu}))\varphi, \{|D^0|, Q_+(\kappa\bar{\nu})\}\varphi \rangle \\ &\quad + 2\alpha \text{Re} \left\langle S \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi, \{|D^0|, Q_+(\kappa\bar{\nu})\}\varphi \right\rangle + \mathcal{O}(\alpha^{3/2}), \end{aligned}$$

$$\begin{aligned} \text{Tr}(|D^0|\{Q_+(\kappa\bar{\nu}), \textcircled{2}\}) &= \frac{\alpha}{1 + \alpha B_\Lambda} \text{Tr}(|D^0|\{Q_+(\kappa\bar{\nu}), (G_{1,0,-}^{(\kappa)} - G_{1,0})(|\varphi|^2)\}) \\ &\quad - \alpha \langle \varphi, R[G_{1,0}(\kappa\bar{\nu})]\varphi \rangle - \alpha \text{Tr}(|D^0|\{Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu}), G_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\}) \\ &+ \alpha \text{Tr}(|D^0|\{G_{1,0}(\kappa\bar{\nu}), (G_{0,1,-}^{(\kappa)} - G_{0,1})(|\varphi\rangle\langle\varphi|)\}) - \frac{\alpha^2}{1 + \alpha B_\Lambda} \text{Tr}(G_{1,0}(|\varphi|^2)R[G_{1,0}(\kappa\bar{\nu})]) \\ &- \frac{\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} D \left( \kappa\bar{\nu}, \frac{U_\Lambda(|k|)}{1 + \alpha B_\Lambda(k)} |\varphi|^2 \right) - 2\alpha^2 B_\Lambda D \left( \kappa\bar{\nu}, \frac{1}{1 + \alpha B_\Lambda(k)} \text{Re}(S(G_{1,0}(\kappa\bar{\nu}))\varphi\bar{\varphi}) \right) \\ &\quad - \frac{\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} D \left( \kappa\bar{\nu}, \frac{1}{1 + \alpha B_\Lambda(k)} \left( 2\text{Re}(S(\rho_+(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu})\varphi\bar{\varphi}) + \rho_{1,0,-,r}^{(\kappa)}(|\varphi|^2) \right) \right) \\ &\quad - 2\alpha^2 B_\Lambda D \left( \kappa\bar{\nu}, \frac{1}{1 + \alpha B_\Lambda(k)} \text{Re} \left( S \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi\bar{\varphi} \right) \right) \\ &\quad + 2\alpha^2 B_\Lambda D \left( \kappa\bar{\nu}, \frac{1}{1 + \alpha B_\Lambda(k)} \text{Re}(S(Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu}))\varphi\bar{\varphi}) \right) \\ &\quad + \alpha^2 B_\Lambda D \left( \kappa\bar{\nu}, \frac{1}{1 + \alpha B_\Lambda(k)} \rho_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|) \right) \\ &\quad + \frac{\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} D \left( \kappa\bar{\nu}, \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(|\varphi|^2)) \right) + \mathcal{O}(\alpha^{3/2}). \end{aligned}$$

For the total kinetic energy we thus find

$$\begin{aligned} \text{Tr}(|D^0|Q_+(\alpha)^2) - \text{Tr}(|D^0|Q_-(\alpha)^2) &= \langle \varphi(\kappa, \Lambda), D^0 \varphi(\kappa, \Lambda) \rangle \\ &\quad - \frac{2\alpha^2}{1 + \alpha B_\Lambda} \text{Tr}(G_{1,0}(|\varphi|^2)R[G_{1,0}(\kappa\bar{\nu})]) + \frac{\alpha^2 B_\Lambda}{(1 + \alpha B_\Lambda)^2} \langle \varphi, V(\rho_-(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu})\varphi \rangle \\ &\quad + \frac{\alpha^2 B_\Lambda}{2(1 + \alpha B_\Lambda)^2} D(|\varphi|^2, |\varphi|^2) + \frac{\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} \left\langle \varphi, V \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi \right\rangle \\ &\quad - 2\alpha \text{Re}\langle S(Q_+(\kappa\bar{\nu}))\varphi, \{|D^0|, Q_+(\kappa\bar{\nu})\}\varphi \rangle + \frac{\alpha}{1 + \alpha B_\Lambda} \text{Tr}(|D^0|\{Q_+(\kappa\bar{\nu}), G_{1,0}(|\varphi|^2)\}) \\ &\quad - 2\alpha \text{Re}\langle G_{0,1,-}^{(\kappa)}(Q_-(\kappa\bar{\nu}))\varphi, |D^0|\varphi \rangle + \frac{2\alpha}{1 + \alpha B_\Lambda} \text{Re}\langle G_{1,0,-}^{(\kappa)}(\rho_-(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu})\varphi, |D^0|\varphi \rangle \end{aligned}$$

$$\begin{aligned}
& + 2\alpha \operatorname{Re} \left\langle G_{1,0,-}^{(\kappa)} \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi, |D^0| \varphi \right\rangle \\
& + \frac{2\alpha}{1 + \alpha B_\Lambda} \operatorname{Re} \langle S(\rho_+(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu}) \varphi, \{|D^0|, Q_+(\kappa\bar{\nu})\} \varphi \rangle \\
& + 2\alpha \operatorname{Re} \left\langle S \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi, \{|D^0|, Q_+(\kappa\bar{\nu})\} \varphi \right\rangle \\
& + \frac{\alpha}{1 + \alpha B_\Lambda} \operatorname{Tr}(|D^0| \{Q_+(\kappa\bar{\nu}), (G_{1,0,-}^{(\kappa)} - G_{1,0})(|\varphi|^2)\}) - \alpha \langle \varphi, R[G_{1,0}(\kappa\bar{\nu})] \varphi \rangle \\
& - \alpha \operatorname{Tr}(|D^0| \{Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu}), G_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\}) \\
& + \alpha \operatorname{Tr}(|D^0| \{G_{1,0}(\kappa\bar{\nu}), (G_{0,1,-}^{(\kappa)} - G_{0,1})(|\varphi\rangle\langle\varphi|)\}) - \frac{\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} D \left( \kappa\bar{\nu}, \frac{U_\Lambda(|k|)}{1 + \alpha B_\Lambda(k)} |\varphi|^2 \right) \\
& - 2\alpha^2 B_\Lambda D \left( \kappa\bar{\nu}, \frac{1}{1 + \alpha B_\Lambda(k)} \operatorname{Re}(S(G_{1,0}(\kappa\bar{\nu})) \varphi \bar{\varphi}) \right) \\
& - \frac{\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} D \left( \kappa\bar{\nu}, \frac{1}{1 + \alpha B_\Lambda(k)} \left( 2\operatorname{Re}(S(\rho_+(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu}) \varphi \bar{\varphi}) + \rho_{1,0,-}^{(\kappa)}(|\varphi|^2) \right) \right) \\
& - 2\alpha^2 B_\Lambda D \left( \kappa\bar{\nu}, \frac{1}{1 + \alpha B_\Lambda(k)} \operatorname{Re} \left( S \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi \bar{\varphi} \right) \right) \\
& + 2\alpha^2 B_\Lambda D \left( \kappa\bar{\nu}, \frac{1}{1 + \alpha B_\Lambda(k)} \operatorname{Re}(S(Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu})) \varphi \bar{\varphi}) \right) \\
& + \alpha^2 B_\Lambda D \left( \kappa\bar{\nu}, \frac{1}{1 + \alpha B_\Lambda(k)} \rho_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|) \right) \\
& + \frac{\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} D \left( \kappa\bar{\nu}, \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(|\varphi|^2)) \right) + \mathcal{O}(\alpha^{3/2}).
\end{aligned}$$

For the last seven terms, we notice that using

$$\frac{1}{1 + \alpha B_\Lambda(k)} = \frac{1}{1 + \alpha B_\Lambda} + \frac{\alpha U_\Lambda(|k|)}{(1 + \alpha B_\Lambda)(1 + \alpha B_\Lambda(k))},$$

we get for instance

$$\begin{aligned}
D \left( \kappa\bar{\nu}, \frac{U_\Lambda(|k|)}{1 + \alpha B_\Lambda(k)} |\varphi|^2 \right) &= \frac{1}{1 + \alpha B_\Lambda} D(\kappa\bar{\nu}, U_\Lambda(|k|) |\varphi|^2) \\
&+ \frac{\alpha}{1 + \alpha B_\Lambda} D \left( U_\Lambda(|k|) \kappa\bar{\nu}, \frac{U_\Lambda(|k|)}{1 + \alpha B_\Lambda(k)} |\varphi|^2 \right),
\end{aligned}$$

the second term being a  $\mathcal{O}(\alpha)$  by the regularity of  $\nu$ . Hence, we can rewrite the kinetic energy by changing only the last seven terms,

$$\begin{aligned}
& \text{Tr}(|D^0|Q_+(\alpha)^2) - \text{Tr}(|D^0|Q_-(\alpha)^2) = \langle \varphi(\kappa, \Lambda), D^0 \varphi(\kappa, \Lambda) \rangle \\
& - \frac{2\alpha^2}{1 + \alpha B_\Lambda} \text{Tr}(G_{1,0}(|\varphi|^2)R[G_{1,0}(\kappa\bar{\nu})]) + \frac{\alpha^2 B_\Lambda}{(1 + \alpha B_\Lambda)^2} \langle \varphi, V(\rho_-(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu}) \varphi \rangle \\
& + \frac{\alpha^2 B_\Lambda}{2(1 + \alpha B_\Lambda)^2} D(|\varphi|^2, |\varphi|^2) + \frac{\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} \left\langle \varphi, V \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi \right\rangle \\
& - 2\alpha \text{Re} \langle S(Q_+(\kappa\bar{\nu})) \varphi, \{|D^0|, Q_+(\kappa\bar{\nu})\} \varphi \rangle + \frac{\alpha}{1 + \alpha B_\Lambda} \text{Tr}(|D^0| \{Q_+(\kappa\bar{\nu}), G_{1,0}(|\varphi|^2)\}) \\
& - 2\alpha \text{Re} \langle G_{0,1,-}^{(\kappa)}(Q_-(\kappa\bar{\nu})) \varphi, |D^0| \varphi \rangle + \frac{2\alpha}{1 + \alpha B_\Lambda} \text{Re} \langle G_{1,0,-}^{(\kappa)}(\rho_-(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu}) \varphi, |D^0| \varphi \rangle \\
& + 2\alpha \text{Re} \left\langle G_{1,0,-}^{(\kappa)} \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi, |D^0| \varphi \right\rangle \\
& + \frac{2\alpha}{1 + \alpha B_\Lambda} \text{Re} \langle S(\rho_+(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu}) \varphi, \{|D^0|, Q_+(\kappa\bar{\nu})\} \varphi \rangle \\
& + 2\alpha \text{Re} \left\langle S \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi, \{|D^0|, Q_+(\kappa\bar{\nu})\} \varphi \right\rangle \\
& + \frac{\alpha}{1 + \alpha B_\Lambda} \text{Tr}(|D^0| \{Q_+(\kappa\bar{\nu}), (G_{1,0,-}^{(\kappa)} - G_{1,0})(|\varphi|^2)\}) - \alpha \langle \varphi, R[G_{1,0}(\kappa\bar{\nu})] \varphi \rangle \\
& - \alpha \text{Tr}(|D^0| \{Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu}), G_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\}) \\
& + \alpha \text{Tr}(|D^0| \{G_{1,0}(\kappa\bar{\nu}), (G_{0,1,-}^{(\kappa)} - G_{0,1})(|\varphi\rangle\langle\varphi|)\}) - \frac{\alpha^2 B_\Lambda}{(1 + \alpha B_\Lambda)^2} \langle \varphi, V(U_\Lambda(|k|)\kappa\bar{\nu}) \varphi \rangle \\
& - \frac{2\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} D(\kappa\bar{\nu}, \text{Re}(S(G_{1,0}(\kappa\bar{\nu}))\varphi\bar{\varphi})) \\
& - \frac{\alpha^2 B_\Lambda}{(1 + \alpha B_\Lambda)^2} D\left(\kappa\bar{\nu}, \left(2\text{Re}(S(\rho_+(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu})\varphi\bar{\varphi}) + \rho_{1,0,-}^{(\kappa)}(|\varphi|^2)\right)\right) \\
& - \frac{2\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} D\left(\kappa\bar{\nu}, \text{Re}\left(S\left(\frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu}))\right)\varphi\bar{\varphi}\right)\right) \\
& + \frac{\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} D\left(\kappa\bar{\nu}, 2\text{Re}(S(Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu}))\varphi\bar{\varphi}) + \rho_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\right) \\
& + \frac{\alpha^2 B_\Lambda}{(1 + \alpha B_\Lambda)^2} D(\kappa\bar{\nu}, \alpha \rho_{0,1}(G_{1,0}(|\varphi|^2))) + \mathcal{O}(\alpha^{3/2}).
\end{aligned}$$

To compute the next term in the energy, that is  $-D(\kappa\nu, \rho_+(\alpha) - \rho_-(\alpha))$ , we need to develop  $\rho_+(\alpha) - \rho_-(\alpha)$  up to  $\mathcal{O}(\alpha^{3/2})$ . We have

$$\rho_+(\alpha) - \rho_-(\alpha) = \frac{1}{1 + \alpha B_\Lambda(k)} |\varphi|^2 + \frac{2\alpha}{1 + \alpha B_\Lambda(k)} \text{Re}(S(G_{1,0}(\kappa\bar{\nu}))\varphi\bar{\varphi})$$



$$\begin{aligned}
& + \frac{\alpha}{1 + \alpha B_\Lambda} \frac{1}{1 + \alpha B_\Lambda(k)} \left( 2\operatorname{Re}(S(\rho_+(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu})\varphi\bar{\varphi}) + \rho_{1,0,-,r}^{(\kappa)}(|\varphi|^2) \right) \\
& \quad + \frac{2\alpha}{1 + \alpha B_\Lambda(k)} \operatorname{Re} \left( S \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi\bar{\varphi} \right) \\
& \quad - \frac{\alpha}{1 + \alpha B_\Lambda(k)} (2\operatorname{Re}(S(Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu}))\varphi\bar{\varphi}) + \rho_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|)) \\
& \quad \quad - \frac{\alpha^2}{1 + \alpha B_\Lambda} \frac{1}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(|\varphi|^2)) + \mathcal{O}^{L^2nc}(\alpha^{3/2}).
\end{aligned}$$

By the same method as above, we have

$$\begin{aligned}
& - D(\kappa\nu, \rho_+(\alpha) - \rho_-(\alpha)) = -\langle\varphi, V(\kappa\bar{\nu})\varphi\rangle - \frac{\alpha}{1 + \alpha B_\Lambda} \langle\varphi, V(U_\Lambda(|k|)\kappa\bar{\nu})\varphi\rangle \\
& \quad - 2\alpha D(\kappa\bar{\nu}, \operatorname{Re}(S(G_{1,0}(\kappa\bar{\nu}))\varphi\bar{\varphi})) \\
& \quad - \frac{\alpha}{1 + \alpha B_\Lambda} D\left(\kappa\bar{\nu}, \left(2\operatorname{Re}(S(\rho_+(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu})\varphi\bar{\varphi}) + \rho_{1,0,-,r}^{(\kappa)}(|\varphi|^2)\right)\right) \\
& \quad \quad - 2\alpha D\left(\kappa\bar{\nu}, \operatorname{Re}\left(S\left(\frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu}))\right)\varphi\bar{\varphi}\right)\right) \\
& \quad + \alpha D\left(\kappa\bar{\nu}, \left(2\operatorname{Re}(S(Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu}))\varphi\bar{\varphi}) + \rho_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\right)\right) \\
& \quad \quad - \frac{\alpha}{1 + \alpha B_\Lambda} D(\kappa\bar{\nu}, \alpha\rho_{0,1}(G_{1,0}(|\varphi|^2)) + \mathcal{O}(\alpha^{3/2})).
\end{aligned}$$

We now pass to the direct term,

$$\frac{\alpha}{2} \left( D(\rho_+(\alpha)) - D(\rho_-(\alpha)) \right) = \frac{\alpha}{2} \left( D(\rho_+(\alpha) - \rho_-(\alpha)) + 2D(\rho_+(\alpha) - \rho_-(\alpha), \rho_-(\alpha)) \right).$$

For the first term, we have to compute  $\rho_+(\alpha) - \rho_-(\alpha)$  up to  $\mathcal{O}(\sqrt{\alpha})$ ,

$$\rho_+(\alpha) - \rho_-(\alpha) = \frac{1}{1 + \alpha B_\Lambda} |\varphi|^2 + \mathcal{O}^{L^2nc}(\alpha),$$

hence

$$\frac{\alpha}{2} D(\rho_+(\alpha) - \rho_-(\alpha)) = \frac{\alpha}{2(1 + \alpha B_\Lambda)^2} D(|\varphi|^2, |\varphi|^2) + \mathcal{O}(\alpha^2).$$

To compute the second term, we use

$$\rho_-(\alpha) = B_\Lambda \kappa\bar{\nu} + \frac{1}{1 + \alpha B_\Lambda} (\rho_-(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu}) + \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) + \mathcal{O}^{L^2nc}(\sqrt{\alpha}),$$

$$\begin{aligned}
\alpha D(\rho_+(\alpha) - \rho_-(\alpha), \rho_-(\alpha)) &= \frac{\alpha B_\Lambda}{1 + \alpha B_\Lambda} \langle \varphi, V(\kappa \bar{\nu}) \varphi \rangle + \frac{\alpha}{(1 + \alpha B_\Lambda)^2} \langle \varphi, V(\rho_-(\kappa \bar{\nu}) - B_\Lambda \kappa \bar{\nu}) \varphi \rangle \\
&+ \frac{\alpha}{(1 + \alpha B_\Lambda)^2} \langle \varphi, V(\alpha \rho_{0,1}(G_{1,0}(\kappa \bar{\nu}))) \varphi \rangle + \frac{\alpha^2 B_\Lambda}{(1 + \alpha B_\Lambda)^2} \langle \varphi, V(U_\Lambda(|k|) \kappa \bar{\nu}) \varphi \rangle \\
&\quad + \frac{2\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} D(\kappa \bar{\nu}, \operatorname{Re}(S(G_{1,0}(\kappa \bar{\nu})) \varphi \bar{\varphi})) \\
&+ \frac{\alpha^2 B_\Lambda}{(1 + \alpha B_\Lambda)^2} D\left(\kappa \bar{\nu}, \left(2\operatorname{Re}(S(\rho_+(\kappa \bar{\nu}) - B_\Lambda \kappa \bar{\nu}) \varphi \bar{\varphi}) + \rho_{1,0,-,r}^{(\kappa)}(|\varphi|^2)\right)\right) \\
&\quad + \frac{2\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} D\left(\kappa \bar{\nu}, \operatorname{Re}\left(S\left(\frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa \bar{\nu}))\right) \varphi \bar{\varphi}\right)\right) \\
&- \frac{\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} D(\kappa \bar{\nu}, (2\operatorname{Re}(S(Q_+(\kappa \bar{\nu}) + G_{1,0}(\kappa \bar{\nu})) \varphi \bar{\varphi}) + \rho_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|))) \\
&\quad - \frac{\alpha^2 B_\Lambda}{(1 + \alpha B_\Lambda)^2} D(\kappa \bar{\nu}, \alpha \rho_{0,1}(G_{1,0}(|\varphi|^2))) + \mathcal{O}(\alpha^{3/2}).
\end{aligned}$$

Hence for the direct term,

$$\begin{aligned}
\frac{\alpha}{2} \left( D(\rho_+(\alpha)) - D(\rho_-(\alpha)) \right) &= \frac{\alpha}{2(1 + \alpha B_\Lambda)^2} D(|\varphi|^2, |\varphi|^2) + \frac{\alpha B_\Lambda}{1 + \alpha B_\Lambda} \langle \varphi, V(\kappa \bar{\nu}) \varphi \rangle \\
&+ \frac{\alpha}{(1 + \alpha B_\Lambda)^2} \langle \varphi, V(\rho_-(\kappa \bar{\nu}) - B_\Lambda \kappa \bar{\nu}) \varphi \rangle + \frac{\alpha}{(1 + \alpha B_\Lambda)^2} \langle \varphi, V(\alpha \rho_{0,1}(G_{1,0}(\kappa \bar{\nu}))) \varphi \rangle \\
&+ \frac{\alpha^2 B_\Lambda}{(1 + \alpha B_\Lambda)^2} \langle \varphi, V(U_\Lambda(|k|) \kappa \bar{\nu}) \varphi \rangle + \frac{2\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} D(\kappa \bar{\nu}, \operatorname{Re}(S(G_{1,0}(\kappa \bar{\nu})) \varphi \bar{\varphi})) \\
&+ \frac{\alpha^2 B_\Lambda}{(1 + \alpha B_\Lambda)^2} D\left(\kappa \bar{\nu}, \left(2\operatorname{Re}(S(\rho_+(\kappa \bar{\nu}) - B_\Lambda \kappa \bar{\nu}) \varphi \bar{\varphi}) + \rho_{1,0,-,r}^{(\kappa)}(|\varphi|^2)\right)\right) \\
&\quad + \frac{2\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} D\left(\kappa \bar{\nu}, \operatorname{Re}\left(S\left(\frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa \bar{\nu}))\right) \varphi \bar{\varphi}\right)\right) \\
&- \frac{\alpha^2 B_\Lambda}{1 + \alpha B_\Lambda} D(\kappa \bar{\nu}, (2\operatorname{Re}(S(Q_+(\kappa \bar{\nu}) + G_{1,0}(\kappa \bar{\nu})) \varphi \bar{\varphi}) + \rho_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|))) \\
&\quad - \frac{\alpha^2 B_\Lambda}{(1 + \alpha B_\Lambda)^2} D(\kappa \bar{\nu}, \alpha \rho_{0,1}(G_{1,0}(|\varphi|^2))) + \mathcal{O}(\alpha^{3/2}).
\end{aligned}$$

Finally, for the exchange term,

$$\begin{aligned}
& - \frac{\alpha}{2} \left( \int_{\mathbb{R}^6} \frac{|[Q_+(\alpha)](x, y)|^2}{|x - y|} dx dy - \int_{\mathbb{R}^6} \frac{|[Q_-(\alpha)](x, y)|^2}{|x - y|} dx dy \right) = \\
& \quad - \frac{\alpha}{2} \int_{\mathbb{R}^6} \frac{|[Q_+(\alpha) - Q_-(\alpha)](x, y)|^2}{|x - y|} dx dy \\
& \quad - \alpha \int_{\mathbb{R}^6} \frac{\operatorname{Tr}_{\mathbb{C}^4}([Q_+(\alpha) - Q_-(\alpha)](x, y)[Q_-(\alpha)](x, y)^*)}{|x - y|} dx dy.
\end{aligned}$$

For the first term, we have to compute  $Q_+(\alpha) - Q_-(\alpha)$  up  $\mathcal{O}^{\mathcal{Q}}(\sqrt{\alpha})$ . We have

$$Q_+(\alpha) - Q_-(\alpha) = |\varphi\rangle\langle\varphi| + \mathcal{O}^{\mathcal{Q}}(\sqrt{\alpha}),$$

so that

$$-\frac{\alpha}{2} \int_{\mathbb{R}^6} \frac{|[Q_+(\alpha) - Q_-(\alpha)](x, y)|^2}{|x - y|} dx dy = -\frac{\alpha}{2} D(|\varphi|^2, |\varphi|^2) + \mathcal{O}(\alpha^{3/2}).$$

To treat the second term we use

$$Q_+(\alpha) - Q_-(\alpha) = |\varphi\rangle\langle\varphi| + \frac{\alpha}{1 + \alpha B_\Lambda} G_{1,0}(|\varphi|^2) + \mathcal{O}^{\text{kin}}(\alpha),$$

$$Q_-(\alpha) = Q_-(\kappa\bar{\nu}) + \mathcal{O}^{\mathcal{Q}}(\sqrt{\alpha}).$$

Hence,

$$\begin{aligned} & -\alpha \int_{\mathbb{R}^6} \frac{\text{Tr}_{\mathbb{C}^4} ([Q_+(\alpha) - Q_-(\alpha)](x, y)[Q_-(\alpha)](x, y)^*)}{|x - y|} dx dy \\ &= -\alpha \langle \varphi, R[Q_-(\kappa\bar{\nu})]\varphi \rangle - \frac{\alpha^2}{1 + \alpha B_\Lambda} \text{Tr}(G_{1,0}(|\varphi|^2)R[Q_-(\kappa\bar{\nu})]) + \mathcal{O}(\alpha^{3/2}). \end{aligned}$$

For the exchange term, we thus obtain

$$\begin{aligned} & -\frac{\alpha}{2} \left( \int_{\mathbb{R}^6} \frac{|[Q_+(\alpha)](x, y)|^2}{|x - y|} dx dy - \int_{\mathbb{R}^6} \frac{|[Q_-(\alpha)](x, y)|^2}{|x - y|} dx dy \right) \\ &= -\frac{\alpha}{2} D(|\varphi|^2, |\varphi|^2) - \alpha \langle \varphi, R[Q_-(\kappa\bar{\nu})]\varphi \rangle - \frac{\alpha^2}{1 + \alpha B_\Lambda} \text{Tr}(G_{1,0}(|\varphi|^2)R[G_{1,0}(\kappa\bar{\nu})]) + \mathcal{O}(\alpha^{3/2}). \end{aligned}$$

For the total energy, we finally have

$$\begin{aligned} F(\kappa, \alpha) &= \lambda_1(\kappa, \Lambda) + \alpha \left\langle \varphi, \left( \frac{1}{1 + \alpha B_\Lambda} V(\rho_-(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu}) - R[Q_-(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu})] \right) \varphi \right\rangle \\ &+ \frac{\alpha}{1 + \alpha B_\Lambda} \langle \varphi, V(\alpha \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})))\varphi \rangle - \frac{3\alpha^2}{1 + \alpha B_\Lambda} \text{Tr}(G_{1,0}(|\varphi|^2)R[G_{1,0}(\kappa\bar{\nu})]) \\ &+ \frac{\alpha}{2(1 + \alpha B_\Lambda)} D(|\varphi|^2, |\varphi|^2) - \frac{\alpha}{1 + \alpha B_\Lambda} \langle \varphi, V(U_\Lambda(|k|)\kappa\bar{\nu})\varphi \rangle \\ &+ \frac{\alpha}{1 + \alpha B_\Lambda} \text{Tr}(|D^0| \{Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu}), G_{1,0}(|\varphi|^2)\}) \\ &- 2\alpha \text{Re} \langle S(Q_+(\kappa\bar{\nu}))\varphi, \{|D^0|, Q_+(\kappa\bar{\nu})\}\varphi \rangle - 2\alpha \text{Re} \langle G_{0,1,-}^{(\kappa)}(Q_-(\kappa\bar{\nu}))\varphi, |D^0|\varphi \rangle \\ &+ \frac{2\alpha}{1 + \alpha B_\Lambda} \text{Re} \langle G_{1,0,-}^{(\kappa)}(\rho_-(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu})\varphi, |D^0|\varphi \rangle \\ &+ 2\alpha \text{Re} \left\langle G_{1,0,-}^{(\kappa)} \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi, |D^0|\varphi \right\rangle \\ &+ \frac{2\alpha}{1 + \alpha B_\Lambda} \text{Re} \langle S(\rho_+(\kappa\bar{\nu}) - B_\Lambda \kappa\bar{\nu})\varphi, \{|D^0|, Q_+(\kappa\bar{\nu})\}\varphi \rangle \end{aligned}$$

$$\begin{aligned}
& + 2\alpha \operatorname{Re} \left\langle S \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \right) \varphi, \{|D^0|, Q_+(\kappa\bar{\nu})\} \varphi \right\rangle \\
& \quad + \frac{\alpha}{1 + \alpha B_\Lambda} \operatorname{Tr}(|D^0| \{Q_+(\kappa\bar{\nu}), (G_{1,0}^{(\kappa)} - G_{1,0})(|\varphi|^2)\}) \\
& \quad - \alpha \operatorname{Tr}(|D^0| \{Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu}), G_{0,1}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\}) \\
& + \alpha \operatorname{Tr}(|D^0| \{G_{1,0}(\kappa\bar{\nu}), (G_{0,1}^{(\kappa)} - G_{0,1})(|\varphi\rangle\langle\varphi|)\}) - 2\alpha D(\kappa\bar{\nu}, \operatorname{Re}(S(G_{1,0}(\kappa\bar{\nu}))\varphi\bar{\varphi})) \\
& - \frac{\alpha}{1 + \alpha B_\Lambda} D\left(\kappa\bar{\nu}, \left(2\operatorname{Re}(S(\rho_+(\kappa\bar{\nu}) - B_\Lambda\kappa\bar{\nu})\varphi\bar{\varphi}) + \rho_{1,0,-}^{(\kappa)}(|\varphi|^2)\right)\right) \\
& \quad - 2\alpha D\left(\kappa\bar{\nu}, \operatorname{Re}\left(S\left(\frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa\bar{\nu}))\right) \varphi\bar{\varphi}\right)\right) \\
& + \alpha D\left(\kappa\bar{\nu}, 2\operatorname{Re}(S(Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu}))\varphi\bar{\varphi}) + \rho_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\right) \\
& \quad - \frac{\alpha}{1 + \alpha B_\Lambda} D(\kappa\bar{\nu}, \alpha\rho_{0,1}(G_{1,0}(|\varphi|^2))) + \mathcal{O}(\alpha^{3/2}).
\end{aligned}$$

Notice that

$$\begin{aligned}
\operatorname{Tr}(G_{1,0}(|\varphi|^2)R[G_{1,0}(\kappa\bar{\nu})]) &= \operatorname{Tr}(V_{|\varphi|^2}G_{0,1}(G_{1,0}(\kappa\bar{\nu}))) \\
&= \int V_{|\varphi|^2}\rho_{0,1}(G_{1,0}(\kappa\bar{\nu})) \\
&= \langle\varphi, V(\rho_{0,1}(G_{1,0}(\kappa\bar{\nu})))\varphi\rangle,
\end{aligned}$$

hence

$$\begin{aligned}
\frac{\alpha}{1 + \alpha B_\Lambda} \langle\varphi, V(\alpha\rho_{0,1}(G_{1,0}(\kappa\bar{\nu})))\varphi\rangle - \frac{3\alpha^2}{1 + \alpha B_\Lambda} \operatorname{Tr}(G_{1,0}(|\varphi|^2)R[G_{1,0}(\kappa\bar{\nu})]) \\
= -\frac{2\alpha}{1 + \alpha B_\Lambda} \langle\varphi, V(\alpha\rho_{0,1}(G_{1,0}(\kappa\bar{\nu})))\varphi\rangle.
\end{aligned}$$

We can add to this term the last term of the energy, since

$$\begin{aligned}
D(\kappa\bar{\nu}, \rho_{0,1}(G_{1,0}(|\varphi|^2))) &= \operatorname{Tr}(V_{\kappa\bar{\nu}}G_{0,1}(G_{1,0}(|\varphi|^2))) \\
&= \operatorname{Tr}(G_{1,0}(\kappa\bar{\nu})R[G_{1,0}(|\varphi|^2)]) \\
&= \operatorname{Tr}(R[G_{1,0}(\kappa\bar{\nu})]G_{1,0}(|\varphi|^2)) \\
&= \operatorname{Tr}(G_{0,1}(G_{1,0}(\kappa\bar{\nu}))V_{|\varphi|^2}) \\
&= \langle\varphi, V(\rho_{0,1}(G_{1,0}(\kappa\bar{\nu})))\varphi\rangle.
\end{aligned}$$

Thus,

$$\begin{aligned}
\frac{\alpha}{1 + \alpha B_\Lambda} \langle\varphi, V(\alpha\rho_{0,1}(G_{1,0}(\kappa\bar{\nu})))\varphi\rangle - \frac{3\alpha^2}{1 + \alpha B_\Lambda} \operatorname{Tr}(G_{1,0}(|\varphi|^2)R[G_{1,0}(\kappa\bar{\nu})]) \\
- \frac{\alpha}{1 + \alpha B_\Lambda} D(\kappa\bar{\nu}, \alpha\rho_{0,1}(G_{1,0}(|\varphi|^2))) = -\frac{3\alpha}{1 + \alpha B_\Lambda} \langle\varphi, V(\alpha\rho_{0,1}(G_{1,0}(\kappa\bar{\nu})))\varphi\rangle.
\end{aligned}$$

Next, we have

$$\begin{aligned} \text{Tr}(|D^0|\{Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu}), G_{1,0}(|\varphi|^2)\}) &= \text{Tr}(G_1(\{|D^0|, Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu})\})V_{|\varphi|^2}) \\ &= \langle \varphi, V(\rho_1(\{|D^0|, Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu})\}))\varphi \rangle, \end{aligned}$$

where for any  $Q$ ,  $\rho_1(Q) := \rho_{G_1(Q)}$  and

$$G_1(Q) := \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D^0 + i\eta} \Pi_{\Lambda} Q \Pi_{\Lambda} \frac{1}{D^0 + i\eta} d\eta.$$

For any  $Q$ , notice that

$$\mathcal{F}[G_1(\{|D^0|, Q\})](p, q) = \frac{1}{2} \left( \frac{D^0(p)}{E(p)} \widehat{Q}(p, q) \frac{D^0(q)}{E(q)} - \widehat{Q}(p, q) \right),$$

thus

$$\begin{aligned} \mathcal{F}[\rho_1(\{|D^0|, Q\})](k) &= \frac{1}{2^{5/2}\pi^{3/2}} \times \\ &\times \int_{\substack{|\ell-k/2| \leq \Lambda \\ |\ell+k/2| \leq \Lambda}} \text{Tr}_{\mathbb{C}^4} \left( \left( \frac{D^0(\ell-k/2)D^0(\ell+k/2)}{E(\ell-k/2)E(\ell+k/2)} - 1 \right) \widehat{Q}(\ell+k/2, \ell-k/2) \right) d\ell. \end{aligned}$$

In the same fashion, we have

$$\text{Tr}(|D^0|\{Q_+(\kappa\bar{\nu}), (G_{1,0,-}^{(\kappa)} - G_{1,0})(|\varphi|^2)\}) = \langle \varphi, V((\rho_{1,-}^{(\kappa)} - \rho_1)(\{|D^0|, Q_+(\kappa\bar{\nu})\}))\varphi \rangle.$$

Using that for any operators  $Q, K$ , we have  $\text{Tr}(R_Q K) = \text{Tr}(R_K Q)$ , we obtain

$$\text{Tr}(|D^0|\{Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu}), G_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|)\}) = \langle \varphi, R[G_{1,-}^{(\kappa)}(\{|D^0|, Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu})\})]\varphi \rangle,$$

$$\text{Tr}(|D^0|\{G_{1,0}(\kappa\bar{\nu}), (G_{0,1,-}^{(\kappa)} - G_{0,1})(|\varphi\rangle\langle\varphi|)\}) = \langle \varphi, R[(G_{1,-}^{(\kappa)} - G_1)(\{|D^0|, G_{1,0}(\kappa\bar{\nu})\})]\varphi \rangle.$$

Next,

$$\begin{aligned} D(\kappa\bar{\nu}, 2\text{Re}(S(G_{1,0}(\kappa\bar{\nu}))\varphi\bar{\varphi})) &= \text{Tr}(V_{\kappa\bar{\nu}}(|S(G_{1,0}(\kappa\bar{\nu}))\varphi\rangle\langle\varphi| + |\varphi\rangle\langle S(G_{1,0}(\kappa\bar{\nu}))\varphi|)) \\ &= \langle \varphi, \{V_{\kappa\bar{\nu}}, S(G_{1,0}(\kappa\bar{\nu}))\}\varphi \rangle, \end{aligned}$$

$$D(\kappa\bar{\nu}, 2\text{Re}(S(\rho_+(\kappa\bar{\nu}) - B_{\Lambda}\kappa\bar{\nu})\varphi\bar{\varphi})) = \langle \varphi, \{V_{\kappa\bar{\nu}}, S(\rho_+(\kappa\bar{\nu}) - B_{\Lambda}\kappa\bar{\nu})\}\varphi \rangle,$$

$$D(\kappa\bar{\nu}, \rho_{1,0,-,r}^{(\kappa)}(|\varphi|^2)) = \langle \varphi, V((\rho_{1,0,-}^{(\kappa)} - \rho_{1,0})(\kappa\bar{\nu}))\varphi \rangle,$$

$$\begin{aligned} D\left(\kappa\bar{\nu}, \text{Re}\left(S\left(\frac{\alpha}{1 + \alpha B_{\Lambda}(k)}\rho_{0,1}(G_{1,0}(\kappa\bar{\nu}))\right)\varphi\bar{\varphi}\right)\right) &= \\ &= \left\langle \varphi, \left\{V_{\kappa\bar{\nu}}, S\left(\frac{\alpha}{1 + \alpha B_{\Lambda}(k)}\rho_{0,1}(G_{1,0}(\kappa\bar{\nu}))\right)\right\}\varphi \right\rangle, \end{aligned}$$

$$D(\kappa\bar{\nu}, 2\text{Re}(S(Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu}))\varphi\bar{\varphi})) = \langle \varphi, \{V_{\kappa\bar{\nu}}, S(Q_+(\kappa\bar{\nu}) + G_{1,0}(\kappa\bar{\nu}))\}\varphi \rangle,$$

$$D(\kappa\bar{\nu}, \rho_{0,1,-}^{(\kappa)}(|\varphi\rangle\langle\varphi|)) = \langle \varphi, R[G_{1,0,-}^{(\kappa)}(\kappa\bar{\nu})]\varphi \rangle.$$

As a consequence, we can write

$$F(\kappa, \alpha) = \lambda_1(\kappa) + \alpha \langle \varphi, H(\kappa \bar{\nu}) \varphi \rangle + \frac{\alpha}{2(1 + \alpha B_\Lambda)} D(|\varphi|^2, |\varphi|^2) + \mathcal{O}_{\alpha \rightarrow 0}(\alpha^{3/2}),$$

where

$$\begin{aligned} H(\kappa \bar{\nu}) &= \frac{1}{1 + \alpha B_\Lambda} V(\rho_-(\kappa \bar{\nu}) - B_\Lambda \kappa \bar{\nu}) - R[Q_-(\kappa \bar{\nu})] + R[(G_{1,0,-}^{(\kappa)} - G_{1,0})(\kappa \bar{\nu})] \\ &\quad - \frac{3}{1 + \alpha B_\Lambda} V(\alpha \rho_{0,1}(G_{1,0}(\kappa \bar{\nu}))) - \frac{1}{1 + \alpha B_\Lambda} V(U_\Lambda(|k|)\kappa \bar{\nu}) \\ &\quad + \frac{1}{1 + \alpha B_\Lambda} V(\rho_1(\{|D^0|, Q_+(\kappa \bar{\nu}) + G_{1,0}(\kappa \bar{\nu})\})) \\ &\quad - \{|D^0|, Q_+(\kappa \bar{\nu})\} S(Q_+(\kappa \bar{\nu})) - S(Q_+(\kappa \bar{\nu}))^* \{|D^0|, Q_+(\kappa \bar{\nu})\} \\ &\quad - \{G_{0,1,-}^{(\kappa)}(Q_-(\kappa \bar{\nu})), |D^0|\} + \frac{1}{1 + \alpha B_\Lambda} \{G_{1,0,-}^{(\kappa)}(\rho_-(\kappa \bar{\nu}) - B_\Lambda \kappa \bar{\nu}), |D^0|\} \\ &\quad + \left\{ G_{1,0,-}^{(\kappa)} \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa \bar{\nu})) \right), |D^0| \right\} \\ &+ \frac{1}{1 + \alpha B_\Lambda} (S(\rho_+(\kappa \bar{\nu}) - B_\Lambda \kappa \bar{\nu})^* \{|D^0|, Q_+(\kappa \bar{\nu})\} + \{|D^0|, Q_+(\kappa \bar{\nu})\} S(\rho_+(\kappa \bar{\nu}) - B_\Lambda \kappa \bar{\nu})) \\ &\quad + S \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa \bar{\nu})) \right)^* \{|D^0|, Q_+(\kappa \bar{\nu})\} \\ &\quad + \{|D^0|, Q_+(\kappa \bar{\nu})\} S \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa \bar{\nu})) \right) \\ &+ \frac{1}{1 + \alpha B_\Lambda} V((\rho_{1,-}^{(\kappa)} - \rho_1)(\{|D^0|, Q_+(\kappa \bar{\nu})\})) - R[G_{1,-}^{(\kappa)}(\{|D^0|, Q_+(\kappa \bar{\nu}) + G_{1,0}(\kappa \bar{\nu})\})] \\ &\quad + R[(G_{1,-}^{(\kappa)} - G_1)(\{|D^0|, G_{1,0}(\kappa \bar{\nu})\})] - S(G_{1,0}(\kappa \bar{\nu})^* V_{\kappa \bar{\nu}} - V_{\kappa \bar{\nu}} S(G_{1,0}(\kappa \bar{\nu}))) \\ &\quad - \frac{1}{1 + \alpha B_\Lambda} (S(\rho_+(\kappa \bar{\nu}) - B_\Lambda \kappa \bar{\nu})^* V_{\kappa \bar{\nu}} + V_{\kappa \bar{\nu}} S(\rho_+(\kappa \bar{\nu}) - B_\Lambda \kappa \bar{\nu})) \\ &\quad - \frac{1}{1 + \alpha B_\Lambda} V((\rho_{1,0,-}^{(\kappa)} - \rho_{1,0})(\kappa \bar{\nu})) \\ &- S \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa \bar{\nu})) \right)^* V_{\kappa \bar{\nu}} - V_{\kappa \bar{\nu}} S \left( \frac{\alpha}{1 + \alpha B_\Lambda(k)} \rho_{0,1}(G_{1,0}(\kappa \bar{\nu})) \right) \\ &\quad + S(Q_+(\kappa \bar{\nu}) + G_{1,0}(\kappa \bar{\nu}))^* V_{\kappa \bar{\nu}} + V_{\kappa \bar{\nu}} S(Q_+(\kappa \bar{\nu}) + G_{1,0}(\kappa \bar{\nu})). \end{aligned}$$



## CHAPTER 3

# Global well-posedness for a nonlinear wave equation coupled to the Dirac sea

The preprint of this article is available online, at *hal-00869201*.

### Abstract

We prove the global well-posedness and we study the linear response for a system of two coupled equations composed of a Dirac equation for an infinite rank operator and a nonlinear wave or Klein-Gordon equation.

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### 1. Introduction

The purpose of this article is to study the time evolution of a classical scalar field propagating in *relativistic* vacuum. The free evolution of a scalar field  $W$  of mass  $m$  in the *non-relativistic* vacuum is governed by a nonlinear wave ( $m = 0$ ) or Klein-Gordon ( $m > 0$ ) equation of the form

$$(\partial_t^2 - \Delta_x + m^2)W = -W^3, \quad t \in \mathbb{R}, x \in \mathbb{R}^3. \quad (3.1.1)$$

The role of the cubic nonlinearity is to take into account some internal phenomena of the field and it is not essential for our analysis. When relativistic effects are taken into account, the structure of the vacuum changes. According to Dirac's picture [Dir34a], the relativistic vacuum is composed of infinitely many virtual particles, whose distribution is uniform in space and thus unobservable. These virtual particles can however react to the presence of the field  $W$ , resulting in a new distribution of particles not uniform anymore: we say that the vacuum becomes *polarized*. The goal of this article is to study mathematically how the scalar field reacts when coupled to the Dirac sea, from a time-dependent point of view.

A rigorous description of an infinite number of Dirac particles is not an easy task, due to the ill-posedness of many-body relativistic quantum mechanics. As a consequence, we use the Hartree-Fock approximation of Quantum Electrodynamics developed by Hainzl, Lewin, and Séré [HLS05a], which provides a well-defined functional setting to describe systems with an infinite number of particles. In this framework, the state of the vacuum is given by a self-adjoint operator  $\gamma = \gamma(t)$  on a Hilbert space  $\mathfrak{H}$  satisfying the constraint  $0 \leq \gamma \leq 1$ . The Hilbert space  $\mathfrak{H}$  we consider is

$$\mathfrak{H} = \mathfrak{H}_\Lambda := \{f \in L^2(\mathbb{R}^3, \mathbb{C}^4), \widehat{f}(k) = 0 \text{ for a.e. } |k| \geq \Lambda\},$$

where  $\Lambda > 0$  is an ultraviolet cut-off, taken to avoid well-known divergences in relativistic theories. Typically,  $\gamma$  is an orthogonal projection of infinite rank, and if  $(\varphi_i)_i$  is an orthonormal basis of  $\text{Ran}(\gamma)$ , then the  $(\varphi_i)_i$  are interpreted as the wavefunctions of the particles present in the vacuum, which here are taken to be fermions. The free evolution of the vacuum is governed by the following von Neumann-type equation

$$i\partial_t \gamma = [D^0, \gamma], \quad (3.1.2)$$

where  $D^0$  denotes the Dirac operator on  $\mathfrak{H}_\Lambda$  given by

$$D^0 := \sum_{k=1}^3 \alpha_k (-i\partial_{x_k}) + \beta,$$

and  $(\alpha_1, \alpha_2, \alpha_3, \beta)$  are the usual Dirac matrices [Tha92]. Notice that  $D^0$  stabilizes  $\mathfrak{H}_\Lambda$  since it is a Fourier multiplier. The vacuum in the absence of fields (the *free* vacuum) is described by the negative spectral projection of the Dirac operator  $\gamma(t) = P_-^0 := \chi_{(-\infty, 0)}(D^0)$ , which is formally the state of lowest possible energy and is a

stationary solution to (3.1.2). When the vacuum reacts to the presence of the scalar field, one has to couple the evolution (3.1.1) of the field to the evolution (3.1.2) of the vacuum. The dynamics of the system is then governed by two coupled Partial Differential Equations

$$\begin{cases} (\partial_t^2 - \Delta_x + m^2)W = f(\gamma, W), \\ i\partial_t\gamma = \Pi_\Lambda [D^0 + g(W), \gamma] \Pi_\Lambda, \end{cases} \quad (3.1.3)$$

where  $\Pi_\Lambda$  is the orthogonal projection from  $L^2(\mathbb{R}^3, \mathbb{C}^4)$  onto  $\mathfrak{H}_\Lambda$ , needed since the term  $g(W)$  may not stabilize the space  $\mathfrak{H}_\Lambda$ . The coupling between the Dirac field  $\gamma$  and the scalar field  $W$  is expressed through the functions  $f$  and  $g$ . These functions must satisfy the crucial property that  $f(P_-^0, 0) = 0$  and  $g(0) = 0$ , meaning that the free vacuum without any field  $(\gamma(t), W(t)) \equiv (P_-^0, 0)$  is a stationary solution to (3.1.3). We could study the general equation (3.1.3) under appropriate assumptions on  $f$  and  $g$ , but we will for shortness restrict ourselves to two physical situations.

**Case 1: Coulomb case.** In the first case,  $W = V$  is a classical Coulomb potential that polarizes the Dirac sea  $\gamma$  composed of an infinity of relativistic electrons. The parameters are given by

$$m = 0, \quad f(\gamma, V) = 4\pi e\rho_{\gamma-1/2}, \quad g(V) = eV, \quad (\text{P1})$$

where  $e > 0$  is the absolute value of the charge of an electron, and  $\rho_{\gamma-1/2}$  is the charge density associated to the state  $\gamma$ , defined formally by

$$\forall x \in \mathbb{R}^3, \rho_{\gamma-1/2}(x) := \text{Tr}_{\mathbb{C}^4} \left( \gamma - \frac{1}{2} \right) (x, x) \in \mathbb{R}.$$

The subtraction of  $1/2$  in  $\gamma - 1/2$  is to ensure charge conjugation symmetry [HLS07]. One can also easily verify that  $\rho_{P_-^0-1/2} \equiv 0$ , so that  $f(P_-^0, 0) = 0$  as desired, and we also have  $\rho_{\gamma-1/2} = \rho_{\gamma-P_-^0}$ . For this set of parameters, the equation is thus

$$\begin{cases} (\partial_t^2 - \Delta_x)V = 4\pi e\rho_{\gamma-1/2}, \\ i\partial_t\gamma = \Pi_\Lambda [D^0 + eV, \gamma] \Pi_\Lambda. \end{cases} \quad (3.1.4)$$

This model describes the polarization of the Dirac sea  $\gamma$  by the *repulsive retarded potential*  $V$  generated by its own charge distribution  $\rho_{\gamma-1/2}$ . This picture is however physically incomplete, because this time-dependent charge distribution should also produce a magnetic field. Including a magnetic field in the Hartree-Fock approximation of QED leads to a much more complicated model [GHLS13], and therefore (3.1.4) is only a toy model for studying retardation effects in the polarized Dirac sea.

**Case 2: Meson case.** The second case concerns a model of nuclear physics, where  $W = U$  represents an attractive classical scalar meson field and  $\gamma$  is a quantum Dirac

nucleon field. The new set of parameters is

$$m > 0, \quad f(\gamma, U) = -U^3 - 4\pi e \rho_{\beta(\gamma - P_-^0)}, \quad g(U) = e\beta U, \quad (\text{P2})$$

where we recall that  $\beta$  is the fourth Dirac matrix. The equation is thus

$$\begin{cases} (\partial_t^2 - \Delta_x + m^2)U = -U^3 - 4\pi e \rho_{\beta(\gamma - P_-^0)}, \\ i\partial_t \gamma = \Pi_\Lambda [D^0 + e\beta U, \gamma] \Pi_\Lambda. \end{cases} \quad (3.1.5)$$

Modelling the meson field by a classical field and adding a nonlinear term  $U^3$  are well-known procedures in the so-called *relativistic mean-field theory* [MTZ<sup>+</sup>06, KR91, Rei89, Rin96]. Here,  $e > 0$  should be interpreted as the square root of the coupling constant  $\alpha = e^2 > 0$  between the two fields.

In both cases, the initial condition for  $\gamma$  is chosen to be of the form  $\gamma|_{t=0} = P_-^0 + Q_0$ , where  $Q_0$  is a Hilbert-Schmidt (hence compact) operator. We show that for all times  $t \geq 0$ ,  $\gamma(t)$  remains of this form, i.e.  $\gamma(t) = P_-^0 + Q(t)$  with  $Q(t)$  Hilbert-Schmidt. We thus study compact perturbations of the stationary state  $P_-^0$ , exactly as in [HLS05a, HLS05b, HLS05c]. Hence, the operator  $\gamma(t)$  is infinite-rank for all  $t$  and really describes a vacuum composed of an infinity of particles. We can rewrite the system (3.1.3) in the variables  $(Q, W)$ :

$$\begin{cases} (\partial_t^2 - \Delta_x + m^2)W = f(P_-^0 + Q, W), \\ i\partial_t Q = \Pi_\Lambda [D^0 + g(W), P_-^0 + Q] \Pi_\Lambda. \end{cases} \quad (3.1.6)$$

The advantage of this formulation is that it has a much nicer functional setting, since  $Q$  is a Hilbert-Schmidt operator on  $\mathfrak{H}_\Lambda$ . In particular, the quantities  $\rho_{\gamma-1/2} = \rho_Q$  and  $\rho_{\beta(\gamma - P_-^0)} = \rho_{\beta Q}$ , which were present in (P1) and (P2), are well-defined square integrable functions [HLS09a, Lemma 1].

The main difference between the Coulomb case and the meson case is the sign of the coupling term  $\pm 4\pi e \rho$  in (P1) and (P2), reminiscent of the fact that the Coulomb potential is repulsive and the meson potential is attractive. While our mathematical treatment of these two types of interactions is essentially the same thanks to the presence of the cut-off  $\Lambda$ , it is worth mentioning that in a model without cut-off, the long time behaviour of the repulsive case looks more mathematically involved than the attractive case, even for simpler models (see Remark 3.3 below).

When  $V$  is instantaneous (i.e. when  $\partial_t^2 - \Delta_x$  is replaced by  $-\Delta_x$  in (3.1.4)), global well-posedness for the equation on  $Q$  has been proved in [HLS05c] via conservation of an energy, after the pioneering works on the so-called *Bogoliubov-Dirac-Fock model* in [HLS05a, HLS05b]. In [HLS05c], it is remarkable that the conservation of energy leads to global well-posedness since usual energies for Dirac equations are unbounded and cannot control any norm of the solution. The coupling of a wave or Klein-Gordon equation with a Schrödinger or Dirac equation for *one* particle has been extensively studied. We mention [Bac84, GV02] and references therein for the study of the

Cauchy problem in the energy space and scattering for the Wave-Schrödinger system, and [MN03] for the local existence theory in the energy space for the much more involved Maxwell-Dirac system, which includes magnetic fields as well. We are not aware of any rigorous work on the coupling between infinitely many Dirac particles and the nonlinear Klein-Gordon equation.

In this article, we prove the global existence and uniqueness of solutions to (3.1.6), for  $(Q, W, \partial_t W)$  in the space  $\mathfrak{S}_2(\mathfrak{H}_\Lambda) \times H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$ . Here,  $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$  denotes the space of Hilbert-Schmidt operators on  $\mathfrak{H}_\Lambda$ . Our two main results are Theorem 3.1 and Theorem 3.2 below. Furthermore, in the Coulomb case, we study the linear response associated to the evolution problem, and compare it with the results of [GLS09] in the time-independent case. Finally, we explain the difficulties of deriving a “time-dependent charge renormalization” formula, which we have not succeeded in proving yet. To our knowledge, this is the first result on global well-posedness for coupled wave-Dirac equations with an infinite number of Dirac particles. Sections 2 and 3 are devoted to the proof of global well-posedness. In Section 4, we study the linear response theory for our system, and discuss the charge renormalization question.

## 2. Local existence theory

For initial conditions  $(Q_0, W_0, W_1) \in \mathfrak{S}_2(\mathfrak{H}_\Lambda) \times H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$ , we prove local existence and uniqueness of solutions

$$(Q, W, \partial_t W) \in \mathcal{C}^0([-T, T], \mathfrak{S}_2 \times H^1 \times L^2) \cap \mathcal{C}^1([-T, T], \mathfrak{S}_2 \times L^2 \times H^{-1})$$

to the system (3.1.6) for some small  $T > 0$ , for both the Coulomb and meson cases, such that  $(Q, W, \partial_t W)|_{t=0} = (Q_0, W_0, W_1)$ . This is equivalent to the existence of  $(Q, W) \in \mathcal{C}^0([-T, T], \mathfrak{S}_2 \times H^1)$  solution to the following Duhamel integral equation:

$$\begin{cases} Q(t) = e^{-itD^0} Q_0 e^{itD^0} - i \int_0^t e^{-i(t-t')D^0} \Pi_\Lambda [g(W(t')), Q(t') + P_-^0] \Pi_\Lambda e^{i(t-t')D^0} dt', \\ W(t) = \cos(tK_m) W_0 + \frac{\sin(tK_m)}{K_m} W_1 + \int_0^t \frac{\sin((t-t')K_m)}{K_m} f(Q(t'), W(t')) dt', \end{cases} \quad (3.2.7)$$

where  $K_m := \sqrt{-\Delta + m^2}$  and we have written  $f(Q, W)$  instead of  $f(P_-^0 + Q, W)$ . We prove local existence of solutions to (3.2.7) by a standard fixed-point argument. In particular, the strategy to handle the nonlinearity  $U^3$  in the meson case (P2) is well-known, and seems to go back to [Jör61]. Hence, the difficulty here is not the nonlinearity  $U^3$  but rather the coupling between the two equations.

**Proposition 3.1** (Local Existence). *Let  $\Lambda > 0$ ,  $m$ ,  $f$ ,  $g$  satisfying either (P1) or (P2), and  $R > 0$ . Then, there exists  $T = T(\Lambda, m, e, R) > 0$  such that for any  $(Q_0, W_0, W_1) \in \mathfrak{S}_2(\mathfrak{H}_\Lambda) \times H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$  satisfying  $\|(Q_0, W_0, W_1)\|_{\mathfrak{S}_2 \times H^1 \times H^2} \leq R$ , there exists  $(Q, W) \in \mathcal{C}^0([-T, T], \mathfrak{S}_2 \times H^1)$  solution to (3.2.7).*

PROOF. Let  $T > 0$  to be chosen later. For any  $(Q, W) \in \mathcal{C}^0([-T, T], \mathfrak{S}_2 \times H^1)$ , we introduce  $\Phi(Q, W) = (\Phi_1(Q, W), \Phi_2(Q))$ , defined for any  $t \in [-T, T]$  by

$$\begin{cases} \Phi_1(Q, W)(t) = e^{-itD^0} Q_0 e^{itD^0} - i \int_0^t e^{-i(t-t')D^0} \Pi_\Lambda [g(W(t')), Q(t') + P_-^0] \Pi_\Lambda e^{i(t-t')D^0} dt', \\ \Phi_2(Q)(t) = \cos(tK_m)W_0 + \frac{\sin(tK_m)}{K_m} W_1 + \int_0^t \frac{\sin((t-t')K_m)}{K_m} f(Q(t'), W(t')) dt'. \end{cases} \quad (3.2.8)$$

We apply a fixed-point argument to  $\Phi$ . We first need to show that  $\Phi$  stabilizes the space  $\mathcal{C}^0([-T, T], \mathfrak{S}_2 \times H^1)$ .

**Lemma 3.1.** *If  $(Q, W) \in \mathcal{C}^0([-T, T], \mathfrak{S}_2 \times H^1)$ , then  $\Phi(Q, W) \in \mathcal{C}^0([-T, T], \mathfrak{S}_2 \times H^1)$ , and we have, for some universal constant  $C > 0$ ,*

$$\begin{aligned} \|\Phi(Q, W)\|_{\mathcal{C}^0([-T, T], \mathfrak{S}_2 \times H^1)} &\leq \|(Q_0, W_0, W_1)\|_{\mathfrak{S}_2 \times H^1 \times L^2} \\ &\quad + Ce\Lambda^{3/2}T(1+T)(1+\|Q\|_{\mathcal{C}^0(\mathfrak{S}_2)})(1+\|W\|_{\mathcal{C}^0(H^1)}). \end{aligned} \quad (3.2.9)$$

PROOF OF LEMMA 3.1. We first prove that

$$t \mapsto \left( e^{-itD^0} Q_0 e^{itD^0}, \cos(tK_m)W_0 + \frac{\sin(tK_m)}{K_m} W_1 \right)$$

belongs to  $\mathcal{C}^0([-T, T], \mathfrak{S}_2 \times H^1)$ . Let us show that  $t \in \mathbb{R} \mapsto e^{-itD^0} Q_0 e^{itD^0} \in \mathfrak{S}_2$  is continuous. Since  $(e^{-itD^0} \cdot e^{itD^0})_{t \in \mathbb{R}}$  is a semi-group of unitary operators on  $\mathfrak{S}_2$ , it is sufficient to show the continuity at  $t = 0$ . We know that for any  $\varphi \in \mathfrak{H}_\Lambda$ ,  $e^{-itD^0} \varphi \rightarrow \varphi$  as  $t \rightarrow 0$  in  $\mathfrak{H}_\Lambda$ . Using this fact, we obtain the continuity at  $t = 0$  of  $t \in \mathbb{R} \mapsto e^{-itD^0} Q_0 e^{itD^0} \in \mathfrak{S}_2$  if  $Q_0$  is finite-rank. Then, continuity for any  $Q_0 \in \mathfrak{S}_2$  is obtained by density of finite rank operators in  $\mathfrak{S}_2$ . The continuity of  $t \in \mathbb{R} \mapsto \cos(tK_m)W_0 + \frac{\sin(tK_m)}{K_m} W_1 \in H^1$  is a well-known fact about the free wave equation: for instance one can write

$$\begin{aligned} &\|\cos(tK_m)W_0 - \cos(t'K_m)W_0\|_{H^1}^2 \\ &= \int_{\mathbb{R}^3} (\cos(tK_m(p)) - \cos(t'K_m(p)))^2 (1+|p|^2) |\widehat{W}_0(p)|^2 dp, \end{aligned}$$

with  $K_m(p) := \sqrt{|p|^2 + m^2}$ , to see that it goes to 0 as  $t \rightarrow t'$  by Lebesgue's dominated convergence theorem. The proof works the same for  $t \mapsto \frac{\sin(tK_m)}{K_m} W_1$ , and we obtain the estimates for all  $t \in [-T, T]$

$$\begin{aligned} \|e^{-itD^0} Q_0 e^{itD^0}\|_{\mathfrak{S}_2} &= \|Q_0\|_{\mathfrak{S}_2}, \quad \|\cos(tK_m)W_0\|_{H^1} \leq \|W_0\|_{H^1}, \\ \left\| \frac{\sin(tK_m)}{K_m} W_1 \right\|_{H^1} &\leq (1+|t|)\|W_1\|_{L^2}. \end{aligned}$$

We now turn to the terms with the time-integrals in (3.2.8). We first show that  $t' \mapsto e^{it'D^0} \Pi_\Lambda [g(W(t')), Q(t') + P_-^0] \Pi_\Lambda e^{-it'D^0} \in L^\infty([-T, T], \mathfrak{S}_2)$ , which is enough to

prove that  $\Phi_1(Q, W) \in \mathcal{C}^0([-T, T], \mathfrak{S}_2)$ . Notice that for any  $U, V \in H^1$ , we have

$$\|\Pi_\Lambda V \Pi_\Lambda\|_{L^2 \rightarrow L^2} \leq \|\Pi_\Lambda V \Pi_\Lambda\|_{\mathfrak{S}_2} \leq \|V \Pi_\Lambda\|_{\mathfrak{S}_2} = C\Lambda^{3/2}\|V\|_{L^2} \leq C\Lambda^{3/2}\|V\|_{H^1},$$

$$\|\Pi_\Lambda \beta U \Pi_\Lambda\|_{L^2 \rightarrow L^2} \leq \|\Pi_\Lambda \beta U \Pi_\Lambda\|_{\mathfrak{S}_2} \leq \|U \Pi_\Lambda\|_{\mathfrak{S}_2} = C\Lambda^{3/2}\|U\|_{L^2} \leq C\Lambda^{3/2}\|U\|_{H^1},$$

where we have used that for all  $f, g \in L^2(\mathbb{R}^3)$ ,

$$\|f(x)g(-i\nabla)\|_{\mathfrak{S}_2}^2 = \text{Tr}(f(x)^2g(-i\nabla)^2) = (2\pi)^{-3}\|f\|_{L^2}^2\|g\|_{L^2}^2.$$

Hence, we have for  $g$  satisfying either (P1) of (P2),

$$\|\Pi_\Lambda g(W(t'))\Pi_\Lambda\|_{L^2 \rightarrow L^2} \leq Ce\Lambda^{3/2}\|W(t')\|_{H^1},$$

$$\|[\Pi_\Lambda g(W(t'))\Pi_\Lambda, P_-^0]\|_{\mathfrak{S}_2} \leq 2\|\Pi_\Lambda g(W(t'))\Pi_\Lambda\|_{\mathfrak{S}_2} \leq Ce\Lambda^{3/2}\|W(t')\|_{H^1}. \quad (3.2.10)$$

Therefore, for all  $t' \in [-T, T]$ ,

$$\begin{aligned} & \|e^{it'D^0}\Pi_\Lambda[g(W(t')), Q(t') + P_-^0]\Pi_\Lambda e^{-it'D^0}\|_{\mathfrak{S}_2} \\ & \leq Ce\Lambda^{3/2}\|W\|_{\mathcal{C}^0([-T, T], H^1)}(1 + \|Q\|_{\mathcal{C}^0([-T, T], \mathfrak{S}_2)}), \end{aligned}$$

and this shows that

$$t' \mapsto e^{it'D^0}\Pi_\Lambda[W(t'), Q(t') + P_-^0]\Pi_\Lambda e^{-it'D^0} \in L^\infty([-T, T], \mathfrak{S}_2) \subset L^1([-T, T], \mathfrak{S}_2),$$

which, in turn, implies that  $\Phi_1(Q, W) \in \mathcal{C}^0([-T, T], \mathfrak{S}_2)$ . Furthermore, we also have

$$\|\Phi_1(Q, W)\|_{\mathcal{C}^0([-T, T], \mathfrak{S}_2)} \leq \|Q_0\|_{\mathfrak{S}_2} + Ce\Lambda^{3/2}T\|W\|_{\mathcal{C}^0([-T, T], H^1)}(1 + \|Q\|_{\mathcal{C}^0([-T, T], \mathfrak{S}_2)}).$$

Finally, for any  $t \in [-T, T]$  and for any  $\rho \in \mathcal{C}^0([-T, T], L^2(\mathbb{R}^3))$ , we have

$$\int_0^t \frac{\sin((t-t')K_m)}{K_m} \rho(t') dt' = t \int_0^1 \frac{\sin(t(1-u)K_m)}{K_m} \rho(tu) du.$$

Since for any  $u \in [0, 1]$ ,  $t \mapsto \frac{\sin(t(1-u)K_m)}{K_m} \rho(tu) \in \mathcal{C}^0([-T, T], H^1)$  with

$$\left\| \frac{\sin(t(1-u)K_m)}{K_m} \rho(tu) \right\|_{H^1} \leq C(1+T)\|\rho\|_{\mathcal{C}^0([-T, T], L^2)}, \quad (3.2.11)$$

we infer again from Lebesgue's dominated convergence theorem that

$$t \mapsto \int_0^t \frac{\sin((t-t')K_m)}{K_m} \rho(t') dt' \in \mathcal{C}^0([-T, T], H^1),$$

for any  $\rho \in \mathcal{C}^0([-T, T], L^2)$ . Notice that, in the bound (3.2.11), the constant  $C(1+T)$  on the right side can be replaced by  $C = C(m)$  if  $m > 0$ . It thus remains to prove that  $t \mapsto f(W(t), Q(t))$  belongs to  $\mathcal{C}^0([-T, T], L^2)$ . The map  $Q \in \mathfrak{S}_2 \mapsto \rho_Q \in L^2$  is linear and continuous with the estimate

$$\|\rho_Q\|_{L^2} \leq C\Lambda^{3/2}\|Q\|_{\mathfrak{S}_2}. \quad (3.2.12)$$

This can be proved by duality:

$$\forall W \in L^2(\mathbb{R}^3), \int_{\mathbb{R}^3} \rho_Q(x)W(x) dx = \text{Tr} WQ,$$

and we have the estimate valid for any  $W \in L^2(\mathbb{R}^3)$ :

$$|\operatorname{Tr} WQ| = |\operatorname{Tr} W\Pi_\Lambda Q| \leq C\Lambda^{3/2}\|W\|_{L^2}\|Q\|_{\mathfrak{S}_2}. \quad (3.2.13)$$

Together with the inequality

$$\|W(t')^3\|_{L^2} = \|W(t')\|_{L^6}^3 \leq C\|W(t')\|_{H^1}^3, \quad (3.2.14)$$

this proves that the maps

$$\begin{aligned} t' &\mapsto 4\pi e\rho_Q(t') \\ t' &\mapsto -4\pi e\rho_{\beta Q}(t') - W(t')^3 \end{aligned}$$

both belong to  $\mathcal{C}^0([-T, T], L^2)$  and we have  $\Phi_2(Q) \in \mathcal{C}^0([-T, T], H^1)$ , with the estimate

$$\begin{aligned} &\|\Phi_2(Q)\|_{\mathcal{C}^0([-T, T], H^1)} \\ &\leq (1+T)\|(W_0, W_1)\|_{H^1 \times L^2} + CT(1+T)(e\Lambda^{3/2}\|Q\|_{\mathcal{C}^0([-T, T], \mathfrak{S}_2)} + \|W\|_{\mathcal{C}^0(\mathbb{R}, H^1)}^3). \end{aligned}$$

This concludes the proof of Lemma 3.1.  $\square$

By Lemma 3.1, we see that for any  $T$  satisfying

$$T(1+T) \leq \frac{1}{CR(1+e\Lambda^{3/2}+R)},$$

$\Phi$  maps  $B(2R) = \{(Q, W), \|(Q, W)\|_{\mathcal{C}^0([-T, T], \mathfrak{S}_2 \times H^1)} \leq 2R\}$  into itself. We are now in position to use the fixed point theorem of Banach-Picard to prove that  $\Phi$  has a unique fixed point on  $B(2R)$ . To do so, it remains to prove that  $\Phi$  is a contraction on  $B(2R)$ , for  $T$  small enough. Let  $(Q, W), (Q', W') \in B(2R)$ . We start with the second term: for any  $t \in [-T, T]$ , we have

$$\begin{aligned} &\|\Phi_2(Q)(t) - \Phi_2(Q')(t)\|_{H^1} \\ &\leq C(1+T) \int_0^t \|f(Q(t'), W(t')) - f(Q'(t'), W'(t'))\|_{L^2} dt' \\ &\leq CT(1+T)(e\Lambda^{3/2}\|Q - Q'\|_{\mathcal{C}^0([-T, T], \mathfrak{S}_2)} + R^2\|W - W'\|_{\mathcal{C}^0([-T, T], H^1)}). \end{aligned}$$

In the previous inequality, we have used the fact that

$$\|W^3 - W'^3\|_{L^2} \leq \|W - W'\|_{L^6}\|W^2 + WW' + W'^2\|_{L^3} \leq CR^2\|W - W'\|_{H^1}.$$

For the term involving  $\Phi_1$ , we have for any  $t \in [-T, T]$

$$\begin{aligned} &\Phi_1(Q, W)(t) - \Phi_1(Q', W')(t) \\ &= -i \int_0^t e^{-i(t-t')D^0} \Pi_\Lambda [g(W(t')), Q(t') - Q'(t')] \Pi_\Lambda e^{i(t-t')D^0} dt' \\ &\quad - i \int_0^t e^{-i(t-t')D^0} \Pi_\Lambda [g(W(t')) - g(W'(t')), Q'(t') + P_-^0] \Pi_\Lambda e^{i(t-t')D^0} dt'. \end{aligned}$$

Hence, by the estimates we already mentioned, we have

$$\|\Phi_1(Q, W)(t) - \Phi_1(Q', W')(t)\|_{\mathfrak{S}_2} \leq Ce\Lambda^{3/2}T(1+R)\|(Q, W) - (Q', W')\|_{C^0([-T, T], \mathfrak{S}_2 \times H^1)}.$$

If we choose  $T$  small enough such that

$$T(1+T) \leq \min \left( \frac{1}{CR(1+e\Lambda^{3/2}+R)}, \frac{1}{2C(e\Lambda^{3/2}+R^2)}, \frac{1}{2Ce\Lambda^{3/2}(1+R)} \right),$$

then, for any  $(Q, W), (Q', W') \in B(2R)$ , we have

$$\|\Phi(Q, W) - \Phi(Q', W')\|_{C^0([-T, T], \mathfrak{S}_2 \times H^1)} \leq \frac{1}{2}\|(Q, W) - (Q', W')\|_{C^0([-T, T], \mathfrak{S}_2 \times H^1)},$$

meaning that we can apply the fixed point theorem of Banach-Picard. This ends the proof of Proposition 3.1.  $\square$

**Remark 3.1.** With the same estimates, we also have Lipschitz continuity of the solution map as a function of the initial data.

We not only have uniqueness of solutions in  $B(2R)$ , but also global uniqueness:

**Proposition 3.2** (Uniqueness). *If  $I = [T_-, T_+]$  is a time interval containing 0, and if  $(Q, W), (Q', W') \in C^0(I, \mathfrak{S}_2 \times H^1)$  are two solutions to (3.2.7), then  $(Q, W) \equiv (Q', W')$  on  $I$ .*

PROOF. The proof relies on a Grönwall-type argument. For any  $t \in I$  we have

$$\begin{aligned} Q(t) - Q'(t) &= -i \int_0^t e^{-i(t-t')D^0} \Pi_\Lambda [g(W(t')), Q(t') - Q'(t')] \Pi_\Lambda e^{i(t-t')D^0} dt' \\ &\quad - i \int_0^t e^{-i(t-t')D^0} \Pi_\Lambda [g(W(t')) - g(W'(t')), Q'(t') + P_-^0] \Pi_\Lambda e^{i(t-t')D^0} dt', \\ W(t) - W'(t) &= \int_0^t \frac{\sin((t-t')K_m)}{K_m} (f(Q(t'), W(t')) - f(Q'(t'), W'(t'))) dt'. \end{aligned}$$

Hence, there exists  $C = C(\Lambda, m, e, T_\pm, \|W\|_{C^0(H^1)}, \|W'\|_{C^0(H^1)}, \|Q'\|_{C^0(\mathfrak{S}_2)})$  such that for any  $t \in I$ ,

$$\|Q(t) - Q'(t)\|_{\mathfrak{S}_2} + \|W(t) - W'(t)\|_{H^1} \leq C \int_0^t (\|Q(t') - Q'(t')\|_{\mathfrak{S}_2} + \|W(t') - W'(t')\|_{H^1}) ds,$$

which implies  $Q \equiv Q'$  and  $W \equiv W'$  on  $I$ .  $\square$

Proposition 3.1 and Proposition 3.2 imply the existence of a unique maximal solution to (3.2.7) belonging to  $C^0((T_-^*, T_+^*), \mathfrak{S}_2 \times H^1)$ ,  $-\infty \leq T_-^* < 0 < T_+^* \leq +\infty$ , with

$$(T_-^*, T_+^*) :=$$

$$\bigcup \{I \text{ open interval containing } 0, \exists (Q, W) \in C^0(I, \mathfrak{S}_2 \times H^1) \text{ satisfying (3.2.7)}\}.$$

We have the following blowup criterion:



**Proposition 3.3** (Blow-Up Criterion). *Let  $(Q, W) \in \mathcal{C}^0((T_-^*, T_+^*), \mathfrak{S}_2 \times H^1)$  be the unique maximal solution to (3.1.6) with initial conditions  $(Q_0, W_0, W_1) \in \mathfrak{S}_2 \times H^1 \times L^2$ . Then we have the following criterion:*

$$T_+^* < +\infty \implies \lim_{\substack{t \rightarrow T_+^* \\ t \in (T_-^*, T_+^*)}} \|(Q(t), W(t), \partial_t W(t))\|_{\mathfrak{S}_2 \times H^1 \times L^2} = +\infty, \quad (3.2.15)$$

$$T_-^* < +\infty \implies \lim_{\substack{t \rightarrow T_-^* \\ t \in (T_-^*, T_+^*)}} \|(Q(t), W(t), \partial_t W(t))\|_{\mathfrak{S}_2 \times H^1 \times L^2} = +\infty. \quad (3.2.16)$$

PROOF. We prove it for  $T_+^*$ , the proof for  $T_-^*$  being the same. Assume that  $T_+^* < +\infty$  and that there exists a sequence of times  $(t_n)$  such that  $t_n \in (T_-^*, T_+^*)$  for all  $n$  and  $t_n \rightarrow T_+^*$  as  $n \rightarrow \infty$ , with  $\|Q(t_n), W(t_n), \partial_t W(t_n)\|_{\mathfrak{S}_2 \times H^1 \times L^2}$  remaining bounded: there exists  $R > 0$  such that for all  $n$ ,

$$\|Q(t_n), W(t_n), \partial_t W(t_n)\|_{\mathfrak{S}_2 \times H^1 \times L^2} \leq R.$$

By Proposition 3.1, from any time  $t_n$ , we can extend the solution to  $t_n + T(\Lambda, m, e, R)$ ,  $T(\Lambda, m, e, R) > 0$  being independent of  $n$ , hence  $t_n \leq T_+^* - T(\Lambda, m, e, R)$ . This contradicts the fact that  $T_+^* < +\infty$  since  $t_n \rightarrow T_+^*$ .  $\square$

### 3. Global existence

Global existence of solutions is obtained by a Grönwall-type argument, based on a Lyapunov functional which depends on whether we work with the Coulomb case (P1) or the meson case (P2).

**3.1. Meson case.** We introduce the following functional

$$F(Q, U) := \frac{1}{2} \operatorname{Tr} Q(t)^2 + \frac{1}{2} \int_{\mathbb{R}^3} ((\partial_t U)^2 + |\nabla U|^2 + m^2 U^2) \, dx + \frac{1}{4} \int_{\mathbb{R}^3} U^4 \, dx.$$

If  $(Q, U)$  is a solution to (3.1.6) for the parameters (P2), then for any  $T_-^* < t < T_+^*$ , the map  $t' \mapsto F(Q(t'), U(t')) \in \mathcal{C}^1([\min(0, t), \max(0, t)], \mathbb{R})$  and we have

$$\frac{d}{dt} F(Q(t'), U(t')) = -ie \operatorname{Tr} Q(t') [\beta U(t'), P_-^0] - 4\pi e \int_{\mathbb{R}^3} \rho_{\beta Q}(t') \partial_t U(t') \, dx.$$

As a consequence, by (3.2.10) and (3.2.12) we have for all  $t' \in [\min(0, t), \max(0, t)]$

$$\begin{aligned} \frac{d}{dt} F(Q(t'), U(t')) &\leq C e \Lambda^{3/2} \|Q(t')\|_{\mathfrak{S}_2} (\|U(t')\|_{H^1} + \|\partial_t U(t')\|_{L^2}) \\ &\leq C_{\Lambda, m, e} F(Q(t'), U(t')). \end{aligned}$$

Hence, by Grönwall's inequality, for all  $t \in (T_-^*, T_+^*)$  we have

$$F(Q(t), U(t)) \leq F(Q(0), U(0)) e^{C_{m, \Lambda} |t|}.$$

Combining this inequality with the blow-up criterion (3.2.15), we deduce the

**Theorem 3.1.** *Let  $m > 0$ ,  $e > 0$  and  $\Lambda > 0$ . Then, for any  $(Q_0, U_0, U_1) \in \mathfrak{S}_2 \times H^1 \times L^2$ , there exists a unique  $(Q, U) \in \mathcal{C}^0(\mathbb{R}, \mathfrak{S}_2 \times H^1) \cap \mathcal{C}^1(\mathbb{R}, \mathfrak{S}_2 \times L^2)$  such that  $\partial_t U \in \mathcal{C}^1(\mathbb{R}, H^{-1})$ , and satisfying for all  $t \in \mathbb{R}$*

$$\begin{cases} (\partial_t^2 - \Delta_x + m^2)U(t) = -4\pi e \rho_{\beta Q(t)} - U(t)^3 & \text{in } H^{-1}(\mathbb{R}^3), \\ i\partial_t Q(t) = \Pi_\Lambda [D^0 + \beta U(t), P_-^0 + Q(t)] \Pi_\Lambda & \text{in } \mathfrak{S}_2(\mathfrak{H}_\Lambda), \end{cases} \quad (3.3.17)$$

with initial conditions  $(Q, U, \partial_t U)|_{t=0} = (Q_0, U_0, U_1)$ .

**Remark 3.2.** The conserved energy of the system is

$$\mathcal{E}_t(Q, U) = \text{Tr}_0(D^0 Q) + e \int \rho_Q U \, dx + \frac{1}{2} \int ((\partial_t U)^2 + |\nabla_x U|^2 + m^2 U^2) \, dx + \frac{1}{4} \int U^4 \, dx,$$

where  $\text{Tr}_0(D^0 Q) := \text{Tr}(|D^0|(Q_{++} - Q_{--})) \geq \text{Tr} Q^2$ , and with the notation  $Q_{++} := (1 - P_-^0)Q(1 - P_-^0)$ ,  $Q_{--} := P_-^0 Q P_-^0$ . The term  $\text{Tr}_0(D^0 Q)$  represents the kinetic energy of  $Q$  [HLS05a]. For it to be well defined and positive, it is enough to know that  $P_-^0 + Q_0$  is an orthogonal projection [HLS05c]. Then, estimating

$$\left| e \int \rho_Q U \, dx \right| \leq C e \Lambda^3 \text{Tr} Q^2 + C e \int U^2 \, dx,$$

we deduce that for  $e$  small enough (depending on  $\Lambda$ ), the conservation of energy also leads to global well-posedness, if  $P_-^0 + Q_0$  is an orthogonal projection. These are stronger assumptions than those of Theorem 3.1, but they imply furthermore that the solution belongs to  $L^\infty(\mathbb{R}, \mathfrak{S}_2 \times H^1)$ .

**3.2. Coulomb case.** In this case, we consider the functional

$$G(Q, V) = \frac{1}{2} \text{Tr} Q^2 + \frac{1}{2} \int_{\mathbb{R}^3} ((\partial_t V)^2 + |\nabla V|^2) \, dx.$$

It verifies

$$\frac{d}{dt} G(Q(t), V(t)) = -ie \text{Tr}(Q(t)[V(t), P_-^0]) + 4\pi e \int_{\mathbb{R}^3} \rho_Q(t) \partial_t V(t) \, dx,$$

for any solution  $(Q, V)$  of (3.1.6) with parameters (P1). By the same estimates as in the previous section, together with the inequality

$$\|[V, P_-^0]\|_{\mathfrak{S}_2(\mathfrak{H}_\Lambda)} \leq C_\Lambda \|\nabla V\|_{L^2}$$

which has been proved in [HLS05c, Lemma 3.1], we also obtain

$$\frac{d}{dt} G(Q(t), V(t)) \leq C_{\Lambda, e} G(Q(t), V(t)).$$

We again deduce

$$\forall t \in (T_-^*, T_+^*), \quad G(Q(t), V(t)) \leq e^{C_{\Lambda, e}|t|}.$$

To use the blow-up criterion (3.2.15), it remains to obtain a control on  $\|V(t)\|_{L^2}$ , but since we have

$$\|V(t)\|_{L^2} \leq \|V(0)\|_{L^2} + \left| \int_0^t \|\partial_t V(s)\|_{L^2} ds \right| \leq \|V(0)\|_{L^2} + \left| \int_0^t \sqrt{2G(Q(s), V(s))} ds \right|,$$

we have proved the

**Theorem 3.2.** *Let  $e > 0$  and  $\Lambda > 0$ . Then, for any  $(Q_0, V_0, V_1) \in \mathfrak{S}_2 \times H^1 \times L^2$ , there exists a unique  $(Q, V) \in \mathcal{C}^0(\mathbb{R}, \mathfrak{S}_2 \times H^1) \cap \mathcal{C}^1(\mathbb{R}, \mathfrak{S}_2 \times L^2)$  such that  $\partial_t V \in \mathcal{C}^1(\mathbb{R}, H^{-1})$ , and satisfying for all  $t \in \mathbb{R}$*

$$\begin{cases} (\partial_t^2 - \Delta_x)V(t) = 4\pi e \rho_{Q(t)} & \text{in } H^{-1}(\mathbb{R}^3), \\ i\partial_t Q(t) = \Pi_\Lambda [D^0 + eV(t), P_-^0 + Q(t)] \Pi_\Lambda & \text{in } \mathfrak{S}_2(\mathfrak{H}_\Lambda), \end{cases} \quad (3.3.18)$$

with initial conditions  $(Q, V, \partial_t V)|_{t=0} = (Q_0, V_0, V_1)$ .

**Remark 3.3.** The main tool to prove global well-posedness is the cut-off  $\Lambda$ . Without the cut-off, it is not clear at all that global well-posedness holds, even for the apparently simpler *repulsive* Schrödinger-Klein-Gordon system

$$\begin{cases} (\partial_t^2 - \Delta + m^2)W = e|u|^2, \\ (i\partial_t + \Delta)u = eWu, \end{cases}$$

which conserved energy has no particular sign. When  $e|u|^2$  is replaced by  $-e|u|^2$  in the equation above (*attractive* case), global well-posedness in the energy space was proved in [Bac84]. It heavily relies on the fact that, in this case, the energy is positive and controls the energy norm.

#### 4. Linear response in the Coulomb case

In this section, we study the linear response of Duhamel's equation

$$Q(t) = e^{itD^0} Q_0 e^{itD^0} - i \int_0^t e^{-i(t-t')D^0} \Pi_\Lambda [eV(t'), Q(t') + P_-^0] \Pi_\Lambda e^{i(t-t')D^0} dt',$$

which corresponds to the first equation of (3.1.6) in the Coulomb case. More precisely, we compute the density  $\rho_{Q_1}$  of the operator  $Q_1$  defined by the formula

$$Q_1(t) = -ie \int_0^t e^{-i(t-t')D^0} [V(t'), P_-^0] e^{i(t-t')D^0} dt', \quad \forall t \in \mathbb{R}.$$

This density  $\rho_{Q_1}$  is relevant since it corresponds to the divergent part (with respect to the cut-off  $\Lambda$ ) of the operator  $Q(t)$ , in analogy with the time-independent version of this equation studied in [GLS09]. As a consequence, controlling this term is a key first step in the process of understanding the limit  $\Lambda \rightarrow +\infty$  of Equation (3.1.6). In Section 4.1, we compute explicitly  $\rho_{Q_1}$  and estimate it. In Section 4.2, we discuss the difficulties of studying the limit  $\Lambda \rightarrow +\infty$  and its link with charge renormalization.

**4.1. Pointwise estimate.** The integral kernel of  $Q_1(t)$  can be computed explicitly in Fourier space,

$$\begin{aligned}\widehat{Q}_1(t; p, q) &= \frac{-ie}{(2\pi)^{\frac{3}{2}}} \int_0^t \widehat{V}(t', p - q) e^{-i(t-t')D^0(p)} (\widehat{P}_-^0(q) - \widehat{P}_-^0(p)) e^{i(t-t')D^0(q)} dt' \\ &= \frac{-ie}{(2\pi)^{\frac{3}{2}}} \int_0^t \widehat{V}(t', p - q) \left( e^{-i(t-t')(E(p)+E(q))} \widehat{P}_+^0(p) \widehat{P}_-^0(q) - e^{i(t-t')(E(p)+E(q))} \widehat{P}_-^0(p) \widehat{P}_+^0(q) \right) dt',\end{aligned}$$

where  $P_+^0 := 1 - P_-^0$  and

$$E(p) := \sqrt{1 + |p|^2}$$

for all  $p \in \mathbb{R}^3$ . Hence, the (space) Fourier transform of the density  $\rho_{Q_1}(t)$  can be written as

$$\begin{aligned}\widehat{\rho_{Q_1}}(t, k) &= \frac{-e}{4\pi^3} \int_0^t \widehat{V}(t', k) \times \\ &\times \int_{\substack{|p+k/2| \leq \Lambda \\ |p-k/2| \leq \Lambda}} \sin((t-t')(E(p+k/2)+E(p-k/2))) \left( 1 - \frac{1 + (p+k/2) \cdot (p-k/2)}{E(p+k/2)E(p-k/2)} \right) dp dt',\end{aligned}$$

for all  $t \in \mathbb{R}$  and  $k \in \mathbb{R}^3$ . Integrating by parts, one finds the formula

$$\begin{aligned}\widehat{\rho_{Q_1}}(t, k) &= -\frac{e}{4\pi} |k|^2 \widehat{V}(t, k) B_\Lambda(0, k) + \frac{e}{4\pi} |k|^2 \widehat{V}(0, k) B_\Lambda(t, k) \\ &\quad + \frac{e}{4\pi} \int_0^t |k|^2 (\partial_t \widehat{V})(t', k) B_\Lambda(t - t', k) dt', \quad (3.4.19)\end{aligned}$$

where

$$\begin{aligned}B_\Lambda(t, k) &= \frac{1}{\pi^2 |k|^2} \times \\ &\times \int_{\substack{|p+k/2| \leq \Lambda \\ |p-k/2| \leq \Lambda}} \frac{\cos(t(E(p+k/2) + E(p-k/2)))}{E(p+k/2) + E(p-k/2)} \left( 1 - \frac{1 + (p+k/2) \cdot (p-k/2)}{E(p+k/2)E(p-k/2)} \right) dp.\end{aligned}$$

This formula is a time-dependent generalization of the function  $B_\Lambda^0$  defined in [GLS09, Eq. (80)], which was rigorously studied in [GLS09, Appendix A] but already present in [HLS05a]. The relation between these two functions is just

$$\forall k \in \mathbb{R}^3, B_\Lambda^0(k) = B_\Lambda(0, k).$$

It is proved in [GLS09] that  $B_\Lambda^0(0)$  is logarithmically divergent:  $B_\Lambda^0(0) \sim \frac{2}{3\pi} \log \Lambda$  as  $\Lambda \rightarrow +\infty$ , which leads to a *charge renormalization* formula [GLS09, Eq. (28)]. In our case, this logarithmic divergence actually disappears as soon as  $t \neq 0$  and it a posteriori justifies the decomposition in (3.4.19):

**Lemma 3.2.** *There exists a universal constant  $C > 0$  such that we have*

$$|B_\Lambda(t, k)| \leq C(1 + |\log(|t|E(k))|), \quad (3.4.20)$$

for all  $\Lambda > 0$ , for all  $t \neq 0$ , and for all  $k \in \mathbb{R}^3$ .

PROOF. Notice that  $B_\Lambda(t, k)$  is an even function of  $t$ , so we may assume  $t > 0$  in the following. Using the same change of variables as in [GLS09, Appendix A], one finds the formula

$$\begin{aligned} B_\Lambda(t, k) &= \frac{|k|}{2\pi} \int_0^{Z_\Lambda(|k|)} \frac{\cos(t(2E(\Lambda) - |k|z))}{E(\Lambda) - |k|z/2} (z - z^2/3) dz \\ &+ \frac{1}{\pi} \int_0^{Z_\Lambda(|k|)} \cos\left(\frac{2t}{\sqrt{1-z^2}} \sqrt{1 + \frac{|k|^2}{4}(1-z^2)}\right) \frac{z^2 - z^4/3}{(1-z^2)(1 + |k|^2(1-z^2)/4)} dz, \end{aligned}$$

with

$$Z_\Lambda(r) = \frac{E(\Lambda) - E(\Lambda - r)}{r}.$$

The function  $B_\Lambda(t, \cdot)$  is supported in the ball  $B(0, 2\Lambda)$ , and for all  $0 \leq r \leq 2\Lambda$ , one has  $0 \leq Z_\Lambda(r) \leq 1$ . Furthermore, for all  $0 \leq z \leq Z_\Lambda(r)$ , one has  $E(\Lambda) - |k|z/2 \geq E(\Lambda)/2$ . Hence, we obtain

$$\left| \frac{|k|}{2\pi} \int_0^{Z_\Lambda(|k|)} \frac{\cos(t(2E(\Lambda) - |k|z))}{E(\Lambda) - |k|z/2} (z - z^2/3) dz \right| \leq C \frac{|k|}{E(\Lambda)} Z_\Lambda(|k|) \leq C.$$

To estimate the second term of  $B_\Lambda(t, k)$ , which we denote by  $I$ , we make the change of variables  $u = \frac{1}{\sqrt{1-z^2}}$ , which leads to

$$I = \frac{1}{3\pi} \int_1^R \cos\left(2tu \sqrt{1 + \frac{|k|^2}{4u^2}}\right) \sqrt{u^2 - 1} \frac{1 + 2u^2}{u^2} \frac{du}{u^2 + |k|^2/4},$$

with  $R = (1 - Z_\Lambda(|k|))^{-1/2}$ . First, we have

$$\begin{aligned} \left| \frac{1}{3\pi} \int_1^R \cos\left(2tu \sqrt{1 + \frac{|k|^2}{4u^2}}\right) \frac{\sqrt{u^2 - 1}}{u^2} \frac{du}{u^2 + |k|^2/4} \right| &\leq C \int_1^\infty \frac{du}{u(u^2 + |k|^2/4)} \\ &\leq C \min\left(1, \frac{1}{|k|}\right). \end{aligned}$$

Then, using that  $|\sqrt{u^2 - 1} - u| \leq 1/(2u)$  for all  $u \geq 1$ , we obtain

$$\begin{aligned} \left| \frac{2}{3\pi} \int_1^R \cos\left(2tu \sqrt{1 + \frac{|k|^2}{4u^2}}\right) (\sqrt{u^2 - 1} - u) \frac{du}{u^2 + |k|^2/4} \right| &\leq C \int_1^\infty \frac{du}{u(u^2 + |k|^2/4)} \\ &= C \min\left(1, \frac{1}{|k|}\right). \end{aligned}$$

Hence,

$$|I| \leq C + \left| \frac{2}{3\pi} \int_1^R \cos \left( 2tu \sqrt{1 + \frac{|k|^2}{4u^2}} \right) \frac{u \, du}{u^2 + |k|^2/4} \right|.$$

Performing the change of variables  $v = \sqrt{u^2 + |k|^2/4}$ , we obtain

$$\begin{aligned} \int_1^R \cos \left( 2tu \sqrt{1 + \frac{|k|^2}{4u^2}} \right) \frac{u \, du}{u^2 + |k|^2/4} &= \int_{E(k/2)}^{\sqrt{R^2 + |k|^2/4}} \frac{\cos(2tv)}{v} \, dv \\ &= \int_{tE(k/2)}^{t\sqrt{R^2 + |k|^2/4}} \frac{\cos(2v)}{v} \, dv. \end{aligned}$$

Assume first  $tE(k/2) \leq 1$ . We distinguish two cases: if  $t\sqrt{R^2 + |k|^2/4} \leq 1$ , then

$$\left| \int_{tE(k/2)}^{t\sqrt{R^2 + |k|^2/4}} \frac{\cos(2v)}{v} \, dv \right| \leq \int_{tE(k/2)}^1 \frac{dv}{v} = |\log(tE(k/2))|.$$

Else, if  $t\sqrt{R^2 + |k|^2/4} \geq 1$ , we have

$$\begin{aligned} \left| \int_{tE(k/2)}^{t\sqrt{R^2 + |k|^2/4}} \frac{\cos(2v)}{v} \, dv \right| &\leq \int_{tE(k/2)}^1 \frac{dv}{v} + \left| \int_1^{t\sqrt{R^2 + |k|^2/4}} \frac{\cos(2v)}{v} \, dv \right| \\ &\leq C + |\log(tE(k/2))|. \end{aligned}$$

On the other hand, if  $tE(k/2) \geq 1$ , then

$$\left| \int_{tE(k/2)}^{t\sqrt{R^2 + |k|^2/4}} \frac{\cos(2v)}{v} \, dv \right| \leq C.$$

In any case, we get

$$\left| \int_{tE(k/2)}^{t\sqrt{R^2 + |k|^2/4}} \frac{\cos(2v)}{v} \, dv \right| \leq C(1 + |\log(tE(k))|).$$

□

**Remark 3.4.** With the same changes of variables, one can easily show that for each  $t \neq 0$  and  $k \in \mathbb{R}^3$  fixed,  $B_\Lambda(t, k)$  has a limit as  $\Lambda \rightarrow +\infty$ , which is

$$\begin{aligned} \lim_{\Lambda \rightarrow +\infty} B_\Lambda(t, k) &= \frac{2}{3\pi} \int_{|t|E(k/2)}^\infty \frac{\cos(2v)}{v} \, dv \\ &\quad + \frac{1}{3\pi} \int_1^\infty \cos \left( 2tu \sqrt{1 + \frac{|k|^2}{4u^2}} \right) \left[ \frac{\sqrt{u^2 - 1}}{u^2} + 2(\sqrt{u^2 - 1} - u) \right] \frac{du}{u^2 + |k|^2/4}. \end{aligned}$$

This has to be compared with the situation at  $t = 0$ , where only  $\lim_{\Lambda \rightarrow +\infty} (B_\Lambda(0, 0) - B_\Lambda(0, k))$  exists.

**4.2. Discussion: time-dependent charge renormalization.** In Equation (3.4.19), we have isolated the logarithmic divergent term  $B_\Lambda(0, k)$  which is independent of  $t$ . The other term is actually uniformly bounded with respect to  $\Lambda$ , which suggests that the limit  $\Lambda \rightarrow +\infty$  of  $\rho_Q(t)$  is divergent. In order to control this divergence, we set  $\alpha = e^2$  the (bare) fine structure constant and fix  $\alpha \log \Lambda$  so that  $\Lambda \rightarrow +\infty$  implies  $\alpha \rightarrow 0$ . In the spirit of [HLS05b, GLS09, GLS11, Sab13a], we expect this limit to be convergent. Let us now explain the difficulties of rigorously proving this convergence. Consider the relation (3.4.19). Then, for all  $t \neq 0$  and for all  $k \in \mathbb{R}^3$ ,

$$4\pi e \widehat{\rho_{Q_1}}(t, k) = -\alpha |k|^2 \widehat{V}(t, k) B_\Lambda^0(0) + \alpha |k|^2 \widehat{V}(t, k) C_\Lambda(|k|) + \alpha |k|^2 \widehat{V}(0, k) B_\Lambda(t, k) \\ + \alpha \int_0^t |k|^2 (\partial_t \widehat{V})(s, k) B_\Lambda(t-s, k) ds,$$

where  $C_\Lambda(|k|) := B_\Lambda^0(0) - B_\Lambda^0(k)$ . The function  $C$  has been studied in [GLS11] and satisfies the estimate

$$\forall \Lambda \geq 1, \forall r \geq 0, \quad 0 \leq C_\Lambda(r) \leq C \log(2 + r^2), \quad (3.4.21)$$

for some universal constant  $C$  (in particular, independent of  $\Lambda$ ). Combining the estimates (3.4.20) and (3.4.21) and assuming that  $\widehat{V}$  and  $\partial_t \widehat{V}$  are decaying rapidly enough, one obtains the following convergence as  $\alpha \rightarrow 0$  with  $\alpha \log \Lambda$  fixed, for fixed time  $t \neq 0$ :

$$4\pi e \rho_{Q_1}(t) \simeq \left( \frac{2}{3\pi} \alpha \log \Lambda \right) \Delta V,$$

for instance in  $L^2(\mathbb{R}^3)$ . Assuming furthermore that  $4\pi(\rho_Q(t) - \rho_{Q_1}(t)) \simeq 0$  in the same limit, we infer that  $V$  satisfies the following wave equation

$$\partial_t^2 V - \left( 1 + \frac{2}{3\pi} \alpha \log \Lambda \right) \Delta_x V = 0, \quad (3.4.22)$$

in the limit  $\alpha \rightarrow 0$  with  $\alpha \log \Lambda$  fixed. We see from this formulation that this limit leads to a renormalization of the propagation speed of the wave in the vacuum, very much alike to the charge renormalization formula in the stationary case. Of course, justifying all the steps leading to this limit is the hard part. In particular, in the spirit of [Sab13a], one should begin with deriving a priori estimates on the solution  $(Q, V)$  to (3.2.7), for instance in the fixed point argument of the proof of Proposition 3.1. The typical a priori estimate one would need is the existence of  $T > 0$  and  $C > 0$  depending only on  $\alpha$  and  $\alpha \log \Lambda$  such that

$$\forall t \in [-T, T], \quad \|\rho_Q(t)\|_{L^2} + \|V(t)\|_{H^1} + \|\partial_t V(t)\|_{L^2} \leq C. \quad (3.4.23)$$

The time  $T$  built in the proof of Proposition 3.1 satisfies  $T \rightarrow 0$  as  $\alpha \rightarrow 0$  with  $\alpha \log \Lambda$  fixed, so that it does not imply (3.4.23). However, as shown by (3.4.19), one cannot expect such a good estimate as (3.4.23) since  $\rho_{Q_1}(t)$  diverges as  $\log \Lambda$ . One

way to circumvent this issue, in the spirit of [**Sab13a**], would be to use a fixed point argument on  $\tilde{Q} := Q - Q_1$  which satisfies the equation

$$\tilde{Q}(t) = e^{-itD^0} \tilde{Q}_0 e^{itD^0} - ie \int_0^t e^{-i(t-t')D^0} \Pi_\Lambda[V(t'), \tilde{Q}(t')] \Pi_\Lambda e^{i(t-t')D^0} dt' + Q_2(t), \quad (3.4.24)$$

where

$$Q_2(t) := -ie \int_0^t e^{-i(t-t')D^0} \Pi_\Lambda[V(t'), Q_1(t')] \Pi_\Lambda e^{i(t-t')D^0} dt'.$$

To build  $\tilde{Q}$  by a fixed point argument, one needs estimates on  $Q_2$  and  $\rho_{Q_2}$  that depend only on  $\alpha$  and  $\alpha \log \Lambda$ , and one also needs to improve estimates as (3.2.11) to control the second term in the right side of (3.4.24). We hope to come back to this problem in the future.





## CHAPTER 4

### The Hartree equation for infinitely many particles.

#### I. Well-posedness theory

This chapter is the subject of a collaboration with Mathieu Lewin. Its preprint is available online, at *hal-00868781*.

**Abstract** We show local and global well-posedness results for the Hartree equation

$$i\partial_t\gamma = [-\Delta + w * \rho_\gamma, \gamma],$$

where  $\gamma$  is a bounded self-adjoint operator on  $L^2(\mathbb{R}^d)$ ,  $\rho_\gamma(x) = \gamma(x, x)$  and  $w$  is a smooth short-range interaction potential. The initial datum  $\gamma(0)$  is assumed to be a perturbation of a translation-invariant state  $\gamma_f = f(-\Delta)$  which describes a quantum system with an infinite number of particles, such as the Fermi sea at zero temperature, or the Fermi-Dirac and Bose-Einstein gases at positive temperature. Global well-posedness follows from the conservation of the relative (free) energy of the state  $\gamma(t)$ , counted relatively to the stationary state  $\gamma_f$ . We indeed use a general notion of relative entropy, which allows to treat a wide class of stationary states  $f(-\Delta)$ . Our results are based on a Lieb-Thirring inequality at positive density and on a recent Strichartz inequality for orthonormal functions, which are both due to Frank, Lieb, Seiringer and the first author of this article.

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## 1. Introduction

The time-dependent Hartree equation

$$\begin{cases} i \partial_t u &= (-\Delta_x + w * |u|^2)u, & (t, x) \in \mathbb{R} \times \mathbb{R}^d \\ u(0, x) &= u_0(x). \end{cases} \quad (4.1.1)$$

describes the dynamics of a Bose-Einstein condensate in  $\mathbb{R}^d$ , in which all the quantum particles are in the same state  $u(t, x)$  (a normalized square integrable function, i.e. with  $\int_{\mathbb{R}^d} |u(t, x)|^2 dx = 1$ ). The equation (4.1.1) can be derived from many-body quantum mechanics in a mean-field limit [**Hep74**, **GV79**, **Spo80**, **EY01**, **RS09**, **KP10**, **Pic11**, **AN08**, **LNS13**]. The nonlinear term  $w * |u|^2$  describes the interactions between the particles, where  $w : \mathbb{R}^d \rightarrow \mathbb{R}$  is the pair interaction potential and  $*$  is a notation for the convolution of two functions in  $\mathbb{R}^d$ . Physically,  $w$  is a short range potential and it is sometimes even taken to be a Dirac  $\delta$ , leading to the so-called Gross-Pitaevskii or cubic nonlinear Schrödinger (NLS) equation.

There is a similar theory for fermions, which is called *reduced Hartree-Fock* in the literature [**Sol91**], or often simply *Hartree* (it corresponds to ignoring the exchange term in the Hartree-Fock model). On the contrary to bosons, fermions cannot occupy the same state and a system of  $N$  particles is then described by a set of  $N$  orthonormal functions  $u_1, \dots, u_N \in L^2(\mathbb{R}^d)$ . Their dynamics is modelled by a system of  $N$  coupled Hartree equations of the previous form:

$$\begin{cases} i \partial_t u_1 &= \left( -\Delta_x + w * \left( \sum_{k=1}^N |u_k|^2 \right) \right) u_1, \\ &\vdots \\ i \partial_t u_N &= \left( -\Delta_x + w * \left( \sum_{k=1}^N |u_k|^2 \right) \right) u_N, \\ u_j(0, x) &= u_{0,j}(x), \quad j = 1, \dots, N. \end{cases} \quad (4.1.2)$$

The function

$$\rho(t, x) := \sum_{j=1}^N |u_j(t, x)|^2$$

is the total density of particles in the system at time  $t$ . Since all the equations (4.1.2) involve the same (so-called *mean-field*) operator  $H(t) = -\Delta + w * \rho(t)$ , it is clear that the system  $(u_1(t), \dots, u_N(t))$  remains orthonormal for every time  $t$ . Indeed, we have  $u_j(t) = U(t, 0)u_j(0)$  where  $U(t, t')$  is the unitary propagator associated with the time-dependent Hamiltonian  $H(t)$ . In particular, the number of particles  $\int_{\mathbb{R}^d} \rho(t) = N$  is conserved for all times. Another conserved quantity along the flow is the nonlinear

Hartree energy

$$\mathcal{E}(u_1, \dots, u_N) := \sum_{j=1}^N \int_{\mathbb{R}^d} |\nabla u_j|^2 + \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y) \rho(t,x) \rho(t,y) dx dy.$$

These two conservation laws can be used to prove global well-posedness of (4.1.2) under suitable assumptions on  $w$  (for instance that  $w \geq 0$ ). The equations (4.1.2) can also be derived from many-body quantum mechanics [BGM03, BEG<sup>+</sup>02, EESY04, FK11, BPS13], in a mean-field or semi-classical limit.

The purpose of this paper is to study the well-posedness of the equation (4.1.2) in the case where  $N = \infty$ , that is, for a gas containing infinitely many particles. In this situation, the total Hartree energy of the system is also infinite. We consider both the zero and positive temperature cases. To our knowledge, the results contained in this article are the first of this kind for the Hartree model with infinitely many particles. A similar problem has been considered before at zero temperature for Dirac particles in [HLS05c] and for crystals in [CS12], but there the mean-field operator  $H(t)$  has a gap in its spectrum, which dramatically simplifies the study.

In order to put the Hartree equation for infinitely many particles on a solid ground, it is easier to use the formalism of *density matrices*. We first explain this for a finite  $N$ , before turning to  $N = \infty$ . The idea is to introduce the operator

$$\gamma(t) := \sum_{j=1}^N |u_j(t)\rangle\langle u_j(t)|,$$

which is the rank- $N$  orthogonal projection<sup>1</sup> onto the  $N$ -dimensional space spanned by the functions  $u_1(t), \dots, u_N(t)$ . The operator  $\gamma(t)$  is our new variable and it is called the *one-particle density matrix*. The equation (4.1.2) can be equivalently re-written in terms of  $\gamma(t)$  as

$$i \partial_t \gamma = [-\Delta + w * \rho_\gamma, \gamma] \tag{4.1.3}$$

with the initial datum

$$\gamma(0) = \sum_{k=1}^N |u_k(0)\rangle\langle u_k(0)|. \tag{4.1.4}$$

Here  $\rho_\gamma(t, x) = \gamma(t, x, x)$  is the density associated with the operator  $\gamma$ , which coincides with the density of particles  $\rho(t, x)$  introduced earlier ( $\gamma(t, x, y)$  is a notation for the integral kernel of  $\gamma(t)$ ). The average particle number and the average energy of the system can now be written in terms of  $\gamma$  only as  $N = \text{Tr}(\gamma)$  and

$$\mathcal{E}(\gamma) = \text{Tr}((-\Delta)\gamma) + \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y) \rho_\gamma(x) \rho_\gamma(y) dx dy.$$

<sup>1</sup>Here and everywhere, we use Dirac's notation  $|u\rangle\langle v|$  for the operator  $f \mapsto \langle v, f \rangle u$ . Our scalar product is always anti-linear with respect to the left argument.

The formulation (4.1.3) is clearly more adapted to the study of infinite systems, in which case we only have to consider a more general initial datum than the finite rank  $\gamma(0)$  in (4.1.4). In principle any non-negative operator  $\gamma(0)$  can be considered, except that for fermions we should not forget the Pauli principle which requires that  $0 \leq \gamma(0) \leq 1$ .

Several authors have already studied the Hartree equation (4.1.3) with  $\gamma(t)$  an *infinite-rank* operator. When  $\gamma(0)$  is a trace-class operator with finite kinetic energy,  $\text{Tr}(1-\Delta)\gamma(0) < \infty$ , Bove, Da Prato and Fano [**BDF74**, **BDF76**] and Chadam [**Cha76**] have simultaneously proved the well-posedness of Equation (4.1.3) (for the more precise Hartree-Fock model which also includes an exchange term). Later, Zagatti obtained the same result by a slightly different method [**Zag92**].

Let us emphasize that, even if  $\gamma(t)$  can have an infinite rank, the trace-class condition in these works means that the total average number of particles  $\text{Tr} \gamma(t)$  is indeed finite for all times. In the present article, we consider an infinite system, for which the average number of particles is infinite:

$$\text{Tr} \gamma(t) = +\infty.$$

In the cases considered in this paper,  $\gamma(t)$  is not even a compact operator and none of the methods used in the previous works [**BDF74**, **BDF76**, **Cha76**, **Zag92**] is applicable.

The equation (4.1.3) has many well-known stationary states with infinitely many particles and we discuss this now. Consider the operator

$$\gamma_f = f(-\Delta)$$

with  $f : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ , which acts in the Fourier variable as a multiplication by the function  $g(p) := f(|p|^2)$ . The integral kernel of  $\gamma_f$  is  $\gamma_f(x, y) = (2\pi)^{-d/2} \check{g}(x - y)$  and hence the corresponding density is uniform in space:

$$\rho_{\gamma_f}(x) = (2\pi)^{-d/2} \check{g}(0) = (2\pi)^{-d} \int_{\mathbb{R}^d} f(|p|^2) dp, \quad \forall x \in \mathbb{R}^d.$$

This integral is finite when  $\int_{\mathbb{R}^d} |f(|p|^2)| dp < \infty$ . As a consequence, we find that the mean-field potential is also uniform,

$$w * \rho_{\gamma_f}(x) = (2\pi)^{-d} \left( \int_{\mathbb{R}^d} f(|p|^2) dp \right) \left( \int_{\mathbb{R}^d} w(x) dx \right),$$

and we get  $[-\Delta + w * \rho_{\gamma_f}, \gamma_f] = [-\Delta, f(-\Delta)] = 0$ . We conclude that any function  $f \geq 0$  such that  $\int_{\mathbb{R}^d} f(|p|^2) dp < \infty$  provides a stationary state  $\gamma_f$  for the Hartree equation. Four important physical examples which are covered by our results, are the

- *Fermi gas at zero temperature and chemical potential  $\mu > 0$ :*

$$f(r) = \mathbf{1}(0 \leq r \leq \mu) \quad \text{and} \quad \gamma_f = \mathbf{1}(-\Delta \leq \mu); \quad (4.1.5)$$

- *Fermi gas at positive temperature  $T > 0$  and chemical potential  $\mu \in \mathbb{R}$ :*

$$f(r) = \frac{1}{e^{(r-\mu)/T} + 1} \quad \text{and} \quad \gamma_f = \frac{1}{e^{(-\Delta-\mu)/T} + 1}; \quad (4.1.6)$$

- *Bose gas at positive temperature  $T > 0$  and chemical potential  $\mu < 0$ :*

$$f(r) = \frac{1}{e^{(r-\mu)/T} - 1} \quad \text{and} \quad \gamma_f = \frac{1}{e^{(-\Delta-\mu)/T} - 1}; \quad (4.1.7)$$

- *Boltzmann gas at positive temperature  $T > 0$  and chemical potential  $\mu \in \mathbb{R}$ :*

$$f(r) = e^{-(r-\mu)/T} \quad \text{and} \quad \gamma_f = e^{(\Delta+\mu)/T}. \quad (4.1.8)$$

Note that, in order to properly define the potential  $w * \rho_{\gamma_f}$ , we have used here both that  $g \in L^1(\mathbb{R}^d)$  and that  $w \in L^1(\mathbb{R}^d)$ . In this paper, we always assume that  $w$  is a (smooth enough) short range potential and we do not discuss possible extensions to, say, the NLS case  $w = a\delta$ .

The main purpose of this article is to prove the global well-posedness of the Hartree equation (4.1.3), for initial data  $\gamma(0)$  which are ‘nice’ perturbations of a reference stationary state  $\gamma_f$ , with  $f$  as before. As usual for Hamiltonian PDEs, after having shown local well-posedness, we use conserved quantities in order to control the possible growth of  $\gamma(t)$  in a suitable space along the flow and prove that the solution is global. We systematically work on the difference  $\gamma(t) - \gamma_f$ , which we think of as the time dependent perturbation of the reference state  $\gamma_f$ . So we have to control  $\gamma(t) - \gamma_f$  in suitable norms.

The situation is much more complicated than for a finite system. For instance, the number of particle is infinite but one can (under suitable assumptions on  $\gamma(0)$ ) give a meaning to the *relative number of particles*  $\delta N(t) = \text{Tr}(\gamma(t) - \gamma_f)$ . We can show that  $\delta N(t)$  is conserved but, since  $\gamma(t) - \gamma_f$  has no sign, this does not seem to yield any bound on  $\gamma(t) - \gamma_f$ .

The energy helps us more, when  $\gamma_f$  is one of the particular Gibbs states in (4.1.5)–(4.1.8). In our approach,  $\gamma(0)$  is assumed to have a finite relative entropy with respect to  $\gamma_f$ . We then prove that the relative free energy is conserved and use it as a Lyapunov function, under suitable assumptions on the potential  $w$ . This is the equivalent of the usual energy methods for finite systems, as we explain in detail in the rest of the paper. The main difference to the usual case is that we only have one conservation law.

Let us remark that if  $\gamma_f \equiv 0$  (vacuum case), then any unitarily invariant norm for  $\gamma(t)$  is also conserved. This includes for instance Schatten norms  $\|\gamma\|_{\mathfrak{S}^p} = (\text{Tr} |\gamma|^p)^{1/p}$  ( $p = 2$  for Hilbert-Schmidt operators). These conservation laws can be used to prove well-posedness for (4.1.3) with  $\gamma_f = 0$  in Schatten spaces with  $p > 1$  (see Appendix A). In our case of  $\gamma_f \neq 0$ , then  $\gamma(t) - \gamma_f$  is not unitarily equivalent to  $\gamma(0) - \gamma_f$  and there is no obvious conserved norm for  $\gamma(t) - \gamma_f$ . Controlling this operator can only

be made through the relative energy, which is an additional difficulty as compared to finite systems.

The article is organized as follows. In the next section we quickly state our main results for the above physical cases (4.1.5)–(4.1.8), even if our results cover more general situations. In Section 3, we construct local solutions in Schatten spaces and which have a sufficiently high regularity. Namely, we require that  $(\gamma(t) - \gamma_f)(1 - \Delta)^{s/2} \in \mathfrak{S}^p$  where  $\mathfrak{S}^p$  is the  $p$ th Schatten space. By using the conservation of the relative Hartree energy and Lieb-Thirring inequalities from [FLLS11, FLLS12], we then completely solve the zero-temperature case (4.1.5) in Section 4, in dimensions  $d \geq 2$ .

The rest of the paper is devoted to the positive temperature case. First, in Section 5, we give another local well-posedness result, useful for gases at positive temperature, and which is based on a recent Strichartz inequality in Schatten spaces from [FLLS13]. Then, in Section 6 we define the relative entropy of two density matrices following [LS13a] and prove Lieb-Thirring inequalities in the spirit of [FLLS11, FLLS12]. We are able to deal with much more than the three examples (4.1.6)–(4.1.8). Finally, in Section 7 we construct solutions around many stationary states  $\gamma_f = f(-\Delta)$  in dimensions  $d = 1, 2, 3$ , which include (4.1.6)–(4.1.8) among others.

## 2. Main results for Bose and Fermi gases

In this section, we quickly state our main results for (4.1.5)–(4.1.8), which are the main cases of physical interest. We refer the reader to the appropriate sections for other results.

**2.1. Fermi gas at zero temperature.** We start by discussing the case of fermions at zero temperature (4.1.5), that is, we take

$$\gamma_f = \mathbf{1}(-\Delta \leq \mu) := \Pi_\mu^-.$$

This state is the formal minimizer of the energy

$$\gamma \mapsto \mathrm{Tr}(-\Delta - \mu)\gamma,$$

among all  $0 \leq \gamma \leq 1$ , but the energy is however infinite. The corresponding Hartree energy

$$\gamma \mapsto \mathrm{Tr}(-\Delta - \mu)\gamma + \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y) \rho_\gamma(x) \rho_\gamma(y) dx dy$$

is also infinite. The correct way to investigate the stability of  $\Pi_\mu^-$  is to introduce the *relative Hartree energy*, which is the formal difference between the energy of  $\gamma$  and that of  $\Pi_\mu^-$  (which are both infinite). In the stationary case, this technique goes back



to [HLS05a, HLS07]. The relative Hartree energy is properly defined in Section 4 and it is formally given by

$$\begin{aligned} \mathcal{E}(\gamma, \Pi_\mu^-) &:= \text{Tr}(-\Delta - \mu)(\gamma - \Pi_\mu^-) \\ &\quad + \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y) \rho_{\gamma - \Pi_\mu^-}(x) \rho_{\gamma - \Pi_\mu^-}(y) dx dy. \end{aligned} \quad (4.2.9)$$

The *relative kinetic energy* is the first term and it is non-negative, since  $\Pi_\mu^-$  formally minimizes  $\gamma \mapsto \text{Tr}(-\Delta - \mu)\gamma$ . It is therefore natural to impose the condition that

$$0 \leq \text{Tr}(-\Delta - \mu)(\gamma - \Pi_\mu^-) < \infty.$$

The trace has to be interpreted in an appropriate way, discussed at length in [FLLS12] and in Section 4.

We emphasize that the function  $\rho_{\gamma - \Pi_\mu^-}$  has no sign *a priori*. Therefore the sign of the nonlinear term appearing in the relative energy (4.2.9)

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y) \rho_{\gamma - \Pi_\mu^-}(x) \rho_{\gamma - \Pi_\mu^-}(y) dx dy = (2\pi)^{d/2} \int_{\mathbb{R}^d} \widehat{w}(k) |\widehat{\rho_{\gamma - \Pi_\mu^-}}(k)|^2 dk \quad (4.2.10)$$

is determined by the sign of  $\widehat{w}$ . In the whole paper we therefore call *defocusing* the case  $\widehat{w} \geq 0$  and *focusing* the case  $\widehat{w} \leq 0$ .

Our main result, proved in Section 4 below, is the following.

**Theorem 4.1** (Global solutions at zero temperature). *Let  $d \geq 2$ ,  $\mu > 0$  and  $\Pi_\mu^- = \mathbf{1}(-\Delta \leq \mu)$ . Assume that  $w \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$  with  $w(x) = w(-x)$  for a.e.  $x \in \mathbb{R}^d$  is such that  $\widehat{w} \geq 0$  or, in dimension  $d = 2$ , that  $\widehat{w} \geq -\varepsilon$  for  $\varepsilon > 0$  small enough.*

*Then, for any  $0 \leq \gamma_0 \leq 1$  with finite kinetic energy relative to  $\Pi_\mu^-$ ,*

$$0 \leq \text{Tr}(-\Delta - \mu)(\gamma_0 - \Pi_\mu^-) < \infty,$$

*the Hartree equation (4.1.1) admits a unique global solution  $\gamma(t)$  such that  $0 \leq \text{Tr}(-\Delta - \mu)(\gamma(t) - \Pi_\mu^-) < \infty$  for all times  $t \in \mathbb{R}$ . Furthermore, the relative Hartree energy is finite, non-negative and conserved:*

$$\mathcal{E}(\gamma(t), \Pi_\mu^-) = \mathcal{E}(\gamma(0), \Pi_\mu^-), \quad \forall t \in \mathbb{R}.$$

Our statement is rather vague with regards to the function space in which the solution  $\gamma(t)$  lives. We refer the reader to Theorem 4.4 for a more precise statement.

The fact that we are unable to deal with dimension  $d = 1$  may sound surprising, but this is due to the lack of a Lieb-Thirring inequality in this case [FLLS12], which is itself related to the Peierls instability of one-dimensional quantum systems [Pei55, Sec. 4.3].

Our assumption that  $w \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$  is probably far from optimal, we have not tried to optimize it. Similarly, we have only stated the result for the “*defocusing case*”  $\widehat{w} \geq 0$  corresponding to having a non-negative potential energy in the relative

Hartree energy (4.2.9). We are indeed able to prove the local existence of solutions without this additional assumption, but then global well-posedness is not known.

**2.2. Bose and Fermi gases at positive temperature.** We have a similar result at positive temperature, which however requires different assumptions on the interaction potential  $w$ , and covers the one-dimensional case.

This time, we take

$$\gamma_{T,\mu}^{\text{fer}} = \frac{1}{e^{(-\Delta-\mu)/T} + 1} \tag{4.2.11}$$

with  $\mu \in \mathbb{R}$  and  $T > 0$  for fermions,

$$\gamma_{T,\mu}^{\text{bos}} = \frac{1}{e^{(-\Delta-\mu)/T} - 1} \tag{4.2.12}$$

with  $\mu < 0$  and  $T > 0$  for bosons, or

$$\gamma_{T,\mu}^{\text{bol}} = e^{(\Delta+\mu)/T} \tag{4.2.13}$$

with  $\mu \in \mathbb{R}$  and  $T > 0$  for “boltzons”. The relative Hartree energy which we have introduced in (4.2.9) is again formally conserved, but it is not the appropriate functional at positive temperature because it does not control the growth of any norm of  $\gamma - \gamma_{T,\mu}$ : the term  $\text{Tr}(-\Delta - \mu)(\gamma - \gamma_{T,\mu})$  has no sign *a priori*. It is more convenient to use the *relative free energy* which contains in addition the difference of the entropies, and is defined as

$$\mathcal{F}(\gamma, \gamma_{T,\mu}) := \mathcal{H}(\gamma, \gamma_{T,\mu}) + \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y) \rho_{\gamma-\gamma_{T,\mu}}(x) \rho_{\gamma-\gamma_{T,\mu}}(y) dx dy \tag{4.2.14}$$

where

$$\mathcal{H}(A, B) = -\text{Tr} \left( S(A) - S(B) - S'(B)(A - B) \right) \geq 0$$

is the *relative entropy*, with

$$S(x) = T \times \begin{cases} -x \log(x) - (1-x) \log(1-x) & \text{for fermions,} \\ -x \log(x) + (1+x) \log(1+x) & \text{for bosons,} \\ -x \log(x) + x & \text{for “boltzons”} \end{cases}$$

The relative entropy  $\mathcal{H}$  is properly defined and studied at length in [LS13a] where we even considered a general concave function  $S$ , leading to many other stationary states  $\gamma_f$  for the Hartree equation. We do not discuss this here for shortness. For the previous gases, our main result is Theorem 4.9 in Section 7, for which we state a simplified version:

**Theorem 4.2** (Global solutions at positive temperature). *Let  $d \in \{1, 2, 3\}$ ,  $T > 0$  and  $\gamma_{T,\mu}$  be given by (4.2.11) or (4.2.13) with  $\mu \in \mathbb{R}$ , or by (4.2.12) with  $\mu < 0$ . Fix  $M = 1$  for fermions, and  $M \geq \max(1, \|\gamma_{T,\mu}\|)$  in the two other cases. Assume that  $w \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$  and that*

- $\widehat{w} \geq 0$  and  $\nabla w \in L^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$  in dimension  $d = 3$ ;
- $\widehat{w} \geq -\kappa_2$  in dimension  $d = 2$ ;
- $\widehat{w} \geq -\sqrt{T} \kappa_1$  in dimension  $d = 1$ ,

where  $\kappa_1$  and  $\kappa_2$  are constants which only depend on  $M$  and  $\mu/T$ .

Then, for any initial datum  $0 \leq \gamma_0 \leq M$  with finite entropy relative to  $\gamma_{T,\mu}$ ,

$$0 \leq \mathcal{H}(\gamma_0, \gamma_{T,\mu}) < \infty,$$

the Hartree equation (4.1.1) admits a unique global solution  $\gamma(t)$  such that  $0 \leq \mathcal{H}(\gamma(t), \gamma_{T,\mu}) < \infty$  for all times  $t \in \mathbb{R}$ . Furthermore, the relative free energy  $\mathcal{F}(\gamma(t), \gamma_{T,\mu})$  is finite, non-negative and conserved.

As compared to the zero temperature case, we are able to deal with the one-dimensional case. The constants  $\kappa_1$  and  $\kappa_2$  appearing in the statement are related to the best constants in the Lieb-Thirring inequality, and they behave differently depending on the statistics. They stay uniformly bounded when  $\mu/T$  varies in a compact set for fermions and boltzons, but they tend to 0 for bosons when  $\mu/T \rightarrow 0^-$ . In dimension  $d = 1$  we gain an additional factor  $\sqrt{T}$  and we can therefore replace the smallness assumption on the negative part of  $\widehat{w}$ , by the requirement that the temperature is large enough and that  $\mu/T$  stays bounded (away from 0 in the bosonic case).

The dimensional restriction  $d \leq 3$  comes from the difficulty to construct local solutions in high dimension. Technically, this is related to a lack of information about the high-momentum decay in Schatten spaces of an operator with a finite relative entropy. Klein's inequality  $\mathcal{H}(\gamma, \gamma_{T,\mu}) \gtrsim \text{Tr}(1 - \Delta)(\gamma - \gamma_{T,\mu})^2$  is the best information that we have (see (4.6.75)). By using only this information we need  $d \leq 3$  in our local well-posedness result in Section 5. In the zero-temperature case we have the additional information that the operator  $(1 - \Pi_{2\mu}^-)(\gamma - \Pi_{\mu}^-)(1 - \Pi_{2\mu}^-)$  is *trace-class*, which is used to deal with  $d \geq 4$ .

That the (free) energy is conserved and positive can be used to prove that the solution does not escape far from the stationary states  $\Pi_{\mu}^-$  and  $\gamma_{T,\mu}^{\text{fer/bos/bol}}$ , which is usually called *orbital stability*. It is an interesting question to investigate the *asymptotic stability* of these states, that is, the weak limit of  $\gamma(t)$  when  $t \rightarrow \infty$ . This is studied in [LS13c].

**Notation.** In the whole paper, we denote by  $\mathcal{B}(\mathfrak{H})$  the space of bounded operators on the Hilbert space  $\mathfrak{H}$ . The corresponding operator norm is  $\|A\|$ . We use the notation  $\mathfrak{S}^p(\mathfrak{H})$  for the Schatten space of all the compact operators  $A$  on  $\mathfrak{H}$  such that  $\text{Tr}|A|^p < \infty$ , with  $|A| = \sqrt{A^*A}$ , and use the norm  $\|A\|_{\mathfrak{S}^p(\mathfrak{H})} := (\text{Tr}|A|^p)^{1/p}$ . We refer to [Sim77] for the properties of Schatten spaces. The spaces  $\mathfrak{S}^2(\mathfrak{H})$  and  $\mathfrak{S}^1(\mathfrak{H})$  correspond to Hilbert-Schmidt and trace-class operators. We often use the shorthand

notation  $\mathcal{B}$  and  $\mathfrak{S}^p$  when the Hilbert space  $\mathfrak{H}$  is clear from the context. We also denote by

$$\Pi_\mu^- := \mathbf{1}(-\Delta \leq \mu) \quad \text{and} \quad \Pi_\mu^+ := \mathbf{1}(-\Delta \geq \mu)$$

the spectral projectors of the Laplacian, which are multiplication operators in Fourier space by the functions  $k \mapsto \mathbf{1}(k^2 \leq \mu)$  and  $k \mapsto \mathbf{1}(k^2 \geq \mu)$ .

### 3. Local well-posedness in Schatten spaces with high regularity

In this section we state and prove the local well-posedness of the Hartree equation (4.1.3), assuming that the initial datum  $\gamma(0)$  is a very smooth perturbation of the reference state  $\gamma_f = f(-\Delta)$ , with  $f$  a general function. Our main theorem uses a fixed point method on the Duhamel formulation of (4.1.3) in Schatten spaces and it is based on estimates on the density  $\rho_{\gamma(t)}$  which are *pointwise* in time. A more involved local well-posedness result based on Strichartz inequalities is later in Section 5.

Let us introduce the new variable

$$Q(t) := \gamma(t) - \gamma_f$$

which represents the variation with respect to the stationary state  $\gamma_f$ . The equation (4.1.3) can be equivalently rewritten as

$$i\partial_t Q = [-\Delta + w * \rho_Q, \gamma_f + Q]. \tag{4.3.15}$$

Here we have used the fact that  $w * \rho_{\gamma_f}$  is a constant function which, as an operator, commutes with  $\gamma = \gamma_f + Q$ . The formulation (4.3.15) is understood in a weak sense: if  $Q \in C^0(I, \mathcal{B}(L^2(\mathbb{R}^d)))$  is such that  $w * \rho_Q \in L^1_{\text{loc}}(I, L^\infty(\mathbb{R}^d))$  for some time interval  $I \ni 0$  (here we assume that  $w * \rho_Q$  is well-defined), then  $Q$  is a solution to (4.3.15) if and only if for all  $f, g \in H^2(\mathbb{R}^d)$  we have the identity

$$i\partial_t \langle f, Q(t)g \rangle = \langle (-\Delta)f, Q(t)g \rangle - \langle Q(t)f, (-\Delta)g \rangle + \langle f, [w * \rho_Q(t), \gamma_f + Q(t)]g \rangle$$

in the sense of distributions on  $I$ . As usual for nonlinear evolution equations, this is equivalent to the Duhamel formulation

$$Q(t) = e^{it\Delta} Q_0 e^{-it\Delta} - i \int_0^t e^{i(t-t')\Delta} [w * \rho_Q(t'), \gamma_f + Q(t')] e^{i(t'-t)\Delta} dt', \tag{4.3.16}$$

for all  $t \in I$ . In this section we use a fixed point procedure to solve (4.3.16). The main difficulty is that we have to deal with operators. Even if the initial datum  $Q_0$  is a finite rank operator, then the rank of  $Q(t)$  is not preserved along the flow, due to the *linear response*  $[w * \rho_Q(t'), \gamma_f]$  which is never finite-rank. So, we have to work in a bigger space. For the usual Hartree equation (4.1.1) one can play with regularity and construct solutions in arbitrary Sobolev spaces (under suitable assumptions on  $w$ ). Here we have two natural parameters at our disposal:  $s$  which determines the

Sobolev regularity on the one hand, and the exponent  $p$  of the Schatten class in which  $Q(t)$  lives on the other hand. This leads to the following Sobolev-like Schatten space

$$\mathfrak{S}^{p,s} = \left\{ Q = Q^* \in \mathcal{B}(L^2(\mathbb{R}^d)) : \right. \\ \left. \|Q(1 - \Delta)^{s/2}\|_{\mathfrak{S}^p}^p = \text{Tr} \left( (1 - \Delta)^{s/2} Q^2 (1 - \Delta)^{s/2} \right)^{p/2} < \infty \right\} \quad (4.3.17)$$

which, for  $s \in \mathbb{R}$  and  $p \geq 1$ , is a Banach space when endowed with the corresponding norm  $\|Q\|_{\mathfrak{S}^{p,s}} := \|Q(1 - \Delta)^{s/2}\|_{\mathfrak{S}^p}$ . The spaces  $\mathfrak{S}^{p,s}$  satisfy the inclusion relation

$$\mathfrak{S}^{p,s} \subset \mathfrak{S}^{q,r} \quad \text{for } s \geq r \text{ and } p \leq q. \quad (4.3.18)$$

Finite rank operators with smooth eigenfunctions are dense in  $\mathfrak{S}^{p,s}$  for all  $1 \leq p < \infty$  and all  $s \geq 0$ .

Another difficulty of our equation is the proper definition of the density  $\rho_Q$  of  $Q$ . Formally,  $\rho_Q(x) = Q(x, x)$  but this only makes sense when the kernel  $Q(x, y)$  of  $Q$  exists and is continuous. Another, better, definition is based on the spectral decomposition of  $Q = \sum_j n_j |u_j\rangle\langle u_j|$ , leading to  $\rho_Q = \sum_j n_j |u_j|^2$ . This is particularly appropriate for trace-class operators, that is, when  $\sum_j |n_j| = \|Q\|_{\mathfrak{S}^1} < \infty$ , in which case  $\rho_Q \in L^1(\mathbb{R}^d)$ . For higher Schatten spaces, we have two strategies at our disposal to deal with  $\rho_Q$ . We can define the density  $\rho_{Q(t)}$  in a weak sense in time, using the time integral in the Duhamel formula (4.3.16) and Strichartz inequalities. This is discussed later in Section 5. The other strategy which is developed in this section is much simpler. It consists in assuming that  $s$  is large enough, which yields a well-defined density for all times, by a variant of the Sobolev inequality for operators.

**Lemma 4.1** (Density  $\rho_Q$  for  $Q$  in  $\mathfrak{S}^{p,s}$ ). *Let  $d \geq 1$ ,  $p \geq 1$  and  $s > d(p - 1)/p$  or  $s \geq 0$  if  $p = 1$ . Then any  $Q \in \mathfrak{S}^{p,s}$  is locally trace-class. Its density  $\rho_Q$  belongs to  $L^q(\mathbb{R}^d)$  and satisfies*

$$\|\rho_Q\|_{L^q(\mathbb{R}^d)} \leq C \|Q\|_{\mathfrak{S}^{p,s}}, \quad \forall Q \in \mathfrak{S}^{p,s}, \quad (4.3.19)$$

for all  $p \leq q < d/(d - s)$  if  $s \leq d$  and for  $p = q = 1$  if  $s = 0$ .

If  $s > d$ , then  $\rho_Q \in L^p(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$  and

$$\|\rho_Q\|_{L^p(\mathbb{R}^d)} + \|\rho_Q\|_{L^\infty(\mathbb{R}^d)} \leq C \|Q\|_{\mathfrak{S}^{p,s}}, \quad \forall Q \in \mathfrak{S}^{p,s}. \quad (4.3.20)$$

The constants depend only on  $d$ ,  $p$ ,  $q$  and  $s$ .

**PROOF.** The result is well-known for  $p = 1$  and  $s = 0$  (see, e.g., the appendix of [GH12]). Furthermore, since  $\mathfrak{S}^{p,s} \subset \mathfrak{S}^{q,s}$  for all  $q \geq p$ , we only have to prove the inequality (4.3.19) for  $q = p$  and for  $q = \infty$  if  $s > d$ .

We compute, for  $Q \in \mathfrak{S}^{p,s}$  and a localization function  $\chi \in L_c^\infty(\mathbb{R}^d)$

$$\chi Q \chi = \chi (1 - \Delta)^{-s/4} (1 - \Delta)^{s/4} Q (1 - \Delta)^{s/4} (1 - \Delta)^{-s/4} \chi.$$

The Kato-Seiler-Simon (KSS) inequality (see [SS75] and [Sim79, Thm 4.1])

$$\|f(x)g(-i\nabla)\|_{\mathfrak{S}^r} \leq (2\pi)^{-d/r} \|f\|_{L^r(\mathbb{R}^d)} \|g\|_{L^r(\mathbb{R}^d)}, \quad \forall r \geq 2, \quad (4.3.21)$$

tells us that

$$\|\chi(1-\Delta)^{-s/4}\|_{\mathfrak{S}^{2p'}} \leq (2\pi)^{-d/p'} \|\chi\|_{L^{2p'}(\mathbb{R}^d)} \left( \int_{\mathbb{R}^d} \frac{dk}{(1+|k|^2)^{sp'/2}} \right)^{\frac{1}{2p'}}$$

where the integral on the right side is finite for  $s > d/p' = d(p-1)/p$ . By Hölder's inequality in Schatten spaces, this proves that

$$\|\chi Q \chi\|_{\mathfrak{S}^1} \leq C \|\chi\|_{L^{2p'}(\mathbb{R}^d)}^2 \|(1-\Delta)^{s/4}|Q|^{1/2}\|_{\mathfrak{S}^{2p}}^2.$$

On the other hand, by the Araki-Lieb-Thirring inequality for operators (see [LT76, Thm 9] and [Ara90, Thm 1]), we have

$$\|(1-\Delta)^{s/4}|Q|^{1/2}\|_{\mathfrak{S}^{2p}}^2 \leq \|(1-\Delta)^{s/2}Q\|_{\mathfrak{S}^p} = \|Q\|_{\mathfrak{S}^{p,s}}.$$

We therefore obtain that  $\chi Q \chi$  is trace-class, for any  $\chi \in L_c^\infty(\mathbb{R}^d)$ , hence that  $Q$  is locally trace-class. In particular,  $\rho_Q(x)$  is well defined in  $L_{\text{loc}}^1(\mathbb{R}^d)$ .

In order to prove that  $\rho_Q \in L^p(\mathbb{R}^d)$ , we argue by duality, starting with a finite rank operator  $Q$  and a potential  $V \in L_c^\infty(\mathbb{R}^d)$ . We find

$$\begin{aligned} \int_{\mathbb{R}^d} \rho_Q V &= \text{Tr}(QV) = \text{Tr} \left( (1-\Delta)^{\frac{s}{4}} Q (1-\Delta)^{\frac{s}{4}} (1-\Delta)^{-\frac{s}{4}} V (1-\Delta)^{-\frac{s}{4}} \right) \\ &\leq \|Q\|_{\mathfrak{S}^{p,s}} \|(1-\Delta)^{-\frac{s}{4}}|V(x)|^{1/2}\|_{\mathfrak{S}^{2p'}}^2 \\ &\leq C \|Q\|_{\mathfrak{S}^{p,s}} \|V\|_{L^{p'}(\mathbb{R}^d)}. \end{aligned}$$

By density of finite rank operators, the final estimate stays true for all  $Q \in \mathfrak{S}^{p,s}$  and all  $V \in L_c^\infty(\mathbb{R}^d)$ . By duality, this finally proves that  $\rho_Q \in L^p(\mathbb{R}^d)$  and that  $\|\rho_Q\|_{L^p(\mathbb{R}^d)} \leq C \|Q\|_{\mathfrak{S}^{p,s}}$ .

If  $s > d$ , the exact same proof shows that

$$\begin{aligned} \int_{\mathbb{R}^d} \rho_Q V &\leq \|(1-\Delta)^{s/4}Q(1-\Delta)^{s/4}\| \|(1-\Delta)^{-s/4}|V|^{1/2}\|_{\mathfrak{S}^2}^2 \\ &\leq C \|Q\|_{\mathfrak{S}^{p,s}} \|V\|_{L^1} \end{aligned}$$

which gives the estimate on  $\|\rho_Q\|_{L^\infty}$ .  $\square$

With Lemma 4.1 at hand, it makes sense to look for solutions of (4.3.16) satisfying  $Q(t) \in \mathfrak{S}^{p,s}$  for all times, since  $\rho_Q$  is well defined in this case.

**Theorem 4.3** (Well-posedness in  $\mathfrak{S}^{p,s}$ ). *Let  $d \geq 1$ ,  $1 \leq p < \infty$  and  $s > d(p-1)/p$  or  $s \geq 0$  if  $p = 1$ . Assume that*

$$w \in W^{s,p'}(\mathbb{R}^d) \quad (4.3.22)$$

and that

$$\int_{\mathbb{R}^d} (1+k^2)^{\frac{np}{2}} |f(k^2)|^p dk < \infty \quad \text{and} \quad w \in W^{n,1}(\mathbb{R}^d) \quad \text{if } p \geq 2, \quad (4.3.23)$$

or that

$$\sum_{z \in \mathbb{Z}^d} \left( \int_{C_z} (1+k^2)^n |f(k^2)|^2 dk \right)^{p/2} < \infty \quad \text{and} \quad \sum_{z \in \mathbb{Z}^d} \|w\|_{W^{n, \frac{2p}{3p-2}}(C_z)} < \infty$$

if  $1 \leq p < 2$ , (4.3.24)

where  $n := \lceil s \rceil$  is the smallest integer  $n \geq s$  and  $C_z = z + [-1/2, 1/2]^d$ .

Then, for any initial datum  $Q_0 \in \mathfrak{S}^{p,s}$  there exists a unique maximal solution  $Q(t) \in C_t^0((-T^-, T^+); \mathfrak{S}^{p,s})$  of (4.3.16) with  $T^\pm > 0$ . Furthermore, we have the blow-up criterion

$$T^\pm < \infty \implies \lim_{t \rightarrow \pm T^\pm} \|Q(t)\|_{\mathfrak{S}^{p,s}} = +\infty. \quad (4.3.25)$$

Finally, the unique solution  $Q(t)$  depends continuously on  $Q_0 \in \mathfrak{S}^{p,s}$ , and on  $w$  and  $f$ : if  $Q_0^{(n)} \rightarrow Q_0$  strongly in  $\mathfrak{S}^{p,s}$ ,  $w_n \rightarrow w$  and  $f_n \rightarrow f$  for the norms corresponding to the above conditions (4.3.22), (4.3.23) and (4.3.24), then the unique solution  $Q^{(n)}(t)$  has maximal times of existence  $T_n^\pm$  such that  $\liminf_{n \rightarrow \infty} T_n^\pm \geq T^\pm$  and  $Q^{(n)}(t) \rightarrow Q(t)$  in  $C_t^0([-T^- + \varepsilon, T^+ - \varepsilon], \mathfrak{S}^{p,s})$  for every  $\varepsilon > 0$ .

Our result requires some stringent conditions (4.3.22), (4.3.23) and (4.3.24) on  $f$  and  $w$ , which are not optimal and which we have not tried to optimize. They are satisfied if for instance  $f$  is bounded and decays fast enough, and if  $w$  is in the Schwartz class. They are also valid in the four physical situations (4.1.5)–(4.1.8) which we have in mind, since  $f$  has a compact support or is exponentially decreasing. We note that when  $1 \leq p < 2$ , the conditions in (4.3.23) are stronger than the ones similar to (4.3.24). Also, we remark that (4.3.23) and (4.3.24) together with  $s > d(p-1)/p$  imply that  $\int_{\mathbb{R}^d} |f(k^2)| dk < \infty$  which is needed to see that  $\rho_{\gamma_f}$  is a well-defined constant.

A natural situation, motivated by the positive temperature case (see Klein's inequality (4.6.75) in Section 6), is the case of Hilbert-Schmidt perturbations with a Sobolev regularity  $s = 1$ , that is of the space  $\mathfrak{S}^{2,1}$ . This situation is covered by the previous result only in dimension  $d = 1$ . By using Strichartz estimates, we will construct solutions in  $\mathfrak{S}^{2,1}$  in dimension  $d = 1, 2, 3$  later in Section 5.

Before turning to the proof of Theorem 4.3, we mention an additional property of the solutions in  $\mathfrak{S}^{p,s}$ . Let  $q \geq p$ ,  $s \geq r > d(q-1)/q$ , and  $Q_0 \in \mathfrak{S}^{p,s} \subset \mathfrak{S}^{q,r}$ . We assume that  $w, f$  satisfy (4.3.22), (4.3.23) and (4.3.24). Then, the unique solution  $Q$  to (4.3.16) has *a priori* distinct maximal times of existence  $T_{p,s}^\pm$  and  $T_{q,r}^\pm$ , corresponding to the two spaces  $\mathfrak{S}^{p,s}$  and  $\mathfrak{S}^{q,r}$ . Since  $\mathfrak{S}^{p,s} \subset \mathfrak{S}^{q,r}$ , they obviously satisfy  $T_{p,s}^\pm \leq T_{q,r}^\pm$ .

The next result, which is sometimes called *persistence of regularity* in the literature, shows that we have  $T_{p,s}^\pm = T_{q,r}^\pm$ . It is a simple corollary of the proof of Theorem 4.3.

**Corollary 4.1** (Persistence of regularity). *Let  $d \geq 1$ ,  $1 \leq p \leq q < \infty$  and  $s \geq r > d(q-1)/q$  or  $s \geq r \geq 0$  if  $p = q = 1$ . Assume that  $w$  and  $f$  satisfy the same assumptions (4.3.22), (4.3.23) and (4.3.24) as in Theorem 4.3. Then, for any  $T_1, T_2 > 0$ , if  $Q \in C_t^0([-T_1, T_2], \mathfrak{S}^{p,s})$  is a solution to (4.3.16), we have the following estimate*

$$\|Q(t)\|_{\mathfrak{S}^{p,s}} \leq \|Q_0\|_{\mathfrak{S}^{p,s}} e^{Ct(1 + \sup_{t' \in [-T_1, T_2]} \|Q(t')\|_{\mathfrak{S}^{q,r}})}, \quad \forall t \in [-T_1, T_2]. \quad (4.3.26)$$

Hence,  $T_{p,s}^\pm = T_{q,r}^\pm$  for all  $1 \leq p \leq q < \infty$  and all  $s \geq r > d(q-1)/q$ .

In the rest of the section we prove Theorem 4.3 and Corollary 4.1.

**PROOF OF THEOREM 4.3.** We use a simple Banach-Picard fixed point theorem in a ball centered at 0 in the space  $\mathfrak{S}^{p,s}$ . To this end, we need two estimates which are stated in the next lemmas.

**Lemma 4.2.** *Let  $d \geq 1$ ,  $1 \leq p < \infty$  and  $s > d(p-1)/p$  or  $s \geq 0$  if  $p = 1$ . Assume that  $f$  and  $w$  satisfy (4.3.23) and (4.3.24). Then we have  $[\rho_Q * w, \gamma_f] \in \mathfrak{S}^{p,s}$  for every  $Q \in \mathfrak{S}^{p,s}$  and*

$$\|[\rho_Q * w, \gamma_f]\|_{\mathfrak{S}^{p,s}} \leq C \|Q\|_{\mathfrak{S}^{p,s}},$$

with a constant  $C$  depending only on  $d, p, s, w$  and  $f$ .

**PROOF.** Denote  $V = \rho_Q * w$ . We first assume  $p \geq 2$ . By the KSS inequality (4.3.21), we have

$$\|V \gamma_f (1 - \Delta)^{s/2}\|_{\mathfrak{S}^p}^2 \leq (2\pi)^{-d/p} \|V\|_{L^p(\mathbb{R}^d)} \left( \int_{\mathbb{R}^d} (1 + k^2)^{sp/2} |f(k^2)|^p dk \right)^{1/p}.$$

For the other term, let  $n = \lceil s \rceil$  be the smallest integer  $n \geq s$ . Then

$$\gamma_f V (1 - \Delta)^{s/2} = \gamma_f V (1 - \Delta)^{n/2} (1 - \Delta)^{(s-n)/2}$$

and, therefore,  $\|V \gamma_f (1 - \Delta)^{s/2}\|_{\mathfrak{S}^p} \leq \|V \gamma_f (1 - \Delta)^{n/2}\|_{\mathfrak{S}^p}$ . Since as before  $\|\gamma_f V\|_{\mathfrak{S}^p} \leq C \|V\|_{L^p(\mathbb{R}^d)}$ , we only have to estimate the  $\mathfrak{S}^p$  norm of

$$\gamma_f V \partial_j^n = \sum_{k=0}^n \binom{n}{k} (-1)^{n-k} (\gamma_f \partial_j^k) (\partial_j^{n-k} V),$$

for all  $j = 1, \dots, d$ . This is done by following again the previous argument, with  $\|V\|_{W^{n,p}(\mathbb{R}^d)}$  appearing on the right side. It remains to use that

$$\|V\|_{W^{n,p}(\mathbb{R}^d)} \leq \|w\|_{W^{n,1}(\mathbb{R}^d)} \|\rho_Q\|_{L^p(\mathbb{R}^d)} \leq C \|w\|_{W^{n,1}(\mathbb{R}^d)} \|Q\|_{\mathfrak{S}^{p,s}}$$

by Lemma 4.1. When  $1 \leq p < 2$ , the argument is the same, except that this time we use the Birman–Solomjak inequality (see [Sim79, Th. 4.5])

$$\|f(x)g(-i\nabla)\|_{\mathfrak{S}^p} \leq C \|f\|_{\ell^p L^2} \|g\|_{\ell^p L^2} \quad (4.3.27)$$



for all  $f, g \in \ell^p(L^2)$ , with

$$\|f\|_{\ell^p L^2}^p := \sum_{z \in \mathbb{Z}^d} \|f\|_{L^2(C_z)}^p,$$

On the right we get the  $\ell^p(L^2)$  norm of the derivatives of  $V$ . They can be estimated by  $\|\rho_Q\|_{L^p(\mathbb{R}^d)}$  using Young's inequality

$$\|f * g\|_{\ell^p L^2} \leq C \|f\|_{\ell^1 L^{\frac{2p}{3p-2}}} \|g\|_{L^p} \quad (4.3.28)$$

and our assumption (4.3.24) on  $w$ .  $\square$

**Lemma 4.3.** *Let  $d \geq 1$ ,  $1 \leq p < \infty$  and  $s > d(p-1)/p$  or  $s \geq 0$  if  $p = 1$ . Assume that  $w \in W^{s,p'}(\mathbb{R}^d)$ . Then, for any  $Q, Q' \in \mathfrak{S}^{p,s}$ , we have  $[\rho_Q * w, Q'] \in \mathfrak{S}^{p,s}$  and*

$$\|[\rho_Q * w, Q']\|_{\mathfrak{S}^{p,s}} \leq C \|Q\|_{\mathfrak{S}^{p,s}} \|Q'\|_{\mathfrak{S}^{p,s}}$$

with a constant  $C$  depending only on  $d, p, s$  and  $w$ .

**PROOF.** Let  $V = \rho_Q * w$ . We have  $\|VQ'(1-\Delta)^{s/2}\|_{\mathfrak{S}^p} \leq \|V\|_{L^\infty} \|Q'\|_{\mathfrak{S}^{p,s}}$  and  $\|Q'V(1-\Delta)^{\frac{s}{2}}\|_{\mathfrak{S}^p} \leq \|Q'\|_{\mathfrak{S}^{p,s}} \|(1-\Delta)^{-\frac{s}{2}}V(1-\Delta)^{\frac{s}{2}}\| = \|Q'\|_{\mathfrak{S}^{p,s}} \|V\|_{H^s \rightarrow H^s}$ . By [GK96, Thm 1.4], one has

$$\|V\|_{H^s \rightarrow H^s} \leq C \|V\|_{W^{s,\infty}} \quad (4.3.29)$$

and the result follows from Young's inequality and Lemma 4.1.  $\square$

Using Lemmas 4.2 and 4.3, we can now finish the proof of Theorem 4.3. Let  $R > 0$  and  $Q_0 \in \mathfrak{S}^{p,s}$  such that  $\|Q_0\|_{\mathfrak{S}^{p,s}} \leq R$ . Note that the first term in Duhamel's formula has a norm independent of  $t$ :  $\|e^{it\Delta}Q_0e^{-it\Delta}\|_{\mathfrak{S}^{p,s}} = \|Q_0\|_{\mathfrak{S}^{p,s}}$ . Let now  $T = T(R) > 0$  to be chosen later. Define the space  $X_T := C_t^0([-T, T], \mathfrak{S}^{p,s})$ . It is a Banach space endowed with the norm  $\|Q\|_{X_T} := \sup_{t \in [-T, T]} \|Q(t)\|_{\mathfrak{S}^{p,s}}$ . For any  $Q \in X_T$ , we denote by  $\Phi(Q)$  the function given by:

$$\Phi(Q)(t) = e^{it\Delta}Q_0e^{-it\Delta} - i \int_0^t e^{i(t-t')\Delta} [w * \rho_Q(t'), \gamma_f + Q(t')] e^{i(t'-t)\Delta} dt'. \quad (4.3.30)$$

From Lemmas 4.2 and 4.3, we deduce that for all  $Q \in X_T$ , we have  $\Phi(Q) \in X_T$  and the estimate  $\|\Phi(Q)\|_{X_T} \leq R + CT\|Q\|_{X_T}(1 + \|Q\|_{X_T})$ . Furthermore, writing for  $Q, Q' \in X_T$  and  $t \in [-T, T]$  that

$$\begin{aligned} \Phi(Q)(t) - \Phi(Q')(t) &= -i \int_0^t e^{i(t-t')\Delta} ([w * (\rho_Q(t') - \rho_{Q'}(t')), \gamma_f + Q(t')] \\ &\quad + [w * \rho_{Q'}(t'), Q(t') - Q'(t')]) e^{i(t'-t)\Delta} dt', \end{aligned} \quad (4.3.31)$$

we infer, using the same estimates, that

$$\|\Phi(Q) - \Phi(Q')\|_{X_T} \leq CT(1 + \|Q\|_{X_T} + \|Q'\|_{X_T})\|Q - Q'\|_{X_T}.$$

As a consequence, if  $T$  is small enough such that  $2CT(1+2R) \leq 1$  and  $CT(1+4R) \leq 1/2$ , we conclude that  $\Phi$  is a contraction on the closed ball  $B_{2R} := \{Q \in X_T, \|Q\|_{X_T} \leq 2R\}$ , and hence admits a unique fixed point on  $B_{2R}$  by the Banach–Picard theorem.

Let us turn to the proof of uniqueness, independently of the size of the solutions (that is, whether they belong to  $B_{2R}$  or not). Let  $Q, Q'$  be two solutions to (4.3.16) in  $C^0([-T_1, T_2], \mathfrak{S}^{p,s})$ , for some  $T_1, T_2 > 0$ . Then, using the equation (4.3.31), we have the refined estimate for all  $t \in [-T_1, T_2]$ ,

$$\|Q(t) - Q'(t)\|_{\mathfrak{S}^{p,s}} \leq C(1 + \|Q\|_{X_T} + \|Q'\|_{X_T}) \int_0^t \|Q(t') - Q'(t')\|_{\mathfrak{S}^{p,s}} dt'.$$

This proves that  $Q \equiv Q'$  on  $[-T_1, T_2]$  by Grönwall's lemma.

The construction of maximal solutions and the stability of the equation follow from standard arguments that can be found for instance in [Tao06, Caz03]. We however do the full proof for completeness. We define  $T^\pm$  as

$$T^+ := \sup\{T > 0, \exists Q \in C_t^0([0, T], \mathfrak{S}^{p,s}) \text{ solution to (4.3.16)}\} \in (0, +\infty),$$

$$T^- := \sup\{T > 0, \exists Q \in C_t^0([-T, 0], \mathfrak{S}^{p,s}) \text{ solution to (4.3.16)}\} \in (0, +\infty).$$

Then, uniqueness of solutions shows that there exists  $Q \in C_t^0((-T^-, T^+), \mathfrak{S}^{p,s})$  solution to (4.3.16). The blow-up criterion is proved by contradiction: assume for instance that  $T^+ < +\infty$  and that there exists a sequence  $(t_n) \subset [0, T^+)$  converging to  $T^+$  with  $(\|Q(t_n)\|_{\mathfrak{S}^{p,s}})_n$  bounded. Then, using local well-posedness theory and defining

$$R = \sup_{n \in \mathbb{N}} \|Q(t_n)\|_{\mathfrak{S}^{p,s}},$$

the solution  $Q$  can be extended to the time interval  $[0, t_n + T(R)]$  for all  $n$ , with  $T(R) > 0$  being independent of  $n$ . Using the fact that  $t_n \rightarrow T^+$ , and the definition of  $T^+$ , this leads to a contradiction. Let us now prove the continuity with respect to  $Q_0, w$ , and  $f$ : let  $(Q_0^{(n)})$  a sequence in  $\mathfrak{S}^{p,s}$  such that  $Q_0^{(n)}$  converges to  $Q_0$  in  $\mathfrak{S}^{p,s}$ ,  $w_n \rightarrow w$  and  $f_n \rightarrow f$  for the norms corresponding to the conditions (4.3.22), (4.3.23) and (4.3.24). These conditions will be referred to abstractly as:

$$\|(w_n, f_n) - (w, f)\|_* \longrightarrow 0.$$

and let  $0 < T < T^+$ . Defining

$$R = 2 \left( \sup_{t \in [0, T]} \|Q(t)\|_{\mathfrak{S}^{p,s}} + \|(w, f)\|_* \right),$$

we know that, for  $n$  large enough,

$$\left\| Q_0^{(n)} \right\|_{\mathfrak{S}^{p,s}} + \|(w_n, f_n)\|_* \leq R$$

and hence  $Q^{(n)}$  is defined on  $[0, T(R)]$  by local well-posedness theory, and that

$$\sup_{t \in [0, T(R)]} \|Q^{(n)}(t)\|_{\mathfrak{S}^{p,s}} \leq 4R.$$

Then, writing for all  $t \in [0, T(R)]$  that

$$\begin{aligned} Q^{(n)}(t) - Q(t) &= e^{it\Delta}(Q_0^{(n)} - Q_0)e^{-it\Delta} \\ &\quad - i \int_0^t e^{i(t-t')\Delta} \left( [(w_n - w) * \rho_{Q^{(n)}(t')}, \gamma_{f_n} + Q^{(n)}(t')] \right. \\ &\quad \left. + [w * (\rho_{Q^{(n)}(t')} - \rho_{Q(t')}), \gamma_{f_n} + Q^{(n)}(t')] \right. \\ &\quad \left. + [w * \rho_{Q(t')}, Q^{(n)}(t') - Q(t') + \gamma_{f_n} - \gamma_f] \right) e^{i(t'-t)\Delta} dt', \end{aligned}$$

we deduce from the estimates of Lemma 4.2 and Lemma 4.3, and Lemma 4.1 that

$$\begin{aligned} \|Q^{(n)}(t) - Q(t)\|_{\mathfrak{S}^{p,s}} &\leq C(R) \left( \|Q_0^{(n)} - Q_0\|_{\mathfrak{S}^{p,s}} + \|(w_n - w, f_n)\|_* + \|(w, f_n - f)\|_* \right) \\ &\quad + C(R) \int_0^t \|Q^{(n)}(t') - Q(t')\|_{\mathfrak{S}^{p,s}} dt'. \end{aligned}$$

Applying Grönwall's Lemma leads to

$$\begin{aligned} \|Q^{(n)}(t) - Q(t)\|_{\mathfrak{S}^{p,s}} &\leq C(R) \left( \|Q_0^{(n)} - Q_0\|_{\mathfrak{S}^{p,s}} + \|(w_n - w, f_n)\|_* + \|(w, f_n - f)\|_* \right) e^{C(R)T(R)}, \end{aligned}$$

and thus  $Q^{(n)} \rightarrow Q$  in  $C_t^0([0, T(R)], \mathfrak{S}^{p,s})$ . In particular,  $Q^{(n)}(T(R)) \rightarrow Q(T(R))$  and thus  $\|Q^{(n)}(T(R))\|_{\mathfrak{S}^{p,s}} \leq R$  for  $n$  large enough. We can repeat the argument on  $[T(R), 2T(R)]$  to show that  $Q^{(n)} \rightarrow Q$  in  $C_t^0([T(R), 2T(R)], \mathfrak{S}^{p,s})$ . The point is that we have extended the interval by a fixed amount  $T(R) > 0$ , and repeating this procedure a finite number of times, we finally cover the whole of  $[0, T]$ .  $\square$

We end this section with the

**PROOF OF COROLLARY 4.1.** For simplicity, we assume  $p \geq 2$ , the argument being similar for  $p < 2$ . From Lemma 4.2 and the proof of Lemma 4.3, we have for all  $t \in [-T_1, T_2]$

$$\|Q(t)\|_{\mathfrak{S}^{p,s}} \leq \|Q_0\|_{\mathfrak{S}^{p,s}} + C \int_0^t (1 + \|\rho_{Q(t')} * w\|_{W^{s,\infty}}) \|Q(t')\|_{\mathfrak{S}^{p,s}} dt'.$$

Since  $q \geq p$ , we have  $w \in W^{s,p'} \cap W^{n,1} \subset W^{s,q'}$ , and therefore, by Young's inequality and Lemma 4.1,  $\|\rho_{Q(t')} * w\|_{W^{s,\infty}} \leq C \|\rho_{Q(t')}\|_{L^q} \leq C \|Q(t')\|_{\mathfrak{S}^{q,r}}$ . We obtain

$$\|Q(t)\|_{\mathfrak{S}^{p,s}} \leq \|Q_0\|_{\mathfrak{S}^{p,s}} + C \left( 1 + \sup_{t'' \in [-T_1, T_2]} \|Q(t'')\|_{\mathfrak{S}^{q,r}} \right) \int_0^t \|Q(t')\|_{\mathfrak{S}^{p,s}} dt',$$

and the estimate (4.3.26) follows from Grönwall's lemma. The equality  $T_{p,s}^\pm = T_{q,r}^\pm$  is a consequence of the blow-up criterion (4.3.25) and of (4.3.26).  $\square$

#### 4. Energy & global well-posedness for the Fermi sea

The purpose of this section is to prove the existence and uniqueness of *global-in-time* solutions in the particular case of the Fermi gas at zero temperature and chemical potential  $\mu > 0$ ,

$$\boxed{\gamma_f = \mathbf{1}(-\Delta \leq \mu) := \Pi_\mu^-}.$$

Our approach is based on the results of the previous section, as well as on a notion of relative energy with respect to  $\Pi_\mu^-$ . Using a recent Lieb-Thirring inequality from [FLLS11, FLLS12], we prove that the energy controls  $Q(t)$  uniformly, leading to global solutions.

Let  $\mu > 0$  and  $\gamma_f = \Pi_\mu^-$ . The *relative Hartree energy* of any density matrix  $0 \leq \gamma \leq 1$  and the reference state  $\Pi_\mu^-$ , is the formal difference between the Hartree energy of  $\gamma$  and that of  $\Pi_\mu^-$ , which are both infinite, leading to the formal expression

$$\mathcal{E}(\gamma, \Pi_\mu^-) := \text{Tr}(-\Delta - \mu)(\gamma - \Pi_\mu^-) + \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} w(x-y) \rho_{\gamma - \Pi_\mu^-}(x) \rho_{\gamma - \Pi_\mu^-}(y) dx dy. \quad (4.4.32)$$

A density matrix  $0 \leq \gamma \leq 1$  is said to live in the energy space when the first (linear) term  $\text{Tr}(-\Delta - \mu)(\gamma - \gamma_f)$  is finite, but it is necessary to interpret this term appropriately, following [HLS05a] and [FLLS12]. When  $\gamma - \Pi_\mu^-$  is finite rank and smooth, then

$$\begin{aligned} 0 \leq \text{Tr}(-\Delta - \mu)(\gamma - \Pi_\mu^-) &= \text{Tr} |-\Delta - \mu|^{\frac{1}{2}} \left( \Pi_\mu^+(\gamma - \Pi_\mu^-) \Pi_\mu^+ - \Pi_\mu^-(\gamma - \Pi_\mu^-) \Pi_\mu^- \right) |-\Delta - \mu|^{\frac{1}{2}} \\ &= \text{Tr} |-\Delta - \mu|^{\frac{1}{2}} \left( \Pi_\mu^+ \gamma \Pi_\mu^+ + \Pi_\mu^-(1 - \gamma) \Pi_\mu^- \right) |-\Delta - \mu|^{\frac{1}{2}}. \end{aligned} \quad (4.4.33)$$

The two formulas on the right side make sense for any  $\gamma$  and they are taken as a definition of the trace  $\text{Tr}(-\Delta - \mu)(\gamma - \Pi_\mu^-)$  in all cases. The set of all the density matrices which have a finite kinetic energy relative to  $\Pi_\mu^-$  is therefore the convex set

$$\mathcal{K}_\mu := \left\{ 0 \leq \gamma = \gamma^* \leq 1 : |\Delta + \mu|^{\frac{1}{2}} (\gamma - \Pi_\mu^-)^{\pm\pm} |\Delta + \mu|^{\frac{1}{2}} \in \mathfrak{S}^1 \right\}, \quad (4.4.34)$$

where  $(\gamma - \Pi_\mu^-)^{++} := \Pi_\mu^+(\gamma - \Pi_\mu^-) \Pi_\mu^+$  and with a similar notation for  $(\gamma - \Pi_\mu^-)^{--}$ . Note that the constraint  $0 \leq \gamma \leq 1$  implies that

$$(\gamma - \Pi_\mu^-)^{++} - (\gamma - \Pi_\mu^-)^{--} \geq (\gamma - \Pi_\mu^-)^2$$

and, hence,

$$\begin{aligned} \left\| (\gamma - \Pi_\mu^-) |-\Delta - \mu|^{\frac{1}{2}} \right\|_{\mathfrak{S}^2}^2 &\leq \text{Tr} |-\Delta - \mu|^{\frac{1}{2}} \left( (\gamma - \Pi_\mu^-)^{++} - (\gamma - \Pi_\mu^-)^{--} \right) |-\Delta - \mu|^{\frac{1}{2}} < \infty. \end{aligned}$$

It is therefore useful to introduce the following Banach space

$$\mathcal{X}_\mu := \left\{ Q = Q^* \in \mathcal{B}(L^2(\mathbb{R}^d)) : Q|\Delta + \mu|^{\frac{1}{2}} \in \mathfrak{S}^2, \right. \\ \left. |\Delta + \mu|^{\frac{1}{2}} Q^{\pm\pm} |\Delta + \mu|^{\frac{1}{2}} \in \mathfrak{S}^1 \right\},$$

endowed with the norm

$$\|Q\|_{\mathcal{X}_\mu} := \|Q\| + \left\| Q|\Delta + \mu|^{\frac{1}{2}} \right\|_{\mathfrak{S}^2} + \left\| |\Delta + \mu|^{\frac{1}{2}} Q^{++} |\Delta + \mu|^{\frac{1}{2}} \right\|_{\mathfrak{S}^1} \\ + \left\| |\Delta + \mu|^{\frac{1}{2}} Q^{--} |\Delta + \mu|^{\frac{1}{2}} \right\|_{\mathfrak{S}^1}.$$

We then have  $\mathcal{K}_\mu = \{0 \leq \gamma = \gamma^* \leq 1 : \gamma - \gamma_f \in \mathcal{X}_\mu\}$ , which realizes  $\mathcal{K}_\mu$  as a convex subset of the affine space  $\gamma_f + \mathcal{X}_\mu$ .

We emphasize that  $|k^2 - \mu|$  vanishes on the Fermi sphere  $|k| = \sqrt{\mu}$ . The fact that operators  $Q$  in  $\mathcal{X}_\mu$  satisfy  $Q|\Delta + \mu|^{1/2} \in \mathfrak{S}^2$  does *not* imply that  $Q$  is Hilbert-Schmidt. Indeed,  $Q$  does not even have to be compact (but it is always bounded by assumption). In particular,  $\mathcal{X}_\mu$  is not included in any of the sets  $\mathfrak{S}^{p,s}$  which we have introduced in the previous section. However, we have  $\mathfrak{S}^{1,s} \subset \mathcal{X}_\mu$  for all  $s \geq 2$ , which will be used later.

A very important property of the relative kinetic energy is the following *Lieb-Thirring inequality*, which was proved in [FLLS12, Thm 2.1]:

$$\mathrm{Tr}(-\Delta - \mu)(\gamma - \Pi_\mu^-) \\ \geq K_{\mathrm{LT}} \int_{\mathbb{R}^d} \left( (\rho_{\Pi_\mu^-} + \rho_Q(x))^{1+\frac{2}{d}} - (\rho_{\Pi_\mu^-})^{1+\frac{2}{d}} - \frac{2+d}{d} (\rho_{\Pi_\mu^-})^{\frac{2}{d}} \rho_Q(x) \right) dx, \quad (4.4.35)$$

for all  $d \geq 2$ ,  $\mu > 0$  and all  $\gamma \in \mathcal{K}_\mu$  with  $Q := \gamma - \Pi_\mu^-$ . The constant  $K_{\mathrm{LT}}$  only depends on the dimension  $d \geq 2$ . The inequality (4.4.35) is *wrong* in dimension  $d = 1$ , see [FLLS12]. The inequality (4.4.35) implies that for any  $\gamma \in \mathcal{K}_\mu$ , the density  $\rho_{\gamma - \Pi_\mu^-}$  belongs to  $L^2(\mathbb{R}^d) + L^{1+2/d}(\mathbb{R}^d)$ . In particular, this shows that the nonlinear term in the relative Hartree energy (4.4.32) is well-defined for any  $\gamma \in \mathcal{K}_\mu$  if  $d \geq 2$  and  $w \in L^1(\mathbb{R}^d) \cap L^{(d+2)/4}(\mathbb{R}^d)$ , in which case we have  $w * \rho_{\gamma - \Pi_\mu^-} \in L^2(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ . We will soon make the stronger assumption that  $w \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$  for simplicity.

We recall that the relative density  $\rho_{\gamma - \Pi_\mu^-}$  has no sign in general. However, by (4.2.10) the second term in (4.4.32) is non-negative when  $\widehat{w} \geq 0$ . Furthermore, when  $d = 2$  and  $\|(\widehat{w})_-\|_{L^\infty} < K_{\mathrm{LT}}/(2\pi)$  we have

$$\mathcal{E}(\gamma, \Pi_\mu^-) \geq \left( 1 - \frac{2\pi \|\widehat{w}_-\|_{L^\infty}}{K_{\mathrm{LT}}} \right) \mathrm{Tr}(-\Delta - \mu)(\gamma - \Pi_\mu^-) \geq 0.$$

We cannot apply the same argument when  $d \geq 3$  because the right side of (4.4.35) behaves as  $(\rho_{\gamma - \Pi_\mu^-})^{1+2/d}$  when  $\rho_{\gamma - \Pi_\mu^-}$  is large, while the second term of (4.4.32) behaves as  $(\rho_{\gamma - \Pi_\mu^-})^2$ . Summarizing our discussion, we have the

**Proposition 4.1** (Coercivity of the relative energy in the defocusing case). *Let  $\gamma \in \mathcal{K}_\mu$ . Then, when  $d \geq 3$  and  $\widehat{w} \geq 0$  we have*

$$\mathcal{E}(\gamma, \Pi_\mu^-) \geq \text{Tr}(-\Delta - \mu)(\gamma - \Pi_\mu^-), \quad (4.4.36)$$

while when  $d = 2$  and  $\|(\widehat{w})_-\|_{L^\infty} < K_{\text{LT}}/(2\pi)$  we have

$$\mathcal{E}(\gamma, \Pi_\mu^-) \geq \left(1 - \frac{2\pi\|\widehat{w}_-\|_{L^\infty}}{K_{\text{LT}}}\right) \text{Tr}(-\Delta - \mu)(\gamma - \Pi_\mu^-). \quad (4.4.37)$$

The interest of the relative free energy  $\mathcal{E}(\gamma, \Pi_\mu^-)$  is that it is a conserved quantity. In the defocusing case it controls the norm of  $\gamma - \Pi_\mu^-$  in  $\mathcal{X}_\mu$  and this can be used to prove global well-posedness.

**Theorem 4.4** (Global well-posedness in energy space at zero temperature). *Assume that  $d \geq 2$  and that  $w \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$  is such that  $w(x) = w(-x)$  for a.e.  $x \in \mathbb{R}^d$ . Let  $Q_0 = \gamma_0 - \Pi_\mu^-$  with  $\gamma_0 \in \mathcal{K}_\mu$ . Then there exists a unique maximal solution  $Q(t) = \gamma(t) - \Pi_\mu^- \in C_t^0((-T^-, T^+), \mathcal{B}) \cap L_{t, \text{loc}}^\infty((-T^-, T^+), \mathcal{X}_\mu)$  of (4.3.16) with  $\gamma(t) \in \mathcal{K}_\mu$  for all  $t$  and  $T^\pm > 0$ . We have the blow-up criterion*

$$T^\pm < \infty \implies \lim_{t \rightarrow \pm T^\pm} \|Q(t)\|_{\mathcal{X}_\mu} = +\infty. \quad (4.4.38)$$

*Its relative Hartree energy is conserved:*

$$\mathcal{E}(\gamma(t), \Pi_\mu^-) = \mathcal{E}(\gamma_0, \Pi_\mu^-), \quad \forall t \in (-T^-, T^+).$$

*Furthermore, when  $d \geq 3$  and  $\widehat{w} \geq 0$  or when  $d = 2$  and  $\|(\widehat{w})_-\|_{L^\infty} < K_{\text{LT}}/(2\pi)$ , then the solution is global:  $T^- = T^+ = +\infty$ .*

Our proof is based on the Lieb-Thirring inequality (4.4.35) and for this reason we do not have a result in dimension  $d = 1$ . The proof is *not* done directly in the energy space  $\mathcal{X}_\mu$ . In order to avoid the difficulty associated with the possible divergence on the Fermi sphere  $k^2 \simeq \mu$ , we rather work in a *larger* space  $\mathcal{Y}_\mu$ , and then prove that solutions which are in the energy space at time 0 remain in it for all times. This strategy is simpler, but it requires the non-optimal condition that  $w \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ .

An immediate consequence of Theorem 4.4 is the orbital stability of the stationary solution  $\Pi_\mu^-$  in the defocusing case.

**Corollary 4.2** (Orbital stability of  $\Pi_\mu^-$  in the defocusing case). *Assume that  $d \geq 2$ , that  $w \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ , and that  $\widehat{w} \geq 0$  when  $d \geq 3$  or  $\|(\widehat{w})_-\|_{L^\infty} < K_{\text{LT}}/(2\pi)$  when  $d = 2$ . We have*

$$\begin{aligned} & \sup_{t \in \mathbb{R}} \text{Tr}(-\Delta - \mu)(\gamma(t) - \Pi_\mu^-) \\ & \leq C \left( \text{Tr}(-\Delta - \mu)(\gamma_0 - \Pi_\mu^-) + \left( \text{Tr}(-\Delta - \mu)(\gamma_0 - \Pi_\mu^-) \right)^{\frac{2d}{d+2}} \right) \end{aligned} \quad (4.4.39)$$

for all  $\gamma_0 \in \mathcal{K}_\mu$  and where  $C$  only depends on  $d$ ,  $\mu$  and  $w$ .

We recall that the relative kinetic energy  $\text{Tr}(-\Delta - \mu)(\gamma - \Pi_\mu^-)$  controls the Hilbert-Schmidt norm of  $(\gamma - \Pi_\mu^-)|\Delta + \mu|^{1/2}$  and the trace norm of  $|\Delta + \mu|^{1/2}(\gamma - \Pi_\mu^-)^{\pm\pm}|\Delta + \mu|^{1/2}$ . Hence the result means that if  $\gamma_0$  is close to  $\Pi_\mu^-$  in these norms, then  $\gamma(t)$  stays close to  $\Pi_\mu^-$  for all times. The energy does not provide a control on the operator norm  $\|\gamma(t) - \Pi_\mu^-\|$ , however.

**PROOF OF COROLLARY 4.2.** The conservation of the relative energy means that

$$\begin{aligned} \text{Tr}(-\Delta - \mu)(\gamma(t) - \Pi_\mu^-) &\leq c\mathcal{E}(\gamma_0, \Pi_\mu^-) \\ &\leq c\text{Tr}(-\Delta - \mu)(\gamma_0 - \Pi_\mu^-) + C\|\rho_{Q_0}\|_{L^2+L^{1+2/d}}^2. \end{aligned}$$

The constant on the first line is  $c = 1$  for  $d \geq 3$  and  $c = K_{\text{LT}}/(K_{\text{LT}} - 2\pi\|\widehat{w}_-\|_{L^\infty})$  for  $d = 2$ . The rest follows from (4.4.35).  $\square$

The rest of the section is devoted to the proof of Theorem 4.4.

**PROOF OF THEOREM 4.4.** Our method is the following: first we show the local well-posedness in a suitable space, which is larger than the energy space  $\mathcal{X}_\mu$ . Then we prove the conservation of the relative Hartree energy for the very smooth solutions which we have constructed in Section 3. By approximating any initial datum with finite energy by a sequence of smooth finite rank operators and passing to the limit, we obtain solutions in the energy space, with a conserved energy. Uniqueness is guaranteed by the first step.

*Step 1. Local well-posedness in a space larger than the energy space.* We start by considering the problem in a space  $\mathcal{Y}_\mu$  which contains  $\mathcal{K}_\mu$  (for  $d \geq 2$ ). As we want to avoid the Fermi sphere  $|k| = \sqrt{\mu}$  at which the operator  $Q$  can fail to be compact, we use the projector  $\Pi_{2\mu}^+$ , and only impose a condition on the density of the operator in the ball of radius  $\sqrt{2\mu}$ . We define

$$\mathcal{Y}_\mu := \left\{ Q = Q^* \in \mathcal{B} : \Pi_{2\mu}^+ Q \Pi_{2\mu}^- \in \mathfrak{S}_2, \Pi_{2\mu}^+ Q \Pi_{2\mu}^+ \in \mathfrak{S}_1, \rho_{\Pi_{2\mu}^- Q \Pi_{2\mu}^-} \in L^2(\mathbb{R}^d) \right\}. \quad (4.4.40)$$

We remark that  $-\|Q\| \Pi_{2\mu}^- \leq \Pi_{2\mu}^- Q \Pi_{2\mu}^- \leq \|Q\| \Pi_{2\mu}^-$  which shows that the density of  $\Pi_{2\mu}^- Q \Pi_{2\mu}^-$  is well defined in  $L^\infty(\mathbb{R}^d)$  and it therefore makes sense to assume that  $\rho_{\Pi_{2\mu}^- Q \Pi_{2\mu}^-} \in L^2(\mathbb{R}^d)$ . The space  $\mathcal{Y}_\mu$  is endowed with the norm

$$\|Q\|_{\mathcal{Y}_\mu} := \|Q\| + \|\Pi_{2\mu}^+ Q \Pi_{2\mu}^-\|_{\mathfrak{S}_2} + \|\Pi_{2\mu}^+ Q \Pi_{2\mu}^+\|_{\mathfrak{S}_1} + \|\rho_{\Pi_{2\mu}^- Q \Pi_{2\mu}^-}\|_{L^2}.$$

The following says that  $\mathcal{K}_\mu - \Pi_\mu^- \subset \mathcal{Y}_\mu$ , that is, the set of density matrices of finite energy is included in  $\mathcal{Y}_\mu$ .

**Lemma 4.4.** *Let  $d \geq 2$  and  $\mu > 0$ . We have*

$$\|Q\|_{\mathcal{Y}_\mu} \leq C \left( \|Q\|_{\mathcal{X}_\mu} + \|Q\|_{\mathcal{X}_\mu}^{1/2} \right) \quad (4.4.41)$$

for all  $Q \in \mathcal{X}_\mu$  satisfying  $-\Pi_\mu^- \leq Q \leq \Pi_\mu^+$  and with  $C = C(d, \mu)$ .

PROOF. We have

$$\|\Pi_{2\mu}^+ Q \Pi_{2\mu}^-\|_{\mathfrak{S}^2} \leq \| |\Delta + \mu|^{1/2} Q \|_{\mathfrak{S}^2} \|\Pi_{2\mu}^+ |\Delta + \mu|^{-1/2}\| = \frac{\| |\Delta + \mu|^{1/2} Q \|_{\mathfrak{S}^2}}{\sqrt{\mu}}$$

and a similar inequality for  $\|\Pi_{2\mu}^+ Q \Pi_{2\mu}^+\|_{\mathfrak{S}^1}$ . On the other hand, since  $-\Pi_\mu^- \leq \Pi_{2\mu}^- Q \Pi_{2\mu}^- \leq \Pi_{2\mu}^-$ , we have  $|\rho_{\Pi_{2\mu}^- Q \Pi_{2\mu}^-}(x)| \leq C\mu^{d/2}$  almost everywhere. The Lieb-Thirring inequality (4.6.78) yields

$$\begin{aligned} \int_{\mathbb{R}^d} |\rho_{\Pi_{2\mu}^- Q \Pi_{2\mu}^-}|^2 &\leq C \int_{\mathbb{R}^d} \min\left(|\rho_{\Pi_{2\mu}^- Q \Pi_{2\mu}^-}|^2, |\rho_{\Pi_{2\mu}^- Q \Pi_{2\mu}^-}|^{1+\frac{2}{d}}\right) \\ &\leq C \operatorname{Tr}(-\Delta - \mu)Q \end{aligned}$$

with constants depending on  $d$  and  $\mu$ , which proves the result.  $\square$

Adapting the proof of Lemma 4.1, it is easy to see that  $\mathcal{Y}_\mu \subset \mathfrak{S}_{1,\text{loc}}$  and thus  $\rho_Q$  is a well-defined function for  $Q \in \mathcal{Y}_\mu$ . We actually have  $\rho_Q \in (L^1 + L^2)(\mathbb{R}^d)$  with the precise estimate

$$\left\| \rho_{\Pi_{2\mu}^- Q \Pi_{2\mu}^-} \right\|_{L^2} + \left\| \rho_{\Pi_{2\mu}^+ Q \Pi_{2\mu}^-} \right\|_{L^2} + \left\| \rho_{\Pi_{2\mu}^- Q \Pi_{2\mu}^+} \right\|_{L^2} + \left\| \rho_{\Pi_{2\mu}^+ Q \Pi_{2\mu}^+} \right\|_{L^1} \leq C \|Q\|_{\mathcal{Y}_\mu}. \quad (4.4.42)$$

It is very important for us that the map

$$Q \in \mathcal{Y}_\mu \mapsto \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y) \rho_Q(x) \rho_Q(y) dx dy$$

is continuous when  $w \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ , which follows from (4.4.42).

**Proposition 4.2** (Local well-posedness in  $\mathcal{Y}_\mu$ ). *Let  $d \geq 1$  and  $w \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ . Let  $Q_0 \in \mathcal{Y}_\mu$  such that*

$$\rho_{e^{it\Delta} \Pi_{2\mu}^- Q_0 \Pi_{2\mu}^- e^{-it\Delta}} \in C_t^0(\mathbb{R}, L_x^2(\mathbb{R}^d)). \quad (4.4.43)$$

*Then there exists a unique maximal solution  $Q \in \mathcal{C}^0((-T^-, T^+), \mathcal{Y}_\mu)$  to the Duhamel principle (4.3.16), with  $T^\pm > 0$ . We have the blow-up criterion*

$$T^\pm < \infty \implies \lim_{t \rightarrow \pm T^\pm} \|Q(t)\|_{\mathcal{Y}_\mu} = +\infty. \quad (4.4.44)$$

*The solution depends continuously on  $Q_0$  in  $\mathcal{Y}_\mu$ , on  $\rho_{e^{it\Delta} \Pi_{2\mu}^- Q_0 \Pi_{2\mu}^- e^{-it\Delta}}$  in the space  $\mathcal{C}_t^0((-T^-, T^+), L_x^2(\mathbb{R}^d))$ , and on  $w$  in  $L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ .*

The assumption (4.4.43) looks complicated but it is automatically satisfied if  $Q_0$  is a smooth finite rank operator, or if  $Q_0 = \gamma_0 - \Pi_\mu^-$  with  $\gamma_0 \in \mathcal{K}_\mu$ , since in this case  $\|e^{it\Delta} Q_0 e^{-it\Delta}\|_{\mathcal{X}_\mu} = \|Q_0\|_{\mathcal{X}_\mu}$  for all  $t$ . This is the situation which we will need later on.



**PROOF OF PROPOSITION 4.2.** The proof of the proposition relies on a fixed point technique, exactly like for the proof of Theorem 4.3 in Section 3. It follows from the estimates:

$$\sup_{t \in \mathbb{R}} \|e^{it\Delta} [\Pi_\mu^-, \rho_Q * w] e^{-it\Delta}\|_{\mathcal{Y}_\mu} \leq C \|Q\|_{\mathcal{Y}_\mu}, \quad (4.4.45)$$

$$\sup_{t \in \mathbb{R}} \|e^{it\Delta} [Q', \rho_Q * w] e^{-it\Delta}\|_{\mathcal{Y}_\mu} \leq C \|Q'\|_{\mathcal{Y}_\mu} \|Q\|_{\mathcal{Y}_\mu}. \quad (4.4.46)$$

All the terms in the definition of  $\|\cdot\|_{\mathcal{Y}_\mu}$  are invariant under the free Schrödinger evolution, except for the one involving the low-momentum density.

We start by proving (4.4.45) and note as a start that

$$\|[\Pi_\mu^-, \rho_Q * w]\| \leq \|\rho_Q * w\|_{L^\infty} \leq C(\|w\|_{L^2} + \|w\|_{L^\infty}) \|Q\|_{\mathcal{Y}_\mu}$$

by (4.4.42). Then we remark that  $\Pi_{2\mu}^+ [\rho_Q * w, \Pi_\mu^-] \Pi_{2\mu}^+ = 0$  since  $\Pi_\mu^- \Pi_{2\mu}^+ = 0$ . Writing for short  $V := \rho_Q * w$ , we turn to

$$\|\Pi_{2\mu}^+ [V, \Pi_\mu^-] \Pi_{2\mu}^-\|_{\mathfrak{S}^2} = \|\Pi_{2\mu}^+ V \Pi_\mu^-\|_{\mathfrak{S}^2} \leq \|V \Pi_\mu^-\|_{\mathfrak{S}^2} = C\mu^{d/4} \|V\|_{L^2},$$

which can be estimated by  $C(\|w\|_{L^1} + \|w\|_{L^2}) \|Q\|_{\mathcal{Y}_\mu}$  by (4.4.42). Finally, we estimate the density of  $e^{it\Delta} \Pi_{2\mu}^- [V, \Pi_\mu^-] \Pi_{2\mu}^- e^{-it\Delta}$  by duality, similarly as in Lemma 4.1:

$$\begin{aligned} \int_{\mathbb{R}^d} \rho_{e^{it\Delta} \Pi_{2\mu}^- V \Pi_\mu^- e^{-it\Delta}} W &= \text{Tr}(e^{it\Delta} \Pi_{2\mu}^- [V, \Pi_\mu^-] \Pi_{2\mu}^- e^{-it\Delta} W) \\ &\leq 2 \|\Pi_{2\mu}^- V\|_{\mathfrak{S}^2} \|\Pi_{2\mu}^- W\|_{\mathfrak{S}^2} \leq C \|V\|_{L^2} \|W\|_{L^2} \end{aligned}$$

where  $C$  is independent of  $t$ .

Next we turn to (4.4.46) and note first that  $\|[V, Q']\| \leq 2 \|V\|_{L^\infty} \|Q'\| \leq C \|Q\|_{\mathcal{Y}_\mu} \|Q'\|_{\mathcal{Y}_\mu}$ . For the Hilbert-Schmidt term, we write

$$\Pi_{2\mu}^+ V Q' \Pi_{2\mu}^- = \Pi_{2\mu}^+ V \Pi_{2\mu}^- Q' \Pi_{2\mu}^- + \Pi_{2\mu}^+ V \Pi_{2\mu}^+ Q' \Pi_{2\mu}^-,$$

and estimate the two terms on the right side. We have  $\|V \Pi_{2\mu}^-\|_{\mathfrak{S}^2} = C\mu^{d/4} \|V\|_{L^2}$ , leading to

$$\|\Pi_{2\mu}^+ V \Pi_{2\mu}^- Q' \Pi_{2\mu}^-\|_{\mathfrak{S}^2} \leq C \|V\|_{L^2} \|Q'\| \leq C \|Q\|_{\mathcal{Y}_\mu} \|Q'\|_{\mathcal{Y}_\mu}.$$

We also have

$$\|\Pi_{2\mu}^+ V \Pi_{2\mu}^+ Q' \Pi_{2\mu}^-\|_{\mathfrak{S}^2} \leq \|V\|_{L^\infty} \|\Pi_{2\mu}^+ Q' \Pi_{2\mu}^-\|_{\mathfrak{S}^2} \leq C \|Q\|_{\mathcal{Y}_\mu} \|Q'\|_{\mathcal{Y}_\mu},$$

and hence  $\|\Pi_{2\mu}^+ V Q' \Pi_{2\mu}^-\|_{\mathfrak{S}^2} \leq C \|Q\|_{\mathcal{Y}_\mu} \|Q'\|_{\mathcal{Y}_\mu}$ . The proof for  $\Pi_{2\mu}^+ Q' V \Pi_{2\mu}^-$  and for  $\Pi_{2\mu}^+ [V, Q'] \Pi_{2\mu}^+$  is similar. Finally,  $\rho[e^{it\Delta} \Pi_{2\mu}^- [V, Q'] \Pi_{2\mu}^- e^{-it\Delta}]$  is estimated by duality as before.

The rest of the proof of Proposition 4.2 goes along the same lines as that of Theorem 4.3. The assumption (4.4.43) on  $Q_0$  is needed to ensure that the term  $e^{it\Delta} Q_0 e^{-it\Delta}$  in Duhamel's formula belongs to  $C_t^0(\mathbb{R}, \mathcal{Y}_\mu)$ . In order to iterate the fixed

point theorem and construct a maximal solution, we need to verify that the condition (4.4.43) is propagated along the flow. So we have to prove that  $\rho_{e^{is\Delta}\Pi_{2\mu}^- Q(t)\Pi_{2\mu}^- e^{-is\Delta}}$  belongs to the space  $C_s^0(\mathbb{R}, L_x^2(\mathbb{R}^d))$ . From Duhamel's formula we have

$$\begin{aligned} \rho [e^{is\Delta}\Pi_{2\mu}^- Q(t)\Pi_{2\mu}^- e^{-is\Delta}] &= \rho [e^{i(t+s)\Delta} Q_0 e^{-i(t+s)\Delta}] \\ &\quad - i \int_0^t \rho [e^{i(s+t-t')\Delta} [w * \rho_Q(t'), \gamma_f + Q(t')] e^{i(t'-t-s)\Delta}] dt'. \end{aligned}$$

The first term is continuous and locally bounded under our assumption (4.4.43) on  $Q_0$ , and the second can be uniformly estimated by  $C \int_0^t (\|Q(t')\|_{\mathcal{Y}_\mu} + \|Q(t')\|_{\mathcal{Y}_\mu}^2) dt'$ . The continuity follows from a density argument.  $\square$

*Step 2. Conservation of relative energy for smooth operators.* In Theorem 4.3 we have constructed smooth solutions to the Hartree equation, in the Sobolev-Schatten spaces  $\mathfrak{S}^{p,s}$ . We remark that  $\mathfrak{S}^{1,s} \subset \mathcal{Y}_\mu$  for  $s > \max(2, d/2)$ , since then  $\rho_Q \in L^2$  by Lemma 4.1. By an argument similar to Corollary 4.1, one can prove that the maximal time of existence of solutions in  $\mathfrak{S}^{1,s}$  is the same as in  $\mathcal{Y}_\mu$ . The purpose of this step is to prove the conservation of the relative Hartree energy  $\mathcal{E}(\gamma(t), \Pi_\mu^-)$  when  $\gamma_0 - \Pi_\mu^- \in \mathfrak{S}^{1,s}$  with  $s$  large enough.

**Proposition 4.3** (Conservation of relative energy in  $\mathfrak{S}^{1,s}$ ). *Let  $d \geq 1$ ,  $s > 2 + \max(2, d/2)$ , and  $w \in L^1 \cap L^\infty$  satisfying all the assumptions of Theorem 4.3, with furthermore  $w(x) = w(-x)$  for a.e.  $x \in \mathbb{R}^d$ . Let  $Q_0 \in \mathfrak{S}^{1,s}$  and consider  $Q \in C_t^0((-T^-, T^+), \mathfrak{S}^{1,s})$  the unique maximal solution to (4.3.16) built in Theorem 4.3 with  $\gamma_f = \Pi_\mu^-$ . Then, the relative particle number and the relative energy are conserved along the flow: we have*

$$\mathcal{E}(\Pi_\mu^- + Q(t), \Pi_\mu^-) = \mathcal{E}(\Pi_\mu^- + Q_0, \Pi_\mu^-) \quad \text{and} \quad \text{Tr } Q(t) = \text{Tr } Q_0$$

for all  $t \in (-T^-, T^+)$ .

PROOF. We abbreviate  $\mathcal{E}(Q) := \mathcal{E}(\Pi_\mu^- + Q, \Pi_\mu^-)$  for shortness:

$$\begin{aligned} \mathcal{E}(Q(t)) &= \text{Tr} | -\Delta - \mu|^{1/2} (Q(t)^{++} - Q(t)^{--}) | -\Delta - \mu|^{1/2} \\ &\quad + \frac{1}{2} \iint \rho_{Q(t)}(x) \rho_{Q(t)}(y) w(x-y) dx dy. \end{aligned}$$

When  $Q \in \mathfrak{S}^{1,s}$  and  $s > \max(2, d/2)$ , then  $V_Q = w * \rho_Q \in (L^2 \cap L^\infty)(\mathbb{R}^d)$  and we infer that

$$\iint \rho_{Q(t)}(x) \rho_{Q(t)}(y) w(x-y) dx dy = \text{Tr}(V_Q Q).$$

From Duhamel's formula we see that  $\partial_t Q \in \mathfrak{S}^{1,s-2}$  and we can differentiate the function  $t \mapsto \mathcal{E}(Q(t))$ . The first term in  $\mathcal{E}(Q(t))$  is differentiable when  $\partial_t Q \in \mathfrak{S}^{1,2}$

which requires  $s \geq 4$ . Similarly, the second term is differentiable when  $s > 2 + d/2$ . Using that  $w(x) = w(-x)$ , we have for all  $t \in (-T^-, T^+)$

$$\partial_t \mathcal{E}(Q(t)) = \text{Tr} |-\Delta - \mu|^{1/2} (\dot{Q}^{++} - \dot{Q}^{--}) |-\Delta - \mu|^{1/2} + \text{Tr}(V_Q \dot{Q}),$$

with

$$\dot{Q}^{++} - \dot{Q}^{--} = (-i) ([-\Delta, Q^{++} - Q^{--}] + [V_Q, Q]^{++} - [V_Q, Q]^{--}).$$

Since  $Q^{++}, Q^{--} \in \mathfrak{S}^{1,4}$ , we have

$$\text{Tr} |-\Delta - \mu|^{1/2} [-\Delta, Q^{++}] |-\Delta - \mu|^{1/2} = 0 = \text{Tr} |-\Delta - \mu|^{1/2} [-\Delta, Q^{--}] |-\Delta - \mu|^{1/2}.$$

We now remark that  $(-\Delta - \mu)[V_Q, Q] \in \mathfrak{S}^1$ . Indeed,  $V_Q \in L^\infty$  and  $Q \in \mathfrak{S}^{1,2}$ , hence  $(-\Delta - \mu)QV_Q \in \mathfrak{S}^1$ . For the other term, we commute the Laplacian as follows

$$(-\Delta)V_Q Q = ((-\Delta V_Q) + 2\nabla V_Q \cdot \nabla)Q + V_Q(-\Delta)Q$$

and we use that  $\Delta V_Q, \nabla V_Q \in L^\infty$ , since  $w \in W^{2,1} \cap W^{2,\infty}$  by assumption. As a consequence,  $(-\Delta - \mu)[V_Q, Q] \in \mathfrak{S}^1$  and we have

$$\text{Tr} |-\Delta - \mu|^{1/2} ([V_Q, Q]^{++} - [V_Q, Q]^{--}) |-\Delta - \mu|^{1/2} = \text{Tr}(-\Delta - \mu)[V_Q, Q].$$

Since we also have  $V_Q Q \in \mathfrak{S}^1$ , then  $\text{Tr}[V_Q, Q] = 0$  and

$$\text{Tr}(-\Delta - \mu)[V_Q, Q] = \text{Tr}(-\Delta)[V_Q, Q] = \text{Tr} V_Q [Q, -\Delta].$$

Summarizing, we thus have proved that

$$\partial_t \text{Tr} |-\Delta - \mu|^{1/2} (Q^{++} - Q^{--}) |-\Delta - \mu|^{1/2} = \text{Tr}[-\Delta, V_Q]Q.$$

Now let us compute the time derivative of the second term in the energy. We have

$$\partial_t \frac{1}{2} \text{Tr}(V_Q Q) = \text{Tr}(V_Q \dot{Q}) = (-i) \text{Tr} V_Q ([-\Delta + V_Q, \gamma_f + Q]).$$

By the proof of Lemma 4.2, we know that  $V_Q \gamma_f \in \mathfrak{S}^{1,s}$ , and therefore the operators  $V_Q^2 \gamma_f$  and  $V_Q \gamma_f V_Q$  are both in  $\mathfrak{S}^1$  since  $V_Q \in L^\infty$ . We deduce that  $\text{Tr} V_Q [V_Q, \gamma_f] = 0$ . We have also seen that  $V_Q Q \in \mathfrak{S}^1$ , hence  $V_Q^2 Q, V_Q Q V_Q \in \mathfrak{S}^1$  and hence  $\text{Tr} V_Q [V_Q, Q] = 0$ . We finally have  $\partial_t \text{Tr}(V_Q Q) = 2 \text{Tr} V_Q [-\Delta, Q]$ , implying that

$$\partial_t \mathcal{E}(Q(t)) = \text{Tr} V_Q [Q, -\Delta] + \text{Tr} V_Q [-\Delta, Q] = 0,$$

and the energy is conserved. The proof for  $\text{Tr} Q(t)$  is similar.  $\square$

*Step 3. A solution starting in  $\mathcal{K}_\mu$  stays in  $\mathcal{K}_\mu$ .* Here we prove that any solution in  $\mathcal{Y}_\mu$  such that  $Q_0 = \gamma_0 - \Pi_\mu^-$  with  $\gamma_0 \in \mathcal{K}_\mu$  stays in the energy space for all times, and that the relative Hartree energy is conserved. Since states in  $\mathcal{K}_\mu$  do not necessarily have a finite particle number relative to  $\Pi_\mu^-$ , we *a priori* lose this conservation law.

**Proposition 4.4** (Conservation of the relative energy). *Assume that  $d \geq 2$  and that  $w \in L^1 \cap L^\infty$  with  $w(x) = w(-x)$  for a.e.  $x \in \mathbb{R}^d$ . Let  $Q_0 = \gamma_0 - \Pi_\mu^-$  with  $\gamma_0 \in \mathcal{K}_\mu$ . Then the unique maximal solution  $Q(t) = \gamma(t) - \Pi_\mu^- \in C_t^0((-T^-, T^+), \mathcal{Y}_\mu)$  satisfies that  $\gamma(t) \in \mathcal{K}_\mu$  for all  $t \in \mathbb{R}$  and the relative energy is conserved:*

$$\mathcal{E}(\gamma(t), \Pi_\mu^-) = \mathcal{E}(\gamma_0, \Pi_\mu^-), \quad \forall t \in (-T^-, T^+).$$

**PROOF.** We start by assuming that  $w$  satisfies all the assumptions of Theorem 4.3, with  $p = 1$  and some  $s > 2 + \max(2, d/2)$ . We will remove this condition at the end of the proof. Let  $\gamma_0 = Q_0 + \Pi_\mu^-$  be any density matrix in  $\mathcal{K}_\mu$ , and denote by  $Q(t)$  the associated maximal solution in  $C^0((-T^-, T^+), \mathcal{Y}_\mu)$ . The following is an improvement of [FLLS12, Lemma 3.2] and it says that one can approximate  $Q_0$  by a sequence of smooth finite-rank operators, with the low-momentum density converging strongly in  $L^2$ .

**Lemma 4.5.** *Let  $\gamma = Q + \Pi_\mu^- \in \mathcal{K}_\mu$  with  $d \geq 2$ . Then there exists a sequence  $-\Pi_\mu^- \leq Q^{(n)} \leq \Pi_\mu^+$  of finite rank operators, compactly supported in Fourier domain, such that*

- For all  $\varphi \in L^2(\mathbb{R}^d)$ ,  $Q^{(n)}\varphi \rightarrow Q\varphi$  in  $L^2(\mathbb{R}^d)$ ;
- $\lim_{n \rightarrow \infty} \|(Q^{(n)} - Q) - \Delta - \mu|^{1/2}\|_{\mathfrak{S}^2} = 0$ ;
- $\lim_{n \rightarrow \infty} \| | - \Delta - \mu|^{1/2} (Q^{(n)} - Q)^{\pm\pm} | - \Delta - \mu|^{1/2} \|_{\mathfrak{S}^1} = 0$ ;
- $\rho_{Q^{(n)}} \rightarrow \rho_Q$  in  $L^1_{\text{loc}}(\mathbb{R}^d)$ ;
- $\rho_{\Pi_{2\mu}^- Q^{(n)} \Pi_{2\mu}^-} \rightarrow \rho_{\Pi_{2\mu}^- Q \Pi_{2\mu}^-}$  strongly in  $L^2(\mathbb{R}^d)$ .

We finish the proof of Proposition 4.3 before turning to that of Lemma 4.5. We take a sequence  $Q_0^{(n)}$  as in Lemma 4.5 and remark that  $Q_0^{(n)} \rightarrow Q_0$  in  $\mathcal{Y}_\mu$ . Furthermore, by the proof of Lemma 4.5, we also have  $\rho[e^{it\Delta} \Pi_{2\mu}^- Q_0^{(n)} \Pi_{2\mu}^- e^{-it\Delta}] \rightarrow \rho[e^{it\Delta} \Pi_{2\mu}^- Q_0 \Pi_{2\mu}^- e^{-it\Delta}]$  strongly in  $L^2(\mathbb{R}^d)$  and uniformly in  $t$  on any compact set of  $\mathbb{R}$ . By Proposition 4.2, this proves that the maximal times of existence of the associated solution  $Q^{(n)}(t)$  satisfy  $\liminf_{n \rightarrow \infty} T_n^\pm \geq T^\pm$  and that  $Q^{(n)}(t) \rightarrow Q(t)$  in  $C_t^0([-T^- + \varepsilon, T^+ - \varepsilon], \mathcal{Y}_\mu)$  for any  $\varepsilon > 0$ . By (4.4.42), this implies in particular that  $\rho_{Q^{(n)}(t)} \rightarrow \rho_{Q(t)}$  strongly in  $C_t^0([-T^- + \varepsilon, T^+ - \varepsilon], L^1 + L^2)$  and, since  $w \in L^1 \cap L^\infty$ , that

$$\begin{aligned} \lim_{n \rightarrow \infty} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y) \rho_{Q^{(n)}(t)}(x) \rho_{Q^{(n)}(t)}(y) dx dy \\ = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y) \rho_{Q(t)}(x) \rho_{Q(t)}(y) dx dy \end{aligned}$$

uniformly in  $t$  on  $[-T^- + \varepsilon, T^+ - \varepsilon]$ . By Proposition 4.3, the relative Hartree energy of  $Q^{(n)}(t)$  is conserved and, therefore,

$$\begin{aligned} & \lim_{n \rightarrow \infty} \operatorname{Tr}(-\Delta - \mu)Q^{(n)}(t) \\ &= \operatorname{Tr}(-\Delta - \mu)Q_0 + \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y)\rho_{Q_0}(x)\rho_{Q_0}(y) dx dy \\ & \quad - \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y)\rho_{Q(t)}(x)\rho_{Q(t)}(y) dx dy \quad (4.4.47) \end{aligned}$$

where the right side is uniformly bounded for  $t \in [-T^- + \varepsilon, T^+ - \varepsilon]$ . Here we have used that  $\lim_{n \rightarrow \infty} \operatorname{Tr}(-\Delta - \mu)Q_0^{(n)} = \operatorname{Tr}(-\Delta - \mu)Q_0$ , by Lemma 4.5.

From (4.4.42) and the assumptions on  $w$ , for  $n$  large enough the potential  $w * \rho_{Q^{(n)}(t)}$  is in  $L^1([-T^- + \varepsilon, T^+ - \varepsilon], L_x^\infty)$ . By [Yaj87], this implies that there exists a unitary operator  $U^{(n)}(t, t')$  on  $L^2(\mathbb{R}^d)$  associated with the time-dependent Hamiltonian  $-\Delta + w * \rho_{Q^{(n)}(t)}$ . Then  $Q^{(n)}(t) = U^{(n)}(t, 0)(\Pi_\mu^- + Q_0^{(n)})U^{(n)}(0, t) - \Pi_\mu^-$ . In particular, since  $0 \leq \Pi_\mu^- + Q_0^{(n)} \leq 1$ , then  $0 \leq \Pi_\mu^- + Q^{(n)}(t) \leq 1$  for all  $t \in (-T^- + \varepsilon, T^+ - \varepsilon)$ . By the same argument, we have  $0 \leq \gamma(t) = \Pi_\mu^- + Q(t) \leq 1$  as well, for all  $t \in (-T^-, T^+)$ . In order to show that  $\gamma(t) \in \mathcal{K}_\mu$ , it suffices to prove that  $\operatorname{Tr}(-\Delta - \mu)Q(t)$  is finite for all  $t$ .

We recall that the relative kinetic energy is defined by  $\operatorname{Tr}(-\Delta - \mu)Q := \operatorname{Tr}|\Delta + \mu|^{1/2}(Q^{++} - Q^{--})|\Delta + \mu|^{1/2}$  and it is weakly lower semi-continuous since  $Q^{++}, -Q^{--} \geq 0$ . From (4.4.47) we deduce that

$$\begin{aligned} \operatorname{Tr}(-\Delta - \mu)Q(t) &\leq \operatorname{Tr}(-\Delta - \mu)Q_0 + \frac{1}{2} \iint w(x-y)\rho_{Q_0}(x)\rho_{Q_0}(y) dx dy \\ & \quad - \frac{1}{2} \iint w(x-y)\rho_{Q(t)}(x)\rho_{Q(t)}(y) dx dy \end{aligned}$$

which proves that  $\gamma(t) \in \mathcal{K}_\mu$  for all  $t$ , and that  $\mathcal{E}(\gamma(t), \Pi_\mu^-) \leq \mathcal{E}(\gamma_0, \Pi_\mu^-)$ , for all  $t \in (-T^-, T^+)$ . In order to derive the other inequality, it suffices to exchange the role of  $t$  and 0. We start the dynamics at  $t$  with initial condition  $\gamma(t) \in \mathcal{K}_\mu$  and, by uniqueness, the so-obtained solution coincides with the other dynamics started at 0. The previous argument provides the reverse inequality  $\mathcal{E}(\gamma_0, \Pi_\mu^-) \leq \mathcal{E}(\gamma(t), \Pi_\mu^-)$ .

Our proof was based on the fact that  $w$  is very smooth, but now that we have shown the conservation of the energy for all solutions in  $\mathcal{K}_\mu$ , we can remove this condition by using the continuity of the solutions in  $\mathcal{Y}_\mu$  with respect to  $w$ . On the other hand, the blow up criterion (4.4.44) follows from the one in  $\mathcal{Y}_\mu$  by (4.4.41). We skip the details.  $\square$

It remains to provide the

**PROOF OF LEMMA 4.5.** Like in [FLLS12, Lemma 3.2], we let  $Q^{(n)} := P_n Q P_n$  with  $P_n := \mathbb{1}(|-\Delta - \mu| \leq n)$ , which localizes away from the Fermi surface and

from infinity. The operator  $Q^{(n)}$  is not yet of finite rank, but it is Hilbert-Schmidt and very smooth, and it can itself be approximated by a finite rank operator by [HLS09a, Thm 6]. The convergence properties of  $Q^{(n)}$  are all proved in [FLLS12, Lemma 3.2], except for the last one, for which we compute

$$\begin{aligned} \Pi_{2\mu}^- Q^{(n)} \Pi_{2\mu}^- - \Pi_{2\mu}^- Q \Pi_{2\mu}^- &= \Pi_{2\mu}^- P_n Q P_n \Pi_{2\mu}^- - \Pi_{2\mu}^- Q \Pi_{2\mu}^- \\ &= -\Pi_{2\mu}^- P_n^\perp Q P_n^\perp \Pi_{2\mu}^- - \Pi_{2\mu}^- P_n^\perp Q P_n \Pi_{2\mu}^- \\ &\quad - \Pi_{2\mu}^- P_n Q P_n^\perp \Pi_{2\mu}^- \end{aligned} \quad (4.4.48)$$

with  $n \geq 2\mu$ . The density of  $\Pi_{2\mu}^- P_n^\perp Q P_n^\perp \Pi_{2\mu}^-$  is in  $L^\infty$  due to the projection  $\Pi_{2\mu}^-$  and, by the Lieb-Thirring inequality (4.4.35), we have

$$\begin{aligned} \int_{\mathbb{R}^d} \rho_{\Pi_{2\mu}^- P_n^\perp Q P_n^\perp \Pi_{2\mu}^-}^2 &\leq C \int_{\mathbb{R}^d} \min(\rho_{\Pi_{2\mu}^- P_n^\perp Q P_n^\perp \Pi_{2\mu}^-}^2, \rho_{\Pi_{2\mu}^- P_n^\perp Q P_n^\perp \Pi_{2\mu}^-}^{1+2/d}) \\ &\leq C \operatorname{Tr} |-\Delta - \mu| \Pi_{2\mu}^- P_n^\perp Q P_n^\perp \Pi_{2\mu}^- \rightarrow 0. \end{aligned}$$

We still need to control the density of the two other terms in (4.4.48) and we only explain how to deal with the first one. We write

$$\begin{aligned} \Pi_{2\mu}^- P_n^\perp Q P_n \Pi_{2\mu}^- &= P_n^\perp Q^{--} P_n + \Pi_{2\mu}^- P_n^\perp Q^{++} P_n \Pi_{2\mu}^- \\ &\quad + \Pi_{\mu}^- P_n^\perp Q P_n \Pi_{2\mu}^- \Pi_{\mu}^+ + \Pi_{\mu}^+ \Pi_{2\mu}^- P_n^\perp Q P_n \Pi_{\mu}^- \end{aligned}$$

Following the proof in [FLLS12, p 456–457], we find that the density of the last two terms can be estimated in  $L^2$  by a constant times

$$\|Q P_n^\perp |\Delta + \mu|^{1/2}\|_{\mathfrak{S}^2}^{1/2} \|Q P_n |\Delta + \mu|^{1/2}\|_{\mathfrak{S}^2}^{1/2}$$

which tends to 0 when  $n \rightarrow \infty$ . We therefore only have to deal with the first two terms. Using that  $Q^{--} \leq 0$ , we write

$$\frac{1}{4\varepsilon} P_n^\perp Q^{--} P_n^\perp + \varepsilon P_n Q^{--} P_n \leq P_n^\perp Q^{--} P_n \leq -\frac{1}{4\varepsilon} P_n^\perp Q^{--} P_n^\perp - \varepsilon P_n Q^{--} P_n$$

and deduce  $|\rho_{P_n^\perp Q^{--} P_n^\perp}| \leq (4\varepsilon)^{-1} |\rho_{P_n^\perp Q^{--} P_n^\perp}| + \varepsilon |\rho_{P_n Q^{--} P_n}|$ . From (4.4.35) and the fact that the density of all the operators appearing in the previous estimates are uniformly bounded, we conclude that

$$\int_{\mathbb{R}^d} |\rho_{P_n^\perp Q^{--} P_n^\perp}|^2 \leq -\frac{1}{4\varepsilon} \operatorname{Tr} |\Delta + \mu| P_n^\perp Q^{--} P_n^\perp - \varepsilon \operatorname{Tr} |\Delta + \mu| Q^{--}.$$

The argument is the same for the term involving  $Q^{++}$  and we get the result by letting first  $n \rightarrow \infty$  and then  $\varepsilon \rightarrow 0$ .  $\square$

*Step 4. Global well-posedness in the defocusing case.* Now we assume that  $d \geq 3$  and  $\widehat{w} \geq 0$  or that  $d = 2$  and  $\|(\widehat{w})_-\|_{L^\infty} < K_{\text{LT}}/(2\pi)$ . Then we deduce from (4.4.36) and (4.4.37) that

$$\text{Tr}(-\Delta - \mu)Q(t) \leq \begin{cases} \mathcal{E}(\gamma_0, \Pi_\mu^-) & \text{for } d \geq 3, \\ \frac{\mathcal{E}(\gamma_0, \Pi_\mu^-)}{1 - \frac{2\pi\|\widehat{w}_-\|_{L^\infty}}{K_{\text{LT}}}} & \text{for } d = 2, \end{cases}$$

and all  $t \in (-T^-, T^+)$ . This shows that  $Q(t)$  is uniformly bounded in  $\mathcal{X}_\mu$  and therefore in  $\mathcal{Y}_\mu$ , by (4.4.41). This implies global well-posedness, by the blow-up criterion (4.4.44) in  $\mathcal{Y}_\mu$ .  $\square$

### 5. Local well-posedness with Strichartz estimates

In Section 3, we have constructed solutions to the Hartree equation (4.1.3) in  $\mathfrak{S}^{p,s}$  with  $s > d(p-1)/p$ . We then used similar techniques in Section 4 to deal with the special case of a Fermi gas at zero temperature,  $\gamma_f = \Pi_\mu^-$ . Our goal is to solve the positive temperature cases (4.1.6)–(4.1.8) as well. Because of Klein's inequality (see (4.6.75) in Section 6), it is natural to look for solutions in the space  $\mathfrak{S}^{2,1}$  of operators  $Q$  such that  $Q(1-\Delta)^{1/2} \in \mathfrak{S}^2$ . This space is covered by Theorem 4.3 only in dimension  $d = 1$ . We treat here the cases  $d = 1, 2, 3$  by a different method.

So far we have only employed estimates relating  $Q(t)$  and  $\rho_{Q(t)}$  which are uniform with respect to the time variable. That is, we have not used the regularization properties of the time-dependent Schrödinger propagator, which are usually expressed by means of *Strichartz inequalities*. The usual inequality of this kind [Str77, KT98, Caz03, Tao06] is of little use in our context and, instead, our results are based on a more precise Strichartz inequality in Schatten spaces, which has recently been proved in [FLLS13].

In this section we take again a general reference state  $\gamma_f = f(-\Delta)$ . We do not assume anymore that  $\gamma_f = \Pi_\mu^-$ . We want to lower the exponent  $s$  measuring the regularity of  $Q$ . For shortness, we only consider two cases in this section:  $\mathfrak{S}^2$  in dimension  $d = 1, 2$  and  $\mathfrak{S}^{2,1}$  in dimension  $d = 1, 2, 3$ . Our method allows to decrease the regularity exponent  $s$  in higher dimensions, but without reaching  $s = 1$ . Also, we can deal with other Schatten exponents  $p$ , but we do not mention this here.

**Theorem 4.5** (Well-posedness in  $\mathfrak{S}^2$  in  $d = 1, 2$ ). *Let  $d \in \{1, 2\}$ ,  $w \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$  and  $f \in L^\infty(\mathbb{R}^+, \mathbb{R})$  such that  $\int_{\mathbb{R}^d} |f(k^2)| dk < \infty$ . Assume that*

$$Q_0 \in \mathfrak{S}^2 \quad \text{and} \quad w * \rho_{e^{it\Delta}Q_0e^{-it\Delta}} \in L_{t,\text{loc}}^{8/d}(\mathbb{R}, L_x^2 \cap L_x^\infty). \quad (4.5.49)$$

*Then there exists a unique maximal solution  $Q(t) \in C^0((-T^-, T^+), \mathfrak{S}^2)$  to (4.3.16) with  $T^\pm > 0$ , such that  $w * \rho_{Q(t)} \in L_{t,\text{loc}}^{8/d}((-T^-, T^+), L_x^2 \cap L_x^\infty)$ . We have the blow up*

*criterion*

$$T^\pm < \infty \implies \lim_{t \rightarrow \pm T^\pm} \int_0^{\pm t} \|w * \rho_{Q(t)}\|_{L_x^2 \cap L_x^\infty}^{8/d} dt = +\infty. \quad (4.5.50)$$

Furthermore, this solution is continuous with respect to  $Q_0$ ,  $w$  and  $f$ : if  $Q_0^{(n)} \rightarrow Q_0$ ,  $w_n \rightarrow w$  and  $f_n \rightarrow f$  for the norms appearing above, then the corresponding unique solution  $Q_n(t)$  has a time of existence such that  $\liminf T_n^\pm \geq T^\pm$ , and we have for every  $\varepsilon > 0$

$$\begin{aligned} \lim_{n \rightarrow \infty} \|w * \rho_{Q(t)} - w_n * \rho_{Q_n(t)}\|_{L^{8/d}((-T^- + \varepsilon, T^+ - \varepsilon), L_x^2 \cap L_x^\infty)} \\ = \lim_{n \rightarrow \infty} \|Q_n(t) - Q(t)\|_{L^\infty((-T^- + \varepsilon, T^+ - \varepsilon), \mathfrak{S}^2)} = 0. \end{aligned}$$

**Theorem 4.6** (Well-posedness in  $\mathfrak{S}^{2,1}$  in  $d = 1, 2, 3$ ). *Let  $d \in \{1, 2, 3\}$ ,  $w, \nabla w \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$  and  $f \in L^\infty(\mathbb{R}^+, \mathbb{R})$  such that  $\int_{\mathbb{R}^d} (|f(k^2)| + k^2 |f(k^2)|^2) dk < \infty$ . Assume that*

$$Q_0 \in \mathfrak{S}^{2,1} \quad \text{and} \quad w * \rho_{e^{it\Delta} Q_0 e^{-it\Delta}} \in L_{t,\text{loc}}^{8/d}(\mathbb{R}, H_x^1 \cap W_x^{1,\infty}). \quad (4.5.51)$$

Then there exists a unique maximal solution  $Q(t) \in C^0((-T^-, T^+), \mathfrak{S}^{2,1})$  to (4.3.16) with  $T^\pm > 0$ , such that  $w * \rho_{Q(t)} \in L_{t,\text{loc}}^{8/d}((-T^-, T^+), H_x^1 \cap W_x^{1,\infty})$ . We have the blow up criterion

$$T^\pm < \infty \implies \lim_{t \rightarrow \pm T^\pm} \int_0^{\pm t} \|w * \rho_{Q(t)}\|_{H_x^1 \cap W_x^{1,\infty}}^{8/d} dt = +\infty. \quad (4.5.52)$$

Furthermore, this solution is continuous with respect to  $Q_0$ ,  $w$  and  $f$ , in the same fashion as in the previous theorem.

As in Proposition 4.2, we need the complicated assumptions (4.5.49) and (4.5.51) on the density of the initial datum  $Q_0$ . This is necessary since an operator  $Q_0 \in \mathfrak{S}^2$  (or  $\in \mathfrak{S}^{2,1}$  for  $d = 3$ ) has no well-defined density in general. The assumption on the density is satisfied if for instance  $Q_0 \in \mathfrak{S}^{8/7}$ , by the Strichartz inequality of [FLLS13] which precisely states that

$$\|\rho_{e^{it\Delta} Q_0 e^{-it\Delta}}\|_{L_t^p L_x^q} \leq C \|Q_0\|_{\mathfrak{S}^{\frac{2q}{q+1}}}, \quad \text{for } 1 \leq q \leq 1 + \frac{2}{d} \text{ and } \frac{2}{p} + \frac{d}{q} = d. \quad (4.5.53)$$

Later, (4.5.51) will be satisfied for another reason, namely because  $\gamma_0 = \gamma_f + Q_0$  will have a finite entropy relative to  $\gamma_f$ .

The strategy to prove Theorems 4.5 and 4.6 is different from our previous proofs of local well-posedness. We use a fixed-point argument on the *potential*  $V_Q = w * \rho_Q$ . To do so, we notice that, if  $Q \in C_t^0([-T, T], \mathfrak{S}_{\text{loc}}^1)$  is such that  $V_Q \in L_t^1((-T, T), L_x^\infty)$ , it is equivalent that  $Q$  solves (4.3.16) and that

$$Q(t) = e^{it\Delta} \mathcal{W}_{V_Q}(t, 0) (\gamma_f + Q_0) \mathcal{W}_{V_Q}(t, 0)^* e^{-it\Delta} - \gamma_f, \quad \forall t \in [-T, T], \quad (4.5.54)$$



where the wave operator  $\mathcal{W}_V(t, 0)$  is defined for any  $V \in L_t^1((-T, T), L_x^\infty)$  via the Dyson series

$$\mathcal{W}_V(t, 0) = 1 + \sum_{n \geq 1} \mathcal{W}_V^{(n)}(t, 0), \quad (4.5.55)$$

with, for all  $t, t_0 \in [-T, T]$ ,

$$\begin{aligned} \mathcal{W}_V^{(n)}(t, t_0) &:= (-i)^n \int_{t_0}^t dt_n \int_{t_0}^{t_n} dt_{n-1} \cdots \int_{t_0}^{t_2} dt_1 \times \\ &\quad \times e^{i(t_0-t_n)\Delta} V(t_n) e^{i(t_n-t_{n-1})\Delta} \cdots e^{i(t_2-t_1)\Delta} V(t_1) e^{i(t_1-t_0)\Delta}. \end{aligned}$$

We recall that this series is absolutely convergent in  $\mathcal{B}(L^2(\mathbb{R}^d))$  for any fixed  $t, t_0$ , since

$$\|\mathcal{W}_V^{(n)}(t, t_0)\| \leq \frac{1}{n!} \|V\|_{L_t^1([-T, T], L_x^\infty(\mathbb{R}^d))}^n$$

for any  $n \geq 1$ . As a consequence, the potential  $V_Q$  solves the equation

$$V_Q(t) = w * (\rho [e^{it\Delta} \mathcal{W}_{V_Q}(t, 0)(\gamma_f + Q_0) \mathcal{W}_{V_Q}(t, 0)^* e^{-it\Delta}] - \rho_{\gamma_f}), \quad (4.5.56)$$

in the space  $L_t^1((-T, T), L_x^\infty)$ . We find a local solution to (4.5.56) in the smaller space  $L_t^{8/d}((-T, T), L_x^2 \cap L_x^\infty)$ , for  $T > 0$  small enough, by a fixed point argument. The solution will then be extended to a maximal time of existence by verifying that the conditions (4.5.49) and (4.5.51) are propagated along the flow.

The rest of this section is devoted to the proof of the two theorems. As usual, we first detail useful estimates before turning to the actual proof. The main ingredient is an estimate from [FLLS13] on the wave operators  $\mathcal{W}_V^{(n)}(t, t_0)$ . For  $n = 1$ , the estimate dual to (4.5.53) is

$$\left\| \mathcal{W}_V^{(1)}(t, t_0) \right\|_{\mathfrak{S}^{2q}} \leq C \|V\|_{L_t^p L_x^q}, \quad (4.5.57)$$

and, for  $n \geq 2$ , it reads

$$\left\| \mathcal{W}_V^{(n)}(t, t_0) \right\|_{\mathfrak{S}^{2\lceil \frac{q}{n} \rceil}} \leq \frac{C^n}{(n!)^{\frac{1}{p}-\varepsilon}} \|V\|_{L_t^p L_x^q}^n. \quad (4.5.58)$$

Here  $t, t_0 \in \mathbb{R}$ ,  $d \geq 1$ ,  $1 + d/2 \leq q < \infty$ ,  $2/p + d/q = 2$  and  $0 < \varepsilon < 1/p$ . The constant  $C$  depends on  $d, p, q, \varepsilon$  but not on  $t, t_0 \in \mathbb{R}$ .

In addition to this result, we need some estimates adapted to the space  $\mathfrak{S}^{2,1}$  (that is, involving derivatives) for the second order term  $\mathcal{W}_V^{(2)}(t, t_0)$ . These estimates are only valid for  $d = 1, 2, 3$ , and this is where the dimensional restriction in Theorem 4.6 comes from.

**Lemma 4.6** (Second order term  $\mathcal{W}^{(2)}$ ). *Let  $d \in \{1, 2, 3\}$ . For any potential functions  $U, V \in L_t^{8/(8-d)}(\mathbb{R}, L_x^2 \cap L_x^4)$ , and for any  $t, t_0 \in \mathbb{R}$ , we define the operator*

$$\mathcal{W}_{(U,V)}^{(2)}(t, t_0) := - \int_{t_0}^t dt_2 \int_{t_0}^{t_2} dt_1 e^{-it_2\Delta} U(t_2) e^{i(t_2-t_1)\Delta} V(t_1) e^{it_1\Delta}.$$

Then, we have the estimate

$$\left\| (1 - \Delta)^{-\frac{1}{4}} \mathcal{W}_{(U,V)}^{(2)}(t, t_0) (1 - \Delta)^{-\frac{1}{4}} \right\|_{\mathfrak{S}^2} \leq C \|U\|_{L_t^{\frac{8}{8-d}}(L_x^2 \cap L_x^4)} \|V\|_{L_t^{\frac{8}{8-d}}(L_x^2 \cap L_x^4)}. \quad (4.5.59)$$

Furthermore, for any  $U, V \in L_t^{\frac{5}{5-d}}(\mathbb{R}, L_x^{5/2}) \cap L_t^{\frac{10}{10-d}}(\mathbb{R}, L_x^{5/2})$ , we have

$$\begin{aligned} & \left\| \mathcal{W}_{(U,V)}^{(2)}(t, t_0) (1 - \Delta)^{-\frac{1}{2}} \right\|_{\mathfrak{S}^2} \\ & \leq C \|U\|_{L_t^{\frac{5}{5-d}}(L_x^{5/2})}^{1/2} \|V\|_{L_t^{\frac{5}{5-d}}(L_x^{5/2})}^{1/2} \|U\|_{L_t^{\frac{10}{10-d}}(L_x^{5/2})}^{1/2} \|V\|_{L_t^{\frac{10}{10-d}}(L_x^{5/2})}^{1/2}. \end{aligned} \quad (4.5.60)$$

The constant  $C > 0$  only depends on the dimension  $d$ .

**PROOF OF LEMMA 4.6.** We start by proving (4.5.59). Let  $U, V \in L_t^{\frac{8}{8-d}}(\mathbb{R}, (L_x^2 \cap L_x^4)(\mathbb{R}^d))$ . The method is the same as the proof of [FLLS13, Thm 2]: noticing that  $e^{-it\Delta} V(x) e^{it\Delta} = V(x + 2tp)$  with  $p := -i\nabla$ , we deduce that

$$\begin{aligned} \left\| (1 - \Delta)^{-\frac{1}{4}} \mathcal{W}_{(U,V)}^{(2)}(t, t_0) (1 - \Delta)^{-\frac{1}{4}} \right\|_{\mathfrak{S}^2}^2 &= \text{Tr} \int_{t_0}^t dt_2 \int_{t_0}^{t_2} dt_1 \int_{t_0}^t dt_4 \int_{t_0}^{t_4} dt_3 \\ & (1 - \Delta)^{-\frac{1}{4}} U(t_2, x + 2t_2 p) V(t_1, x + 2t_1 p) (1 - \Delta)^{-\frac{1}{2}} \times \\ & \times V(t_3, x + 2t_3 p) U(t_4, x + 2t_4 p) (1 - \Delta)^{-\frac{1}{4}}, \end{aligned}$$

which can be estimated by

$$\begin{aligned} & \int_{\mathbb{R}^4} dt_1 dt_2 dt_3 dt_4 \left\| (1 - \Delta)^{-\frac{1}{4}} |U|^{\frac{1}{2}}(t_2, x + 2t_2 p) \right\|_{\mathfrak{S}^8} \times \\ & \times \left\| |U|^{\frac{1}{2}}(t_2, x + 2t_2 p) |V|^{\frac{1}{2}}(t_1, x + 2t_1 p) \right\|_{\mathfrak{S}^4} \left\| |V|^{\frac{1}{2}}(t_1, x + 2t_1 p) (1 - \Delta)^{-\frac{1}{4}} \right\|_{\mathfrak{S}^8} \times \\ & \times \left\| (1 - \Delta)^{-\frac{1}{4}} |V|^{\frac{1}{2}}(t_3, x + 2t_3 p) \right\|_{\mathfrak{S}^8} \left\| |V|^{\frac{1}{2}}(t_3, x + 2t_3 p) |U|^{\frac{1}{2}}(t_4, x + 2t_4 p) \right\|_{\mathfrak{S}^4} \times \\ & \times \left\| |U|^{\frac{1}{2}}(t_4, x + 2t_4 p) (1 - \Delta)^{-\frac{1}{4}} \right\|_{\mathfrak{S}^8}. \end{aligned}$$

Using that  $k \mapsto (1 + k^2)^{-1/4} \in L^8(\mathbb{R}^d)$  for  $d = 1, 2, 3$  and the estimate

$$\|f(\alpha x + \beta p) g(\gamma x + \delta p)\|_{\mathfrak{S}^r} \leq (2\pi)^{-d/r} \frac{\|f\|_{L^r(\mathbb{R}^d)} \|g\|_{L^r(\mathbb{R}^d)}}{|\alpha\delta - \beta\gamma|^{\frac{d}{r}}} \quad (4.5.61)$$

valid for all  $r \geq 2$  by [FLLS13, Lemma 1], we deduce that

$$\begin{aligned} \left\| (1 - \Delta)^{-\frac{1}{4}} \mathcal{W}_{(U,V)}^{(2)}(t, t_0) (1 - \Delta)^{-\frac{1}{4}} \right\|_{\mathfrak{S}^2}^2 &\leq C \int_{\mathbb{R}^4} dt_1 dt_2 dt_3 dt_4 \times \\ & \times \frac{\|U(t_1)\|_{L_x^2 \cap L_x^4} \|U(t_2)\|_{L_x^2 \cap L_x^4} \|V(t_3)\|_{L_x^2 \cap L_x^4} \|V(t_4)\|_{L_x^2 \cap L_x^4}}{|t_1 - t_2|^{\frac{d}{4}} |t_3 - t_4|^{\frac{d}{4}}}. \end{aligned}$$

The inequality (4.5.59) follows from the multilinear Hardy-Littlewood-Sobolev (HLS) inequality [FLLS13, Thm 4]. To prove (4.5.60), we use the same method:

$$\begin{aligned} & \left\| \mathcal{W}_{(U,V)}^{(2)}(t, t_0)(1 - \Delta)^{-\frac{1}{2}} \right\|_{\mathfrak{S}^2}^2 \\ & \leq \int_{\mathbb{R}^4} dt_1 dt_2 dt_3 dt_4 \|(1 - \Delta)^{-\frac{1}{2}} |V|^{\frac{1}{2}}(t_3, x + 2t_3 p)\|_{\mathfrak{S}^5} \times \\ & \quad \times \| |V|^{\frac{1}{2}}(t_3, x + 2t_3 p) |U|^{\frac{1}{2}}(t_4, x + 2t_4 p) \|_{\mathfrak{S}^5} \times \\ & \quad \times \| |U|^{\frac{1}{2}}(t_4, x + 2t_4 p) |U|^{\frac{1}{2}}(t_2, x + 2t_2 p) \|_{\mathfrak{S}^5} \times \\ & \quad \times \| |U|^{\frac{1}{2}}(t_2, x + 2t_2 p) |V|^{\frac{1}{2}}(t_1, x + 2t_1 p) \|_{\mathfrak{S}^5} \| |V|^{\frac{1}{2}}(t_1, x + 2t_1 p) (1 - \Delta)^{-1/2} \|_{\mathfrak{S}^5}. \end{aligned}$$

Then, again by (4.5.61), we have

$$\begin{aligned} & \left\| \mathcal{W}_{(U,V)}^{(2)}(t, t_0)(1 - \Delta)^{-\frac{1}{2}} \right\|_{\mathfrak{S}^2}^2 \\ & \leq \int_{\mathbb{R}^4} dt_1 dt_2 dt_3 dt_4 \frac{\|U(t_1)\|_{L_x^{5/2}} \|U(t_2)\|_{L_x^{5/2}} \|V(t_3)\|_{L_x^{5/2}} \|V(t_4)\|_{L_x^{5/2}}}{|t_1 - t_2|^{\frac{d}{5}} |t_2 - t_4|^{\frac{d}{5}} |t_3 - t_4|^{\frac{d}{5}}}, \end{aligned}$$

which leads to (4.5.60) by the multilinear HLS inequality.  $\square$

**Lemma 4.7.** *Let  $d \geq 1$ . We have*

$$\|\mathcal{W}_V^{(n)}(t, t_0)g(-i\nabla)\|_{\mathfrak{S}^2} \leq (2\pi)^{d/2} \frac{\|V\|_{L_t^1 L_x^\infty}^{n-1}}{(n-1)!} \|V\|_{L_t^1 L_x^2} \|g\|_{L^2}, \quad \forall t, t_0 \in \mathbb{R}$$

for any  $V \in L_t^1(\mathbb{R}, L_x^2 \cap L_x^\infty)$ ,  $g \in L^2(\mathbb{R}^d)$ , and all  $n \geq 1$ .

PROOF. We write

$$\begin{aligned} & \|\mathcal{W}_V^{(n)}(t, t_0)g(-i\nabla)\|_{\mathfrak{S}^2} \\ & \leq \int_{t_0}^t dt_n \int_{t_0}^{t_n} dt_{n-1} \cdots \int_{t_0}^{t_2} dt_1 \|V(t_n)\|_{L_x^\infty} \cdots \|V(t_2)\|_{L_x^\infty} \|V(t_1, x)g(-i\nabla)\|_{\mathfrak{S}^2} \\ & \leq (2\pi)^{\frac{d}{2}} \|V\|_{L_t^1 L_x^2} \|g\|_{L^2} \int_{t_0}^t dt_n \int_{t_0}^{t_n} dt_{n-1} \cdots \int_{t_0}^{t_2} dt_1 \|V(t_n)\|_{L_x^\infty} \cdots \|V(t_2)\|_{L_x^\infty} \\ & \leq (2\pi)^{\frac{d}{2}} \frac{\|V\|_{L_t^1 L_x^\infty}^{n-1}}{(n-1)!} \|V\|_{L_t^1 L_x^2} \|g\|_{L^2}. \end{aligned} \quad \square$$

By using the previous estimates, we are now able to get local solutions to the potential equation (4.5.56).

**Proposition 4.5** (Solving the potential equation (4.5.56)). *Let  $d \in \{1, 2, 3\}$ ,  $w \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$  and  $f \in L^\infty(\mathbb{R}^+, \mathbb{R})$  such that  $\int_{\mathbb{R}^d} |f(k^2)| dk < \infty$ . Assume that*

$$Q_0 \in \mathfrak{S}^2 \quad \text{and} \quad w * \rho_{e^{it\Delta} Q_0 e^{-it\Delta}} \in L_{t,\text{loc}}^{8/d}(\mathbb{R}, L_x^2 \cap L_x^\infty) \quad (4.5.62)$$

with the additional condition that  $Q_0 \in \mathfrak{S}^{2,1}$  if  $d = 3$ . Then there exists a time  $T > 0$  and a solution  $V \in L_t^{8/d}((-T, T), L_x^2 \cap L_x^\infty)$  of (4.5.56). The corresponding density satisfies

$$\begin{aligned} \rho [e^{it\Delta} \mathcal{W}_V(t, 0)(\gamma_f + Q_0) \mathcal{W}_V(t, 0)^* e^{-it\Delta}] - \rho_{\gamma_f} - \rho [e^{it\Delta} Q_0 e^{-it\Delta}] \\ \in L_t^{8/d}((-T, T), L_x^1 + L_x^2). \end{aligned} \quad (4.5.63)$$

Furthermore, if

$$\begin{aligned} \|Q_0\|_{\mathfrak{S}^2 / \mathfrak{S}^{2,1}} + \|w * \rho_{e^{it\Delta} Q_0 e^{-it\Delta}}\|_{L_t^{8/d}((-1, 1), L_x^2 \cap L_x^\infty)} + \|w\|_{L^1 \cap L^\infty} \\ + \|f\|_{L^\infty} + \int_{\mathbb{R}^d} |f(k^2)| dk \leq R, \end{aligned}$$

then the time  $T > 0$  can be chosen to depend only on  $R$ .

PROOF OF PROPOSITION 4.5. Let  $Q_0$  be as in the statement,  $0 < T \leq 1$  to be chosen later and  $R \geq \|Q_0\|_{\mathfrak{S}^2 / \mathfrak{S}^{2,1}} + \|w * \rho_{e^{it\Delta} Q_0 e^{-it\Delta}}\|_{L_t^{8/d}((-1, 1), L_x^2 \cap L_x^\infty)}$  where the norm for  $Q_0$  is that of  $\mathfrak{S}^2$  when  $d = 1, 2$  and  $\mathfrak{S}^{2,1}$  when  $d = 3$ . For any  $V \in L_t^{8/d}((-T, T), L_x^2 \cap L_x^\infty)$ , define

$$\Phi(V)(t) = w * (\rho [e^{it\Delta} \mathcal{W}_V(t, 0)(\gamma_f + Q_0) \mathcal{W}_V(t, 0)^* e^{-it\Delta}] - \rho_{\gamma_f}),$$

for all  $t \in (-T, T)$ . We now provide the necessary estimates to apply a fixed-point argument to  $\Phi$ . First, we perform the decomposition

$$\begin{aligned} e^{it\Delta} \mathcal{W}_V(t, 0)(\gamma_f + Q_0) \mathcal{W}_V(t, 0)^* e^{-it\Delta} &= \gamma_f + e^{it\Delta} Q_0 e^{-it\Delta} \\ &+ e^{it\Delta} (\mathcal{W}_V^{(1)}(t, 0) Q_0 + Q_0 \mathcal{W}_V^{(1)}(t, 0)^*) e^{-it\Delta} \\ &+ \sum_{n \geq 1} e^{it\Delta} (\mathcal{W}_V^{(n)}(t, 0) \gamma_f + \gamma_f \mathcal{W}_V^{(n)}(t, 0)^*) e^{-it\Delta} + A_V(t). \end{aligned} \quad (4.5.64)$$

Let us now show that  $A_V \in C_t^0([-T, T], \mathfrak{S}^1)$ , which will imply that  $\rho_{A_V}$  belongs to  $C_t^0([-T, T], L^1)$ . From the definition of  $A_V$ , we have

$$\begin{aligned} A_V(t) &= \sum_{n \geq 2} e^{it\Delta} (\mathcal{W}_V^{(n)}(t, 0) Q_0 + Q_0 \mathcal{W}_V^{(n)}(t, 0)^*) e^{-it\Delta} \\ &+ e^{it\Delta} \mathcal{W}_V^{(1)}(t, 0) Q_0 \mathcal{W}_V^{(1)}(t, 0)^* e^{-it\Delta} \\ &+ \sum_{\max(n, m) \geq 2} e^{it\Delta} \mathcal{W}_V^{(n)}(t, 0) Q_0 \mathcal{W}_V^{(m)}(t, 0)^* e^{-it\Delta} \\ &+ \sum_{n, m \geq 1} e^{it\Delta} \mathcal{W}_V^{(n)}(t, 0) \gamma_f \mathcal{W}_V^{(m)}(t, 0)^* e^{-it\Delta}. \end{aligned}$$

We estimate the last term using Lemma 4.7:

$$\begin{aligned} \sum_{n,m \geq 1} \|e^{it\Delta} \mathcal{W}_V^{(n)}(t,0) \gamma_f \mathcal{W}_V^{(m)}(t,0)^* e^{-it\Delta}\|_{\mathfrak{S}^1} &\leq \left( \sum_{n \geq 1} \|\mathcal{W}_V^{(n)}(t,0) |\gamma_f|^{1/2}\|_{\mathfrak{S}^2} \right)^2 \\ &\leq C \left( \sum_{n \geq 1} \frac{\|V\|_{L_t^1(L_x^2 \cap L_x^\infty)}^n}{(n-1)!} \right)^2. \end{aligned}$$

Notice that we used here that  $T \leq 1$  to have  $\|V\|_{L_t^1} \leq \|V\|_{L_t^{8/d}}$ . The terms in  $A_V(t)$  involving  $Q_0$  are treated differently according to the dimension and we first deal with  $d = 1, 2$ . Let  $0 < \varepsilon = \varepsilon(d) < 1 - d/4$ . Then, by (4.5.58), we have for all  $n \geq 1$  and for  $d = 1$ ,

$$\|\mathcal{W}_V^{(n)}(t)\|_{\mathfrak{S}^{2\lceil 2/n \rceil}} \leq \frac{C^n}{(n!)^{\frac{3}{4}-\varepsilon}} \|V\|_{L_t^{\frac{4}{3}} L_x^2}^n \leq \frac{C^n}{(n!)^{1-\frac{d}{4}-\varepsilon}} \|V\|_{L_t^{8/d}(L_x^2 \cap L_x^\infty)}^n,$$

while for  $d = 2$  we have

$$\|\mathcal{W}_V^{(n)}(t)\|_{\mathfrak{S}^{2\lceil 2/n \rceil}} \leq \frac{C^n}{(n!)^{\frac{1}{2}-\varepsilon}} \|V\|_{L_{t,x}^2}^n \leq \frac{C^n}{(n!)^{1-\frac{d}{4}-\varepsilon}} \|V\|_{L_t^{8/d}(L_x^2 \cap L_x^\infty)}^n.$$

Therefore, using that

$$\|e^{it\Delta} \mathcal{W}_V^{(1)}(t,0) Q_0 \mathcal{W}_V^{(1)}(t,0)^* e^{-it\Delta}\|_{\mathfrak{S}^1} \leq C \|\mathcal{W}_V^{(1)}(t,0)\|_{\mathfrak{S}^4}^2 \|Q_0\|_{\mathfrak{S}^2},$$

$$\sum_{n \geq 2} \|e^{it\Delta} (\mathcal{W}_V^{(n)}(t,0) Q_0 + Q_0 \mathcal{W}_V^{(n)}(t,0)^*) e^{-it\Delta}\|_{\mathfrak{S}^1} \leq 2 \|Q_0\|_{\mathfrak{S}^2} \sum_{n \geq 2} \|\mathcal{W}_V^{(n)}(t,0)\|_{\mathfrak{S}^2},$$

and

$$\begin{aligned} \sum_{\max(n,m) \geq 2} \|e^{it\Delta} \mathcal{W}_V^{(n)}(t,0) Q_0 \mathcal{W}_V^{(m)}(t,0)^* e^{-it\Delta}\|_{\mathfrak{S}^1} \\ \leq C \|Q_0\|_{\mathfrak{S}^2} \sum_{n \geq 2} \|\mathcal{W}_V^{(n)}(t,0)\|_{\mathfrak{S}^2} \sum_{m \geq 1} \|\mathcal{W}_V^{(m)}(t,0)\|, \end{aligned}$$

we deduce the estimate uniform in  $t \in [-T, T]$ :

$$\begin{aligned} \|A_V(t)\|_{\mathfrak{S}^1} &\leq 2 \|Q_0\|_{\mathfrak{S}^2} \left( \sum_{n \geq 0} \frac{C^n}{(n!)^{1-\frac{d}{4}-\varepsilon}} \|V\|_{L_t^{8/d}(L_x^2 \cap L_x^\infty)}^n \right)^2 \\ &\quad + C \left( \sum_{n \geq 1} \frac{1}{(n-1)!} \|V\|_{L_t^{8/d}(L_x^2 \cap L_x^\infty)}^n \right)^2. \end{aligned} \quad (4.5.65)$$

If  $d = 3$ , we have  $\|\mathcal{W}_V^{(1)}(t)\|_{\mathfrak{S}^5} \leq C \|V\|_{L_{t,x}^{5/2}}$  by (4.5.57) and

$$\forall n \geq 2, \|\mathcal{W}_V^{(n)}(t)\|_{\mathfrak{S}^{2\lceil 5/(2n) \rceil}} \leq \frac{C^n}{(n!)^{\frac{2}{5}-\varepsilon}} \|V\|_{L_{t,x}^{5/2}}^n \leq \frac{C^n}{(n!)^{\frac{2}{5}-\varepsilon}} \|V\|_{L_t^{8/3}(L_x^2 \cap L_x^\infty)}^n,$$

by (4.5.58). In particular,  $\mathcal{W}_V^{(n)}(t, 0) \in \mathfrak{S}^2$  only for  $n \geq 3$ , while  $\mathcal{W}_V^{(2)}(t, 0) \in \mathfrak{S}^4$ . Hence, the operators  $\mathcal{W}_V^{(n)}(t, 0)Q_0$  is trace-class when  $n \geq 3$  and  $\mathcal{W}_V^{(n)}(t, 0)Q_0\mathcal{W}^{(m)}(t, 0)^*$  is trace-class when  $\max(n, m) \geq 3$ , by Hölder's inequality. Furthermore, using the KSS inequality (4.3.21), we infer that

$$\|\mathcal{W}_V^{(1)}(t)(1 - \Delta)^{-1/2}\|_{\mathfrak{S}^{10/3}} \leq C \int_0^t \|V(s)\|_{L_x^{10/3}} ds \leq C \|V\|_{L_t^{3/2}(L_x^2 \cap L_x^\infty)}$$

for all  $t \in [-T, T]$ . Hence, the operator

$$\mathcal{W}_V^{(1)}(t)Q_0\mathcal{W}_V^{(1)}(t)^* = \mathcal{W}_V^{(1)}(t)(1 - \Delta)^{-1/2}(1 - \Delta)^{1/2}Q_0\mathcal{W}_V^{(1)}(t)^*$$

belongs to  $\mathfrak{S}^1$  since  $1 = 3/10 + 1/2 + 1/5$ . Finally, by (4.5.60), we have  $\mathcal{W}_V^{(2)}(t)Q_0 \in \mathfrak{S}^1$  for all  $t \in [-T, T]$  with

$$\begin{aligned} \|\mathcal{W}_V^{(2)}(t)Q_0\|_{\mathfrak{S}^1} &\leq C \|V\|_{L_{t,x}^{5/2}} \|V\|_{L_t^{10/7} L_x^{5/2}} \|Q_0\|_{\mathfrak{S}^{2,1}} \\ &\leq C \|V\|_{L_t^{8/3}(H_x^1 \cap W_x^{1,\infty})}^2 \|Q_0\|_{\mathfrak{S}^{2,1}}. \end{aligned}$$

As a consequence, we find that  $A_V(t) \in \mathfrak{S}^1$  also for  $d = 3$ , with the same estimate (4.5.65), because  $(n!)^{-2/5} \leq (n!)^{-1/4} = (n!)^{-1+d/4}$ , except that  $\|Q_0\|_{\mathfrak{S}^2}$  is replaced by  $\|Q_0\|_{\mathfrak{S}^{2,1}}$ . From the fact that  $A_V(t) \in \mathfrak{S}^1$  with an estimate uniform in  $t \in [-T, T]$ , we deduce that

$$\begin{aligned} \|w * \rho_{A_V(t)}\|_{L_t^{8/d}(L_x^2 \cap L_x^\infty)} &\leq C \|w\|_{L^1 \cap L^2} \|\rho_{A_V(t)}\|_{L_t^{8/d} L_x^1} \\ &\leq CT^{d/8} \|\rho_{A_V(t)}\|_{L_t^\infty L_x^1} \leq CT^{d/8} \|A_V(t)\|_{L_t^\infty \mathfrak{S}^1}. \end{aligned}$$

In order to estimate  $\|\Phi(V)\|_{L_t^{8/d}(L_x^2 \cap L_x^\infty)}$ , it only remains to bound

$$\left\| w * \rho \left[ e^{it\Delta} (\mathcal{W}_V^{(1)}(t, 0)Q_0 + Q_0\mathcal{W}_V^{(1)}(t, 0)^*) e^{-it\Delta} \right] \right\|_{L_t^{8/d}(L_x^2 \cap L_x^\infty)}$$

and

$$\sum_{n \geq 1} \left\| w * \rho \left[ e^{it\Delta} (\mathcal{W}_V^{(n)}(t, 0)\gamma_f + \gamma_f\mathcal{W}_V^{(n)}(t, 0)^*) e^{-it\Delta} \right] \right\|_{L_t^{8/d}(L_x^2 \cap L_x^\infty)}.$$

We treat these terms by duality. Let  $U \in L_x^2$ . Then by Lemma 4.7 and our assumption on  $f$ , the operator  $\mathcal{W}^{(n)}(t, 0)\gamma_f U(x)$  is trace-class with

$$\begin{aligned} \|\mathcal{W}^{(n)}(t, 0)\gamma_f U(x)\|_{\mathfrak{S}^1} &\leq \|\mathcal{W}^{(n)}(t, 0)|\gamma_f|^{1/2}\|_{\mathfrak{S}^2} \| |\gamma_f|^{1/2} U(x) \|_{\mathfrak{S}^2} \\ &\leq \frac{C}{(n-1)!} \|V\|_{L_t^{8/d}(L_x^2 \cap L_x^\infty)}^n \|U\|_{L^2}. \end{aligned}$$

As a consequence, we have

$$\begin{aligned} \sum_{n \geq 1} \left\| \rho \left[ e^{it\Delta} (\mathcal{W}_V^{(n)}(t, 0) \gamma_f + \gamma_f \mathcal{W}_V^{(n)}(t, 0)^*) e^{-it\Delta} \right] \right\|_{L_t^\infty L_x^2} \\ \leq C \sum_{n \geq 1} \frac{1}{(n-1)!} \|V\|_{L_t^{8/d} (L_x^2 \cap L_x^\infty)}^n, \end{aligned}$$

and hence by Young's inequality

$$\begin{aligned} \sum_{n \geq 1} \left\| w * \rho \left[ e^{it\Delta} (\mathcal{W}_V^{(n)}(t, 0) \gamma_f + \gamma_f \mathcal{W}_V^{(n)}(t, 0)^*) e^{-it\Delta} \right] \right\|_{L_t^{8/d} (L_x^2 \cap L_x^\infty)} \\ \leq CT^{d/8} \|w\|_{L^1 \cap L^2} \sum_{n \geq 1} \frac{1}{(n-1)!} \|V\|_{L_t^{8/d} (L_x^2 \cap L_x^\infty)}^n. \end{aligned}$$

Note that

$$\begin{aligned} \int_{-T}^T dt \int_{\mathbb{R}^d} dx \rho \left[ e^{it\Delta} \mathcal{W}_V^{(1)}(t) Q_0 e^{-it\Delta} \right] (x) U(t, x) \\ = i \operatorname{Tr} \left[ \left( \mathcal{W}_{(U,V)}^{(2)}(T, 0) + \mathcal{W}_{(U,V)}^{(2)}(-T, 0) \right) Q_0 \right]. \end{aligned}$$

In dimensions  $d = 1, 2$ , we obtain

$$\begin{aligned} \left| \int_{-T}^T dt \int_{\mathbb{R}^d} dx \rho \left[ e^{it\Delta} \mathcal{W}_V^{(1)}(t) Q_0 e^{-it\Delta} \right] (x) U(t, x) \right| \\ \leq C \|Q_0\|_{\mathfrak{S}^2} \left\| \mathcal{W}_{(U,V)}^{(2)}(T, 0) \right\|_{\mathfrak{S}^2} \leq C \|Q_0\|_{\mathfrak{S}^2} \|U\|_{L_t^{\frac{8}{8-d}} (L_x^4)} \|V\|_{L_t^{\frac{8}{8-d}} (L_x^4)} \end{aligned}$$

by (4.5.58), and this proves that

$$\begin{aligned} \left\| \rho \left[ e^{it\Delta} \mathcal{W}_V^{(1)}(t) Q_0 e^{-it\Delta} \right] \right\|_{L_t^{8/d} (L_x^{4/3})} &\leq C \|Q_0\|_{\mathfrak{S}^2} \|V\|_{L_t^{\frac{8}{8-d}} (L_x^4)} \\ &\leq CT^{1-\frac{d}{4}} \|Q_0\|_{\mathfrak{S}^2} \|V\|_{L_t^{\frac{8}{d}} (L_x^4)}. \end{aligned}$$

In dimension  $d = 3$ , we have to use that  $Q_0 \in \mathfrak{S}^{2,1}$  through Lemma 4.6 and we obtain by the exact same method

$$\begin{aligned} \left\| \rho \left[ e^{it\Delta} \mathcal{W}_V^{(1)}(t) Q_0 e^{-it\Delta} \right] \right\|_{L_t^{8/d} (L_x^2 + L_x^{4/3})} &\leq C \|Q_0\|_{\mathfrak{S}^{2,1}} \|V\|_{L_t^{\frac{8}{8-d}} (L_x^2 \cap L_x^4)} \\ &\leq CT^{1-\frac{d}{4}} \|Q_0\|_{\mathfrak{S}^{2,1}} \|V\|_{L_t^{\frac{8}{d}} (L_x^2 \cap L_x^4)}. \end{aligned}$$

In all cases, we get

$$\begin{aligned} \left\| w * \rho \left[ e^{it\Delta} (\mathcal{W}_V^{(1)}(t) Q_0 + Q_0 \mathcal{W}_V^{(1)}(t)^*) e^{-it\Delta} \right] \right\|_{L_t^{\frac{8}{d}} (L_x^2 \cap L_x^\infty)} \\ \leq CT^{1-\frac{d}{4}} \|w\|_{L^1 \cap L^\infty} \|V\|_{L_t^{\frac{8}{d}} (L_x^2 \cap L_x^\infty)}. \end{aligned}$$

Gathering all our bounds, we obtain the final estimate

$$\begin{aligned}
\|\Phi(V)\|_{L_t^{\frac{8}{d}}(L_x^2 \cap L_x^\infty)} &\leq R + CT^{1-\frac{d}{4}}\|V\|_{L_t^{\frac{8}{d}}(L_x^2 \cap L_x^\infty)} \\
&+ CT^{d/8} \sum_{n \geq 1} \frac{1}{(n-1)!} \|V\|_{L_t^{8/d}(L_x^2 \cap L_x^\infty)}^n \\
&+ CT^{d/8} \|Q_0\|_{\mathfrak{S}^2 / \mathfrak{S}^{2,1}} \left( \sum_{n \geq 0} \frac{C^n}{(n!)^{1-\frac{d}{4}-\varepsilon}} \|V\|_{L_t^{8/d}(L_x^2 \cap L_x^\infty)}^n \right)^2 \\
&+ CT^{d/8} \left( \sum_{n \geq 1} \frac{1}{(n-1)!} \|V\|_{L_t^{8/d}(L_x^2 \cap L_x^\infty)}^n \right)^2.
\end{aligned}$$

This implies that for  $T = T(R) > 0$  small enough,  $\Phi$  stabilizes the ball

$$\{\|V\|_{L_t^{8/d}(L_x^2 \cap L_x^\infty)} \leq 2R\}.$$

Using very similar estimates, we can also show that  $\Phi$  is a contraction on this ball, decreasing  $T$  if necessary. We do not detail these estimates here for brevity. This ends the proof of Proposition 4.5.  $\square$

By using the local existence result of Proposition 4.5, we are now able to prove the main theorems of this section. We start with the

**PROOF OF THEOREM 4.5.** From Proposition 4.5 we can construct a potential  $V \in L_t^{8/d}(L_x^2 \cap L_x^\infty)$  solving (4.5.56) for some small enough time  $T > 0$ . We have to show that the condition (4.5.49) is propagated and the result will then follow from an iteration argument. So we define the operator

$$Q(t) := e^{it\Delta} \mathcal{W}_V(t, 0) (\gamma_f + Q_0) \mathcal{W}_V(t, 0)^* e^{-it\Delta} - \gamma_f,$$

and prove that  $Q \in L_t^\infty((-T, T), \mathfrak{S}^2)$ . The continuity then follows from the fact that  $Q$  satisfies (4.3.16). Indeed, since  $\mathcal{W}_V(t, 0)$  is unitary, we have

$$\|e^{it\Delta} \mathcal{W}_V(t, 0) Q_0 \mathcal{W}_V(t, 0)^* e^{-it\Delta}\|_{\mathfrak{S}^2} \leq \|Q_0\|_{\mathfrak{S}^2}.$$

On the other hand,

$$\begin{aligned}
&e^{it\Delta} \mathcal{W}_V(t, 0) \gamma_f \mathcal{W}_V(t, 0)^* e^{-it\Delta} - \gamma_f \\
&= e^{it\Delta} \left( (\mathcal{W}_V(t, 0) - 1) \gamma_f \mathcal{W}_V(t, 0)^* + \gamma_f (\mathcal{W}_V(t, 0)^* - 1) \right) e^{-it\Delta}
\end{aligned}$$

which is Hilbert-Schmidt (uniformly for  $t$  in compact sets), by Lemma 4.7 and the assumptions on  $f$ . We then have to show that  $w * \rho[e^{is\Delta} Q(t^*) e^{-is\Delta}] \in L_{s, \text{loc}}^{8/d}(\mathbb{R}, L_x^2 \cap L_x^\infty)$



for any  $t^* \in (-T, T)$ . To do so, we recall (4.5.64):

$$\begin{aligned} Q(t^*) &= e^{it^*\Delta} Q_0 e^{-it^*\Delta} + e^{it^*\Delta} (\mathcal{W}_V^{(1)}(t^*, 0) Q_0 + Q_0 \mathcal{W}_V^{(1)}(t^*, 0)^*) e^{-it^*\Delta} \\ &\quad + \sum_{n \geq 1} e^{it^*\Delta} (\mathcal{W}_V^{(n)}(t^*, 0) \gamma_f + \gamma_f \mathcal{W}_V^{(n)}(t^*, 0)^*) e^{-it^*\Delta} + A_V(t^*). \end{aligned}$$

Here  $A_V(t^*) \in \mathfrak{S}^1$ , therefore  $e^{is\Delta} A_V(t^*) e^{-is\Delta} \in L_s^\infty(\mathbb{R}, \mathfrak{S}^1)$  and  $w * \rho[e^{is\Delta} A_V(t^*) e^{-is\Delta}]$  belongs to  $L_s^\infty(\mathbb{R}, L_x^2 \cap L_x^\infty)$ . By our assumption (4.5.49) on  $Q_0$ , we have that  $w * \rho[e^{i(s+t^*)\Delta} Q_0 e^{-i(s+t^*)\Delta}]$  belongs to  $L_{s,\text{loc}}^{8/d}(\mathbb{R}, L_x^2 \cap L_x^\infty)$ . The other terms in the decomposition of  $Q(t^*)$  are treated by duality as in the proof of Proposition 4.5. At this point we have constructed a maximal solution.

Let us now prove uniqueness. If  $Q, Q' \in C_t^0([-T^-, T^+], \mathfrak{S}^2)$  are two solutions to (4.3.16) such that  $V_Q$  and  $V_{Q'}$  belong to  $L_t^{8/d}((-T^-, T^+), L_x^2 \cap L_x^\infty)$ , then  $Q = Q'$  will obviously follow from  $V_Q = V_{Q'}$ . We cannot use a Grönwall-type argument due to the fact that we lack *pointwise* estimates in  $t$  on  $\Phi(V_Q)(t) - \Phi(V_{Q'})(t)$ . Instead, we use a continuity argument: let  $t^*$  be the largest time  $\leq T$  for which  $V_{Q(t)} = V_{Q'(t)}$  for all  $0 \leq t \leq t^*$ . From the fixed point argument of Proposition 4.5, we know that  $t^* > 0$ . Indeed, let

$$\begin{aligned} R &\geq \|Q_0\|_{\mathfrak{S}^2 / \mathfrak{S}^{2,1}} + \|w * \rho_{e^{it\Delta} Q_0 e^{-it\Delta}}\|_{L_t^{8/d}((-1,1), L_x^2 \cap L_x^\infty)} \\ &\quad + \|V_Q\|_{L_t^{8/d}((-1,1), L_x^2 \cap L_x^\infty)} + \|V_{Q'}\|_{L_t^{8/d}((-1,1), L_x^2 \cap L_x^\infty)}. \end{aligned}$$

We have proved that there exists  $t' = t'(R) > 0$  small enough such that (4.5.56) has a unique solution on the ball  $\{\|V\|_{L_t^{8/d}(L_x^2 \cap L_x^\infty)} \leq 2R\}$ . Since both  $V_Q$  and  $V_{Q'}$  belong to this ball, we have  $V_Q \equiv V_{Q'}$  a.e. on  $[-t', t']$ , and therefore  $t^* > 0$ . We now argue by contradiction: assume that  $t^* < T$ . Since  $V_Q \equiv V_{Q'}$  a.e. on  $(-t^*, t^*)$ ,  $Q \equiv Q'$  on  $[-t^*, t^*]$  and in particular  $Q(t^*) = Q'(t^*)$ ,  $Q(-t^*) = Q'(-t^*)$  (we use here the continuity of  $t \mapsto Q(t)$  in  $\mathfrak{S}^2$ ). Also, the density  $\rho_{e^{is\Delta} Q(t^*) e^{-is\Delta}}$  belongs to  $L_{s,\text{loc}}^{8/d}(\mathbb{R}, L_x^2 \cap L_x^\infty)$ , as we have already proved. Hence we can apply Proposition 4.5 again at  $t^*$ , leading to a contradiction. The argument is the same for negative times.

The argument for the continuity with respect to  $Q_0$ ,  $f$  and  $w$  is similar. Let  $(Q_0^{(n)}, f_n, w_n) \rightarrow (Q_0, f, w)$ , and  $V_n$  the associated solutions. First assume that  $V_n$  and  $V$  are defined on  $[0, T]$  for all  $n$  and some  $T > 0$ , and that  $(V_n)$  is uniformly bounded in  $L_t^{8/d}([0, T], L_x^2 \cap L_x^\infty)$ . Let us show that  $V_n \rightarrow V$ . From the fixed point technique in Proposition 4.5, we deduce that  $\|V_n - V\|_{L_t^{8/d}([0, T'], L_x^2 \cap L_x^\infty)} \rightarrow 0$  for  $T' > 0$  small enough. Note that  $t \mapsto \|V_n - V\|_{L_t^{8/d}([0, t], L_x^2 \cap L_x^\infty)}$  is increasing, hence has a subsequence which converges everywhere, to a non-decreasing function. Let now  $t^*$  be the first time such that the limit fails to be 0 and assume that  $t^* < T$ . We choose  $\varepsilon > 0$  small enough such that the time of existence for the problem in the ball of radius  $2\|(Q(t^* - \varepsilon), f, w)\|$  is  $> 2\varepsilon$ . Since for  $n$  large enough,  $(Q_n(t^* - \varepsilon), f_n, w_n)$  falls into this ball, we get again a contradiction. Hence,  $V_n \rightarrow V$  in  $L_t^{8/d}([0, T], L_x^2 \cap L_x^\infty)$ , from which

we deduce that  $Q_n \rightarrow Q$  in  $C_t^0([0, T], \mathfrak{S}^2)$  and that  $w * \rho_{e^{it\Delta} Q_n(s)e^{-it\Delta}} \rightarrow w * \rho_{e^{it\Delta} Q(s)e^{-it\Delta}}$  in  $L_{t,\text{loc}}^{8/d}(\mathbb{R}, L_x^2 \cap L_x^\infty)$  for all  $s \in [0, T]$ . Now let  $0 < T < T^+$ , and let

$$\begin{aligned} \frac{R}{2} = & \sup_{s \in [0, T]} \|Q(s)\|_{\mathfrak{S}^2} + \|V\|_{L_t^{8/d}([0, T], L_x^2 \cap L_x^\infty)} + \|w\|_{L_x^1 \cap L_x^\infty} + \|f\|_{L^\infty} \\ & + \int_{\mathbb{R}^d} |f(k^2)| dk + \sup_{s \in [0, T]} \|w * \rho_{e^{it\Delta} Q(s)e^{-it\Delta}}\|_{L_t^{8/d}([0, T], L_x^2 \cap L_x^\infty)}, \end{aligned}$$

which is finite by the estimates provided before. By Proposition 4.5, for  $n$  large enough,  $V_n$  and  $V$  are defined up to time  $0 < T(R) \leq T$  and uniformly bounded on  $[0, T(R)]$ . By the previous argument, this implies that  $V_n \rightarrow V$ ,  $Q_n \rightarrow Q$ , and  $w * \rho_{e^{it\Delta} Q_n(s)e^{-it\Delta}} \rightarrow w * \rho_{e^{it\Delta} Q(s)e^{-it\Delta}}$  on  $[0, T(R)]$ . In particular, for  $n$  large enough

$$\|Q_n(T(R))\|_{\mathfrak{S}^2} + \|w * \rho_{e^{it\Delta} Q_n(T(R))e^{-it\Delta}}\|_{L_t^{8/d}([0, T(R)], L_x^2 \cap L_x^\infty)} \leq R$$

and we can again extend the solutions up to  $[0, 2T(R)]$ . Repeating this procedure a finite number of times, we can cover the whole  $[0, T]$ . This ends the proof of Theorem 4.5.  $\square$

We finally turn to the

**PROOF OF THEOREM 4.6.** The proof is the same as for Theorem 4.5, with some minor differences. First we remark that, by (4.5.63), the solution  $V(t)$  constructed in Proposition 4.5 is automatically in  $L^{8/d}((-T, T), H_x^1 \cap W_x^{1, \infty})$  when  $\nabla w \in L^1 \cap L^\infty$  and when  $\rho_{e^{it\Delta} Q_0 e^{-it\Delta}} \in L_{t,\text{loc}}^{8/d}(H_x^1 \cap W_x^{1, \infty})$ . So, in order to mimic the proof of Theorem 4.5, we only have to show that  $Q \in C_t^0(\mathfrak{S}^{2,1})$ . First, by (4.3.29), we have  $\|(1 - \Delta)^{1/2} V (1 - \Delta)^{-1/2}\| \leq C \|V\|_{W^{1, \infty}}$ , hence

$$\|(1 - \Delta)^{1/2} \mathcal{W}_V(t, 0) (1 - \Delta)^{-1/2}\| \leq C \sum_{n \geq 0} \frac{\|V\|_{L_t^1 W_x^{1, \infty}}^n}{n!},$$

which is finite when  $V \in L_{t,\text{loc}}^{8/d}(W_x^{1, \infty})$ . This implies that

$$\|e^{it\Delta} \mathcal{W}_V(t) Q_0 \mathcal{W}_V(t)^* e^{-it\Delta}\|_{\mathfrak{S}^{2,1}} \leq C \left( \sum_{n \geq 0} \frac{\|V\|_{L_t^1 W_x^{1, \infty}}^n}{n!} \right) \|Q_0\|_{\mathfrak{S}^{2,1}}.$$

Using that  $\|\gamma_f V (1 - \Delta)^{1/2}\|_{\mathfrak{S}^2} \leq C \|V\|_{H_x^1}$  as we have proved in Lemma 4.2, we infer that, for  $n \geq 1$ ,

$$\begin{aligned} \|\gamma_f \mathcal{W}_V^{(n)}(0, t) (1 - \Delta)^{1/2}\|_{\mathfrak{S}^2} & \leq C \frac{1}{(n-1)!} \|V\|_{L_t^1 W_x^{1, \infty}}^{n-1} \|\gamma_f V (1 - \Delta)^{1/2}\|_{L_t^1 \mathfrak{S}^2} \\ & \leq C \frac{1}{(n-1)!} \|V\|_{L_t^1 W_x^{1, \infty}}^{n-1} \|V\|_{L_t^1 H_x^1}. \end{aligned}$$

Hence, we have  $e^{it\Delta} \mathcal{W}_V(t) \gamma_f \mathcal{W}_V(t)^* e^{-it\Delta} - \gamma_f \in L_t^\infty((-T, T), \mathfrak{S}^{2,1})$ , which finishes the proof of Theorem 4.6.  $\square$

## 6. Inequalities on the relative entropy

The purpose of this section is to provide the necessary tools to prove global well-posedness for a large class of functions  $f$ 's, including the gases at positive temperature (4.1.6)–(4.1.8). We use a general concept of relative entropy  $\mathcal{H}(\gamma, \gamma_f)$  of two one-particle density matrices  $\gamma$  and  $\gamma_f$  which has been recently introduced in [LS13a]. The purpose of this section is to prove some useful lower bounds on this relative entropy. We particularly discuss *Lieb-Thirring inequalities* in the spirit of [FLLS11, FLLS12], which are important to get bounds on the density  $\rho_\gamma$ , as we have already seen in the zero temperature case.

**6.1. Generalized relative entropy.** Before turning to the general definition of the relative entropy, let us recall the usual case of the von Neumann entropy. To simplify our exposition, we start by working in a finite-dimensional space  $\mathfrak{K}$ . The entropy of the system takes the form

$$\boxed{\mathcal{S}(\gamma) = \text{Tr}_{\mathfrak{K}}(S(\gamma))}$$

where

$$S(x) = \begin{cases} -x \log(x) - (1-x) \log(1-x), & x \in [0, 1], & \text{(fermions),} \\ -x \log(x) + (1+x) \log(1+x), & x \in [0, M], & \text{(bosons),} \\ -x \log(x) + x, & x \in [0, M], & \text{(boltzons).} \end{cases} \quad (4.6.66)$$

We always work with bounded operators and  $M > 0$  could in principle be any positive number. Later we will restrict ourselves to  $M = 1$  for simplicity. The function  $S$  is concave in these cases, hence so is  $\mathcal{S}$  (see, e.g., [OP93, Chap. 3]). It is important to remember that  $\gamma$  is the *one-particle density matrix* of the system, and not the state itself. Both for fermions and bosons, there is a unique quasi-free state associated with  $\gamma$ , which is an operator  $D \geq 0$  acting on the Fock space  $d\Gamma(\mathfrak{K})$ , such that  $\text{Tr}_{d\Gamma(\mathfrak{K})}(D) = 1$  and which has  $\gamma$  as one-particle density matrix [BLS94]. Then, the usual von Neumann entropy of  $D$  coincides with the above formulas:  $-\text{Tr}_{d\Gamma(\mathfrak{K})}(D \log(D)) = \mathcal{S}(\gamma) = \text{Tr}_{\mathfrak{K}}(S(\gamma))$ . The situation is similar for boltzons.

Consider now any self-adjoint operator  $h$  on  $\mathfrak{K}$ . The corresponding density matrices are obtained by minimizing the free energy, which is by definition the difference between the energy and the entropy:

$$\gamma_f = \underset{0 \leq \gamma = \gamma^* \leq M}{\text{argmin}} \left\{ \text{Tr}_{\mathfrak{K}}(h\gamma - S(\gamma)) \right\}.$$

The optimal state is

$$\gamma_f = \begin{cases} \frac{1}{e^h + 1} & \text{for fermions,} \\ \frac{1}{e^h - 1} & \text{for bosons,} \\ e^{-h} & \text{for boltzons.} \end{cases}$$

In the bosonic case, it is necessary to have  $h \geq \log(1 + 1/M)$ . Normally we should multiply  $S$  by the temperature  $T$ , in which case we get  $h/T$  instead of  $h$  in the previous formulas, but we can always think of including  $T$  in the definition of  $h$ .

Now that we have found the minimizer of the free energy, it is useful to look at the difference between the free energy of any state  $\gamma$  and that of the minimizer  $\gamma_f$ . This difference is precisely the *relative entropy*

$$\mathcal{H}(\gamma, \gamma_f) := \text{Tr}_{\mathfrak{K}} (h(\gamma - \gamma_f) - S(\gamma) + S(\gamma_f)). \quad (4.6.67)$$

That the relative entropy  $\mathcal{H}(\gamma, \gamma_f)$  is non-negative is an obvious consequence of the fact that  $\gamma_f$  minimizes the free energy. The relevance of  $\mathcal{H}(\gamma, \gamma_f)$  comes from the fact that it can make sense for infinite systems, even if the three terms in (4.6.67) do not make sense separately.

Here we have prescribed the Hamiltonian  $h$  and we got the Gibbs state  $\gamma_f$ . But we can turn the matter around and find  $h$  from  $\gamma_f$ . Indeed, writing that the derivative of the free energy vanishes at the point  $\gamma_f$ , we find that  $h = S'(\gamma_f)$ . Therefore, we can re-write the relative entropy as

$$\mathcal{H}(\gamma, \gamma_f) := - \text{Tr}_{\mathfrak{K}} \left( S(\gamma) - S(\gamma_f) - S'(\gamma_f)(\gamma - \gamma_f) \right). \quad (4.6.68)$$

In this formula,  $S$  is given by (4.6.66). In [LS13a], the relative entropy (4.6.68) was studied for  $S$  a general concave function, and several properties were proved. First by Klein's lemma (see [OP93, Prop. 3.16] and [LS13a, Lem. 1]), it is known that  $\mathcal{H}(\gamma, \gamma_f) \geq 0$  for any  $0 \leq \gamma, \gamma_f \leq 1$ , on a finite-dimensional space  $\mathfrak{K}$ . The main contribution of [LS13a] was to prove that  $\mathcal{H}$  is monotone, that is

$$\mathcal{H}(PAP, PBP) \leq \mathcal{H}(A, B)$$

for every orthogonal projection, if and only if  $-S'$  is operator-monotone. Monotonicity is a natural concept which allows to define the relative entropy in infinite dimension as is always done in statistical mechanics, that is, by a thermodynamic limit. In mathematical terms, the proper definition in infinite dimension is

$$\mathcal{H}(\gamma, \gamma_f) := \lim_{k \rightarrow \infty} \mathcal{H}(P_k \gamma P_k, P_k \gamma_f P_k) \quad (4.6.69)$$

where  $P_k$  is any increasing sequence of finite-rank orthogonal projections such that  $P_k \rightarrow 1$  strongly. The limit always exist in  $\mathbb{R}^+ \cup \{+\infty\}$  since the right side is monotone,

and it can be shown to be independent of the chosen sequence  $(P_k)$ , see [LS13a, Thm. 2].

In this paper we always assume that

$$S : [0, 1] \rightarrow \mathbb{R}^+ \text{ is continuous on } [0, 1] \quad (4.6.70)$$

and that

$$-S' \text{ is operator monotone on } (0, 1) \text{ and not constant.} \quad (4.6.71)$$

Recall that an operator monotone function on an interval  $(a, b)$  is always  $C^\infty$  [Bha97, Chap. V]. Here we work on the interval  $[0, 1]$  for simplicity but, by a simple change of variable, the results are all exactly the same on an interval  $[0, M]$  with  $M < \infty$ . Of course, in the three usual physical cases (4.6.66), the assumptions (4.6.70) and (4.6.71) are fulfilled (only for  $\mu < -\log(2)$  in the bosonic case). Other examples of functions  $S$  satisfying (4.6.70) and (4.6.71) are provided in [AHP10] and include

$$S(x) = \begin{cases} -(t+x) \log(t+x), & t \geq 0 \\ \log(t+x), & t > 0, \\ x^m, & 0 < m \leq 1, \\ -x^m, & 1 \leq m \leq 2. \end{cases}$$

**Remark 4.1.** Any function  $S$  satisfying (4.6.70) and (4.6.71) can be written as

$$\begin{aligned} S(x) = a'x + c' + b \int_0^\infty \left( \log(t+x) - \log(t+1/2) - \frac{2x-1}{2t+1} \right) d\nu_1(t) \\ + b \int_0^\infty \left( \log(t+1-x) - \log(t+1/2) + \frac{2x-1}{2t+1} \right) d\nu_2(t) \end{aligned} \quad (4.6.72)$$

with  $\nu_1$  and  $\nu_2$  two positive Borel measures satisfying  $2 \int_0^\infty (2t+1)^{-2} (d\nu_1 + d\nu_2)(t) = 1$  (see [LS13a]). The constraint that  $S$  admits limits at 0 and 1 means that

$$- \int_0^1 \log(t) (d\nu_1 + d\nu_2)(t) < \infty$$

and it implies  $\nu_1(\{0\}) = \nu_2(\{1\}) = 0$ , as well as

$$\lim_{x \rightarrow 0^+} xS'(x) = \lim_{x \rightarrow 1^-} (1-x)S'(x) = 0. \quad (4.6.73)$$

The usual Fermi-Dirac distribution is obtained by taking  $d\nu_1 = d\nu_2 = dt/2$ ,  $a' = 0 = c'$ ,  $b = 2$ .

**6.2. Klein inequality.** From now on we work again in the Hilbert space  $\mathfrak{H} = L^2(\mathbb{R}^d)$  and we consider a reference state of the form  $\gamma_f = f(-\Delta)$  coming from an entropy  $S$  as before, which requires  $f = (S')^{-1}$  (the inverse function of  $x \in (0, 1) \mapsto$

$S'(x)$ . In order to have  $0 \leq \gamma_f \leq 1$ , we need that  $S'((0, 1)) \supset (0, \infty)$ . Because we assume that  $-S'$  is operator monotone,  $S'$  is decreasing and therefore we need to have

$$\lim_{x \rightarrow 0^+} S'(x) = +\infty \quad \text{and} \quad \lim_{x \rightarrow 1^-} S'(x) \leq 0. \tag{4.6.74}$$

We think of including the chemical potential  $\mu$  in the function  $f$ . Of course, replacing  $f(-\Delta)$  by  $f(-\Delta - \mu)$  amounts to replacing  $S(x)$  by  $S(x) + \mu x$ . We see that, by choosing  $\mu$  sufficiently negative, we can always ensure that  $S'(1) \leq 0$ . In the case of the Bose-Einstein entropy, any  $\mu \leq -\log(2)$  will do, if we work on  $[0, 1]$  with a temperature  $T = 1$ . In the Fermi-Dirac case, we have  $S'(x) \rightarrow -\infty$  when  $x \rightarrow 1$  and one can take any  $\mu \in \mathbb{R}$ .

The first important information that we have when  $\mathcal{H}(\gamma, \gamma_f) < \infty$ , is that  $\gamma - \gamma_f \in \mathfrak{S}^{2,1}$ . This is stated in the following result, inspired of [HLS08, Thm 1] and [FHSS12, Lemma 1].

**Lemma 4.8** (Klein inequality). *We assume that  $d \geq 1$  and that  $S$  satisfies (4.6.70), (4.6.71), (4.6.74). Let  $\gamma_f = f(-\Delta)$  with  $f = (S')^{-1}$ . Then there exists a constant  $C > 0$  (depending only on  $S$ ) such that*

$$\mathcal{H}(\gamma, \gamma_f) \geq C \operatorname{Tr} (1 - \Delta)(\gamma - \gamma_f)^2, \tag{4.6.75}$$

for all  $0 \leq \gamma \leq 1$ .

PROOF. It was proved in [LS13a, Thm. 3] that  $\mathcal{H}(A, B) \geq C \operatorname{Tr} (1 + |S'(B)|)(A - B)^2$  for all  $A, B$ . Since  $-\Delta = S'(\gamma_f)$ , the result follows.  $\square$

The result can be used to approximate  $A$  by a finite-rank perturbation of  $B$  in a suitable sense, see [LS13a, Cor. 1].

**6.3. Lieb-Thirring inequality.** We have seen in the previous section that the relative entropy  $\mathcal{H}(\gamma, \gamma_f)$  controls the  $\mathfrak{S}^{2,1}$  norm. Except in dimension  $d = 1$ , this does not tell us anything about the density  $\rho_{\gamma - \gamma_f}$ . Here we discuss Lieb-Thirring inequalities in the spirit of [FLLS11, FLLS12], which give an information of this type.

First, in order that  $\gamma_f$  has a finite density  $\rho_{\gamma_f}$ , we need

$$\int_{\mathbb{R}^d} f(|p|^2) dp = \frac{|S^{d-1}|}{2} \int_0^{f(0)} \lambda |S''(\lambda)| S'(\lambda)^{\frac{d}{2}-1} d\lambda < \infty.$$

By using Löwner's formula (4.6.72), this is the same as

$$\int_0^1 S'(\lambda)_+^{\frac{d}{2}} d\lambda < \infty. \tag{4.6.76}$$

The integrability condition (4.6.76) is satisfied for the Fermi-Dirac and Bose-Einstein distributions, since  $S'$  diverges logarithmically at 0 in those cases. It is simple to

verify that (4.6.76) is satisfied for  $S(x) = x^m$  with  $0 < m < 1$  in dimension  $d \leq 2$  and  $1 - 2/d < m < 1$  in dimension  $d \geq 3$ .

By using Klein's inequality (4.6.75), it is easy to verify that, in dimension  $d = 1$ , the relative density  $\rho_\gamma - \rho_{\gamma_f}$  is in  $L^q(\mathbb{R})$  for all  $2 \leq q < \infty$ . The following is very similar to Lemma 4.1.

**Lemma 4.9** (Density in 1D). *We assume that  $d = 1$  and that  $S$  satisfies (4.6.70), (4.6.71), (4.6.74) and (4.6.76). Let  $\gamma_f = f(-\Delta)$  with  $f = (S')^{-1}$ . Then we have*

$$\mathcal{H}(\gamma, \gamma_f) \geq \begin{cases} K_{\text{LT,S}} \int_{\mathbb{R}} |\rho_\gamma - \rho_{\gamma_f}|^q & \text{for } 2 \leq q < 3 \\ K_{\text{LT,S}} \left( \int_{\mathbb{R}} |\rho_\gamma - \rho_{\gamma_f}|^q \right)^{\frac{2}{q-1} - \varepsilon} & \text{for } 3 \leq q < \infty \text{ and } \varepsilon > 0. \end{cases} \quad (4.6.77)$$

for all  $0 \leq \gamma \leq 1$ , with constants  $K_{\text{LT,S}}$  which only depends on  $S$ ,  $q$  and  $\varepsilon$ .

**PROOF OF LEMMA 4.9.** By [LS13a, Cor. 1], it suffices to prove the result for  $Q := \gamma - \gamma_f$  a smooth finite rank operator. We write

$$\int_{\mathbb{R}} \rho_Q V = \text{Tr}(QV) = \text{Tr} \left( (1 - \Delta)^{\frac{1}{2q}} Q (1 - \Delta)^{\frac{1}{2q}} \frac{1}{(1 - \Delta)^{\frac{1}{2q}}} V \frac{1}{(1 - \Delta)^{\frac{1}{2q}}} \right)$$

with  $2 \leq q < 3$ . Similarly as in Lemma 4.1, we have by the Araki-Lieb-Thirring inequality  $\|(1 - \Delta)^{1/(2q)} |Q|^{1/q}\|_{\mathfrak{S}^{2q}} \leq \|(1 - \Delta)^{1/2} Q\|_{\mathfrak{S}^2}^{1/q}$ . On the other hand, since  $\|Q\| \leq 1$  we have  $\||Q|^{1-2/q}\| \leq 1$  as well, for  $q \geq 2$ . We then obtain, from the KSS inequality (4.3.21),

$$\int_{\mathbb{R}} \rho_Q V \leq (2\pi)^{1/q-1} (\text{Tr}(1 - \Delta) Q^2)^{1/q} \|V\|_{L^{q'}(\mathbb{R})} \left( \int_{\mathbb{R}} \frac{dp}{(1 + p^2)^{\frac{1}{q-1}}} \right)^{1/q'}.$$

The integral on the right is finite for  $q < 3$ . This ends the proof of the first inequality, by duality and by (4.6.75). When  $q \geq 3$ , we write, instead,

$$\int_{\mathbb{R}} \rho_Q V = \text{Tr} \left( (1 - \Delta)^{\frac{1}{4q'} + \varepsilon} Q (1 - \Delta)^{\frac{1}{4q'} + \varepsilon} \frac{1}{(1 - \Delta)^{\frac{1}{4q'} + \varepsilon}} V \frac{1}{(1 - \Delta)^{\frac{1}{4q'} + \varepsilon}} \right)$$

and get, similarly as before,

$$\begin{aligned} \|\rho_Q\|_{L^q(\mathbb{R})} &\leq C \left\| (1 - \Delta)^{\frac{1}{4q'} + \varepsilon} Q (1 - \Delta)^{\frac{1}{4q'} + \varepsilon} \right\|_{\mathfrak{S}^q} \\ &\leq C \left\| (1 - \Delta)^{\frac{1}{4q'} + \varepsilon} Q (1 - \Delta)^{\frac{1}{4q'} + \varepsilon} \right\|_{\mathfrak{S}^{\frac{2q'}{1+4\varepsilon q'}}} \\ &\leq C (\text{Tr}(1 - \Delta) Q^2)^{\frac{1+4\varepsilon q'}{2q'}}. \end{aligned}$$

We have used here that  $2q' \leq q$  for  $q \geq 3$ . □

In higher dimensions the previous argument does not work any more, since  $(1 + |p|^2)^{-1}$  is not integrable. However, we can derive a similar bound by using the Lieb-Thirring inequality of [FLLS11, FLLS12].

**Theorem 4.7** (Lieb-Thirring inequality). *We assume that  $d \geq 2$  and that  $S$  satisfies (4.6.70), (4.6.71), (4.6.74) and (4.6.76). Then, with  $\gamma_f = f(-\Delta)$  and  $f = (S')^{-1}$ , we have the Lieb-Thirring inequality*

$$\mathcal{H}(\gamma, \gamma_f) \geq K_{\text{LT,S}} \int_{\mathbb{R}^d} \left( (\rho_{\gamma_f} + \rho_{\gamma - \gamma_f}(x))^{1 + \frac{2}{d}} - (\rho_{\gamma_f})^{1 + \frac{2}{d}} - \frac{2 + d}{d} (\rho_{\gamma_f})^{\frac{2}{d}} \rho_{\gamma - \gamma_f}(x) \right) dx \quad (4.6.78)$$

for all  $0 \leq \gamma \leq 1$  and with a constant  $K_{\text{LT,S}}$  depending only on  $S$  and  $d$ . In particular,  $\rho_{\gamma - \gamma_f} \in L^2(\mathbb{R}^d) + L^{1+2/d}(\mathbb{R}^d)$  when  $\mathcal{H}(\gamma, \gamma_f) < \infty$ .

The inequality dual to (4.6.78) (that is, expressed in terms of a potential  $V(x)$ ) has been derived in [FLLS12, Thm. 5.4]. Instead of getting (4.6.78) from this result, we prove (4.6.78) directly using the zero temperature inequality (4.1.5). A similar approach is used in [FLLS12].

Since  $\rho_\gamma - \rho_{\gamma_f}$  belongs to  $L^2(\mathbb{R}^d) + L^{1+2/d}(\mathbb{R}^d)$  when  $\mathcal{H}(\gamma, \gamma_f) < \infty$  and  $\rho_{\gamma_f}$  is a constant by (4.6.76), we deduce that  $\rho_\gamma \in L^1_{\text{loc}}(\mathbb{R}^d)$ , hence that  $\gamma$  is locally trace-class.

**PROOF.** By [LS13a, Cor. 1], it suffices to prove the theorem for  $\gamma$  a smooth finite rank perturbation of  $\gamma_f = f(-\Delta)$ , and we make this assumption throughout the proof. Let us start by deriving a useful integral representation formula for  $\mathcal{H}(A, B)$ , when  $A$  and  $B$  are finite matrices. Inserting

$$S(x) = S(0) + \int_0^1 S'(\lambda) \mathbf{1}(x \geq \lambda) d\lambda,$$

in the definition of  $\mathcal{H}(A, B)$ , we obtain

$$\mathcal{H}(A, B) = \int_0^1 \text{Tr} (S'(B) - S'(\lambda)) (\mathbf{1}(A \geq \lambda) - \mathbf{1}(B \geq \lambda)) d\lambda.$$

We remark that  $\mathbf{1}(B \geq \lambda) = \mathbf{1}(S'(B) \leq S'(\lambda))$ , since  $S'$  is a decreasing function. So we obtain

$$\begin{aligned} & \text{Tr} (S'(B) - S'(\lambda)) (\mathbf{1}(A \geq \lambda) - \mathbf{1}(B \geq \lambda)) \\ &= -\text{Tr} |S'(B) - S'(\lambda)| \mathbf{1}(B \geq \lambda) (\mathbf{1}(A \geq \lambda) - \mathbf{1}(B \geq \lambda)) \mathbf{1}(B \geq \lambda) \\ & \quad + \text{Tr} |S'(B) - S'(\lambda)| \mathbf{1}(B \leq \lambda) (\mathbf{1}(A \geq \lambda) - \mathbf{1}(B \geq \lambda)) \mathbf{1}(B \leq \lambda). \end{aligned}$$



A simple calculation shows that

$$\begin{aligned} (\mathbf{1}(A \geq \lambda) - \mathbf{1}(B \geq \lambda))^2 &= -\mathbf{1}(B \geq \lambda)(\mathbf{1}(A \geq \lambda) - \mathbf{1}(B \geq \lambda))\mathbf{1}(B \geq \lambda) \\ &\quad + \mathbf{1}(B \leq \lambda)(\mathbf{1}(A \geq \lambda) - \mathbf{1}(B \geq \lambda))\mathbf{1}(B \leq \lambda) \end{aligned}$$

and therefore we arrive at

$$\mathcal{H}(A, B) = \int_0^1 \text{Tr} |S'(B) - S'(\lambda)| (\mathbf{1}(A \geq \lambda) - \mathbf{1}(B \geq \lambda))^2 d\lambda.$$

The formula is still true in infinite dimension, but proving it requires some work. In our particular case we only need the lower bound

$$\mathcal{H}(\gamma, \gamma_f) \geq \int_0^1 \text{Tr} |S'(\gamma_f) - S'(\lambda)| (\mathbf{1}(\gamma \geq \lambda) - \mathbf{1}(\gamma_f \geq \lambda))^2 d\lambda. \quad (4.6.79)$$

To prove (4.6.79), we take an increasing sequence of finite-dimensional projections  $P_k$ , with  $P_k \rightarrow 1$  strongly in  $H^1(\mathbb{R}^d)$ . We can use the formula in finite dimension and that  $\mathcal{H}(P_k \gamma P_k, P_k \gamma_f P_k) \nearrow \mathcal{H}(\gamma, \gamma_f)$  when  $k \rightarrow \infty$ , by the definition of  $\mathcal{H}$  in (4.6.69). The right term is slightly more complicated to deal with. First,  $|S'(P_k \gamma_f P_k) - S'(\lambda)|^{1/2} \rightarrow |S'(\gamma_f) - S'(\lambda)|^{1/2}$  and  $\mathbf{1}(P_k \gamma_f P_k \geq \lambda) \rightarrow \mathbf{1}(\gamma_f \geq \lambda)$  strongly in  $H^1(\mathbb{R}^d)$ . By [RS72, Thm VIII.24], this follows from the fact that, since  $S'$  is strictly decreasing on  $(0, 1)$ ,  $\lambda$  can never be an eigenvalue of  $\gamma_f$ . Similarly, we have that  $\mathbf{1}(P_k \gamma P_k \geq \lambda) \rightarrow \mathbf{1}(\gamma \geq \lambda)$  strongly if  $\lambda$  is not an eigenvalue of  $\gamma$ , and in this case we get

$$\begin{aligned} \liminf_{k \rightarrow \infty} \text{Tr} |S'(P_k \gamma_f P_k) - S'(\lambda)| (\mathbf{1}(P_k \gamma P_k \geq \lambda) - \mathbf{1}(P_k \gamma_f P_k \geq \lambda))^2 \\ \geq \text{Tr} |S'(\gamma_f) - S'(\lambda)| (\mathbf{1}(\gamma \geq \lambda) - \mathbf{1}(\gamma_f \geq \lambda))^2 \end{aligned} \quad (4.6.80)$$

by Fatou's lemma for operators. The strong convergence of  $\mathbf{1}(P_k \gamma P_k \geq \lambda)$  can however fail if  $\lambda$  happens to be an eigenvalue of  $\gamma$ . Fortunately, the set of eigenvalues is at most countable and it is therefore of Lebesgue measure zero. Applying Fatou's theorem for the integral over  $\lambda$ , this ends the proof of the lower bound (4.6.79).

Let us estimate the terms in the integral for every  $\lambda$ . In dimension  $d \geq 2$ , we use the Lieb-Thirring inequality (4.4.35) and obtain

$$\begin{aligned} \mathcal{H}(\gamma, \gamma_f) \geq K(d) \int_{\mathbb{R}^d} dx \int_0^{f(0)} S'(\lambda)^{1+\frac{d}{2}} F \left( \frac{\rho_\lambda(x)}{S'(\lambda)^{\frac{d}{2}}} \right) d\lambda \\ + K(d) \int_{\mathbb{R}^d} dx \int_{f(0)}^1 \rho_\lambda(x)^{1+\frac{2}{d}} d\lambda \end{aligned} \quad (4.6.81)$$

with  $\rho_\lambda := \rho_{\mathbf{1}(\gamma \geq \lambda)} - \rho_{\mathbf{1}(-\Delta \leq S'(\lambda))}$  and  $F(t) := (c_d + t)_+^{1+2/d} - c_d^{1+2/d} - \frac{2+d}{d} c_d^{2/d} t$  and where  $c_d = \rho_{\mathbf{1}(-\Delta \leq 1)}$ . The function  $F(t)$  is controlled from above and below by  $G(t) := \min(t^2, |t|^{1+2/d})$ , for  $t \geq -c_d$ . The estimates are a bit simpler with  $G$  and we

shall use it in the rest of the proof. So we can bound from below the first integral in (4.6.81) by a constant times

$$\int_0^{f(0)} S'(\lambda)^{1+\frac{d}{2}} \left( \frac{\rho_\lambda(x)^2}{S'(\lambda)^d} \mathbf{1}(\rho_\lambda(x) \leq S'(\lambda)^{\frac{d}{2}}) + \frac{\rho_\lambda(x)^{1+\frac{2}{d}}}{S'(\lambda)^{1+\frac{d}{2}}} \mathbf{1}(\rho_\lambda(x) \geq S'(\lambda)^{\frac{d}{2}}) \right) d\lambda.$$

By the Cauchy-Schwarz inequality, we have

$$\begin{aligned} \int_0^{f(0)} \mathbf{1}(\rho_\lambda(x) \leq S'(\lambda)^{\frac{d}{2}}) S'(\lambda)^{1-\frac{d}{2}} \rho_\lambda(x)^2 d\lambda &\geq \frac{\left( \int_0^{f(0)} \rho_\lambda(x) \mathbf{1}(\rho_\lambda(x) \leq S'(\lambda)^{\frac{d}{2}}) d\lambda \right)^2}{\int_0^{f(0)} S'(\lambda)^{\frac{d}{2}-1} d\lambda} \end{aligned}$$

where the denominator is finite by our assumption (4.6.76) and since  $d \geq 2$ . On the other hand, by Jensen's inequality we have

$$\begin{aligned} \int_0^{f(0)} \mathbf{1}(\rho_\lambda(x) \geq S'(\lambda)^{\frac{d}{2}}) \rho_\lambda(x)^{1+\frac{2}{d}} d\lambda &\geq f(0)^{-\frac{2}{d}} \left( \int_0^{f(0)} \rho_\lambda(x) \mathbf{1}(\rho_\lambda(x) \geq S'(\lambda)^{\frac{d}{2}}) d\lambda \right)^{1+\frac{2}{d}}. \end{aligned}$$

The integral with  $f(0) \leq \lambda \leq 1$  is similar. Let us now denote

$$\rho_1(x) = \int_{f(0)}^1 \rho_\lambda(x) d\lambda, \quad \rho_2(x) := \int_0^{f(0)} \rho_\lambda(x) \mathbf{1}(\rho_\lambda(x) \leq S'(\lambda)^{\frac{d}{2}}) d\lambda,$$

and

$$\rho_3(x) := \int_0^{f(0)} \rho_\lambda(x) \mathbf{1}(\rho_\lambda(x) \geq S'(\lambda)^{\frac{d}{2}}) d\lambda,$$

which are such that  $\rho_1(x) + \rho_2(x) + \rho_3(x) = \int_0^1 \rho_\lambda(x) d\lambda = \rho_\gamma(x) - \rho_{\gamma_f}(x)$ . Then we have proved that

$$\mathcal{H}(\gamma, \gamma_f) \geq c \int_{\mathbb{R}^d} \left( \rho_1(x)^{1+\frac{2}{d}} + \rho_2(x)^2 + \rho_3(x)^{1+\frac{2}{d}} \right) dx.$$

Note that, by convexity of  $F$ ,

$$\begin{aligned} \rho_1(x)^{1+\frac{2}{d}} + \rho_2(x)^2 + \rho_3(x)^{1+\frac{2}{d}} &\geq G(\rho_1(x)) + G(\rho_2(x)) + G(\rho_3(x)) \\ &\geq c\left(F(\rho_1(x)) + F(\rho_2(x)) + F(\rho_3(x))\right) \\ &\geq 3c F\left(\frac{\rho_1(x) + \rho_2(x) + \rho_3(x)}{3}\right) \\ &= 3c F\left(\frac{\rho_{\gamma-\gamma_f}(x)}{3}\right). \end{aligned}$$

The last term can be estimated by a constant times the one appearing on the left of (4.6.78) and this concludes the proof of Theorem 4.7.  $\square$

**6.4. High momentum estimate and consequences.** In this section we prove a uniform estimate on the high-momentum density of a matrix  $\gamma$  such that  $\mathcal{H}(\gamma, \gamma_f) < \infty$ .

**Theorem 4.8** (High momentum estimate). *We assume that  $d \geq 2$  and that  $S$  satisfies (4.6.70), (4.6.71), (4.6.74) and (4.6.76). We denote as before  $\gamma_f = f(-\Delta)$  with  $f = (S')^{-1}$ . Let  $1 \leq r \leq 1 + 2/d$  and  $0 \leq \theta \leq 1$  be such that  $r^{-1} = (1 - \theta)d/(d + 2) + \theta$ . Then*

$$\begin{aligned} \left\| \rho_{\Pi_A^+ Q \Pi_A^+} \right\|_{L^r + L^2} &\leq C \frac{\mathcal{H}(\gamma_f + Q, \gamma_f)^{\frac{1}{r}}}{A^\theta} \\ &\quad + C \mathcal{H}(\gamma_f + Q, \gamma_f)^{1/2} \left( \int_0^{f(A/2)} |S'(\lambda)|^{\frac{d}{2}-1} d\lambda \right)^{1/2}, \end{aligned} \quad (4.6.82)$$

and

$$\begin{aligned} \left\| \rho_{\Pi_A^+ Q \Pi_A^-} \right\|_{L^r + L^2} + \left\| \rho_{\Pi_A^- Q \Pi_A^+} \right\|_{L^r + L^2} &\leq C \frac{\mathcal{H}(\gamma_f + Q, \gamma_f)^{\frac{1}{r}} + \mathcal{H}(\gamma_f + Q, \gamma_f)^{\frac{1}{2}}}{A^{\frac{\theta}{2}}} \\ &\quad + C \mathcal{H}(\gamma_f + Q, \gamma_f)^{1/2} \left( \int_0^{f(A/2)} |S'(\lambda)|^{\frac{d}{2}-1} d\lambda \right)^{1/2}, \end{aligned} \quad (4.6.83)$$

for all  $A \geq C$  and a constant  $C$  depending only on  $S$  and  $r$ .

When  $r < 1 + 2/d$ , the terms on the right side are small for large  $A$ , since  $S$  satisfies the integrability condition (4.6.76) and since  $f(A/2) \rightarrow 0$  when  $A \rightarrow \infty$ . Our bound is not small for  $r = 1 + 2/d$ , however.

An estimate similar to (4.6.82) and (4.6.83) can easily be derived in dimension  $d = 1$  by arguing as in Lemma 4.9:

$$\left\| \Pi_A^+ Q \Pi_A^+ \right\|_{L^2(\mathbb{R})} + \left\| \Pi_A^+ Q \Pi_A^- \right\|_{L^2(\mathbb{R})} + \left\| \Pi_A^- Q \Pi_A^+ \right\|_{L^2(\mathbb{R})} \leq \frac{C}{\sqrt{A}} \mathcal{H}(\gamma_f + Q, \gamma_f)^{1/2}. \quad (4.6.84)$$

Before turning to the proof of Theorem 4.8, we mention a corollary. It concerns the approximation of operators with finite relative entropy by means of operators in  $\mathfrak{S}^{2,s}$  for a large  $s$ . It is similar to [LS13a, Cor. 1] but includes in addition an information about the density  $\rho$ .

**Corollary 4.3** (Approximation by operators in  $\mathfrak{S}^{2,s}$ ). *Let  $d \geq 1$ . We assume that  $S$  satisfies (4.6.70), (4.6.71), (4.6.74) and (4.6.76). We denote as before  $\gamma_f = f(-\Delta)$  with  $f = (S')^{-1}$ . Let  $0 \leq \gamma \leq 1$  be such that  $\mathcal{H}(\gamma, \gamma_f) < \infty$ , and let  $Q = \gamma - \gamma_f$  and  $\Pi_A^- = \mathbf{1}(-\Delta \leq A)$ . Then we have*

- $\lim_{A \rightarrow \infty} \|\Pi_A^- Q \Pi_A^- - Q\|_{\mathfrak{S}^{2,1}} = 0$ ;
- $\lim_{A \rightarrow \infty} \mathcal{H}(\gamma_f + \Pi_A^- Q \Pi_A^-, \gamma_f) = \mathcal{H}(\gamma, \gamma_f)$ ;
- $\lim_{A \rightarrow \infty} \left\| \rho_{\Pi_A^- Q \Pi_A^-} - \rho_Q \right\|_{L^r + L^2} = 0$  for all  $1 \leq r < 1 + 2/d$ .

The last limit is uniform in  $\gamma$ , for  $\mathcal{H}(\gamma, \gamma_f) \leq C$  and  $r \leq 1 + 2/d - 1/C$ .

**PROOF OF COROLLARY 4.3.** For the first two items see [LS13a, Cor. 1], only the limit of the density is new. We write  $Q - \Pi_A^- Q \Pi_A^- = \Pi_A^+ Q \Pi_A^+ + \Pi_A^- Q \Pi_A^+ + \Pi_A^+ Q \Pi_A^-$ . These terms are estimated in  $L^r + L^2$  in Theorem 4.8, with a bound uniform for  $\mathcal{H}(\gamma, \gamma_f) \leq C$  and  $r \leq 1 + 2/d - 1/C$ .  $\square$

It remains to write the

**PROOF OF THEOREM 4.8.** We write the proof for  $Q$  a smooth finite rank operator and we use (4.6.79) as in the proof of Theorem 4.7. We have as before

$$Q = \int_0^1 (\mathbf{1}(\gamma \geq \lambda) - \mathbf{1}(-\Delta \leq S'(\lambda))) d\lambda,$$

and introduce for simplicity  $\mu := S'(\lambda)$ ,  $P_\mu := \mathbf{1}(\gamma \geq \lambda)$  and  $Q_\mu := P_\mu - \Pi_\mu^-$ , in such a way that  $\Pi_A^+ Q \Pi_A^+ = \int_0^1 \Pi_A^+ Q_\mu \Pi_A^+ d\lambda$ . We use the notation  $Q_\mu^{++} := \Pi_\mu^+ Q_\mu \Pi_\mu^+$ ,  $Q_\mu^{+-} := \Pi_\mu^+ Q_\mu \Pi_\mu^-$  and so on. We estimate the density of  $\Pi_A^+ Q_\mu \Pi_A^+$  for every fixed  $\mu$ , before integrating with respect to  $\lambda = (S')^{-1}(\mu)$ .

We first deal with the case  $\mu \leq A/2$ . Then  $\Pi_\mu^- \Pi_A^+ = 0$  and, using that  $(p^2 - \mu)\mathbf{1}(p^2 \geq A) \geq A/2$  for  $\mu \leq A/2$ , we get

$$\int_{\mathbb{R}^d} \rho_{\Pi_A^+ Q_\mu \Pi_A^+} = \int_{\mathbb{R}^d} \rho_{\Pi_A^+ Q_\mu^{++} \Pi_A^+} \leq \frac{2}{A} \text{Tr}(-\Delta - \mu) Q_\mu^{++} \leq \frac{2}{A} \text{Tr}|\Delta + \mu| Q_\mu^2.$$

On the other hand, by the usual Lieb-Thirring inequality, we have

$$\int_{\mathbb{R}^d} \rho_{\Pi_A^+ Q_\mu \Pi_A^+}^{1+2/d} \leq C \text{Tr}(-\Delta) \Pi_A^+ Q_\mu^{++} \leq 2C \text{Tr}|\Delta + \mu| Q_\mu^2.$$

By Hölder's inequality we deduce that

$$\left\| \rho_{\Pi_A^+ Q_\mu \Pi_A^+} \right\|_{L^r} \leq \frac{C}{A^\theta} (\text{Tr}|\Delta + \mu| Q_\mu^2)^{\frac{1}{r}},$$

with  $r^{-1} = (1 - \theta)d/(d + 2) + \theta$ .

Assume now that  $\mu \geq A/2$ . Then we are not going to use  $A$ , but we perform a similar decomposition using  $2\mu$ . We write

$$\Pi_A^+ Q_\mu \Pi_A^+ = \Pi_{2\mu}^+ Q_{\mu,A} \Pi_{2\mu}^+ + \Pi_{2\mu}^+ Q_{\mu,A} \Pi_{2\mu}^- + \Pi_{2\mu}^- Q_{\mu,A} \Pi_{2\mu}^+ + \Pi_{2\mu}^- Q_{\mu,A} \Pi_{2\mu}^-$$

and  $Q_{\mu,A} := \Pi_A^+ Q_\mu \Pi_A^+$ . The previous argument gives

$$\left\| \rho_{\Pi_{2\mu}^+ Q_{\mu,A} \Pi_{2\mu}^+} \right\|_{L^r} \leq C \frac{(\text{Tr} |\Delta + \mu| Q_\mu^2)^{\frac{1}{r}}}{\mu^\theta} \leq C \frac{(\text{Tr} |\Delta + \mu| Q_\mu^2)^{\frac{1}{r}}}{A^\theta}. \quad (4.6.85)$$

On the other hand, we have  $\|\rho_{\Pi_{2\mu}^- Q_{\mu,A} \Pi_{2\mu}^-}\|_{L^\infty} \leq C\mu^{d/2}$  and, by the Lieb-Thirring inequality (4.4.35),

$$\int_{\mathbb{R}^d} \min \left( |\rho_{\Pi_{2\mu}^- Q_{\mu,A} \Pi_{2\mu}^-}|^{1+2/d}, \mu^{1-\frac{d}{2}} |\rho_{\Pi_{2\mu}^- Q_{\mu,A} \Pi_{2\mu}^-}|^2 \right) \leq C \text{Tr} |\Delta + \mu| Q_\mu^2.$$

From these two bounds we deduce that

$$\left\| \rho_{\Pi_{2\mu}^- Q_{\mu,A} \Pi_{2\mu}^-} \right\|_{L^2} \leq C\mu^{\frac{d}{4}-\frac{1}{2}} (\text{Tr} |\Delta + \mu| Q_\mu^2)^{1/2}. \quad (4.6.86)$$

Finally, the density of  $\Pi_{2\mu}^+ Q_{\mu,A} \Pi_{2\mu}^-$  can be estimated in  $L^2$  by duality:

$$\begin{aligned} \text{Tr} (\Pi_{2\mu}^+ Q_{\mu,A} \Pi_{2\mu}^- V) &\leq \|\Pi_{2\mu}^+ Q\|_{\mathfrak{S}^2} \|\Pi_{2\mu}^- V\|_{\mathfrak{S}^2} \\ &\leq C\mu^{\frac{d}{4}-\frac{1}{2}} (\text{Tr} |\Delta + \mu| Q_\mu^2)^{\frac{1}{2}} \|V\|_{L^2}. \end{aligned} \quad (4.6.87)$$

So for  $\mu \geq A/2$  we obtain

$$\left\| \rho_{\Pi_A^+ Q_\mu \Pi_A^+} \right\|_{L^r + L^2} \leq C\mu^{\frac{d}{4}-\frac{1}{2}} (\text{Tr} |\Delta + \mu| Q_\mu^2)^{1/2} + C \frac{(\text{Tr} |\Delta + \mu| Q_\mu^2)^{\frac{1}{r}}}{A^\theta}.$$

Now we integrate with respect to  $\lambda$  and appeal to (4.6.79). We use the concavity of  $x \mapsto x^{1/r}$  and the Cauchy-Schwarz inequality for the integral over  $\lambda$  involving  $\mu^{\frac{d}{4}-\frac{1}{2}}$ . We obtain

$$\begin{aligned} \left\| \rho_{\Pi_A^+ Q_\mu \Pi_A^+} \right\|_{L^r + L^2} &\leq C \frac{\mathcal{H}(\gamma_f + Q, \gamma_f)^{\frac{1}{r}}}{A^\theta} \\ &\quad + C \mathcal{H}(\gamma_f + Q, \gamma_f)^{1/2} \left( \int_0^1 |S'(\lambda)|^{\frac{d}{2}-1} \mathbf{1}(S'(\lambda) \geq A/2) d\lambda \right)^{1/2}, \end{aligned}$$

which is the desired result.

We estimate the cross terms  $\Pi_A^\pm Q_\mu \Pi_A^\mp$  by using similar arguments. We start with  $\mu \leq A/2$  and therefore look at  $\Pi_A^+ Q_\mu \Pi_A^- = \Pi_A^+ Q_\mu^{++} \Pi_A^- + \Pi_A^+ Q_\mu^{+-}$ . The second term is estimated by duality like in (4.6.87), leading to

$$\left\| \rho_{\Pi_A^+ Q_\mu^{+-}} \right\|_{L^2} \leq \frac{C\mu^{\frac{d}{4}}}{\sqrt{A}} (\text{Tr} |\Delta + \mu| Q_\mu^2)^{1/2}.$$

For the first term, we remark that for every  $V \geq 0$

$$\begin{aligned} |\operatorname{Tr}(\Pi_A^+ Q_\mu^{++} \Pi_A^- V)| &\leq \left\| \sqrt{V} \Pi_A^+ \sqrt{Q_\mu^{++}} \right\|_{\mathfrak{S}^2} \left\| \sqrt{Q_\mu^{++}} \Pi_A^- \sqrt{V} \right\|_{\mathfrak{S}^2} \\ &\leq A^{\frac{\theta}{2}} \operatorname{Tr}(\Pi_A^+ Q_\mu^{++} \Pi_A^- V) + \frac{1}{4A^{\frac{\theta}{2}}} \operatorname{Tr}(\Pi_A^- Q_\mu^{++} \Pi_A^- V), \end{aligned}$$

which implies the pointwise inequality

$$|\rho_{\Pi_A^+ Q_\mu^{++} \Pi_A^-}| \leq A^{\frac{\theta}{2}} \rho_{\Pi_A^+ Q_\mu^{++} \Pi_A^+} + \frac{1}{4A^{\frac{\theta}{2}}} \rho_{\Pi_A^- Q_\mu^{++} \Pi_A^-}.$$

We have shown before that  $\|\rho_{\Pi_A^+ Q_\mu^{++} \Pi_A^+}\|_{L^r} \leq CA^{-\theta} (\operatorname{Tr} |\Delta + \mu|Q_\mu^2|)^{1/r}$  and, by the Lieb-Thirring inequality (4.4.35), we have

$$\left\| \rho_{\Pi_A^- Q_\mu^{++} \Pi_A^-} \right\|_{L^{1+2/d+L^2}} \leq C \left( (\operatorname{Tr} |\Delta + \mu|Q_\mu^2|)^{\frac{d}{d+2}} + \mu^{\frac{d}{4}-\frac{1}{2}} (\operatorname{Tr} |\Delta + \mu|Q_\mu^2|)^{\frac{1}{2}} \right).$$

So we get, for  $\mu \leq A/2$ ,

$$\left\| \rho_{\Pi_A^+ Q_\mu \Pi_A^-} \right\|_{L^r+L^2} \leq \frac{C}{A^{\frac{\theta}{2}}} \left( (\operatorname{Tr} |\Delta + \mu|Q_\mu^2|)^{\frac{1}{r}} + (1 + \mu^{\frac{d}{4}-\frac{1}{2}}) (\operatorname{Tr} |\Delta + \mu|Q_\mu^2|)^{\frac{1}{2}} \right).$$

Finally, we deal with the case  $\mu \geq A/2$  in a similar fashion. We write

$$\begin{aligned} \Pi_A^+ Q_\mu \Pi_A^- &= \Pi_{2\mu}^+ Q_\mu \Pi_A^- + \Pi_A^+ \Pi_{2\mu}^- Q_\mu^{++} \Pi_A^- + \Pi_A^+ Q_\mu^{--} \Pi_A^- \\ &\quad + \Pi_A^+ Q_\mu^{-+} \Pi_A^- + \Pi_A^+ \Pi_{2\mu}^- Q_\mu^{+-} \Pi_A^-. \end{aligned} \quad (4.6.88)$$

The density of  $\Pi_{2\mu}^+ Q_\mu \Pi_A^-$  is estimated exactly as in (4.6.87). The density of the operator  $\Pi_A^+ \Pi_{2\mu}^- Q_\mu^{++} \Pi_A^-$  is bounded as before by using

$$2|\rho_{\Pi_A^+ \Pi_{2\mu}^- Q_\mu^{++} \Pi_A^-}| \leq \rho_{\Pi_A^- Q_\mu^{++} \Pi_A^-} + \rho_{\Pi_A^+ \Pi_{2\mu}^- Q_\mu^{++} \Pi_A^-}.$$

The two densities on the right can be estimated in  $L^\infty$  by  $C\mu^{d/2}$  and in  $L^{1+2/d} + L^2$  by the Lieb-Thirring inequality. Like in (4.6.86), this leads to

$$\left\| \rho_{\Pi_A^+ \Pi_{2\mu}^- Q_\mu^{++} \Pi_A^-} \right\|_{L^2} \leq C\mu^{\frac{d}{4}-\frac{1}{2}} (\operatorname{Tr} |\Delta + \mu|Q_\mu^2|)^{1/2}.$$

The argument is the same for the term involving  $Q^{--}$  in (4.6.88). Finally, the two terms involving  $Q^{+-}$  and  $Q^{-+}$  in (4.6.88) are bounded by using directly [FLLS12, Eq. (3.11)–(3.12)], leading to

$$\left\| \rho_{\Pi_A^+ Q_\mu^{-+} \Pi_A^-} \right\|_{L^2} + \left\| \rho_{\Pi_A^+ \Pi_{2\mu}^- Q_\mu^{+-} \Pi_A^-} \right\|_{L^2} \leq C\mu^{\frac{d}{4}-\frac{1}{2}} (\operatorname{Tr} |\Delta + \mu|Q_\mu^2|)^{1/2}.$$

The final bound is

$$\left\| \rho_{\Pi_A^+ Q_\mu \Pi_A^-} \right\|_{L^2} \leq C\mu^{\frac{d}{4}-\frac{1}{2}} (\operatorname{Tr} |\Delta + \mu|Q_\mu^2|)^{1/2} \quad (4.6.89)$$

for  $\mu \geq A/2$  and (4.6.83) follows after integrating with respect to  $\lambda$ .  $\square$

### 7. Free energy & global well-posedness for generalized Gibbs states

We have proved the existence of local-in-time solutions to the nonlinear Hartree equation

$$i\dot{\gamma} = [-\Delta + w * \rho_\gamma, \gamma],$$

in various situations in Section 3, and of global-in-time solutions when  $\gamma$  is a local perturbation of the Fermi sea  $\gamma_f = \mathbf{1}(-\Delta \leq \mu)$  in Section 4. The purpose of this section is to derive a similar result for more general reference states  $\gamma_f$ , including (4.1.6)–(4.1.8).

Consider a reference state  $\gamma_f = f(-\Delta)$  with  $f = (S')^{-1}$  and  $S$  satisfying (4.6.70), (4.6.71), (4.6.74) and (4.6.76). The following *relative free energy*, analogous to the relative energy of Section 4, is formally conserved and will be used as a Lyapunov function to get global solutions:

$$\mathcal{F}_f(\gamma, \gamma_f) := \mathcal{H}(\gamma, \gamma_f) + \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y) \rho_{\gamma-\gamma_f}(x) \rho_{\gamma-\gamma_f}(y) dx dy. \quad (4.7.90)$$

This functional is defined on the *free energy space*

$$\mathcal{K}_f := \left\{ 0 \leq \gamma = \gamma^* \leq 1 : \mathcal{H}(\gamma, \gamma_f) < \infty \right\}. \quad (4.7.91)$$

From Klein's inequality (4.6.75), we know that any  $\gamma \in \mathcal{K}_f$  satisfies  $(1-\Delta)^{1/2}(\gamma-\gamma_f) \in \mathfrak{S}^2$  and from Lemma 4.9 and the Lieb-Thirring inequality in Theorem 4.7, we know that  $\rho_\gamma - \rho_{\gamma_f} \in L^2(\mathbb{R}^d) + L^{1+\min(1,2/d)}(\mathbb{R}^d)$ . We infer that the last term is well-defined, provided that  $w$  decays fast enough. The condition is  $w \in L^1(\mathbb{R}^d)$  for  $d = 1, 2$ , and  $w \in L^1(\mathbb{R}^d) \cap L^{(d+2)/4}(\mathbb{R}^d)$  for  $d \geq 3$ . We have the equivalent of Proposition 4.1 for the relative free energy:

**Proposition 4.6** (Coercivity of the relative free energy in the defocusing case). *Let  $\gamma \in \mathcal{K}_f$ . Then, when  $d \geq 3$  and  $\widehat{w} \geq 0$  we have*

$$\mathcal{F}_f(\gamma, \gamma_f) \geq \mathcal{H}(\gamma, \gamma_f), \quad (4.7.92)$$

while when  $d = 1, 2$  and  $\|\widehat{w}_-\|_{L^\infty} < K_{\text{LT},S}/(2\pi)^{d/2}$  we have

$$\mathcal{F}_f(\gamma, \gamma_f) \geq \left( 1 - \frac{(2\pi)^{d/2} \|\widehat{w}_-\|_{L^\infty}}{K_{\text{LT},S}} \right) \mathcal{H}(\gamma, \gamma_f), \quad (4.7.93)$$

where  $K_{\text{LT},S}$  is the Lieb-Thirring constant of Lemma 4.9 and Theorem 4.7.

We use this result to globalize the local-in-time solutions to the Hartree equation with finite relative free energy built in Theorem 4.3.

**Theorem 4.9** (Global well-posedness at positive temperature for  $d = 1, 2, 3$ ). *Assume that  $d = 1, 2, 3$  and that  $w \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$  if  $d = 1, 2$  with furthermore  $|\nabla w| \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$  if  $d = 3$ . Assume also that  $w(x) = w(-x)$  for a.e.  $x \in \mathbb{R}^d$ . Let  $\gamma_f = f(-\Delta)$  with  $f = (S')^{-1}$  and  $S$  satisfying (4.6.70), (4.6.71), (4.6.74) and*

(4.6.76). Let  $Q_0 = \gamma_0 - \gamma_f$  with  $\gamma_0 \in \mathcal{K}_f$ . Then there exists a unique maximal solution  $Q(t) = \gamma(t) - \gamma_f \in C_t^0((-T^-, T^+), \mathfrak{S}^2)$  if  $d = 1, 2$ , and  $Q(t) \in C_t^0((-T^-, T^+), \mathfrak{S}^{2,1})$  if  $d = 3$ , of (4.3.16) with initial datum  $Q_0$ , such that  $\gamma(t) \in \mathcal{K}_f$  for almost all  $t \in (-T^-, T^+)$  and  $T^\pm > 0$ . We have the blow-up criterion

$$T^\pm < \infty \implies \lim_{t \rightarrow \pm T^\pm} \mathcal{H}(\gamma(t), \gamma_f) = +\infty. \quad (4.7.94)$$

The relative free energy is constant for almost every  $t \in (-T^-, T^+)$ . Furthermore, when  $d = 3$  and  $\widehat{w} \geq 0$  or when  $d = 1, 2$  and  $\|(\widehat{w})_-\|_{L^\infty} < K_{\text{LT,S}}/(2\pi)^{d/2}$ , then the solution is global,  $T^- = T^+ = +\infty$ .

This result holds for a fixed function  $S$  and for  $0 \leq \gamma_0, \gamma_f \leq 1$ . By scaling and multiplication by a constant we can deal with the general situation and, in particular, get Theorem 4.2 stated in the introduction. For instance, in order to deal with density matrices satisfying  $\leq M$ , it suffices to multiply the time-dependent equation by  $1/M$  and to consider the operators  $\gamma_f/M$  and  $\gamma_0/M$ . This changes  $w$  into  $Mw$  and the entropy  $S$  into  $M^{-1}S(Mx)$ . In dimensions  $d = 1, 2$  the condition on  $\widehat{w}$  then involves  $M$  through the constant  $K_{\text{LT,S}}$ . Similarly, in the physical examples (4.1.6)–(4.1.8), the entropy  $S$  includes the temperature  $T$  and the chemical potential  $\mu$ . By a scaling argument, we can always reduce the problem to  $T = 1$  with chemical potential  $\mu/T$  and then  $K_{\text{LT,S}}$  only depends on  $\mu/T$ . Indeed, if  $\gamma_f = f(-\Delta/T)$ , then defining the unitary operator  $(U_T f) := T^{d/4} f(\sqrt{T}x)$ , we see that the time-dependent equation satisfied by  $\tilde{\gamma}(t) := U_T^* \gamma U_T(t/T)$  is

$$\begin{cases} i \partial_t \tilde{\gamma} = [-\Delta + w_T * \rho_{\tilde{\gamma}}, \tilde{\gamma}], \\ \tilde{\gamma}(0) = f(-\Delta) + U_T^* Q(0) U_T, \end{cases} \quad (4.7.95)$$

with  $w_T(x) = T^{-1}w(x/\sqrt{T})$  and, hence,  $\widehat{w}_T(k) = T^{d/2-1}\widehat{w}(\sqrt{T}k)$ . In the Boltzmann and Fermi-Dirac cases, it is easy to verify that the Lieb-Thirring constant  $K_{\text{LT,S}}$  stays positive when  $\mu$  varies in an interval around 0. This is not true in the Bose-Einstein case since the operator norm of  $\gamma_{1,\mu/T}^{\text{bos}}$  diverges when  $\mu/T \rightarrow 0^-$ , in which case we have to divide the equation by a large constant, as explained before. Thus the constants  $\kappa_1$  and  $\kappa_2$  appearing in Theorem 4.2 stay bounded away from 0 when  $\mu/T$  stays in a compact set for fermions and boltzons, but it converges to 0 when  $\mu/T \rightarrow 0^-$  for bosons.

The rest of the section is devoted to the proof of Theorem 4.9. As in Section 4, we begin by showing conservation of energy for ‘regular’ solutions, namely those belonging to the space  $\mathfrak{S}^{1,4}$ .

**Proposition 4.7** (Conservation of the relative free energy for regular solutions). *Let  $d \geq 1$  and  $w \in (\ell^1(L^2) \cap L^\infty)(\mathbb{R}^d)$  such that  $\partial^\alpha w \in (\ell^1(L^2) \cap L^\infty)(\mathbb{R}^d)$  for all multi-indices  $|\alpha| \leq 4$ . Assume also  $w(x) = w(-x)$  for a.e.  $x \in \mathbb{R}^d$ . Let  $\gamma_f = f(-\Delta)$  with*



$f = (S')^{-1}$  and  $S$  satisfying (4.6.70), (4.6.71), (4.6.74) and (4.6.76) with furthermore  $(1 + |\cdot|^4)g(\cdot) \in \ell^1(L^2)(\mathbb{R}^d)$  where  $g = f(|\cdot|^2)$ . Let  $Q_0 \in \mathfrak{S}^{1,4}$  be such that  $\gamma_f + Q_0 \in \mathcal{K}_f$ . Let  $Q \in C_t^0((-T^-, T^+), \mathfrak{S}^{1,4})$  be the maximal solution to the Hartree equation with initial condition  $Q_0$  built in Theorem 4.3. Then, for all  $t \in (-T^-, T^+)$ ,  $\gamma_f + Q(t) \in \mathcal{K}_f$  and the relative free energy is conserved:  $\mathcal{F}_f(\gamma_f + Q(t), \gamma_f) = \mathcal{F}_f(\gamma_f + Q_0, \gamma_f)$ .

**Remark 4.2.** The assumption that  $k \mapsto (1 + k^4)f(k^2) \in \ell^1 L^2$  is satisfied if, for instance,  $(1 + k^2)^{2+\delta/2}f(k^2) \in L^2(\mathbb{R}^d)$  for some  $\delta > d/2$ , by [Sim77, Chap. 4]. A sufficient condition for this to hold is  $\int_0^1 \lambda(1 + S'(\lambda)_+)^{\delta+4} S'(\lambda)_+^{d/2} d\lambda < \infty$  which, by (4.6.76), is itself implied by the boundedness of  $\lambda \mapsto \lambda^{\frac{1}{\delta+4}} S'(\lambda)$  as  $\lambda \rightarrow 0$ . In Lemma 4.10, we will show that any  $S$  satisfying (4.6.70), (4.6.71), (4.6.74) and (4.6.76) can be approximated by a monotone sequence  $(S_n)$  satisfying this.

**PROOF OF PROPOSITION 4.7.** Let  $Q(t)$  be the solution to the Hartree equation with initial datum  $Q_0$ . We prove that for all  $t \in (-T^-, T^+)$

$$\mathcal{H}(\gamma_f + Q(t), \gamma_f) = \mathcal{H}(\gamma_f + Q_0, \gamma_f) + \text{Tr}(-\Delta)(Q(t) - Q_0) \quad (4.7.96)$$

where we recall that  $(-\Delta)(Q(t) - Q_0) \in \mathfrak{S}^1$ . The proof that the relative free energy is conserved then follows by the same method as for Theorem 4.3, using that  $Q(t)$  belongs to  $C_t^0 \mathfrak{S}^{1,4} \cap C_t^1 \mathfrak{S}^{1,2}$  for all times. The rest of the argument is therefore devoted to the proof (4.7.96).

Since  $\rho_Q(t)$  belongs to  $L_{t,\text{loc}}^\infty((-T^-, T^+), L_x^1(\mathbb{R}^d))$ , then  $V(t) = w * \rho_Q(t)$  belongs to  $L_{t,\text{loc}}^{p'}((-T^-, T^+), L_x^{q'}(\mathbb{R}^d))$  for any  $2/p' + d/q' = 2$ . By [FLS13], we deduce that for all  $t \in (-T^-, T^+)$ ,  $\gamma_f + Q(t) = U_V(t)(\gamma_f + Q_0)U_V(t)^*$ , where  $U_V(t) - 1 \in C^0(\mathfrak{S}^{d+2})$ , with  $U_V(t)$  a strongly continuous family of unitary operators on  $L^2(\mathbb{R}^d)$  with  $U_V(0) = 1$ . In particular,  $0 \leq \gamma_f + Q(t) \leq 1$  for all  $t$ . From the proof of Theorem 4.3, we also know that  $(U_V(t) - 1)\gamma_f(1 - \Delta) \in C^0(\mathfrak{S}^1)$  and that  $[\nabla, U_V(t) - 1] \in C^0(\mathfrak{S}^{d+2})$ . Indeed, computing the last commutator we get a sum of terms in which one of the potentials  $V$  is replaced by  $\nabla V$ , and the estimate is the same as for  $U_V(t) - 1$  using our assumptions on  $w$ . In the following we denote  $K(t) := U_V(t) - 1$ .

We only prove (4.7.96) for short times, the proof in the general case follows by iterating the argument below. For  $t \ll 1$  we have the additional information that  $\|K(t)\|_{\mathfrak{S}^{d+2}} < 1$  and this implies that we can write  $U_V(t) = \exp(iB(t))$  where  $t \mapsto B(t) \in C^0(\mathfrak{S}^{d+2})$ , with  $B(t) = B(t)^*$ . The operator  $B(t)$  satisfies the same properties as  $K(t)$ , namely  $B(t)\gamma_f(1 - \Delta) \in C^0(\mathfrak{S}^1)$  and  $[\nabla, B(t)] \in C^0(\mathfrak{S}^{d+2})$ . We now proceed in two steps. First we replace  $B(t)$  by an operator  $B_n$  of finite rank and prove (4.7.96) with  $Q_n := e^{iB_n}(\gamma_f + Q_0)e^{-iB_n} - \gamma_f$  in place of  $Q(t)$ . Then we let  $n \rightarrow \infty$ .

The approximation sequence  $B_n = B_n^*$  is chosen such as to have

$$\begin{aligned} \lim_{n \rightarrow \infty} \|B_n - B(t)\|_{\mathfrak{S}^{d+2}} &= \lim_{n \rightarrow \infty} \|(B_n - B(t))\gamma_f(1 - \Delta)\|_{\mathfrak{S}^1} \\ &= \lim_{n \rightarrow \infty} \|[\nabla, B_n - B(t)]\|_{\mathfrak{S}^{d+2}} = 0. \end{aligned}$$

One simple way to construct such a sequence  $B_n$ , is to first truncate the large momenta by looking at  $B'_A := \Pi_A^- B(t) \Pi_A^-$ . Since  $\gamma_f$ ,  $\nabla$  and  $\Delta$  commute with  $\Pi_A^-$  it is clear that  $B'_A$  converges to  $B(t)$  in the above norms as  $A \rightarrow \infty$ . Furthermore, we have  $B'_A \in \mathfrak{S}^1$  for the same reason as for  $B(t)\gamma_f \in \mathfrak{S}^1$ . Then  $\Delta B'_A \in \mathfrak{S}^1$  since  $\Delta$  is bounded on the range of  $\Pi_A^-$ . Now we can approximate  $B'_A$  in  $\mathfrak{S}^1(\Pi_A^- L^2)$  by a finite-rank operator and all the other properties follow immediately. We will use in the proof that  $K_n := e^{iB_n} - 1$  is also a finite rank operator with range in  $\Pi_A^- L^2$  and that it converges to  $K = e^{iB} - 1$  for the same norms as for  $B$ .

We turn to the proof of (4.7.96) with  $Q_n$  in place of  $Q(t)$ . Let  $P_k$  be an increasing sequence of finite-rank orthogonal projectors whose range contains the range of  $B_n$ , such that  $P_k \rightarrow 1$  strongly. We choose  $P_k$  such as to have  $P_k(1 - \Delta)P_k \leq C(1 - \Delta)$  for all  $k$  (the constant can depend on  $B_n$ ). Since  $B_n$  lives over the space  $\Pi_A^- L^2$ , it suffices to take projections adapted to the decomposition of the momentum space into shells,  $NA \leq -\Delta \leq (N + 1)A$ ,  $N \geq 0$ . By definition of the relative entropy, we have

$$\begin{aligned} &\mathcal{H}(\gamma_f + Q_n, \gamma_f) - \mathcal{H}(\gamma_f + Q_0, \gamma_f) = \\ &\lim_{k \rightarrow \infty} \text{Tr}_{P_k \mathfrak{H}} \left[ S(P_k(\gamma_f + Q_0)P_k) - S(P_k(\gamma_f + Q_n)P_k) + S'(P_k \gamma_f P_k) P_k (Q_n - Q_0) P_k \right]. \end{aligned}$$

By construction of  $P_k$ , we have  $P_k e^{iB_n} = e^{iB_n} P_k$  and hence

$$\begin{aligned} \text{Tr}_{P_k \mathfrak{H}} [S(P_k(\gamma_f + Q_n)P_k)] &= \text{Tr}_{P_k \mathfrak{H}} [e^{iB_n} S(P_k(\gamma_f + Q_0)P_k) e^{-iB_n}] \\ &= \text{Tr}_{P_k \mathfrak{H}} [S(P_k(\gamma_f + Q_0)P_k)]. \end{aligned}$$

Therefore we obtain

$$\mathcal{H}(\gamma_f + Q_n, \gamma_f) - \mathcal{H}(\gamma_f + Q_0, \gamma_f) = \lim_{k \rightarrow \infty} \text{Tr}_{\mathfrak{H}} [P_k S'(P_k \gamma_f P_k) P_k (Q_n - Q_0)]. \quad (4.7.97)$$

Using the integral representation (4.6.72) for  $S'$  and the inequality

$$\frac{1}{P_k(t + \gamma_f)P_k} \leq P_k \frac{1}{t + \gamma_f} P_k$$

for all  $t > 0$  (which follows from the Schur complement formula), we get

$$-C(1 - \Delta) \leq -C P_k(1 - \Delta)P_k \leq S'(P_k \gamma_f P_k) \leq C P_k(1 - \Delta)P_k \leq C(1 - \Delta).$$

Again from the representation (4.6.72) for  $S'$ , we can then show by Lebesgue's dominated convergence theorem that

$$P_k S'(P_k \gamma_f P_k) P_k \rightarrow S'(\gamma_f) = -\Delta$$

strongly as quadratic forms on  $H^1(\mathbb{R}^d)$ . The operator

$$Q_n - Q_0 = K_n Q_0 + Q_0 K_n + K_n Q_0 K_n + K_n \gamma_f + \gamma_f K_n + K_n \gamma_f K_n$$

has a finite rank and its eigenfunctions are in  $H^1$ , due to our assumption that  $Q_0 \in \mathfrak{S}^{1,4}$ . We can therefore pass to the limit  $k \rightarrow \infty$  in (4.7.97) and get

$$\mathcal{H}(e^{iB_n}(\gamma_f + Q_0)e^{-iB_n}, \gamma_f) = \mathcal{H}(\gamma_f + Q_0, \gamma_f) + \text{Tr}(-\Delta)(Q_n - Q_0).$$

In a second step we take the limit  $n \rightarrow \infty$ . If we can show that

$$\lim_{n \rightarrow \infty} \text{Tr}(-\Delta)(Q_n - Q(t)) = 0, \quad (4.7.98)$$

then we find, using the lower semi-continuity of  $\mathcal{H}$ , that

$$\mathcal{H}(\gamma_f + Q(t), \gamma_f) \leq \mathcal{H}(\gamma_f + Q_0, \gamma_f) + \text{Tr}(-\Delta)(Q(t) - Q_0).$$

Exchanging the roles of  $t$  and 0 gives the other inequality and this concludes the proof of (4.7.96) for short times.

So it remains to show (4.7.98). We can write (abbreviating  $Q = Q(t)$ )

$$\begin{aligned} Q_n - Q &= (K_n - K)Q_0 + Q_0(K_n - K) + (K_n - K)Q_0K_n + KQ_0(K_n - K) \\ &\quad + (K_n - K)\gamma_f + \gamma_f(K_n - K) + (K_n - K)\gamma_fK_n + K\gamma_f(K_n - K). \end{aligned}$$

That  $\text{Tr}(-\Delta)(K_n - K)Q_0 = \text{Tr}(K_n - K)Q_0(-\Delta) \rightarrow 0$  is obvious, since  $Q_0(-\Delta) \in \mathfrak{S}^1$  and  $K_n \rightarrow K$  in  $\mathfrak{S}^{d+2}$ . Let us look at

$$\begin{aligned} &\text{Tr}(-\Delta)KQ_0(K_n - K) \\ &= \sum_{j=1}^d \text{Tr} p_j K Q_0 (K_n - K) p_j \\ &= \sum_{j=1}^d \text{Tr} [p_j, K] Q_0 [K_n - K, p_j] + \text{Tr} [p_j, K] Q_0 p_j (K_n - K) \\ &\quad + \text{Tr} K p_j Q_0 [K_n - K, p_j] + \text{Tr} K p_j Q_0 p_j (K_n - K). \end{aligned}$$

This converges to 0, since  $\|[p_j, K_n - K]\|_{\mathfrak{S}^{d+2}} \rightarrow 0$ ,  $\|K_n - K\|_{\mathfrak{S}^{d+2}} \rightarrow 0$ ,  $Q_0 p_j \in \mathfrak{S}^1$  and  $p_j Q_0 p_j \in \mathfrak{S}^1$ . The last assertion follows from the property that  $|p||Q_0|^{1/2} \in \mathfrak{S}^2$ , by the Araki-Lieb-Thirring inequality and the fact that  $Q_0 \in \mathfrak{S}^{1,4}$ . The argument is similar for all the other terms, and this finishes our proof of Proposition 4.7.  $\square$

Global well-posedness in the energy space  $\mathcal{K}_f$  follows by approximating the initial datum  $\gamma_0 \in \mathcal{K}_f$ , the interaction potential  $w$  and the reference state  $\gamma_f$  by a sequence  $(\gamma_{0,n}, w_n, \gamma_{f,n})$  satisfying the assumptions of Proposition 4.7. The following lemma deals with the construction of  $(\gamma_{0,n})$  and  $(\gamma_{f,n})$ .

**Lemma 4.10.** *Let  $d \geq 1$ . We assume that  $S$  satisfies (4.6.70), (4.6.71), (4.6.74) and (4.6.76). We denote as before  $\gamma_f = f(-\Delta) = (S')^{-1}(-\Delta)$ . Let  $\gamma \in \mathcal{K}_f$  and  $Q := \gamma - \gamma_f$ . Then, there exist two sequences  $(S_n)$  and  $(\gamma_n)$  such that*

- $S_n$  satisfies (4.6.70), (4.6.71), (4.6.74) and (4.6.76) with additionally  $k \mapsto (1 + k^4)f_n(k^2) \in \ell^1 L^2(\mathbb{R}^d)$ , where  $f_n := (S'_n)^{-1}$ ;
- $\gamma_n \in \mathcal{K}_{f_n}$  and  $Q_n := \gamma_n - \gamma_{f_n} \in \mathfrak{S}^{1,4}$ ;
- $\lim_{n \rightarrow \infty} \int_{\mathbb{R}^d} |f_n(k^2) - f(k^2)| dk = \lim_{n \rightarrow \infty} \int_{\mathbb{R}^d} k^2 |f_n(k^2) - f(k^2)|^2 dk = 0$ ;
- $\lim_{n \rightarrow \infty} \mathcal{H}_n(\gamma_n, \gamma_{f_n}) = \mathcal{H}(\gamma, \gamma_f)$ ;
- $\lim_{n \rightarrow \infty} \|Q_n - Q\|_{\mathfrak{S}^{2,1}} = \lim_{n \rightarrow \infty} \|\rho_{e^{it\Delta} Q_n e^{-it\Delta}} - \rho_{e^{it\Delta} Q e^{-it\Delta}}\|_{L_t^\infty(L^1 + L^2)} = 0$ .

Here  $\mathcal{H}_n$  and  $\mathcal{H}$  are the relative entropies of  $S_n$  and  $S$ , respectively.

**PROOF OF LEMMA 4.10.** We begin by constructing the sequence  $(S_n)$ . A change of variables leads to the estimate

$$\int_{\mathbb{R}^d} |f_n(k^2) - f(k^2)| dk \leq C \int_0^{f(0)} |\lambda - (S'_n)^{-1}(S'(\lambda))| S'(\lambda)^{\frac{d}{2}-1} |S''(\lambda)| d\lambda. \quad (4.7.99)$$

Let  $\nu_1$  and  $\nu_2$  be the Löwner measures associated with  $S$ , as in (4.6.72). We define  $S_n$  by the same formula (4.6.72) as  $S$ , except that we replace  $a'$  by  $a'_n \leq a'$  and the measure  $d\nu_1$  by  $d\nu_{1,n}(t) := (t^{1-\bar{\alpha}} \mathbb{1}_{0 \leq t \leq 1/n} + \mathbb{1}_{t > 1/n}) d\nu_1(t)$ , where  $0 \leq \bar{\alpha} \leq 1$  is defined in the following fashion. First we look at

$$\alpha^* = \sup \left\{ 0 \leq \alpha \leq 1, \int_0^1 \frac{d\nu_1(t)}{t^\alpha} < +\infty \right\},$$

which is finite since  $\int_0^1 d\nu_1(t) < +\infty$ . We distinguish two cases. If  $\alpha^* > (d+6)/(d+8)$ , then we set  $\bar{\alpha} = 1$ , that is,  $\nu_{1,n} = \nu_1$  and we claim that we already have  $k \mapsto (1 + k^4)f(k^2) \in \ell^1 L^2$ . Indeed, by definition of  $\alpha^*$ , there exists  $\alpha > (d+6)/(d+8)$  such that  $\int_0^1 t^{-\alpha} d\nu_1(t) < \infty$ . Defining  $\delta = \frac{1}{1-\alpha} - 4$ , the condition  $\alpha > (d+6)/(d+8)$  implies that  $\delta > d/2$ . Using that  $S'(\lambda) \sim C + \int_0^1 (t + \lambda)^{-1} d\nu_1(t)$  we see that  $\lambda \mapsto \lambda^{\frac{1}{\delta+4}} S'(\lambda)$  is bounded when  $\lambda \rightarrow 0$ . By Remark 4.2 we deduce that  $k \mapsto (1 + k^4)f(k^2) \in \ell^1 L^2$ , and there is nothing to do.

Now, let us assume that  $\alpha^* \leq (d+6)/(d+8)$ . This implies that  $\alpha^* + 2/(d+8) \leq 1$ , and we pick any number  $\bar{\alpha}$  such that  $0 \leq \alpha^* < \bar{\alpha} < \alpha^* + 2/(d+8) \leq 1$ . The sequence  $a'_n \leq a'$  is chosen in the following fashion: we choose any sequence  $a'_n \rightarrow a'$  satisfying the property that  $a' - a'_n \geq 4b \int_0^{1/n} d\nu_1(t)$ . Since for all  $n$ ,  $\nu_{1,n} \leq \nu_1$  as positive Borel measures,  $S_n$  satisfies conditions (4.6.70) and (4.6.71). By the monotone convergence theorem, we have for all  $x > 0$ ,

$$\int_0^\infty \frac{d\nu_{1,n}(t)}{(t+x)(1+2t)} \rightarrow \int_0^\infty \frac{d\nu_1(t)}{(t+x)(1+2t)}$$

and hence  $S'_n(x) \rightarrow S'(x)$  as  $n \rightarrow \infty$ . Furthermore, using only  $a'_n \leq a'$  and  $\nu_{1,n} \leq \nu_1$ , we infer that  $S'_n(x) \leq S'(x)$  for all  $0 \leq x \leq 1/2$ . When  $1/2 \leq x \leq 1$ , we have

$$\begin{aligned} S'(x) - S'_n(x) &= (a' - a'_n)x - b(2x - 1) \int_0^{1/n} \frac{(1 - t^{1-\bar{\alpha}})d\nu_1(t)}{(t+x)(2t+1)} \\ &\geq \frac{a' - a'_n}{2} - 2b \int_0^{1/n} d\nu_1(t) \geq 0. \end{aligned}$$

Hence,  $S'_n(x) \leq S'(x)$  for all  $0 \leq x \leq 1$ , and since  $S'_n$  and  $S'$  are decreasing, we deduce that  $(S'_n)^{-1}(\lambda) \leq (S')^{-1}(\lambda)$  for all  $\lambda$ . By the monotone convergence theorem, we deduce that

$$\lim_{n \rightarrow \infty} \int_0^{f(0)} |\lambda - (S'_n)^{-1}(S'(\lambda))| S'(\lambda)^{\frac{d}{2}-1} |S''(\lambda)| d\lambda = 0.$$

From the fact that  $S'_n \leq S'$ , we also deduce that  $S_n$  satisfies condition (4.6.76) and condition (4.6.74) for all  $n$ . Because  $\bar{\alpha} < \alpha^* + 2/(d+8)$ , there exists  $d/2 < \delta < 1/(\bar{\alpha} - \alpha^*) - 4$ , and

$$\int_0^1 \frac{d\nu_{1,n}(t)}{t^{1-\frac{1}{\delta+4}}} = \int_0^{1/n} \frac{d\nu_1(t)}{t^{\bar{\alpha}-\frac{1}{\delta+4}}} + \int_{1/n}^1 \frac{d\nu_1(t)}{t^{1-\frac{1}{\delta+4}}} < +\infty$$

since  $\bar{\alpha} - 1/(\delta+4) < \alpha^*$ . As before this implies that  $(1+k^4)f_n(k^2) \in \ell^1 L^2$ . Finally, we have the inequality

$$\begin{aligned} &\int_{\mathbb{R}^d} k^2 |f_n(k^2) - f(k^2)|^2 dk \\ &\leq \left( \|k^2 f(k^2)\|_{L_k^\infty} + \sup_n \|k^2 f_n(k^2)\|_{L_k^\infty} \right) \int_{\mathbb{R}^d} |f_n(k^2) - f(k^2)| dk. \end{aligned}$$

Now  $\|k^2 f(k^2)\|_{L_k^\infty} = \|xS'(x)_+\|_{L_x^\infty} < \infty$  by (4.6.73), and it is also clear that we have  $\sup_n \|xS'_n(x)_+\|_{L_x^\infty} < +\infty$  since  $S'_n \leq S'$ .

We now construct the sequence  $(\gamma_n)$ . Corollary 4.3 and Theorem 4.8 show that we can find a sequence  $(\tilde{Q}_n) \subset \mathfrak{S}^{2,s}$  for all  $s \geq 0$ , with furthermore  $Q_n = \Pi_{A_n}^- \tilde{Q}_n \Pi_{A_n}^-$  for all  $n$ , for some sequence  $A_n \rightarrow +\infty$ , and such that  $\mathcal{H}(\gamma_f + \tilde{Q}_n, \gamma_f) \rightarrow \mathcal{H}(\gamma, \gamma_f)$ ,  $\tilde{Q}_n \rightarrow Q$  in  $\mathfrak{S}^{2,1}$ , and  $\rho_{e^{it\Delta} \tilde{Q}_n e^{-it\Delta}} \rightarrow \rho_{e^{it\Delta} Q e^{-it\Delta}}$  in  $L^\infty(\mathbb{R}, L^1 + L^2)$ . By [LS13a, Cor. 1], we can assume that each  $\tilde{Q}_n$  has finite-rank and hence belongs to  $\mathfrak{S}^{1,4}$  since it is compactly supported in Fourier space. By the formula defining  $S'_n$ , we see that  $s - S_n$  also satisfies conditions (4.6.70) and (4.6.71). Hence

$$\mathcal{H}(\gamma_f + \tilde{Q}_n, \gamma_f) - \mathcal{H}_n(\gamma_f + \tilde{Q}_n, \gamma_f) = \mathcal{H}_{s-S_n}(\gamma_f + \tilde{Q}_n, \gamma_f) \geq 0.$$

Defining  $X_n = (\gamma_{f_n}/\gamma_f)^{1/2}$  which satisfies  $0 \leq X_n \leq 1$  for all  $n$  since  $(S_n)^{-1} \leq (S')^{-1}$ , we also have by the monotony of the relative entropy (see [LS13a, Thm. 1])

$$\mathcal{H}_n(\gamma_f + \tilde{Q}_n, \gamma_f) \geq \mathcal{H}_n(X_n(\gamma_f + \tilde{Q}_n)X_n, X_n \gamma_f X_n) = \mathcal{H}_n(\gamma_{f_n} + X_n \tilde{Q}_n X_n, \gamma_{f_n}).$$

We thus set  $Q_n := X_n \tilde{Q}_n X_n$  and  $\gamma_n := \gamma_{f,n} + Q_n$ . By the previous inequality, we have  $\limsup_{n \rightarrow \infty} \mathcal{H}_n(\gamma_n, \gamma_{f,n}) \leq \mathcal{H}(\gamma, \gamma_f)$ . Using the weak lower semi-continuity of the relative entropy in finite dimension gives the reverse inequality with a liminf, and hence  $\mathcal{H}_n(\gamma_n, \gamma_{f,n}) \rightarrow \mathcal{H}(\gamma, \gamma_f)$ . Since  $X_n$  is a multiplication in Fourier space and since  $X_n \rightarrow 1$  strongly in  $L^2(\mathbb{R}^d)$ , we also deduce that  $Q_n \rightarrow Q$  in  $\mathfrak{S}^{2,1}$ . Finally, Lemma 4.1 gives that  $\rho[e^{it\Delta} Q_n e^{-it\Delta}] - \rho[e^{it\Delta} \tilde{Q}_n e^{-it\Delta}] \rightarrow 0$  in  $L^\infty(\mathbb{R}, L^1 + L^2)$ .  $\square$

PROOF OF THEOREM 4.9. Let  $(\gamma_0, w, \gamma_f)$  be as in the statement of the theorem. Let  $(\gamma_{0,n}, \gamma_{f,n})$  be given by Lemma 4.10. Let also  $(w_n) \subset (\ell^1 L^2 \cap L^\infty)(\mathbb{R}^d)$  be such that  $\partial^\alpha w_n \in (\ell^1 L^2 \cap L^\infty)(\mathbb{R}^d)$  for all multi-indices  $|\alpha| \leq 4$  and all  $n$ , with furthermore  $w_n(x) = w_n(-x)$  for a.e.  $x \in \mathbb{R}^d$ ,  $w_n \rightarrow w$  in  $(L^1 \cap L^\infty)(\mathbb{R}^d)$  if  $d = 1, 2$ , and additionally  $\nabla w_n \rightarrow \nabla w$  in  $(L^1 \cap L^\infty)(\mathbb{R}^d)^d$  when  $d = 3$ . Let  $Q_n \in \mathcal{C}^0((-T_n^-, T_n^+), \mathfrak{S}^{1,4})$  be the unique solution to (4.3.16) associated to the triplet  $(\gamma_{0,n}, w_n, \gamma_{f,n})$  given by Proposition 4.7. Let also  $Q \in \mathcal{C}^0((-T^-, T^+), \mathfrak{S}^2)$  if  $d = 1, 2$  and  $Q \in \mathcal{C}^0((-T^-, T^+), \mathfrak{S}^{2,1})$  if  $d = 3$  the solution to (4.3.16) built in Theorem 4.5 and Theorem 4.6. By these theorems, for all  $\varepsilon > 0$  and for all  $n$  large enough,  $T_n^\pm \geq T^\pm - \varepsilon$  and we have  $V_{Q_n} \rightarrow V_Q$  in  $L_t^{8/d}([-T^- + \varepsilon, T^+ - \varepsilon], L_x^2 \cap L_x^\infty)$ ,  $Q_n(t) \rightarrow Q(t)$  in  $\mathcal{C}^0([-T^- + \varepsilon, T^+ - \varepsilon], \mathfrak{S}^2)$ . Using the weak lower semi continuity of the relative entropy in finite dimension, we infer that for all  $t$

$$\mathcal{H}(\gamma_f + Q(t), \gamma_f) \leq \liminf_{n \rightarrow \infty} \mathcal{H}_n(\gamma_{f,n} + Q_n(t), \gamma_{f,n}).$$

The estimate

$$\left| \iint w(x-y) \rho_{Q_n(t)}(x) \rho_{Q_n(t)}(y) dx dy - \iint w(x-y) \rho_{Q(t)}(x) \rho_{Q(t)}(y) dx dy \right| \leq \|\rho_Q + \rho_{Q_n}\|_{L^1+L^2} \|V_{Q_n(t)} - V_{Q(t)}\|_{L^2 \cap L^\infty},$$

together with Hölder's inequality give

$$\iint w(x-y) \rho_{Q_n(t)}(x) \rho_{Q_n(t)}(y) dx dy \rightarrow \iint w(x-y) \rho_{Q(t)}(x) \rho_{Q(t)}(y) dx dy$$

in  $L_t^{4/d}([-T^- + \varepsilon, T^+ - \varepsilon])$ , and thus almost everywhere up to a subsequence. Taking the limit  $n \rightarrow \infty$  in the relative free energy of  $Q_n$ , we find that

$$\mathcal{F}_f(\gamma_f + Q(t), \gamma_f) \leq \mathcal{F}_f(\gamma_0, \gamma_f)$$

almost everywhere. Putting the initial time at any  $t$  for which there is convergence gives the reverse inequality. The blow-up criterion (4.7.94) follows from the Lieb-Thirring inequality and the blow-up criterion of Theorem 4.5 and Theorem 4.6. Assuming the defocusing conditions on  $\widehat{w}$ , using Proposition 4.6 and the Lieb-Thirring inequality, we deduce that the solution  $Q$  is global:  $T^\pm = +\infty$ . This concludes the proof of our main theorem.  $\square$

**Remark 4.3.** The defocusing condition also implies that the energy is constant everywhere (and not only almost everywhere): for all  $t \in \mathbb{R}$  and for all  $n$ , we have  $\mathcal{H}_n(\gamma_{f,n} + Q_n(t), \gamma_{f,n}) \leq c_n \mathcal{F}_{f_n}(\gamma_{f_n} + Q_n(t), \gamma_{f_n})$ , with  $(c_n)$  bounded. Thanks to Theorem 4.8 and since  $Q_n(t) \rightarrow Q(t)$  in  $\mathfrak{S}^2$ , this implies that  $\rho_{Q_n(t)} \rightarrow \rho_{Q(t)}$  in  $L^1 + L^2$  for *all*  $t$  (and not only on a full measure set). Hence,  $\mathcal{F}_f(\gamma_f + Q(t), \gamma_f) \leq \mathcal{F}_f(\gamma_0, \gamma_f)$  for all  $t$  and we have conservation of the energy by exchanging  $t$  and 0.

### A. Application of the generalized Strichartz estimates of Frank, Lewin, Lieb, and Seiringer: Well-posedness in $\mathfrak{S}^q$ , $q > 1$ , and decay for the Hartree and NLS equations

As we mentioned in the introduction, the well-posedness theory for the Hartree equation

$$i \partial_t \gamma = [-\Delta + w * \rho_\gamma, \gamma]$$

is well-known when the initial data  $\gamma_0$  belongs to the Schatten space  $\mathfrak{S}^1$ . This is mainly due to the uniform estimate

$$\|\rho_\gamma\|_{L^1(\mathbb{R}^d)} \leq \|\gamma\|_{\mathfrak{S}^1},$$

valid for all  $\gamma \in \mathfrak{S}^1$ . However, if  $\gamma \in \mathfrak{S}^q$  with  $q > 1$ , the density  $\rho_\gamma$  is not a well-defined object. Reflecting the dispersive properties of the propagator  $e^{it\Delta}$ , the generalized Strichartz inequality of [FLLS13] allows to define it almost everywhere though, in the following sense: for all  $1 \leq q \leq (d+2)/(d+1)$  and for all  $\gamma \in \mathfrak{S}^q$ , we have the inequality

$$\|\rho_{e^{it\Delta}\gamma e^{-it\Delta}}\|_{L_t^{q'/d}(\mathbb{R}, L_x^{q/(2-q)}(\mathbb{R}^d))} \leq C \|\gamma\|_{\mathfrak{S}^q}.$$

This is still not enough to find local solutions to the Hartree equation with initial data in  $\mathfrak{S}^q$ : writing its Duhamel formulation

$$\gamma(t) = e^{it\Delta}\gamma_0 e^{-it\Delta} - i \int_0^t e^{i(t-s)\Delta} [w * \rho_{\gamma(s)}, \gamma(s)] e^{i(s-t)\Delta} ds,$$

we see that the Strichartz estimate allows to control only the density of the first term  $e^{it\Delta}\gamma_0 e^{-it\Delta}$ . The density of the second term, though, cannot be controlled directly by this inequality. One can use the *inhomogeneous* Strichartz inequality of [FLLS13], which states that

$$\begin{aligned} \left\| \rho \left[ i \int_0^t e^{i(t-s)\Delta} [w * \rho_{\gamma(s)}, \gamma(s)] e^{i(s-t)\Delta} ds \right] \right\|_{L_t^{q'/d} \left( \mathbb{R}, L_x^{\frac{q}{2-q}}(\mathbb{R}^d) \right)} \\ \leq C \left\| \int_{\mathbb{R}} e^{is\Delta} |i[w * \rho_{\gamma(s)}, \gamma(s)]| e^{-is\Delta} ds \right\|_{\mathfrak{S}^q}. \end{aligned}$$

In particular, if  $\gamma \in C_t^0([0, T], \mathfrak{S}^q)$  is such that  $\rho_\gamma \in L_t^{q'/d}([0, T], L_x^{q/(2-q)}(\mathbb{R}^d))$ , then

$$\begin{aligned} & \left\| \rho \left[ i \int_0^t e^{i(t-s)\Delta} [w * \rho_{\gamma(s)}, \gamma(s)] e^{i(s-t)\Delta} ds \right] \right\|_{L_t^{\frac{q'}{d}}(\mathbb{R}, L_x^{\frac{q}{2-q}}(\mathbb{R}^d))} \\ & \leq CT^{1-\frac{d}{q'}} \|w\|_{L_x^{q'/2}} \|\rho_\gamma\|_{L_t^{q'/d} L_x^{q/(2-q)}} \|\gamma\|_{C_t^0 \mathfrak{S}^q}. \end{aligned}$$

Here, we used that  $w \in L_x^{q'/2}(\mathbb{R}^d)$  and  $\rho_\gamma \in L_x^{q/(2-q)}(\mathbb{R}^d)$  to infer that  $w * \rho_\gamma \in L_x^\infty(\mathbb{R}^d)$ , almost everywhere in the time variable. Using these estimates and a standard fixed point argument, we easily obtain local well-posedness for the Hartree equation in  $\mathfrak{S}^q$ . Furthermore, since the potential  $w * \rho_\gamma$  belongs to  $L_t^1 L_x^\infty$ , we know that there exists a unitary operator  $U(t)$  on  $L^2(\mathbb{R}^d)$  such that

$$\gamma(t) = U(t)\gamma_0 U(t)^*$$

for all times of existence  $t$ . This shows that  $\|\gamma(t)\|_{\mathfrak{S}^q}$  is actually conserved, which naturally leads to global well-posedness.

**Theorem 4.10.** *Let  $d \geq 1$  and  $1 \leq q \leq (d+2)/(d+1)$ . Let  $w \in L_x^{q'/2}(\mathbb{R}^d)$ . Then, for all  $\gamma_0 \in \mathfrak{S}^q$ , there exists  $\gamma \in C_t^0(\mathbb{R}, \mathfrak{S}^q)$  with  $\rho_\gamma \in L_{t,\text{loc}}^{q'/d}(\mathbb{R}, L_x^{q/(2-q)}(\mathbb{R}^d))$  solution to the equation*

$$\begin{cases} i \partial_t \gamma &= [-\Delta + w * \rho_\gamma, \gamma], \\ \gamma_{t=0} &= \gamma_0. \end{cases} \quad (4.A.100)$$

Furthermore, this solution is unique among all  $\gamma \in C_t^0(\mathbb{R}, \mathfrak{S}^q)$  satisfying the property that  $\rho_\gamma \in L_{t,\text{loc}}^{q'/d}(\mathbb{R}, L_x^{q/(2-q)}(\mathbb{R}^d))$ .

By a refined method, we also have information about the decay of these solutions for large times.

**Theorem 4.11.** *Let  $d \geq 2$ ,  $\gamma_0 \in \mathfrak{S}^{2d/(2d-1)}$  and  $w \in (L_x^{d/2} \cap L_x^d)(\mathbb{R}^d)$ . Then, there exists  $\varepsilon > 0$  such that if  $\|\gamma_0\|_{\mathfrak{S}^{2d/(2d-1)}} \leq \varepsilon$ , the density  $\rho_\gamma$  of the solution to the Hartree equation built in the previous theorem satisfies*

$$\rho_\gamma \in L_t^2 L_x^{d/(d-1)}(\mathbb{R} \times \mathbb{R}^d).$$

PROOF. Let  $T > 0$ . We develop the solution as a Dyson series as in Section 5

$$\rho_\gamma(t) = \sum_{n,m \geq 0} \rho \left[ e^{it\Delta} \mathcal{W}_V^{(n)}(t) \gamma_0 \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta} \right],$$



where  $V := w * \rho_\gamma$ . We estimate these terms by duality: let  $U \in L_t^2 L_x^d([0, T] \times \mathbb{R}^d)$ . Then,

$$\begin{aligned} \int_0^T \int_{\mathbb{R}^d} \rho \left[ e^{it\Delta} \mathcal{W}_V^{(n)}(t) \gamma_0 \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta} \right] (t, x) U(t, x) dt dx \\ = \int_0^T \text{Tr} \left[ e^{it\Delta} \mathcal{W}_V^{(n)}(t) \gamma_0 \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta} U(t, x) \right] dt \\ = \int_0^T \text{Tr} \left[ \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta} U(t, x) e^{it\Delta} \mathcal{W}_V^{(n)}(t) \gamma_0 \right] dt. \end{aligned}$$

Now by a straightforward generalization of [FLLS13, Thm. 3] we have the estimate

$$\left\| \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta} U(t, x) e^{it\Delta} \mathcal{W}_V^{(n)}(t) \right\|_{\mathfrak{S}^{2d}} \leq C \|U\|_{L_t^2 L_x^d} \frac{C^{n+m} \|V\|_{L_t^2 L_x^d}^{n+m}}{(n!)^{\frac{1}{2d}} (m!)^{\frac{1}{2d}}},$$

with  $C$  independent of  $T$ ,  $n$ , and  $m$ . Using that  $\gamma_0 \in \mathfrak{S}^{2d/(2d-1)}$  and the Hölder inequality, we deduce that

$$\left\| \rho \left[ e^{it\Delta} \mathcal{W}_V^{(n)}(t) \gamma_0 \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta} \right] \right\|_{L_t^2 L_x^{d/(d-1)}} \leq C \|\gamma_0\|_{\mathfrak{S}^{2d/(2d-1)}} \frac{C^{n+m} \|V\|_{L_t^2 L_x^d}^{n+m}}{(n!)^{\frac{1}{2d}} (m!)^{\frac{1}{2d}}}.$$

Using that  $\|V\|_{L_t^2 L_x^d} \leq C \|w\|_{L_x^{d/2}} \|\rho_\gamma\|_{L_t^2 L_x^{d/(d-1)}}$  leads to the estimate

$$\|\rho_\gamma\|_{L_t^2 L_x^{d/(d-1)}} \leq C \|\gamma_0\|_{\mathfrak{S}^{2d/(2d-1)}} \left[ 1 + \|\rho_\gamma\|_{L_t^2 L_x^{d/(d-1)}} + f_w \left( \|\rho_\gamma\|_{L_t^2 L_x^{d/(d-1)}} \right) \right],$$

where

$$f_w(z) = \sum_{n+m \geq 2} \frac{\left( C \|w\|_{L_x^{d/2}} z \right)^{n+m}}{(n!)^{\frac{1}{2d}} (m!)^{\frac{1}{2d}}}.$$

The function  $z \mapsto f_w(z)$  is a  $o(z^2)$  as  $z \rightarrow 0$ . In particular, for  $\|\gamma_0\|_{\mathfrak{S}^{2d/(2d-1)}} \leq \varepsilon$  with  $\varepsilon > 0$  small enough, there exists  $z_\varepsilon \geq 0$  such that

$$0 \leq z \leq z_\varepsilon \implies \frac{C \|\gamma_0\|_{\mathfrak{S}^{2d/(2d-1)}}}{1 - C \|\gamma_0\|_{\mathfrak{S}^{2d/(2d-1)}}} (1 + f_w(z)) \geq z$$

and

$$z_\varepsilon < z < z_\varepsilon + \eta \implies \frac{C \|\gamma_0\|_{\mathfrak{S}^{2d/(2d-1)}}}{1 - C \|\gamma_0\|_{\mathfrak{S}^{2d/(2d-1)}}} (1 + f_w(z)) < z$$

if  $\eta > 0$  is small enough. Since the map  $T \mapsto \|\rho_\gamma\|_{L_t^2 L_x^{d/(d-1)}([0, T] \times \mathbb{R}^d)}$  is continuous, this shows that

$$\|\rho_\gamma\|_{L_t^2 L_x^{d/(d-1)}([0, T] \times \mathbb{R}^d)} \leq z_\varepsilon$$

for all  $T \geq 0$  and hence  $\rho_\gamma \in L_t^2 L_x^{d/(d-1)}(\mathbb{R}_+ \times \mathbb{R}^d)$ . Repeating this argument for negative times shows the result.  $\square$

The same method allows to build solutions to the NLS version of our equation, in dimension 2:

**Theorem 4.12** (Global Well-Posedness for NLS in  $d = 2$ ). *There exists  $\varepsilon > 0$  such that for any  $\gamma_0 \in \mathfrak{S}^{4/3}(L^2(\mathbb{R}^2))$  with  $\|\gamma_0\|_{\mathfrak{S}^{4/3}} \leq \varepsilon$ , there exists a unique  $\gamma \in C_t^0(\mathbb{R}, \mathfrak{S}^{4/3})$  with  $\rho_\gamma \in L_{t,x}^2(\mathbb{R} \times \mathbb{R}^2)$  which is solution to the NLS equation*

$$\begin{cases} i \partial_t \gamma &= [-\Delta + \rho_\gamma, \gamma], \\ \gamma_{t=0} &= \gamma_0. \end{cases} \quad (4.A.101)$$

Notice that  $d = 2$  is the only dimension that we can attain with this method, since we need to put  $\rho_\gamma$  in  $L_t^p L_x^q$  with  $(p, q)$  admissible for both the Strichartz inequality and its dual, and furthermore verifies  $(p, q) = (p', q')$ . The only couple satisfying this condition is  $(p, q) = (2, 2)$  in  $d = 2$ . We did not have this issue for the Hartree equation since the convolution with  $w$  could always raise the exponent  $q$ . Let us also mention that scattering for these solutions follows immediately from the fact that  $\rho_\gamma \in L_t^p L_x^q(\mathbb{R} \times \mathbb{R}^d)$ , by [Yaj87, FLLS13].



## CHAPTER 5

# The Hartree equation for infinitely many particles.

## II. Dispersion and scattering in 2D

This chapter is the subject of a collaboration with Mathieu Lewin. Its preprint is available online, at *hal-00868782*.

### Abstract

We consider the nonlinear Hartree equation for an interacting gas containing infinitely many particles and we investigate the large-time stability of the stationary states of the form  $f(-\Delta)$ , describing an homogeneous Fermi gas. Under suitable assumptions on the interaction potential and on the momentum distribution  $f$ , we prove that the stationary state is asymptotically stable in dimension 2. More precisely, for any initial datum which is a small perturbation of  $f(-\Delta)$  in a Schatten space, the system weakly converges to the stationary state for large times.

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### 1. Introduction

This article is the continuation of the previous work [LS13b] where we considered the nonlinear Hartree equation for infinitely many particles (but the main result of the present article does not rely on [LS13b]).

The Hartree equation can be written using the formalism of density matrices as

$$\begin{cases} i\partial_t \gamma &= [-\Delta + w * \rho_\gamma, \gamma], \\ \gamma(0) &= \gamma_0. \end{cases} \quad (5.1.1)$$

Here  $\gamma(t)$  is the one-particle density matrix of the system, which is a bounded non-negative self-adjoint operator on  $L^2(\mathbb{R}^d)$  with  $d \geq 1$ , and  $\rho_\gamma(t, x) = \gamma(t, x, x)$  is the density of particles in the system at time  $t$ . On the other hand  $w$  is the interaction potential between the particles, which we assume to be smooth and fastly decaying at infinity.

The starting point of [LS13b] was the observation that (5.1.1) has many stationary states. Indeed, if  $f \in L^\infty(\mathbb{R}_+, \mathbb{R})$  is such that

$$\int_{\mathbb{R}^d} |f(|k|^2)| dk < +\infty,$$

then the operator

$$\gamma_f := f(-\Delta)$$

(the Fourier multiplier by  $k \mapsto f(|k|^2)$ ) is a bounded self-adjoint operator which commutes with  $-\Delta$  and whose density

$$\rho_{\gamma_f}(x) = (2\pi)^{-d} \int_{\mathbb{R}^d} f(|k|^2) dk, \quad \forall x \in \mathbb{R}^d,$$

is constant. Hence, for  $w \in L^1(\mathbb{R}^d)$ ,  $w * \rho_{\gamma_f}$  is also constant, and  $[w * \rho_{\gamma_f}, \gamma_f] = 0$ . Therefore  $\gamma(t) \equiv \gamma_f$  is a stationary solution to (5.1.1). The purpose of [LS13b] and of this article is to investigate the stability of these stationary states, under “local perturbations”. We do not necessarily think of small perturbations in norm, but we typically think of  $\gamma(0) - \gamma_f$  being compact.

The simplest choice is  $f \equiv 0$  which corresponds to the vacuum case. We are interested here in the case of  $f \neq 0$ , describing an infinite, homogeneous gas containing infinitely many particles and with positive constant density  $\rho_{\gamma_f} > 0$ . Four important physical examples are the

- *Fermi gas at zero temperature:*

$$\gamma_f = \mathbf{1}(-\Delta \leq \mu), \quad \mu > 0; \quad (5.1.2)$$

- *Fermi gas at positive temperature  $T > 0$ :*

$$\gamma_f = \frac{1}{e^{(-\Delta - \mu)/T} + 1}, \quad \mu \in \mathbb{R}; \quad (5.1.3)$$

- *Bose gas at positive temperature*  $T > 0$ :

$$\gamma_f = \frac{1}{e^{(-\Delta-\mu)/T} - 1}, \quad \mu < 0; \quad (5.1.4)$$

- *Boltzmann gas at positive temperature*  $T > 0$ :

$$\gamma_f = e^{(\Delta+\mu)/T}, \quad \mu \in \mathbb{R}. \quad (5.1.5)$$

In the density matrix formalism, the number of particles in the system is given by  $\text{Tr } \gamma$ . It is clear that  $\text{Tr } \gamma_f = +\infty$  in the previous examples since  $\gamma_f$  is a translation-invariant (hence non-compact) operator. Because they contain infinitely many particles, these systems also have an infinite energy. In [LS13b], we proved the existence of global solutions to the equation (5.1.1) in the defocusing case  $\widehat{w} \geq 0$ , when the initial datum  $\gamma_0$  has a finite *relative energy* counted with respect to the stationary states  $\gamma_f$  given in (5.1.2)–(5.1.5), in dimensions  $d = 1, 2, 3$ . We also proved the orbital stability of  $\gamma_f$ .

In this work, we are interested in the *asymptotic stability* of  $\gamma_f$ . As usual for Schrödinger equations, we cannot expect strong convergence in norm and we will rather prove that  $\gamma(t) \rightharpoonup \gamma_f$  weakly as  $t \rightarrow \pm\infty$ , if the initial datum  $\gamma_0$  is small enough. Physically, this means that a small defect added to the translation-invariant state  $\gamma_f$  disappears for large times due to dispersive effects, and the system locally relaxes towards the homogeneous gas. More precisely, we are able to describe the exact behavior of  $\gamma(t)$  for large times, by proving that

$$e^{-it\Delta}(\gamma(t) - \gamma_f)e^{it\Delta} \xrightarrow[t \rightarrow \pm\infty]{} Q_{\pm}$$

strongly in a Schatten space (hence for instance for the operator norm). This nonlinear scattering result means that the perturbation  $\gamma(t) - \gamma_f$  of the homogeneous gas evolves for large times as in the case of free particles:

$$\gamma(t) - \gamma_f \underset[t \rightarrow \pm\infty]{\simeq} e^{it\Delta} Q_{\pm} e^{-it\Delta} \underset[t \rightarrow \pm\infty]{\rightarrow} 0.$$

If  $f \equiv 0$  and  $\gamma_0 = |u_0\rangle\langle u_0|$  is a rank-one orthogonal projection, then (5.1.1) reduces to the well-known Hartree equation for one function

$$\begin{cases} i\partial_t u = (-\Delta + w * |u|^2)u, \\ u(0) = u_0. \end{cases} \quad (5.1.6)$$

There is a large literature about scattering for the nonlinear equation (5.1.6), see for instance [GV80, Str81, HT87, Moc89, GV00, Nak99]. The intuitive picture is that the nonlinear term is negligible for small  $u$ , since  $w * |u|^2 u$  is formally of order 3. It is important to realize that this intuition does not apply in the case  $f \neq 0$  considered in this paper. Indeed the nonlinear term is not small and it behaves linearly with respect to the small parameter  $\gamma - \gamma_f$ :

$$[w * \rho_{\gamma}, \gamma] = [w * \rho_{\gamma - \gamma_f}, \gamma] \simeq [w * \rho_{\gamma - \gamma_f}, \gamma_f] \neq 0. \quad (5.1.7)$$

One of the main purpose of this paper is to rigorously study the linear response of the homogeneous Hartree gas  $\gamma_f$  (the last term in (5.1.7)), which is a very important object in the physical literature, called the Lindhard function (see [Lin54] and [GV05, Chap. 4]). For a general  $f$ , our main result requires that the interaction potential  $w$  is small enough, in order to control the linear term. Under the natural assumption that  $f$  is strictly decreasing (as it is in the three physical examples (5.1.3)–(5.1.5)), the condition can be weakened in the defocusing case  $\widehat{w} \geq 0$ .

The paper is organized as follows. In the next section we state our main result and make several comments. In Section 3 we study the linear response in detail, before turning to the higher order terms in the expansion of the wave operator in Section 4. Apart from the linear response, our method requires to treat separately the next  $d-1$  terms of this expansion, in spacial dimension  $d$ . Even if all the other estimates are valid in any dimension, in this paper we only deal with the second order in dimension  $d = 2$ .

## 2. Main result

In the whole paper, we denote by  $\mathcal{B}(\mathfrak{H})$  the space of bounded operators on the Hilbert space  $\mathfrak{H}$ . The corresponding operator norm is  $\|A\|$ . We use the notation  $\mathfrak{S}^p(\mathfrak{H})$  for the Schatten space of all the compact operators  $A$  on  $\mathfrak{H}$  such that  $\text{Tr}|A|^p < \infty$ , with  $|A| = \sqrt{A^*A}$ , and use the norm  $\|A\|_{\mathfrak{S}^p(\mathfrak{H})} := (\text{Tr}|A|^p)^{1/p}$ . We refer to [Sim77] for the properties of Schatten spaces. The spaces  $\mathfrak{S}^2(\mathfrak{H})$  and  $\mathfrak{S}^1(\mathfrak{H})$  correspond to Hilbert-Schmidt and trace-class operators. We often use the shorthand notation  $\mathcal{B}$  and  $\mathfrak{S}^p$  when the Hilbert space  $\mathfrak{H}$  is clear from the context.

Our main result is the following.

**Theorem 5.1** (Dispersion and scattering in 2D). *Let  $f : \mathbb{R}_+ \rightarrow \mathbb{R}$  be such that*

$$\int_0^\infty (1+r^{\frac{k}{2}})|f^{(k)}(r)| dr < \infty \quad \text{for } k = 0, \dots, 4 \quad (5.2.8)$$

and  $\gamma_f := f(-\Delta)$ . Denote by  $\check{g}$  the Fourier inverse on  $\mathbb{R}^2$  of  $g(k) = f(|k|^2)$ . Let  $w \in W^{1,1}(\mathbb{R}^2)$  be such that

$$\|\check{g}\|_{L^1(\mathbb{R}^2)} \|\widehat{w}\|_{L^\infty(\mathbb{R}^2)} < 4\pi \quad (5.2.9)$$

or, if  $f' < 0$  a.e. on  $\mathbb{R}_+$ , such that

$$\max\left(\varepsilon_g \widehat{w}(0)_+, \|\check{g}\|_{L^1(\mathbb{R}^2)} \|(\widehat{w})_-\|_{L^\infty(\mathbb{R}^2)}\right) < 4\pi \quad (5.2.10)$$

where  $(\widehat{w})_-$  is the negative part of  $\widehat{w}$  and  $0 \leq \varepsilon_g \leq \|\check{g}\|_{L^1(\mathbb{R}^2)}$  is a constant depending only on  $g$  (defined later in Section 3).

Then, there exists a constant  $\varepsilon_0 > 0$  (depending only on  $w$  and  $f$ ) such that, for any  $\gamma_0 \in \gamma_f + \mathfrak{S}^{4/3}$  with

$$\|\gamma_0 - \gamma_f\|_{\mathfrak{S}^{4/3}} \leq \varepsilon_0,$$

there exists a unique  $\gamma \in \gamma_f + C_t^0(\mathbb{R}, \mathfrak{S}^2)$  solution to the Hartree equation (5.1.1) with initial datum  $\gamma_0$ , such that

$$\rho_\gamma - \rho_{\gamma_f} \in L_{t,x}^2(\mathbb{R} \times \mathbb{R}^2).$$

Furthermore,  $\gamma(t)$  scatters around  $\gamma_f$  at  $t = \pm\infty$ , in the sense that there exists  $Q_\pm \in \mathfrak{S}^4$  such that

$$\begin{aligned} \lim_{t \rightarrow \pm\infty} \|e^{-it\Delta}(\gamma(t) - \gamma_f)e^{it\Delta} - Q_\pm\|_{\mathfrak{S}^4} \\ = \lim_{t \rightarrow \pm\infty} \|\gamma(t) - \gamma_f - e^{it\Delta}Q_\pm e^{-it\Delta}\|_{\mathfrak{S}^4} = 0. \end{aligned} \quad (5.2.11)$$

Before explaining our strategy to prove Theorem 5.1, we make some comments.

First we notice that the gases at positive temperature (5.1.3), (5.1.4) and (5.1.5) are all covered by the theorem with the condition (5.2.10), since the corresponding  $f$  is smooth, strictly decreasing and exponentially decaying at infinity. Our result does not cover the Fermi gas at zero temperature (5.1.2), however. We show in Section 3 that its linear response is unbounded and it is a challenging task to better understand its dynamical stability.

The next remark concerns the assumption (5.2.9) which says that the interactions must be small or, equivalently, that the gas must contain few particles having a small momentum (if  $\check{g} \geq 0$ , then the condition can be written  $f(0) \|\widehat{w}\|_{L^\infty(\mathbb{R}^2)} < 2$  and hence  $f(|k|^2)$  must be small for small  $k$ ). Our method does not work without the condition (5.2.9) if no other information on  $w$  and  $f$  is provided. However, under the natural additional assumption that  $f$  is strictly decreasing, we can replace the condition (5.2.9) by the weaker condition (5.2.10). The latter says that the negative part of  $\widehat{w}$  and the value at zero of the positive part should be small (with a better constant for the latter). We will explain later where the condition (5.2.10) comes from, but we mention already that we are not able to deal with an arbitrary large potential  $\widehat{w}$  in a neighborhood of the origin, even in the defocusing case. We also recall that the focusing or defocusing character of our equation is governed by the sign of  $\widehat{w}$  and not of  $w$ , as it is for (5.1.6). This is seen from the sign of the nonlinear term

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y) \rho_{\gamma-\gamma_f}(x) \rho_{\gamma-\gamma_f}(y) dx dy = (2\pi)^{d/2} \int_{\mathbb{R}^d} \widehat{w}(k) |\widehat{\rho_{\gamma-\gamma_f}}(k)|^2 dk$$

which appears in the relative energy of the system (see [LS13b, Eq. (9)–(10)]).

Let us mention that our results hold for *small* initial data, where the smallness is not only qualitative (meaning that  $\gamma_0 - \gamma_f \in \mathfrak{S}^{4/3}$  for instance), but also quantitative since we need that  $\|\gamma_0 - \gamma_f\|_{\mathfrak{S}^{4/3}}$  be small enough. This is a well-known restriction, coming from our method of proof, based on a fixed point argument. The literature on nonlinear Schrödinger equations suggests that, in order to remove this smallness assumption, one would need some assumption on  $w$  like  $\widehat{w} \geq 0$ , as well as some



additional (almost) conservation laws [**Caz03**]. Our study of the linear response operator however indicates that the situation is involved and more information on the momentum distribution  $f$  is certainly also necessary.

We finally note that in our previous article [**LS13b**], we proved the existence of global solutions under the assumption that the initial state  $\gamma_0$  has a finite relative entropy with respect to  $\gamma_f$  (and for  $f$  being one of the physical examples (5.1.2)–(5.1.5)). By the Lieb-Thirring inequality (see [**FLLS11**, **FLLS12**] and [**LS13b**]), this implies that  $\rho_{\gamma(t)} - \rho_{\gamma_f} \in L_t^\infty(L_x^2)$ . By interpolation we therefore get that  $\rho_{\gamma(t)} - \rho_{\gamma_f} \in L_t^p(L_x^2)$  for every  $2 \leq p \leq \infty$ . This requires of course that the initial perturbation  $\gamma_0 - \gamma_f$  be small in  $\mathfrak{S}^{4/3}$ . Our method does not allow to replace this condition by the fact that  $\gamma_0$  has a small relative entropy with respect to  $\gamma_f$ .

We now explain our strategy for proving Theorem 5.1. The idea of the proof relies on a fixed point argument, in the spirit of [**LS13b**, Sec. 5]. If we can prove that  $\rho_\gamma - \rho_{\gamma_f} \in L_{t,x}^2(\mathbb{R}_+ \times \mathbb{R}^2)$ , then we deduce from [**Yaj87**, **FLLS13**] that there exists a family of unitary operators  $U_V(t) \in C_t^0(\mathbb{R}_+, \mathcal{B})$  on  $L^2(\mathbb{R}^2)$  such that

$$\gamma(t) = U_V(t)\gamma_0U_V(t)^*,$$

for all  $t \in \mathbb{R}_+$ . We furthermore have

$$U_V(t) = e^{it\Delta}\mathcal{W}_V(t),$$

where  $\mathcal{W}_V(t)$  is the wave operator. By iterating Duhamel's formula, the latter can be expanded in a series as

$$\mathcal{W}_V(t) = 1 + \sum_{n \geq 1} \mathcal{W}_V^{(n)}(t) \tag{5.2.12}$$

with

$$\begin{aligned} \mathcal{W}_V^{(n)}(t) := & (-i)^n \int_0^t dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_2} dt_1 \times \\ & \times e^{-it_n\Delta}V(t_n)e^{i(t_n-t_{n-1})\Delta} \cdots e^{i(t_2-t_1)\Delta}V(t_1)e^{it_1\Delta}. \end{aligned}$$

The idea is to find a solution to the nonlinear equation

$$\rho_Q(t) = \rho \left[ e^{it\Delta}\mathcal{W}_{w*\rho_Q}(t)(\gamma_f + Q_0)\mathcal{W}_{w*\rho_Q}(t)^*e^{-it\Delta} \right] - \rho_{\gamma_f}, \tag{5.2.13}$$

by a fixed point argument on the variable  $\rho_Q \in L_{t,x}^2(\mathbb{R} \times \mathbb{R}^2)$ , where  $Q := \gamma - \gamma_f$  and  $Q_0 = \gamma_0 - \gamma_f$ .

Inserting the expansion (5.2.12) of the wave operator  $\mathcal{W}_V$ , the nonlinear equation (5.2.14) may be written as

$$\rho_Q = \rho \left[ e^{it\Delta}Q_0e^{-it\Delta} \right] - \mathcal{L}(\rho_Q) + \mathcal{R}(\rho_Q), \tag{5.2.14}$$

where  $\mathcal{L}$  is linear and  $\mathcal{R}(\rho_Q)$  contains higher order terms. The sign convention for  $\mathcal{L}$  is motivated by the stationary case [FLLS12]. The linear operator  $\mathcal{L}$  can be written

$$\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2$$

where

$$\mathcal{L}_1(\rho_Q) = -\rho \left[ e^{it\Delta} (\mathcal{W}_{w*\rho_Q}^{(1)}(t)\gamma_f + \gamma_f \mathcal{W}_{w*\rho_Q}^{(1)}(t)^*) e^{-it\Delta} \right]$$

and

$$\mathcal{L}_2(\rho_Q) = -\rho \left[ e^{it\Delta} (\mathcal{W}_{w*\rho_Q}^{(1)}(t)Q_0 + Q_0 \mathcal{W}_{w*\rho_Q}^{(1)}(t)^*) e^{-it\Delta} \right].$$

Note that  $\mathcal{L}_2$  depends on  $Q_0$  and it can always be controlled by adding suitable assumptions on  $Q_0$ . On the other hand, the other linear operator  $\mathcal{L}_1$  does not depend on the studied solution, it only depends on the functions  $w$  and  $f$ .

In Section 3, we study the linear operator  $\mathcal{L}_1$  in detail, and we prove that it is a space-time Fourier multiplier of the form  $\widehat{w}(k)m_f(\omega, k)$  where  $m_f$  is a famous function in the physics literature called the *Lindhard function* [Lin54, Mih11, GV05]), which only depends on  $f$  and  $d$ . We particularly investigate when  $\mathcal{L}_1$  is bounded on  $L^p_{t,x}(\mathbb{R} \times \mathbb{R}^2)$  and we show it is the case when  $w$  and  $f$  are sufficiently smooth. For the Fermi sea (5.1.2), we prove that  $\mathcal{L}_1$  is unbounded on  $L^2_{t,x}$ .

The next step is to invert the linear part by rewriting the equation (5.2.14) in the form

$$\rho_Q = (1 + \mathcal{L})^{-1} \left( \rho \left[ e^{it\Delta} Q_0 e^{-it\Delta} \right] + \mathcal{R}(\rho_Q) \right) \tag{5.2.15}$$

and to apply a fixed point method. In the time-independent case, a similar technique was used for the Dirac sea in [HLS05a]. In order to be able to invert the Fourier multiplier  $\mathcal{L}_1$ , we need that

$$\boxed{\min_{(\omega,k) \in \mathbb{R} \times \mathbb{R}^2} |\widehat{w}(k)m_f(\omega, k) + 1| > 0.} \tag{5.2.16}$$

Then  $1 + \mathcal{L} = 1 + \mathcal{L}_1 + \mathcal{L}_2$  is invertible if  $Q_0$  is small enough. In Section 3 we prove the simple estimate

$$|m_f(\omega, k)| \leq (4\pi)^{-1} \|\check{g}\|_{L^1(\mathbb{R}^2)}$$

and this leads to our condition (5.2.9). If  $f$  is strictly decreasing, then we are able to prove that the imaginary part of  $m_f(k, \omega)$  is never 0 for  $k \neq 0$  or  $\omega \neq 0$ . Since  $m_f(\omega, k)$  has a fixed sign for  $\omega = 0$  and  $k = 0$ , everything boils down to investigating the properties of  $m_f$  at  $(\omega, k) = (0, 0)$ . At this point  $m_f$  will usually not be continuous, and it can take both positive and negative values. We have

$$\limsup_{(\omega,k) \rightarrow (0,0)} \Re m_f(\omega, k) = (4\pi)^{-1} \|\check{g}\|_{L^1(\mathbb{R}^2)}$$

and we denote

$$\liminf_{(\omega,k) \rightarrow (0,0)} \Re m_f(\omega, k) := -(4\pi)^{-1} \varepsilon_g,$$

leading to our condition (5.2.10). It is well-known in the physics literature that the imaginary part of the Lindhard function plays a crucial role in the dynamics of the homogeneous Fermi gas. In our rigorous analysis it is used to invert the linear response operator outside of the origin. The behavior of  $m_f(\omega, k)$  for  $(\omega, k) \rightarrow (0, 0)$  is however involved and  $1 + \mathcal{L}_1$  is not invertible if  $\widehat{w}(0) > 4\pi/\varepsilon_g$  or  $\widehat{w}(0) < -4\pi/\|\check{g}\|_{L^1(\mathbb{R}^2)}$ .

For the Fermi gas at zero temperature (5.1.2) we will prove that the minimum in (5.2.16) is always zero, except when  $\widehat{w}$  vanishes sufficiently fast at the origin, this means that  $1 + \mathcal{L}_1$  is never invertible. It is an interesting open question to understand the asymptotic stability of the Fermi sea.

Once the linear response  $\mathcal{L}$  has been inverted, it remains to study the zeroth order term  $\rho[e^{it\Delta}Q_0e^{-it\Delta}]$  and the higher order terms contained in  $\mathcal{R}(\rho_Q)$ . At this step we use a recent Strichartz estimate in Schatten spaces which is due to Frank, Lieb, Seiringer and the first author.

**Theorem 5.2** (Strichartz estimate on wave operator [FLLS13, Thm 3]). *Let  $d \geq 1$ ,  $1 + d/2 \leq q < \infty$ , and  $p$  such that  $2/p + d/q = 2$ . Let also  $0 < \varepsilon < 1/p$ . Then, there exists  $C = C(d, p, \varepsilon) > 0$  such that for any  $V \in L_t^p(\mathbb{R}, L_x^q(\mathbb{R}^d))$  and any  $t \in \mathbb{R}$ , we have the estimates*

$$\left\| \mathcal{W}_V^{(1)}(t) \right\|_{\mathfrak{S}^{2q}} \leq C \|V\|_{L_t^p L_x^q} \quad (5.2.17)$$

and

$$\forall n \geq 2, \quad \left\| \mathcal{W}_V^{(n)}(t) \right\|_{\mathfrak{S}^{2\lceil \frac{d}{n} \rceil}} \leq \frac{C^n}{(n!)^{\frac{1}{p}-\varepsilon}} \|V\|_{L_t^p L_x^q}^n. \quad (5.2.18)$$

The estimate (5.2.17) is the dual version of

$$\left\| \rho_{e^{it\Delta} A e^{-it\Delta}} \right\|_{L^p(\mathbb{R}, L^q(\mathbb{R}^d))} \leq C \|A\|_{\mathfrak{S}^{\frac{2q}{q+1}}}, \quad (5.2.19)$$

for any  $(p, q)$  such that  $2/p + d/q = d$  and  $1 \leq q \leq 1 + 2/d$ , see [FLLS13, Thm. 1]. The estimate (5.2.19) is useful to deal with the first order term involving  $Q_0$  in (5.2.15), leading to the natural condition that  $Q_0 \in \mathfrak{S}^{4/3}$  in dimension  $d = 2$  with  $p = q = 2$ .

In dimension  $d$ , it seems natural to prove that  $\rho_Q \in L_{t,x}^{1+2/d}(\mathbb{R} \times \mathbb{R}^d)$ . The estimate (5.2.18) turns out to be enough to deal with the terms of order  $\geq d+1$  but it does not seem to help for the terms of order  $\leq d$ , because the wave operators  $\mathcal{W}_V^{(n)}$  with small  $n$  belong to a Schatten space with a too large exponent. Apart from the linear response, we are therefore left with  $d-1$  terms for which a more detailed computation is necessary. We are not able to do this in any dimension (the number of such terms grows with  $d$ ), but we can deal with the second order term in dimension  $d = 2$ ,

$$\rho \left[ e^{it\Delta} (\mathcal{W}_{w^* \rho_Q}^{(2)}(t) \gamma_f + \mathcal{W}_{w^* \rho_Q}^{(1)}(t) \gamma_f \mathcal{W}_{w^* \rho_Q}^{(1)}(t)^* + \gamma_f \mathcal{W}_{w^* \rho_Q}^{(2)}(t)^*) e^{-it\Delta} \right],$$

which then finishes the proof of the theorem in this case. The second-order term is the topic of Section 5.

Even if our final result only covers the case  $d = 2$ , we have several estimates in any dimension  $d \geq 2$ . With the results of this paper, only the terms of order 2 to  $d$  remain to be studied to obtain a result similar to Theorem 5.1 (with  $\rho_\gamma - \rho_{\gamma_f} \in L_{t,x}^{1+2/d}(\mathbb{R} \times \mathbb{R}^d)$ ) in dimensions  $d \geq 3$ .

### 3. Linear response theory

**3.1. Computation of the linear response operator.** As we have explained before, we deal here with the linear response  $\mathcal{L}_1$  associated with the homogeneous state  $\gamma_f$ . The first order in Duhamel's formula is defined by

$$Q_1(t) := -i \int_0^t e^{i(t-t')\Delta} [w * \rho_{Q(t')}, \gamma_f] e^{i(t'-t)\Delta} dt'.$$

We see that it is a linear expression in  $\rho_Q$ , and we compute its density as a function of  $\rho_Q$ .

**Proposition 5.1** (Uniform bound on  $\mathcal{L}_1$ ). *Let  $d \geq 1$ ,  $f \in L^\infty(\mathbb{R}_+, \mathbb{R})$  such that  $\int_{\mathbb{R}^d} |f(k^2)| dk < +\infty$ , and  $w \in L^1(\mathbb{R}^d)$ . Then, the linear operator  $\mathcal{L}_1$  defined for all  $\varphi \in \mathcal{D}(\mathbb{R}_+ \times \mathbb{R}^d)$  by*

$$\mathcal{L}_1(\varphi)(t) := -\rho[Q_1(t)] = \rho \left[ i \int_0^t e^{i(t-t')\Delta} [w * \varphi(t'), \gamma_f] e^{i(t'-t)\Delta} dt' \right]$$

is a space-time Fourier multiplier by the kernel  $K^{(1)} = \widehat{w}(k) m_f(\omega, k)$ , where

$$\boxed{[\mathcal{F}_\omega^{-1} m_f](t, k) := 2\mathbf{1}_{t \geq 0} \sqrt{2\pi} \sin(t|k|^2) \check{g}(2tk)} \quad (5.3.20)$$

(we recall that  $g(k) := f(k^2)$  and that  $\check{g}$  is its Fourier inverse). This means that for all  $\varphi \in \mathcal{D}(\mathbb{R}_+ \times \mathbb{R}^d)$ , we have

$$\mathcal{F}_{t,x}[\mathcal{L}_1(\varphi)](\omega, k) = \widehat{w}(k) m_f(\omega, k) [\mathcal{F}_{t,x}\varphi](\omega, k), \quad \forall (\omega, k) \in \mathbb{R} \times \mathbb{R}^d$$

where  $\mathcal{F}_{t,x}$  is the space-time Fourier transform. Furthermore, if  $\int_0^\infty |x|^{2-d} |\check{g}(x)| dx < \infty$ , then  $m_f \in L_{\omega,k}^\infty(\mathbb{R} \times \mathbb{R}^d)$  and we have the explicit estimates

$$\|m_f\|_{L_{\omega,k}^\infty} \leq \frac{1}{2|\mathbb{S}^{d-1}|} \left( \int_{\mathbb{R}^d} \frac{|\check{g}(x)|}{|x|^{d-2}} dx \right) \quad (5.3.21)$$

and

$$\|\mathcal{L}_1\|_{L_{t,x}^2 \rightarrow L_{t,x}^2} \leq \frac{\|\widehat{w}\|_{L^\infty}}{2|\mathbb{S}^{d-1}|} \left( \int_{\mathbb{R}^d} \frac{|\check{g}(x)|}{|x|^{d-2}} dx \right). \quad (5.3.22)$$

PROOF. Let  $\varphi \in \mathcal{D}(\mathbb{R}_+ \times \mathbb{R}^d)$ . In order to compute  $\mathcal{L}(\varphi)$ , we use the relation

$$\int_0^\infty \text{Tr}[W(t, x) Q_1(t)] dt = \int_0^\infty \int_{\mathbb{R}^d} W(t, x) \rho_{Q_1}(t, x) dx dt,$$

valid for any function  $W \in \mathcal{D}(\mathbb{R}_+ \times \mathbb{R}^d)$ . This leads to

$$\begin{aligned} \int_0^\infty \int_{\mathbb{R}^d} W(t, x) \rho_{Q_1}(t, x) dx dt &= \frac{-i}{(2\pi)^d} \int_0^\infty \int_0^t \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} e^{-2i(t-t')k \cdot \ell} \times \\ &\quad \times \widehat{W}(t, -k) \widehat{V}(t', k) (g(\ell - k/2) - g(\ell + k/2)) d\ell dk dt' dt, \end{aligned}$$

where  $g(k) := f(k^2)$  and  $V = w * \varphi$ . Computing the  $\ell$ -integral gives

$$\begin{aligned} \int_{\mathbb{R}^d} e^{-2i(t-t')k \cdot \ell} (g(\ell - k/2) - g(\ell + k/2)) d\ell \\ = -(2\pi)^{d/2} 2i \sin((t-t')|k|^2) \check{g}(2(t-t')k). \end{aligned}$$

Hence, using that  $\widehat{V} = (2\pi)^{d/2} \widehat{w} \widehat{\varphi}$ , we find that

$$\begin{aligned} \int_0^\infty \int_{\mathbb{R}^d} W(t, x) \rho_{Q_1}(t, x) dx dt \\ = -2 \int_0^\infty \int_0^t \int_{\mathbb{R}^d} \sin((t-t')|k|^2) \check{g}(2(t-t')k) \widehat{w}(k) \widehat{W}(t, -k) \widehat{\varphi}(t', k) dk dt' dt. \end{aligned}$$

Since  $g$  is radial, then  $\check{g}$  is also radial and we have

$$\begin{aligned} |m_f(\omega, k)| &\leq 2 \int_0^\infty |\sin(t|k|^2)| |\check{g}(2t|k|)| dt \\ &\leq 2 \int_0^\infty \frac{|\sin(t|k|)|}{|k|} |\check{g}(2t)| dt \\ &\leq \frac{1}{2} \int_0^\infty r |\check{g}(r)| dr. \end{aligned}$$

This ends the proof of the proposition.  $\square$

We now make several remarks about the previous result.

First, the physical examples for  $g$  are

$$g(k) = \begin{cases} \mathbf{1}(|k|^2 \leq \mu), & \mu > 0, \\ e^{-(|k|^2 - \mu)/T}, & T > 0, \mu \in \mathbb{R}, \\ \frac{1}{e^{(|k|^2 - \mu)/T} + 1}, & T > 0, \mu \in \mathbb{R}, \\ \frac{1}{e^{(|k|^2 - \mu)/T} - 1}, & T > 0, \mu < 0. \end{cases}$$

In the last three choices,  $g$  is a Schwartz function hence  $\check{g} \in L^1(\mathbb{R}^d)$ . For the first choice of  $g$  (Fermi sea at zero temperature), we have  $\check{g}(r) \sim r^{-1} \sin r$ , which obviously does not verify  $r\check{g}(r) \in L^1(0, +\infty)$ .

Then, we remark that (5.3.21) is optimal without more assumptions on  $f$ . Indeed, for  $\omega = 0$  and small  $k$  we find

$$m_f(0, k) = 2 \int_0^\infty \sin(t|k|^2) \check{g}(2tk) dt$$

$$\xrightarrow{k \rightarrow 0} \frac{1}{2} \int_0^\infty r \check{g}(r) dr = \frac{1}{2|\mathbb{S}^{d-1}|} \int_{\mathbb{R}^d} \frac{\check{g}(x)}{|x|^{d-2}} dx.$$

We conclude that (5.3.21) is optimal if  $\check{g}$  has a constant sign (for instance  $f$  is decreasing, as in the physical examples (5.1.3)–(5.1.5)). Similarly, (5.3.22) is optimal if both  $\check{g}$  and  $w$  have a constant sign (then  $|\widehat{w}(0)| = \|\widehat{w}\|_{L^\infty}$ ).

In general, the function  $m_f$  is complex-valued and it is not an easy task to determine when  $\widehat{w}(k)m_f(\omega, k)$  stays far from  $-1$ . Since the stationary linear response is real,  $\Im m_f(0, k) \equiv 0$ , the condition should at least involve the maximum or the minimum of  $m_f$  on the set  $\{\omega = 0\}$ , depending on the sign of  $\widehat{w}$ . Even if the function  $m_f$  is bounded on  $\mathbb{R} \times \mathbb{R}^d$  by (5.3.21), it will usually not be continuous at the point  $(0, 0)$ . Under the additional condition that  $f$  is strictly decreasing, we are able to prove that

$$\{\Im m_f(\omega, k) = 0\} = \{\omega = 0\} \cup \{k = 0\}$$

and this can be used to replace the assumption on  $\widehat{w}$  by one on  $(\widehat{w})_-$  and  $\widehat{w}(0)_+$ . In order to explain this, we first compute  $m_f$  in the case of a Fermi gas at zero temperature,  $f(k^2) = \mathbb{1}(|k|^2 \leq \mu)$ .

**Proposition 5.2** (Linear response at zero temperature). *Let  $d \geq 1$  and  $\mu > 0$ . Then, for the Fermi sea at zero temperature  $\gamma_f = \mathbb{1}(-\Delta \leq \mu)$ , the corresponding Fourier multiplier  $m_f(\omega, k) := m_d^F(\mu, \omega, k)$  of the linear response operator in dimension  $d$  is given by*

$$m_1^F(\mu, \omega, k) = \frac{1}{2\sqrt{2\pi}|k|} \log \left| \frac{(|k|^2 + 2|k|\sqrt{\mu})^2 - \omega^2}{(|k|^2 - 2|k|\sqrt{\mu})^2 - \omega^2} \right|$$

$$+ i \frac{\sqrt{\pi}}{2\sqrt{2}|k|} \left\{ \mathbb{1}(|\omega + |k|^2| \leq 2\sqrt{\mu}|k|) - \mathbb{1}(|\omega - |k|^2| \leq 2\sqrt{\mu}|k|) \right\} \quad (5.3.23)$$

for  $d = 1$ , by

$$m_2^F(\mu, \omega, k) = \frac{1}{4} \left\{ 2 - \frac{\operatorname{sgn}(|k|^2 + \omega)}{|k|^2} \left( (|k|^2 + \omega)^2 - 4\mu|k|^2 \right)_+^{\frac{1}{2}} \right.$$

$$\left. - \frac{\operatorname{sgn}(|k|^2 - \omega)}{|k|^2} \left( (|k|^2 - \omega)^2 - 4\mu|k|^2 \right)_+^{\frac{1}{2}} \right\}$$

$$+ i \frac{1}{2|k|^2} \left\{ \left( (|k|^2 + \omega)^2 - 4\mu|k|^2 \right)_-^{\frac{1}{2}} - \left( (|k|^2 - \omega)^2 - 4\mu|k|^2 \right)_-^{\frac{1}{2}} \right\}. \quad (5.3.24)$$

for  $d = 2$ , and by

$$\begin{aligned} m_d^{\text{F}}(\mu, \omega, k) &= \frac{|\mathbb{S}^{d-2}| \mu^{\frac{d-1}{2}}}{(2\pi)^{\frac{d-1}{2}}} \int_0^1 m_1^{\text{F}}(\mu(1-r^2), \omega, k) r^{d-2} dr, \quad \text{for } d \geq 2, \\ &= \frac{|\mathbb{S}^{d-3}| \mu^{\frac{d-2}{2}}}{(2\pi)^{\frac{d-2}{2}}} \int_0^1 m_2^{\text{F}}(\mu(1-r^2), \omega, k) r^{d-3} dr, \quad \text{for } d \geq 3. \end{aligned} \quad (5.3.25)$$

The formula for  $m_d^{\text{F}}$  is well known in the physics literature (see [Lin54], [Mih11] and [GV05, Chap. 4]). It is also possible to derive an explicit expression for  $m_3^{\text{F}}(\mu, \omega, k)$ , see [GV05, Chap. 4]. We remark that  $m_d^{\text{F}}(\mu, 0, k)$  coincides with the time-independent linear response computed in [FLLS12, Thm 2.5].

From the formulas we see that the real part of  $m_d^{\text{F}}$  can have both signs. It is always positive for  $\omega = 0$  and it can take negative values for  $\omega \neq 0$ . For instance, in dimension  $d = 2$ , on the curve  $\omega = |k|^2 + 2\sqrt{\mu}|k|$  the imaginary part vanishes and we get

$$m_2^{\text{F}}(\mu, |k|^2 + 2\sqrt{\mu}|k|, k) = \frac{1}{2} \left( 1 - \sqrt{1 + \frac{2\sqrt{\mu}}{|k|}} \right) \xrightarrow[k \rightarrow 0]{} -\infty. \quad (5.3.26)$$

In particular, if  $\widehat{w}(k)/\sqrt{|k|} \rightarrow +\infty$  when  $k \rightarrow 0$ , then  $\widehat{w}(k)m_f(|k|^2 + 2\sqrt{\mu}|k|, k) \rightarrow -\infty$  when  $|k| \rightarrow 0$ . Since on the other hand  $\widehat{w}(k)m_f(|k|^2 + 2\sqrt{\mu}|k|, k) \rightarrow 0$  when  $|k| \rightarrow \infty$ , we conclude that the function must cross  $-1$ , and  $(1 + \mathcal{L}_1)^{-1}$  is not bounded.

An important feature of  $m_d^{\text{F}}$  which we are going to use in the positive temperature case, is that the imaginary part  $\Im m_d^{\text{F}}(\mu, \omega, k)$  has a constant sign on  $\{\omega > 0\}$  and on  $\{\omega < 0\}$ . Before we discuss this in detail, we provide the proof of the proposition.

PROOF. First, a calculation shows that the Fourier inverse  $\check{g}_1$  of the radial  $g$  in dimension  $d = 1$  is given by

$$\check{g}_1(\mu, x) = \sqrt{\frac{2}{\pi}} \frac{\sin(\sqrt{\mu}|x|)}{|x|}. \quad (5.3.27)$$

In dimension  $d \geq 2$  we can write

$$\begin{aligned} \check{g}_d(\mu, |x|) &= \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathbf{1}(|k|^2 \leq \mu) e^{ik \cdot x} \\ &= \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}} dk_1 \int_{\mathbb{R}^{d-1}} dk_{\perp} \mathbf{1}(|k_1|^2 \leq \mu - |k_{\perp}|^2) e^{ik_1|x|} \\ &= \frac{|\mathbb{S}^{d-2}| \mu^{\frac{d-1}{2}}}{(2\pi)^{d/2}} \int_{\mathbb{R}} dk_1 \int_0^1 \mathbf{1}(|k_1|^2 \leq \mu(1-r^2)) e^{ik_1|x|} r^{d-2} dr \\ &= \frac{|\mathbb{S}^{d-2}| \mu^{\frac{d-1}{2}}}{(2\pi)^{\frac{d-1}{2}}} \int_0^1 \check{g}_1(\mu(1-r^2), |x|) r^{d-2} dr \\ &= \frac{2|\mathbb{S}^{d-2}| \mu^{\frac{d-1}{2}}}{(2\pi)^{d/2} |x|} \int_0^1 \sin(\sqrt{\mu}|x|\sqrt{1-r^2}) r^{d-2} dr. \end{aligned} \quad (5.3.28)$$

Similarly, we have in dimension  $d \geq 3$

$$\check{g}_d(\mu, |x|) = \frac{|\mathbb{S}^{d-3}| \mu^{\frac{d-2}{2}}}{(2\pi)^{\frac{d-2}{2}}} \int_0^1 \check{g}_2(\mu(1-r^2), |x|) r^{d-3} dr. \tag{5.3.29}$$

Now we can compute the multiplier  $m_d^F(\mu, \omega, k)$  for  $d = 1, 2$ . We start with  $d = 1$  for which we have

$$[\mathcal{F}_\omega^{-1} m_{f,1}](t, k) = 4 \mathbb{1}_{t \geq 0} \frac{\sin(t|k|^2) \sin(2\sqrt{\mu t}|k|)}{2t|k|}.$$

There remains to compute the time Fourier transform. We use the formula valid for any  $a, b \in \mathbb{R}$ ,

$$\begin{aligned} \int_0^\infty \frac{\sin(at) \sin(bt)}{t} e^{-it\omega} dt &= \frac{1}{4} \log \left| \frac{(a+b)^2 - \omega^2}{(a-b)^2 - \omega^2} \right| \\ &+ i \frac{\pi}{8} (\operatorname{sgn}(a-b-\omega) - \operatorname{sgn}(a+b-\omega) + \operatorname{sgn}(a+b+\omega) - \operatorname{sgn}(a-b+\omega)), \end{aligned}$$

and obtain (5.3.23). To provide the more explicit expression in dimension 2, we use this time the formula

$$\forall a \in \mathbb{R}, \quad \frac{1}{a} \int_0^1 \log \frac{|a + 2\sqrt{1-r^2}|}{|a - 2\sqrt{1-r^2}|} dr = \frac{\pi}{2} - \frac{\pi}{2} \left( 1 - \frac{4}{a^2} \right)_+^{1/2},$$

which leads to the claimed form (5.3.24) of  $m_2^F(\mu, \omega, k)$ . □

Now we will use the imaginary part of  $m_d^F$  to show that  $1 + \mathcal{L}_1$  is invertible with bounded inverse when  $\widehat{w} \geq 0$  with  $\widehat{w}(0)$  not too large, and when  $f$  is strictly decreasing.

**Corollary 5.1** ( $1 + \mathcal{L}_1$  is always invertible in the defocusing case). *Let  $d \geq 1$  and  $f \in L^\infty(\mathbb{R}_+, \mathbb{R})$  such that  $\int_0^\infty (r^{d/2-1}|f(r)| + |f'(r)|) dr < \infty$  and  $f'(r) < 0$  for all  $r > 0$ . Assume furthermore that  $\int_{\mathbb{R}^d} |x|^{2-d} |\check{g}(x)| dx < \infty$  with  $g(k) = f(|k|^2)$ . If  $w \in L^1(\mathbb{R}^d)$  is an even function such that*

$$\|(\widehat{w})_-\|_{L^\infty} \left( \int_{\mathbb{R}^d} \frac{|\check{g}(x)|}{|x|^{d-2}} dx \right) < 2|\mathbb{S}^{d-1}|, \tag{5.3.30}$$

and such that

$$\varepsilon_g \widehat{w}(0)_+ < 2|\mathbb{S}^{d-1}|, \quad \text{where} \quad \varepsilon_g := - \liminf_{(\omega, k) \rightarrow (0,0)} \frac{\Re m_f(\omega, k)}{2|\mathbb{S}^{d-1}|}, \tag{5.3.31}$$

then we have

$$\min_{(\omega, k) \in \mathbb{R} \times \mathbb{R}^d} |\widehat{w}(k) m_f(\omega, k) + 1| > 0$$

and  $(1 + \mathcal{L}_1)$  is invertible on  $L^2_{t,x}(\mathbb{R} \times \mathbb{R}^d)$  with bounded inverse.



PROOF. First we recall that  $m_f$  is uniformly bounded by (5.3.21). Therefore we only have to look at the set

$$A = \left\{ k \in \mathbb{R}^d : |\widehat{w}(k)| \geq \frac{1}{4|\mathbb{S}^{d-1}|} \left( \int_{\mathbb{R}^d} \frac{|\check{g}(x)|}{|x|^{d-2}} dx \right) \right\}.$$

On the complement of  $A$ , we have  $|\widehat{w} m_f + 1| \geq 1/2$ . Since  $\widehat{w}(k) \rightarrow 0$  when  $|k| \rightarrow \infty$ , then  $A$  is a compact set. Next, from the integral formula

$$f(|k|^2) = - \int_0^\infty \mathbf{1}(|k|^2 \leq s) f'(s) ds,$$

we infer that

$$m_f(\omega, k) = - \int_0^\infty m_d^F(s, \omega, k) f'(s) ds.$$

This integral representation can be used to prove that  $m_f$  is continuous on  $\mathbb{R} \times \mathbb{R}_+ \setminus \{(0, 0)\}$ . In general, the function  $m_f$  is not continuous at  $(0, 0)$ , however.

Since  $m_d^F(s, 0, k) \geq 0$  for all  $k$  and  $s \geq 0$ , we conclude that  $m_f(0, k) \geq 0$  and that

$$m_f(0, k) \widehat{w}(k) \geq -m_f(0, k) \widehat{w}(k)_- \geq -\|\widehat{w}_-\|_{L^\infty} \frac{1}{2|\mathbb{S}^{d-1}|} \left( \int_{\mathbb{R}^d} \frac{|\check{g}(x)|}{|x|^{d-2}} dx \right),$$

due to (5.3.21). In particular,

$$|m_f(0, k) \widehat{w}(k) + 1| \geq 1 - \|\widehat{w}_-\|_{L^\infty} \frac{1}{2|\mathbb{S}^{d-1}|} \left( \int_{\mathbb{R}^d} \frac{|\check{g}(x)|}{|x|^{d-2}} dx \right) > 0$$

due to our assumption on  $(\widehat{w})_-$ . Similarly, we have  $m_f(\omega, 0) = 0$  for all  $\omega \neq 0$  and therefore  $m_f(\omega, 0) \widehat{w}(0) + 1 = 1$  is invertible on  $\{k = 0, \omega \neq 0\}$ .

Now we look at  $k \neq 0$  and  $\omega > 0$  and we prove that the imaginary part of  $m_f$  never vanishes. We write the argument for  $d = 1$ , as it is very similar for  $d \geq 2$ , using the integral representation (5.3.24). We have

$$\begin{aligned} \Im m_f(\omega, k) &= \frac{\sqrt{\pi}}{2\sqrt{2}|k|} \times \\ &\times \int_0^\infty \left\{ \mathbf{1}((\omega - |k|^2)^2 \leq 4s|k|^2) - \mathbf{1}((\omega + |k|^2)^2 \leq 4s|k|^2) \right\} f'(s) ds. \end{aligned}$$

The difference of the two Heaviside functions is always  $\geq 0$  for  $\omega > 0$ . Furthermore, it is equal to 1 for all  $s$  in the interval

$$\frac{(\omega - |k|^2)^2}{4|k|^2} \leq s \leq \frac{(\omega + |k|^2)^2}{4|k|^2}.$$

Therefore we have

$$\Im m_f(\omega, k) \leq \frac{\sqrt{\pi}}{2\sqrt{2}|k|} \int_{\frac{(\omega - |k|^2)^2}{4|k|^2}}^{\frac{(\omega + |k|^2)^2}{4|k|^2}} f'(s) ds < 0$$

for all  $\omega > 0$  and  $k \neq 0$ . For  $\omega < 0$  we can simply use that  $\Im m_f(\omega, k) = -\Im m_f(-\omega, k)$  and this concludes the proof that the imaginary part does not vanish outside of  $\{k = 0\} \cup \{\omega = 0\}$ .

From the previous argument, we see that everything boils down to understanding the behavior of  $\Re m_f$  in a neighborhood of  $(0, 0)$ . At this point the maximal value is  $\frac{1}{2} \int_0^\infty r \check{g}(r) dr$  and the minimal value is  $-\varepsilon_g 2|\mathbb{S}^{d-1}|$  by definition, hence the result follows.  $\square$

We remark that

$$\Re m_f(\omega, k) \underset{\substack{k \rightarrow 0 \\ \omega \rightarrow 0}}{\simeq} \frac{1}{2} \int_0^\infty t \check{g}(t) \cos\left(\frac{\omega}{2|k|}t\right) dt$$

and therefore we can express

$$-\varepsilon_g := \frac{1}{4|\mathbb{S}^{d-1}|} \min_{a \in \mathbb{R}} \int_0^\infty t \check{g}(t) \cos(at) dt.$$

In the three physical cases (5.1.3)–(5.1.5), the function  $f$  satisfies the assumptions of the corollary, and therefore  $1 + \mathcal{L}_1$  is invertible with bounded inverse when  $w$  satisfies (5.3.30) and (5.3.31). Numerical computations show that  $\varepsilon_g$  is always  $> 0$ , but usually smaller than the maximum, by a factor 2 to 10. As an illustration, we display the function  $\Re m_f(\omega, k)$  for  $T = 100$  and  $\mu = 1$  in Figure 1 below.

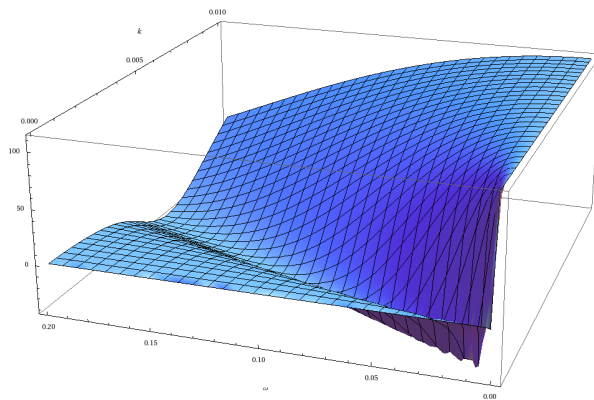


FIGURE 1. Plot of  $\Re m_f(\omega, k)$  in the fermionic case (5.1.3) for  $d = 2$ ,  $T = 100$  and  $\mu = 1$

**3.2. Boundedness of the linear response in  $L^p_{t,x}$ .** We have studied the boundedness of  $\mathcal{L}_1$  from  $L^2_{t,x}$  to  $L^2_{t,x}$ . This is useful in dimension  $d = 2$ , where the density  $\rho_Q$  naturally belongs to  $L^2_{t,x}$ . However, in other space dimensions, we would like to prove that  $\rho_Q$  belongs to  $L^{1+2/d}_{t,x}$  and hence, it makes sense to ask whether  $\mathcal{L}_1$  is bounded

from  $L^p_{t,x}$  to  $L^p_{t,x}$ . This is the topic of this section. The study of Fourier multipliers acting on  $L^p$  is a classical subject in harmonic analysis. We use theorems of Stein and Marcinkiewicz to infer the required boundedness.

**Proposition 5.3** (Boundedness of the linear response on  $L^p$ ). *Let  $w \in L^1(\mathbb{R}^d)$  be such that  $|x|^{d+2}w \in L^1(\mathbb{R}^d)$  and such that*

$$\left( \prod_{i \in I} |k_i|^2 \prod_{j \in J} \partial_{k_j} \right) \widehat{w}(k) \in L^\infty_k(\mathbb{R}^d), \quad \forall I \subset \{1, \dots, d\}, \quad \forall J \subset I.$$

Let also  $h : \mathbb{R}^d \rightarrow \mathbb{R}$  be an even function such that

$$\forall \alpha \in \mathbb{N}^d, \quad |\alpha| \leq d + 3, \quad \int_{\mathbb{R}^d} (1 + |k|^{d+4}) |\partial^\alpha h(k)| dk < +\infty$$

and

$$\left( \prod_{i \in I} \partial_{k_i} \right) h \in L^\infty_k(\mathbb{R}^d), \quad \text{for all } I \subset \{1, \dots, d\}.$$

Then the Fourier multiplier

$$\mathcal{F}_t \{ \mathbf{1}(t \geq 0) \sin(t|k|^2) h(2tk) \}$$

defines a bounded operator from  $L^p_{t,x}$  to itself, for every  $1 < p < \infty$ .

The conditions on  $h$  are fulfilled if for instance  $h$  is a Schwartz function, hence they are fulfilled for our physical examples (5.1.3)–(5.1.5), where we take  $h = \check{g}$ .

PROOF. We define

$$m_1(t, k) = \mathbf{1}(t \geq 1) \widehat{w}(k) \sin(t|k|^2) h(2tk)$$

and

$$m_2(t, k) = \mathbf{1}(0 \leq t \leq 1) \widehat{w}(k) \sin(t|k|^2) h(2tk),$$

and use a different criterion for these two multipliers.

To show that  $m_1$  defines a bounded operator on  $L^p$ , we use the criterion of Stein [Ste70, Thm. 1, II.2]. We write  $m_1(t, k) = \widehat{w}(k) \widetilde{m}_1(t, k)$ . We first prove estimates on  $\widetilde{m}_1$ , which then imply that  $m_1$  defines a bounded Fourier multiplier on  $L^p$  by Stein's theorem. Computing the inverse Fourier transform of  $\widetilde{m}_1$ , one has

$$M_1(t, x) := [\mathcal{F}_k^{-1} \widetilde{m}_1](t, x) = \mathbf{1}(t \geq 1) (2\pi)^{-d/2} \int_{\mathbb{R}^d} \sin(t|k|^2) h(2tk) e^{ix \cdot k} dk.$$

Then, we have

$$\nabla_x M_1(t, x) = \mathbf{1}(t \geq 1) \frac{(2\pi)^{-d/2}}{(2t)^{d+1}} i \int_{\mathbb{R}^d} kh(k) \sin\left(\frac{|k|^2}{4t}\right) e^{i\frac{x \cdot k}{2t}} dk. \quad (5.3.32)$$

From this formula, we see that for all  $(t, x)$ ,

$$t^{d+2} |\nabla_x M_1(t, x)| \leq C \int_{\mathbb{R}^d} |k|^3 |h(k)| dk. \quad (5.3.33)$$

Next, let  $1 \leq j \leq d$  and notice that

$$x_j^{d+2} e^{i \frac{x \cdot k}{2t}} = \frac{d^{d+2}}{dk_j^{d+2}} (2t)^{d+2} (-i)^{d+2} e^{i \frac{x \cdot k}{2t}},$$

and hence by an integration by parts we obtain

$$\begin{aligned} x_j^{d+2} \nabla_x M_1(t, x) &= \mathbf{1}(t \geq 1) (2\pi)^{-d/2} 2ti (-i)^{d+2} \int_{\mathbb{R}^d} \frac{d^{d+2}}{dk_j^{d+2}} \left[ kh(k) \sin\left(\frac{|k|^2}{4t}\right) \right] e^{i \frac{x \cdot k}{2t}} dk. \end{aligned}$$

When the  $k_j$ -derivative hits at least once  $\sin(|k|^2/4t)$ , one gains at least  $1/4t$  compensating the  $2t$  before the integral; the only term for which we have to prove that it is bounded in  $t$  is when all the  $k_j$ -derivatives hit the term  $kh(k)$ , which is

$$\mathbf{1}(t \geq 1) (2\pi)^{-d/2} 2it (-i)^{d+2} \int_{\mathbb{R}^d} \frac{d^{d+2}}{dk_j^{d+2}} [kh(k)] \sin\left(\frac{|k|^2}{4t}\right) e^{i \frac{x \cdot k}{2t}} dk.$$

It is also bounded since  $|\sin(|k|^2/4t)| \leq |k|^2/4t$ . We deduce that for all  $(t, x)$ ,

$$|x|^{d+2} |\nabla_x M_1(t, x)| \leq C \sup_{\substack{\alpha \in \mathbb{N}^d \\ |\alpha| \leq d+2}} \int_{\mathbb{R}^d} (1 + |k|^{d+3}) |\partial^\alpha h(k)| dk. \quad (5.3.34)$$

For the time derivative we use the form

$$M_1(t, x) = \mathbf{1}(t \geq 1) (2\pi)^{-d/2} \int_{\mathbb{R}^d} h(2tk) \sin(t|k|^2) \cos(x \cdot k) dk$$

to infer that for  $t \neq 1$ ,

$$\begin{aligned} \partial_t M_1(t, x) &= 2\mathbf{1}(t \geq 1) (2\pi)^{-d/2} \int_{\mathbb{R}^d} k \cdot \nabla_k h(2tk) \sin(t|k|^2) \cos(x \cdot k) dk \\ &\quad + \mathbf{1}(t \geq 1) (2\pi)^{-d/2} \int_{\mathbb{R}^d} |k|^2 h(2tk) \cos(t|k|^2) \cos(x \cdot k) dk \\ &= \frac{2\mathbf{1}(t \geq 1)}{(2t)^{d+1}} (2\pi)^{-d/2} \int_{\mathbb{R}^d} k \cdot \nabla_k h(k) \sin\left(\frac{|k|^2}{4t}\right) \cos\left(\frac{x \cdot k}{2t}\right) dk \\ &\quad + \frac{\mathbf{1}(t \geq 1)}{(2t)^{d+2}} (2\pi)^{-d/2} \int_{\mathbb{R}^d} |k|^2 h(k) \cos\left(\frac{|k|^2}{4t}\right) \cos\left(\frac{x \cdot k}{2t}\right) dk. \end{aligned} \quad (5.3.35)$$

By the same method as before, we infer

$$\|(t, x)\|^{d+2} |\partial_t M_1(t, x)| \leq C \sup_{\substack{\alpha \in \mathbb{N}^d \\ |\alpha| \leq d+3}} \int_{\mathbb{R}^d} (1 + |k|^{d+4}) |\partial^\alpha h(k)| dk. \quad (5.3.36)$$

Now let us go back to the multiplier  $m_1$ . We have

$$\mathcal{F}_x^{-1}m_1(t, x) = (2\pi)^{d/2}(w \star M_1(t, \cdot))(x),$$

and hence

$$\nabla_{t,x}\mathcal{F}_x^{-1}m_1(t, x) = (2\pi)^{d/2}(w \star \nabla_{t,x}M_1(t, \cdot))(x).$$

First we have

$$|t^{d+2}\nabla_{t,x}\mathcal{F}_x^{-1}m_1(t, x)| \leq C\|w\|_{L_x^1}\|t^{d+2}\nabla_{t,x}M_1(t, x)\|_{L_{t,x}^\infty},$$

which is finite thanks to (5.3.33), (5.3.34), and (5.3.36). Next,

$$\begin{aligned} |x|^{d+2}|\nabla_{t,x}\mathcal{F}_x^{-1}m_1(t, x)| &\leq C\|\cdot\|^{d+2}w\|_{L_x^1}\|\nabla_{t,x}M_1(t, x)\|_{L_{t,x}^\infty} \\ &\quad + C\|w\|_{L_x^1}\|x|^{d+2}\nabla_{t,x}M_1(t, x)\|_{L_{t,x}^\infty}. \end{aligned}$$

The second term is finite also from (5.3.33) and (5.3.34), while the first term is finite by the expressions (5.3.32) and (5.3.35). As a consequence, we can apply Stein's theorem to  $m_1$  and we deduce that the corresponding operator is bounded on  $L_{t,x}^p$  for all  $1 < p < \infty$ .

The multiplier  $m_2$  is treated differently. We show that

$$m_2 \in L_t^1(\mathbb{R}, \mathcal{B}(L_x^p \rightarrow L_x^p)),$$

which is enough to show that  $m_2$  defines a bounded operator on  $L_{t,x}^p$ . Indeed, for any  $\varphi \in L_{t,x}^p$ , define the Fourier multiplication operator  $T_{m_2}$  by

$$(T_{m_2}\varphi)(t, x) = \int_{\mathbb{R}} \mathcal{F}_x^{-1}[m_2(t-t', \cdot)(\mathcal{F}_x\varphi)(t', \cdot)](x) dt'.$$

Then, we have

$$\begin{aligned} \|T_{m_2}\varphi(t)\|_{L_x^p} &\leq \int_{\mathbb{R}} \|\mathcal{F}_x^{-1}[m_2(t-t', \cdot)(\mathcal{F}_x\varphi)(t', \cdot)]\|_{L_x^p} dt' \\ &\leq \int_{\mathbb{R}} \|m_2(t-t')\|_{\mathcal{B}(L_x^p \rightarrow L_x^p)} \|\varphi(t')\|_{L_x^p} dt', \end{aligned}$$

and hence

$$\|T_{m_2}\varphi\|_{L_{t,x}^p} \leq \|m_2\|_{L_t^1(\mathbb{R}, \mathcal{B}(L_x^p \rightarrow L_x^p))} \|\varphi\|_{L_{t,x}^p}.$$

Hence, let us show that  $\|m_2\|_{L_x^p \rightarrow L_x^p} \in L_t^1$ . We estimate  $\|m_2\|_{L_x^p \rightarrow L_x^p}$  by the Marcinkiewicz theorem [GA08, Cor. 5.2.5]. Namely, we have to show that for all  $1 \leq i_1, \dots, i_\ell \leq d$  all different indices, we have

$$k_{i_1} \cdots k_{i_\ell} \partial_{k_{i_1}} \cdots \partial_{k_{i_\ell}} m_2(t, k) \in L_k^\infty,$$

and if so the Marcinkiewicz theorem tells us that

$$\|m_2(t)\|_{L_x^p \rightarrow L_x^p} \leq C \sup_{i_1, \dots, i_\ell} \|k_{i_1} \cdots k_{i_\ell} \partial_{k_{i_1}} \cdots \partial_{k_{i_\ell}} m_2(t, k)\|_{L_k^\infty}.$$

A direct computation shows that

$$\begin{aligned} & |k_{i_1} \cdots k_{i_\ell} \partial_{k_{i_1}} \cdots \partial_{k_{i_\ell}} m_2(t, k)| \\ & \leq C \mathbf{1}_{0 \leq t \leq 1} \sum_{I \subset \{i_1, \dots, i_\ell\}} \sum_{J \subset I} |k_{i_1}|^2 \cdots |k_{i_\ell}|^2 |\partial_I \widehat{w}(k)| |(\partial_J h)(2tk)|, \end{aligned}$$

where we used the notation  $\partial_J h := \prod_{j \in J} \partial_{k_j} h$ . Hence,

$$\begin{aligned} & \|k_{i_1} \cdots k_{i_\ell} \partial_{k_{i_1}} \cdots \partial_{k_{i_\ell}} m_2(t, k)\|_{L_k^\infty} \\ & \leq C \mathbf{1}_{0 \leq t \leq 1} \sup_{I, J \subset \{i_1, \dots, i_\ell\}} \| |k_{i_1}|^2 \cdots |k_{i_\ell}|^2 |\partial_I \widehat{w}(k)| \|_{L_k^\infty} \| \partial_J h \|_{L_k^\infty}, \end{aligned}$$

which is obviously a  $L_t^1$ -function.  $\square$

#### 4. Higher order terms

In this section, we explain how to treat the higher order terms in (5.2.14). We recall the decomposition of the solution for all  $t \geq 0$ :

$$\rho_Q(t) = \rho \left[ e^{it\Delta} \mathcal{W}_{w^* \rho_Q}(t) (\gamma_f + Q_0) \mathcal{W}_{w^* \rho_Q}(t)^* e^{-it\Delta} \right] - \rho_{\gamma_f}.$$

We first estimate the terms involving  $Q_0$ , in dimension 2.

**Lemma 5.1.** *Let  $Q_0 \in \mathfrak{S}^{4/3}(L^2(\mathbb{R}^2))$  and  $V \in L_{t,x}^2(\mathbb{R}_+ \times \mathbb{R}^2)$ . Then, we have the following estimate for all  $n, m \geq 0$*

$$\left\| \rho \left[ e^{it\Delta} \mathcal{W}_V^{(n)}(t) Q_0 \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta} \right] \right\|_{L_{t,x}^2(\mathbb{R}_+ \times \mathbb{R}^2)} \leq C \|Q_0\|_{\mathfrak{S}^{4/3}} \frac{C^{n+m} \|V\|_{L_{t,x}^2}^{n+m}}{(n!)^{\frac{1}{4}} (m!)^{\frac{1}{4}}},$$

for some  $C > 0$  independent of  $Q_0$ ,  $n$ ,  $m$ , and  $V$ .

PROOF. Defining  $\mathcal{W}_V^{(0)}(t) := 1$ , for  $n, m \geq 0$ , the density of

$$e^{it\Delta} \mathcal{W}_V^{(n)}(t) Q_0 \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta}$$

is estimated by duality in the following fashion. Let  $U \in L_{t,x}^2(\mathbb{R}_+ \times \mathbb{R}^2)$ . The starting point is the formula

$$\begin{aligned} & \int_0^\infty \int_{\mathbb{R}^2} U(t, x) \rho \left[ e^{it\Delta} \mathcal{W}_V^{(n)}(t) Q_0 \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta} \right] (t, x) dx dt \\ & = \int_0^\infty \text{Tr} \left[ U(t, x) e^{it\Delta} \mathcal{W}_V^{(n)}(t) Q_0 \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta} \right] dt. \end{aligned}$$

By cyclicity of the trace, we have

$$\begin{aligned} & \text{Tr} \left[ U(t, x) e^{it\Delta} \mathcal{W}_V^{(n)}(t) Q_0 \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta} \right] \\ & = \text{Tr} \left[ \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta} U(t, x) e^{it\Delta} \mathcal{W}_V^{(n)}(t) Q_0 \right] \end{aligned}$$

A straightforward generalization of Theorem 5.2 shows that we have

$$\left\| \int_0^\infty \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta} U(t, x) e^{it\Delta} \mathcal{W}_V^{(n)}(t) dt \right\|_{\mathfrak{S}^4} \leq \|U\|_{L^2_{t,x}} \frac{C^n \|V\|_{L^2_{t,x}}^n}{(n!)^{1/4}} \frac{C^m \|V\|_{L^2_{t,x}}^m}{(m!)^{1/4}},$$

and hence using that  $Q_0 \in \mathfrak{S}^{4/3}$  and Hölder's inequality, we infer that

$$\left\| \rho \left[ e^{it\Delta} \mathcal{W}_V^{(n)}(t) Q_0 \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta} \right] \right\|_{L^2_{t,x}} \leq \|Q_0\|_{\mathfrak{S}^{4/3}} \frac{C^n \|V\|_{L^2_{t,x}}^n}{(n!)^{1/4}} \frac{C^m \|V\|_{L^2_{t,x}}^m}{(m!)^{1/4}}.$$

This concludes the proof of the lemma. □

When  $d \geq 2$ , the corresponding result is

**Lemma 5.2.** *Let  $d \geq 2$ ,  $Q_0 \in \mathfrak{S}^{\frac{d+2}{d+1}}(L^2(\mathbb{R}^d))$ ,  $1 < q \leq 1 + 2/d$  and  $p$  such that  $2/p + d/q = d$ . Let  $V \in L^p_t L^q_x(\mathbb{R}_+ \times \mathbb{R}^d)$ . Then, we have the following estimate for any  $n, m \geq 0$*

$$\left\| \rho \left[ e^{it\Delta} \mathcal{W}_V^{(n)}(t) Q_0 \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta} \right] \right\|_{L^p_t L^q_x(\mathbb{R}_+ \times \mathbb{R}^d)} \leq C \|Q_0\|_{\mathfrak{S}^{\frac{d+2}{d+1}}} \frac{C^{n+m} \|V\|_{L^p_t L^q_x}^{n+m}}{(n!)^{\frac{1}{2q'}} (m!)^{\frac{1}{2q'}}},$$

for some  $C > 0$  independent of  $Q_0, n, m$ , and  $V$ .

The proof follows the same lines as in  $d = 2$ , and relies on the following estimate for any  $n, m$

$$\begin{aligned} \left\| \int_0^\infty \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta} U(t, x) e^{it\Delta} \mathcal{W}_V^{(n)}(t) dt \right\|_{\mathfrak{S}^{d+2}} \\ \leq \|U\|_{L^p_t L^q_x} \frac{C^n \|V\|_{L^p_t L^q_x}^n}{(n!)^{\frac{1}{2q'}}} \frac{C^m \|V\|_{L^p_t L^q_x}^m}{(m!)^{\frac{1}{2q'}}}. \end{aligned}$$

We see that the terms involving  $Q_0$  can be treated in any dimension, provided that  $Q_0$  is in an adequate Schatten space. This is not the case for the terms involving  $\gamma_f$ , for which we can only deal with the higher orders.

**Lemma 5.3.** *Let  $d \geq 1$ ,  $g : \mathbb{R}^d \rightarrow \mathbb{R}$  such that  $\check{g} \in L^1(\mathbb{R}^d)$ ,  $1 < q \leq 1 + 2/d$  and  $p$  such that  $2/p + d/q = d$ . Let  $V \in L^p_t L^q_x(\mathbb{R}_+ \times \mathbb{R}^d)$ . Then, for all  $n, m$  such that*

$$n + m + 1 \geq 2q',$$

we have

$$\left\| \rho \left[ e^{it\Delta} \mathcal{W}_V^{(n)}(t) \gamma_f \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta} \right] \right\|_{L^p_t L^q_x} \leq C \|\check{g}\|_{L^1} \frac{C^n \|V\|_{L^p_t L^q_x}^n}{(n!)^{\frac{1}{2q'}}} \frac{C^m \|V\|_{L^p_t L^q_x}^m}{(m!)^{\frac{1}{2q'}}}.$$

where  $\gamma_f = g(-i\nabla)$ .

PROOF. We again argue by duality. Let  $U \in L_t^{p'} L_x^{q'}$ . Without loss of generality, we can assume that  $U, V \geq 0$ . Then, we evaluate

$$\begin{aligned} & \int_0^\infty \text{Tr} \left[ U(t, x) e^{it\Delta} \mathcal{W}_V^{(n)}(t) \gamma_f \mathcal{W}_V^{(m)}(t)^* e^{-it\Delta} \right] dt \\ &= (-i)^n i^m \int_0^\infty dt \int_{0 \leq s_1 \leq \dots \leq s_m \leq t} ds_1 \cdots ds_m \int_{0 \leq t_1 \leq \dots \leq t_n \leq t} dt_1 \cdots dt_n \times \\ & \quad \times \text{Tr} [V(s_1, x - 2is_1 \nabla) \cdots V(s_m, x - 2is_m \nabla) U(t, x - 2it \nabla) \times \\ & \quad \times V(t_n, x - 2it_n \nabla) \cdots V(t_1, x - 2it_1 \nabla) \gamma_f], \end{aligned}$$

where we used the relation

$$e^{-it\Delta} W(t, x) e^{it\Delta} = W(t, x - 2it \nabla).$$

In the spirit of [FLLS13], we gather the terms using the cyclicity of the trace as

$$\begin{aligned} & \text{Tr} [V(s_1, x - 2is_1 \nabla) \cdots V(s_m, x - 2is_m \nabla) U(t, x - 2it \nabla) \times \\ & \quad \times V(t_n, x - 2it_n \nabla) \cdots V(t_1, x - 2it_1 \nabla) \gamma_f] \\ &= \text{Tr} \left[ V(s_1, x - 2is_1 \nabla)^{\frac{1}{2}} V(s_2, x - 2is_2 \nabla)^{\frac{1}{2}} \cdots \times \right. \\ & \quad \left. V(s_m, x - 2is_m \nabla)^{\frac{1}{2}} U(t, x - 2it \nabla)^{\frac{1}{2}} U(t, x - 2it \nabla)^{\frac{1}{2}} V(t_n, x - 2it_n \nabla)^{\frac{1}{2}} \times \right. \\ & \quad \left. \times \cdots V(t_1, x - 2it_1 \nabla)^{\frac{1}{2}} \gamma_f V(s_1, x - 2is_1 \nabla)^{\frac{1}{2}} \right]. \quad (5.4.37) \end{aligned}$$

The first ingredient to estimate this trace is [FLLS13, Lemma 1], which states that

$$\|\varphi_1(\alpha x - i\beta \nabla) \varphi_2(\gamma x - i\delta \nabla)\|_{\mathfrak{S}^r} \leq \frac{\|\varphi_1\|_{L^r(\mathbb{R}^d)} \|\varphi_2\|_{L^r(\mathbb{R}^d)}}{(2\pi)^{\frac{d}{r}} |\alpha\delta - \beta\gamma|^{\frac{d}{r}}}, \quad \forall r \geq 2. \quad (5.4.38)$$

The second ingredient, to treat the term with  $\gamma_f$ , is a generalization of this inequality involving  $\gamma_f$ .

**Lemma 5.4.** *There exists a constant  $C > 0$  such that for all  $t, s \in \mathbb{R}$  we have*

$$\|\varphi_1(x + 2it \nabla) g(-i \nabla) \varphi_2(x + 2is \nabla)\|_{\mathfrak{S}^r} \leq \frac{\|\check{g}\|_{L^1(\mathbb{R}^d)} \|\varphi_1\|_{L^r(\mathbb{R}^d)} \|\varphi_2\|_{L^r(\mathbb{R}^d)}}{(2\pi)^{\frac{d}{2}} (2\pi)^{\frac{d}{r}} |t - s|^{\frac{d}{r}}} \quad (5.4.39)$$

for all  $r \geq 2$ .

We remark that (5.4.39) reduces to (5.4.38) when  $g = 1$  and  $\check{g} = (2\pi)^{d/2} \delta_0$ . We postpone the proof of this lemma, and use it to estimate (5.4.37) in the following way:

$$\begin{aligned} & |\text{Tr} [V(s_1, x - 2is_1 \nabla) \cdots V(s_m, x - 2is_m \nabla) U(t, x - 2it \nabla) \times \\ & \quad \times V(t_n, x - 2it_n \nabla) \cdots V(t_1, x - 2it_1 \nabla) \gamma_f]| \\ & \leq C \|\check{g}\|_{L^1} \frac{\|V(s_1)\|_{L^{q'}} \cdots \|V(s_m)\|_{L^{q'}} \|U(t)\|_{L^{q'}} \|V(t_n)\|_{L^{q'}} \|V(t_1)\|_{L^{q'}}}{|s_1 - t_1|^{\frac{d}{2q'}} \cdots |s_m - t|^{\frac{d}{2q'}} |t - t_n|^{\frac{d}{2q'}} \cdots |t_2 - t_1|^{\frac{d}{2q'}}}. \end{aligned}$$



Here, we have used the condition  $n + m + 1 \geq 2q'$  to ensure that the operator inside the trace is trace-class by Hölder's inequality. From this point the proof is identical to the proof of [FLLS13, Thm. 3].  $\square$

**PROOF OF LEMMA 5.4.** The inequality is immediate if  $r = \infty$ . Hence, by complex interpolation, we only have to prove it for  $r = 2$ . We have

$$\begin{aligned} & \|\varphi_1(t, x + 2it\nabla)g(-i\nabla)\varphi_2(s, x + 2is\nabla)\|_{\mathfrak{S}^2}^2 \\ &= \text{Tr} [\varphi_1(x)^2 e^{i(t-s)\Delta} g(-i\nabla) \varphi_2(x)^2 e^{i(s-t)\Delta} g(-i\nabla)] \\ &= \frac{(2\pi)^{-2d}}{|t-s|^d} \iint \varphi_1(x)^2 \left| \left( \check{g} * e^{-i\frac{|x|^2}{4(t-s)}} \right) (x-y) \right|^2 \varphi_2(y)^2 dx dy \\ &\leq \frac{(2\pi)^{-2d}}{|t-s|^d} \|\check{g}\|_{L^1}^2 \|\varphi_1\|_{L^2}^2 \|\varphi_2\|_{L^2}^2. \end{aligned}$$

$\square$

In dimension  $d$ , we want to prove that  $\rho_Q$  belongs to  $L_{t,x}^{1+2/d}$ , hence we consider  $q = 1 + 2/d$  and  $q' = 1 + d/2$ . The previous result estimates the terms of order  $n + m + 1 \geq d + 2$ , that is  $n + m \geq d + 1$ . The case  $n + m = 1$  corresponds exactly to the linear response studied in the previous section. In dimension  $d = 2$ , we see that we are still lacking the case  $n + m = 2$ , which is what we call the second order. The next section is devoted to this order. We are not able to treat the terms with  $1 < n + m \leq d$  in other dimensions.

## 5. Second order in 2D

The study of the linear response is not enough to prove dispersion for the Hartree equation in 2D. We also have to estimate the second order term, that we first compute explicitly in any dimension, and then study only in dimension 2.

**5.1. Exact computation in any dimension.** Define the second order term in the Duhamel expansion of  $Q(t)$ ,

$$Q_2(t) := (-i)^2 \int_0^t ds \int_0^s dt_1 e^{i(t-s)\Delta} [V(s), e^{i(s-t_1)\Delta} [V(t_1), \gamma_f] e^{i(t_1-s)\Delta}] e^{i(s-t)\Delta},$$

where we again used the notation  $V = w * \rho_Q$ . We compute explicitly its density. To do so, we let  $W \in \mathcal{D}(\mathbb{R}_+ \times \mathbb{R}^d)$  and use the relation

$$\int_0^\infty \int_{\mathbb{R}^d} W(t, x) \rho_{Q_2}(t, x) dx dt = \int_0^\infty \text{Tr}[W(t)Q_2(t)] dt.$$

For any  $(p, q) \in \mathbb{R}^d \times \mathbb{R}^d$  we have

$$\begin{aligned} \widehat{Q}_2(t, p, q) = & -\frac{1}{(2\pi)^d} \int_0^t ds \int_0^s dt_1 \int_{\mathbb{R}^d} dq_1 e^{i(t-s)(q^2-p^2)} \times \\ & \times \left[ \widehat{V}(s, p - q_1) e^{i(s-t_1)(q^2-q_1^2)} \widehat{V}(t_1, q_1 - q) (g(q) - g(q_1)) \right. \\ & \left. - \widehat{V}(s, q_1 - q) e^{i(s-t_1)(q_1^2-p^2)} \widehat{V}(t_1, p - q_1) (g(q_1) - g(p)) \right]. \end{aligned}$$

Using that

$$\text{Tr}[W(t)Q_2(t)] = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d \times \mathbb{R}^d} \widehat{W}(t, q - p) \widehat{Q}_2(t, p, q) dp dq,$$

we arrive at the formula

$$\begin{aligned} \int_0^\infty \int_{\mathbb{R}^d} W(t, x) \rho_{Q_2}(t, x) dx dt = & \int_0^\infty \int_0^\infty \int_0^\infty \int_{\mathbb{R}^d \times \mathbb{R}^d} dt ds dt_1 dk d\ell \times \\ & \times K^{(2)}(t - s, s - t_1; k, \ell) \widehat{W}(t, -k) \widehat{\rho}_Q(s, k - \ell) \widehat{\rho}_Q(t_1, \ell), \end{aligned}$$

with

$$\begin{aligned} K^{(2)}(t, s; k, \ell) \\ = \mathbf{1}_{t \geq 0} \mathbf{1}_{s \geq 0} \frac{4\widehat{w}(\ell)\widehat{w}(k - \ell)}{(2\pi)^{d/2}} \sin(tk \cdot (k - \ell)) \sin(\ell \cdot (tk + s\ell)) \check{g}(2(tk + s\ell)). \end{aligned}$$

## 5.2. Estimates in 2D.

**Proposition 5.4.** *Assume that  $g \in L^1(\mathbb{R}^2)$  is such that  $|x|^a |\check{g}(x)| \in L^\infty(\mathbb{R}^2)$  for some  $a > 3$ . Assume also that  $w$  is such that  $(1 + |k|^{1/2}) |\widehat{w}(k)| \in L^\infty(\mathbb{R}^2)$ . Then, if  $\rho_Q \in L^2_{t,x}(\mathbb{R} \times \mathbb{R}^2)$  we have*

$$\|\rho_{Q_2}\|_{L^2_{t,x}(\mathbb{R} \times \mathbb{R}^2)} \leq C \|(1 + |\cdot|^2)^{a/2} \check{g}\|_{L^\infty} \|(1 + |\cdot|^{1/2}) \widehat{w}\|_{L^\infty} \|\rho_Q\|_{L^2_{t,x}(\mathbb{R} \times \mathbb{R}^2)}^2, \quad (5.5.40)$$

for some constant  $C(g, w)$  only depending on  $g$  and  $w$ .

PROOF. First, we have the estimate

$$\left| \int_{\mathbb{R}^3} G(t_1 - t_2, t_2 - t_3) f_1(t_1) f_2(t_2) f_3(t_3) dt_1 dt_2 dt_3 \right| \leq C \|G\|_{L^2 L^1} \prod_{i=1}^3 \|f_i\|_{L^2},$$

for any  $G$ , and hence

$$\begin{aligned} \left| \int_{\mathbb{R}^3} K^{(2)}(t_1 - t_2, t_2 - t_3; k, \ell) \widehat{W}(t_1, -k) \widehat{\rho}_Q(t_2, k - \ell) \widehat{\rho}_Q(t_3, \ell) dt_1 dt_2 dt_3 \right| \\ \leq \|K^{(2)}(t, s; k, \ell)\|_{L^2_t L^1_s} \|\widehat{W}(\cdot, -k)\|_{L^2} \|\widehat{\rho}_Q(\cdot, k - \ell)\|_{L^2} \|\widehat{\rho}_Q(\cdot, \ell)\|_{L^2}. \end{aligned}$$

Let us thus estimate  $\|K^{(2)}(t, s; k, \ell)\|_{L_t^2 L_s^1}$ . To do so, we use  $|\sin(tk \cdot (k - \ell))| \leq 1$ ,  $|\sin(\ell \cdot (tk + s\ell))| \leq |\ell| |tk + s\ell|$  and get

$$\|K^{(2)}(t, s; k, \ell)\|_{L_t^2 L_s^1}^2 \leq \frac{16\widehat{w}(\ell)^2 \widehat{w}(k - \ell)^2}{(2\pi)^d} \ell^2 \int_{\mathbb{R}} dt \left| \int_{\mathbb{R}} ds |tk + s\ell| |\check{g}(2(tk + s\ell))| \right|^2.$$

We let

$$u = \ell s + t \frac{k \cdot \ell}{\ell} \quad \text{and} \quad v = \sqrt{k^2 - \frac{(k \cdot \ell)^2}{\ell^2}} t$$

and notice that

$$|tk + s\ell| = \left( \ell^2 \left( s + t \frac{k \cdot \ell}{\ell^2} \right)^2 + \left( k^2 - \frac{(k \cdot \ell)^2}{\ell^2} \right) t^2 \right)^{1/2} = \sqrt{u^2 + v^2}.$$

Since  $\check{g}$  is a radial function we find that

$$\begin{aligned} \ell^2 \int_{\mathbb{R}} dt \left| \int_{\mathbb{R}} ds |tk + s\ell| |\check{g}(2(tk + s\ell))| \right|^2 \\ = \frac{|\ell|}{(k^2 \ell^2 - (k \cdot \ell)^2)^{1/2}} \int_{\mathbb{R}} dv \left| \int_{\mathbb{R}} du \sqrt{u^2 + v^2} |\check{g}(2\sqrt{u^2 + v^2})| \right|^2. \end{aligned}$$

The double integral on the right is finite under some mild decay assumptions on  $\check{g}$ , for instance it is finite if  $|\check{g}(r)| \leq C(1 + r^2)^{-a/2}$ , for some  $a > 3$ . Noticing that  $(k^2 \ell^2 - (k \cdot \ell)^2)^{1/2} = |\det(k, \ell)|$ , we thus have

$$\begin{aligned} |\langle W, \rho_{Q_2} \rangle| &\leq C \|(1 + |\cdot|^2)^{a/2} \check{g}\|_{L^\infty} \int_{\mathbb{R}^{2d}} dk d\ell \times \\ &\quad \times \frac{\|\widehat{W}(\cdot, -k)\|_{L^2} \|\widehat{w}(k - \ell)\| \|\widehat{\rho}_Q(\cdot, k - \ell)\|_{L^2} |\ell|^{1/2} \|\widehat{w}(\ell)\| \|\widehat{\rho}_Q(\cdot, \ell)\|_{L^2}}{|\det(k, \ell)|^{1/2}}. \end{aligned}$$

We prove the following inequality of Hardy-Littlewood-Sobolev type:

**Lemma 5.5.** *For any functions  $f, g, h$  we have*

$$\left| \int_{\mathbb{R}^2 \times \mathbb{R}^2} \frac{f(k)g(k - \ell)h(\ell)}{|\det(k, \ell)|^{1/2}} dk d\ell \right| \leq C \|f\|_{L^2} \|g\|_{L^2} \|h\|_{L^2}. \quad (5.5.41)$$

PROOF. Since  $\det(k, \ell) = k_1 \ell_2 - k_2 \ell_1$ , we first fix  $k_1 \neq 0$ ,  $\ell_1 \neq 0$ ,  $k_1 \neq \ell_1$  and estimate

$$\begin{aligned} & \left| \int_{\mathbb{R}^2} \frac{f(k_1, k_2)g(k_1 - \ell_1, k_2 - \ell_2)h(\ell_1, \ell_2)}{|k_1 \ell_2 - k_2 \ell_1|^{1/2}} dk_2 d\ell_2 \right| \\ & \leq \left( \int_{\mathbb{R}^2} \frac{|f(k_1, k_2)|^{3/2}|g(k_1 - \ell_1, k_2 - \ell_2)|^{3/2}}{|k_1 \ell_2 - k_2 \ell_1|^{1/2}} dk_2 d\ell_2 \right)^{1/3} \times \\ & \quad \times \left( \int_{\mathbb{R}^2} \frac{|f(k_1, k_2)|^{3/2}|h(\ell_1, \ell_2)|^{3/2}}{|k_1 \ell_2 - k_2 \ell_1|^{1/2}} dk_2 d\ell_2 \right)^{1/3} \times \\ & \quad \times \left( \int_{\mathbb{R}^2} \frac{|g(k_1 - \ell_1, k_2 - \ell_2)|^{3/2}|h(\ell_1, \ell_2)|^{3/2}}{|k_1 \ell_2 - k_2 \ell_1|^{1/2}} dk_2 d\ell_2 \right)^{1/3}. \end{aligned}$$

We then have

$$\begin{aligned} & \int_{\mathbb{R}^2} \frac{|f(k_1, k_2)|^{3/2}|g(k_1 - \ell_1, k_2 - \ell_2)|^{3/2}}{|k_1 \ell_2 - k_2 \ell_1|^{1/2}} dk_2 d\ell_2 \\ & = \int_{\mathbb{R}^2} \frac{|f(k_1, k_2)|^{3/2}|g(k_1 - \ell_1, \ell_2)|^{3/2}}{|k_2(k_1 - \ell_1) - \ell_2 k_1|^{1/2}} dk_2 d\ell_2 \\ & = \frac{1}{|k_1||k_1 - \ell_1|} \int_{\mathbb{R}^2} \frac{|f(k_1, k_2/(k_1 - \ell_1))|^{3/2}|g(k_1 - \ell_1, \ell_2/k_1)|^{3/2}}{|k_2 - \ell_2|^{1/2}} dk_2 d\ell_2 \\ & \leq \frac{C}{|k_1||k_1 - \ell_1|} \|f(k_1, \cdot/(k_1 - \ell_1))\|_{L^2}^{3/2} \|g(k_1 - \ell_1, \cdot/k_1)\|_{L^2}^{3/2} \\ & \leq \frac{C}{|k_1|^{1/4}|k_1 - \ell_1|^{1/4}} \|f(k_1, \cdot)\|_{L^2}^{3/2} \|g(k_1 - \ell_1, \cdot)\|_{L^2}^{3/2}, \end{aligned}$$

and in the same fashion

$$\begin{aligned} & \int_{\mathbb{R}^2} \frac{|f(k_1, k_2)|^{3/2}|h(\ell_1, \ell_2)|^{3/2}}{|k_1 \ell_2 - k_2 \ell_1|^{1/2}} dk_2 d\ell_2 \leq \frac{C}{|k_1|^{1/4}|\ell_1|^{1/4}} \|f(k_1, \cdot)\|_{L^2}^{3/2} \|h(\ell_1, \cdot)\|_{L^2}^{3/2}, \\ & \int_{\mathbb{R}^2} \frac{|g(k_1 - \ell_1, k_2 - \ell_2)|^{3/2}|h(\ell_1, \ell_2)|^{3/2}}{|k_1 \ell_2 - k_2 \ell_1|^{1/2}} dk_2 d\ell_2 \\ & \leq \frac{C}{|\ell_1|^{1/4}|k_1 - \ell_1|^{1/4}} \|g(k_1 - \ell_1, \cdot)\|_{L^2}^{3/2} \|h(\ell_1, \cdot)\|_{L^2}^{3/2}. \end{aligned}$$

As a consequence, we have

$$\begin{aligned} & \left| \int_{\mathbb{R}^2} \frac{f(k_1, k_2)g(k_1 - \ell_1, k_2 - \ell_2)h(\ell_1, \ell_2)}{|k_1 \ell_2 - k_2 \ell_1|^{1/2}} dk_2 d\ell_2 \right| \\ & \leq C \frac{\|f(k_1, \cdot)\|_{L^2} \|g(k_1 - \ell_1, \cdot)\|_{L^2} \|h(\ell_1, \cdot)\|_{L^2}}{|k_1|^{1/6}|\ell_1|^{1/6}|k_1 - \ell_1|^{1/6}}. \end{aligned}$$

We now need a multilinear Hardy-Littlewood-Sobolev-type inequality. Integrating over  $(k_1, \ell_1)$  we find that

$$\begin{aligned}
& \left| \int_{\mathbb{R}^2 \times \mathbb{R}^2} \frac{f(k)g(k-\ell)h(\ell)}{|\det(k, \ell)|^{1/2}} dk d\ell \right| \\
& \leq C \int_{\mathbb{R}^2} \frac{\|f(k_1, \cdot)\|_{L^2} \|g(k_1 - \ell_1, \cdot)\|_{L^2} \|h(\ell_1, \cdot)\|_{L^2}}{|k_1|^{1/6} |\ell_1|^{1/6} |k_1 - \ell_1|^{1/6}} dk_1 d\ell_1 \\
& \leq C \left( \frac{\|g(k_1 - \ell_1, \cdot)\|_{L^2}^{3/2} \|h(\ell_1, \cdot)\|_{L^2}^{3/2}}{|k_1|^{1/2}} dk_1 d\ell_1 \right)^{1/3} \times \\
& \quad \times \left( \frac{\|f(k_1, \cdot)\|_{L^2}^{3/2} \|g(k_1 - \ell_1, \cdot)\|_{L^2}^{3/2}}{|\ell_1|^{1/2}} dk_1 d\ell_1 \right)^{1/3} \times \\
& \quad \times \left( \frac{\|f(k_1, \cdot)\|_{L^2}^{3/2} \|h(\ell_1, \cdot)\|_{L^2}^{3/2}}{|k_1 - \ell_1|^{1/2}} dk_1 d\ell_1 \right)^{1/3} \\
& \leq C \|f\|_{L^2} \|g\|_{L^2} \|h\|_{L^2}
\end{aligned}$$

where in the last line we have used the 2D Hardy-Littlewood-Sobolev inequality.  $\square$

From the lemma, we deduce that

$$|\langle W, \rho_{Q_2} \rangle| \leq C \|(1 + |\cdot|^2)^{a/2} \check{g}\|_{L^\infty} \|(1 + |\cdot|^{1/2}) \widehat{w}\|_{L^\infty} \|\rho_Q\|_{L^2_{t,x}},$$

which ends the proof of the proposition.  $\square$

## 6. Proof of the main theorem

PROOF OF THEOREM 5.1. Let  $T > 0$ . Assume also that  $\|Q_0\|_{\mathfrak{S}^{4/3}} \leq 1$ . We solve the equation

$$\begin{aligned}
\rho_Q(t) &= \rho \left[ e^{it\Delta} \mathcal{W}_{w^* \rho_Q}(t) (\gamma_f + Q_0) \mathcal{W}_{w^* \rho_Q}(t)^* e^{-it\Delta} \right] - \rho_{\gamma_f} \\
&= \rho \left[ e^{it\Delta} Q_0 e^{-it\Delta} \right] - \mathcal{L}(\rho_Q) + \mathcal{R}(\rho_Q)
\end{aligned}$$

by a fixed-point argument. Here  $\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2$  where  $\mathcal{L}_1$  was studied in Section 3 and

$$\mathcal{L}_2(\rho_Q) = -\rho \left[ e^{it\Delta} (\mathcal{W}_{w^* \rho_Q}^{(1)}(t) Q_0 + Q_0 \mathcal{W}_{w^* \rho_Q}^{(1)}(t)^*) e^{-it\Delta} \right].$$

As explained in Proposition 5.1 and in Corollary 5.1, under the assumption (5.2.9) (or (5.2.10) when  $f$  is strictly decreasing),  $(1 + \mathcal{L}_1)$  is invertible with bounded inverse on  $L^2_{t,x}$ . The operator  $1 + \mathcal{L} = 1 + \mathcal{L}_1 + \mathcal{L}_2$  is invertible with bounded inverse when

$$\|\mathcal{L}_2\| < \frac{1}{\|(1 + \mathcal{L}_1)^{-1}\|}.$$

By Lemma 5.1, we have

$$\|\mathcal{L}_2\| \leq C \|w\|_{L^1} \|Q_0\|_{\mathfrak{S}^{4/3}}$$

and therefore a sufficient condition can be expressed as

$$\|Q_0\|_{\mathfrak{S}^{4/3}} < \frac{1}{C \|w\|_{L^1} \|(1 + \mathcal{L}_1)^{-1}\|}.$$

Then we can write

$$\rho_Q(t) = (1 + \mathcal{L})^{-1} (\rho [e^{it\Delta} Q_0 e^{-it\Delta}] + \mathcal{R}(\rho_Q)).$$

For any  $\varphi \in L^2_{t,x}([0, T] \times \mathbb{R}^2)$ , define

$$F(\varphi)(t) = \rho [e^{it\Delta} Q_0 e^{-it\Delta}] + \mathcal{R}(\varphi).$$

We apply the Banach fixed-point theorem on the map  $(1 + \mathcal{L})^{-1}F$ . To do so, we expand  $F$  as

$$\begin{aligned} F(\varphi)(t) &= \rho [e^{it\Delta} Q_0 e^{-it\Delta}] + \sum_{n+m \geq 2} \rho [e^{it\Delta} \mathcal{W}_{w*\varphi}(t) Q_0 \mathcal{W}_{w*\varphi}(t)^* e^{-it\Delta}] \\ &\quad + \sum_{n+m=2} \rho [e^{it\Delta} \mathcal{W}_{w*\varphi}^{(n)}(t) \gamma_f \mathcal{W}_{w*\varphi}^{(m)}(t)^* e^{-it\Delta}] \\ &\quad + \sum_{n+m \geq 3} \rho [e^{it\Delta} \mathcal{W}_{w*\varphi}^{(n)}(t) \gamma_f \mathcal{W}_{w*\varphi}^{(m)}(t)^* e^{-it\Delta}]. \end{aligned}$$

By the Strichartz estimate (5.2.19), we have

$$\|\rho [e^{it\Delta} Q_0 e^{-it\Delta}]\|_{L^2_{t,x}} \leq C \|Q_0\|_{\mathfrak{S}^{4/3}}.$$

By Lemma 5.1, we have

$$\left\| \sum_{n+m \geq 2} \rho [e^{it\Delta} \mathcal{W}_{w*\varphi}(t) Q_0 \mathcal{W}_{w*\varphi}(t)^* e^{-it\Delta}] \right\|_{L^2_{t,x}} \leq C \|Q_0\|_{\mathfrak{S}^{4/3}} \sum_{n+m \geq 2} \frac{C^{n+m} \|w * \varphi\|_{L^2_{t,x}}^{n+m}}{(n!)^{\frac{1}{4}} (m!)^{\frac{1}{4}}}.$$

By Proposition 5.4, we have

$$\begin{aligned} &\left\| \sum_{n+m=2} \rho [e^{it\Delta} \mathcal{W}_{w*\varphi}^{(n)}(t) \gamma_f \mathcal{W}_{w*\varphi}^{(m)}(t)^* e^{-it\Delta}] \right\|_{L^2_{t,x}} \\ &\leq C \|(1 + |\cdot|^2)^{a/2} \check{g}\|_{L^\infty} \|(1 + |\cdot|^{1/2}) \widehat{w}\|_{L^\infty} \|\varphi\|_{L^2_{t,x}}^2. \end{aligned}$$

Finally, by Lemma 5.3 we have

$$\left\| \sum_{n+m \geq 3} \rho [e^{it\Delta} \mathcal{W}_{w*\varphi}^{(n)}(t) \gamma_f \mathcal{W}_{w*\varphi}^{(m)}(t)^* e^{-it\Delta}] \right\|_{L^2_{t,x}} \leq C \|\check{g}\|_{L^1} \sum_{n+m \geq 3} \frac{C^{n+m} \|w * \varphi\|_{L^2_{t,x}}^{n+m}}{(n!)^{\frac{1}{4}} (m!)^{\frac{1}{4}}}.$$

We deduce that for all  $\varphi \in L^2_{t,x}([0, T] \times \mathbb{R}^2)$ , we have the estimate

$$\|(1 + \mathcal{L})^{-1} F(\varphi)\|_{L^2_{t,x}} \leq C \|(1 + \mathcal{L})^{-1}\| \left( \|Q_0\|_{\mathfrak{S}^{4/3}} + A(\|\varphi\|_{L^2_{t,x}}) \right),$$

where we used the notation

$$A(z) = C \sum_{n+m \geq 2} \frac{C^{n+m} (\|w\|_{L^1} z)^{n+m}}{(n!)^{\frac{1}{4}} (m!)^{\frac{1}{4}}} + C \|(1 + |\cdot|^2)^{a/2} \check{g}\|_{L^\infty} \|(1 + |\cdot|^{1/2}) \widehat{w}\|_{L^\infty} z^2 \\ + C \|\check{g}\|_{L^1} \sum_{n+m \geq 3} \frac{C^{n+m} (\|w\|_{L^1} z)^{n+m}}{(n!)^{\frac{1}{4}} (m!)^{\frac{1}{4}}}.$$

We have  $A(z) = O(z^2)$  as  $z \rightarrow 0$ . As a consequence, there exists  $C_0, z_0 > 0$  only depending on  $\|w\|_{L^1}$ ,  $\|(1 + |\cdot|^2)^{a/2} \check{g}\|_{L^\infty}$ ,  $\|(1 + |\cdot|^{1/2}) \widehat{w}\|_{L^\infty}$ , and  $\|\check{g}\|_{L^1}$  such that

$$|A(z)| \leq C_0 z^2,$$

for all  $|z| \leq z_0$ . Choosing

$$R = \min \left( z_0, \frac{1}{2C_0 \|(1 + \mathcal{L})^{-1}\|} \right)$$

and

$$\|Q_0\|_{\mathfrak{S}^{4,3}} \leq \min \left( 1, \frac{R}{2C \|(1 + \mathcal{L})^{-1}\|} \right),$$

leads to the estimate

$$\|(1 + \mathcal{L})^{-1} F(\varphi)\|_{L_{t,x}^2} \leq R,$$

for all  $\|\varphi\|_{L_{t,x}^2} \leq R$ , independently of the maximal time  $T > 0$ . Similar estimates show that  $F$  is also a contraction on this ball, up to diminishing  $R$  if necessary. The Banach fixed point theorem shows that there exists a solution for any time  $T > 0$ , with a uniform estimate with respect to  $T$ . Having built this solution  $\varphi_0 \in L_{t,x}^2(\mathbb{R}_+ \times \mathbb{R}^2)$ , we define the operator  $\gamma$  as

$$\gamma(t) = e^{it\Delta} \mathcal{W}_{w*\varphi_0}(t) (\gamma_f + Q_0) \mathcal{W}_{w*\varphi_0}(t)^* e^{-it\Delta}.$$

We have  $\varphi_0 = \rho_\gamma - \rho_{\gamma_f}$  by definition. Uniqueness of solutions independently of whether they belong to the ball where we performed the fixed point argument follows from the same arguments as in the proof of [LS13b, Thm. 5].

From [FLLS13, Thm. 3] we know that  $\mathcal{W}_{w*\varphi_0} - 1 \in C_t^0(\mathbb{R}_+, \mathfrak{S}^4)$  and that  $\mathcal{W}_{w*\varphi_0} - 1$  admits a strong limit in  $\mathfrak{S}^4$  when  $t \rightarrow \infty$ , which gives that  $\gamma - \gamma_f \in C^0(\mathbb{R}_+, \mathfrak{S}^4)$  and our scattering result (5.2.11). Next, we remark that since  $w \in W^{1,1}(\mathbb{R}^2) \subset L^2(\mathbb{R}^2)$ , we have  $w*\varphi_0 \in L_t^2(L_x^\infty \cap L_x^2)$ . From [LS13b, Lemma 7] and the fact that  $g \in L^2(\mathbb{R}^2)$  (due to (5.2.8)), we deduce that  $(\mathcal{W}_{w*\varphi_0}(t) - 1)\gamma_f \in C^0(\mathbb{R}_+, \mathfrak{S}^2)$ . This now shows that  $\gamma - \gamma_f \in C^0(\mathbb{R}_+, \mathfrak{S}^2)$ . Of course, we can perform the same procedure for negative times and this finishes the proof of Theorem 5.1.  $\square$

## CHAPTER 6

### A family of monotone quantum relative entropies

This chapter is the subject of a collaboration with Mathieu Lewin. Its preprint is available online, at *arXiv:1309.4046*.

#### Abstract

We study here the elementary properties of the relative entropy  $\mathcal{H}(A, B) = \text{Tr}[\varphi(A) - \varphi(B) - \varphi'(B)(A - B)]$  for  $\varphi$  a convex function and  $A, B$  bounded self-adjoint operators. In particular, we prove that this relative entropy is monotone if and only if  $\varphi'$  is operator monotone. We use this to appropriately define  $\mathcal{H}(A, B)$  in infinite dimension.

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In this paper we introduce a relative entropy  $\mathcal{H}(A, B)$  of two bounded operators  $A$  and  $B$  on a Hilbert space and discuss its elementary properties. Our relative entropy  $\mathcal{H}(A, B)$  could be useful in many practical situations including quantum information theory. In a separate work [LS13b], we will use it to discuss the orbital stability of certain stationary states for the Hartree equation of an interacting gas containing infinitely many quantum particles.

For simplicity we work on the interval  $I = [0, 1]$  but all our results can be generalized to any finite interval. We consider two  $N \times N$  hermitian matrices  $A, B$  whose spectrum is a subset of  $I$ . For  $\varphi \in C^0([0, 1], \mathbb{R}) \cap C^1((0, 1), \mathbb{R})$  a *convex* function, we introduce the following relative entropy<sup>1</sup>

$$\mathcal{H}(A, B) = \text{Tr} \left( \varphi(A) - \varphi(B) - \varphi'(B)(A - B) \right). \quad (6.0.1)$$

We remind the reader of Klein's lemma.

**Lemma 6.1** (Klein [OP93, Prop. 3.16], [Rue99, Thm 2.5.2]). *If  $f_k, g_k : [a, b] \rightarrow \mathbb{R}$  are  $K$  measurable functions such that  $\sum_{k=1}^K f_k(x)g_k(y) \geq 0$  for all  $x, y \in [a, b]$ , then we have  $\sum_{k=1}^K \text{Tr} (f_k(A)g_k(B)) \geq 0$  for all hermitian matrices  $a \leq A, B \leq b$ .*

Because of our assumption that  $\varphi$  is convex, we obtain from the lemma that the trace in (6.0.1) is always non-negative. If  $\varphi$  is strictly convex, it can be proved that  $\mathcal{H}(A, B) = 0$  only when  $A = B$ . Therefore,  $\mathcal{H}(A, B)$  is an appropriate object to measure how  $A$  is close to  $B$ .

The formula (6.0.1) is motivated by several physical situations. First, the usual von Neumann entropy

$$\mathcal{H}_{\text{vN}}(A, B) = \text{Tr} A(\log A - \log B)$$

corresponds to taking

$$\varphi_{\text{vN}}(x) = x \log(x), \quad x \in [0, 1].$$

This is not the only function of interest, however. If we take two quasi-free states  $\alpha$  and  $\beta$  on the CAR (resp. CCR) algebra of a (finite-dimensional) Hilbert space  $\mathfrak{H}$ , then the corresponding von Neumann entropy can be expressed in terms of the one-particle density matrices  $A$  and  $B$  of  $\alpha$  and  $\beta$ , leading to the expression (6.0.1) with, this time,

$$\varphi_{\text{CAR}}(x) = x \log(x) + (1 - x) \log(1 - x), \quad x \in [0, 1]$$

and

$$\varphi_{\text{CCR}}(x) = x \log(x) - (1 + x) \log(1 + x), \quad x \in [0, 1],$$

---

<sup>1</sup>This expression always makes sense if  $0 < B < 1$ . If the spectrum of  $B$  contains 0 or 1 and if  $\varphi$  is not differentiable at these points, then we let  $\mathcal{H}(A, B) = +\infty$  except when  $A = B$  on  $\ker B$ ,  $\ker(1 - B)$ , or  $\ker B \oplus \ker(1 - B)$ . In this case the trace is by definition taken on the orthogonal to these subspaces.

respectively [BLS94]. It seems therefore natural to study the properties of  $\mathcal{H}$  for a general convex function  $\varphi$ , and this is the main purpose of this paper. We will particularly study the possibility to define  $\mathcal{H}$  for two bounded operators in an *infinite* dimensional Hilbert space  $\mathfrak{H}$ . *Monotonicity* then plays a crucial role and we discuss it in the next section.

### 1. Monotonicity

Our goal is to define  $\mathcal{H}(A, B)$  for  $A$  and  $B$  two bounded operators on an infinite dimensional Hilbert space. The usual technique employed in statistical mechanics is to first project the system into a finite dimensional space and then to take the limit when the dimension goes to  $+\infty$ . This means that we will define

$$\mathcal{H}(A, B) := \lim_{k \rightarrow \infty} \mathcal{H}(P_k A P_k, P_k B P_k) \quad (6.1.2)$$

where  $P_k$  is an increasing sequence of finite-rank orthogonal projectors on  $\mathfrak{H}$ . For a general (convex) function  $\varphi$ , the limit is not guaranteed to exist. Furthermore, the limit could be different for two sequences  $P_k$  and  $P'_k$ . One natural way to ensure a good behavior is to add the constraint that  $\mathcal{H}$  is *monotone*, that is, satisfies the inequality

$$\boxed{\mathcal{H}(PAP, PBP) \leq \mathcal{H}(A, B)} \quad (6.1.3)$$

for every finite self-adjoint matrices  $0 \leq A, B \leq 1$  and every orthogonal projector  $P$ . The limit on the right of (6.1.2) is then monotone and  $\mathcal{H}(A, B)$  is well defined in  $\mathbb{R}^+ \cup \{+\infty\}$ . Our purpose in this section is to characterize the convex functions  $\varphi$  for which  $\mathcal{H}$  is monotone in the sense of (6.1.3).

Let us emphasize that another notion of monotonicity is often used in the literature. Assume that our (finite-dimensional) Hilbert space is the tensor product  $\mathfrak{H} = \mathfrak{H}_1 \otimes \mathfrak{H}_2$ . Define  $\Phi(A) = \text{Tr}_{\mathfrak{H}_2}(A)$ , the partial trace with respect to the second Hilbert space. Then the von Neumann relative entropy (corresponding to  $\varphi = \varphi_{\text{vN}}$ ) satisfies that

$$\mathcal{H}_{\text{vN}}(\Phi(A), \Phi(B)) \leq \mathcal{H}_{\text{vN}}(A, B) \quad (6.1.4)$$

for every  $0 \leq A, B \leq 1$  with  $\text{Tr}(A) = \text{Tr}(B)$ . Indeed, the property holds for any trace-preserving completely positive map  $\Phi$  between two Hilbert spaces [OP93]. Since  $A \mapsto PAP + P^\perp A P^\perp$  is completely positive and trace-preserving, it is easy to deduce that the von Neumann entropy also satisfies (6.1.3). Furthermore, it can be shown (see [OP93, Chap. 2]) that  $\varphi(x) = ax \log(x) + bx + c$  with  $a \geq 0$  are the only functions for which (6.1.4) is satisfied.

The weaker monotonicity property (6.1.3) is associated with a decomposition of the Hilbert space  $\mathfrak{H}$  into a direct sum  $\mathfrak{H} = \mathfrak{H}_1 \oplus \mathfrak{H}_2$ , instead of a tensor product. Indeed, if we have a quasi-free state on the CCR (resp. CAR) algebra of a Hilbert space  $\mathfrak{H}$ , the restriction of this state to a sub-algebra of observables in  $\mathfrak{H}_1 \subset \mathfrak{H}$  is obtained by

taking a *partial trace for the state* and by *replacing the one-particle density matrix  $A$  by  $P_1AP_1$* . The tensor structure at the level of states is transformed into a direct sum at the level of density matrices. From this discussion we conclude that the relative entropy associated with  $\varphi_{\text{CCR/CAR}}$  (defined above) must also satisfy the monotonicity property (6.1.3), even if they do not satisfy the stronger monotonicity (6.1.4).

In this section we want to characterize the convex functions  $\varphi$  for which  $\mathcal{H}$  is monotone in the sense of (6.1.3). In a recent paper [AHP10], Audenaert, Hiai and Petz have studied the strong sub-additivity of the generalized entropy  $A \mapsto -\text{Tr } \varphi(A)$  when  $\varphi'$  is operator monotone. Petz then conjectured that the operator monotonicity of  $\varphi'$  is necessary. Here we express everything in terms of the relative entropy (6.0.1) and we prove Petz's conjecture in this setting.

**Theorem 6.1** (Monotonicity). *Let  $\varphi \in C^0([0, 1], \mathbb{R}) \cap C^1((0, 1), \mathbb{R})$  be a convex function. Then the following are equivalent*

- (1)  $\varphi'$  is operator monotone on  $(0, 1)$ ;
- (2) For any linear map  $X : \mathfrak{H}_1 \rightarrow \mathfrak{H}_2$  on finite-dimensional spaces  $\mathfrak{H}_1$  and  $\mathfrak{H}_2$  with  $X^*X \leq 1$ , and for any  $0 \leq A, B \leq 1$  on  $\mathfrak{H}_1$ , we have

$$\mathcal{H}(XAX^*, XBX^*) \leq \mathcal{H}(A, B), \quad (6.1.5)$$

with  $\mathcal{H}(A, B)$  defined in (6.0.1).

Typical functions  $\varphi$  satisfying the conditions in Theorem 6.1 are provided in [AHP10] and include

$$\varphi(x) = \begin{cases} (t+x) \log(t+x), & t \geq 0 \\ -\log(t+x), & t > 0, \\ -x^m, & 0 < m \leq 1, \\ x^m, & 1 \leq m \leq 2. \end{cases}$$

By using Löwner's characterization of operator-monotone functions, it is possible to write an integral representation formula for the allowed functions  $\varphi$ . This is done later in the proof, see (6.1.8).

**PROOF.** As a preliminary we remark that  $x \mapsto x\varphi'(x)$  possesses a limit when  $x \rightarrow 0^+$ . Indeed, since  $\varphi$  is convex by assumption, then  $x \mapsto x\varphi'(x) - \varphi(x)$  must be increasing on  $(0, 1)$ . Also,  $x\varphi'(x) - \varphi(x) \geq -\varphi(0)$  and we conclude that  $x \mapsto x\varphi'(x) - \varphi(x)$  possesses a limit when  $x \rightarrow 0^+$ . Since  $\varphi$  is continuous by assumption, then  $x\varphi'(x)$  must have a limit as well, and this limit is  $\geq 0$ . The same argument shows that  $(1-x)\varphi'(x)$  has a limit when  $x \rightarrow 1^-$ .

Next we prove that (2) implies (1). Let  $A$  be any matrix such that  $0 < \eta < A < 1 - \eta$ , and  $P$  be any orthogonal projector. We use the shorthand notation  $A_{11} = PAP$ ,  $A_{22} = P^\perp AP^\perp$  and so on. Let  $X$  be any self-adjoint matrix such that

$P^\perp X = XP^\perp = P^\perp$  and  $0 < X \leq 1$ . Then we have by assumption

$$\begin{aligned} \mathcal{H}(XAX, XA_{11}X + A_{22}) &= \mathcal{H}(XAX, X(A_{11} + A_{22})X) \\ &\leq \mathcal{H}(A, A_{11} + A_{22}). \end{aligned}$$

Note that

$$\begin{aligned} \text{Tr}_{\mathfrak{H}} \varphi'(A_{11} + A_{22})(A - A_{11} - A_{22}) \\ = \text{Tr}_{P\mathfrak{H} \oplus P^\perp\mathfrak{H}} \begin{pmatrix} \varphi'(A_{11}) & 0 \\ 0 & \varphi'(A_{22}) \end{pmatrix} \begin{pmatrix} 0 & A_{12} \\ A_{21} & 0 \end{pmatrix} = 0. \end{aligned}$$

A similar argument for the term involving  $X$  gives

$$\begin{aligned} 0 &\leq \mathcal{H}(A, A_{11} + A_{22}) - \mathcal{H}(XAX, XA_{11}X + A_{22}) \\ &= \text{Tr}_{\mathfrak{H}} \left( \varphi(A) - \varphi(A_{11} + A_{22}) - \varphi(XAX) + \varphi(XA_{11}X + A_{22}) \right) \\ &= \text{Tr}_{\mathfrak{H}} \left( \varphi(A) - \varphi(XAX) \right) - \text{Tr}_{P\mathfrak{H}} \left( \varphi(A_{11}) - \varphi((XAX)_{11}) \right). \end{aligned}$$

Now we choose  $X := \exp(-\varepsilon C)$  for some  $C > 0$  living in the range of  $P$  and  $\varepsilon > 0$ . We remark that  $XAX = A - \varepsilon(CA + AC) + O(\varepsilon^2)$ . Using the differentiability of  $A \mapsto \text{Tr} \varphi(A)$ , we obtain

$$\text{Tr}_{\mathfrak{H}} \left( \varphi(A) - \varphi(e^{-\varepsilon C} A e^{-\varepsilon C}) \right) = 2\varepsilon \text{Tr}_{\mathfrak{H}} (CA\varphi'(A)) + o(\varepsilon).$$

The same argument for the other term and the fact that the inequality is valid for all  $C > 0$  on  $P\mathfrak{H}$  and all  $\varepsilon > 0$  gives

$$(A\varphi'(A))_{11} \geq A_{11}\varphi'(A_{11}).$$

This inequality is valid for all  $0 < A < 1$ . We have already seen that  $x \mapsto x\varphi'(x)$  can be extended by continuity at  $x = 0$ . So the property stays true for all  $0 \leq A < 1$ . By [Bha97, Thm V.2.3 & Thm V.2.9], this exactly proves that the function  $\varphi'$  is operator monotone on  $I$ . These results give us the additional information that  $\lim_{x \rightarrow 0^+} x\varphi'(x) \leq 0$ , and since we already had the other inequality we deduce that  $\lim_{x \rightarrow 0^+} x\varphi'(x) = 0$ .

Next we turn to the proof that (1) implies (2), for which we follow arguments from [AP09, AHP10]. By Löwner's theorem (see [Bha97, Corollary V.4.5]), we can write  $\varphi'$  as

$$\varphi'(x) = a + b \int_{-1}^1 \frac{2x - 1}{1 - \lambda(2x - 1)} d\nu(\lambda) \tag{6.1.6}$$

with  $b \geq 0$  and  $\nu$  a Borel probability measure on  $[-1, 1]$ . Integrating this formula, we find

$$\varphi(x) = ax + c - \frac{b}{2} \int_{-1}^1 \left( \frac{2x - 1}{\lambda} + \frac{\log(1 + \lambda(1 - 2x))}{\lambda^2} \right) d\nu(\lambda).$$

The fact that  $\varphi$  possesses a limit at 0 and 1 implies that  $\nu(\{-1\}) = \nu(\{1\}) = 0$ . From this we can actually prove that

$$\lim_{x \rightarrow 0^+} x\varphi'(x) = \lim_{x \rightarrow 1^-} (1-x)\varphi'(x) = 0. \quad (6.1.7)$$

After letting  $t = -(1+\lambda)/(2\lambda)$  for  $\lambda \in (-1, 0)$  and  $t = (1-\lambda)/(2\lambda)$  for  $\lambda \in (0, 1)$ ,  $\varphi$  can also be written as

$$\begin{aligned} \varphi(x) = a'x + c' - b \int_0^\infty \left( \log(t+x) - \log(t+1/2) - \frac{2x-1}{2t+1} \right) d\nu_1(t) \\ - b \int_0^\infty \left( \log(t+1-x) - \log(t+1/2) + \frac{2x-1}{2t+1} \right) d\nu_2(t) \end{aligned} \quad (6.1.8)$$

with  $\nu_1$  and  $\nu_2$  two positive Borel measures satisfying

$$2 \int_0^\infty \frac{(d\nu_1 + d\nu_2)(t)}{(2t+1)^2} = 1.$$

The constraint that  $\varphi$  admits limits at 0 and 1 now means that

$$- \int_0^1 \log(t)(d\nu_1 + d\nu_2)(t) < \infty \quad (6.1.9)$$

and it implies  $\nu_1(\{0\}) = \nu_2(\{1\}) = 0$ , as we have already said before. The usual Fermi-Dirac distribution is obtained by taking  $d\nu_1 = d\nu_2 = dt/2$ ,  $a' = 0 = c'$ ,  $b = 2$ .

It suffices to prove the monotonicity for  $\varphi(x) = -\log(t+x)$  and for  $\varphi(x) = -\log(t+1-x)$  with  $t \geq 0$ . We start by considering the case  $t = 0$  and we let  $\varphi(x) = -(1/2)\log(x)$ . We follow the method of [AP09]. For  $A$  a positive  $n \times n$  matrix, we introduce the corresponding normalized Gaussian, defined by

$$f_A(x) := \frac{\sqrt{\det(A)}}{(2\pi)^{n/2}} \exp\left(-\frac{x^T A x}{2}\right).$$

A simple calculation shows that the *classical* entropy of  $f_A$  is

$$\begin{aligned} - \int_{\mathbb{R}^n} f_A(x) \log f_A(x) dx &= -\frac{\log \det(A)}{2} + \frac{n \log(2\pi e)}{2} \\ &= \frac{\text{Tr} \log(A^{-1})}{2} + \frac{n \log(2\pi e)}{2}, \end{aligned}$$

and that the *classical* relative entropy of two Gaussians  $f_A$  and  $f_B$  is

$$\mathcal{H}_{\text{class}}(f_A, f_B) = \int_{\mathbb{R}^n} f_A(x) \log \frac{f_A(x)}{f_B(x)} dx = \mathcal{H}(A^{-1}, B^{-1}),$$

see [AP09, Eq. (21)–(22)]. Now, let  $P$  be any orthogonal projection on  $\mathfrak{H}$ . Up to a change of variables we may assume for simplicity that  $x = (x_1, x_2)$  with  $Px = (x_1, 0)$

for all  $x \in \mathbb{R}^n$ . The marginal of a Gaussian is computed in [AP09, Lemma 4] and it is equal to

$$\int f_A(x_1, x_2) dx_2 = f_{A_{11} - A_{12}A_{22}^{-1}A_{21}}(x_1)$$

where we have used the decomposition

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}.$$

Noticing that  $(A_{11} - A_{12}A_{22}^{-1}A_{21})^{-1} = (A^{-1})_{11}$  by the Schur complement formula, we deduce that

$$\mathcal{H}_{\text{class}} \left( \int f_{A^{-1}} dx_2, \int f_{B^{-1}} dx_2 \right) = \mathcal{H}(A_{11}, B_{11}) = \mathcal{H}(PAP, PBP).$$

The inequality  $\mathcal{H}(PAP, PBP) \leq \mathcal{H}(A, B)$  now follows from the well-known monotonicity of the classical relative entropy in terms of marginals. The argument is exactly the same if  $\log(x)$  is replaced by  $\log(t+x)$  and  $\log(t+1-x)$ , since  $(t+A)_{11} = t+A_{11}$  and  $(t+1-A)_{11} = t+1-A_{11}$ .

We have proved the monotonicity for a projection  $P$ . If  $U : \mathfrak{H}_1 \rightarrow \mathfrak{H}_2$  is a partial isometry between two spaces such that  $U^*U = 1_{\mathfrak{H}_1}$  and  $UU^* \leq 1_{\mathfrak{H}_2}$ , it is obvious that  $\mathcal{H}(UAU^*, UBU^*) = \mathcal{H}(A, B)$  since  $U\mathfrak{H}_1$  is then isometric to a subspace of  $\mathfrak{H}_2$ . On the other hand, if we have  $UU^* = 1_{\mathfrak{H}_2}$  and  $U^*U \leq 1_{\mathfrak{H}_1}$ , then  $\mathcal{H}(UAU^*, UBU^*) \leq \mathcal{H}(A, B)$  by the previous result on projections, since  $U^*\mathfrak{H}_2$  is now isometric to a subspace of  $\mathfrak{H}_1$ .

In order to deduce the result for an arbitrary operator  $X : \mathfrak{H} \rightarrow \mathfrak{H}$  with  $X^*X \leq 1$ , we double the dimension of the space, that is, we introduce the partial isometry

$$\begin{aligned} U : \mathfrak{H} &\rightarrow \mathfrak{H} \oplus \mathfrak{H} \\ f &\mapsto Xf \oplus \sqrt{1 - X^*X}f \end{aligned}$$

and we infer  $\mathcal{H}(UAU^*, UBU^*) = \mathcal{H}(A, B)$ , since  $U^*U = 1_{\mathfrak{H}}$ . Note that

$$UAU^* = \begin{pmatrix} XAX & XA\sqrt{1 - X^*X} \\ \sqrt{1 - X^*X}AX & \sqrt{1 - X^*X}A\sqrt{1 - X^*X} \end{pmatrix}.$$

If we project onto the first Hilbert space of  $\mathfrak{H} \oplus \mathfrak{H}$ , this decreases the relative entropy and we obtain the result. The case of  $X : \mathfrak{H}_1 \rightarrow \mathfrak{H}_2$  with different Hilbert spaces and  $X^*X \leq 1$  follows from the polar decomposition  $X = UY$  with  $U$  a partial isometry and  $0 \leq Y = \sqrt{X^*X} \leq 1$ . This concludes our proof that (1) implies (2).  $\square$

After having characterized the functions  $\varphi$  for which  $\mathcal{H}$  is monotone, we quickly mention the consequences on the entropy  $S(A) = -\text{Tr } \varphi(A)$ , for completeness.

One of the fundamental properties of the von Neumann entropy (defined with  $\varphi_{\text{vN}}(x) = x \log(x)$ ) is its strong subadditivity (SSA), which was proved by Lieb and Ruskai in [LR73a, LR73b]. The fact that SSA is very important for large quantum systems was first remarked by Robinson and Ruelle in [RR67], see also

[Weh78] and [HLS09b]. It is well-known that SSA is equivalent to the monotonicity of the relative von Neumann entropy  $\mathcal{H}$  under completely positive trace-preserving maps [OP93, Car10, Weh78], as in (6.1.4).

The usual definition of SSA is expressed using a decomposition of the ambient Hilbert space  $\mathfrak{H}$  into a tensor product of the form  $\mathfrak{H} = \mathfrak{H}_1 \otimes \mathfrak{H}_2 \otimes \mathfrak{H}_3$ , and we do not recall it here. In our setting there is another concept of SSA, which is associated with a decomposition of  $\mathfrak{H}$  into a direct sum  $\mathfrak{H} = \mathfrak{H}_1 \oplus \mathfrak{H}_2 \oplus \mathfrak{H}_3$  of three spaces (instead of a tensor product), and which was considered before in [AHP10]. For  $\varphi = \varphi_{\text{CCR/CAR}}$ , this is just the usual SSA for quasi-free states, expressed in terms of the corresponding one-particle density matrices. We denote by  $P_j$  the corresponding orthogonal projections, as well as  $P_{12} = P_1 + P_2$  and  $P_{123} = 1$ .

**Corollary 6.1** (SSA for the entropy). *We assume that  $\varphi \in C^0([0, 1], \mathbb{R})$  and that  $\varphi'$  is operator monotone on  $(0, 1)$ . Let  $S(A) = -\text{Tr}_{\mathfrak{H}} \varphi(A)$ , with  $\dim(\mathfrak{H}) < \infty$ . Then we have*

$$S(P_{123}AP_{123}) + S(P_2AP_2) \leq S(P_{12}AP_{12}) + S(P_{23}AP_{23}),$$

for all self-adjoint matrices  $0 \leq A \leq 1$  on  $\mathfrak{H}$ .

**PROOF.** By using the monotonicity of the relative entropy, we deduce that we have  $\mathcal{H}(P_{123}AP_{123}, P_{23}AP_{23}) \geq \mathcal{H}(P_{12}AP_{12}, P_2AP_2)$ . It is straightforward to verify that  $\mathcal{H}(P_{123}AP_{123}, P_{23}AP_{23}) = S(P_{123}AP_{123}) - S(P_{23}AP_{23})$  and that  $\mathcal{H}(P_{12}AP_{12}, P_2AP_2) = S(P_{12}AP_{12}) - S(P_2AP_2)$  and the result follows.  $\square$

**Remark 6.1.** Since an operator monotone function is always  $C^\infty$ , there is no need to assume anymore that  $\varphi \in C^1$ .

## 2. Definition in infinite-dimensional spaces

We now turn to the definition of  $\mathcal{H}(A, B)$  in an infinite-dimensional space  $\mathfrak{H}$ . For any two self-adjoint operators  $0 \leq A, B \leq 1$ , we let

$$\mathcal{H}(A, B) := \lim_{k \rightarrow \infty} \mathcal{H}(P_k A P_k, P_k B P_k) \quad (6.2.10)$$

where  $P_k$  is any increasing sequence of finite-dimensional projections on  $\mathfrak{H}$ , such that  $P_k \rightarrow 1$  strongly. The following result says that the limit exists in  $[0, \infty]$  and provides important properties of  $\mathcal{H}$ .

**Theorem 6.2** (Generalized relative entropy in infinite dimension). *We assume that  $\varphi \in C^0([0, 1], \mathbb{R})$  and that  $\varphi'$  is operator monotone on  $(0, 1)$ .*

• ( $\mathcal{H}$  is well-defined). *For any increasing sequence  $P_k$  of finite-dimensional projections on  $\mathfrak{H}$  such that  $P_k \rightarrow 1$  strongly, the sequence  $\mathcal{H}(P_k A P_k, P_k B P_k)$  is monotone and possesses a limit in  $\mathbb{R}^+ \cup \{+\infty\}$ . This limit does not depend on the chosen sequence  $P_k$  and hence  $\mathcal{H}(A, B)$  is well-defined in  $\mathbb{R}^+ \cup \{+\infty\}$ .*

- (Monotonicity). *The so-defined relative entropy  $\mathcal{H}(A, B)$  is monotone: for any linear map  $X : \mathfrak{H}_1 \rightarrow \mathfrak{H}_2$  such that  $X^*X \leq 1$  and any  $0 \leq A, B \leq 1$  on  $\mathfrak{H}_1$ , we have*

$$\mathcal{H}(A, B) \geq \mathcal{H}(XAX^*, XBX^*). \quad (6.2.11)$$

- (Approximation). *If  $X_k : \mathfrak{H}_1 \rightarrow \mathfrak{H}_k$  is a sequence such that  $X_k^*X_k \leq 1$  and  $X_k^*X_k \rightarrow 1$  strongly in  $\mathfrak{H}_1$ , then*

$$\mathcal{H}(A, B) = \lim_{k \rightarrow \infty} \mathcal{H}(X_kAX_k^*, X_kBX_k^*). \quad (6.2.12)$$

- (Weak lower semi-continuity). *The relative entropy is weakly lower semi-continuous: if  $0 \leq A_n, B_n \leq 1$  are two sequences such that  $A_n \rightarrow A$  and  $B_n \rightarrow B$  weakly-\* in  $\mathcal{B}(\mathfrak{H})$ , then*

$$\mathcal{H}(A, B) \leq \liminf_{n \rightarrow \infty} \mathcal{H}(A_n, B_n). \quad (6.2.13)$$

Most of the statements of the theorem easily follow from the monotonicity in finite dimension proved in Theorem 6.1, showing the importance of this concept.

PROOF. We split the proof into several steps.

*Step 1. Lower semi-continuity in finite dimension.* We want to prove that we have  $\mathcal{H}(A, B) \leq \liminf_{n \rightarrow \infty} \mathcal{H}(A_n, B_n)$  if  $A_n \rightarrow A$  and  $B_n \rightarrow B$  are convergent sequences of hermitian matrices. All the terms in the definition of  $\mathcal{H}(A, B)$  are continuous, except possibly for  $(A, B) \mapsto \text{Tr } \varphi'(B)(A - B)$ . We write this term as

$$\begin{aligned} & \text{Tr } \varphi'(B)(B - A) \\ &= -\text{Tr } \varphi'(B)\mathbf{1}(\varphi'(B) \leq 0)A + \text{Tr } \varphi'(B)\mathbf{1}(\varphi'(B) \geq 0)(1 - A) \\ & \quad + \text{Tr } B\varphi'(B)\mathbf{1}(\varphi'(B) \leq 0) - \text{Tr } (1 - B)\varphi'(B)\mathbf{1}(\varphi'(B) \geq 0). \end{aligned}$$

Using that the first two terms involve non-negative matrices and that the next ones are continuous by (6.1.7), we obtain the result.

*Step 2. The definition in infinite dimension does not depend on  $(P_k)$ .* Let us consider two sequences  $(P_k)$  and  $(P'_\ell)$  of increasing orthogonal projections, such that  $P_k \rightarrow 1$  and  $P'_\ell \rightarrow 1$  strongly. By the monotonicity in finite dimension, we have  $\mathcal{H}(P_kP'_\ell AP'_\ell P_k, P_kP'_\ell BP'_\ell P_k) \leq \mathcal{H}(P'_\ell AP'_\ell, P'_\ell BP'_\ell)$ . Taking first  $\ell \rightarrow \infty$  using that  $P_kP'_\ell AP'_\ell P_k \rightarrow P_kP'_\ell BP'_\ell P_k$  and the lower semi-continuity of  $\mathcal{H}$  in the finite dimensional space  $\text{Ran}(P_k)$ , we get

$$\mathcal{H}(P_kAP_k, P_kBP_k) \leq \lim_{\ell \rightarrow \infty} \mathcal{H}(P'_\ell AP'_\ell, P'_\ell BP'_\ell).$$

Taking then  $k \rightarrow \infty$  shows that

$$\lim_{k \rightarrow \infty} \mathcal{H}(P_kAP_k, P_kBP_k) \leq \lim_{\ell \rightarrow \infty} \mathcal{H}(P'_\ell AP'_\ell, P'_\ell BP'_\ell).$$

Exchanging  $P_k$  and  $P'_\ell$  gives the other inequality.



*Step 3. Monotonicity in infinite dimension.* Let  $X : \mathfrak{H}_1 \rightarrow \mathfrak{H}_2$  be such that  $X^*X \leq 1_{\mathfrak{H}_1}$ . For fixed sequences  $(P_k)$  and  $(P'_\ell)$  of finite-rank projections on  $\mathfrak{H}_1$  and  $\mathfrak{H}_2$  respectively, we have

$$\begin{aligned} \mathcal{H}(P'_\ell X P_k A P_k X^* P'_\ell, P'_\ell X P_k B P_k X^* P'_\ell) &\leq \mathcal{H}(X P_k A P_k X^*, X P_k B P_k X^*) \\ &\leq \mathcal{H}(P_k A P_k, P_k B P_k). \end{aligned}$$

Taking first  $k \rightarrow \infty$  using that  $P'_\ell X P_k A P_k X^* P'_\ell \rightarrow P'_\ell X A X^* P'_\ell$  with the finite rank projection  $P'_\ell$  fixed, and only then  $\ell \rightarrow \infty$ , gives the monotonicity.

*Step 4. Weak lower semi-continuity.* If  $A_n \rightarrow A$  and  $B_n \rightarrow B$  weakly-\* in  $\mathcal{B}(\mathfrak{H})$ , then

$$\mathcal{H}(P_k A P_k, P_k B P_k) \leq \liminf_{n \rightarrow \infty} \mathcal{H}(P_k A_n P_k, P_k B_n P_k) \leq \liminf_{n \rightarrow \infty} \mathcal{H}(A_n, B_n)$$

for any fixed sequence  $(P_k)$  as before. Here we have used that  $P_k A_n P_k \rightarrow P_k A P_k$  for a finite-rank projection and the lower semi-continuity in finite dimension. Taking  $k \rightarrow \infty$  gives the weak lower semi-continuity.

*Step 5. Convergence for any sequence  $X_k \rightarrow 1$ .* Let  $X_k : \mathfrak{H} \rightarrow \mathfrak{H}$  be any sequence of self-adjoint operators, such that  $X_k^* X_k \leq 1$  and  $X_k^* X_k \rightarrow 1$  strongly. We want to prove that  $\mathcal{H}(X_k A X_k^*, X_k B X_k^*) \rightarrow \mathcal{H}(A, B)$  but, by the polar decomposition  $X_k = U_k Y_k$ , we can always assume that  $X_k$  is self-adjoint, hence that  $X_k \rightarrow 1$  strongly. We have  $\mathcal{H}(X_k A X_k, X_k B X_k) \leq \mathcal{H}(A, B)$ . On the other hand,  $X_k A X_k \rightarrow A$  strongly and thus the weak lower semi-continuity implies the reverse inequality. If  $X_k : \mathfrak{H}_1 \rightarrow \mathfrak{H}_2$ , the argument is similar.  $\square$

### 3. Klein inequalities and consequences

In this last section, we derive some useful bounds on  $A - B$  when the relative entropy  $\mathcal{H}(A, B)$  is finite. For instance, we will prove that  $A - B$  must be a Hilbert-Schmidt (hence compact) operator. Our main result is inspired of [HLS08, Thm 1] and of [FHSS12, Lemma 1] and it is mainly based on Klein's Lemma 6.1, hence the name "Klein inequalities".

**Theorem 6.3** (Klein inequalities). *We assume that  $\varphi \in C^0([0, 1], \mathbb{R})$ , and that  $\varphi'$  is operator monotone on  $(0, 1)$  and not constant.*

- (Lower bound). *There exists  $C > 0$  (depending only on  $\varphi$ ) such that*

$$\mathcal{H}(A, B) \geq C \operatorname{Tr} (1 + |\varphi'(B)|)(A - B)^2, \quad (6.3.14)$$

*for all  $0 \leq A, B \leq 1$ . Hence,  $A - B$  is Hilbert-Schmidt when  $\mathcal{H}(A, B) < \infty$ .*

- (Upper bound). *Similarly, we have*

$$\mathcal{H}(A, B) \leq C \operatorname{Tr} \left( \frac{1}{B^2} + \frac{1}{(1 - B)^2} \right) (A - B)^2, \quad (6.3.15)$$

*for all  $0 \leq A, B \leq 1$ .*

- (Regularity). If  $0 \leq A \leq 1$  and  $0 < \varepsilon \leq A', B \leq 1 - \varepsilon$  are such that  $A - A'$  and  $A' - B$  are Hilbert-Schmidt operators, then

$$|\mathcal{H}(A, B) - \mathcal{H}(A', B)| \leq C_\varepsilon \left( \|A - A'\|_{\mathfrak{S}^2}^2 + \|A' - B\|_{\mathfrak{S}^2} \|A - A'\|_{\mathfrak{S}^2} \right) \quad (6.3.16)$$

where  $C_\varepsilon$  depends on  $\varphi$  and on  $\varepsilon$ .

We remark that the inequality (6.3.15) is far from optimal if  $\varphi(x)$  is very smooth at 0 or 1. Similarly, (6.3.16) holds without the assumptions that the density matrices have their spectrum in  $[\varepsilon, 1 - \varepsilon]$ , if  $\varphi''$  is bounded on  $[0, 1]$ .

PROOF OF THEOREM 6.3. We have

$$-\frac{\log(t+x) - \log(t+y) - \frac{x-y}{t+y}}{(x-y)^2} = \frac{1}{(t+y)^2} \frac{h - \log(1+h)}{h^2},$$

with  $h = (x-y)/(t+y)$ . Using that  $h \mapsto h^{-2}(h - \log(1+h))$  is decreasing, we deduce that

$$\min_{0 \leq x \leq 1} \left( -\frac{\log(t+x) - \log(t+y) - \frac{x-y}{t+y}}{(x-y)^2} \right) = \frac{\frac{1-y}{t+y} - \log\left(1 + \frac{1-y}{t+y}\right)}{(1-y)^2}.$$

Using now that

$$\frac{h - \log(1+h)}{h^2} \geq \frac{1}{2(h+1)}$$

for all  $h \geq 0$ , we conclude that

$$-\left( \log(t+x) - \log(t+y) - \frac{x-y}{t+y} \right) \geq \frac{(x-y)^2}{2(1+t)(t+y)}. \quad (6.3.17)$$

By replacing  $x$  by  $1-x$  and  $y$  by  $1-y$ , we get the same estimate with  $t+1-y$  in place of  $t+y$  in the denominator on the right side. Inserting in (6.1.8) we find that, for all  $0 < x, y < 1$ ,

$$\begin{aligned} & \varphi(x) - \varphi(y) - \varphi'(y)(x-y) \\ & \geq \frac{b}{2} \left( \int_0^\infty \frac{d\nu_1(t)}{(1+t)(t+y)} + \int_0^\infty \frac{d\nu_2(t)}{(1+t)(t+1-y)} \right) (x-y)^2 \\ & \geq C \left( \int_1^\infty \frac{d\nu_1(t) + d\nu_2(t)}{(2t+1)^2} + \int_0^1 \frac{d\nu_1(t)}{t+y} + \int_0^1 \frac{d\nu_2(t)}{t+1-y} \right) (x-y)^2. \end{aligned}$$

From the integral representation of  $\varphi$  in (6.1.8), we see that

$$\varphi'(x) \underset{x \rightarrow 0^+}{\sim} -b \int_0^1 \frac{d\nu_1(t)}{(t+x)} + C, \quad \varphi'(x) \underset{x \rightarrow 1^-}{\sim} b \int_0^1 \frac{d\nu_2(t)}{(t+1-x)} + C.$$

Therefore we have proved that

$$\forall 0 \leq x, y \leq 1, \quad \varphi(x) - \varphi(y) - \varphi'(y)(x-y) \geq C(1 + |\varphi'(y)|)(x-y)^2.$$

The result follows for finite matrices by Klein’s Lemma 6.1, and for general operators by the definition of  $\mathcal{H}$  using projections on finite-dimensional spaces.

Maximizing instead of minimizing in (6.3.17), we find

$$\begin{aligned} -\left(\log(t+x) - \log(t+y) - \frac{x-y}{t+y}\right) &\leq (x-y)^2 \frac{-\frac{y}{t+y} - \log\left(1 - \frac{y}{t+y}\right)}{y^2} \\ &\leq (x-y)^2 \frac{1 - \log\left(\frac{t}{t+y}\right)}{(t+y)^2} \end{aligned}$$

and a similar estimate for  $1-x$  and  $1-y$ . After integrating with respect to  $t$ , we see that the integral converges for large  $t$ , uniformly in  $y$ . The only possibly diverging terms are

$$\int_0^1 \frac{\log\left(\frac{t}{t+y}\right)}{(t+y)^2} d\nu_1(t) + \int_0^1 \frac{\log\left(\frac{t}{t+1-y}\right)}{(t+1-y)^2} d\nu_2(t)$$

and they can always be estimated by a constant times  $y^{-2} + (1-y)^{-2}$ , by (6.1.9). (This is far from optimal if  $\nu_1$  or  $\nu_2$  vanish sufficiently fast at 0).

Now we turn to the proof of (6.3.16), which only has to be done in finite dimension, by the definition of  $\mathcal{H}$ . We remark that

$$\mathcal{H}(A, B) - \mathcal{H}(A', B) = \mathcal{H}(A, A') + \text{Tr}(\varphi'(A) - \varphi'(B'))(A - A').$$

Since  $\varphi''$  is bounded on  $[\varepsilon, 1 - \varepsilon]$ , we have

$$\text{Tr}(\varphi'(A) - \varphi'(B'))^2 \leq C \text{Tr}(A' - B)^2,$$

by Klein’s Lemma 6.1. By Hölder’s inequality this gives

$$|\text{Tr}(\varphi'(A) - \varphi'(B'))(A - A')| \leq C \|A' - B\|_{\mathfrak{S}^2} \|A - A'\|_{\mathfrak{S}^2}.$$

Using (6.3.15) and the assumption that  $\varepsilon \leq A' \leq 1 - \varepsilon$  to estimate  $\mathcal{H}(A, A')$  gives (6.3.16). □

Using the previous Klein inequalities, we can get some information on the set of one-particle density matrices  $A$  which have a finite relative entropy with respect to a given  $B$ . Of particular interest is fact that any operator  $A$  such that  $\mathcal{H}(A, B) < \infty$  can be approximated in an appropriate sense by a sequence of finite rank perturbations of  $B$ .

**Corollary 6.2** (Density of finite rank perturbations). *We assume that  $\varphi \in C^0([0, 1], \mathbb{R})$  and that  $\varphi'$  is operator monotone on  $(0, 1)$  and that  $0 \leq A, B \leq 1$  have a finite relative entropy,  $\mathcal{H}(A, B) < \infty$ . Then for every  $\varepsilon > 0$ , there exists  $0 \leq A' \leq 1$  such that*

- $A' - A$  has a finite rank and its eigenvectors belong to  $\ker(B)$ , to  $\ker(1 - B)$ , or to the domain of  $B^{-2} + (1 - B)^{-2}$  in the orthogonal of these two subspaces;
- $\text{Tr}(1 + |\varphi'(B)|)(A - A')^2 \leq \varepsilon$ ;

- $|\mathcal{H}(A, B) - \mathcal{H}(A', B)| \leq \varepsilon$ .

PROOF. We have several cases to look at, depending whether  $\varphi'$  diverges at the end points 0 and 1 and depending whether  $B$  has the end points as eigenvalues or not. First we note that if  $\varphi'$  diverges at 0 and  $\ker B \neq \{0\}$ , then  $A = B$  on  $\ker B$  and therefore there is nothing to do on this subspace and we can argue on the orthogonal of  $\ker B$ . So let us now assume that  $\ker B = \ker(1 - B) = \{0\}$ . We introduce the spectral projector  $\Pi_\eta := \mathbf{1}(\eta \leq B \leq 1 - \eta)$ . By the spectral theorem, we have  $\Pi_\eta \rightarrow 1$  strongly when  $\eta \rightarrow 0$ . By Theorem 6.2, we deduce that

$$\lim_{\eta \rightarrow 0} \mathcal{H}(\Pi_\eta A \Pi_\eta, \Pi_\eta B \Pi_\eta) = \lim_{\eta \rightarrow 0} \mathcal{H}(B + \Pi_\eta(A - B)\Pi_\eta, B) = \mathcal{H}(A, B).$$

In the first equality we have used that

$$\begin{aligned} \mathcal{H}(B + \Pi_\eta(A - B)\Pi_\eta, B) &= \mathcal{H}(\Pi_\eta^\perp B \Pi_\eta^\perp + \Pi_\eta A \Pi_\eta, \Pi_\eta^\perp B \Pi_\eta^\perp + \Pi_\eta B \Pi_\eta) \\ &= \mathcal{H}(\Pi_\eta A \Pi_\eta, \Pi_\eta B \Pi_\eta) + \mathcal{H}(\Pi_\eta^\perp B \Pi_\eta^\perp, \Pi_\eta^\perp B \Pi_\eta^\perp) \\ &= \mathcal{H}(\Pi_\eta A \Pi_\eta, \Pi_\eta B \Pi_\eta), \end{aligned}$$

since  $\Pi_\eta$  commutes with  $B$ . By Klein's inequality (6.3.14), we know that  $(1 + |\varphi'(B)|)^{1/2}(A - B)$  is a Hilbert-Schmidt operator, and it is then clear that

$$\lim_{\eta \rightarrow 0} \text{Tr}(1 + |\varphi'(B)|) \left( \Pi_\eta(A - B)\Pi_\eta - (A - B) \right)^2 = 0.$$

The density matrix  $A_\eta := B + \Pi_\eta(A - B)\Pi_\eta$  satisfies all the desired properties, except for the finite rank one, and we need to approximate it further.

In order to approximate  $A_\eta$ , we will work in the space  $\mathfrak{H}_\eta := \Pi_\eta \mathfrak{H}$ . We first remark that, by Klein's inequality,  $\Pi_\eta A \Pi_\eta$  is a Hilbert-Schmidt perturbation of  $\Pi_\eta B$  and, therefore, the essential spectrum of  $\Pi_\eta A \Pi_\eta$  (restricted to  $\mathfrak{H}_\eta$ ) is included in the interval  $[\eta, 1 - \eta]$ . The end points 0 and 1 can only be isolated eigenvalues of finite multiplicity. Let us denote by  $P_0$  and  $P_1$  the associated projections (if they exist). Then  $A'_\eta := \Pi_\eta A \Pi_\eta + \varepsilon P_0 - \varepsilon P_1$  is a finite rank perturbation of  $A_\eta$  and a simple calculation shows that

$$\begin{aligned} \mathcal{H}(\Pi_\eta A \Pi_\eta + \varepsilon P_0 - \varepsilon P_1, \Pi_\eta B) - \mathcal{H}(\Pi_\eta A \Pi_\eta, \Pi_\eta B) &= (\varphi(\varepsilon) - \varphi(0)) \text{Tr } P_0 \\ &\quad + (\varphi(1 - \varepsilon) - \varphi(1)) \text{Tr } P_1 + \varepsilon \text{Tr} (\Pi_\eta \varphi'(B)(P_1 - P_0)) \end{aligned}$$

(the computation must be done in a finite sequence of dimensional spaces  $V_k \nearrow \mathfrak{H}_\eta$  and it is simpler to assume that the eigenvectors of  $\Pi_\eta A \Pi_\eta$  corresponding to the end points belong to these spaces). This goes to 0 as  $\varepsilon \rightarrow 0$  with  $\eta$  fixed. At this step we have approximated  $\Pi_\eta A \Pi_\eta$  by an operator  $A'_\eta$  which has its spectrum away from 0 and 1, and which is a Hilbert-Schmidt perturbation of  $\Pi_\eta B$ . Now we can take any sequence  $Q_k$  of smooth finite rank operators which converges to  $A'_\eta - \Pi_\eta B$  in the Hilbert-Schmidt norm. For large  $k$  the operator  $A_k := \Pi_\eta B + Q_k$  satisfies  $0 \leq A_k \leq 1$

and its relative entropy converges to that of  $A'_\eta$ , by (6.3.16) in Theorem 6.3. This concludes the proof in the case where  $\ker B = \ker(1 - B) = \{0\}$ .

When 0 or 1 is an eigenvalue of  $B$  and  $\varphi'$  is bounded at these points, the argument is exactly the same and we leave it to the reader. The projection  $P_\eta$  must include all (if the multiplicity is finite) or a sequence of eigenvectors (if the multiplicity is infinite) at the end points.  $\square$

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