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Mean Field Limits in Quantum Mechanics

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DE L'UNIVERSITÉ PSL

Préparée à l'Université Paris-Dauphine

Limites de champ moyen en mécanique quantique

Soutenue par

Arnaud TRIAY

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Mean-field limits in quantum mechanics

Thèse dirigée par Mathieu LEWIN

Mots clés: variational methods, partial differential equations, spectral theory, mathematical physics, quantum mechanics, quantum gases

Keywords: méthodes variationnelles, équations aux dérivées partielles, théorie spectrale, physique mathématique, mécanique quantique, gaz quantique

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À mes grands-parents.

Le linéaire, ça dure pas toute la vie.

Michel Alfaro

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LIMITES DE CHAMP MOYEN EN MÉCANIQUE QUANTIQUE**Mean-field limits in quantum mechanics****Résumé**

Cette thèse est consacrée à la dérivation et à l'étude de différents modèles non-linéaires en mécanique quantique. Ces modèles décrivent des systèmes à grand nombre de particules dans l'approximation de champ moyen. Dans une première partie, nous étudions la validité de modèles effectifs décrivant un gaz de bosons dipolaires. Nous montrons que les minimiseurs ainsi que les solutions de l'équation dépendante du temps sont correctement décrits au premier ordre par la théorie de Gross-Pitaevskii. Pour la dynamique, nous montrons également que le second ordre est donné par la théorie de Bogoliubov. Nous étudions aussi la fonctionnelle de Gross-Pitaevskii dipolaire avec un terme de correction quintique prenant en compte les corrections de Lee-Huang-Yang. La seconde partie de la thèse est consacrée à l'étude de limites semi-classiques pour les grands systèmes fermioniques. Nous nous intéressons d'abord à un gaz de fermions à température positive dans la limite semi-classique et nous montrons que l'énergie libre, ainsi que les états de Gibbs approchés, sont donnés par la théorie de Vlasov. Nous étudions ensuite l'énergie d'un atome lourd dans la limite non-relativiste où nous calculons le second ordre de son développement, la correction de Scott, pour le modèle de Dirac-Fock.

Mots clés : variational methods, partial differential equations, spectral theory, mathematical physics, quantum mechanics, quantum gases

Abstract

This thesis is devoted to the derivation and the study of several non-linear models in quantum mechanics. These models describe systems consisting of a large number of particles in the mean-field approximation. In the first part we study the validity of some effective models describing a gas of dipolar bosons. We show that the ground state as well as the time-evolved solutions are correctly described by the Gross-Pitaevskii theory, at first order. For the dynamics, we also show that the second order is given by Bogoliubov's theory. Moreover, we study a modified Gross-Pitaevskii functional including a quintic term accounting for the Lee-Huang-Yan corrections. The second part of this thesis is devoted to the study of large fermionic systems. We first analyse a fermionic gas at positive temperature in the semi-classical limit and we show that the latter and the approximate Gibbs states are given by Vlasov's theory. Then, we study the energy of heavy atoms in the non-relativistic limit where we compute the second term of its expansion, the Scott correction, for the Dirac-Fock model.

Keywords: méthodes variationnelles, équations aux dérivées partielles, théorie spectrale, physique mathématique, mécanique quantique, gaz quantique

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Introduction

Cette thèse est consacrée à la dérivation, dans l'approximation de champ moyen et depuis les principes de la mécanique quantique, de plusieurs modèles non-linéaires.

La mécanique quantique prétend décrire l'ensemble du comportement de la matière à l'échelle microscopique. C'est une théorie intrinsèquement linéaire pour laquelle il serait possible, a priori, d'accéder facilement à ses prédictions. Cependant, il devient très rapidement impossible de trouver des solutions exactes aux problèmes impliquant plus de 3 corps, et pour des systèmes composés d'un très grand nombre de particules, il est vain d'espérer pouvoir se reposer sur l'outil informatique. La dimension de l'espace des états à N particules croît généralement de manière exponentielle en N . Ce phénomène est couramment appelé la *malédiction de la dimension*. Pour cette raison, il est important de trouver des modèles simplifiés, comportant peu de degrés de liberté tout en donnant une description au moins qualitative des phénomènes en jeu. Une telle procédure est souvent appelée réduction de la dimensionalité. Les modèles ainsi dérivés sont qualifiés de *ad hoc* en opposition aux principes fondamentaux qui sont eux *ab initio*. Contrairement à ces derniers, les modèles effectifs sont souvent non-linéaires : c'est là une conséquence inéluctable de la réduction de la dimension. Cette thèse s'articule autour de l'étude du Hamiltonien dans \mathbb{R}^{dN}

$$H_N = \sum_{j=1}^N (|i\hbar\nabla_j + A(x_j)|^2 + V(x_j)) + \lambda \sum_{1 \leq j < k \leq N} w_N(x_j - x_k), \quad (1)$$

décrivant N particules quantiques évoluant dans \mathbb{R}^d . Ici A est un potentiel magnétique et V un potentiel électrique qui sont ressentis par chaque particule tandis que w est un potentiel d'interaction et $w_N = N^{d\eta}w(N^\eta)$. L'exposant η représente le caractère dilué du gaz considéré, il fera l'objet d'une plus ample discussion dans la suite. Le facteur λ est un paramètre de champ moyen que l'on prendra égal à

$$\lambda \sim \frac{1}{N}.$$

Il est choisi de telle sorte que les deux sommes dans (1) soient du même ordre de grandeur N . Plus précisément nous voulons décrire l'état fondamental de H_N

$$H_N \Psi = \lambda \Psi$$

ainsi que les solutions à l'équation d'évolution

$$i\partial_t \Psi = H_N \Psi.$$

Les systèmes de particules quantiques sont divisés en deux familles : les bosons et les fermions. Les premiers sont décrits par une fonction d'onde Ψ symétrique tandis que les seconds par une fonction d'onde antisymétrique. Plus précisément, si N particules indiscernables sont dans un état représenté par Ψ alors

$$\begin{aligned} \Psi(x_1, \dots, x_N) &= (\pm 1)^{\varepsilon(\sigma)} \Psi(x_{\sigma(1)}, \dots, x_{\sigma(N)}), \\ \forall \sigma \in \mathfrak{S}(\{1, \dots, N\}), \quad \forall x_1, \dots, x_N \in \mathbb{R}^d \end{aligned}$$

avec $+1$ pour les bosons et -1 pour les fermions, où $\varepsilon(\sigma)$ est la signature de la permutation σ . C'est une simple conséquence de l'indiscernabilité de particules identiques : si \mathbb{P} est la probabilité de présence des particules alors

$$\mathbb{P}(x_1, \dots, x_N) = \mathbb{P}(x_{\sigma(1)}, \dots, x_{\sigma(N)}),$$

pour toute permutation σ et $x_1, \dots, x_N \in \mathbb{R}^3$, ainsi que de la représentation hilbertienne des fonctions d'onde. En apparence anodine, cette propriété définit deux types de comportements très différents.

Les bosons ont la capacité de "se condenser", une telle situation est décrite par une fonction factorisée

$$\Psi \simeq u^{\otimes N}. \quad (2)$$

L'énergie de cet ansatz est donnée par la fonctionnelle de Gross-Pitaevskii,

$$\frac{\langle u^{\otimes N}, H_N u^{\otimes N} \rangle}{N} = \int_{\mathbb{R}^3} |(i\hbar\nabla + A)u|^2 + \int_{\mathbb{R}^3} V|u|^2 + \frac{(N-1)\lambda}{2} \int_{\mathbb{R}^3} w_N * |u|^2 |u|^2.$$

Elle fut largement étudiée depuis les années 1970-80 pour décrire la dynamique [Hep74; Spo81] et l'énergie fondamentale [BL83; LY87; LNR14].

Les fermions, quant à eux, vérifient le principe d'exclusion de Pauli et les fonctions antisymétriques les plus simples sont données par les déterminants de Slater

$$\Psi \simeq \frac{1}{\sqrt{N!}} \det(\varphi_i(x_j)) = \varphi_1 \wedge \dots \wedge \varphi_N$$

où $(\varphi_i) \subset L^2(\mathbb{R}^3)$ est une famille orthogonale. Les φ_i s'appellent les orbitales. L'utilisation de cet ansatz donne le modèle de Hartree-Fock. Cette fonctionnelle fut étudiée dans les années 1970 par Lieb et Simon [LS77a]. Dû au principe de Pauli, les orbitales forment un système orthonormé ce qui impose au terme d'énergie cinétique d'être d'ordre $\hbar^2 N^{1+2/d}$ comme le montre l'inégalité de Lieb-Thirring

$$\left\langle \Psi, \left(\sum_{j=1}^N -\Delta_j \right) \Psi \right\rangle \geq C \int_{\Omega} (\rho_{\Psi}^{(1)})^{1+2/d} \geq C \left(\int_{\Omega} \rho_{\Psi}^{(1)} \right)^{1+2/d} |\Omega|^{-\frac{1+2/d}{1+d/2}} \geq CN^{1+2/d},$$

où $\rho_{\Psi}^{(1)}(x) = N \int_{\mathbb{R}^{3(N-1)}} |\Psi|^2(x, x') dx'$ est la densité de particules et $\Psi \in \bigwedge^N H^1(\Omega)$. Pour obtenir une limite non triviale quand $N \rightarrow \infty$, il est donc nécessaire de prendre $\hbar \sim N^{-1/d}$. Ce choix de paramètre pour \hbar peut être justifié dans certaines situations par changement d'échelle. Les modèles limites sont celui de Vlasov qui décrit la dynamique et celui de Thomas-Fermi pour l'énergie fondamentale. Ils furent étudiés respectivement par Braun et Hepp [BH77] et Lieb et Simon [LS77b]. Le modèle de Hartree-Fock est valable dans ce régime mais il converge vers celui de Vlasov.

Cette thèse est constituée de deux parties : la première a pour objet l'étude et la dérivation de la théorie de Gross-Pitaevskii pour le gaz dipolaire, quant à la seconde nous y étudions des limites semi-classiques de grand systèmes fermioniques. Nous allons maintenant donner une description sommaire des résultats obtenus par chapitre.

Partie I : Le gaz de bosons dipolaires

Dans la première partie, nous étudions la dérivation du modèle de Gross-Pitaevskii pour des particules dipolaires. Ce modèle décrit l'état commun des particules d'un gaz de bosons en régime dilué à très basse température. Cette partie est composée de trois chapitres. La dérivation de l'énergie et de l'état fondamental fait l'objet du premier chapitre, et celle de l'évolution temporelle, du second chapitre. Enfin dans le troisième chapitre, nous étudions les minimiseurs de la fonctionnelle de Gross-Pitaevskii comprenant un terme supplémentaire quintique tenant compte des corrections de Lee-Huang-Yang.

L'interaction dipolaire est anisotrope et à longue portée, mais la difficulté principale réside dans le fait qu'elle est partiellement attractive. Les techniques habituelles ne permettent pas de contrôler la partie négative du potentiel. Le modèle effectif associé, en plus du terme d'interaction ponctuel, comprend un terme non-local tenant compte de la longue portée de l'interaction. Le gaz d'atomes dipolaires fait l'objet d'une grande attention en physique expérimentale et en physique théorique où de multiples propriétés exotiques sont attendues. Il a été récemment observé que le spectre d'excitation d'un gaz d'atomes d'erbium comporte un minimum local connu sous le nom de *roton* [CBPF+18]. Ce concept fut introduit par Landau pour expliquer le caractère superfluide de l'hélium.

Chapitre 1 : L'énergie fondamentale d'un gaz de bosons dipolaires. Dans ce premier chapitre, nous considérons le hamiltonien H_N (1) agissant sur $\otimes_s^N L^2(\mathbb{R}^3)$ et nous prenons $\hbar = 1$, $\lambda = N^{-1}$, $\eta > 0$ (les hypothèses précises sur η seront données ultérieurement), $V(x) \rightarrow \infty$ quand $|x| \rightarrow \infty$ et

$$w = w_0 + b\mathbb{1}_{|x|>R}K \quad (3)$$

où $R, b > 0$, $w_0 \in L^1(\mathbb{R}^3)$ et K est le potentiel dipolaire défini par

$$K(x) = \frac{1 - 3\cos^2(\theta_x)}{|x|^3},$$

avec $\cos(\theta_x) = x \cdot \vec{n}/|x|$, où $\vec{n} \in \mathbb{R}^3$ est un vecteur unitaire fixé. C'est le potentiel d'interaction entre deux dipôles alignés dans la direction \vec{n} . Nous montrons que l'énergie fondamentale et les minimiseurs approchés sont donnés par le minimum et les minimiseurs de la fonctionnelle de Gross-Pitaevskii dipolaire

$$\mathcal{E}_{\text{GP}}^{\text{dip}}(u) := \int_{\mathbb{R}^3} |(i\nabla + A)u|^2 + \int_{\mathbb{R}^3} V|u|^2 + \frac{a}{2} \int_{\mathbb{R}^3} |u|^4 + \frac{b}{2} \int_{\mathbb{R}^3} K * |u|^2 |u|^2,$$

où $a = \int_{\mathbb{R}^3} w_0$. Plus précisément, si $e_N = \inf \sigma(H_N/N)$ alors nous montrons

$$\lim_{N \rightarrow \infty} e_N = \inf_{\int_{\mathbb{R}^3} |u|^2 = 1} \mathcal{E}_{\text{GP}}^{\text{dip}}(u)$$

et que les minimiseurs approchés $\langle \Psi_N, H_N \Psi_N \rangle \leq N e_N + o(N)$ vérifient

$$|\Psi_N\rangle\langle\Psi_N| \simeq \int_{\mathcal{M}} |u^{\otimes N}\rangle\langle u^{\otimes N}| d\mu(u)$$

où \mathcal{M} est l'ensemble des minimiseurs de \mathcal{E} et μ est une mesure de probabilité sur cet ensemble. Le sens précis de cette approximation sera expliqué dans la suite. Les techniques utilisées reposent sur des méthodes développées dans [LNR15a], notamment l'utilisation des théorèmes de de Finetti en mécanique quantique.

Chapitre 2 : La dynamique d'un gaz de bosons dipolaires. Ici nous considérons à nouveau le hamiltonien H_N , toujours en prenant $\hbar = 1, \lambda = N^{-1}$ et w donné par (3) mais $A = V = 0$. Nous étudions l'évolution temporelle de la fonction d'onde Ψ_N solution de l'équation de Schrödinger

$$\begin{cases} i\partial_t \Psi_N(t) = H_N \Psi_N(t) \\ \Psi_N(0) = \Psi_{0,N} \end{cases}$$

avec

$$\Psi_{0,N} = u^{\otimes N} \varphi_0 + u^{\otimes N-1} \otimes_s \varphi_1 + u^{\otimes N-2} \otimes_s \varphi_2 + \dots + \varphi_N$$

où $\varphi_k \in \bigotimes_s^k \{u\}^\perp$ pour tout $k \geq 0$. La fonction u représente le condensat tandis que les fonctions φ_k sont des excitations. Nous montrons que dans la limite $N \rightarrow \infty$ cette évolution est donnée par

$$\Psi_N(t) \simeq u(t)^{\otimes N} \varphi_0(t) + u(t)^{\otimes N-1} \otimes_s \varphi_1(t) + u(t)^{\otimes N-2} \otimes_s \varphi_2(t) + \dots + \varphi_N(t)$$

où $u(t)$ est solution de l'équation de Gross-Pitaevskii

$$i\partial_t u(t) = (-\Delta + a|u(t)|^2 + bK * |u(t)|^2)u(t),$$

et l'évolution des excitations est donnée par l'équation de Bogoliubov

$$i\partial_t \Phi(t) = \mathbb{H}(t)\Phi(t)$$

où $\Phi(t) = \bigoplus_{k=1}^{\infty} \varphi_k(t)$ et $\mathbb{H}(t)$ est le hamiltonien de Bogoliubov dont on donnera la définition ultérieurement. La preuve de ce résultat utilise des techniques développées dans [LNSS13; LNS15; NN17].

Chapitre 3 : La fonctionnelle de Gross-Pitaevskii dipolaire quintique Dans ce chapitre nous analysons l'existence de minimiseurs pour la fonctionnelle de Gross-Pitaevskii dipolaire quintique. Elle est donnée par la formule suivante

$$\mathcal{E}_b(u) = \int_{\mathbb{R}^3} |\nabla u|^2 + \frac{1}{2} \int_{\mathbb{R}^3} |u|^4 + \frac{b}{2} \int_{\mathbb{R}^3} K * |u|^2 |u|^2 + \int_{\mathbb{R}^3} |u|^5,$$

où u vérifie la contrainte $\int_{\mathbb{R}^3} |u|^2 = \lambda \geq 0$. Le dernier terme rend la fonctionnelle \mathcal{E}_b bornée inférieurement pour tout choix de b , il permet de tenir compte des corrections dites de Lee-Huang-Yang (LHY). La minimisation de \mathcal{E}_b est utilisée dans la littérature physique pour décrire un état méta-stable dans le régime habituellement instable où le potentiel dipolaire domine l'interaction à courte portée répulsive. Nous montrons l'existence d'une masse critique $\lambda_c(b)$ telle que l'existence de minimiseur soit équivalente à $\lambda \geq \lambda_c(b)$. Nous montrons aussi la régularité de ces minimiseurs.

Partie II : Limites semi-classiques de grands systèmes fermioniques

Le comportement des fermions est entièrement différent de celui des bosons. Le principe d'exclusion de Pauli, qui se traduit par l'anti-symétrie de la fonction d'onde, contraint l'énergie cinétique à croître comme $N^{1+2/d}$ où N est le nombre de particules. On note $\bigwedge_1^N L^2(\mathbb{R}^3) \subset L^2(\mathbb{R}^3)^{\otimes N}$ l'espace des fonctions d'onde antisymétriques. Pour obtenir une limite finie, en plus de prendre $\lambda \sim N^{-1}$ dans le hamiltonien H_N (1) comme précédemment pour les bosons, il est aussi nécessaire que $\hbar \sim N^{-2/d}$. Ce dernier paramètre définit le régime semi-classique dans lequel on décompose l'espace des phases en petits cubes de taille $\sqrt{\hbar}$. Cette heuristique sera rendue rigoureuse plus loin dans cette introduction.

Chapitre 4 : Limite semi-classique de grands systèmes fermioniques à température positive Ce chapitre présente un travail réalisé en collaboration avec Mathieu Lewin et Peter Madsen où l'on étudie un gaz de fermions dans un potentiel confinant à température positive en régime semi-classique. Ce travail est la continuation de l'étude du même système à température nulle [FLS18]. Nous partons à nouveau du hamiltonien H_N et nous considérons l'énergie libre dans l'ensemble canonique

$$\mathcal{E}_{\text{Can}}^{N,\hbar}(\Gamma) = \text{Tr}(H_{N,\hbar}\Gamma) + \frac{1}{\beta} \text{Tr}(\Gamma \log \Gamma),$$

où $\beta > 0$ est la température inverse et $0 \leq \Gamma$ est un opérateur, appelé matrice densité, sur $\bigwedge_1^N L^2(\mathbb{R}^3)$ vérifiant $\text{Tr} \Gamma = 1$. Cet opérateur Γ est la généralisation de la fonction d'onde à température positive, en effet celui-ci peut se décomposer comme

$$\Gamma = \sum_{j \geq 1} \lambda_j |\Psi_j\rangle \langle \Psi_j|$$

où $\Psi_j \in \bigwedge_1^N L^2(\mathbb{R}^3)$, $\lambda_j \geq 0$ pour tout $j \geq 1$ et $\sum_{j \geq 1} \lambda_j = 1$. Le Hamiltonien H_N est donné par (1) où l'on prend pour simplifier cette introduction $\eta = 0$ mais nous traitons aussi le cas dilué $\eta > 0$ comme nous l'expliquerons plus loin.

Le minimiseur de ce problème est donnée par $\Gamma_{N,\hbar,\beta} = Z^{-1} e^{-\beta H_{N,\hbar}}$ où Z est une constante de normalisation appelée fonction de partition. Nous montrons que les minimiseurs approchés Γ_N vérifient

$$\Gamma_N \simeq m_0^{\otimes N} \tag{4}$$

quand $N \rightarrow \infty$, $\lambda N \rightarrow 1$ et $\hbar^d N \rightarrow \rho > 0$ et où m_0 est la mesure sur l'espace des phases $L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ qui minimise la fonctionnelle de Vlasov

$$\begin{aligned} \mathcal{E}_{\text{Vla}}^{\beta,\rho}(m) &= \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} (|p + A(x)|^2 + V(x)) m(x, p) \, dx \, dp \\ &+ \frac{1}{2\rho} \iint_{\mathbb{R}^{2d}} w(x - y) \rho_m(x) \rho_m(y) \, dx \, dy \\ &+ \frac{1}{(2\pi)^d \beta} \iint_{\mathbb{R}^{2d}} s(m(x, p)) \, dx \, dp, \end{aligned}$$

où $0 \leq m \leq 1$ vérifie $(2\pi)^{-d} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} m = \rho$ et $s(x) = x \log x + (1 - x) \log(1 - x)$ est l'entropie fermionique. La contrainte ponctuelle sur m et la forme de l'entropie sont ce qu'il reste, à la limite, de la nature fermionique des systèmes initiaux, autrement dit du principe de Pauli. Ce modèle est utilisé pour décrire des atomes lourds ou encore les étoiles à neutron.

Chapitre 5 : La correction de Scott pour le modèle de Dirac-Fock Ce dernier chapitre est la présentation d'un travail réalisé en collaboration avec Søren Fournais et Mathieu Lewin. Nous donnons la dérivation de la correction de Scott pour le modèle de Dirac-Fock.

Considérons le hamiltonien H_N (1) avec $A = 0$, $V(x) = N/|x|$, $w(x) = 1/|x|$, $\eta = 0$, $\lambda = 1$ et $\hbar^2 = 1/2$. Le premier ordre est donné par la très célèbre théorie de Thomas-Fermi qui fut dérivée des premiers principes par Lieb et Simon dans les années 1970 [LS73; LS77a; LS77b; Lie81a] :

$$E(N, Z = N) = e_{\text{TF}} Z^{7/3} + \frac{1}{2} Z^2 + o(N^2),$$

où e_{TF} est l'énergie de Thomas-Fermi et est définie par

$$e_{\text{TF}} = \min_{\substack{\rho \geq 0 \\ \int_{\mathbb{R}^3} \rho = 1}} \left\{ \frac{3}{10} (3\pi^2)^{2/3} \int_{\mathbb{R}^3} \rho(x)^{5/3} dx - \int_{\mathbb{R}^3} \frac{\rho(x)}{|x|} dx + \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho(x)\rho(y)}{|x-y|} dx dy \right\}.$$

Le second terme est appelé la correction de Scott. Cette dernière est créée par un petit nombre d'électrons proches de la singularité du potentiel coulombien à l'origine où se trouve le noyau. Ces électrons ont par conséquent une très grande vitesse, il n'est donc pas satisfaisant de les considérer comme des particules non-relativistes. Pour cela, nous considérons ce nouveau Hamiltonien

$$\sum_{j=1}^N \left(c\boldsymbol{\alpha} \cdot \mathbf{p} + c^2\beta - \frac{Z}{|x|} - c^2 \right)_j + \sum_{1 \leq j < k \leq N} \frac{1}{|x_j - x_k|}, \quad (5)$$

où c est la vitesse de la lumière. L'opérateur $D_0 := c\boldsymbol{\alpha} \cdot \mathbf{p} + c^2\beta$ est non borné inférieurement, son spectre est donné par $\sigma(D_0) =]-\infty, -1] \cup [1, \infty[$ et une des conséquences est que l'opérateur à de Dirac à N corps (48) n'est pas bien défini pour l'interaction coulombienne. Pour cette raison, nous considérons directement la fonctionnelle de Dirac-Fock réduite

$$\mathcal{E}_{\text{DF}}(\gamma) = \text{Tr} \left(D_0 - \frac{1}{|x|} - 1 \right) \gamma + \frac{1}{2N} D(\rho_\gamma, \rho_\gamma)$$

où $\rho_\gamma(x) = \gamma(x, x)$. La matrice densité γ vérifie $0 \leq \gamma \leq 1$, $\text{Tr} \gamma \leq N$ ainsi que la contrainte non-linéaire suivante

$$0 \leq \gamma \leq \mathbf{1} \left(D_0 - \frac{\kappa}{|x|} + \alpha \rho_\gamma * \frac{1}{|x|} \right).$$

Cette dernière s'interprète comme le fait que l'espace d'état des électrons correspond au sous-espace d'énergies positives de l'opérateur de Dirac. Ici nous avons choisi de prendre l'espace d'énergies positives de l'opérateur de Dirac-Coulomb auquel est ajouté le champ moyen créé par les électrons eux-mêmes. Précédemment, des modèles avec les projecteurs associés à l'opérateur de Dirac libre et à l'opérateur de Dirac-Coulomb ont été étudiés. Nous montrons que dans la limite $N \rightarrow \infty$ et $\alpha N \rightarrow 1$, la correction de Scott du modèle de Dirac-Fock coïncide avec celle donnée par le modèle de Dirac-Coulomb

$$c_{\text{Scott}}(\kappa) := \frac{\kappa^2}{2} + \sum_{n \geq 1} \left\{ \lambda_n \left(D_0 - \frac{\kappa}{|x|} - 1 \right) - \lambda_n \left(-\frac{\Delta}{2} - \frac{\kappa}{|x|} \right) \right\},$$

où les λ_n sont les valeurs propres dans $[-2, 0]$ de l'opérateur entre parenthèses, répétées en cas de multiplicité, et dans l'ordre croissant.

Avant de passer à une présentation plus en profondeur de ces différentes parties, nous synthétisons les différentes situations évoquées jusqu'ici par le schéma suivant.

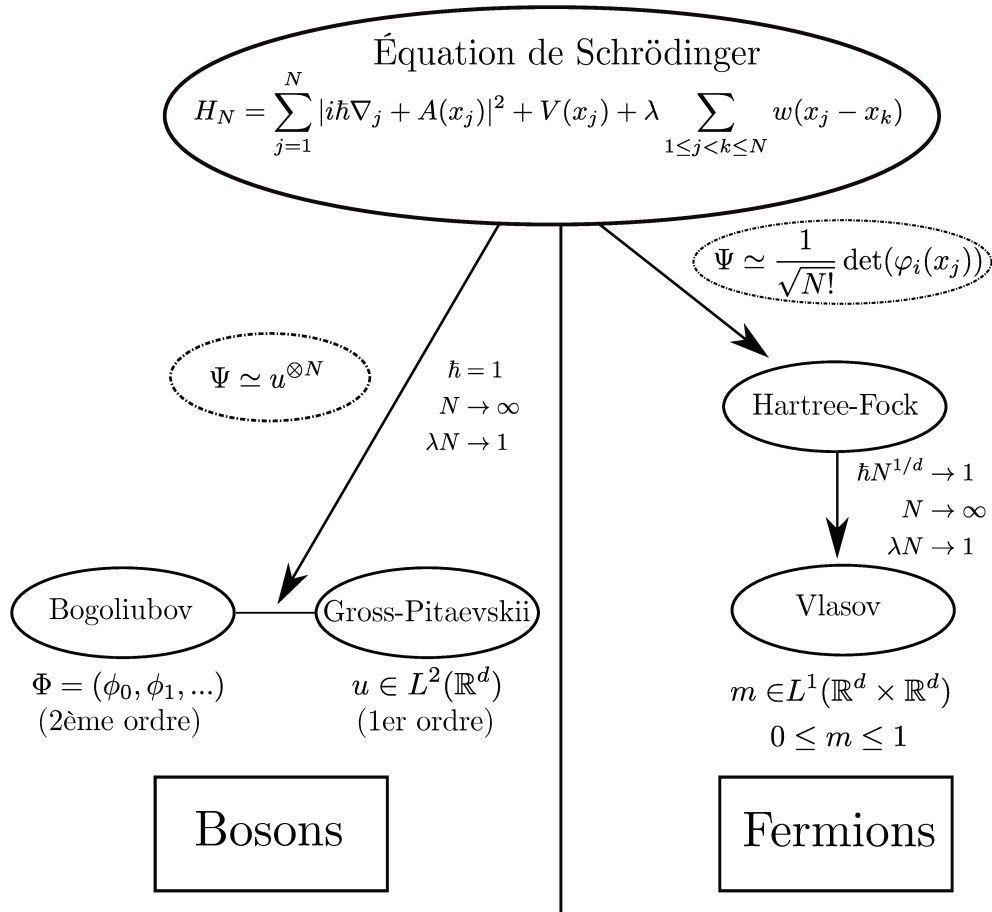


Figure 1 – Les différents régimes et les modèles effectifs associés

Nous passons maintenant à une présentation plus détaillée des résultats ainsi que du contexte dans lequel ils se placent. Dans la partie I nous regroupons les travaux concernant les gaz de bosons. Nous débutons par une introduction à la théorie de Gross-Pitaevskii suivie d'une discussion sur la stabilité des systèmes de particules dipolaires. Ensuite nous présentons successivement, les résultats des chapitres 1, 2 et 3 de la thèse concernant respectivement la dérivation de l'énergie fondamentale, de la dynamique et l'étude de la fonctionnelle de Gross-Pitaevskii dipolaire avec corrections de Lee-Huang-Yang. La partie II concerne nos travaux sur les limites semi-classiques de grands systèmes fermioniques. Plus précisément nous donnons d'abord les résultats obtenus au chapitre 4 sur les limites semi-classiques à température positive ainsi que ceux obtenus au chapitre 5 sur la correction de Scott pour le modèle de Dirac-Fock.

I. Condensation de Bose-Einstein : la théorie de Gross-Pitaevskii

La condensation de Bose-Einstein est un phénomène quantique où dans un gaz de bosons, en-deçà d'une température critique, un état particulier est occupé par une proportion macroscopique des particules et tend à contenir l'ensemble des particules quand la température continue de décroître. Il fut prédit par Bose pour les photons et généralisé par Einstein pour un gaz de particules idéales, c'est-à-dire sans interaction. Comme expliqué précédemment, la fonction d'onde d'un système bosonique est, par définition, invariante par permutation des particules.

$$\Psi(x_1, \dots, x_N) = \Psi(x_{\sigma(1)}, \dots, x_{\sigma(N)}), \quad \forall \sigma \in \mathfrak{S}(\{1, \dots, N\})$$

Pour un système sans interaction, où le hamiltonien d'une particule est h , l'énergie et l'état fondamentaux du Hamiltonien à N corps

$$\sum_{j=1}^N \mathbf{1} \otimes \dots \otimes h \otimes \dots \mathbf{1}$$

où dans le j^{me} terme de la somme h apparaît en j^{me} position, sont donnés respectivement par $N\lambda_0$ et $\Psi = \psi_0^{\otimes N}$ où $\lambda_0 = \inf \sigma(h)$ et ψ_0 le vecteur propre associé (en supposant λ_0 non dégénérée). Mais qu'en est-il dans les systèmes réels où les particules interagissent (faiblement) et sont corrélées ? Dans les années 1960, on calcule par des méthodes perturbatives des modèles décrivant le gaz avec interaction, en particulier l'équation de Gross-Pitaevskii qui est l'objet de notre étude. Mais il a fallu attendre 1995 et l'expérience de Cornell et Wieman [AEMWC95], pour observer pour la première fois un condensat d'atomes de Rubidium. Outre l'exploit expérimental et l'attribution du prix Nobel de Physique à ses auteurs, cette expérience est une victoire pour la mécanique quantique fondamentale qui voit ses prédictions validées. Elle crée aussi un regain d'intérêt dans la communauté mathématique pour la dérivation à partir des premiers principes de modèles effectifs déjà utilisés dans la communauté physique. Dès 1998, Lieb et Yngvason obtiennent de manière rigoureuse l'expression de l'énergie fondamentale d'un condensat de Bose-Einstein [LY98] améliorant le résultat de Dyson [Dys57] qui donnait une borne inférieure du bon ordre de grandeur mais trop petite d'un facteur 14. Il s'ensuit un engouement très fort et une quantité très importante de travaux sur la dérivation du modèle de Gross-Pitaevskii et du modèle de Bogoliubov, qui décrivent respectivement le premier et le second ordre d'un gaz de bosons. Parmi les problématiques usuelles, on peut citer la dérivation de l'énergie fondamentale, de l'état fondamental ou des minimiseurs approchés, la description de l'évolution temporelle ou encore le calcul du spectre d'excitation.

I.1 Le modèle de Gross-Pitaevskii

Considérons un gaz de N bosons soumis à un potentiel confinant $V : \mathbb{R}^3 \rightarrow \mathbb{R}$, tel que $V(x) \rightarrow \infty$ quand $|x| \rightarrow \infty$ et interagissant via un potentiel $w : \mathbb{R}^3 \rightarrow \mathbb{R}$. Le hamiltonien du système est le suivant

$$H_N = \sum_{j=1}^N -\Delta_{x_j} + V(x_j) + \lambda \sum_{1 \leq j < k \leq N} w(x_j - x_k), \quad (6)$$

où λ est un paramètre de couplage. Il agit sur $\bigvee_{j=1}^N L^2(\mathbb{R}^3)$, le produit tensoriel symétrique de N copies de $L^2(\mathbb{R}^3)$. Un état totalement condensé est de la forme $\Psi = u^{\otimes N}$, où u est une fonction

d'onde à un corps dans $L^2(\mathbb{R}^3)$, son énergie par particule est donnée par l'énergie de Hartree

$$\frac{\langle u^{\otimes N}, H_N u^{\otimes N} \rangle}{N} = \int_{\mathbb{R}^3} |\nabla u|^2 + \int_{\mathbb{R}^3} V|u|^2 + \frac{(N-1)\lambda}{2} \int_{\mathbb{R}^3} w * |u|^2 |u|^2 =: \mathcal{E}_{\text{Hartree}}(u). \quad (7)$$

Il apparaît qu'une condition nécessaire à ce que la quantité ci-dessus possède une limite quand le nombre de particules N croît est de choisir

$$\lambda \sim \frac{1}{N},$$

c'est l'approximation de champ moyen. Cet artefact mathématique peut néanmoins trouver sa justification en invoquant des arguments de dilatations de l'espace, par exemple si w est le potentiel coulombien. Dans ce régime, dit de Hartree, la distance interparticulaire moyenne $N^{-1/3}$ est beaucoup plus petite que la portée de l'interaction qui est d'ordre 1 : les collisions sont fréquentes mais de faible intensité à cause du facteur λ .

Dans le régime dilué, ou régime de Gross-Pitaevskii, les particules interagissent plus rarement mais fortement. Cela est modélisé en dilatant le potentiel d'interaction

$$w_N(x-y) = N^3 w(N(x-y)).$$

Remarquons tout d'abord que cette dilatation préserve la norme $L^1(\mathbb{R}^3)$. La portée de l'interaction est alors d'ordre N^{-1} , ce qui est petit comparé à la distance moyenne entre les particules. Insérons ce potentiel modifié dans la fonctionnelle de Hartree et prenons la limite $N \rightarrow \infty$, on obtient alors la fonctionnelle de Gross-Pitaevskii :

$$\mathcal{E}_{\text{GP}}(u) := \int_{\mathbb{R}^3} |\nabla u|^2 + \int_{\mathbb{R}^3} V|u|^2 + \frac{a}{2} \int_{\mathbb{R}^3} |u|^4,$$

où $a = \int_{\mathbb{R}^3} w$. En réalité, le gaz de bosons en interaction ne se comporte pas exactement comme $u^{\otimes N}$ et en conséquence la constante a apparaissant dans les modèles physiques n'est pas $\int_{\mathbb{R}^3} w$ mais la longueur de diffusion du potentiel w qui est strictement plus petite [LSSY05].

Enfin, il existe une classe d'interpolation entre ces deux régimes que l'on peut paramétrer par $0 \leq \beta \leq 1$, en prenant

$$w_N(x-y) = N^{3\beta} w(N^\beta(x-y)).$$

Il est suspecté (et parfois établi) que tant que $\beta < 1$, le paramètre a devant le terme d'interaction dans \mathcal{E}^{GP} est donné par $\int_{\mathbb{R}^3} w$.

La théorie de Gross-Pitaevskii prétend prédire l'énergie fondamentale

$$e_N := \inf \sigma \left(\frac{H_N}{N} \right),$$

l'état fondamental

$$H_N \Psi_N = N e_N \Psi_N,$$

ainsi que l'évolution temporelle d'un condensat de Bose-Einstein

$$i\partial_t \Psi_N(t) = H_N \Psi_N(t). \quad (8)$$

Supposons que le potentiel d'interaction soit donné par w_N et que $\lambda \sim N^{-1}$ dans (6). Les

problématiques suivantes ont fait l'objet d'une grande attention dans la littérature. Nous les rappelons avant d'expliquer en quoi nous voulons les généraliser.

1. Montrer que

$$\lim_{N \rightarrow \infty} e_N = \inf_{\int_{\mathbb{R}^3} |u|^2 = 1} \mathcal{E}^{\text{GP}}(u).$$

2. Montrer que si (Ψ_N) est une suite de minimiseurs approchés, c'est-à-dire

$$\langle \Psi_N, H_N \Psi_N \rangle \leq N e_N + o(N),$$

alors

$$\lim_{N \rightarrow \infty} \text{Tr}_{2 \rightarrow N} |\Psi_N\rangle \langle \Psi_N| = |u_0\rangle \langle u_0|,$$

où $\text{Tr}_{2 \rightarrow N}$ est la trace partielle sur toutes les variables sauf une et u_0 est le minimiseur de \mathcal{E}^{GP} .

3. Montrer que si

$$\text{Tr}_{2 \rightarrow N} |\Psi_N(0)\rangle \langle \Psi_N(0)| = |u(0)\rangle \langle u(0)| + o(1)$$

pour un certain $u(0) \in H^1(\mathbb{R}^3)$ en norme de trace (par exemple), alors

$$\text{Tr}_{2 \rightarrow N} |\Psi_N(t)\rangle \langle \Psi_N(t)| = |u(t)\rangle \langle u(t)| + o(1)$$

où respectivement $\Psi_N(t)$ est solution de l'équation de Schrödinger (8) et $u(t)$ est la solution à l'équation de Gross-Pitaevskii

$$i\partial_t u(t) = (-\Delta + V + a|u(t)|^2) u(t).$$

4. Donner une description dans $L^2(\mathbb{R}^{3N})$ de la fonction d'onde $\Psi_N(t)$.

La trace partielle intervenant dans ces énoncés est la bonne manière de comparer Ψ à u . Une compréhension plus fine de u (question 4) est plus délicate.

I.2 L'interaction dipolaire

Pour le moment, nous sommes resté assez vague sur les hypothèses concernant le potentiel d'interaction w . L'heuristique que l'on vient de présenter pour justifier la pertinence de \mathcal{E}_{GP} supposait tout de même $w \in L^1(\mathbb{R}^3)$ de sorte que $w_N * |u|^2 \rightarrow (\int_{\mathbb{R}^3} w) |u|^2$. Dans le régime dilué, si le potentiel d'interaction est à courte portée il devient à la limite une interaction de contact. L'objet de notre travail a été d'étendre les résultats mentionnés dans la partie précédente au cas de particules dipolaires. Rappelons que le potentiel d'interaction entre deux dipôles alignés dans la même direction, fixée par $\vec{n} \in \mathbb{R}^3$, est donné par

$$K(x) = \frac{1 - 3 \cos^2(\theta_x)}{|x|^3}, \quad (9)$$

où $\cos(\theta_x) = x \cdot \vec{n} / |x|$. Remarquons dans un premier temps que ce potentiel n'est pas dans $L^1(\mathbb{R}^3)$ et que la dilatation appliquée précédemment à w laisse K invariant. En réalité, l'expression ci-dessus est l'approximation au premier ordre d'un système de 4 charges coulombiennes, constituant les dipôles, quand les dipôles sont éloignés d'une distance grande devant leur taille. Pour cette raison, nous nous intéressons aux potentiels donnés de la forme

$$w = w_0 + \mathbb{1}_{|x| > R} K(x) \quad (10)$$

où $w_0 \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ et où $R > 0$ est choisi arbitrairement. La fonctionnelle de Hartree pour ce nouveau potentiel converge vers la fonctionnelle de Gross-Pitaevskii généralisée (ou dipolaire)

$$\mathcal{E}_{\text{GP}}^{\text{dip}}(u) := \int_{\mathbb{R}^3} |\nabla u|^2 + \int_{\mathbb{R}^3} V|u|^2 + \frac{a}{2} \int_{\mathbb{R}^3} |u|^4 + \frac{b}{2} \int_{\mathbb{R}^3} K * |u|^2 |u|^2, \quad (11)$$

où b est un paramètre qui dans les modèles physiques est proportionnel au carré du moment des dipôles. On remarquera que la fonctionnelle limite ne dépend pas du choix de $R > 0$, ceci est dû au fait que

$$\int_{\mathbb{S}^2} (1 - 3 \cos^2(\theta_x)) d\sigma(x) = 0$$

et que la partie L^1 (à courte portée) du potentiel se réduit, à la limite, à $\int_{\mathbb{R}^3} w_0$ dans le régime considéré. Ce potentiel ne satisfait pas aux hypothèses habituellement utilisées dans la littérature mathématique. Tout d'abord, ni le potentiel K , ni le potentiel tronqué $\mathbf{1}_{|x|>R}K$, ne sont intégrables. Par ailleurs, le potentiel total w est partiellement attractif et cela complique l'analyse mathématique mais est aussi à l'origine des propriétés atypiques du gaz dipolaire.

Malgré la non intégrabilité du potentiel dipolaire, la convolution par K est une opération continue dans tous les $L^p(\mathbb{R}^3)$ pour $1 < p < \infty$. En particulier, pour $p = 2$, elle est unitairement équivalente à la multiplication par une fonction bornée, autrement dit $\widehat{K} \in L^\infty(\mathbb{R}^3)$.

Une seconde difficulté, et beaucoup plus grande, provient de la nature attractive de l'interaction. Elle met en jeu la stabilité du système. En effet, il est non trivial de montrer que pour un potentiel non positif w , il existe une constante $C > 0$, indépendante de N , telle que

$$H_N \geq -CN. \quad (12)$$

Cette condition est en particulier nécessaire pour espérer pouvoir obtenir la fonctionnelle de Gross-Pitaevskii $\mathcal{E}_{\text{dip}}^{\text{GP}}$ à la limite. La propriété ci-dessus est en réalité très importante car elle garantit que l'énergie cinétique par particule reste bornée. En plus d'être une condition physique raisonnable, cela permet, d'un point de vue mathématique, de montrer la compacité des suites minimisantes.

Les systèmes coulombiens, même entre particules de charges opposées, sont naturellement très stables. Cela s'explique par la positivité de la transformée de Fourier de $1/|x|$:

$$\mathcal{F}\left(\frac{1}{|x|}\right)(k) = \frac{1}{4\pi|k|^2} \geq 0.$$

En effet, remplaçons pour simplifier $1/|x|$ par un potentiel plus lisse $0 \leq \widehat{w} \in L^1(\mathbb{R}^3)$, ce qui revient à enlever la singularité à l'origine, alors le potentiel d'interaction de N particules, positionnées en $x_1, \dots, x_N \in \mathbb{R}^3$, de charges respectives $e_1, \dots, e_N \in \{\pm 1\}$ est donné par

$$\sum_{1 \leq j < k \leq N} e_j e_k w(x_j - x_k) = \int_{\mathbb{R}^3} \widehat{w}(p) \left| \sum_{j=1}^N e^{ip \cdot x_j} \right|^2 dp - w(0)N.$$

Un tel potentiel vérifie la propriété suivante, que l'on nomme *stabilité classique*,

$$\sum_{1 \leq j < k \leq N} w(x_j - x_k) \geq -CN, \quad (13)$$

pour une certaine constante $C > 0$ indépendante de N . Malgré les $N(N-1)$ termes dans la

sommes ci-dessus, celle-ci ne peut diverger vers $-\infty$ qu'au plus proportionnellement à N . Un exemple simple de potentiel classiquement stable est donné par $w = w_1 + w_2$ où $w_1 \geq 0$ et $0 \leq \widehat{w}_2 \in L^1(\mathbb{R}^3)$.

Comme énoncé précédemment, le potentiel dipolaire est l'approximation au premier ordre d'un système coulombien. Il est donc naturel de considérer des potentiels w_0 tels que le potentiel défini par (5) soit classiquement stable. Nous montrerons que, sous certaines hypothèses génériques sur w_0 , le potentiel w est en effet classiquement stable.

Dans le régime qui nous intéresse, où le potentiel apparaissant dans le Hamiltonien H_N est $w_N = N^{3\beta}w(N^\beta \cdot)$, la stabilité classique de w assure la stabilité du second type (12) pour $\beta \leq 1/3$. Nous montrerons qu'un système confiné est stable pour des valeurs de β légèrement supérieures.

I.3 La dérivation de la théorie de Gross-Pitaevskii pour l'énergie fondamentale

Dans cette section nous présentons les résultats obtenus dans le Chapitre 1 et qui font l'objet de la publication [Tri18].

L'originalité de notre travail consiste à étudier la dérivation de la théorie de Gross-Pitaevskii pour une classe particulière de potentiels à longue portée, dont le potentiel dipolaire défini en (9) est un cas particulier. Nous commençons par définir cette classe, soit $q > 1$ et $\Omega \in L^q(\mathbb{S}^2)$ une fonction paire vérifiant

$$\int_{\mathbb{S}^2} \Omega(x) d\sigma(x) = 0, \quad (14)$$

on définit

$$K(x) = \frac{\Omega(x/|x|)}{|x|^3}. \quad (15)$$

Alors pour tout $f \in L^p(\mathbb{R}^3)$, pour tout $p \in]1, \infty[$ il existe une constante $C_p > 0$ telle que pour tout $\varepsilon > 0$

$$\|(K\mathbb{1}_{|x|>\varepsilon}) * f\|_{L^p(\mathbb{R}^3)} \leq C_p \|\Omega\|_{L^q(\mathbb{S}^2)} \|f\|_{L^p(\mathbb{R}^3)}$$

et pour presque tout $x \in \mathbb{R}^3$ la limite suivante existe

$$\lim_{\varepsilon \rightarrow 0} (K\mathbb{1}_{|x|>\varepsilon}) * f(x) =: K * f(x).$$

On a aussi

$$\|K * f\|_{L^p(\mathbb{R}^3)} \leq C_p \|\Omega\|_{L^q(\mathbb{S}^2)} \|f\|_{L^p(\mathbb{R}^3)}.$$

En particulier $\widehat{K} \in L^\infty(\mathbb{R}^3)$.

Nous pouvons maintenant présenter notre premier résultat sur les propriétés de la fonctionnelle de Gross-Pitaevskii généralisée. Pour le cas dipolaire, elle a déjà fait l'objet de travaux théoriques et numériques [CMS08; BCW10; BAC12; CH15a]. Le théorème suivant est donc une généralisation aux potentiels de la forme (3). Nous commençons par quelques définitions. Pour $a, b \in \mathbb{R}$, $V \in L^1_{\text{loc}}(\mathbb{R}^3)$ et $A \in L^2_{\text{loc}}(\mathbb{R}^3)$, définissons la fonctionnelle de Gross-Pitaevskii généralisée (ou dipolaire)

$$\mathcal{E}_{a,b}^{\text{GP}}(u) := \int_{\mathbb{R}^3} |(i\nabla + A)u|^2 + \int_{\mathbb{R}^3} V|u|^2 + \frac{a}{2} \int_{\mathbb{R}^3} |u|^4 + \frac{b}{2} \int_{\mathbb{R}^3} K * |u|^2 |u|^2, \quad (16)$$

ainsi que son énergie fondamentale

$$e_{\text{GP}}(a, b) = \inf_{\int_{\mathbb{R}^3} |u|^2 = 1} \mathcal{E}_{a,b}^{\text{GP}}(u).$$

Le premier résultat du Chapitre 1 est le suivant.

Théorème 1 (Minimisation de la fonctionnelle de Gross-Pitaevskii généralisée, [Tri18]). *Soient $V \in L^1_{\text{loc}}(\mathbb{R}^3)$, $A \in L^2_{\text{loc}}(\mathbb{R}^3)$ tels qu'il existe $s, C > 0$ tel que $V(x) \geq C^{-1}(|A(x)|^2 + |x|^s) - C$.*

1. Si

$$\begin{cases} b > 0 \text{ et } a \geq b (\inf \widehat{K})_-, \\ \text{ou} \\ b < 0 \text{ et } a \geq -b (\sup \widehat{K})_+, \end{cases} \quad (17)$$

alors $e_{\text{GP}}(a, b) > -\infty$ et $\mathcal{E}_{a,b}^{\text{GP}}$ possède des minimiseurs.

2. Si

$$\begin{cases} b > 0 \text{ and } a < b (\inf \widehat{K})_-, \\ \text{ou} \\ b < 0 \text{ and } a < -b (\sup \widehat{K})_+, \end{cases} \quad (18)$$

alors $e_{\text{GP}}(a, b) = -\infty$.

Ce résultat donne une caractérisation de la stabilité de $\mathcal{E}_{\text{GP}}^{a,b}$, il faut que l'interaction à courte portée soit suffisamment répulsive pour contrebalancer l'attraction due aux dipôles. En fait, cette condition de stabilité est comparable à la stabilité classique (13) du problème à N corps. Considérons la fonctionnelle de Hartree (7), avec w_N , qui est l'énergie par particule d'un état entièrement factorisé $u^{\otimes N}$ pour $u \in H^1(\mathbb{R}^3)$ et fournit par conséquence une borne supérieure à l'énergie fondamentale du problème à N corps. Par un argument de dilatation, on observe que la stabilité de la fonctionnelle de Hartree équivaut à

$$\iint_{\mathbb{R}^3 \times \mathbb{R}^3} w(x-y) |u(x)|^2 |u(y)|^2 dx dy \geq 0, \quad \forall u \in H^1(\mathbb{R}^3). \quad (19)$$

Cette condition se déduit de stabilité classique (13) en testant avec $u^{\otimes N}$ et en prenant la limite $N \rightarrow \infty$. Réciproquement, si $w(0) < \infty$, on peut retrouver (13) à partir de (19) en prenant

$$u(x) = \sum_{j=1}^N \lambda^{-3/2} f(\lambda^{-1}(x - x_j))$$

dans (19), où f est une fonction C^∞ à support compact, et en passant à la limite $\lambda \rightarrow 0$. Pour conclure, en prenant dans (19) la fonction $\lambda^{-3/2} u(\lambda^{-1} \cdot)$ et en passant à la limite $\lambda \rightarrow \infty$ on retrouve la condition de stabilité du Théorème 1.

Considérons le Hamiltonien

$$H_N = \sum_{j=1}^N |i\nabla_j + A(x_j)|^2 + V(x_j) + \frac{1}{N} \sum_{1 \leq j < k \leq N} N^{3\beta} w(N^\beta(x_j - x_k)). \quad (20)$$

Le résultat principal du Chapitre 1 est le suivant.

Théorème 2 (Dérivation de la théorie de Gross-Pitaevskii dipolaire, [Tri18]). *Soit $A \in L^2_{loc}(\mathbb{R}^3)$ et $0 \leq V \in L^1_{loc}(\mathbb{R}^3)$ tels que*

$$V(x) \geq C^{-1}(|A(x)|^2 + |x|^s) - C, \quad \forall x \in \mathbb{R}^3.$$

Soit $K = \Omega(x/|x|)|x|^{-3}$ avec $\Omega \in L^q(\mathbb{S}^2)$, où $q \geq 2$, une fonction paire vérifiant (14). Soit w , $R > 0$ et $b \in \mathbb{R}$, tels que

$$w - b\mathbb{1}_{|x|>R}K \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3).$$

Nous supposons que w est classiquement stable (13).

Si

$$\beta < \frac{1}{3} + \frac{s}{45 + 42s} \quad (21)$$

alors

$$\boxed{\lim_{N \rightarrow \infty} e_N = e_{GP}(a, b),} \quad (22)$$

où

$$a = \int_{\mathbb{R}^3} (w(x) - b\mathbb{1}_{|x|>R}K(x)) \, dx.$$

De plus, a et b vérifient la condition (17).

Nous montrons aussi la convergence des minimiseurs qui est en fait une conséquence de la convergence de l'énergie fondamentale. Toutes les particules ne sont pas dans le même état $u_0 \in L^2(\mathbb{R}^3)$ mais seulement une proportion macroscopique d'entre elles. De plus, $\Psi_N \in \mathcal{H}^{\otimes_s N}$ n'est pas dans le même espace pour tout $N \geq 1$. Pour ces raisons, nous exprimons la convergence des minimiseurs en terme des traces partielles qui sont l'équivalent quantique des marginales pour les probabilités classiques. Nous notons $\gamma_{\Psi}^{(k)} := \text{Tr}_{k+1 \rightarrow N} |\Psi\rangle \langle \Psi|$ la matrice densité à k corps de Ψ , elle est définie par dualité

$$\text{Tr}_{\mathcal{H}^{\otimes_s k}} (A \gamma_{\Psi}^{(k)}) = \langle \Psi, A \otimes 1_{N-k} \Psi \rangle,$$

pour tout opérateur borné A sur $\mathcal{H}^{\otimes_s k}$.

Theorem 3 (Convergence des états, [Tri18]). *Sous les hypothèses du Théorème 2, si (Ψ_N) est une suite de minimiseurs, alors il existe une mesure de probabilité de Borel μ supportée sur $\mathcal{M}_{GP}(a, b)$, l'ensemble des minimiseurs de $\mathcal{E}_{GP}^{a,b}$, et une sous-suite (N') telle que,*

$$\gamma_{\Psi_{N'}}^{(k)} \xrightarrow{N' \rightarrow \infty} \int_{\mathcal{M}_{GP}} |u^{\otimes k}\rangle \langle u^{\otimes k}| \, d\mu(u), \quad \forall k \geq 1, \quad (23)$$

où la convergence est en norme de trace. De plus, si $\mathcal{E}_{GP}^{a,b}$ possède un unique minimiseur alors la suite $(\gamma_{\Psi_N}^{(k)})_N$ converge entièrement dans (23).

La méthode utilisée pour prouver le Théorème 2 utilise le résultat suivant de [LNR17], initialement prouvé par [CKMR07]. Tout d'abord notons $\gamma_{\Psi}^{(k)} = \text{Tr}_{k+1 \rightarrow N} |\Psi\rangle \langle \Psi|$ la matrice densité d'ordre k de $\Psi \in \mathcal{H}^N := \otimes_s^N L^2(\mathbb{R}^3)$, pour $k \geq 1$.

Théorème 4 (Théorème de de Finetti quantique en dimension finie avec estimée, [LNR17]). *Soit $\Psi \in \mathcal{H}^N$ et P un projecteur orthogonal de rang fini. Alors, il existe une mesure de Borel*

positive $d\mu_\Psi$ sur la sphère unité $SP\mathcal{H}$ telle que

$$\mathrm{Tr}_{\mathcal{H}} \left| P^{\otimes 2} \gamma_\Psi^{(2)} P^{\otimes 2} - \int_{SP\mathcal{H}} |u^{\otimes 2}\rangle \langle u^{\otimes 2}| d\mu_\Psi(u) \right| \leq \frac{8 \dim P\mathcal{H}}{N} \quad (24)$$

et

$$\int_{SP\mathcal{H}} d\mu_\Psi(u) \geq \left(\mathrm{Tr} P \gamma_\Psi^{(1)} \right)^2.$$

Les théorèmes de de Finetti nous indiquent que les états bosoniques, quand le nombre de particules est grand, convergent *naturellement* vers des moyennes d'états produits. Pour une revue de l'utilisation de ces théorèmes en mécanique des atomes ultra-froids, le lecteur est invité à lire [Rou15b]. Le Théorème 4 donne une estimée sur la distance entre la matrice densité à deux corps d'un état à N particules et une combinaison convexe d'états produits. Ainsi, en reformulant

$$\frac{\langle \Psi_N H_N \Psi_N \rangle}{N} = \frac{1}{2} \mathrm{Tr}_{\mathcal{H}^2} \gamma_{\Psi_N}^{(2)} (|i\nabla_x + A(x)|^2 + V(x) + |i\nabla_y + A(y)|^2 + V(y) + N^{3\beta} w(N^\beta(x-y)))$$

il ne reste plus qu'à projeter $\gamma_{\Psi_N}^{(2)} \simeq P^{\otimes 2} \gamma_{\Psi_N}^{(2)} P^{\otimes 2}$ sur un sous-espace de dimension finie pour pouvoir appliquer le Théorème 4. Un choix naturel de projecteur est $P = \mathbb{1}_{(-\infty, L)}(|i\nabla_x + A(x)|^2 + V(x))$ et $L > 0$, puisqu'il est raisonnable de supposer que l'énergie cinétique des particules reste bornée. Puisque l'opérateur $|i\nabla_x + A(x)|^2 + V(x)$ est à résolvante compacte, le seul défaut de compacité pour les suites minimisantes provient du terme d'interaction. Cet éventuel défaut de compacité permettrait au système de vivre sur un grand espace, obligeant à choisir un niveau d'énergie L grand, et affaiblissant l'estimée (24). Ceci souligne l'importance de l'hypothèse de stabilité classique (13).

I.4 Théorie de Gross-Pitaevskii et de Bogolyubov : dérivation de la dynamique

Cette section présente les résultats de l'article soumis [Tri19a] et faisant l'objet du Chapitre 2.

Nous considérons l'évolution temporelle de N particules dipolaires décrites par une fonction d'onde $\Psi_N(t) \in \bigoplus_s^N L^2(\mathbb{R}^3)$ vérifiant l'équation de Schrödinger

$$i\partial_t \Psi_N(t) = H_N \Psi_N(t), \quad (25)$$

où le Hamiltonien est donné par

$$H_N = \sum_{j=1}^N \Delta_j + \frac{1}{N} \sum_{j < k} w_N(x_j - x_k)$$

où $w_N = N^{3\beta} w(N^\beta \cdot)$, $w - b\mathbb{1}_{|x| > R} K \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$, $R > 0$ et $0 < \beta < 1$.

Nous nous intéressons à la validité de la théorie de Gross-Pitaevskii et de celle de Bogolyubov. Elles prétendent décrire respectivement le premier et le second ordre de l'évolution temporelle de la fonction d'onde d'un gaz condensé $\Psi_N(t)$. De manière heuristique, si le système est à l'instant initial dans l'état $\Psi_N(0) \simeq u(0)^{\otimes N}$ pour un certain $u \in H^1(\mathbb{R}^3)$, nous voulons montrer que cette factorisation est préservée au premier ordre par l'équation de Schrödinger (25) : $\Psi_N(t) \simeq u(t)^{\otimes N}$

où $u(0) = u_0$ est $u(t, x)$ vérifie l'équation de Gross-Pitaevskii

$$i\partial_t u(t) = (-\Delta + a|u(t)|^2 + bK * |u(t)|^2) u(t).$$

Une manière rigoureuse de formuler cette approximation est d'estimer la distance en norme de trace entre la matrice densité réduite à 1 corps de $\Psi_N(t)$ et le projecteur orthogonal $|u(t)\rangle\langle u(t)|$:

$$\|\gamma_{\Psi_N}^{(1)} - |u(t)\rangle\langle u(t)|\|_{\mathfrak{S}_1} \leq C(t)\varepsilon(N)$$

où $\varepsilon(N) \rightarrow 0$ quand $N \rightarrow \infty$. Nous rappelons que pour $p \geq 1$, l'espace de Schatten \mathfrak{S}_p est défini ainsi

$$\mathfrak{S}_p = \left\{ A \in \mathcal{B}(\mathcal{H}), \|A\|_{\mathfrak{S}_p} = \left(\text{Tr}(A^*A)^{p/2} \right)^{1/p} < \infty \right\},$$

où $\mathcal{B}(\mathcal{H})$ est l'espace des opérateurs bornés de \mathcal{H} . L'information que donne l'estimation ci-dessus est *marginale* et n'indique en rien que $\Psi_N(t)$ est proche de $u(t)^{\otimes N}$ dans $L^2(\mathbb{R}^3)^{\otimes N}$. Ce n'est d'ailleurs pas le cas. En réalité des collisions à l'intérieur du condensat peuvent créer des excitations et respectivement des particules excitées peuvent, en se rencontrant, réduire leurs moments cinétiques respectifs et retourner dans la partie condensée du gaz. L'approximation de Bogolyubov prétend décrire cette dynamique, c'est-à-dire donner une approximation dans $L^2(\mathbb{R}^3)^{\otimes N}$ de $\Psi_N(t)$. Nous avons d'abord besoin de quelques notations. Suivant [LNSS13], où la théorie de Bogolyubov pour l'énergie fondamentale d'un gaz de bosons dans la limite de champ moyen est prouvée rigoureusement, nous remarquons que tout $u \in \mathcal{H}$ fixé, $\Psi_N \in \mathcal{H}^{\otimes_s N}$ se décompose de manière unique de la façon suivante

$$\Psi_N = u^{\otimes N} \varphi_0 + u^{\otimes N-1} \otimes_s \varphi_1 + u^{\otimes N-2} \otimes_s \varphi_2 + \dots + \varphi_N, \quad (26)$$

où $\varphi_k \in \mathcal{H}_+^{\otimes_s k}$ avec $\mathcal{H}_+ = \{u\}^\perp$. Cela permet de définir la transformation unitaire suivante

$$\begin{aligned} U_N : \mathcal{H}^N &\longrightarrow \mathcal{F}^{\leq N}(\mathcal{H}_+) := \bigoplus_{k=0}^N \mathcal{H}_+^{\otimes_s k} \\ \Psi_N &\longmapsto \Phi_N := \bigoplus_{k=0}^N \varphi_k. \end{aligned} \quad (27)$$

Ici \otimes_s est le produit tensoriel symétrique. L'équation de Schrödinger (25) est alors réécrite dans l'espace de Fock des excitations du gaz

$$\begin{cases} i\partial_t \Phi_N(t) = \mathcal{G}_N(t) \Phi_N(t) \\ \Phi_N(0) = U_N(0) \Psi_N(0). \end{cases}$$

À la limite on peut montrer que $\mathcal{G}_N(t) \rightarrow \mathbb{H}(t)$, l'hamiltonien de Bogoliubov, et considérer l'évolution effective suivante

$$i\partial_t \Phi(t) = \mathbb{H}(t) \Phi(t) \quad (28)$$

où, dans le formalisme de la seconde quantification,

$$\begin{aligned} \mathbb{H}(t) = & \int_{\mathbb{R}^3} (\nabla a_x^* \nabla a_x + w_N * |u(t)|^2(x)) a_x^* a_x dx - \mu_N(t) \mathcal{N} \\ & + \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \left(K_1(t, x, y) a_x^* a_y + \frac{1}{2} \left(K_2(t, x, y) a_x^* a_y^* + \overline{K_2(t, x, y)} a_x a_y \right) \right) dx dy, \end{aligned}$$

où $\mu_N(t)$ est un potentiel chimique, $K_1(t, x, y)$ est le noyau de l'opérateur $Q(t)u(t, x)\widehat{w_N}(i\nabla)u(t, x)Q(t)$ où $Q(t) = 1 - P(t) = 1 - |u(t)\rangle\langle u(t)|$, et $K_2(t) = Q(t) \otimes Q(t) w_N(x - y)u(t) \otimes u(t) \in L^2(\mathbb{R}^3)^{\otimes_s 2}$. Le lecteur peut se référer à [Lew11] pour les notations et définitions

concernant le formalisme de la seconde quantification et les espaces de Fock. Nous rappelons néanmoins que \mathcal{N} est l'opérateur nombre de particules, vérifiant

$$\mathcal{N} = \bigoplus_{n \geq 0} n = \int_{\mathbb{R}^3} a_x^* a_x dx,$$

où a_x^* et a_x sont respectivement les opérateurs de création et d'annihilation au point $x \in \mathbb{R}^3$ et vérifiant les relations de commutation canoniques

$$[a_x, a_y^*] = a_x a_y^* - a_y^* a_x = \delta(x - y),$$

for all $x, y \in \mathbb{R}^3$.

Par commodité, nous prenons comme condensat de référence dans la décomposition (26) la fonction $u_N(t)$ solution de l'équation de Gross-Pitaevskii approchée

$$\begin{cases} i\partial_t u_N = (-\Delta + w_N * |u_N|^2 - \mu_N(t)) u_N \\ u_N(0) = u_0. \end{cases} \quad (29)$$

Les solutions $u_N(t)$ et $u(t)$ sont proches dans $L^2(\mathbb{R}^3)$, leur distance dépend de la régularité du potentiel d'interaction w . Notamment, on peut montrer sous certaines hypothèses que

$$\|u_N(t)\|_{H^1(\mathbb{R}^3)} + \|u(t)\|_{H^1(\mathbb{R}^3)} \leq C, \quad (30)$$

$$\|u_N(t)\|_{H^k(\mathbb{R}^3)} + \|u(t)\|_{H^k(\mathbb{R}^3)} \leq C e^{C't}, \text{ si de plus } u_0 \in H^k(\mathbb{R}^3), \quad (31)$$

où dans la seconde inégalité C ne dépend que de $\|u_0\|_{H^k(\mathbb{R}^3)}$ et C' de $\|u_0\|_{H^1(\mathbb{R}^3)}$. De plus si $u_0 \in H^2(\mathbb{R}^3)$ alors

$$\|u_N(t) - u(t)\|_{L^2(\mathbb{R}^3)} \leq C \frac{\exp(c_1 \exp(c_2 t))}{N^\beta}, \quad (32)$$

où $C, c_1, c_2 > 0$ dépendent de $\|u_0\|_{H^2(\mathbb{R}^3)}$.

Nous pouvons énoncer le résultat principal du Chapitre 2.

Théorème 5 (Dérivation de la dynamique, [Tri19a]). *Soit $\beta > 0$ et $w = w_0 + b\mathbf{1}_{|x| > RK}$ avec $w_0 \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$, $b \geq 0$, $R > 0$ et où $K = \Omega(x/|x|)|x|^{-3}$ avec $\Omega \in L^q(\mathbb{S}^2)$, où $q \geq 2$, une fonction paire vérifiant (14). Soit u_N la solution de l'équation de Gross-Pitaevskii (29) sur un intervalle $[0, T)$ avec $T \in \mathbb{R}_+ \cup \{\infty\}$ telle que (30) et (31) soient vérifiées. Soit $\Phi(t) = (\varphi_k(t))_{k \geq 0}$ la solution de l'équation de Bogoliubov (28) telle que*

$$\sum_{k=1}^{\infty} \|\varphi_k(0)\|_{L^2(\mathbb{R}^3)^{\otimes k}}^2 = 1, \quad \text{et} \quad \sum_{k=1}^{\infty} k \langle \varphi_k(0), (1 - \Delta_{x_1}) \varphi_k(0) \rangle < \infty.$$

Soit

$$\Psi_N(0) = \sum_{k=1}^N u_N(0) \otimes_s \varphi_k(0)$$

et $\Psi_N(t)$ la solution de l'équation de Schrödinger (25) avec condition initiale $\Psi_N(0)$.

1. Si $0 < \beta < 1/6$ alors pour tout $0 < \alpha < \min((1 - 6\beta)/4, (2 - 7\beta)/4)$ on a

$$\left\| \Psi_N(t) - \sum_{k=0}^N u_N(t)^{\otimes k} \otimes_s \varphi_k(t) \right\|_{L^2(\mathbb{R}^{3N})}^2 \leq C_\alpha e^{C't} N^{-\alpha}, \quad (33)$$

où C_α dépend de α , C_0 et $\|u(0)\|_{H^4(\mathbb{R}^3)}$ et où C' dépend de $\|u(0)\|_{H^1(\mathbb{R}^3)}$.

2. Si $0 < \beta < 1/4$ alors pour tout $0 < \alpha < \min((3 - 10\beta)/4, (1 - 4\beta)/4)$ on a

$$\|\Gamma_{\Psi_N(t)}^{(1)} - |u_N(t)\rangle \langle u_N(t)|\|_{\mathfrak{S}_1} \leq C_\alpha e^{C't} N^{-\alpha}, \quad (34)$$

où C_α dépend de α , C_0 , et $\|u(0)\|_{H^4(\mathbb{R}^3)}$ et C' dépend de $\|u(0)\|_{H^1(\mathbb{R}^3)}$.

3. Si par ailleurs w est classiquement stable, c'est-à-dire vérifie (13), alors

(a) Si $0 < \beta < 1/5$ alors on a (33) pour $0 < \alpha < \min((3 - 10\beta)/4, (1 - 5\beta)/4)$.

(b) Si $0 < \beta < 3/8$ alors on a (34) pour $0 < \alpha < \min((1 - \beta)/2, (2 - 5\beta)/2, (3 - 8\beta)/4)$.

L'estimée (34) est un développement au premier ordre, tandis que (33) est un développement au second ordre. Il est aisément vérifiable que le (33) implique (34).

De même que pour l'étude de l'énergie fondamentale, la nature attractive du potentiel peut générer des instabilités. Pour pallier à ce problème, nous adaptons une méthode dite de localisation de [NN17] où l'on considère une évolution auxiliaire sur un espace de Fock restreint où le nombre d'excitations ne peut dépasser une certaine valeur. Le gain de cette méthode s'explique de la manière suivante. Le résultat escompté (33), est une estimation dans $L^2(\mathbb{R}^{3N})$ et découle d'estimées sur l'énergie cinétique du système. Le système auxiliaire, quant à lui, est proche du système réel dans $L^2(\mathbb{R}^{3N})$ mais est plus stable car seul un nombre restreint de particules peuvent être dans un état excité.

1.5 La fonctionnelle de Gross-Pitaevskii dipolaire avec corrections de Lee-Huang-Yang

Cette section présente les résultats de l'article suivant, qui fait l'objet du Chapitre 3.

A. Triay. "Existence of minimizers in generalized Gross-Pitaevskii theory with the Lee-Huang-Yang correction". 2019.

De récentes expériences [FKSWP16; KSWW+16; SWBFP16; CBPM+16] montrent la formation de gouttelettes d'atomes dipolaires auto-confinées dans le régime normalement instable où l'interaction dipolaire est dominante par rapport à l'interaction courte portée répulsive (Théorème 6). Cet état méta-stable est atteint à partir de l'état fondamental du régime stable (interactions répulsives dominantes) en réduisant lentement (adiabatiquement) la longueur de diffusion a [CBPM+16]. La stabilisation est expliquée par les corrections de Lee-Huang-Yang [LHY57] et sont prises en compte par l'ajout d'un terme quintique dans la fonctionnelle de Gross-Pitaevskii dipolaire [BWBB16a]

$$\mathcal{E}_{\text{dip}}^{GP}(\psi) = \int_{\mathbb{R}^3} |\nabla\psi|^2 + \frac{a}{2} \int_{\mathbb{R}^3} |\psi|^4 + \frac{a_{\text{dd}}}{2} \int_{\mathbb{R}^3} K \star |\psi|^2 |\psi|^2 + \frac{2}{5} \gamma_{\text{QF}} \int_{\mathbb{R}^3} |\psi|^5,$$

où a est la longueur de diffusion, a_{dd} est une constante proportionnelle au carré des moments dipolaires des particules et γ_{QF} paramètre l'intensité de la correction de LHY (aussi appelées *quantum fluctuations* en anglais). Afin d'étudier l'existence de minimiseurs, on se ramène par

changement d'échelle à étudier la fonctionnelle

$$\mathcal{E}_b(\psi) := \int_{\mathbb{R}^3} |\nabla\psi|^2 + \frac{1}{2} \int_{\mathbb{R}^3} |\psi|^4 + \frac{b}{2} \int_{\mathbb{R}^3} K_{\text{dip}} \star |\psi|^2 |\psi|^2 + \frac{2}{5} \int_{\mathbb{R}^3} |\psi|^5,$$

et on note $E(\lambda, b) = \inf_{\int |\psi|^2 = \lambda} \mathcal{E}_b(\psi)$. Nous nous intéressons au cas d'un potentiel à longue portée général défini par (3) et nous montrons à l'aide de méthodes de type concentration compacité [Lio84a; Lio84b; Lie83] qu'il existe une masse critique nécessaire et suffisante à l'existence de minimiseurs.

Théorème 6 (Minimisation de \mathcal{E}_b). *Pour tout $b > 1$, la fonction*

$$\lambda \in \mathbb{R}_+ \mapsto E(\lambda, b)$$

est décroissante et il existe $0 < \lambda_c(b) < \infty$ tel que

- *si $0 < \lambda < \lambda_c(b)$, alors $E(\lambda, b) = 0$ et il n'y a pas de minimiseur*
- *la fonction $\lambda \mapsto E(\lambda, b)$ est strictement décroissante sur $[\lambda_c(b), +\infty)$. Pour tout $\lambda \geq \lambda_c(b)$ elle possède au moins un minimiseur qui vérifie l'équation d'Euler-Lagrange*

$$(-\Delta + |\psi|^2 + bK \star |\psi|^2 + |\psi|^3 - \mu) \psi = 0, \quad (35)$$

où $\mu < 0$. De plus ψ est C^∞ et décroît exponentiellement vite.

Par ailleurs, on a l'estimée suivante pour $\lambda_c(b)$

$$\frac{2^{1/2} 5^{1/2} 3\pi}{(b-1)^{5/2}} \leq \lambda_c(b),$$

et dans le cas dipolaire (9) nous avons la borne supérieure suivante

$$\lambda_c(b) \leq 84.437 \frac{1}{(b-1)^{5/2}}.$$

II. Limites semi-classiques de grands systèmes fermioniques

II.1 Le gaz de fermions à température positive

Cette section présente un travail [LMT19] réalisé en collaboration avec Mathieu Lewin et Peter Madsen et qui fait l'objet du Chapitre 4.

Nous nous intéressons dans cette partie à l'énergie libre d'un gaz de fermions à température positive dans la limite semi-classique et dans l'approximation de champ moyen. Nous rappelons que les fermions vérifient le principe d'exclusion de Pauli, qui se traduit mathématiquement par l'antisymétrie de la fonction d'onde par rapport aux permutations des particules

$$\Psi(x_1, \dots, x_N) = (-1)^{\varepsilon(\sigma)} \Psi(x_{\sigma(1)}, \dots, x_{\sigma(N)}).$$

On note $\bigwedge^N L^2(\mathbb{R}^d)$ l'espace de Hilbert constitué des fonctions antisymétriques de $L^2(\mathbb{R}^d)^{\otimes N}$, où $d \geq 1$. Sur cet espace agit le Hamiltonien suivant

$$H_{N, \hbar} = \sum_{j=1}^N (i\hbar \nabla_{x_j} + A(x_j))^2 + V(x_j) + \frac{1}{N} \sum_{1 \leq j < k \leq N} w_N(x_j - x_k) \quad (36)$$

où

$$|A|^2, w \in L^{1+\frac{d}{2}}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d), V \in L_{\text{loc}}^{1+d/2}(\mathbb{R}^d),$$

$V(x) \rightarrow \infty$ quand $|x| \rightarrow \infty$, et \hbar est la constante de Planck. Pour $p \geq 1$, $f \in L^p(\mathbb{R}^3) + L^\infty_\varepsilon(\mathbb{R}^3)$ signifie que pour tout $\varepsilon > 0$, il existe $g \in L^p(\mathbb{R}^3)$ et $h \in L^\infty(\mathbb{R}^3)$ telles que $\|h\|_{L^\infty(\mathbb{R}^3)} \leq \varepsilon$ et $f = g + h$. On note

$$E(N) = \inf \sigma_{\wedge^N L^2(\mathbb{R}^3)}(H_{N,\hbar}),$$

l'énergie fondamentale du Hamiltonien $H_{N,\hbar}$. De même que le paramètre de champ moyen N^{-1} devant le terme d'interaction renormalise la double somme pour qu'elle soit d'ordre N , nous rappelons que pour les systèmes fermioniques nous prenons

$$\hbar \sim N^{-1/d}$$

pour que le terme d'énergie cinétique soit lui aussi d'ordre N . C'est ce que l'on nomme régime semi-classique, cela revient à affaiblir le principe d'incertitude d'Heisenberg ($\hbar \rightarrow 0$) de sorte que l'observable quantité de mouvement et l'observable position commutent à la limite :

$$[x, p] = [x, -i\hbar\nabla] = i\hbar \text{Id} \xrightarrow{\hbar \rightarrow 0} 0.$$

La dynamique et l'énergie associée à (10) convergent vers celles du modèle de Vlasov dont l'énergie est donnée par

$$\begin{aligned} \mathcal{E}_{\text{Vla}}^\rho(m) &= \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} (|p + A(x)|^2 + V(x)) m(x, p) \, dx \, dp \\ &\quad + \frac{1}{2\rho} \iint_{\mathbb{R}^{2d}} w(x - y) \rho_m(x) \rho_m(y) \, dx \, dy \end{aligned}$$

où

$$\rho_m(x) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} m(x, p) \, dp$$

est la densité spatiale de particules. Ici m est une mesure sur l'espace des phases $\mathbb{R}^d \times \mathbb{R}^d$, avec pour convention que

$$\frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} m(x, p) \, dx \, dp = \int_{\mathbb{R}^d} \rho_m(x) \, dx = \rho,$$

de plus m vérifie le principe de Pauli $0 \leq m \leq 1$. En fait, on peut minimiser la fonctionnelle de Vlasov à densité spatiale fixée $\nu \in L^1(\mathbb{R}^d)$, $\int_{\mathbb{R}^d} \nu = \rho$ et obtenir la fonctionnelle de Thomas-Fermi

$$\inf_{\substack{\int_{\mathbb{R}^d} m(\cdot, p) \, dp = \nu \\ 0 \leq m \leq 1}} \mathcal{E}_{\text{Vla}}^\rho(m) = \mathcal{E}_{\text{TF}}^\rho(\nu)$$

où

$$\mathcal{E}_{\text{TF}}^\rho(\nu) = \int_{\mathbb{R}^d} \nu(x)^{1+2/d} + V(x)\nu(x) + \frac{1}{2\rho} \iint_{\mathbb{R}^{2d}} w(x - y) \nu(x) \nu(y) \, dx \, dy.$$

De même, on note

$$e_{\text{TF}}(\rho) = \inf_{\substack{\iint_{\mathbb{R}^d \times \mathbb{R}^d} m = (2\pi)^d \\ 0 \leq m \leq 1}} \mathcal{E}_{\text{Vla}}^\rho(m)$$

le minimum de l'énergie de Vlasov (et donc aussi de Thomas-Fermi).

Dans [FLS18], les auteurs montrent que l'énergie fondamentale $E(N)$ ainsi que les suites minimisantes du problème à N corps convergent vers les minimiseurs du modèle de Vlasov. Plus précisément, si $f \in L^2(\mathbb{R}^d)$ fixée telle que $\int_{\mathbb{R}^3} |f|^2 = 1$, et pour tout $x, p \in \mathbb{R}^d$ on définit les états cohérents $f_{x,p}^{\hbar}(y) = \hbar^{-d/4} f(\hbar^{-1/2}(y-x)) e^{ip \cdot y/\hbar}$. On définit la mesure de Husimi à k particules de Ψ par

$$m^{(k)}(x_1, p_1, \dots, x_k, p_k) = \langle \Psi P_{x_1, p_1} \otimes \dots \otimes P_{x_k, p_k} \otimes 1_{N-k} \Psi \rangle, \quad \text{où } P_{x,p} = |f_{x,p}^{\hbar}\rangle \langle f_{x,p}^{\hbar}|,$$

pour $1 \leq k \leq N$, $x_1, p_1, \dots, x_k, p_k \in \mathbb{R}^d$. Cette mesure détecte comment Ψ est corrélé avec les déterminants de Slater de la forme $\det(f_{x_i, p_i}(y_j))$ où les f_{x_i, p_i} sont localisés dans des petites boîtes de tailles $\sqrt{\hbar}$ dans l'espace des phases. Alors, il est montré dans [FLS18], dans différentes situations et sous certaines hypothèses que nous n'allons pas détailler ici, que

$$\lim_{\substack{N \rightarrow \infty \\ \hbar^d N \rightarrow \rho}} \frac{E(N)}{N} = e_{\text{TF}}(\rho)$$

et que pour tout $\varphi \in L^1(\mathbb{R}^{2dk}) + L_{\varepsilon}^{\infty}(\mathbb{R}^{2dk})$

$$\int_{\mathbb{R}^{2dk}} m^{(k)} \varphi \longrightarrow \int_{\mathcal{M}} \left(\int_{\mathbb{R}^{2dk}} m^{\otimes k} \varphi \right) d\mathcal{P}(m),$$

où \mathcal{P} est une mesure de probabilité sur \mathcal{M} , l'ensemble des minimiseurs de $\mathcal{E}_{\text{Vla}}^{\rho}$. Ce résultat doit être mis en comparaison avec la convergence des états bosoniques du Théorème 8. Mais parce que les fonctions d'onde fermioniques sont antisymétriques les matrices densités réduites ne peuvent pas satisfaire à une convergence directement, il faut pour cela considérer les mesures de Husimi ou de Wigner.

Notre but est d'étendre le résultat précédent au cas de la température positive dans l'ensemble canonique : nous désirons étudier l'énergie libre et ces minimiseurs. Dans l'ensemble canonique le nombre de particules N est donné, contrairement à l'ensemble grand-canonique où le nombre de particules est inconnu (aléatoire). Le système est alors décrit par un opérateur $\Gamma \in \mathfrak{S}_1(\bigwedge^N L^2(\mathbb{R}^3))$ positif de trace 1:

$$0 \leq \Gamma, \quad \text{Tr}_{\bigwedge^N L^2(\mathbb{R}^3)} \Gamma = 1.$$

L'énergie libre est donnée par la fonctionnelle suivante

$$\mathcal{E}_{\text{Can}}^{N, \hbar}(\Gamma) = \text{Tr}(H_{N, \hbar} \Gamma) + \frac{1}{\beta} \text{Tr}(\Gamma \log \Gamma), \quad (37)$$

où $\beta > 0$ est la température inverse. Le minimum de cette fonctionnelle est atteint uniquement pour

$$\Gamma_{N, \hbar, \beta} = Z^{-1} e^{-\beta H_{N, \hbar}},$$

où $Z = \text{Tr} e^{-\beta H_{N, \hbar}}$, et dont l'énergie libre est

$$e_{\text{Can}}^{\beta}(\hbar, N) := \min_{\Gamma} \mathcal{E}_{\text{Can}}^{N, \hbar}(\Gamma) = -\frac{1}{\beta} \log \text{Tr} e^{-\beta H_{N, \hbar}}.$$

La fonctionnelle de Vlasov à température positive est donnée par

$$\begin{aligned} \mathcal{E}_{\text{Vla}}^{\beta,\rho}(m) &= \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} (|p + A(x)|^2 + V(x)) m(x, p) \, dx \, dp \\ &\quad + \frac{1}{2\rho} \iint_{\mathbb{R}^{2d}} w(x - y) \rho_m(x) \rho_m(y) \, dx \, dy \\ &\quad + \frac{1}{(2\pi)^d \beta} \iint_{\mathbb{R}^{2d}} s(m(x, p)) \, dx \, dp, \end{aligned}$$

où $s(x) = x \log x + (1 - x) \log(1 - x)$ est l'entropie fermionique. On dénote

$$e_{\text{Vla}}^{\beta}(\rho) = \inf_{\substack{0 \leq m \leq 1 \\ (2\pi)^{-d} \iint_{\mathbb{R}^{2d}} m = \rho}} \mathcal{E}_{\text{Vla}}^{\beta,\rho}(m). \quad (38)$$

l'énergie minimum de Vlasov. Le premier résultat du Chapitre 4 porte sur la minimisation de $\mathcal{E}_{\text{Vla}}^{\beta,\rho}$ et l'étude de ses minimiseurs.

Théorème 7 (Minimisation de $\mathcal{E}_{\text{Vla}}^{\beta,\rho}$, [LMT19]). *Soient $\rho, \beta_0 > 0$. Nous supposons que A, V vérifient les hypothèses décrites plus haut et qu'en plus $\int_{\mathbb{R}^d} e^{-\beta_0 V_+(x)} \, dx < \infty$. Soit*

$$w \in L^{1+\frac{d}{2}}(\mathbb{R}^d) + L_{\varepsilon}^{\infty}(\mathbb{R}^d) + \mathbb{R}_+ \delta_0.$$

Alors, pour tout $\beta > \beta_0$, le problème (2) admet des minimiseurs. Tout minimiseur m_0 est solution de l'équation non-linéaire

$$m_0(x, p) = \frac{1}{1 + \exp\left(\beta(|p + A(x)|^2 + V(x) + \rho^{-1} w * \rho_{m_0}(x) - \mu)\right)}, \quad (39)$$

où μ est un multiplicateur de Lagrange. Le minimum s'exprime en fonction de m_0 et de μ par

$$\begin{aligned} e_{\text{Vla}}^{\beta}(\rho) &= -\frac{1}{(2\pi)^d \beta} \iint_{\mathbb{R}^{2d}} \log\left(1 + e^{-\beta(|p|^2 + V(x) + \rho^{-1} w * \rho_{m_0}(x) - \mu)}\right) \, dx \, dp \\ &\quad + \mu \rho - \frac{1}{2\rho} \iint_{\mathbb{R}^{2d}} w(x - y) \rho_{m_0}(x) \rho_{m_0}(y) \, dx \, dy. \end{aligned} \quad (40)$$

Si de plus $\widehat{w} \geq 0$, alors $\mathcal{E}_{\text{Vla}}^{\beta,\rho}$ est strictement convexe et possède un unique minimiseur

Le lecteur assidu aura pu constater que nous considérons aussi le cas où w est une mesure de Dirac positive. Le modèle en question apparaît alors dans le régime dilué comme nous l'expliquons plus loin. Nous pouvons énoncer notre principal résultat du Chapitre 4

Théorème 8 (Dérivation de la théorie de Vlasov à température positive, [LMT19]). *Sous les hypothèses du Théorème 7 et sous l'hypothèse supplémentaire que $\widehat{w} \geq 0$, pour tout $\beta > \beta_0$ on a*

$$\lim_{\substack{N \rightarrow \infty \\ \hbar^d N \rightarrow \rho}} \hbar^d e_{\text{Can}}^{\beta}(\hbar, N) = e_{\text{Vla}}^{\beta}(\rho). \quad (41)$$

De plus, si (Γ_N) est une suite d'états de Gibbs approchés, c'est-à-dire,

$$\mathcal{E}_{\text{Can}}^{N,\hbar}(\Gamma_N) = e_{\text{Can}}^\beta(\hbar, N) + o(\hbar^{-d}),$$

alors la densité spatiale à 1 particule de Γ_N vérifie

$$\hbar^d \rho_{\Gamma_N}^{(1)} \rightharpoonup \rho_{m_0} \text{ faiblement dans } L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d),$$

et

$$m_{f,\Gamma_N}^{(1)} \longrightarrow m_0 \text{ fortement dans } L^1(\mathbb{R}^{2d}), \quad (42)$$

$$\rho_{m_{f,\Gamma_N}^{(1)}} \longrightarrow \rho_{m_0} \text{ fortement dans } L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d), \quad (43)$$

où m_0 est l'unique minimiseur de la fonctionnelle de Vlasov.

Si de plus,

$$\mathcal{E}_{\text{Can}}^{N,\hbar}(\Gamma_N) = e_{\text{Can}}^\beta(\hbar, N) + o(1),$$

alors

$$\int_{\mathbb{R}^{2dk}} m_{f,\Gamma_N}^{(k)} \varphi \rightarrow \int_{\mathbb{R}^{2dk}} m_0^{\otimes k} \varphi \quad (44)$$

pour tout $\varphi \in L^1(\mathbb{R}^{2dk}) + L^\infty(\mathbb{R}^{2dk})$.

Ce régime peut par exemple décrire un atome lourd confiné dans un potentiel harmonique puissant ou encore le noyau d'une étoile à neutrons. Nous traitons aussi le cas d'un gaz dilué, comme dans le cas bosonique, où l'interaction est dilatée ainsi $N^{d\eta}w(N^\eta(x-y))$ où $0 < \eta$. Dans ce régime nous distinguons deux comportements différents, quand $0 < \eta < 1/d$ l'interaction devient ponctuelle tandis que lorsque $1/d < \eta$ celle-ci disparaît du modèle limite. Ce dernier phénomène traduit le fait que la portée de l'interaction $N^{-\eta}$ est d'un ordre de grandeur plus petit que la distance minimale entre deux fermions qui est dictée par le principe d'incertitude $\hbar \sim N^{-1/d}$. Cette disparition totale de l'interaction est notamment due à l'absence de spin des particules considérées. Dans [Sei06], l'auteur étudie le cas $\eta > 1/d$, pour $d = 3$, dans le cas grand-canonique, et montre que seules les particules de spins différents contribuent à l'énergie d'interaction. Notre résultat est présenté ci-après.

Théorème 9 (Dérivation de $\mathcal{E}_{\text{Vla}}^{\beta,\rho}$ dans le régime dilué, [LMT19]). *Soit $\beta_0, \rho > 0$. Soient V et A vérifiant les hypothèses du Théorème 8. Soit $w \in L^1(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ une fonction paire,*

- Si $0 < \eta < 1/d$ et $\hat{w} \geq 0$ alors, pour tout $\beta > \beta_0$,

$$\lim_{\substack{N \rightarrow \infty \\ \hbar^d N \rightarrow \rho}} \hbar^d e_{\text{Can}}^\beta(\hbar, N) = e_{\text{Vla}}^{\beta, (\int_{\mathbb{R}^d} w) \delta_0}(\rho)$$

où $e_{\text{Vla}}^{\beta, (\int_{\mathbb{R}^d} w) \delta_0}(\rho)$ est le minimum de l'énergie de Vlasov avec comme potentiel d'interaction $(\int_{\mathbb{R}^d} w) \delta_0$.

- Si $\eta > 1/d$, $d \geq 3$ et $w \geq 0$ est à support compact, alors pour $\beta > \beta_0$,

$$\lim_{\substack{N \rightarrow \infty \\ \hbar^d N \rightarrow \rho}} \hbar^d e_{\text{Can}}^\beta(\hbar, N) = e_{\text{Vla}}^{\beta, 0}(\rho)$$

où $e_{\text{Can}}^{\beta, 0}(\rho)$ est le minimum de l'énergie de Vlasov sans interaction.

Dans les deux cas, les états de Gibbs approchés vérifient les mêmes conclusions que celles du Théorème 8.

La preuve du Théorème 8 est constituée de trois parties. La démonstration de la borne inférieure de l'énergie, celle de la borne supérieure et finalement la convergence des états de Gibbs approchés. L'hypothèse la plus forte apparaissant dans ce théorème est $\hat{w} \geq 0$ et n'est utilisée que pour déduire la borne inférieure. Un tel potentiel, supposons qu'en plus $\hat{w} \in L^1(\mathbb{R}^d)$, vérifie l'inégalité

$$\sum_{1 \leq i < j \leq N} w(x_i - x_j) \geq \sum_{i=1}^N w * \varphi(x_i) - \frac{1}{2} \int_{\mathbb{R}^d} (\varphi * w) \varphi - \frac{N}{2} w(0). \quad (45)$$

pour tout $\varphi \in C_c^\infty(\mathbb{R}^d)$ et $x_1, \dots, x_N \in \mathbb{R}^d$. Il est ainsi possible de minorer le terme d'interaction à deux corps par un terme d'interaction à un corps composé du champ moyen créé par une distribution de particules donnée par φ . En une deuxième étape, nous minorons le problème sans interaction obtenu dans l'ensemble canonique par le même problème dans l'ensemble grand-canonique où des calculs exacts sont possibles et donnent l'énergie libre en terme de la matrice densité à un corps de l'état de Gibbs. Cet état grand-canonique est appelé dans le cas d'un système idéal (sans interaction) état quasi-libre. Cela se résume par l'emploi de l'inégalité suivante [BLS94; Thi02]

$$\mathrm{Tr}_{\wedge^N \mathcal{H}} \Gamma \log \Gamma \geq \mathrm{Tr}_{\mathcal{H}} \left(\Gamma^{(1)} \log \Gamma^{(1)} + \left(1 - \Gamma^{(1)}\right) \log \left(1 - \Gamma^{(1)}\right) \right) = \mathrm{Tr}_{\mathcal{H}} s \left(\Gamma^{(1)} \right)$$

qui est vérifiée pour tout état grand-canonique (et donc canonique) Γ et où $\Gamma^{(1)} = N \mathrm{Tr}_{2 \rightarrow N} \Gamma$ (dans le cas canonique seulement) est la matrice densité à 1 corps de Γ . Le reste de la preuve de la borne inférieure est donné par une analyse semi-classique [Sim80] usuelle utilisant la résolution de l'identité en états cohérents

$$\frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^{2d}} |f_{x,p}^\hbar\rangle \langle f_{x,p}^\hbar| = \mathrm{Id}_{L^2(\mathbb{R}^d)}.$$

La borne supérieure est obtenue en construisant un état canonique convergeant, dans un sens approprié, c'est-à-dire où tous les termes composants l'énergie libre convergent, vers un état semi-classique. Nous utilisons fortement l'équivalence des ensembles à la limite thermodynamique dans la preuve. Enfin, la convergence des mesures de Husimi pour les états de Gibbs approchés est prouvée grâce à un argument à la Feynman-Hellmann, en perturbant l'énergie à l'ordre 1, et en utilisant un théorème de de Finetti [FLS18, Theorem 2.1] donnant la limite des mesures de Husimi comme combinaison convexe de mesures produits. Ce théorème est inspiré de [LNR14] où une version faible du théorème de de Finetti quantique fut introduite pour étudier une limite de champ moyen dans le cas bosonique.

II.2 Dérivation de la correction de Scott pour le modèle de Dirac-Fock

Cette section présente les résultats du Chapitre 5 qui ont été obtenus en collaboration avec Søren Fournais et Mathieu Lewin. Nous étudions le développement asymptotique de l'énergie d'un atome lourd en fonction du nombre de ses électrons. Nous nous plaçons dans l'approximation de Born-Oppenheimer dans laquelle les nucléons, dont la masse est beaucoup plus grande que celle des électrons, sont supposés fixes dans l'espace et ponctuels. Le système étudié est donc le gaz d'électrons autour d'un noyau composé de Z protons. Le Hamiltonien du système, après

changement d'échelle, est le suivant

$$H_N = \sum_{j=1}^N \left(-\frac{1}{2} \Delta_j + \frac{Z}{|x_j|} \right) + \sum_{1 \leq j < k \leq N} \frac{1}{|x_j - x_k|},$$

agissant sur $\bigwedge^N L^2(\mathbb{R}^3, \mathbb{C}^2)$. Notons l'énergie fondamentale $E(N, Z) = \inf \sigma(H_N)$. Remarquons que le changement de variable $x = N^{-1/3} x'$ montre que H_N est unitairement équivalent à

$$N^{4/3} \left(\sum_{j=1}^N \left(-\frac{N^{-2/3}}{2} \Delta_j + \frac{ZN^{-1}}{|x_j|} \right) + \frac{1}{N} \sum_{1 \leq j < k \leq N} \frac{1}{|x_j - x_k|} \right) \sim N^{4/3} H_{N, \hbar}$$

où $H_{N, \hbar}$ est le Hamiltonien considéré le Chapitre 4 avec $\hbar \sim N^{-1/3}$. Pour cette raison, le premier ordre du développement $E(N)$ est donné par l'énergie de Thomas-Fermi. Améliorer l'ordre de ce développement a été l'objet d'un grand nombre de travaux et actuellement le meilleur résultat est le suivant

$$E(N, N) = e_{\text{TF}} Z^{7/3} + \frac{Z^2}{2} + Z^{5/3} c_{\text{DS}} + o(Z^{5/3}).$$

Le second ordre, en Z^2 , est appelé la correction de Scott et c'est là l'objet de notre travail. Elle fut rigoureusement prouvée dans [SW87a; SW87b; SW89; Hug90; ILS96; IS93]. L'ordre suivant, en $Z^{5/3}$, fut prédit par Dirac et Schwinger [Dir30; Sch51; ES84a; ES84c; ES84b] et prouvé dans une série de travaux par Fefferman et Seco [FS89; FS90; FS92; FS93; FS94a; FS94b; FS94c; FS95]. Si le premier ordre ne dépend pas de la nature du potentiel d'interaction, les deux corrections sont, quant à elles, dues à la singularité Coulombienne. Plus précisément, ce sont les électrons proches du noyau, qui malgré leur faible nombre, affectent l'énergie à ces ordres supérieurs. Cette proximité au noyau leur attribue une très grande énergie cinétique et il est alors justifié de se demander si ces corrections dépendent de l'approximation non-relativiste qui est réalisée ici. Les effets relativistes modifient de manière importante les propriétés des éléments chimiques, et pas seulement des plus lourds. La relativité donne sa couleur à l'or [GA10], qui sans elle partagerait celle de l'argent, elle explique aussi pourquoi le mercure est liquide à température ambiante [CPWS13], ou même encore, elle nous permet de démarrer notre voiture [ZP11].

La relation de dispersion d'une particule relativiste est donnée par

$$E_c = \sqrt{p^2 c^2 + c^4} - c^2,$$

en comparaison avec celle d'une particule non-relativiste $E = p^2/2$. Ainsi une première amélioration consiste à remplacer $-\Delta$ par l'opérateur pseudo-relativiste de Chandrasekhar $\sqrt{-c^2 \Delta + c^4} - c^2$, ce qui n'affecte pas le premier ordre mais modifie la correction de Scott [FSW08]. Ce dernier opérateur donne une bonne description qualitative de particules relativistes mais souffre de plusieurs défauts. Il n'est pas invariant par le groupe de Lorentz et en particulier n'est pas un opérateur local. Pour remédier à cela, Dirac proposa l'opérateur suivant

$$D_0 = c\alpha_1 p_1 + c\alpha_2 p_2 + c\alpha_3 p_3 + \beta c^2$$

où $p_j = -i\nabla_{x_j}$,

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

et

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

sont les matrices de Pauli. On notera simplement $D_0 = \boldsymbol{\alpha} \cdot \mathbf{p} + \beta$ où $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ et $\mathbf{p} = (p_1, p_2, p_3)$. On remarquera que cet opérateur agit sur $L^2(\mathbb{R}^3, \mathbb{C}^4)$ et qu'il vérifie $D_0^2 = \mathbf{p}^2 + 1$, $\sigma(D_0) =]-\infty, -1[\cup]1, \infty[$. Le sous-espace spectral d'énergies négatives est vu comme l'espace d'état des positrons, l'anti-particule de l'électron, tandis que ce dernier vit dans le sous-espace d'énergies positives. Le fait que D_0 n'est pas borné inférieurement est à l'origine de plusieurs difficultés. Tout d'abord, il faut adapter les formulations variationnelles habituelles et notamment la caractérisation de Courant-Fisher des valeurs propres [GLS99; DES00]. On ne connaît pas d'extension auto-adjointe pour l'opérateur de Dirac à N corps en interaction coulombienne [Der93]. Par ailleurs, l'ajout d'un potentiel V pose des problèmes difficiles d'auto-adjonction [Nen76; ELS17] et modifie la mer de Dirac. En effet, si

$$D_V = D_0 + V$$

où V est un potentiel, le sous-espace d'énergies positives devient

$$\mathbf{1}_{[0, \infty[}(D_V)L^2(\mathbb{R}^3, \mathbb{C}^4) \neq \mathbf{1}_{[0, \infty[}(D_0)L^2(\mathbb{R}^3, \mathbb{C}^4).$$

Le Hamiltonien du système est donné par

$$H_N = \sum_{j=1}^N \left(c\boldsymbol{\alpha} \cdot \mathbf{p} + c^2\beta - \frac{Z}{|x|} - c^2 \right)_j + \sum_{1 \leq j < k \leq N} \frac{1}{|x_j - x_k|} \quad (46)$$

$$= c^2 \mathcal{U}^* \left(\sum_{j=1}^N \left(\boldsymbol{\alpha} \cdot \mathbf{p} + \beta - \frac{\kappa}{|x|} - 1 \right)_j + \alpha \sum_{1 \leq j < k \leq N} \frac{1}{|x_j - x_k|} \right) \mathcal{U} \quad (47)$$

où c est la vitesse de la lumière, $\alpha = \frac{1}{c}$ (dans nos unités) est la constante de structure fine de Sommerfeld, $\kappa = Z/c$ et \mathcal{U} est la transformation unitaire $\mathcal{U}\Psi = c^{3N/2}\Psi(c)$.

D'une part, à la limite non-relativiste, $c \rightarrow \infty$, l'opérateur de Dirac $D_0 := c\boldsymbol{\alpha} \cdot \mathbf{p} + c^2\beta$ converge vers $-\Delta/2$. D'autre part, nous pouvons aussi faire apparaître par changement d'échelle les paramètres semi-classique et de champ-moyen. En effet, réalisons par le changement de variable $x \rightarrow Z^{1/3}x$ dans (46), nous obtenons alors le hamiltonien suivant

$$N^{4/3} \left(\sum_{j=1}^N \left(\tilde{c}\boldsymbol{\alpha} \cdot (\hbar\mathbf{p}) + \tilde{c}^2\beta - \frac{1}{|x|} - \tilde{c}^2 \right)_j + \frac{1}{N} \sum_{1 \leq j < k \leq N} \frac{1}{|x_j - x_k|} \right), \quad (48)$$

où $\hbar = N^{-1/3}$ et $\tilde{c} = N^{1/3}$. Nous considérons des atomes donc nous prendrons aussi $N = Z$. Pour résumer, le régime considéré est composé d'une limite non-relativiste $c \rightarrow \infty$, $\alpha \rightarrow 0$, d'une limite semi-classique $\hbar \rightarrow 0$ et champ moyen $N \rightarrow \infty$, $\alpha = \lambda \sim N^{-1}$.

Rappelons que l'opérateur de Dirac à N corps (46) n'admet pas d'extension auto-adjointe connue. On considère un sous-espace \mathcal{H} de $L^2(\mathbb{R}^3, \mathbb{C}^4)$ sur lequel l'opérateur de Dirac (avec ou sans potentiel extérieur) est borné inférieurement et on définit l'espace d'état du système à N corps par $\bigwedge^N \mathcal{H}$. Le choix $\mathcal{H} = \mathbf{1}_{[0, \infty[}(D_0)L^2(\mathbb{R}^3, \mathbb{C}^4)$ est appelé la description de Brown-Ravenhall et le calcul de la correction de Scott dans ce cas a été réalisé dans [FSW09]. Cette correction se trouve être différente de celle donnée par l'opérateur de Chandrasekhar. Un second référentiel est donnée par la description de Furry-Oppenheimer où l'espace d'état à 1 corps est

$\mathcal{H} = \mathbb{1}_{[0, \infty[}(D_0 - \kappa|x|^{-1})L^2(\mathbb{R}^3, \mathbb{C}^4)$ et amène à encore une autre correction de Scott [HS15]. Dans notre travail, nous démarrons directement avec le modèle de Dirac-Fock, qui est la version relativiste du modèle de Hartree-Fock. Cela revient à commencer un cran en dessous dans le schéma de la figure 1. Dans ce modèle, la mer de Dirac est définie par rapport au total du champ provenant du noyau (comme dans l'opérateur de Furry) mais aussi du champ moyen créé par les électrons eux-mêmes.

Plus précisément, si le système est décrit par une matrice densité, c'est-à-dire un opérateur positif auto-adjoint dont la trace vaut N : $0 \leq \gamma$, $\text{Tr } \gamma = N$, et nous imposons la contrainte non-linéaire suivante

$$\mathbb{1}_{]-\infty, 0]} \left(D_0 - \frac{\kappa}{|x|} + \alpha \rho_\gamma * \frac{1}{|x|} \right) \gamma = 0, \quad (49)$$

où ρ_γ est la densité de particules $\rho_\gamma(x) = \gamma(x, x)$. Dans nos unités $c = 1$, $\alpha = e^2 \sim 1/137$.

Nous commençons par fixer $\rho \in L^1(\mathbb{R}^3)$ tel que $\rho \geq 0$, $\int_{\mathbb{R}^3} \rho = 1$ et $D(\rho, \rho) = \int_{\mathbb{R}^3} \rho * |x|^{-1} \rho < \infty$, et nous déduisons des conditions sur $\kappa \geq 0$ et $\nu \geq 0$ assurant l'existence d'un trou spectral pour l'opérateur

$$D_\rho := D_0 - \frac{\kappa}{|x|} + \nu \rho * \frac{1}{|x|}.$$

Pour cela nous utilisons un principe de continuation dans l'idée de [DES00]. Définissons, pour $\nu \geq 0$

$$\mu(\nu) := \inf_{\substack{0 \leq \rho, \int \rho = 1 \\ D(\rho, \rho) < \infty}} \sigma \left(D_0 - \nu \rho * \frac{1}{|x|} \right) \cap [0, \infty)$$

et $\nu_c := \sup\{\nu \geq 0 \mid \mu(\nu) > 0\}$. D'après [Tix98] nous savons que $\nu_c \geq 2/(2/\pi + \pi/2) \simeq 0.9$ mais nous conjecturons que $\nu_c = 1$. La connaissance a priori du trou spectral nous permet de comparer D_ρ et D_0 pour pouvoir ensuite utiliser les inégalités de Sobolev. Nous montrons le résultat suivant.

Theorem 10 (Trou spectral pour opérateurs de Dirac-Coulomb généralisés). *Pour tout $0 \leq \kappa < 1$ et tout $0 \leq \nu < \nu_c$, alors*

$$\sigma(D_0 - \kappa|x|^{-1} + \nu \rho * |x|^{-1}) \cap (-\mu(\nu), \sqrt{1 - \kappa^2}) = \emptyset$$

et il existe une constante universelle $c_{\kappa, \nu} > 0$ telle que

$$c_{\kappa, \nu} |D_0| \leq |D_{\kappa, \rho}| \quad (50)$$

pour tout ρ positif tel que $\sqrt{\rho} \in H^{1/2}(\mathbb{R}^3)$ et $\int_{\mathbb{R}^3} \rho = \nu$. On peut prendre

$$c_{\kappa, \nu} = \frac{2(c_\kappa)^2}{\pi(\nu + \kappa)} \left(1 + \frac{\pi}{2c_\kappa} \frac{\nu \nu_c}{\nu_c - \nu} \right)^{-2} \quad (51)$$

où c_κ est telle que $c_\kappa |D_0| \leq |D_\kappa|$.

Avant d'énoncer le résultat principal du Chapitre 5, nous donnons quelques définitions. Soit $0 < \kappa < 1$, de sorte que $\inf |\sigma(D_\kappa)| > 0$, posons

$$\Gamma_{N, \kappa} := \left\{ 0 \leq \gamma \leq 1, \text{Tr } \gamma \leq N, |D_\kappa|^{1/2} \gamma |D_\kappa|^{1/2} \in \mathfrak{S}_1 \right\}$$

de sorte que pour $\gamma \in \Gamma_{N,\kappa}$, l'énergie de Dirac-Fock associée à cet état est donnée par

$$\begin{aligned}\mathcal{E}_{\text{DF}}(\gamma) &= \text{Tr} \left(D_0 - \frac{\kappa}{|x|} - 1 \right) \gamma + \frac{\alpha}{2} D(\rho_\gamma, \rho_\gamma) \\ &= \text{Tr}(D_\gamma - 1)\gamma - \frac{\alpha}{2} D(\rho_\gamma, \rho_\gamma).\end{aligned}$$

La constante de structure fine α sera notre paramètre de champ moyen, nous prendrons $\alpha \sim \kappa/N$ avec $\nu = \kappa$. L'énergie fondamentale est alors

$$E_{\text{DF}}(N) = \inf_{\substack{\gamma \in \Gamma_{N,\kappa} \\ \mathbb{1}_{(-\infty,0)}(D_\gamma)\gamma=0}} \mathcal{E}_{\text{DF}}(\gamma).$$

Nous montrons le théorème suivant.

Théorème 11 (Correction de Scott). *Si $\lim_{N \rightarrow \infty} \alpha N = \kappa < \nu_c$ alors*

$$E_{\text{DF}}(N) = e_{\text{TF}} \alpha^2 N^{7/3} + c_{\text{Scott}}(\kappa) + o(1).$$

où $c_{\text{Scott}}(\kappa)$ est donnée par

$$c_{\text{Scott}}(\kappa) := \frac{\kappa^2}{2} + \sum_{n \geq 1} \left\{ \lambda_n \left(D_0 - \frac{\kappa}{|x|} - 1 \right) - \lambda_n \left(-\frac{\Delta}{2} - \frac{\kappa}{|x|} \right) \right\},$$

La démonstration de la borne inférieure consiste à se ramener à l'opérateur Dirac-Coulomb et à contrôler, pour des suites minimisantes γ_N , la distance Hilbert-Schmidt entre les projecteurs sur la mer de Dirac des opérateurs de Dirac-Coulomb D_κ et de Dirac-Fock $D_\kappa + \alpha \rho_{\gamma_N} * |x|^{-1}$.

Pour la borne supérieure, nous devons trouver un ansatz vérifiant (49) et ayant une énergie appropriée. Dans [Sér05], Éric Séré construit une rétraction θ pour projeter les matrices densité sur la sous-variété des états vérifiant la contrainte non-linéaire (49), et ainsi trouver des minimiseurs à la fonctionnelle de Dirac-Fock. Cette dernière est définie par

$$\theta(\gamma) = \lim_{N \rightarrow \infty} \gamma_n$$

où γ_n est définie par récurrence par

$$\gamma_{n+1} = P_n \gamma_n P_n, \quad \text{où } P_n = \mathbb{1}(D_0 - \frac{\kappa}{|x|} + \alpha \rho_{\gamma_n} * \frac{1}{|x|} \geq 0).$$

Nous considérons alors l'ansatz défini pour le modèle de Furry défini en [HS15] dont l'énergie est connue au second ordre. Grâce à la rétraction définie ci-dessus, nous construisons un nouvel état vérifiant (49) et dont la distance au premier est contrôlée pour la norme $\| |D_\kappa|^{1/2} \cdot |D_\kappa|^{1/2} \|_{\mathfrak{S}_1}$ permettant de contrôler de son énergie.

Notre résultat est restreint au cas des atomes $\nu = \kappa$ car nous nous basons sur des travaux existant qui pour la plupart ne considèrent que cette situation particulière mais nous conjecturons que la généralisation aux ions est aussi valide.

Première partie

La théorie de Gross-Pitaevskii pour
des bosons dipolaires

Chapitre 1

Derivation of the dipolar Gross-Pitaevskii energy

Ce chapitre reprend l'intégralité de l'article publié dont le préprint est accessible en ligne sur arXiv / Hal. Les hypothèses du Lemme 13 ont toutefois été élargies et sa preuve simplifiée grâce des remarques de Rémi Carles et Benjamin Schlein que nous remercions.

A. Triay. "Derivation of the dipolar Gross-Pitaevskii energy". *SIAM J. Math. Anal.* 50.1 (2018), pp. 33–63

Abstract

We consider N trapped bosons in \mathbb{R}^3 interacting via a pair potential w which has a long range of dipolar type. We show the convergence of the energy and of the minimizers for the many-body problem towards those of the dipolar Gross-Pitaevskii functional, when N tends to infinity. In addition to the usual cubic interaction term, the latter has the long range dipolar interaction. Our results hold under the assumption that the two-particle interaction is scaled in the form $N^{3\beta-1}w(N^\beta x)$ for some $0 \leq \beta < \beta_{\max}$ with $\beta_{\max} = 1/3 + s/(45 + 42s)$ where s is related to the growth of the trapping potential.

Résumé

Nous étudions N bosons confinés dans \mathbb{R}^3 et interagissant via un potentiel w à longue portée de type dipolaire. Nous montrons que l'énergie et les minimiseurs du problème à N corps convergent vers ceux de la fonctionnelle de Gross-Pitaevskii dipolaire quand N tend vers l'infini. En plus du terme d'interaction cubique, cette dernière possède aussi un terme d'interaction non-local dipolaire. Nos résultats sont valides pour le régime dans lequel l'interaction est dilatée de la forme $N^{3\beta-1}w(N^\beta x)$ avec $0 \leq \beta < \beta_{\max}$ vérifiant $\beta_{\max} = 1/3 + s/(45 + 42s)$ et où s est lié à la croissance du potentiel confinant.

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1 Introduction

Bose-Einstein Condensation (BEC) is a phenomenon occurring at very low temperature for a highly dilute gas of bosons. In the proper experimental conditions, most of the particles get to occupy the same quantum state. In 1925, Bose [Bos24] and Einstein [Ein24] proved condensation for ideal particles, that is, under the important assumption that the particles do not interact with each other. Seventy years later, Cornell and Wieman [AEMWC95] obtained the first experimental realization of a full BEC with Rubidium atoms. This major achievement has triggered a new interest in the theoretical study of condensation. In 1999, the first rigorous derivation of the expression for the ground state energy was provided by Lieb, Seiringer and Yngvason [LSY00], while in 2002 was given the first proof of BEC (derivation of the ground state) [LS02]. In these works, the particles are confined by a trapping potential and interact via a positive, radial and short range interaction.

The experimental study of BEC remains a very active field of research today. A challenging task is to realize condensates of particles with diverse interactions. In 2005, a first dipolar condensate has been observed by Griesmaier *et al* using Chromium particles [GWHSP05]. The dipolar interaction differs in many points from the ones encountered before. It is long range, anisotropic and has an attractive and a repulsive part. Its study is both experimentally and mathematically intricate but it opens the way to new physical effects. For instance, it is believed that dipolar condensates exhibit a roton-maxon excitation spectrum [SSL03] which is not observed for simpler interactions. See for example [LMSLP09] for a review of the physical properties of the dipolar Bose gas.

In this article, we give the first derivation of the Gross-Pitaevskii (GP) theory for dipolar Bose gases, starting from the many-particle linear Schrödinger problem. Our method is based on mean field limits and de Finetti theorems introduced in [LNR14; LNR15a] as well as new techniques developed to deal with negative pair interaction that can be found in [NRS15; LNR15b].

More precisely, we will show that the particles in the condensate have a common state which can be computed by minimizing the dipolar Gross-Pitaevskii functional:

$$\begin{aligned} \mathcal{E}_{GP}^{a,b}(u) = & \int_{\mathbb{R}^3} |(\nabla + iA(x))u(x)|^2 dx + \int_{\mathbb{R}^3} V(x)|u(x)|^2 dx + \frac{a}{2} \int_{\mathbb{R}^3} |u(x)|^4 dx \\ & + \frac{b}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} (K \star |u|^2(x))|u(x)|^2 dx. \end{aligned} \quad (1)$$

The first term in (1) represents the kinetic energy where $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ is a vector potential (modeling a magnetic field or the Coriolis force due to the rotation of the atoms). The second term is the one-body potential energy where $V : \mathbb{R}^3 \rightarrow \mathbb{R}$ is a trapping potential, that is, $V(x) \rightarrow \infty$ when $|x| \rightarrow \infty$. The third term is the short range interaction in the gas where $a \in \mathbb{R}$ is proportional to the scattering length or an approximation of it. The last term is the dipolar energy and $b \in \mathbb{R}$ is proportional to the norm of the dipoles. The dipolar interaction potential

$$K_{dip}(x) = \frac{1 - 3 \cos^2(\theta_x)}{|x|^3} = \frac{\Omega_{dip}(x/|x|)}{|x|^3}, \quad (2)$$

represents the interaction between two aligned dipoles located at distance $|x|$. The parameter θ_x is the angle between x and the direction n of all the dipoles, namely $\cos(\theta_x) = n \cdot x/|x|$. In this paper we consider more general long-range potentials of the form

$$K(x) = \frac{\Omega(x/|x|)}{|x|^3} \quad (3)$$

where Ω is an even function satisfying the cancellation property on \mathbb{S}^2 , the unit sphere of \mathbb{R}^3 ,

$$\int_{\mathbb{S}^2} \Omega(\omega) d\sigma(\omega) = 0, \quad (4)$$

where $d\sigma$ denotes the Lebesgue measure on \mathbb{S}^2 . Note that the convolution

$$K \star |u|^2(x) = \int_{\mathbb{R}^3} \frac{\Omega(y/|y|)}{|y|^3} |u(x-y)|^2 dy = \lim_{\varepsilon \rightarrow 0} \int_{|y|>\varepsilon} \frac{\Omega(y/|y|)}{|y|^3} |u(x-y)|^2 dy$$

is an improper integral which is not absolutely convergent. It will be discussed later in Lemma 11. If all the particles share the same quantum state u , the latter should minimize the functional in (1) under the normalization constraint

$$\int_{\mathbb{R}^3} |u(x)|^2 dx = 1.$$

We therefore introduce the ground state energy

$$e_{GP}(a, b) := \inf_{\|u\|_{L^2}=1} \mathcal{E}_{GP}^{a,b}(u). \quad (5)$$

This variational problem has been extensively studied, both theoretically [CMS08; CH15b; AS11; BJ16] and numerically [BAC12; BCW10] in the dipolar case (2).

Our aim is to justify the validity of the Gross-Pitaevskii minimization (5), starting with the exact many-body problem based on the Hamiltonian

$$H_N = \sum_{j=1}^N \left(-(\nabla_{x_j} + iA(x_j))^2 + V(x_j) \right) + \frac{1}{N-1} \sum_{1 \leq i < j \leq N} N^{3\beta} w(N^\beta(x_i - x_j)), \quad (6)$$

where

$$w = w_0 + b\mathbb{1}_{|x| \geq R} K,$$

for some $R > 0$ and $w_0 \in L^1(\mathbb{R}^3)$. We will need further assumptions on w which will be stated later. This operator, H_N , acts on $\bigotimes_s^N L^2(\mathbb{R}^3)$, the symmetric tensor product of N copies of $L^2(\mathbb{R}^3)$. We denote by

$$e_N := \inf_{\substack{\Psi \in \bigotimes_s^N L^2(\mathbb{R}^3) \\ \|\Psi\|_{L^2}=1}} \frac{\langle \Psi, H_N \Psi \rangle}{N}$$

the many-body ground state energy per particle. We investigate the limit of a large number of particles, $N \rightarrow \infty$. In (13), the scaling chosen for the interaction between the particles is very common. On the one hand, the L^1 -preserving scaling of the potential

$$w_N(x) := N^{3\beta} w(N^\beta x)$$

will retain in the limit only its short and long range parts. In our case, we will have

$$w_N \rightharpoonup a\delta + bK,$$

since K and δ behave the same under scaling. On the other hand, the coupling factor $(N-1)^{-1}$ is typical of mean field limits and ensures that the potential is of the same order as the kinetic energy. The function w is the real interaction between the atoms in the gas. It will be assumed to be repulsive at short distances (hence $a > 0$) and of dipolar type (close to bK) at large distances.

The parameter $\beta \in [0, 1]$ interpolates between the pure mean-field regime $\beta = 0$ and the Gross-Pitaevskii regime $\beta = 1$ which is more difficult to handle. The value $\beta = 1/3$, called self-interaction threshold [EESY06], plays a special role in this problem. The case $\beta < 1/3$ corresponds to a high density regime with the interaction length $N^{-\beta}$ being larger than the mean distance $N^{-1/3}$ between the particles. This is a natural setting for the law of large numbers to apply. The case $\beta > 1/3$ is more subtle and corresponds to a low density regime where the particles meet rarely but interact with intensity proportional to $N^{3\beta-1}$. The difficulties culminate at $\beta = 1$ where now the details of the scattering process play a role.

To deal with the negativity of w , we will assume in this article that it is classically stable, which means that

$$\sum_{1 \leq i < j \leq N} w(x_i - x_j) \geq -CN, \quad (7)$$

for all $N \geq 2$ and all space configurations $x_1, \dots, x_N \in \mathbb{R}^3$ of the N particles [Rue99]. The compatibility of above property with the dipolar potential will be discussed in Appendix B. Real atoms in the laboratory do not interact with such simple two-body forces but it is convenient and physically reasonable to restrict to this case. This is perfectly justified at long distances and less clear at short distances, where the internal structure of the atoms starts to matter. In the physics literature, it is often assumed that w is very repulsive close to the origin in order to avoid any unphysical instability phenomenon. Such potentials are always classically stable, which justifies our assumption (7). The techniques used in this paper seem to fail without (7) but we have not tried to overcome this mathematical problem. Notice that when w is continuous at the origin and $\beta > 0$, then (7) turns out to be a necessary condition for the energy e_N to be bounded below, see the comments after (22).

The classical stability (7) ensures automatically that e_N is bounded from below when $\beta \leq 1/3$. The case $\beta > 1/3$ is particularly difficult and the proof that e_N is bounded from below requires to use the kinetic energy, that is, some quantum feature of the system. The scaled interaction alone is unstable.

For $\beta = 0$ the convergence of e_N to the Hartree energy was proven in [LNR14]. In this paper, we prove that

$$\lim_{N \rightarrow \infty} e_N = e_{GP}(a, b) \quad (8)$$

as $N \rightarrow \infty$ for

$$0 < \beta < \frac{1}{3} + \frac{s}{45 + 42s}$$

under the sole assumption that w is stable as in (7) and that $V(x) \geq C|x|^s$ at infinity. In that case, we are able to show that $e_N \geq -C$ but it is unclear if additional assumptions on w are needed for higher β 's. Under the additional condition that $e_N \geq -C$ our result (8) applies up to $\beta < 2/3$. In addition to the convergence of the energy, we are also able to prove the convergence of the minimizers. Loosely speaking, we prove that the ground state of (5) factorizes in the limit, that is,

$$\Psi(x_1, \dots, x_N) \simeq u(x_1) \cdots u(x_N) \text{ as } N \rightarrow \infty, \quad (9)$$

where u is a minimizer of the dipolar Gross-Pitaevskii functional. The meaning of (9) is in the sense of density matrices and not in L^2 norm as we will recall.

In this work, we focus on the ground state problem. There is a very large literature on the time-dependent equation, see for instance [BPS16] for a review of recent results. To our knowledge, none of these works cover the case of dipolar interactions. The derivation of the dipolar Gross-Pitaevskii equation is carried out in Chapter 2.

The paper is organized as follows. In Section 2 we state our main contributions, including some results on the existence and uniqueness of minimizers of the Gross-Pitaevskii functional (1) as well as our main convergence property (8). In Section 3 we prove our main result, Theorem 6.

2 Main results

2.1 Properties of the dipolar Gross-Pitaevskii functional

As discussed before, the dipolar GP equation has already been widely studied and we slightly extend the results of [BCW10; CH15b] to deal with more general K and V as well as a magnetic potential or a Coriolis force A . The main adjustment concerns the uniqueness of minimizers which, in order to remain true, requires some extra assumptions on the intensity of the magnetic field.

Theorem 1 (Existence of GP minimizers). *Let us assume that $V \in L^1_{\text{loc}}(\mathbb{R}^3)$, $A \in L^2_{\text{loc}}(\mathbb{R}^3)$ and that there is some $s > 0$ such that*

$$V(x) \geq C^{-1}(|A(x)|^2 + |x|^s) - C, \quad \forall x \in \mathbb{R}^3 \quad (10)$$

for some $C > 0$. Let

$$K(x) = \frac{\Omega(x/|x|)}{|x|^3}$$

with $\Omega \in L^q(\mathbb{S})$, for some $q > 1$, an even function satisfying the cancellation property

$$\int_{\mathbb{S}^2} \Omega(w) d\sigma(w) = 0.$$

Let \widehat{K} be the Fourier transform of K in the sense of the principal value (as defined later in Lemma 11).

i) If

$$\begin{cases} b > 0 \text{ and } a \geq b (\inf \widehat{K})_-, \\ \text{or} \\ b < 0 \text{ and } a \geq -b (\sup \widehat{K})_+, \end{cases} \quad (11)$$

then $e_{GP}(a, b) > -\infty$ and \mathcal{E}_{GP} has minimizers.

ii) If

$$\begin{cases} b > 0 \text{ and } a < b (\inf \widehat{K})_-, \\ \text{or} \\ b < 0 \text{ and } a < -b (\sup \widehat{K})_+, \end{cases} \quad (12)$$

then $e_{GP}(a, b) = -\infty$.

Remark 2. In the dipolar case where $\Omega(x/|x|) = 1 - 3 \cos^2(\theta_x)$, then $\widehat{K}(k) = \frac{4\pi}{3} (3 \cos^2(\theta_k) - 1)$, $(\inf \widehat{K})_- = 4\pi/3$ and $(\sup \widehat{K})_+ = 8\pi/3$.

Remark 3. *We always assume $a > 0$, since the short range part of the interaction is needed to stabilize its dipolar part.*

The understanding of the effective theory is necessary to grasp the forthcoming difficulties in the derivation from the many-body theory. The condition *i*) on a and b aims to make the interaction stable which in this case is equivalent to be positive, mainly because then $a + b\widehat{K} \geq 0$. Indeed, one can easily see that if the interaction term is negative for some configuration (a, b) and some wave function u , then by scaling one gets that $e_{GP}(a, b) = -\infty$.

In fact, most of our results remain true if we change $(\nabla + iA(x))^2 + V(x)$ by any abstract self-adjoint operator h such that $h \geq C^{-1}(-\Delta + |x|^s) - C$.

We first state some lemma that will be useful in the proof of Theorem 1.

Lemma 4 (Magnetic Laplacian). *Under assumption (10), one has the operator inequality on $L^2(\mathbb{R}^3)$*

$$C^{-1}(-\Delta + V) - C \leq (-i\nabla + A)^2 + V \leq C(-\Delta + V + 1),$$

for some constant $C > 0$.

Proof of Lemma 4. Using the Cauchy-Schwarz inequality for operators (44) and inequality (10), we have the upper bound

$$(p + A)^2 = p^2 + pA + Ap + |A|^2 \leq C(p^2 + V) + C.$$

To get the lower bound, we choose some $0 < \eta < 1$ sufficiently close to 1 but fixed and we use again the Cauchy-Schwarz inequality

$$(p + A)^2 + V \geq (1 - \eta)p^2 + (1 - \eta^{-1})|A|^2 + V \geq C^{-1}(p^2 + V) - C.$$

□

Proof of Theorem 1. We start by proving *i*). First, since $V \in L^1_{\text{loc}}(\mathbb{R}^3)$ and $A \in L^2_{\text{loc}}(\mathbb{R}^3)$ the quadratic form associated with the first two terms of the energy $\mathcal{E}_{GP}^{a,b}$ is closed on a domain included in $H^1(\mathbb{R}^3)$ and provides a self-adjoint realization of $H_0 = -(\nabla + iA)^2 + V$ by the method of Friedrichs [LS81]. Then, to prove *i*), it suffices to follow the same proof as in [CH15b] and to use, when necessary, that $H_0 = -(\nabla + iA)^2 + V$ has compact resolvent [Iwa86]. More precisely, let us take a minimizing sequence (u_n) for \mathcal{E}_{GP} . The condition on a and b ensures that the interaction part of the energy is non-negative

$$a \int |u|^4 + b \int K \star |u|^2 |u|^2 = \int (a + b\widehat{K}) |\widehat{|u|^2}|^2 \geq 0.$$

Thus \mathcal{E}_{GP} is bounded below on the unit sphere of $L^2(\mathbb{R}^3)$ and $\langle u_n, H_0 u_n \rangle$ is bounded. We can then extract of (u_n) a converging subsequence in $L^2 \cap L^4$. Indeed, thanks to Lemma 4, H_0 has compact resolvent. We can write $u_n = H_0^{-1/2} H_0^{1/2} u_n$ and since $(H_0^{1/2} u_n)$ is bounded in $L^2(\mathbb{R}^3)$, because (u_n) is a minimizing sequence of $\mathcal{E}_{GP}^{a,b}$, then (u_n) is precompact in $L^2(\mathbb{R}^3)$. We can then extract a converging subsequence that we still denote by (u_n) and we write u its limit. Fatou's lemma gives $\mathcal{E}(u) \leq \liminf \mathcal{E}_{GP}(u_n) = \inf \mathcal{E}_{GP}$.

For *ii*), it suffices to employ Lemma 4 above to adapt the proof of [CH15b]. Without loss of generality, we can assume that $e_3 \in \{a + b\widehat{K} < -\delta\} \neq \emptyset$. Let f be a smooth function compactly supported with $\|f\|_{L^2} = 1$ and let us denote by $\rho(x) = |f|^2(x)$ and $f_\lambda(x) = f(\lambda x_1, \lambda x_2, \lambda^{-2} x_3)$. We have $\|f_\lambda\|_{L^2} = \|f\|_{L^2} = 1$, $\|\widehat{\rho}_\lambda\|_{L^1} = \|\widehat{\rho}^2\|_{L^1} = \|f\|_{L^4}^4$ and $\|\widehat{\rho}_\lambda\|_{L^\infty} \leq \|\rho_\lambda\|_{L^1} = 1$ for all

$\lambda > 0$. For any $r > 0$ we denote by C_r the cone with vertex at the origin, with direction e_3 and with angle r . For any $\eta > 0$, there exists λ_0 such that for any $0 < \lambda \leq \lambda_0$, we have

$$\int_{\mathbb{R}^3 \setminus C_r} \rho_\lambda^2 < \eta. \quad (13)$$

According to Lemma 11 below, \widehat{K} is an homogeneous function which is continuous except at the origin. Since \widehat{K} is continuous at e_3 , we can find $r > 0$ such that $B(e_3, r) \subset \{a + b\widehat{K} < -\delta\}$. Now for any $\eta > 0$, there exists some $\lambda_0 > 0$ such that for all $\lambda \leq \lambda_0$ we have (13), then

$$\begin{aligned} \int (a + b\widehat{K}) |\widehat{\rho}_\lambda|^2 &= \int_{\mathbb{R}^3 \setminus C_r} (a + b\widehat{K}) |\widehat{\rho}_\lambda|^2 + \int_{C_r} (a + b\widehat{K}) |\widehat{\rho}_\lambda|^2 \\ &\leq \eta \|a + b\widehat{K}\|_{L^\infty} - (\|f\|_{L^4}^4 - \eta)\delta. \end{aligned}$$

If we take $\eta < \delta \|f\|_{L^4}^4 / (2\delta + 2\|a + b\widehat{K}\|_{L^\infty})$, we obtain

$$\int a|f_\lambda|^4 + bK \star |f_\lambda|^2 |f_\lambda|^2 = \int (a + b\widehat{K}) \widehat{\rho}_\lambda^2 \leq -\frac{\|f\|_{L^4}^4 \delta}{2} < 0.$$

Now, let us denote by $\varphi = f_{\lambda_0}$ and by $\varphi_\ell = \ell^{3/2} \varphi(\ell x)$. Since V is L^1_{loc} and φ is compactly supported, with, say, $\text{supp } \varphi \subset B(0, R)$, we have

$$\left| \int_{\mathbb{R}^3} V |\varphi_\ell|^2 \right| \leq \ell^3 \int_{B(0, R\ell^{-1})} |V| = o(\ell^3).$$

Applying Lemma 4 we obtain

$$\mathcal{E}_{GP}(\varphi_\ell) \leq C \left(\int |\nabla \varphi_\ell|^2 + V |\varphi_\ell|^2 \right) + \int a |\varphi_\ell|^4 + bK \star |\varphi_\ell|^2 |\varphi_\ell|^2.$$

And for ℓ large enough, we have

$$\begin{aligned} e_{GP}(a, b) &\leq C\ell^2 \int |\nabla \varphi|^2 + \ell^3 \int_{B(0, R\ell^{-1})} |V| + \ell^3 \left(\int a |\varphi|^4 + bK \star |\varphi|^2 |\varphi|^2 \right) \\ &\leq C\ell^2 - \frac{\|f\|_{L^4}^4 \delta}{2} \ell^3. \end{aligned}$$

Taking the limit $\ell \rightarrow \infty$, the last inequality gives $e_{GP}(a, b) = -\infty$. \square

If $A = 0$, we can assume $u > 0$, because $|\nabla u| \geq |\nabla |u||$ almost everywhere. Then since $a + b\widehat{K} \geq 0$, the functional is strictly convex with respect to $|u|^2$ and uniqueness follows as in [BCW10] where the case $K = K_{dip}$ was considered. On the other hand, if $A \neq 0$, the functional is no longer convex and uniqueness can fail. Indeed, a strong magnetic field can create vortices which are a sign of rotational symmetry breaking. This situation was already encountered in the non dipolar case $K = 0$ in [Sei02; Sei03]. A small magnetic field A does not create any vortex and uniqueness remains true, as we will show in Theorem 5.

In the non-dipolar case $K = 0$, uniqueness has been shown in several situations [LSSY05; Sei02; Sei03]. These works can all be adapted to the dipolar case $K \neq 0$ but here for shortness we only discuss an extension of [LSSY05, Ch. 7]. In the following result we apply the implicit function theorem for A small enough without getting any information on how small A has to be.

The second part deal with a radial magnetic field and gives an explicit range of validity as in [LSSY05, Ch. 7].

Theorem 5 (Uniqueness of the minimizer for GP functional with magnetic field). *Let A, V and K satisfy the assumptions of Theorem 1 and let (a, b) be admissible parameters as in (11).*

1. *For $t \in \mathbb{R}$, we denote by $\mathcal{E}_{GP}^{a,b,t}$ the Gross-Pitaevskii functional where A has been replaced by tA . Then, there exists $t_0 > 0$ such that for all $|t| < t_0$, $\mathcal{E}_{GP}^{a,b,t}$ has a unique minimizer, up to a phase factor, in the sector of mass $\int_{\mathbb{R}^3} |u|^2 = 1$.*
2. *Assume $A(x) = a(r, z)e_\theta$, $V(x) = V(r, z)$ where (r, θ, z) are the cylindrical coordinates with $e_z = n$ (the common direction of all the dipolar moments). If $\|ra\|_\infty < 1/2$ then \mathcal{E}_{GP} has a unique minimizer, up to a phase factor, in the sector of mass $\int_{\mathbb{R}^3} |u|^2 = 1$. It is non negative and axially symmetric, with axis $e_z = n$.*

The proof is given in Appendix C.

2.2 Derivation of the dipolar Gross-Pitaevskii energy and minimizers

The phenomenon of condensation can be detected through the convergence of the ground state and the ground state energy towards those predicted by the Gross-Pitaevskii theory. We want to give general assumptions on w to be stable and to behave like the dipolar interaction at long distances. Investigating this problem, one can first notice that taking $w = w_0 + K$ with $w_0 \in L^1$ is not permitted. Indeed, the two particles hamiltonian H_2 would be ill defined due to the singularity of K at the origin. Taking $w = w_0 + b\mathbb{1}_{|x|>R}K$ removes the singularity and still is physically relevant since the dipolar interaction is anyway the large distance approximation of the true Coulomb interaction of two neutral charge distributions.

Theorem 6 (Convergence of the energy). *Let $A \in L^2_{loc}(\mathbb{R}^3)$ and $0 \leq V \in L^1_{loc}(\mathbb{R}^3)$ satisfying*

$$V(x) \geq C^{-1}(|A(x)|^2 + |x|^s) - C, \quad \forall x \in \mathbb{R}^3.$$

Let $K = \Omega(x/|x|)|x|^{-3}$ with $\Omega \in L^q(\mathbb{S}^2)$, for some $q \geq 2$, an even function satisfying the cancellation property (3). Let $w, R > 0$ and $b \in \mathbb{R}$, be such that

$$w - b\mathbb{1}_{|x|>R}K \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3). \quad (14)$$

We also assume w to be classically stable, that is

$$\sum_{1 \leq i < j \leq N} w(x_i - x_j) \geq -CN, \quad \forall N \geq 2, \quad \forall x_1, \dots, x_N \in \mathbb{R}^3, \quad (15)$$

for some $C > 0$ independent of N .

If

$$\beta < \frac{1}{3} + \frac{s}{45 + 42s} \quad (16)$$

then

$$\boxed{\lim_{N \rightarrow \infty} e_N = e_{GP}(a, b),} \quad (17)$$

for

$$a = \int_{\mathbb{R}^3} (w(x) - b\mathbb{1}_{|x|>R}K(x)) dx.$$

In addition, a and b satisfy the stability property (11).

Remark 7. *The convergence rate given by the proof is the sum of the error in (61) and of another one depending on w (see Lemma 17) which comes from the approximation of the Gross-Pitaevskii energy by the Hartree one. We do not state any quantitative estimate here for shortness.*

Notice that the value of the constant $R > 0$ in the definition of w in (14) has no importance because of the cancellation property of K , see Lemma 11 below.

If $V(x) \rightarrow \infty$ when $|x| \rightarrow \infty$ faster than any polynomial (e.g. $V = +\infty$ outside a bounded domain) then the condition (16) reduces to

$$\beta < \frac{1}{3} + \frac{1}{42}.$$

We now turn to the convergence of states, which is expressed in terms of the k -particle reduced density matrices. For $\Psi \in \bigotimes_s^N L^2(\mathbb{R}^3)$, let us define its k -particle density matrix by

$$\gamma_\Psi^{(k)} := \text{Tr}_{k+1 \rightarrow N} |\Psi\rangle \langle \Psi|,$$

or, in terms of its kernel,

$$\begin{aligned} \gamma_\Psi^{(k)}(x_1, \dots, x_k, y_1, \dots, y_k) \\ = \int_{(\mathbb{R}^3)^{N-k}} \Psi(x_1, \dots, x_k, z_{k+1}, \dots, z_N) \overline{\Psi(y_1, \dots, y_k, z_{k+1}, \dots, z_N)} dz_{k+1} \dots dz_N. \end{aligned}$$

From now on, when we consider a ground state Ψ_N of H_N , we will denote by $\gamma_N^{(k)}$ its k -particle reduced density matrix for simplicity.

Theorem 8 (Convergence of states). *Under the assumptions of Theorem 6, for any sequence of ground states (Ψ_N) , there exists a Borel probability measure μ supported on $\mathcal{M}_{GP}(a, b)$, the set of ground states of $\mathcal{E}_{GP}^{a,b}$, such that, up to a subsequence (N') ,*

$$\gamma_{N'}^{(k)} \xrightarrow{N' \rightarrow \infty} \int_{\mathcal{M}_{GP}} |u^{\otimes k}\rangle \langle u^{\otimes k}| d\mu(u), \quad \forall k \geq 1, \quad (18)$$

where the convergence is in the trace norm. Besides, if $\mathcal{E}_{GP}^{a,b}$ has a unique minimizer, then there is convergence of the whole sequence $(\gamma_N^{(k)})_N$ in (18).

Proof. Since the energy per particle is bounded by Theorem 6, the convergence of states can be proved exactly as in [LNR15a, Theorem 2.5]. \square

We now make several remarks concerning our two main results, Theorem 6 and Theorem 8.

The main novelty of these two results is that the interaction potential has a negative part, is anisotropic and long range. Furthermore the derivation holds for some $\beta > 1/3$ where the stability is of quantum nature (due to the kinetic term). Unfortunately, we are not yet able to push the analysis to larger β 's, but we conjecture that similar results hold for $\beta < 1$, possibly under more stringent assumptions on w .

In fact, the assumption (15) is not essential. What we need is that a kind of 2nd moment kinetic energy per particle is bounded, more precisely,

$$\text{Tr} \left(h \otimes h \gamma_{\Psi_N}^{(2)} \right) \leq C \quad (19)$$

for all N , where $h = (-i\nabla + A)^2 + V$. The idea of using such a bound in the time dependent case originates from works by [EY01; ESY07; ESY10], was recently adapted to the ground state problem and the stability of H_N in [NRS15; CH17; LNR15b]. For example, if $H_{N,\varepsilon} \geq -CN$, where $H_{N,\varepsilon}$ is defined as H_N but replacing w by $(1 - \varepsilon)^{-1}w$ in (13), for some $\varepsilon > 0$, we can prove (19) for any $\beta < 2/3$ and therefore have convergence of both the ground states and ground state energies. If, on the other hand, we assume (15), the boundedness of the moment (19) holds immediately for $\beta \leq 1/3$ and with a bootstrap argument borrowed from [LNR15b] we extend it to $\beta < 1/3 + s/(45 + 42s)$.

If a potential w satisfies $w - b\mathbb{1}_{|x|>R}K_{dip} \in L^1 \cap L^2$ then by increasing its value in a neighborhood of the origin, we can make it classically stable as in (15). We explain this in Appendix B.

A natural question arises: are all admissible configurations (a, b) (i.e. those satisfying (11) of Theorem 1) reachable by the derivation? In the case of the dipolar potential

$$K_{dip}(x) = \frac{1 - 3\cos^2(\theta_x)}{|x|^3},$$

the answer is yes. We are able to construct a potential w_{dip} (resp. \widetilde{w}_{dip}) satisfying the assumptions of Theorem 6 in the case $b > 0$ (resp. $b < 0$) and such that the corresponding a and b satisfy the equality case $a = \frac{4\pi}{3}b$ (resp. $a = -\frac{8\pi}{3}b$). Then, any configuration (a, b) satisfying the strict inequality (11) is reached by adding a well chosen non negative function to w_{dip} (resp. \widetilde{w}_{dip}). The interaction w_{dip} is defined as follows. Let $d \in \mathbb{R}$,

$$w_{dip}(x) := 2W(x) - W(x + dn) - W(x - dn) \quad (20)$$

where

$$W(x) = \frac{1 - e^{-|x|}}{|x|}.$$

The potential w_{dip} represents the interaction of a couple of dipoles interacting with the smeared Coulomb potential W . The potential \widetilde{w}_{dip} is defined in Appendix A, in the proof of the following proposition. One could think that the case $b < 0$ has less physical meaning as it will turn out that $b = d^2$, but it is experimentally feasible to tune the parameter b to be negative [GGP02].

Proposition 9 (Full range of parameters in the dipolar GP functional). *For any admissible parameters (a, b) , i.e. satisfying (11), there exists a potential w satisfying the assumptions of Theorem 6 and in particular $a = \int (w - b\mathbb{1}_{|x|>R}K_{dip})$. Hence we have*

$$\lim_{N \rightarrow \infty} e_N = e_{GP}(a, b).$$

The proof is provided in Appendix A. The rest of the paper is dedicated to the proof of our main result.

3 Proof of Theorem 6: derivation of the dipolar Gross-Pitaevskii energy

This section is dedicated to the proof of Theorem 6.

3.1 Preliminaries

Our method in this paper is to follow the path exposed in [LNR15a] which consists in a two steps argument. We first approximate the N -body theory by Hartree's theory and then pass from the latter to the Gross-Pitaevskii theory. We use and adapt techniques developed in [NRS15; LNR15b] for the non-negative short range 3D case and the short range 2D case to our 3D dipolar problem. We denote by $h = -(\nabla_x + iA(x))^2 + V(x)$ the one body operator which is the Friedrichs extension of the operator defined similarly on $C_0^\infty(\mathbb{R}^3)$. Furthermore, h has a compact resolvent under the assumption that V is confining: $\lim_{|x| \rightarrow \infty} V(x) = \infty$, which we make, see [Iwa86] for more details on h .

The Hartree functional is given by the energy of a condensed state

$$\begin{aligned} \mathcal{E}_H^N(u) &= \frac{\langle u^{\otimes N}, H_N u^{\otimes N} \rangle}{N} \\ &= \int_{\mathbb{R}^3} |(\nabla + iA)u|^2 + \int_{\mathbb{R}^3} V|u|^2 + \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} (w_N \star |u|^2)|u|^2. \end{aligned} \quad (21)$$

We denote by

$$e_{H,N} := \inf_{\|u\|_{L^2}=1} \mathcal{E}_H^N(u)$$

the Hartree ground state energy. If a potential W is classically stable then it is Hartree stable [LNR15a]:

$$\iint_{\mathbb{R}^3 \times \mathbb{R}^3} W(x-y)\rho(x)\rho(y)dx dy \geq 0, \quad \forall \rho \geq 0. \quad (22)$$

It is easy to see that Hartree stability (15) is needed to have $\liminf e_{H,N} \geq \liminf e_N > -\infty$. The kinetic energy can never help here. Indeed, if the quantity in (22) is negative for some $\rho \geq 0$, by taking $u_N(x) = \sqrt{\rho_N(x)} = N^{3\beta/2} \sqrt{\rho(N^\beta x)}$, one can see that $e_{H,N} \rightarrow -\infty$ as $N \rightarrow \infty$. If besides, W is continuous at the origin, Hartree stability implies classical stability: taking $\rho = \sum_i \delta_{x_i}$ in (22) gives (15) with $C = w(0)/2$.

Notice that both in the Hartree functional and in the GP functional, stability is equivalent to the non negativity of the interaction energy, compare Lemma 11 and condition (11) of Theorem 1.

The two steps of the proof are as follows. The derivation of the Hartree theory follows arguments of [LNR14], using de Finetti theorems combined with a stability argument. The way from Hartree theory to Gross-Pitaevskii theory is essentially based on the observation that for $w \in L^1$, $w_N \rightarrow \delta_0 \int w$ in the sense of measures.

Estimating the pair-potential by the kinetic energy

This section is dedicated to the proof of Proposition 10 which is a generalization of [NRS15, Lemma 3.2] to a larger class of interactions including the dipolar potential. The latter has a slow decay at infinity and is therefore not a L^1 function as in [NRS15].

Proposition 10 (Domination of the interaction potential by the kinetic energy). *Define $w = w_0 + \mathbf{1}_{|x| \geq R} K$ with $w_0 \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$, K as in Theorem 6 and $R > 0$. Denote $w_N = N^{3\beta} w(N^\beta \cdot)$ for any $0 \leq \beta \leq 1$. We have the following estimates.*

$$|w_N(x-y)| \leq CN^\beta h_x \quad (23)$$

$$\pm w_N(x-y) \leq C_\varepsilon (h_x)^{3/4+\varepsilon} \otimes (h_y)^{3/4+\varepsilon}, \quad \forall \varepsilon > 0, \quad (24)$$

$$\pm (h_x w_N(x-y) + w_N(x-y) h_x) \leq CN^{3\beta/2} h_x \otimes h_y. \quad (25)$$

We will first state some lemmas to deal with the dipolar potential K . The first two have been adapted from [Duo01] and their proof will not be given here. In this paper we use the following Fourier transform $\widehat{f}(k) = \int_{\mathbb{R}^3} f(x)e^{-ik \cdot x} dx$.

Lemma 11 (Fourier transform of the potential K , Corollary 4.5 of [Duo01]). *Let $q > 1$ and $\Omega \in L^q(\mathbb{S}^2)$ be an even function satisfying the cancellation property*

$$\int_{\mathbb{S}^2} \Omega(\omega) d\sigma(\omega) = 0.$$

For any $R' > R \geq 0$ we define

$$K_R^{R'}(x) = \mathbb{1}_{R' > |x| > R} \frac{\Omega(x/|x|)}{|x|^3}. \quad (26)$$

Then for any $R' > R > 0$,

$$\begin{aligned} \widehat{K}_R^{R'}(k) &= \int_{\mathbb{S}^2} \int_R^{R'} \frac{\cos(rk \cdot \omega)}{r} \Omega(\omega) dr d\sigma(\omega) \\ &= \int_{\mathbb{S}^2} \int_R^{R'} \frac{\cos(rk \cdot \omega) - \cos(r|k|)}{r} \Omega(\omega) dr d\sigma(\omega), \end{aligned}$$

and as $R' \rightarrow \infty$ and $R \rightarrow 0$ it converges for $k \neq 0$ to

$$\widehat{K}(k) = \int_{\mathbb{S}^2} \log \left(\frac{|k|}{|k \cdot \omega|} \right) \Omega(\omega) d\sigma(\omega). \quad (27)$$

Moreover

$$\|\widehat{K}_R^{R'}\|_{L^\infty(\mathbb{R}^3)} \leq C_q \|\Omega\|_{L^q(\mathbb{S}^2)}$$

for some constant $C_q > 0$ independent of $R' > R \geq 0$ and therefore

$$\|\widehat{K}\|_{L^\infty(\mathbb{R}^3)} \leq C_q \|\Omega\|_{L^q(\mathbb{S}^2)}$$

Note that the function \widehat{K} defined in (27) is homogeneous of degree zero and continuous except at the origin.

Lemma 12 (Definition and continuity in L^p , Theorem 4.12 of [Duo01]). *Under the assumptions of the previous lemma, for any $1 < p < \infty$, we define for $f \in L^p(\mathbb{R}^3)$*

$$K \star f(x) := \lim_{\substack{R' \rightarrow \infty \\ R \rightarrow 0}} K_R^{R'} \star f(x)$$

which exists for almost every $x \in \mathbb{R}^3$. Then, there exists some constant $C_p > 0$, independent of $0 \leq R < R' \leq \infty$ such that

$$\|K_R^{R'} \star f\|_{L^p(\mathbb{R}^3)} \leq C_p C_q \|\Omega\|_{L^q(\mathbb{S}^2)} \|f\|_{L^p(\mathbb{R}^3)}, \quad \forall f \in L^p(\mathbb{R}^3).$$

Now we prove an inequality allowing to control long range interactions having bounded Fourier transform, by the kinetic energy.

Lemma 13 (Domination of the long range potential by the kinetic energy). *Let $W \in L^2_{\text{loc}}(\mathbb{R}^3)$ be such that $\widehat{W} \in L^\infty(\mathbb{R}^3)$. Then, for all $\varepsilon > 0$, there exists a constant $C_\varepsilon > 0$, independent of*

W , such that the following operator inequality holds

$$\pm W(x-y) \leq C_\varepsilon \|\widehat{W}\|_{L^\infty(\mathbb{R}^3)} (1-\Delta_x)^{3/4+\varepsilon} \otimes (1-\Delta_y)^{3/4+\varepsilon}. \quad (28)$$

Proof. We follow and adapt the proof of [ESY09][Lemma 10.1]. Let take $f \in \mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3)$ and $w \in \mathcal{S}(\mathbb{R}^3)$ where \mathcal{S} is the Schwartz class and conclude by a density argument. We rewrite the following quantity in Fourier space and use the Cauchy-Schwarz inequality

$$\begin{aligned} & \left| \int_{\mathbb{R}^6} |f(x,y)|^2 w(x-y) dx dy \right| \\ &= \left| \int_{\mathbb{R}^{12}} \overline{\widehat{f}(p_1, p_2)} \widehat{w}(q_1 - p_1) \widehat{f}(q_1, q_2) \delta(p_1 + p_2 - q_1 - q_2) dp_1 dp_2 dq_1 dq_2 \right| \\ &\leq \|\widehat{w}\|_{L^\infty(\mathbb{R}^3)} \left(\int_{\mathbb{R}^9} |\widehat{f}(p_1, p_2)|^2 \frac{(1+|p_1|^2)^{3/4+\varepsilon} (1+|p_2|^2)^{3/4+\varepsilon}}{(1+|q_1|^2)^{3/4+\varepsilon} (1+|p_1+p_2-q_1|^2)^{3/4+\varepsilon}} dp_1 dp_2 dq_1 \right)^{1/2} \\ &\quad \times \left(\int_{\mathbb{R}^9} |\widehat{f}(q_1, q_2)|^2 \frac{(1+|q_1|^2)^{3/4+\varepsilon} (1+|q_2|^2)^{3/4+\varepsilon}}{(1+|p_1|^2)^{3/4+\varepsilon} (1+|q_1+q_2-p_1|^2)^{3/4+\varepsilon}} dp_1 dq_1 dq_2 \right)^{1/2} \\ &\leq \|\widehat{w}\|_{L^\infty(\mathbb{R}^3)} \|(1-\Delta_x)^{3/8+\varepsilon/2} f\|_{L^2(\mathbb{R}^6)}^2 \sup_{k \in \mathbb{R}^3} \int_{\mathbb{R}^3} \frac{1}{(1+|k-q|^2)^{3/4+\varepsilon} (1+|q|^2)^{3/4+\varepsilon}} dq, \end{aligned}$$

where δ is the Dirac delta function. The result follows from the fact that

$$\sup_{k \in \mathbb{R}^3} \int_{\mathbb{R}^3} \frac{1}{(1+|k-q|^2)^{3/4+\varepsilon} (1+|q|^2)^{3/4+\varepsilon}} dq \leq \int_{\mathbb{R}^3} \frac{1}{(1+|q|^2)^{3/2+2\varepsilon}} dq < \infty,$$

where we have used again Cauchy-Schwarz inequality. \square

Thanks to Lemma 13 and Lemma 4 we are now able to prove Proposition 10.

Proof of Proposition 10. The first inequality (23) is exactly the same as in [NRS15, Lemma 3.2] and the last inequality (25) is easily adapted from [NRS15]. The major improvement concerns (24) where in [NRS15] the potential was assumed to be in L^1 which the dipolar potential is not.

Proof of (23).

Using the Sobolev inequality one has

$$|W(x-y)| \leq C \|W\|_{L^{3/2}(-\Delta_x)},$$

for any $W \in L^{3/2}(\mathbb{R}^3)$. Then using $\|w_N\|_{L^{3/2}} = N^\beta \|w\|_{L^{3/2}}$ and Lemma 4 we obtain (23).

Proof of (24).

Let us write $w(x) = w_0(x) + \mathbf{1}_{|x|>R} K(x)$ with $w_0 \in L^1$. Then, $\|\widehat{w}\|_{L^\infty} \leq \|\widehat{w}_0\|_{L^\infty} + \|\widehat{K}_R\|_{L^\infty} \leq \|w_0\|_{L^1} + C_q \|\Omega\|_{L^q(\mathbb{S}^2)}$ thanks to Lemma 11. We can now apply Lemma 13 which proves (24).

Proof of (25).

The proof of [NRS15, Lemma 3.2] gives

$$\pm (h_x W(x-y) + W(x-y) h_x) \leq C(\|W\|_{L^{3/2}} + \|W\|_{L^2}) h_x \otimes h_y.$$

and since $\|w_N\|_{L^{3/2}} = N^\beta \|w\|_{L^{3/2}}$ and $\|w_N\|_{L^2} = N^{3\beta/2} \|w\|_{L^2}$, inequality (25) follows. \square

3.2 From the many-body problem to Hartree theory

Our proof is inspired of the one for the 2D case of [LNR15b] with techniques first introduced in [LNR15a]. The method is the following: we derive a lower bound on the many-body energy per particle e_N making two approximations. First we project the ground state on a finite (but varying) number of low energy levels of the one-body operator, and then we use the quantitative de Finetti theorem in finite dimension to approximate the projection of the ground state by a Hartree state. The error terms involve L (the dimension of the low energy subspace the ground state has been projected on), N the number of particles and $e_{N,\varepsilon}$ the energy per particle itself (with kinetic energy decreased by a factor $(1-\varepsilon)$) which is not yet known to be bounded. But, by a bootstrap argument, first introduced in [LNR15b], we get a condition on β ensuring the boundedness of e_N . As in [NRS15; LNR15b] the main improvement regarding [LNR15a] is the use of moment estimates on ground states rather than pure operator estimates.

Moment estimates

Now, we prove some moment estimates which will be useful to control the errors. Namely, we adapt [LNR15b, Lemma 5] to the 3D case, the main difference being the assumption $0 < \beta < 1$ which has to be strengthened due to the negative part of the potential w . We define the Hamiltonian

$$H_{N,\varepsilon} := H_N - \varepsilon \sum_{j=1}^N h_j$$

and we denote by $N \times e_{N,\varepsilon}$ its ground state energy.

Lemma 14 (Moments estimates). *Let $0 < \beta < 2/3$ and $\Psi_N \in \mathfrak{h}^N$ be a ground state of H_N . Then for all $\varepsilon \in (0, 1)$ we have*

$$\mathrm{Tr} \left(h \gamma_{\Psi_N}^{(1)} \right) \leq C \frac{1 + |e_{N,\varepsilon}|}{\varepsilon} \quad (29)$$

and

$$\mathrm{Tr} \left(h \otimes h \gamma_{\Psi_N}^{(2)} \right) \leq C \frac{(1 + |e_{N,\varepsilon}|)^2}{\varepsilon^2}, \quad (30)$$

for N sufficiently large, and where the constant C is independent of N .

Proof. We have

$$H_{N,\varepsilon} = H_N - \varepsilon \sum_{j=1}^N h_j \geq N e_{N,\varepsilon} \quad (31)$$

since $N e_{N,\varepsilon}$ is the ground state energy for $H_{N,\varepsilon}$. Because $H_N \Psi_N = N e_N \Psi_N$, by taking the trace of (31) against $\gamma = |\Psi_N\rangle \langle \Psi_N|$ we get

$$e_N - \varepsilon \mathrm{Tr}(h\gamma) \geq e_{N,\varepsilon}$$

which shows the first moment estimate since e_N is upper bounded by a constant. For the second inequality, let us write

$$\begin{aligned} & \frac{1}{N^2} \left\langle \Psi_N, \left(\left(\sum_{j=1}^N h_j \right) H_N + H_N \left(\sum_{j=1}^N h_j \right) \right) \Psi_N \right\rangle \\ &= 2 \frac{e_N}{N} \left\langle \Psi_N, \sum_{j=1}^N h_j \Psi_N \right\rangle \leq C \frac{(1 + |e_{N,\varepsilon}|)^2}{\varepsilon} \end{aligned} \quad (32)$$

where we used that $|e_N| \lesssim 1 + |e_{N,\varepsilon}|$ and the first moment estimate. Let us find a lower bound on (32). One has

$$\begin{aligned} & \frac{1}{N^2} \left[\left(\sum_{j=1}^N h_j \right) H_N + H_N \left(\sum_{j=1}^N h_j \right) \right] \\ &= \frac{2}{N^2} \left(\sum_{j=1}^N h_j \right)^2 + \frac{1}{N^2(N-1)} \sum_{i=1}^N \sum_{j < k} (h_i w_N(x_j - x_k) + w_N(x_j - x_k) h_i). \end{aligned} \quad (33)$$

We split the second term in (33) in two terms, depending whether $i \neq j < k \neq i$ or $i \in \{j, k\}$. For any $1 \leq i_0 \leq N$, we have

$$\begin{aligned} & \frac{1}{N-1} \sum_{\substack{1 \leq j < k \leq N \\ j \neq i_0, k \neq i_0}} w_N(x_j - x_k) = H_{N,\varepsilon} - (1 - \varepsilon) \sum_{j=1}^N h_j - \frac{1}{N-1} \sum_{j \neq i_0} w_N(x_{i_0} - x_j) \\ & \geq N e_{N,\varepsilon} - \left(1 - \varepsilon + C \frac{N^\beta}{N-1} \right) \left(\sum_{j=1}^N h_j \right), \end{aligned} \quad (34)$$

where (23) of Proposition 10 has been used. Then multiplying (34) by h_i , we obtain

$$\begin{aligned} & \frac{1}{N^2(N-1)} \sum_{i=1}^N \sum_{i \neq j < k \neq i} h_i w_N(x_j - x_k) + w_N(x_j - x_k) h_i \\ & \geq 2 \frac{e_{N,\varepsilon}}{N} \left(\sum_{j=1}^N h_j \right) - \frac{2}{N^2} \left(1 - \varepsilon + C \frac{N^\beta}{N} \right) \left(\sum_{j=1}^N h_j \right)^2. \end{aligned} \quad (35)$$

On the other hand, for $j \neq k$, we have by (25)

$$h_j w_N(x_j - x_k) + w_N(x_j - x_k) h_j \geq -CN^{3\beta/2} h_j h_k$$

and, after summing for $1 \leq j < k \leq N$, we obtain

$$\sum_{j < k} h_j w_N(x_j - x_k) + w_N(x_j - x_k) h_j \geq -CN^{3\beta/2} \left(\sum_{j=1}^N h_j \right)^2. \quad (36)$$

Combining (35) and (36) we arrive at the estimate

$$\begin{aligned} \frac{1}{N^2} \left\{ \left(\sum_{j=1}^N h_j \right) H_N + H_N \left(\sum_{j=1}^N h_j \right) \right\} &\geq \frac{2}{N^2} \left(\varepsilon - C \frac{N^\beta}{N} - C \frac{N^{3\beta/2}}{N} \right) \left(\sum_{j=1}^N h_j \right)^2 \\ &\quad - C \frac{1 + |e_{N,\varepsilon}|}{N} \left(\sum_{j=1}^N h_j \right). \end{aligned} \quad (37)$$

Taking the trace of (37) against $|\Psi_N\rangle\langle\Psi_N|$ and using the first moment estimate, we conclude that

$$\left(\varepsilon - C \frac{N^\beta}{N} - C \frac{N^{3\beta/2}}{N} \right) \text{Tr} \left(h \otimes h \gamma_{\Psi_N}^{(2)} \right) \leq C \frac{(1 + |e_{N,\varepsilon}|)^2}{\varepsilon}.$$

Now, if $\beta < 2/3$, for N large enough one has $\varepsilon - CN^{\beta-1} - CN^{3\beta/2-1} \geq \varepsilon/2 > 0$ and the second moment estimate is proved. \square

Lower bound via de Finetti

We now state some quantitative version of the de Finetti theorem [LNR15b, Lemma 3] originally proven in [CKMR07] (see also [Chi10; Har13; LNR14] for variants of the proof and [FV06] for new results). For a summary of the use of de Finetti theorems in the mathematics of ultracold atomic gases, see [Rou15b]. Heuristically, the result states that the density matrices of symmetric wave functions are well approximated by convex combinations of product states when N is large.

Theorem 15 (Quantitative quantum de Finetti in finite dimension). *Let $\Psi \in \mathfrak{H}^N = \bigotimes_s^N L^2(\mathbb{R}^3)$ and P be an orthogonal projection of finite rank. Then, there exists a positive Borel measure $d\mu_\Psi$ on the unit sphere $SP\mathfrak{H}$ such that*

$$\text{Tr}_{\mathfrak{H}} \left| P^{\otimes 2} \gamma_{\Psi}^{(2)} P^{\otimes 2} - \int_{SP\mathfrak{H}} |u^{\otimes 2}\rangle\langle u^{\otimes 2}| d\mu_\Psi(u) \right| \leq \frac{8 \dim P\mathfrak{H}}{N}$$

and

$$\int_{SP\mathfrak{H}} d\mu_\Psi(u) \geq \left(\text{Tr} P \gamma_{\Psi}^{(1)} \right)^2.$$

Let us introduce the two-body operator $K_2^N = h \otimes 1 + 1 \otimes h + \frac{1}{2} w_N(x - y)$. Define $P := P(L) = \mathbf{1}_{(-\infty, L]}(h)$, for any $L > 0$, the projection onto the subspace of energy levels lower than L of the one-particle operator. The ground state energy can be written

$$\begin{aligned} \frac{\langle \Psi_N, H_N \Psi_N \rangle}{N} &= \text{Tr} \left(K_2 \gamma_{\Psi_N}^{(2)} \right) \\ &= \int_{\mathbb{S}L^2} \langle u^{\otimes 2}, K_2 u^{\otimes 2} \rangle d\mu_{\Psi_N}(u) + \text{Tr} K_2 \left(\gamma_{\Psi_N}^{(2)} - P^{\otimes 2} \gamma_{\Psi_N}^{(2)} P^{\otimes 2} \right) \\ &\quad + \text{Tr} K_2 \left(P^{\otimes 2} \gamma_{\Psi_N}^{(2)} P^{\otimes 2} - \int_{\mathbb{S}L^2} |u^{\otimes 2}\rangle\langle u^{\otimes 2}| d\mu_{\Psi_N}(u) \right). \end{aligned}$$

Where we have denoted the unit sphere of $L^2(\mathbb{R}^3)$ by SL^2 . The first term is the sought after approximation leading to the Hartree energy :

$$\mathcal{E}_H^N(u) = \langle u^{\otimes 2}, K_2^N u^{\otimes 2} \rangle.$$

The two others are error terms which have to be controlled. We summarize our estimates in the following lemma.

Lemma 16 (Lower bound via de Finetti). *For any $0 < \beta \leq 1$ and any $L, \varepsilon, \delta > 0$, there exists a constant $C > 0$ and $N_0 > 0$ such that, we have for all $N \geq N_0$*

$$\int_{\mathbb{S}L^2} \langle u^{\otimes 2}, K_2 u^{\otimes 2} \rangle d\mu_{\Psi_N}(u) \geq e_{H,N} - C \frac{(1 + |e_{N,\varepsilon}|)}{\varepsilon L}, \quad (38)$$

$$\mathrm{Tr} \left(K_2 \left(P^{\otimes 2} \gamma_{\Psi_N}^{(2)} P^{\otimes 2} - \int_{\mathbb{S}L^2} |u^{\otimes 2}\rangle \langle u^{\otimes 2}| d\mu_{\Psi_N}(u) \right) \right) \geq -C_\delta \frac{L^{3(1+\frac{1}{s})+2\delta}}{N} \quad (39)$$

and

$$\mathrm{Tr} K_2 \left(\gamma_{\Psi_N}^{(2)} - P^{\otimes 2} \gamma_{\Psi_N}^{(2)} P^{\otimes 2} \right) \geq -C_\delta \frac{(1 + |e_{N,\varepsilon}|)^{\frac{13}{8} + \frac{3\delta}{2}}}{\varepsilon L^{\frac{1}{8} - \frac{\delta}{2}}}. \quad (40)$$

Combining the inequalities (38), (39) and (40) we find

$$e_N \geq e_{H,N} - C \frac{(1 + |e_{N,\varepsilon}|)}{\varepsilon L} - C_\delta \left(\frac{L^{3(1+\frac{1}{s})+2\delta}}{N} + \frac{(1 + |e_{N,\varepsilon}|)^{\frac{13}{8} + \frac{3\delta}{2}}}{\varepsilon^{\frac{13}{8} + \frac{3\delta}{2}} L^{\frac{1}{8} - \frac{\delta}{2}}} \right).$$

Proof. Let us take $0 < \beta \leq 1$, $L, \varepsilon, \delta > 0$ and $N_0 > 0$ such that Lemma 14 holds.

Main term (38).

Since $\langle u^{\otimes 2}, K_2 u^{\otimes 2} \rangle = \mathcal{E}_H(u)$, we have

$$\int_{\mathbb{S}L^2} \langle u^{\otimes 2}, K_2 u^{\otimes 2} \rangle d\mu_{\Psi_N}(u) \geq e_{H,N} \int_{\mathbb{S}L^2} d\mu_{\Psi_N}(u).$$

But $\int_{\mathbb{S}L^2} d\mu_{\Psi_N}(u) \leq \left(\mathrm{Tr} P \gamma_{\Psi_N}^{(1)} \right)^2$ and $Q := 1 - P \leq L^{-1}h$ and therefore

$$\int_{\mathbb{S}L^2} d\mu_{\Psi_N}(u) \geq (1 - \mathrm{Tr} Q \gamma_{\Psi_N}^{(1)})^2 \geq 1 - \frac{2}{L} \mathrm{Tr} h \gamma_{\Psi_N}^{(1)}.$$

So we obtain

$$\int_{\mathbb{S}L^2} \langle u^{\otimes 2}, K_2 u^{\otimes 2} \rangle d\mu_{\Psi_N}(u) \geq e_{H,N} - \frac{C}{L} \mathrm{Tr} h \gamma_{\Psi_N}^{(1)} \geq e_{H,N} - C \frac{(1 + |e_{N,\varepsilon}|)}{\varepsilon L} \quad (41)$$

where we have used (29).

First error term (39).

Using the quantitative quantum de Finetti Theorem 15 and the bound $Ph \leq LP$ we obtain

$$\left| \mathrm{Tr} (h_1 + h_2) \left(P^{\otimes 2} \gamma_{\Psi_N}^{(2)} P^{\otimes 2} - \int_{\mathbb{S}L^2} |u^{\otimes 2}\rangle \langle u^{\otimes 2}| d\mu_{\Psi_N}(u) \right) \right| \leq C \frac{Ld_L}{N}, \quad (42)$$

where $d_L = \dim \text{Ran } P$. Besides, from (24) in Proposition 10 we deduce that for $\delta > 0$,

$$\pm P^{\otimes 2} w_N(x_1 - x_2) P^{\otimes 2} \leq C_\delta (Ph_1 \otimes Ph_2)^{3/4+\delta} \leq C_\delta L^{3/2+2\delta} P^{\otimes 2}$$

which, combined with (42), gives

$$\text{Tr} \left(K_2 \left(P^{\otimes 2} \gamma_{\Psi_N}^{(2)} P^{\otimes 2} - \int_{\mathbb{S}L^2} |u^{\otimes 2}\rangle \langle u^{\otimes 2}| d\mu_{\Psi_N}(u) \right) \right) \geq -C_\delta \frac{L^{3/2+2\delta} \dim P\mathfrak{H}}{N}. \quad (43)$$

We now use [CSS78, Theorem 2.1] according to which there is some constant $C > 0$ such that $\dim P\mathfrak{H} \leq CL^{3(1/2+1/s)}$ and which shows (39).

Second error term (40).

The operator inequality $h \geq Ph$ gives

$$\text{Tr} \left((h_1 + h_2) \left(\gamma_{\Psi_N}^{(2)} - P^{\otimes 2} \gamma_{\Psi_N}^{(2)} P^{\otimes 2} \right) \right) = \text{Tr} \left[\left((h_1 + h_2) - P^{\otimes 2} (h_1 + h_2) P^{\otimes 2} \right) \gamma_{\Psi_N}^{(2)} \right] \geq 0.$$

Then, we follow and adapt [LNR15b]. Using the Cauchy-Schwarz inequality for operators

$$\pm (AB + B^*A^*) \leq \eta^{-1}AA^* + \eta B^*B, \quad \forall \eta > 0, \quad (44)$$

we obtain

$$\begin{aligned} & \pm 2 \left(\gamma_{\Psi_N}^{(2)} - P^{\otimes 2} \gamma_{\Psi_N}^{(2)} P^{\otimes 2} \right) \\ &= \pm \left((1 - P^{\otimes 2}) \gamma_{\Psi_N}^{(2)} + \gamma_{\Psi_N}^{(2)} (1 - P^{\otimes 2}) + P^{\otimes 2} \gamma_{\Psi_N}^{(2)} (1 - P^{\otimes 2}) + (1 - P^{\otimes 2}) \gamma_{\Psi_N}^{(2)} P^{\otimes 2} \right) \\ &\leq 2\eta^{-1} (1 - P^{\otimes 2}) \gamma_{\Psi_N}^{(2)} (1 - P^{\otimes 2}) + \eta \left(\gamma_{\Psi_N}^{(2)} + P^{\otimes 2} \gamma_{\Psi_N}^{(2)} P^{\otimes 2} \right), \quad \forall \eta > 0. \end{aligned} \quad (45)$$

On the other hand, using (24) and the fact that

$$t^r = \inf_{\rho > 0} (r\rho^{-1}t + (1-r)\rho^{\frac{r}{1-r}}), \quad \forall t \geq 0, \quad \forall r \in (0, 1), \quad (46)$$

we get

$$\pm w_N(x - y) \leq C_\delta (h_x h_y)^{3/4+\delta} \leq C_\delta \left(\rho^{-1} h_x h_y + \rho^{\frac{3+4\delta}{1-4\delta}} \right). \quad (47)$$

Now, combining (45) and (47) we have

$$\begin{aligned} 2 \text{Tr} \left(w_N \left(\gamma_{\Psi_N}^{(2)} - P^{\otimes 2} \gamma_{\Psi_N}^{(2)} P^{\otimes 2} \right) \right) &\geq \\ &-2C_\delta \eta^{-1} \text{Tr} \left((h_x h_y)^{3/4+\delta} \right) \left((1 - P^{\otimes 2}) \gamma_{\Psi_N}^{(2)} (1 - P^{\otimes 2}) \right) \\ &-C_\delta \eta \text{Tr} \left(\rho^{-1} h_x h_y + \rho^{\frac{3+4\delta}{1-4\delta}} \right) \left(\gamma_{\Psi_N}^{(2)} + P^{\otimes 2} \gamma_{\Psi_N}^{(2)} P^{\otimes 2} \right). \end{aligned}$$

After optimizing over $\eta > 0$ we find

$$\begin{aligned} \text{Tr} \left(w_N (\gamma_{\Psi_N}^{(2)} - P^{\otimes 2} \gamma_{\Psi_N}^{(2)} P^{\otimes 2}) \right) &\geq \\ &- C_\delta \left[\text{Tr} \left((h_x h_y)^{3/4+\delta} \left((1 - P^{\otimes 2}) \gamma_{\Psi_N}^{(2)} (1 - P^{\otimes 2}) \right) \right)^{1/2} \right. \\ &\quad \times \left. \text{Tr} \left(\rho^{-1} h_x h_y + \rho^{\frac{3+4\delta}{1-4\delta}} \right) \left(\gamma_{\Psi_N}^{(2)} + P^{\otimes 2} \gamma_{\Psi_N}^{(2)} P^{\otimes 2} \right) \right]^{1/2}. \end{aligned} \quad (48)$$

Let us deal with the second factor in (48), we have

$$\left| \text{Tr} \left(\rho^{-1} h_x h_y + \rho^{\frac{3+4\delta}{1-4\delta}} \right) \left(\gamma_{\Psi_N}^{(2)} + P^{\otimes 2} \gamma_{\Psi_N}^{(2)} P^{\otimes 2} \right) \right| \leq C \left(\rho^{-1} \text{Tr} \left(h_1 h_2 \gamma_{\Psi_N}^{(2)} \right) + \rho^{\frac{3+4\delta}{1-4\delta}} \right)$$

and by optimizing over $\rho > 0$, we obtain

$$\left| \text{Tr} \left(\rho_0^{-1} h_x h_y + \rho_0^{\frac{3+4\delta}{1-4\delta}} \right) \left(\gamma_{\Psi_N}^{(2)} + P^{\otimes 2} \gamma_{\Psi_N}^{(2)} P^{\otimes 2} \right) \right| \leq C \text{Tr} \left(h_1 h_2 \gamma_{\Psi_N}^{(2)} \right)^{3/4+\delta}. \quad (49)$$

Now, let us find an upper bound of the first factor in (48). We define $Q := 1 - P$ and we notice that

$$\begin{aligned} 1 - P^{\otimes 2} &= 1 - (1 - Q) \otimes (1 - Q) = Q \otimes 1 + 1 \otimes Q - Q \otimes Q \\ &\leq Q \otimes 1 + 1 \otimes Q. \end{aligned} \quad (50)$$

This allows us to write

$$(1 - P^{\otimes 2}) (h \otimes h)^{3/4+\delta} (1 - P^{\otimes 2}) \leq C \left(Q h^{3/4+\delta} \otimes h^{3/4+\delta} + h^{3/4+\delta} \otimes Q h^{3/4+\delta} \right) \quad (51)$$

$$\leq C \frac{1}{L^{1/4-\delta}} \left(h \otimes h^{3/4+\delta} + h^{3/4+\delta} \otimes h \right) \quad (52)$$

$$\leq C \frac{1}{L^{1/4-\delta}} \left(\eta^{-1} h \otimes h + \eta^{\frac{3+4\delta}{1-4\delta}} (h \otimes 1 + 1 \otimes h) \right), \quad (53)$$

for all $\eta > 0$. In (51), we used (50), whereas in (52) we used that $Q \leq L^{-1}h$. Finally, in (53) we used (46). Now, taking the trace of (53) against $\gamma_{\Psi_N}^{(2)}$ and optimizing over $\eta > 0$ we get

$$\begin{aligned} \text{Tr} \left((h_x h_y)^{3/4+\delta} (1 - P^{\otimes 2}) \gamma_{\Psi_N}^{(2)} (1 - P^{\otimes 2}) \right) &\leq \\ &\frac{1}{L^{\frac{1}{4}-\delta}} \left(\text{Tr} h \otimes h \gamma_{\Psi_N}^{(2)} \right)^{3/4+\delta} \left(\text{Tr} h \gamma_{\Psi_N}^{(1)} \right)^{1/4-\delta}. \end{aligned} \quad (54)$$

Finally, from (49) and (54) we get

$$\begin{aligned} \text{Tr} \left(w_N \left(\gamma_{\Psi_N}^{(2)} - P^{\otimes 2} \gamma_{\Psi_N}^{(2)} P^{\otimes 2} \right) \right) &\geq \\ &- \frac{C_\delta}{L^{1/8-\delta/2}} \left(\text{Tr} h \otimes h \gamma_{\Psi_N}^{(2)} \right)^{3/4+\delta/2} \left(\text{Tr} h \gamma_{\Psi_N}^{(1)} \right)^{1/8-\delta/2}. \end{aligned} \quad (55)$$

Now, using the moment estimates (29) and (30) of Lemma 14 the result follows. \square

Final energy estimates and stability of the second kind

We follow the bootstrap argument of [LNR15b]. From Lemma 16 we have

$$e_{H,N} \geq e_N \geq e_{H,N} - C \frac{(1 + |e_{N,\varepsilon}|)}{\varepsilon L} - C_\delta \left(\frac{L^{3(1+s^{-1})+2\delta}}{N} + \frac{(1 + |e_{N,\varepsilon}|)^{13/8+3\delta/2}}{\varepsilon^{13/8+3\delta/2} L^{1/8-\delta/2}} \right). \quad (56)$$

We want to prove that $e_{N,\varepsilon}$ is bounded, otherwise, since we take $L \geq 1$ we have

$$\frac{(1 + |e_{N,\varepsilon}|)}{\varepsilon L} \leq \frac{(1 + |e_{N,\varepsilon}|)^{13/8+3\delta/2}}{\varepsilon^{13/8+3\delta/2} L^{1/8-\delta/2}}. \quad (57)$$

We can therefore omit the left side of (57) in inequality (56). Now, let us rewrite (56), replacing w by $(1 - \varepsilon)^{-1}w$, we get

$$e_{H,N}^\varepsilon \geq e_{N,\varepsilon} \geq e_{H,N}^\varepsilon - C_\delta \left(\frac{L^{3(1+\frac{1}{s})+2\delta}}{N} + \frac{(1 + |e_{N,\varepsilon'}|)^{\frac{13}{8} + \frac{3\delta}{2}}}{(\varepsilon' - \varepsilon)^{\frac{13}{8} + \frac{3\delta}{2}} L^{\frac{1}{8} - \frac{\delta}{2}}} \right), \quad (58)$$

for all $1 > \varepsilon' > \varepsilon > 0$. Note as well that $e_{H,N}^\varepsilon \geq 0$. Thanks to the classical stability of w (15), we know that for all $0 \leq \varepsilon \leq 1$ we have $e_{N,\varepsilon} \geq -CN^{3\beta-1}$. Now, as in [LNR15b], this leads us to make the following induction hypothesis, denoted I_η , for $\eta \geq 0$,

$$\limsup_{N \rightarrow \infty} \frac{|e_{N,\varepsilon}|}{1 + N^\eta} < \infty, \quad \forall \varepsilon \in (0, 1).$$

It is clear that I_η holds for $\eta = 3\beta - 1$, and we would like to prove I_0 . By choosing $L = N^\tau$, for $\tau > 0$, we see that if I_η holds, then $I_{\eta'}$ also holds as soon as

$$\eta' > \max \left\{ 3\tau(1 + s^{-1}) - 1, \frac{13\eta - \tau}{8} \right\}. \quad (59)$$

Optimizing over τ , (59) becomes

$$\eta' > \eta - \frac{s - \eta(15 + 14s)}{24 + 25s}.$$

In order to choose some $\eta' < \eta$, the condition $\eta < s/(15 + 14s)$ must be fulfilled. In term of β (in order to start the induction) this means

$$\beta < \frac{1}{3} + \frac{s}{45 + 42s}. \quad (60)$$

If condition (60) is fulfilled, we can show that (I_0) holds, after applying (58) finitely many times. Namely, we have convergence of the energy per particle with the following estimate on the rate of convergence

$$e_N \geq e_{H,N} - C_\delta N^{-\frac{1}{(25+24/s)+12\delta}}. \quad (61)$$

3.3 From Hartree theory to Gross-Pitaevskii

We have shown above that the many-body ground state energy e_N is well approximated by Hartree's energy $e_{H,N}$. It remains to show that $e_{H,N}$ is a good approximation of the Gross-Pitaevskii energy $e_{GP}(a, b)$. This is easier than the approximation of the many body energy by the Hartree energy. The case $w \in L^1(\mathbb{R}^3)$ follows from standard arguments [LNR15a; LNR15b] and it remains to adapt the proof to deal with K .

Lemma 17 (From Hartree to Gross-Pitaevskii). *Let $w_0 \in L^1(\mathbb{R}^3)$ and $K(x) = \Omega(x)/|x|^3$ satisfying the assumptions of Theorem 6. Let $b \in \mathbb{R}$ and $a = \int_{\mathbb{R}^3} w_0$, let us define $w = w_0 + b\mathbb{1}_{|x|>R}K$ for some $R > 0$. Then*

$$\begin{aligned} \lim_{N \rightarrow \infty} \sup_{\substack{u \in H^1 \\ u \neq 0}} \|u\|_{H^1}^{-4} \left| \iint w_N(x-y) |u(x)|^2 |u(y)|^2 dx dy \right. \\ \left. - a \int |u(x)|^4 dx - b \iint K(x-y) |u(x)|^2 |u(y)|^2 dx dy \right| = 0. \end{aligned} \quad (62)$$

We have not stated here any rate of convergence as it depends on the properties of the short range potential w_0 . The dipolar part of the Hartree energy converges with an error of $O(N^{-\beta})$ towards the dipolar part of the Gross-Pitaevskii energy. As an example, under the extra assumption $|x|w_0(x) \in L^1(\mathbb{R}^3)$, the short range part of the energy converges also with an error of $O(N^{-\beta})$.

Lemma 17 shows that $e_{H,N} = e_{GP} + o(1)$ as $N \rightarrow \infty$ and ends the proof of Theorem 6.

Proof. For the L^1 part of the potential, the proof of convergence is the same as in [LNR15b, Lemma 7] except that the integration domain is \mathbb{R}^3 and not \mathbb{R}^2 . We quickly recall it here: let $w_0 \in L^1(\mathbb{R}^3)$ and $A > 0$. We have

$$\begin{aligned} & \left| \iint w_{0,N}(x-y) |u(x)|^2 |u(y)|^2 dx dy - a \int |u(y)|^4 dy \right| \\ &= \left| \iint w_0(x) |u(y)|^2 (|u(N^{-\beta}x+y)|^2 - |u(y)|^2) dx dy \right| \\ &\leq 2 \iint \mathbb{1}_{|x|<A} |w_0(x)| |u(y)|^2 \int_0^1 |u \nabla u(tN^{-\beta}x+y) \cdot x| N^{-\beta} dt dx dy \\ &\quad + 2 \left(\int \mathbb{1}_{|x|>A} |w_0(x)| dx \right) \|u\|_{L^4}^4 \\ &\leq 2 \left(AN^{-\beta} + 2 \left(\int \mathbb{1}_{|x|>A} |w_0(x)| dx \right) \right) \|u\|_{H^1}^4. \end{aligned}$$

Taking $A = N^{\beta/2}$ gives the desired result. For the dipolar part, the same proof will not work since the potential is not integrable both at the origin and at infinity. Nevertheless, as we saw in Lemma 11, the convolution by K extends to a bounded operator on $L^2(\mathbb{R}^3)$ and coincides in Fourier space with the multiplication by a bounded function $\widehat{K} \in L^\infty(\mathbb{R}^3)$. By definition, for $f \in L^p(\mathbb{R}^3)$,

$$K \star f := \lim_{\substack{\varepsilon \rightarrow 0 \\ \eta \rightarrow \infty}} K_\varepsilon^\eta \star f \text{ where } K_\varepsilon^\eta(x) = K(x) \mathbb{1}_{\varepsilon \leq |x| \leq \eta}(x), \quad \forall x \in \mathbb{R}^3.$$

As computed in Lemma 11

$$\widehat{K}_\varepsilon^\eta = \int_{\mathbb{S}^2} \int_\varepsilon^\eta (\cos(rp \cdot \omega) - 1) \Omega(\omega) \frac{dr}{r} d\sigma(\omega). \quad (63)$$

In order to prove (62), we seek to find a bound on the error $\int (K_0^{RN^{-\beta}} \star |u|^2) |u|^2$. First, let us notice that for $p \in \mathbb{R}^3$

$$\left| \widehat{K}_0^{RN^{-\beta}}(p) \right| \leq C \int_{\mathbb{S}^2} \int_0^{RN^{-\beta}} |\cos(rp \cdot \omega) - 1| \frac{dr}{r} d\sigma(\omega) \leq C |p| N^{-\beta}. \quad (64)$$

Then,

$$\begin{aligned} \left| \int_{\mathbb{R}^3} (K_N \mathbb{1}_{|x| \geq RN^{-\beta}} \star |u|^2) |u|^2 - \int_{\mathbb{R}^3} (K \star |u|^2) |u|^2 \right| &\leq \int_{\mathbb{R}^3} \widehat{K}_0^{RN^{-\beta}} \left| \widehat{|u|^2} \right|^2 \\ &\leq C N^{-\beta} \int_{\mathbb{R}^3} |p| \left| \widehat{|u|^2}(p) \right|^2. \end{aligned} \quad (65)$$

By a density argument we can assume that u is smooth and use that $\widehat{|u|^2} = \widehat{|u|} \star \widehat{|u|}$, we obtain

$$\begin{aligned} \int_{\mathbb{R}^3} |p| \left| \widehat{|u|^2}(p) \right|^2 &\leq \int |p| \widehat{|u|}(p-k) \widehat{|u|}(k) \widehat{|u|}(p-q) \widehat{|u|}(q) dq dk dp \\ &\leq 2 \int |p-k| \widehat{|u|}(p-k) \widehat{|u|}(k) \widehat{|u|}(p-q) \widehat{|u|}(q) dq dk dp, \end{aligned}$$

where we used that $|p| \leq |p-k| + |k|$ and the symmetry of the integrand. We now define $f = \mathcal{F}^{-1}(\widehat{|u|})$ and $g = \mathcal{F}^{-1}(|p| \widehat{|u|})$ such that $\|f\|_{H^1} = \|u\|_{H^1} \leq \|u\|_{H^1}$ and $\|g\|_{L^2} \leq \|\nabla u\|_{L^2}$. And finally,

$$\begin{aligned} \int_{\mathbb{R}^3} |p| \left| \widehat{|u|^2} \right|^2 &\leq \int |g(x)| |f(x)|^3 dx \\ &\leq C \|g\|_{L^2} \|f\|_{L^6}^3 \leq C \|g\|_{L^2} \|f\|_{H^1}^3 \leq C \|u\|_{H^1}^4 \end{aligned} \quad (66)$$

Inequality (66) inserted in (65) concludes the proof of Lemma 17. \square

Appendix A Proof of Proposition 9

Here, we show that in the dipolar case $K = K_{dip}$, any admissible (a, b) , i.e satisfying the condition (11) of Theorem 1, comes from a pair potential in the many-body problem. The proof uses two well chosen potentials w_{dip} and \widetilde{w}_{dip} which give the case of equality in (11) respectively for $b > 0$ and $b < 0$. Higher a 's are then achieved by adding a non negative pair function having the correct mass. First, we need the following lemma in order to build a classically stable potential behaving like the dipolar one at large distances.

Lemma 18 ([Lew04], Dipolar approximation). *There is a constant $C > 0$ such that for all $x, h \in \mathbb{R}^3$ with $R + h \neq 0$,*

$$\left| \frac{1}{|x+h|} - \left(\frac{1}{|x|} - \frac{e_x \cdot h}{|x|^2} + \frac{3(e_x \cdot h)^2 - |h|^2}{2|x|^3} \right) \right| \leq \frac{C|h|^3}{|x|^3|x+h|}$$

with $e_x = x/|x|$.

We now recall the definition of w_{dip} ,

$$w_{dip}(x) = 2W(x) - W(x + dn) - W(x - dn) \text{ with } W(x) = \frac{1 - e^{-|x|}}{|x|}. \quad (67)$$

The potential w_{dip} represents the total interaction of two dipoles given by four charged particles interacting via the smeared Coulomb potential W whose position and charge are $(\mathcal{O}, 1)$, $(dn, -1)$ (for the first dipole) and $(x, 1)$, $(x + dn, -1)$ (for the second dipole). The dipolar moment d is a characteristic of the system and is parallel to n , the common direction of the dipoles. In particular, by Lemma 18, if we fix some $R > 0$, the potential w_{dip} can be written

$$w_{dip} = w_0 + d^2 \mathbb{1}_{|x| \geq R} K \quad (68)$$

with $w_0 \in L^1 \cap L^\infty$. Furthermore, w_{dip} is of positive type since

$$\begin{aligned} \widehat{w_{dip}}(k) &= 2\widehat{W}(k) - \widehat{W(\cdot + dn)}(k) - \widehat{W(\cdot - dn)}(k) \\ &= \frac{8\pi}{|k|^2(1 + |k|^2)} (1 - \cos(k \cdot dn)) \geq 0. \end{aligned} \quad (69)$$

Computation of the short range parameter a

Now, let us compute the short range strength $a = \int w_0$, defined in (68). Recall that this quantity is independent of the choice of $R > 0$. We have

$$\int_{\mathbb{R}^3} w_0 = \int_{\mathbb{R}^3} (w_{dip} - d^2 \mathbb{1}_{|x| > R} K) = \lim_{A \rightarrow \infty} \int_{B(0, A)} w_{dip},$$

thanks to the cancellation property (3).

Lemma 19 (Computation of the short range strength). *The short range parameter of w_{dip} is given by*

$$\int_{\mathbb{R}^3} w_0 = \frac{4\pi}{3} d^2.$$

Proof. Recall that $w - d^2 \mathbb{1}_{|x| > R} K \in L^1$, we can consider

$$\mathcal{F}(w_{dip} - d^2 \mathbb{1}_{|x| > R} K) = \widehat{w_{dip}} - d^2 \left(\widehat{K} - K \widehat{\mathbb{1}_{|x| > R}} \right) \quad (70)$$

which is a continuous function and satisfies $\mathcal{F}(w_{dip} - d^2 \mathbb{1}_{|x| > R} K)(0) = \int w_0$. Now, we compute the limit when $p \rightarrow 0$ of the right side of (70). The third term is an error term and according to (64), it is a $\mathcal{O}(p)$ as $p \rightarrow 0$. On the other hand, for any $p \in \mathbb{R}^3$, we can write the first term as

$$\mathcal{F}(w_{dip})(p) - d^2 \mathcal{F}(K)(p) = 4\pi \left[\frac{2}{(1 + |p|^2)|p|^2} (1 - \cos(p \cdot dn)) - \frac{(p \cdot dn)^2}{|p|^2} + \frac{d^2}{3} \right],$$

which tends to $\frac{4\pi}{3} d^2$ as $p \rightarrow 0$. \square

Now, using w_{dip} , we will show that any a and b satisfying assumptions (11) are reached for some potential w . For this purpose, let us distinguish two cases.

Case 1: $b > 0$

Let (a, b) satisfy condition (11) with $b > 0$. Let us take $d^2 = b$ and $a \geq 4\pi b/3$. Define

$$w = f + w_{dip},$$

with $f \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ of positive type, such that $\int f = a - 4\pi b/3$. Then, the potential w is classically stable, since $w \geq w_{dip}$ and w_{dip} is. It satisfies the assumptions of Theorem 6, and so the result holds for $b > 0$.

Case 2: $b < 0$

Without loss of generality, let us assume $n = e_3$ and let us take $d^2 = -b$. Define

$$\widetilde{w}_{dip} = f - w_{dip}$$

with f being the inverse Fourier transform of

$$\widehat{f}(p) = \frac{4\pi}{(1 + |p|^2) \left(d^{-2} + \frac{p_1^2 + p_2^2}{4} \right)}.$$

We have $\widehat{f} \in L^1$, since

$$\int_{\mathbb{R}^3} \frac{1}{(1 + |p|^2)(1 + p_1^2 + p_2^2)} dp_1 dp_2 dp_3 = \int_{\mathbb{R}} \frac{dp_3}{1 + p_3^2} \int_{\mathbb{R}^2} \frac{dp_1 dp_2}{(1 + p_1^2 + p_2^2)^{3/2}} < \infty,$$

where we used the change of variable $p_3 = \sqrt{1 + p_1^2 + p_2^2}$. One can verify that $(1 - \Delta)^2 \widehat{f} \in L^1$ and therefore $f \in L^1$. Furthermore, the inequality

$$2(1 - \cos(p_3 d)) \left(d^{-2} + \frac{p_1^2 + p_2^2}{4} \right) \leq p^2,$$

implies $\widetilde{w}_{dip} = \widehat{f} - \widehat{w}_{dip} \geq 0$. Moreover, since $\widehat{f} \in L^1$, $f \in L^1 \cap L^2$ the potential \widetilde{w}_{dip} satisfies the assumptions of Theorem 6 and its short range parameter is given by $a = (\widehat{f} - \widehat{w}_0)(0) = -8\pi b/3$.

This concludes the case of equality of Proposition 9, the other cases are obtained by adding positive functions to the potential \widetilde{w}_{dip} .

Appendix B Stabilization of the long range potential

Here we show that given a potential $K = \Omega(x/|x|)|x|^{-3}$, with Ω an even function satisfying the cancellation property (3) and some regularity condition, there always exists a classically stable potential w_{stab} behaving like K at infinity (Proposition 20). Moreover, if some potential w has the long range behavior of K , we show that one can always make it classically stable by increasing its value in a fixed neighborhood of the origin (Proposition 21).

Proposition 20 (Existence of stable potential). *Let $K = \Omega(x/|x|)|x|^{-3}$ with $\Omega \in W^{4,q}(\mathbb{S}^2)$, an even function, satisfying the cancellation property (3), for some $q > 1$. Then, for any $R > 0$, there exists some continuous function $w_{stab} \in L^p(\mathbb{R}^3)$, for $1 < p \leq \infty$, of positive type (hence classically stable), such that $w_{stab} - \mathbb{1}_{|x| > R} K \in L^1(\mathbb{R}^3)$. Moreover, we can choose w_{stab} such that $|w_{stab}(x) - \mathbb{1}_{|x| > R} K(x)| = \mathcal{O}(e^{-\mu|x|})$, for some $\mu > 0$, as x tends to infinity.*

Proposition 21 (Long range stability). *Let K be as in Proposition 20, $R > 0$ and $w \in L^1(\mathbb{R}^3)$ with $(w)_- \in L^\infty(\mathbb{R}^3)$ and such that $w(x) - \mathbb{1}_{|x|>R}K(x) \in L^1(\mathbb{R}^3)$. For all $\delta > 0$ there exists $\eta > 0$ such that $w + \eta\mathbb{1}_{|x|<\delta}$ is classically stable.*

To show the properties above we need the following lemma whose proof will be postponed.

Lemma 22 (Stabilisation by a short range potential). *Let $w_0 \in L^1_{\text{loc}}(\mathbb{R}^3)$, $w_0 > \eta > 0$ and $w_1 \in L^\infty(\mathbb{R}^3)$ such that*

$$|w_1(x)| \leq C_0 1/|x|^{3+\varepsilon} \quad (71)$$

for all $x \in \mathbb{R}^3$, where $\eta, \varepsilon, C_0 > 0$. Let us define for $R > 0$

$$\varphi_R = w_0 \mathbb{1}_{|x| \leq R} + w_1 \mathbb{1}_{|x| \geq R}.$$

Then, there is come constant C_ε , given by (80), such that, if

$$C_\varepsilon \leq \frac{R^{2+\varepsilon} \eta}{C_0(1 + R^{-6(1+\frac{2}{\varepsilon})})}, \quad (72)$$

then, there exists $\psi \in L^1(\mathbb{R}^3)$ such that $\varphi_R \geq \psi$, $\widehat{\psi} \geq 0$ and $\widehat{\psi} \in L^1$. In particular, φ_R is classically stable.

If Lemma 22 and Proposition 20 hold, then Proposition 21 is easily verified.

Proof of Proposition 21. Let us consider w_{stab} as in Proposition 20. Let us write $w = w_0 \mathbb{1}_{|x| \leq R} + \mathbb{1}_{|x| > R}K$ and rewrite w as,

$$w = w_0 \mathbb{1}_{|x| \leq R} - w_{stab} \mathbb{1}_{|x| < R} + (K - w_{stab}) \mathbb{1}_{|x| > R} + w_{stab}. \quad (73)$$

The second term in (73) is smaller than $\|w_{stab}\|_{L^\infty}$, the third term is a $\mathcal{O}(e^{-|x|})$ and the last term is of positive type according to Proposition 20. Then, by increasing w_0 sufficiently in some fixed neighborhood of the origin, one can make w classically stable by using Lemma 22. The idea of the proof is based on a result of Ruelle [Rue99, Proposition 3.2.8]. \square

Now we prove Lemma 22 and Proposition 20.

Proof of Lemma 22. The strategy of the proof is to increase the function φ_R , by adding a function ψ_1 whose Fourier transform is well controlled, and such that $\varphi_R + \psi_1$ is positive. We will then look for conditions on R, η and C_0 to bound $\varphi_R + \psi_1$ from below by a function of positive type ψ_2 , such that $\psi := \psi_2 - \psi_1$ is classically stable.

Let α be a smooth positive function with support in $B(0, 1)$ and such that $\int \alpha = 1$. Let us denote $\alpha_R(x) = (R/2)^{-3} \alpha(2x/R)$. For $|x| > R$, we have

$$\begin{aligned} \int_{B(0, R/2)} \frac{1}{|x - x'|^{3+\varepsilon}} \alpha_R(x') dx' &\geq \frac{1}{(|x| + R/2)^{3+\varepsilon}} \geq \frac{R^{3+\varepsilon}}{(R + R/2)^{3+\varepsilon}} \frac{1}{|x|^{3+\varepsilon}} \\ &\geq \left(\frac{2}{3}\right)^{3+\varepsilon} \frac{1}{|x|^{3+\varepsilon}}. \end{aligned} \quad (74)$$

Let us define

$$\psi_1(x) = C_0 \left(\frac{3}{2}\right)^{3+\varepsilon} \left(\frac{1}{|x'|^{3+\varepsilon}} \mathbb{1}_{|x'| \geq R/2}\right) \star \alpha_R(x),$$

from (71) and (74) we deduce

$$|w_1(x)|\mathbb{1}_{|x|>R} \leq C_0 \frac{1}{|x|^{3+\varepsilon}} \mathbb{1}_{|x|>R} \leq \psi_1(x)$$

and in particular we obtain

$$\psi_1 \leq w_1 \mathbb{1}_{|x|>R} + 2\psi_1. \quad (75)$$

We now look for a bound on $\widehat{\psi}_1$, we have

$$\|(1+p^2)^3 \widehat{\psi}_1\|_\infty \leq \|(1-\Delta)^3 \psi_1\|_{L^1}$$

from which we obtain

$$|\widehat{\psi}_1(p)| \leq \frac{C_0 3^{3+\varepsilon} \|(1-\Delta)^3 \alpha_R\|_{L^1} \|\mathbb{1}_{|x| \geq R} 1/|x|^{3+\varepsilon}\|_{L^1}}{2^{3+\varepsilon} (1+p^2)^3} = \frac{4\pi C_0 3^{3+\varepsilon} \|(1-\Delta)^3 \alpha_R\|_{L^1}}{2^{3+\varepsilon} R^\varepsilon (1+p^2)^3}. \quad (76)$$

Let us define for $\mu > 0$, $\lambda > 1$,

$$\psi_\lambda^\mu(x) = \mu \frac{e^{-\lambda|x|/2} - e^{-\lambda|x|}}{|x|}.$$

We have

$$\widehat{\psi}_\lambda^\mu(p) = \mu \left(\frac{1}{|p|^2 + \lambda^2/4} - \frac{1}{|p|^2 + \lambda^2} \right) = \frac{\frac{3}{4}\lambda^2 \mu}{(|p|^2 + \lambda^2/4)(|p|^2 + \lambda^2)} \geq \frac{\frac{3}{4}\lambda^2 \mu}{(|p|^2 + \lambda^2)^2}. \quad (77)$$

We want to find a condition on λ and μ such that $\psi_\lambda^\mu(x) \leq \psi_1(x)$ for $|x| > R$, and since it is sufficient to have

$$\psi_\lambda^\mu(x) = \mu \frac{e^{-\lambda|x|/2} - e^{-\lambda|x|}}{|x|} \leq \mu \frac{e^{-\lambda|x|/2}}{|x|} \leq C_0 \frac{1}{|x|^{3+\varepsilon}} \leq \psi_1(x) \quad \forall |x| > R,$$

it is then sufficient to assume $\mu \leq C_0 C_\varepsilon \lambda^{2+\varepsilon}$ where $C_\varepsilon = (4 + 2\varepsilon)^{2+\varepsilon} e^{-(2+\varepsilon)}$. Therefore, with (75) we obtain

$$\psi_\lambda^\mu(x) - 2\psi_1(x) \leq w_1(x), \quad \forall |x| > R. \quad (78)$$

On the other hand for $\mu \leq \eta$, we have

$$\psi_\lambda^\mu(x) - 2\psi_1(x) \leq \mu \leq \eta \leq w_0(x), \quad \forall |x| < R.$$

From (76) and (77) we deduce that if $\mu R^\varepsilon \geq 3^4 \pi \lambda^2 C_0 \|(1-\Delta)^3 \alpha_R\|_{L^1}$ and $\lambda > 1$, then

$$0 \leq \widehat{\psi}_\lambda^\mu - 2\widehat{\psi}_1.$$

Gathering the conditions, we deduce that if

$$3^4 \pi \frac{\|(1-\Delta)^3 \alpha_R\|_{L^1}^{1+\frac{2}{\varepsilon}}}{(4+2\varepsilon)^\frac{4+2\varepsilon}{\varepsilon} e^{-\frac{4+2\varepsilon}{\varepsilon}}} < \frac{R^{2+\varepsilon} \eta}{C_0} \quad (79)$$

then we can find some $\lambda, \mu > 0$ such that $\psi := \psi_\lambda^\mu - 2\psi_1 \leq \varphi_R$ where ψ fulfills the assumptions

of the lemma. We define

$$C_{\varepsilon,0} = \frac{3^4 \pi e^{\frac{4+2\varepsilon}{\varepsilon}}}{(4+2\varepsilon)^{\frac{4+2\varepsilon}{\varepsilon}}} \sup_{R>0} \inf_{\alpha} \frac{\|(1-\Delta)^3 \alpha_R\|_{L^1}^{1+\frac{2}{\varepsilon}}}{1+R^{-6(1+\frac{2}{\varepsilon})}}. \quad (80)$$

□

Proof of Proposition 20. Let $0 \leq \chi \leq 1$ be a smooth function such that $\chi(x) = 0$ for $|x| \leq 1/2$ and $\chi(x) = 1$ for $|x| \geq 1$. Let us denote by $\chi_R(x) = \chi(x/R)$ and $g = \chi_R K$. We have $(1-\Delta)^2 g = (1+|p|^2)^2 \widehat{g}$ and

$$\begin{aligned} (1+|p|^2)^2 |\widehat{g}(p)| &\leq \|\widehat{g}\|_{L^\infty} + 2\| |p|^2 \widehat{g} \|_{L^\infty} + \| |p|^4 \widehat{g} \|_{L^\infty} \\ &\leq \|(1-\chi_R) \mathbf{1}_{|x|<R} K\|_{L^1} + \|\widehat{\mathbf{1}_{|x|<R} K}\|_{L^\infty} + 2\| -\Delta g \|_{L^1} + \|(-\Delta)^2 g\|_{L^1} \\ &\leq C_R \|\Omega\|_{W^{4,q}}. \end{aligned}$$

Now, for $\mu > 0$, consider $\psi_1^\mu \in L^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ as defined in the proof of Lemma 22. It satisfies

$$\widehat{\psi_1^\mu}(p) \geq \frac{\frac{3}{4}\mu}{(1+|p|^2)^2}.$$

Taking $\mu \geq 4C_R \|\Omega\|_q / 3$, we define $w_{stab} = \psi_1^\mu + (1-\chi_R)K$. Because of Sobolev embeddings $\Omega \in L^\infty$ and therefore $w_{stab} - \mathbf{1}_{|x|>R} K \in L^\infty(\mathbb{R}^3)$. Moreover $\psi_1^\mu(x) = \mathcal{O}(e^{-\mu|x|})$ as $x \rightarrow \infty$, this concludes the proof of Proposition 20. □

Appendix C Proof of Theorem 5: uniqueness

Proof of 1)

We use the implicit function theorem to prove the uniqueness of the ground state of the Gross-Pitaevskii energy in some neighborhood of $\varphi = 0$. This method does not allow to give an explicit value of φ_0 in the lemma.

Let us fix some admissible parameters (a, b) , i.e. satisfying condition (11), and let us define

$$\mathcal{E}(u, \varphi) := \int_{\mathbb{R}^3} |(\nabla + i\varphi A)u|^2 + \int_{\mathbb{R}^3} V|u|^2 + a \int_{\mathbb{R}^3} |u|^4 + b \int_{\mathbb{R}^3 \times \mathbb{R}^3} (K \star |u|^2)|u|^2.$$

We assume without loss of generality that $V \geq 0$. A minimizer of $\mathcal{E}(\cdot, \varphi)$ satisfies the Euler-Lagrange equation

$$\Phi(u_1, u_2, \varphi) := h^\varphi u + 2a|u|^2 u + 2bK \star |u|^2 u - \mu(u, \varphi)u = 0$$

where $u = u_1 + iu_2$ with u_1, u_2 are real valued,

$$h^\varphi = (i\nabla + \varphi A)^2 + V$$

and $\mu(u, \varphi) = \mathcal{E}(u, \varphi) + a \int |u|^4 + b \int K \star |u|^2 |u|^2$. We want to apply the implicit function on Φ in a neighborhood of $(u_0, 0)$. For that, we first need the following lemma.

Lemma 23. *Define the operator*

$$L^- = -\Delta + V + 2au_0^2 + 2bK \star u_0^2 - \mu(u_0, 0)$$

with domain $\mathcal{D}(h_0)$. Then L^- is a non-negative self-adjoint operator with compact resolvent. Moreover, its ground state is u_0 and it is non-degenerate.

Proof. Thanks to Lemma 11 and Sobolev embeddings we have $f := 2au_0^2 + 2b(K \star u_0^2) \in L^2(\mathbb{R}^3)$. The self-adjointness and the compactness of the resolvent of H_0 follow from Sobolev inequality. The uniqueness and the non-negativity of the ground state up to a constant phase follow from [LL01, Theorem 7.8]. Now, since u_0 minimizes $\mathcal{E}(\cdot, 0)$, we know that $H_0 u_0 = \mu_0 u_0$ and also that for any $v \in \mathcal{D}(h_0^{1/2})$ we have $\frac{d^2}{dt^2} \mathcal{E}(u_0 + tv)|_{t=0} \geq 0$. The latter is equivalent to

$$\begin{aligned} & \left\langle v \left| -\Delta + V + 2au_0^2 + 2bK \star u_0^2 \right| v \right\rangle \\ & + 4a \int u_0(x)^2 \Re(v(x))^2 dx + 4b \iint K(x-y) u_0(x) \Re(v(x)) u_0(y) \Re(v(y)) dx dy \\ & \geq \mu(u_0, 0) \|v\|_{L^2(\mathbb{R}^3)}^2. \end{aligned}$$

Taking iv with v real in the last inequality shows that $L^- \geq 0$ (since we know the ground state of L^- is real up to a constant phase). Taking $v = u_0$ shows that u_0 is the ground state. \square

To verify the assumptions of the implicit function theorem we must compute

$$\begin{aligned} d_1 \Phi_{(u_0, 0, 0)} \xi &:= L^+ \xi \\ &= L^- \xi + 4au_0^2 \xi + 4b(K \star u_0 \xi) u_0 \\ &\quad - 4 \left(a \int u_0^3 \xi + b \int (K \star u_0^2) u_0 \xi \right) u_0 - 2\mu(u_0, 0) \langle u_0, \xi \rangle_{L^2} u_0 \end{aligned}$$

and

$$d_2 \Phi_{(u_0, 0, 0)} \xi = L^- \xi = h^0 \xi + 2au_0^2 \xi + 2b(K \star u_0^2) \xi - \mu(u_0, 0) \xi.$$

Define $\mathcal{V} := \mathcal{D}(h_0^{1/2})$ endowed with the norm $\|u\|_{\mathcal{V}} = \|u\|_{L^2} + \|h_0^{1/2} u\|_{L^2}$ and denote by $\{u_0\}^\perp$ the orthogonal space in $L^2(\mathbb{R}^3)$ to u_0 with respect to the L^2 scalar product. We emphasize that the latter are spaces composed of real valued functions. Using Sobolev inequality and Lemma 11, it is elementary that Φ , $d_1 \Phi$ and $d_2 \Phi$ are continuous functions. In order to apply the implicit function theorem, we want to prove that $(L^+)^{-1} : (L^2(\mathbb{R}^3), \|\cdot\|_{L^2}) \rightarrow (\mathcal{V}, \|\cdot\|_{\mathcal{V}})$ and $(L^-)^{-1} : (\{u_0\}^\perp, \|\cdot\|_{L^2}) \rightarrow (\mathcal{V} \cap \{u_0\}^\perp, \|\cdot\|_{\mathcal{V}})$ are bounded linear operators. Since, L^\pm have compact resolvents, it is sufficient to prove that 0 is not an eigenvalue of L^+ and that $\ker(L^-) = \text{span}\{u_0\}$. We prove this by contradiction, let $\xi \in \ker(L^+)$, writing $\xi = \lambda u_0 + \xi^\perp$ with $\xi^\perp \in \{u_0\}^\perp$, we have

$$\begin{aligned} & \langle \xi^\perp, L^+ \xi \rangle = 0 \\ & = \langle \xi^\perp, L^- \xi^\perp \rangle + 4 \left(a \int (u_0 \xi^\perp)^2 + b \int K \star (u_0 \xi^\perp) u_0 \xi^\perp \right) - 2\lambda \langle u_0, h^0 \xi^\perp \rangle, \end{aligned} \tag{81}$$

$$\langle u_0, L^+ \xi \rangle = 0 = -2\lambda \mu(u_0, 0). \tag{82}$$

From (82), and since $\mu(u_0, 0) > 0$ because we assumed $V \geq 0$, we deduce that $\lambda = 0$ and then

from (81) together with Lemma 23 and the admissibility of (a, b) we obtain that $\xi^\perp = 0$ which is the contradiction we seek. Similar arguments gives that $\ker(L^-) = \text{span}(u_0)$. We in fact only proved that $(L^+)^{-1} : (L^2(\mathbb{R}^3), \|\cdot\|_{L^2}) \rightarrow (\mathcal{V}, \|\cdot\|_{L^2})$ is continuous, but since $\|\cdot\|_{L^2} \lesssim \|\cdot\|_{\mathcal{V}}$ the desired continuity property holds. Now, we can use [Cha06, Theorem 1.2.1 & 1.2.3] and claim that there is some neighborhood $X \times]-\varphi_0, \varphi_0[\ni (u_0, 0)$ in $\mathcal{H} := \mathcal{V} \oplus (\{u_0\}^\perp \cap \mathcal{V}) \times \mathbb{R}$ and some function $h :]-\varphi_0, \varphi_0[\rightarrow X$ such that for any $(u, \varphi) \in X \times]-\varphi_0, \varphi_0[$

$$\Phi(u, \varphi) = 0 \iff u = h(\varphi).$$

Hence, there is uniqueness of the minimizer in X . Now we must prove that there is some other neighborhood of 0 which we will still denote by $] -\varphi_0, \varphi_0[$ such that for all $|\varphi| < \varphi_0$, any minimizer of $\mathcal{E}(\cdot, \varphi)$ (restricted to the unit sphere of $L^2(\mathbb{R}^3)$) belongs to X (up to a constant phase). We prove it by contradiction, assume there is a sequence $\varphi_n \rightarrow 0$ with $u_n \in (\mathcal{V} \oplus \mathcal{V}) \setminus X$ minimizing $\mathcal{E}(\cdot, \varphi_n)$ for all n . First, notice that for all $u \in L^2(\mathbb{R}^3)$ there is some $\theta \in \mathbb{R}$ such that

$$\Im(ue^{i\theta}) = \Re(u) \sin(\theta) + \Im(u) \cos(\theta) \in \{u_0\}^\perp.$$

It suffices to take $\theta = -\tan^{-1}(\langle \Im(u), u_0 \rangle / \langle \Re(u), u_0 \rangle)$. Hence, we can assume that $u_n \in \mathcal{H}$ for all n . Then, notice that (u_n) is bounded in \mathcal{H} it is thus precompact in $L^2(\mathbb{R}^3)$ and we can assume without loss of generality that it converges to some function $u_\infty \in L^2(\mathbb{R}^3)$. Besides, for any u and $|\varphi| \leq C$ we have

$$|\mathcal{E}(u, \varphi) - \mathcal{E}(u, 0)| \leq |\varphi| |\langle u, (\nabla A + A\nabla)u \rangle| + |\varphi|^2 |\langle u, A^2u \rangle| \leq C|\varphi| |\langle u, (h_0 + 1)u \rangle|.$$

So that

$$\mathcal{E}(u_n, 0) = \mathcal{E}(u_n, \varphi_n) + o(1) \leq \mathcal{E}(u_0, \varphi_n) + o(1) = \mathcal{E}(u_0, 0) + o(1).$$

And since $\mathcal{E}(\cdot, 0)$ is lower semi-continuous, by passing to the limit above we obtain $\mathcal{E}(u_\infty, 0) \leq \mathcal{E}(u_0, 0)$ hence $u_\infty = u_0$ by uniqueness. We recall that X is a \mathcal{H} -neighborhood of u_0 so we must prove the convergence of u_n in the topology of \mathcal{H} . We know that $(h_0^{1/2}u_n)$ is bounded in $L^2(\mathbb{R}^3)$ thus, without loss of generality, we assume it converges weakly to some limit we denote by v_∞ . Then, for any $\xi \in \mathcal{V} \oplus \mathcal{V}$ we have

$$\langle h_0^{1/2}u_n, \xi \rangle = \langle u_n, h_0^{1/2}\xi \rangle \rightarrow \langle u_0, h_0^{1/2}\xi \rangle = \langle h_0^{1/2}u_0, \xi \rangle$$

proving that $v_\infty = h_0^{1/2}u_0$ since $\mathcal{V} \oplus \mathcal{V}$ is a dense subset of $L^2(\mathbb{R}^3)$. Now, let us prove that the convergence is strong. For that, it suffices to prove the conservation of mass in the limit: $\|h_0^{1/2}u_n\| \rightarrow \|h_0^{1/2}u_0\|$ as $n \rightarrow \infty$. We have, by the Euler-Lagrange equation,

$$\begin{aligned} \left| \|h_0^{1/2}u_n\| - \|h_0^{1/2}u_0\| \right| &\leq |\mathcal{E}(u_n, 0) - \mathcal{E}(u_0, 0)| \\ &+ \int \left| |u_n|^4 - |u_0|^4 \right| + \int |K \star u_n^2 u_n^2 - K \star u_0^2 u_0^2| \rightarrow 0, \end{aligned}$$

as $n \rightarrow \infty$. We already know that the first term tends to 0, for the two other, it comes from Sobolev embeddings and Lemma 11. Hence $u_n \rightarrow u_0$ in \mathcal{H} and this is the contradiction we seek : there is some $\varphi_0 > 0$ such that if u is a minimizer of $\mathcal{E}(\cdot, \varphi)$ then $u \in X$. This ends the proof.

Proof of 2)

This result is stated for the case $K = 0$ in a remark of [LSSY05, Ch. 7]. Here, we give a proof working for any K satisfying the assumption of Lemma (11) using the fact that the interaction term is convex in $\rho = |u|^2$. We write the Fourier decomposition of u in cylindrical coordinates

$$u(r, \theta, z) = \sum_{n \in \mathbb{Z}} c_n(r, z) e^{in\theta}, \quad \forall r, z > 0, \theta \in [0, 2\pi[,$$

where

$$c_n(r, z) = \frac{1}{2\pi} \int_0^{2\pi} u(r, \theta, z) e^{-in\theta} d\theta, \quad \forall n \in \mathbb{Z}.$$

Then, we have

$$\begin{aligned} \int_{\mathbb{R}^3} \left| \left(\frac{i}{r} \partial_\theta + a \right) u \right|^2 &= \int_{-\infty}^{\infty} \int_0^{\infty} \int_0^{2\pi} \sum_{n \in \mathbb{Z}} |c_n(r, z)|^2 \left(\frac{n}{r} + a \right)^2 r dr dz \\ &\geq \int_{-\infty}^{\infty} \int_0^{\infty} \int_0^{2\pi} \sum_{n \in \mathbb{Z}} |c_n(r, z) a|^2 r dr dz = \int_{\mathbb{R}^3} |au|^2 \end{aligned} \quad (83)$$

where we used that if $\|ra\|_\infty \leq 1/2$ then $|n/r + a| \geq |a|$ for any $n \in \mathbb{Z}$. From inequality (83), we know that taking $\langle |u|^2 \rangle_\theta^{1/2}$, where $\langle \cdot \rangle_\theta$ stands for the θ -average, can only lower the θ -component of kinetic energy. We know that it also lowers the other components of the kinetic energy which are convex in $\rho = |u|^2$ since they are not affected by A [LL01, Theorem 7.8] and proves that minimizers are non negative up to a constant phase. Besides, the interaction term is strictly convex in ρ , indeed using that $a + b\widehat{K} \geq 0$ and denote by $\langle F(\rho) \rangle_\rho = (F(\rho_1) + F(\rho_2))/2$ for some ρ_1, ρ_2 and any function F , we have

$$\begin{aligned} \left\langle a \int \rho^2 + b \int (K \star \rho) \rho \right\rangle_\rho &= \int (a + b\widehat{K}) \langle |\widehat{\rho}|^2 \rangle_\rho \\ &\geq \int (a + b\widehat{K}) |\langle \widehat{\rho} \rangle_\rho|^2 = \int (a + b\widehat{K}) |\langle \widehat{\rho} \rangle_\rho|^2 \\ &= a \int \langle \rho \rangle_\rho^2 + b \int K \star \langle \rho \rangle_\rho \langle \rho \rangle_\rho. \end{aligned}$$

The strict convexity of the functional gives the uniqueness of the minimizer by standard means.

Chapitre 2

Derivation of the Gross-Pitaevskii and Bogoliubov equations for dipolar gases

Ce chapitre reprend l'intégralité de l'article soumis dont le préprint est accessible en ligne sur arXiv / Hal.

A. Triay. "Derivation of the time-dependent Gross-Pitaevskii equation for the dipolar gases". *arXiv preprint arXiv:1904.04000* (2019)

Abstract

We derive the time-dependent dipolar Gross-Pitaevskii (GP) equation and the Bogoliubov equation from the N -body Schrödinger equation. More precisely, we show a norm approximation for the solution of the many body equation as well as the convergence of its one-body reduced density matrix towards the orthogonal projector onto the solution of the dipolar GP equation. We consider the interpolation regime where interaction potential is scaled like $N^{3\beta-1}w(N^\beta(x-y))$, the range of validity of β depends on the stability of the ground state problem. In particular, we can prove the convergence on the one-body density matrix assuming $\hat{w} \geq 0$ and $\beta < 3/8$.

Résumé

Nous dérivons l'équation de Gross-Pitaevskii (GP) dépendante du temps ainsi que l'équation de Bogoliubov à partir de l'équation de Schrödinger à N corps. Plus précisément, nous montrons une approximation en norme de la solution de l'équation à N corps ainsi que la convergence de la matrice densité réduite à 1 corps vers la projection orthogonale sur la solution de l'équation de Gross-Pitaevskii dipolaire. Nous considérons le régime dans lequel l'interaction est dilatée de la forme $N^{3\beta-1}w(N^\beta(x-y))$, la plage de validité de β dépend de la stabilité du système dans l'état fondamental. En particulier, nous montrons la convergence des matrices densités sous l'hypothèse $\hat{w} \geq 0$ et $\beta < 3/8$.

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1 Introduction

The phenomenon of Bose-Einstein Condensation (BEC) predicted in 1924 [Bos24; Ein24] and experimentally observed in 1995 [AEMWC95], has triggered a vast interest in the mathematical physics community. Initially analyzed for a gas of ideal particles, it has been a mathematical challenge to prove its persistence in the presence of interactions. Most of the first studies on BEC focused on the repulsive case, where the interaction is assumed to be non-negative or, at least, with a non-negative scattering length. Alongside, as experimental physicists mastered the creation process of condensates, it has been made possible to condense chemical elements with more complex interactions. In particular, the realization of dipolar BEC was achieved in 2005 for Chromium by Griesmaier et al [GWHSP05] and is still an active domain of research [BCZL+08; LBYL11; AFMB+12].

The nature of the dipolar interaction opened the way to a great variety of new properties such as a stable/unstable regime, the roton-maxon shape of the excitation spectrum [SSL03; HNP10] or the existence of a droplet state [CBPM+16; BWBB16a]. See [LMSLP09] for a survey. Yet, the dipolar interaction rarely fits the framework of the standard mathematical analysis of Bose-Einstein condensation as it is long-range and partially attractive.

In this work we give the first derivation of the dipolar Gross-Pitaevskii (GP) equation from the N -body Schrödinger dynamics. The GP equation determines the evolution of the common wave function of all the particles in the condensate. In the 3D case and in the Gross-Pitaevskii regime, the rigorous derivation for a repulsive interaction was proven in a series of works by Erdős, Schlein and Yau [ESY06; ESY07; ESY09; ESY10]. This is the regime where the scattering length is of order N^{-1} , it corresponds in the N body setting to a scaled interaction potential of the form $N^2 w(N \cdot)$ for some fixed $w \in L^1(\mathbb{R}^3)$. In this regime, the scattering process plays an important role and has to be precisely taken into account. Like many other works in the subject, we will focus on an interpolation regime between the Gross Pitaevskii and the Hartree regime where the potential is scaled like $N^{3\beta-1} w(N^\beta \cdot)$ with $0 < \beta < 1$. This case is easier because no significant correlation structure is expected to take place. In our setting, the difficulty comes from the attractive part of the interaction potential that may cause instabilities, as we will discuss. The derivation for the mean-field regime $\beta = 0$ was carried out in [BGM00; EY01] and later in a more general framework in [AN08; AN09; AN11].

Removing the non-negativity assumption on the interacting potential or studying the attractive case is a difficult task since the system may not be stable of the second kind that is $H_N \geq -CN$ for a constant $C > 0$ independent of N and where H_N is the Hamiltonian of the system. For this reason, the focusing case $w \leq 0$ is only globally well-posed in low dimensions ($d \leq 2$) [NN17]. The derivation of the 1D and 2D focusing cases was provided by Chen and Holmer [CH16; CH17] using the BBGKY hierarchy method. It relies on compactness arguments and therefore does not give any information on the rate of convergence. Later Jeblick and Pickl [JP18b] using a method of Pickl [Pic11] gave another proof in the 2D case yielding a precise estimate on the rate of convergence in trace norm for the density matrices. Then Nam and Napiórkowski [NN17] obtained the norm approximation of the N -body wave function. This result gives the fluctuations around the condensate and implies the convergence in trace class of the density matrices. In these works, the range of β depends on the stability of the second kind analyzed in [LNR15a; LNR17].

For the 3D case, Pickl [Pic10] could deal with $0 < \beta < 1/6$ assuming the interaction w is compactly supported, spherically symmetric and bounded. In [Cho16], Chong gave, under the same assumptions and additionally that $w \leq 0$, another proof of the convergence of the density matrices. Later, Jeblick and Pickl [JP18a] proved the convergence of the density matrices in the GP regime ($\beta = 1$) for a class of non-purely non positive potentials, namely, for which one has

stability of the second kind. The class of potentials treated in this last work is quite specific and does not include long-range interaction of the type considered here.

In this paper, we show, in the case of long-range interactions, the norm approximation in $L^2(\mathbb{R}^{3N})$ of the solution of the N -body Schrödinger equation by the solution of the Bogoliubov evolution as well as the convergence in trace norm of one-body reduced density matrix towards the orthogonal projector onto the solution of the dipolar GP equation. In particular, we remove the non-negativity assumption on the interaction potential and we are able to consider the dipole-dipole interaction (DDI), given by

$$K_{\text{dip}}(x) = \frac{1 - 3 \cos(\theta_x)^2}{|x|^3},$$

where θ_x is the angle between x and a fixed direction along which the dipoles are aligned. The exact type of potentials we consider will be detailed later. The derivation of the Gross-Pitaevskii energy for the ground state of a Bose gas with dipolar interaction was studied in [Tri18].

A quantitative method developed in [Pic11] consists in applying the Grönwall lemma on the expectation of the average number of particles outside the condensate which controls the distance of the one-body density matrix to the orthogonal projection onto the solution of the Gross-Pitaevskii equation. The next order, i.e. the norm approximation of the N body wave function, requires the study of the fluctuations around the condensate. To do so and following the work of Lewin, Nam, Serfaty and Solovej [LNSS15] where the authors analyzed the second order of the ground state energy of a Bose gas, one re-writes the N -body Schrödinger evolution in the Fock space of excitations and study their dynamics. In this new setting, one tries to verify Bogoliubov's approximation according to which the evolution of the fluctuation can be obtained by neglecting the terms of order 3 and 4 in creation and annihilation operators. This transformation was used in [LNS15] to prove the norm approximation in the mean-field regime by the solution of the Bogoliubov's equation. In this paper, we follow the same method together with the localization method of [NN17] where the idea is to use an auxiliary evolution equation defined on the restricted Fock space of at most M excitations. This type of localization in the number of excitations was already present in [LS01; LNSS15] and also in [Pic11].

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2 Setting and main result

2.1 The effective equation

The purpose of this study is to prove the convergence to the dipolar Gross-Pitaevskii time-dependent equation given by

$$i\partial_t \varphi(t) = (-\Delta + a|\varphi(t)|^2 + bK * |\varphi(t)|^2 - \mu(t)) \varphi(t), \quad (1)$$

where $a \in \mathbb{R}$ accounts for the strength of the short range interaction, $b \in \mathbb{R}$ is proportional to the norm of the dipoles and

$$\mu(t) = \frac{1}{2} \left(a \int_{\mathbb{R}^3} |\varphi(t)|^4 + b \int_{\mathbb{R}^3} K * |\varphi(t)|^2 |\varphi(t)|^2 \right).$$

The chemical potential $\mu(t)$ is just a phase factor that we add for convenience but that can be removed by a gauge transformation. The dipolar part is given by

$$K(x) = \frac{\Omega(x/|x|)}{|x|^3} \quad (2)$$

where $\Omega \in L^q(\mathbb{S}^2)$, for some $q \geq 2$, is a pair function satisfying the following cancellation property on \mathbb{S}^2 , the unit sphere of \mathbb{R}^3 ,

$$\int_{\mathbb{S}^2} \Omega(\omega) d\sigma(\omega) = 0, \quad (3)$$

with $d\sigma$ denoting the Haar measure on \mathbb{S}^2 . This includes the dipolar potential with $\Omega_{dip}(x) = 1 - 3\cos^2(\theta_x)$ where $\cos(\theta_x) = n \cdot x/|x|$ and where n is a fixed unit vector aligned with all the dipoles. The dipolar interaction is a large distance approximation of a system of Coulomb charges where the size of the dipoles is small compared to the distance between the dipoles. Hence, it is physically relevant to consider interaction looking like K outside of a ball of fixed radius. The convolution with K (in the sense of the principal values) defines a bounded operator in $L^p(\mathbb{R}^3)$, $1 < p < \infty$ [Duo01] and corresponds to the multiplication in Fourier space by some function $\widehat{K} \in L^\infty(\mathbb{R}^3)$.

In order to simplify the computations to come, it is easier to work with the following approximate Gross-Pitaevskii equation

$$\begin{cases} i\partial_t u_N = (-\Delta + w_N * |u_N|^2 - \mu_N(t)) u_N \\ u_N(0) = u_0, \end{cases} \quad (4)$$

where,

$$\mu_N(t) = \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} |u_N(t, x)|^2 w_N(x - y) |u_N(t, y)|^2 dx dy,$$

and $w_N(x) = N^{3\beta} w(N^\beta x)$ for some interaction potential $w : \mathbb{R}^3 \rightarrow \mathbb{R}$ and some $\beta > 0$. Choosing

$$w = w_0 + b\mathbb{1}_{|x|>R}K \quad (5)$$

where $w_0 \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$, $b \geq 0$, $R > 0$ with $a = \int_{\mathbb{R}^3} w_0$, one can show that the solutions of (1) and (4) are close in L^2 -norm as is stated in Proposition 1 below. For the truncated dipolar potential, we also have (for instance see [Duo01]) the existence for all $1 < p < \infty$ of some constant C_p independent of $R > 0$ such that for all $f \in L^p(\mathbb{R}^3)$

$$\|(\mathbb{1}_{|x|>R}K) * f\|_{L^p(\mathbb{R}^3)} \leq C_p \|f\|_{L^p(\mathbb{R}^3)}. \quad (6)$$

The regularity of the solutions of (1) and (4) has already been well studied. But since (4) depends on N , one has to make sure that the Sobolev norms of the solution can be bounded independently of N . We do so in the following proposition which is an easy adaptation of [BdS15, Proposition 3.1].

Proposition 1. *Let $a, b \in \mathbb{R}$ and let w satisfy (5), then the Cauchy problems (4), respectively (1)*

(with initial date u_0), admit unique maximal solutions respectively $u_N, \varphi \in C^1([0, T], L^2(\mathbb{R}^3)) \cap C^0([0, T], H^1(\mathbb{R}^3))$ for some $T > 0$. If $\widehat{w} \geq 0$ (respectively $a \geq \text{binf } \widehat{K}$) or if $\|\nabla u_0\|_{L^2(\mathbb{R}^3)}$ is small enough, the solutions u_N and φ are global in time, $T = +\infty$, and we have the following bounds

$$\|u_N(t)\|_{H^1(\mathbb{R}^3)} + \|\varphi(t)\|_{H^1(\mathbb{R}^3)} \leq C, \quad (7)$$

$$\|u_N(t)\|_{H^k(\mathbb{R}^3)} + \|\varphi(t)\|_{H^k(\mathbb{R}^3)} \leq Ce^{C't}, \text{ when moreover } u_0 \in H^k(\mathbb{R}^3), \quad (8)$$

where in the last equation C depends only on $\|u_0\|_{H^k(\mathbb{R}^3)}$ and C' on $\|u_0\|_{H^1(\mathbb{R}^3)}$. If moreover, we have

$$|\widehat{w_0}(k) - a| \leq C|k|, \quad (9)$$

for some constant $C > 0$, where $a = \int_{\mathbb{R}^3} w_0$, and if $u_0 \in H^2(\mathbb{R}^3)$ then

$$\|u_N(t) - \varphi(t)\|_{L^2(\mathbb{R}^3)} \leq C \frac{\exp(c_1 \exp(c_2 t))}{N^\beta}, \quad (10)$$

where $C, c_1, c_2 > 0$ depend on $\|u_0\|_{H^2(\mathbb{R}^3)}$.

Remark 2. The assumption (9) is technical and could be reduced with a trade off on the rate of convergence in (10). This condition holds for instance as soon as $|x|^2 w_0(x) \in L^1(\mathbb{R}^3)$. Assuming the latter, the parity of w actually implies (9) with on the right-hand side $|k|^{1+\alpha}$ for all $\alpha < 1$. In a similar way, we have automatically

$$\left| \mathbf{1}_{|x| \leq R} \widehat{K}(k) \right| \leq CR^2 k^2 \quad (11)$$

with a constant C independent of R and k . This can be deduced from the following formula [Tri18, Lemma 9]

$$\mathbf{1}_{|x| \leq R} \widehat{K}(k) = \int_{\mathbb{S}^2} \int_0^R \frac{\cos(rk \cdot \omega) - 1}{r} \Omega(\omega) dr d\sigma(\omega).$$

Proof of Proposition 1. The existence and uniqueness are standard, see [Caz03], and come from the regularity properties of the convolution with K [Ste70]. We also have from usual techniques the blow-up alternative, that is if $T < \infty$ then $\|u_N(t)\|_{H^1(\mathbb{R}^3)} \rightarrow \infty$ as $t \rightarrow T$. Hence if $\widehat{w} \geq 0$ then we have

$$C = \int_{\mathbb{R}^3} |\nabla u_N(t)|^2 + \iint_{\mathbb{R}^3 \times \mathbb{R}^3} |u_N(t)|^2 w_N * |u_N(t)|^2 \geq \|\nabla u_N(t)\|_{L^2(\mathbb{R}^3)}^2,$$

and similarly for $\varphi(t)$. From this and the blow-up alternative we deduce global existence in this case. If $\|\nabla u_0\|_{L^2(\mathbb{R}^3)}$ is small enough, it is also standard that $\|u_N(t)\|_{H^1(\mathbb{R}^3)}$ and $\|\varphi(t)\|_{H^1(\mathbb{R}^3)}$ have to remain bounded [CMS08]. Hence the global existence yields in this case too.

The bounds on the growth of $\|u_N(t)\|_{H^k(\mathbb{R}^3)}$ and $\|\varphi(t)\|_{H^k(\mathbb{R}^3)}$ are obtained via the same proof of [BdS15, Proposition 3.1] where the authors only used that $w \in L^p(\mathbb{R}^3)$, for $p > 1$ and $\widehat{w} \in L^\infty(\mathbb{R}^3)$. Finally, the bound on $\|u_N(t) - \varphi(t)\|_{L^2(\mathbb{R}^3)}$ is also obtained the same way as in [BdS15, Proposition 3.1] using (9) and Remark 2. \square

2.2 Main result: derivation of the Gross-Pitaevskii equation

We consider N bosons in \mathbb{R}^3 interacting via a pair potential $w_N(x-y) := N^{3\beta} w(N^\beta(x-y))$, where $w \in L^{6/5}(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ is such that $\widehat{w} \in L^\infty(\mathbb{R}^3)$. Note that the interaction potential is

possibly long-range and is allowed to be (partly) attractive. The system is entirely described at any time t by its wave function $\Psi_N(t)$ evolving in $L^2(\mathbb{R}^3)^{\otimes_s N}$, the symmetric tensor product of N copies of $L^2(\mathbb{R}^3)$, whose dynamics is given by the Schrödinger equation

$$i\partial_t \Psi_N = H_N \Psi_N. \quad (12)$$

Here H_N is the Hamiltonian of the system given by

$$H_N = \sum_{j=1}^N -\Delta_{x_j} + \frac{1}{N-1} \sum_{1 \leq i < j \leq N} w_N(x_i - x_j). \quad (13)$$

Even though we are interested in the dynamics, the behavior of the ground state energy plays an important role. In such a system where the interaction has a negative part, proving stability of the second kind (that is, $H_N \geq -CN$ for some constant $C > 0$ independent of N) is a difficult problem. In [Tri18], it was proven that in the presence of an external confining potential $V(x) \geq C|x|^s$ for some $s > 0$, if w satisfies (5) and $\beta < 1/3 + s/(45 + 42s)$ the Hamiltonian H_N is stable of the second kind. Note that with the only assumption that $\hat{w} \geq 0$, $\hat{w} \in L^1(\mathbb{R}^3)$ we automatically have $H_N \geq -CN$ for all $\beta \leq 1/3$. For the evolved system, stability of the second kind allows to control the interaction term by the kinetic one, and the latter by the energy itself which is preserved by the Hamiltonian evolution.

The goal of this paper, loosely speaking, is to show that if the initial wave function $\Psi_N(0)$ is close to a product state $\varphi(0)^{\otimes N}$, then the propagated wave function $\Psi_N(t)$ remains well approximated by the product state $\varphi(t)^{\otimes N}$, where $\varphi(t)$ solves the non-linear Gross-Pitaevskii equation (1). This *approximation* is true at first order, that is we can prove that the one-body reduced density matrix of $\Psi_N(t)$ converges towards the orthogonal projector onto $\varphi(t)$. But this fails as a norm approximation in $L^2(\mathbb{R}^{3N})$ since Ψ_N is never a pure condensate and contains fluctuations around it. The dynamics of these fluctuations is encoded in the time-dependent Bogoliubov equation that we define later on.

Before stating our main result, we recall the definition of the k -particle reduced density matrix of a pure state $\Psi \in L^2(\mathbb{R}^3)^{\otimes_s N}$,

$$\Gamma_{\Psi}^{(k)} := \text{Tr}_{k+1 \rightarrow N} |\Psi\rangle \langle \Psi| \quad (14)$$

where $|\Psi\rangle \langle \Psi|$ is the orthogonal projection onto Ψ , or in terms of kernel,

$$\Gamma_{\Psi}^{(k)}(x_1, \dots, x_k, y_1, \dots, y_k) = \int \Psi(x_1, \dots, x_k, z_{k+1}, \dots, z_N) \overline{\Psi(y_1, \dots, y_k, z_{k+1}, \dots, z_N)} dz_{k+1} \dots dz_N.$$

In the following we denote by $\Psi_N(t, x)$ the solution to (12) and $u_N(t, x)$ the solution to (4). We will denote by $\mathcal{H} := L^2(\mathbb{R}^3)$ the one particle space and by $\mathcal{H}^N := L^2(\mathbb{R}^3)^{\otimes_s N}$ the N particle bosonic space. We define $P(t) = |u_N(t)\rangle \langle u_N(t)|$ the orthogonal projector onto $u_N(t) \in L^2(\mathbb{R}^3)$ and $Q(t) = 1 - P(t)$.

To describe the excitations orthogonal to the condensate, we follow the technique of [LNSS15; LNS15]. Let us denote by $\mathcal{H}_+ = \{u_N\}^\perp$ the orthogonal space of u_N in \mathcal{H} , then note that the N -body wave function Ψ_N admits the unique decomposition

$$\Psi_N = u_N^{\otimes N} \varphi_0 + u_N^{\otimes N-1} \otimes_s \varphi_1 + u_N^{\otimes N-2} \otimes_s \varphi_2 + \dots + \varphi_N$$

with $\varphi_k \in \mathcal{H}_+^{\otimes_s k}$ for all $k \geq 0$ with the convention that $\varphi_0 \in \mathbb{C}$. The above decomposition allows

to define the unitary map

$$\begin{aligned} U_N : \mathcal{H}^N &\longrightarrow \mathcal{F}(\mathcal{H}_+) \\ \Psi_N &\longmapsto \Phi_N := \bigoplus_{k=0}^N \varphi_k. \end{aligned} \quad (15)$$

The unitary transformation U_N is a one-to-one correspondance between a N particle state and its excitations orthogonal to the condensate.

In the sequel we will denote by $\Phi_N(t) = U_N(t)\Psi_N(t)$ the corresponding state describing the excitations in the truncated Fock space $\mathcal{F}^{\leq N}(\mathcal{H}_+)$. The Bogoliubov approximation consists in approximating $\Phi_N(t)$ by the solution $\Phi(t)$ of the time dependent Bogoliubov equation

$$\begin{cases} i\partial_t \Phi(t) = \mathbb{H}(t)\Phi(t) \\ \Phi(0) = U_N(0)\Psi_N(0), \end{cases} \quad (16)$$

where the Bogoliubov Hamiltonian \mathbb{H} is the operator acting on the entire Fock space $\mathcal{F}(\mathcal{H})$ (not only $\mathcal{F}(\mathcal{H}_+)$) given by

$$\mathbb{H}(t) = d\Gamma(h(t)) + \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \left(K_2(t, x, y) a_x^* a_y^* + \overline{K_2(t, x, y)} a_x a_y \right) dx dy.$$

Where

$$h(t) = -\Delta + w_N * |u_N(t, x)|^2 + Q(t)\tilde{K}_1(t)Q(t) - \mu_N(t), \quad K_2(t) = Q(t) \otimes Q(t)\tilde{K}_2(t) \in \mathcal{H}^2,$$

with $\tilde{K}_1(t) \in \mathcal{B}(\mathcal{H})$ is the operator of kernel

$$\tilde{K}_1(t)(x, y) = u_N(t, x)w_N(x - y)\overline{u_N(t, y)},$$

and $\tilde{K}_2(t) \in \mathcal{H}^2$ is the function given by

$$\tilde{K}_2(t, x, y) = u_N(t, x)w_N(x - y)u_N(t, y).$$

We have used the formalism of the second quantification, see [Lew11] for instance for definitions, and we have denoted

$$d\Gamma(A) = 0 \oplus \bigoplus_{n \geq 1} \left(\sum_{k=1}^n A_k \right)$$

for any operator A on $L^2(\mathbb{R}^3)$ where $A_k = 1 \otimes \dots \otimes A \otimes \dots \otimes 1$ with A in k th position. The bosonic creation and annihilation operators a_x^* and a_y satisfy the Canonical Commutation Relation (CCR)

$$[a_y, a_x^*] = \delta(x - y)$$

where δ is the Dirac delta function. We also recall the number operator

$$\mathcal{N} = d\Gamma(1) = \bigoplus_{n \geq 0} n = \int_{\mathbb{R}^3} a_x^* a_x dx.$$

It was proven in [LNS15] that the Cauchy problem (16) is well posed when $\langle \Phi(0), d\Gamma(1 - \Delta)\Phi(0) \rangle < \infty$ and when $u_N \in C^0([0, T], H^1(\mathbb{R}^3)) \cap C^1([0, T], H^{-1}(\mathbb{R}^3))$. Then there is unique corresponding solution of (16), $\Phi \in C^0([0, T], \mathcal{F}(\mathcal{H})) \cap L_{\text{loc}}^\infty([0, T], \mathcal{Q}(d\Gamma(1 - \Delta)))$. We emphasize that even if the Cauchy problem (16) is posed in $\mathcal{F}(\mathcal{H})$, the solution satisfies $\Phi(t) \in \mathcal{F}(\mathcal{H}_+)$

as one can verify by computing the time-derivative of the quantity $\|a(u_N(t))\Phi(t)\|_{L^2(\mathbb{R}^{3N})}$ and observe that it vanishes.

The norm approximation of $\Psi_N(t)$ by $U_N^*\Phi(t)$ is stronger than the convergence in trace norm of the one body reduced density matrix $\Gamma^{(1)}$ towards $|u_N(t)\rangle\langle u_N(t)|$. This is why in our result below the range of validity for the parameter β is wider when we look at the convergence of the one-body reduced density matrix. We recall that for $p \geq 1$, the p th Schatten class is defined as

$$\mathfrak{S}_p(\mathcal{H}) = \left\{ A \in \mathcal{B}(\mathcal{H}) \mid \|A\|_{\mathfrak{S}_p(\mathcal{H})} := \left(\text{Tr}(\sqrt{A^*A})^p \right)^{1/p} < \infty \right\}.$$

We can now state our main result.

Theorem 3 (Main Theorem). *Let $\beta > 0$ and let $w = w_0 + b\mathbb{1}_{|x| > R}K$ where $w_0 \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$, $b \geq 0$, $R > 0$ and where K is given by (2). Let u_N be a solution of the Gross-Pitaevskii equation (4) on some interval $[0, T]$ with $T \in \mathbb{R}_+ \cup \{\infty\}$ such that (7) and (8) hold on $[0, T]$. Let $(\Psi_N(0))_N$ be such that*

$$\text{Tr}((-\Delta)^{1/2}Q(0)\Gamma_{\Psi_N(0)}^{(1)}Q(0)(-\Delta)^{1/2}) \leq C_0N^{-1} \quad (17)$$

for some constant $C_0 > 0$ and $\Psi_N(t)$ be the solution to the Schrödinger equation (12) with initial condition $\Psi_N(0)$. Let $\Phi(t) = (\varphi_k(t))_{k \geq 0}$ be the solution of the Bogoliubov equation (16).

1. If $0 < \beta < 1/6$ then for all $0 < \alpha < \min((1 - 6\beta)/4, (2 - 7\beta)/4)$ we have

$$\left\| \Psi_N(t) - \sum_{k=0}^N u_N(t)^{\otimes k} \otimes_s \varphi_k(t) \right\|_{L^2(\mathbb{R}^{3N})} \leq C_\alpha e^{C't} N^{-\alpha}, \quad (18)$$

where C_α depends on α , C_0 and $\|u(0)\|_{H^4(\mathbb{R}^3)}$ and where C' depends on $\|u(0)\|_{H^1(\mathbb{R}^3)}$.

2. If $0 < \beta < 1/4$ then for all $0 < \alpha < \min((3 - 10\beta)/4, (1 - 4\beta)/4)$ we have

$$\|\Gamma_{\Psi_N(t)}^{(1)} - |u_N(t)\rangle\langle u_N(t)|\|_{\mathfrak{S}_1} \leq C_\alpha e^{C't} N^{-\alpha}, \quad (19)$$

where C_α depends on α , C_0 , and $\|u(0)\|_{H^4(\mathbb{R}^3)}$ and C' depends on $\|u(0)\|_{H^1(\mathbb{R}^3)}$.

3. Let moreover assume that $\widehat{w} \geq 0$ and that $\widehat{w} \in L^1(\mathbb{R}^3)$.

(a) If $0 < \beta < 1/5$ then we have (18) for $0 < \alpha < \min((3 - 10\beta)/4, (1 - 5\beta)/4)$.

(b) If $0 < \beta < 3/8$ then we have (19) for $0 < \alpha < \min((1 - \beta)/2, (2 - 5\beta)/2, (3 - 8\beta)/4)$.

Remark 4. *As said earlier, a priori estimates on the kinetic energy are crucial in our proof. This is why the assumption $\widehat{w} \geq 0$ allows us to extend the range of β . Assuming stability of the second kind, one could improve it again.*

Remark 5. *Note that the range of β includes regimes where the stability of the second kind is not established. In particular, when $\widehat{w} \geq 0$ we allow $0 < \beta < 3/8$ which is above the threshold $1/3$. In such a regime $\beta > 1/3$, the system is very dilute since the range of the interaction is much smaller than the mean distance between particles.*

The rest of the paper is devoted to the proof of Theorem 3.

3 The localization method

3.1 Presentation of the method

To simplify notations, we will in the sequel denote by $u_N(t)$ the solution of modified Gross-Pitaevskii equation (4). The Schrödinger evolution (12) is unitarily equivalent to the following dynamics for the excitations outside the condensate. Recalling that $\Phi_N(t) = U_N(t)\Psi_N(t)$, we have

$$\begin{cases} i\partial_t \Phi_N(t) = \mathcal{G}_N(t)\Phi_N(t) \\ \Phi_N(0) = U_N(0)\Psi_N(0), \end{cases}$$

with

$$\mathcal{G}_N(t) = \mathbf{1}^{\leq N} (\mathbb{H}(t) + \mathcal{E}_N(t)) \mathbf{1}^{\leq N} = U_N H_N U_N^*$$

and $\mathcal{E}_N(t)$ is an error term which is given by

$$\mathcal{E}_N(t) = \frac{1}{2} \sum_{j=0}^4 (R_j + R_j^*),$$

$$\begin{aligned} R_0 &= R_0^* = d\Gamma(Q(t)[w_N * |u_N(t)|^2 + \tilde{K}_1(t) - \mu_N(t)]Q(t)) \frac{1 - \mathcal{N}}{N - 1}, \\ R_1 &= -2 \frac{\mathcal{N}\sqrt{N - \mathcal{N}}}{N - 1} a(Q(t)[w_N * |u_N(t)|^2]u_N(t)), \\ R_2 &= \iint K_2(t, x, y) a_x^* a_y^* dx dy \left(\frac{\sqrt{(N - \mathcal{N})(N - \mathcal{N} - 1)}}{N - 1} - 1 \right) \\ R_3 &= \frac{\sqrt{N - \mathcal{N}}}{N - 1} \iiint (1 \otimes Q(t)w_N Q(t) \otimes Q(t))(x, y, x', y') \overline{u(t, x)} a_y^* a_{x'} a_{y'} dx dy dx' dy', \\ R_4 &= R_4^* = \frac{1}{2(N - 1)} \iiint (Q(t) \otimes Q(t)w_N Q(t) \otimes Q(t))(x, y, x', y') a_x^* a_{x'}^* a_{y'} dx dy dx' dy'. \end{aligned}$$

This computation can be found in [LNS15]. Besides this reformulation of the Schrödinger equation, we will use the localization method which consists in using an auxiliary dynamics localized in the truncated Fock space $\mathcal{F}^{\leq M}(\mathcal{H}_+)$ for $M = N^{1-\delta}$, for some $\delta > 0$. Having an *a priori* bound on the number of excitations allows to control accurately the error terms above and hence also the expectation of the kinetic energy $d\Gamma(1 - \Delta)$, which itself controls the expectation of the number of excitations \mathcal{N}_+ . More precisely, the localized dynamics is given, for $1 \leq M \leq N$, by

$$\begin{cases} i\partial_t \Phi_{N,M}(t) = \mathbf{1}^{\leq M} \mathcal{G}_N(t) \mathbf{1}^{\leq M} \Phi_{N,M}(t) \\ \Phi_{N,M}(0) = U_N(0)\Psi_N(0). \end{cases} \quad (20)$$

We have denoted by $\mathbf{1}^{\leq M} := \mathbf{1}(\mathcal{N} \leq M)$ the spectral projection associated to the number operator \mathcal{N} . The existence and uniqueness of the solution of (20) follows from [LNS15, Theorem 7]. Here as well, a direct computation shows that the time derivative of $\|a(u_N(t))\Phi_{N,M}(t)\|_{L^2(\mathbb{R}^3N)}^2$, $\|a(u_N(t))\Phi_N(t)\|_{L^2(\mathbb{R}^3N)}^2$ and $\|\mathbf{1}^{\leq M}\Phi_{N,M}(t)\|_{L^2(\mathbb{R}^3N)}^2$ vanish, see [NN17; LNS15], implying that $\Phi_N(t) \in \mathcal{F}(\mathcal{H}_+)$ and $\Phi_{N,M}(t) \in \mathcal{F}^{\leq M}(\mathcal{H}_+)$ for all $t \geq 0$.

3.2 Estimate on the kinetic energy

We start by proving that the assumption (17) is enough to bound the whole energy of $\Psi_N(t)$.

Proposition 6. *Assume (17) then for all $t \in [0, T]$*

$$\langle \Psi_N(t), H_N \Psi_N(t) \rangle = \langle \Psi_N(0), H_N \Psi_N(0) \rangle \leq CN.$$

Proof. The equality follows from differentiating $\langle \Psi_N(t), H_N \Psi_N(t) \rangle$ and the use of (12). We now prove the inequality. By the Cauchy-Schwarz inequality we have that

$$\begin{aligned} \mathrm{Tr}_{\mathcal{H}}(-\Delta \Gamma_{\Psi_N}^{(1)}) &\leq 2 \mathrm{Tr}_{\mathcal{H}}(P(0)(-\Delta)P(0)\Gamma_{\Psi_N}^{(1)}) + 2 \mathrm{Tr}_{\mathcal{H}}(Q(0)(-\Delta)Q(0)\Gamma_{\Psi_N}^{(1)}) \\ &\leq 2\|\nabla u(0)\|_{L^2(\mathbb{R}^3)}^2 + 2\frac{C_0}{N} \leq C, \end{aligned} \quad (21)$$

where we have used assumption (17). Similarly

$$\begin{aligned} w_N(x-y) &= P(0) \otimes 1 w_N(x-y) P(0) \otimes 1 + P(0) \otimes 1 w_N(x-y) Q(0) \otimes 1 \\ &\quad + Q(0) \otimes 1 w_N(x-y) P(0) \otimes 1 + Q(0) \otimes 1 w_N(x-y) Q(0) \otimes 1 \\ &\leq w_N * |u_N(t)|^2(y) + \eta |w_N| * |u_N(t)|^2(y) + (1 + \eta^{-1}) Q(0) \otimes 1 |w_N(x-y)| Q(0) \otimes 1 \\ &\leq 2 \left(\|w_N * |u_N(t)|^2\|_{L^{3/2}(\mathbb{R}^3)} + \eta \|w_N * |u_N(t)|^2\|_{L^{3/2}(\mathbb{R}^3)} \right) (-\Delta_y) \\ &\quad + (1 + \eta^{-1}) \|w_N\|_{L^{3/2}(\mathbb{R}^3)} Q(0) \otimes 1 (-\Delta_x) Q(0) \otimes 1 \end{aligned}$$

for all $\eta > 0$, where we used Sobolev's inequality in the last inequality. Recall that w is not an L^1 function and that the continuity properties of the convolution by w rely mainly on cancellations, hence we cannot estimate in the same way $w_N * |u_N(t)|^2$ and $|w_N| * |u_N(t)|^2$. Since w satisfies (5) and (6), we have

$$\|w_N * |u_N(t)|^2\|_{L^{3/2}} \leq (\|w_0\|_{L^1(\mathbb{R}^3)} + C) \|u_N(t)\|_{L^3(\mathbb{R}^3)}^2 \leq C$$

for some constant $C > 0$ depending only on $\|u(0)\|_{H^1(\mathbb{R}^3)}$ and

$$\||w_N| * |u_N(t)|^2\|_{L^{3/2}} \leq \|w_N\|_{L^{1+\varepsilon}(\mathbb{R}^3)} \|u_N\|_{L^{3-2\varepsilon'}(\mathbb{R}^3)}^2 \leq CN^{3\beta\varepsilon/(1+\varepsilon)} \|w\|_{L^{1+\varepsilon}(\mathbb{R}^3)}$$

where $\varepsilon, \varepsilon' > 0$, $\varepsilon' \leq 1/2$ are such that

$$\frac{1}{1+\varepsilon} + \frac{1}{3/2-\varepsilon'} = 1 + \frac{2}{3},$$

and where $C > 0$ is some other constant depending only $\|u(0)\|_{H^1(\mathbb{R}^3)}$. Hence we obtain

$$w_N(x-y) \leq C(1 + \eta N^{3\beta\varepsilon/(1+\varepsilon)}) (-\Delta_y) + (1 + \eta^{-1}) Q(0) \otimes 1 (-\Delta_x) Q(0) \otimes 1,$$

for all $\varepsilon, \eta > 0$. From this, we deduce

$$\begin{aligned} \langle \Psi_N H_N \Psi_N \rangle &= N \left(\text{Tr}_{\mathcal{H}}(-\Delta \Gamma_{\Psi_N}^{(1)}) + \text{Tr}_{\mathcal{H}^2}(w_N(x-y) \Gamma_{\Psi_N}^{(2)}) \right) \\ &\leq 2N \text{Tr}_{\mathcal{H}}(-\Delta \Gamma_{\Psi_N}^{(1)}) + CN \text{Tr}_{\mathcal{H}^2}((1 + \eta N^{3\beta\varepsilon/(1+\varepsilon)})(-\Delta_y) \Gamma_{\Psi_N}^{(2)}) \\ &\quad + C \text{Tr}_{\mathcal{H}^2}((1 + \eta^{-1} Q(0) \otimes 1(-\Delta_x) Q(0) \otimes 1) \Gamma_{\Psi_N}^{(2)}) \\ &\leq CN(1 + \eta N^{3\beta\varepsilon/(1+\varepsilon)}) \text{Tr}_{\mathcal{H}}(-\Delta \Gamma_{\Psi_N}^{(1)}) + (1 + \eta^{-1}) \text{Tr}_{\mathcal{H}}(Q(0)(-\Delta)Q(0) \Gamma_{\Psi_N}^{(1)}) \end{aligned}$$

for all $\varepsilon, \eta > 0$. Now using the assumption (21) and (17) we obtain

$$\langle \Psi_N H_N \Psi_N \rangle \leq CN(1 + \eta N^{3\beta\varepsilon/(1+\varepsilon)}) + (1 + \eta^{-1}) C_0 N^{-1}$$

and taking $\eta = N^{-3\beta\varepsilon/(1+\varepsilon)}$ for $\varepsilon \leq (3\beta)^{-1}$ proves the result. \square

Denote by

$$e_N = \inf \sigma \left(\frac{1}{2} \sum_{k=1}^N -\Delta_{x_k} + \frac{1}{N-1} \sum_{1 \leq j < k \leq N} w_N(x_j - x_k) \right).$$

A computation shows the following.

Corollary 7. *For all $t \in [0, T]$,*

$$\langle \Phi_N(t), d\Gamma(1 - \Delta)\Phi_N(t) \rangle \leq 2\langle \Psi_N(t), H_N \Psi_N(t) \rangle - 2e_N \leq C(|e_N| + N), \quad (22)$$

We will need the following two intermediate results. But first, we establish the convention that throughout the rest of the paper $C_{t,\varepsilon}$ denotes a constant that can always be bounded by $C_\varepsilon e^{C't}$ where C_ε depends on $\varepsilon > 0$ and $\|u(0)\|_{H^4(\mathbb{R}^3)}$ and $C' > 0$ depends on $\|u(0)\|_{H^1(\mathbb{R}^3)}$. It is easily verified in the proofs using Proposition 1. In this way we can retrieve the right hand-side of the estimates of Theorem 3.

Proposition 8 (Kinetic estimate for the truncated dynamics). *Let $0 < \beta < 1$ and $M = N^\alpha$ with $0 < \alpha < 1 - \beta$, let $\varepsilon > 0$, then, for N large enough, we have*

$$\langle \Phi_{N,M}(t), d\Gamma(1 - \Delta)\Phi_{N,M}(t) \rangle \leq C_{t,\varepsilon} N^{\beta+\varepsilon},$$

for some constant $C_{t,\varepsilon} > 0$.

Proposition 9 (Kinetic estimate for the Bogoliubov dynamics). *Let $0 < \beta < 1$ and let $\varepsilon > 0$, we have*

$$\langle \Phi(t), d\Gamma(1 - \Delta)\Phi(t) \rangle \leq C_{t,\varepsilon} N^{\beta+\varepsilon},$$

for some constant $C_{t,\varepsilon} > 0$.

The proofs of Proposition 8 and Proposition 9 are similar and we will only give the one of Proposition 8. It is a consequence of the following lemmas whose proofs are postponed until the end of the proof of Proposition 8.

Lemma 10. *Let $\beta, \varepsilon > 0$. There exists some constant $C_{t,\varepsilon} > 0$ such that for $A \in \{\mathbb{H}(t) + d\Gamma(\Delta), \partial_t \mathbb{H}(t), i[\mathbb{H}, \mathcal{N}]\}$, we have*

$$\pm A \leq C_{t,\varepsilon} (\mathcal{N} + \eta N^{\beta+\varepsilon} + \eta^{-1} d\Gamma(1 - \Delta)),$$

for any $\eta > 0$.

Lemma 11. *Let $0 < \beta < 1$. For every $1 \leq m \leq N$, $\varepsilon > 0$ and for $A \in \{\mathcal{E}_N(t), \partial_t \mathcal{E}_N(t), i[\mathcal{E}_N(t), \mathcal{N}]\}$ we have*

$$\pm \mathbf{1}^{\leq m} A \mathbf{1}^{\leq m} \leq C_{t,\varepsilon} \sqrt{\frac{m}{N^{1-\beta-\varepsilon}}} d\Gamma(1-\Delta) \text{ in } \mathcal{F}(\mathcal{H}_+). \quad (23)$$

Proof of Proposition 8. Let $\varepsilon > 0$ and define $\varepsilon_\alpha = (1 - \beta - \alpha)/2$. We use Lemma 11 with ε_α and Lemma 10 with ε . For N large enough we have

$$A(t) := C_{t,\varepsilon} \mathbf{1}^{\leq M} (\mathcal{N} + N^{\beta+\varepsilon}) + \mathbf{1}^{\leq M} \mathcal{G}_N(t) \mathbf{1}^{\leq M} \geq \frac{1}{2} \mathbf{1}^{\leq M} d\Gamma(1-\Delta),$$

hence we only need to control the left-hand side to show the proposition. For this we use Grönwall's lemma

$$\begin{aligned} & \frac{d}{dt} \langle \Phi_{N,M}(t), A(t) \Phi_{N,M}(t) \rangle \\ &= \langle \Phi_{N,M}(t), \partial_t A(t) \Phi_{N,M}(t) \rangle + i \langle \Phi_{N,M}(t), [\mathbf{1}^{\leq M} \mathcal{G}_N(t) \mathbf{1}^{\leq M}, A(t)] \Phi_{N,M}(t) \rangle \\ &= \langle \Phi_{N,M}(t), (\partial_t \mathbb{H}(t) + \partial_t \mathcal{E}_N(t) + \partial_t C_{t,\varepsilon} (N^{\beta+\varepsilon} + \mathcal{N})) \Phi_{N,M}(t) \rangle \\ &\quad + i \langle \Phi_{N,M}(t), [\mathbf{1}^{\leq M} \mathcal{G}_N(t) \mathbf{1}^{\leq M}, C_{t,\varepsilon} \mathcal{N}] \Phi_{N,M}(t) \rangle \\ &\leq C_{t,\varepsilon} \langle \Phi_{N,M}(t), A(t) \Phi_{N,M}(t) \rangle, \end{aligned}$$

where we used Lemma 10 and Lemma 11 in the last inequality. \square

The proofs of Lemma 10 and Lemma 11 require the following intermediate results. The first one, Lemma 12 is a slightly adapted version of [NNS16, Lemma 9]. And the second one, Lemma 13 is an estimate on the three body term of the error in the Bogoliubov approximation.

Lemma 12. *Let $H > 0$ be a self-adjoint operator on \mathfrak{H} . Let $K : \bar{\mathfrak{H}} \equiv \mathfrak{H}^* \rightarrow \mathfrak{H}$ be an operator with kernel $K(x, y) \in \mathfrak{H}^2$. Assume that $KH^{-1}K^* \leq H$ and that $H^{-1/2}K$ is Hilbert-Schmidt. Let $\chi_1, \chi_2 : \mathbb{R} \rightarrow [0, 1]$ then*

$$\begin{aligned} \tilde{\mathbb{H}} &:= d\Gamma(H) + \frac{1}{2} \iint \left(K(x, y) \chi_1(\mathcal{N}) a_x^* a_y^* \chi_2(\mathcal{N}) + \overline{K(x, y)} \chi_1(\mathcal{N}) a_x a_y \chi_2(\mathcal{N}) \right) dx dy \\ &\geq -\frac{1}{2} \|H^{-1/2}K\|_{HS}^2. \quad (24) \end{aligned}$$

Proof. The proof is a simple adaptation of the one of [NNS16]. For $\Psi \in D(\tilde{\mathbb{H}})$ we have

$$\langle \Psi, \tilde{\mathbb{H}} \Psi \rangle = \text{Tr}(H^{1/2} \gamma_\Psi H^{1/2}) + \Re \text{Tr}(K^* \tilde{\alpha}_\Psi),$$

where the operators $\gamma_\Psi : \mathfrak{H} \rightarrow \mathfrak{H}$ and $\tilde{\alpha}_\Psi : \mathfrak{H} \rightarrow \mathfrak{H}^*$ are defined in the following way. For all $f, g \in \mathfrak{H}$,

$$\langle f, \gamma_\Psi g \rangle = \langle \Psi, a^*(g) a(f) \Psi \rangle, \quad \langle f, \tilde{\alpha}_\Psi g \rangle = \langle \Psi, \chi_1(\mathcal{N}) a^*(g) a^*(f) \chi_2(\mathcal{N}) \Psi \rangle.$$

Here $a^*(f)$ and $a(f)$ for $f \in \mathfrak{H}$ are the creation and annihilation operators in Fock space. Let

$J : \mathfrak{H} \rightarrow \mathfrak{H}^*$ defined by $J(f)(g) = \langle f, g \rangle$ for all $f, g \in \mathfrak{H}$, then we have

$$\begin{aligned} & \left\langle \begin{pmatrix} f \\ Jg \end{pmatrix}, \begin{pmatrix} \gamma_\Psi & \tilde{\alpha}_\Psi^* \\ \tilde{\alpha}_\Psi & 1 + J\gamma_\Psi J^* \end{pmatrix} \begin{pmatrix} f \\ Jg \end{pmatrix} \right\rangle \\ &= \left\langle \Psi, \left\{ \left(\chi_1(\mathcal{N})a^*(g) + \chi_2(\mathcal{N})a(f) \right) \left((a(g)\chi_1(\mathcal{N}) + a^*(f)\chi_2(\mathcal{N})) \right) \right. \right. \\ & \quad \left. \left. + (1 - \chi_1(\mathcal{N})^2)a^*(g)a(g) + (1 - \chi_2(\mathcal{N})^2)a^*(f)a(f) \right\} \Psi \right\rangle \geq 0. \end{aligned}$$

Hence we have by [NNS16, Lemma 3] that

$$\gamma_\Psi \geq 0 \quad \text{and} \quad \gamma_\Psi \geq \tilde{\alpha}_\Psi^*(1 + J\gamma_\Psi J^*)^{-1}\tilde{\alpha}_\Psi. \quad (25)$$

The rest of the proof proceeds as in [NNS16]. We only need to prove it for Ψ such that γ_Ψ and $\tilde{\alpha}_\Psi$ are finite-rank operator, in which case we have

$$\begin{aligned} |\text{Tr}(K^*\tilde{\alpha}_\Psi)| &= |\text{Tr}(\tilde{\alpha}_\Psi K^*)| = \left| \text{Tr}((1 + J\gamma_\Psi J^*)^{-1/2}\tilde{\alpha}_\Psi H^{1/2}H^{-1/2}K^*(1 + J\gamma_\Psi J^*)^{1/2}) \right| \\ &\leq \|(1 + J\gamma_\Psi J^*)^{-1/2}\tilde{\alpha}_\Psi H^{1/2}\|_{\text{HS}} \|H^{-1/2}K^*(1 + J\gamma_\Psi J^*)^{1/2}\|_{\text{HS}} \\ &\leq \text{Tr}(H^{1/2}\tilde{\alpha}_\Psi^*(1 + J\gamma_\Psi J^*)^{-1}\tilde{\alpha}_\Psi H^{1/2})^{1/2} \\ &\quad \times \text{Tr}((1 + J\gamma_\Psi J^*)^{1/2}KH^{-1}K^*(1 + J\gamma_\Psi J^*)^{1/2})^{1/2} \\ &\leq \left(\text{Tr}(H^{1/2}\gamma_\Psi H^{1/2}) \right)^{1/2} \left(\text{Tr}(KH^{-1}K^*) + \text{Tr}(H^{1/2}\gamma_\Psi H^{1/2}) \right)^{1/2} \\ &\leq \text{Tr}(H^{1/2}\gamma_\Psi H^{1/2}) + \text{Tr}(KH^{-1}K^*), \end{aligned}$$

where we used (25) and the assumption $KH^{-1}K^* \leq JHJ^*$. Inserting this in (24) concludes the proof. \square

We now turn to another standard intermediate result.

Lemma 13. *Let $w \in L^{6/5}(\mathbb{R}^3)$, $f \in L^\infty(\mathbb{R}^3)$, $\chi_1, \chi_2 \in L^\infty(\mathbb{R})$. Then we have for all $\eta > 0$*

$$\begin{aligned} & \pm \left(\chi_1(\mathcal{N}) \iint f(x)w(x-y)a_y^*a_xa_y dx dy \chi_2(\mathcal{N}) + h.c. \right) \\ & \leq \|w\|_{L^{6/5}(\mathbb{R}^3)} \|f\|_{L^\infty(\mathbb{R}^3)} \left(\eta\chi_1(\mathcal{N})^2\mathcal{N} + \eta^{-1}\chi_2(\mathcal{N})^2\mathcal{N} d\Gamma(-\Delta) \right). \end{aligned}$$

Here *h.c.* means *hermitian conjugate* so that $A + h.c. = A + A^*$ for any operator A (with dense domain).

Proof. We recall the Cauchy-Schwarz inequality for operator:

$$\pm(AB + B^*A^*) \leq \eta AA^* + \eta^{-1}B^*B, \quad \forall \eta > 0.$$

We will use it for $A = \chi_1(\mathcal{N})a_y^*$ and $B = f(x)w(x-y)a_x a_y \chi_2(\mathcal{N})$, we obtain for all $\eta > 0$

$$\begin{aligned} & \pm \left(\iint \chi_1(\mathcal{N})f(x)w(x-y)a_y^* a_x a_y dx dy \chi_2(\mathcal{N}) + h.c. \right) \\ & \leq \eta \int \chi_1(\mathcal{N})a_y^* a_y \chi_1(\mathcal{N}) dy \\ & \quad + \eta^{-1} \int \left(\iint w(x-y)f(x)\overline{f(x')w(x'-y)}\chi_2(\mathcal{N})a_x^* a_y^* a_x a_y \chi_2(\mathcal{N}) dx dx' \right) dy. \end{aligned} \quad (26)$$

The second term above is $\chi_2(\mathcal{N})\mathbb{T}\chi_2(\mathcal{N})$ where \mathbb{T} is the second quantization of the operator T defined by

$$T(\varphi)(x, y) = w(x-y)f(x) \int \overline{w(x'-y)f(x')} \varphi(x', y) dx',$$

for all $\varphi \in H^1(\mathbb{R}^3 \times \mathbb{R}^3)$. It satisfies

$$\begin{aligned} \langle \varphi, T\varphi \rangle_{L^2(\mathbb{R}^3 \times \mathbb{R}^3)} &= \int \left| \int \overline{w(x-y)f(x)} \varphi(x, y) dx \right|^2 dy \\ &\leq \int \|w\|_{L^{6/5}(\mathbb{R}^3)}^2 \|f\|_{L^\infty(\mathbb{R}^3)}^2 \|\varphi(\cdot, y)\|_{L^6(\mathbb{R}^3)}^2 dy \\ &\leq \|w\|_{L^{6/5}(\mathbb{R}^3)}^2 \|f\|_{L^\infty(\mathbb{R}^3)}^2 \int \|\nabla_1 \varphi(\cdot, y)\|_{L^2(\mathbb{R}^3)}^2 dy \\ &\leq \|w\|_{L^{6/5}(\mathbb{R}^3)}^2 \|f\|_{L^\infty(\mathbb{R}^3)}^2 \langle \varphi, (-\Delta \otimes 1)\varphi \rangle_{L^2(\mathbb{R}^3 \times \mathbb{R}^3)}. \end{aligned}$$

Hence this yields the bound

$$(26) \leq \eta \mathcal{N} \chi_1(\mathcal{N})^2 + C\eta^{-1} \|w\|_{L^{6/5}(\mathbb{R}^3)}^2 \|f\|_{L^\infty(\mathbb{R}^3)}^2 \mathcal{N} \chi_2(\mathcal{N})^2 d\Gamma(-\Delta)$$

from which we obtain the desired result, using that $\mathcal{N} = d\Gamma(1) \leq d\Gamma(1 - \Delta)$ and optimizing over η . \square

Bogoliubov's approximation: proof of Lemma 11

We follow the proof [NN17]. We emphasize that the inequalities (23) hold in $\mathcal{F}^{\leq m}(\mathcal{H}_+)$, that is

$$\langle \Phi, A\Phi \rangle \leq \mathbb{1}^{\leq m} \leq C_{\varepsilon, t} \sqrt{\frac{m}{N^{1-\beta-\varepsilon}}} \langle \Phi, d\Gamma(1 - \Delta)\Phi \rangle, \quad \forall \Phi \in \mathcal{F}^{\leq m}(\mathcal{H}_+).$$

Nevertheless, when possible, we will try to obtain first general estimates in $\mathcal{F}(\mathcal{H})$ and then take the projection on $\mathcal{F}^{\leq m}(\mathcal{H}_+)$.

Let us begin by noting that $[R_0, \mathcal{N}] = [R_4, \mathcal{N}] = 0$, $[R_1, \mathcal{N}] = R_1$, $[R_2, \mathcal{N}] = -2R_2$ and $[R_3, \mathcal{N}] = R_3$. It is therefore sufficient to prove (23) only for $A \in \{\mathcal{E}_N(t), \partial_i \mathcal{E}_N(t)\}$. From Hölder's inequality and the continuity property of the dipolar kernel K , see for instance [Duo01, Theorem 4.12], for all $2 \leq p < \infty$, there exists some constant $C_p > 0$ such that for all $f \in L^p(\mathbb{R}^3)$ we have for all $N \geq 1$,

$$\|w_N * f\|_{L^p(\mathbb{R}^3)} \leq C_p \|f\|_{L^p(\mathbb{R}^3)}.$$

From this it follows that

$$\begin{aligned}\|\tilde{K}_1(t)\|_{op} &\leq C_2 \|u_N(t)\|_{L^\infty(\mathbb{R}^3)}^2, \\ \|\partial_t \tilde{K}_1(t)\|_{op} &\leq C_2 \|u_N(t)\|_{L^\infty(\mathbb{R}^3)} \|\partial_t u_N(t)\|_{L^\infty(\mathbb{R}^3)}.\end{aligned}$$

Similarly we have

$$\|w_N * f\|_{L^\infty(\mathbb{R}^3)} \leq C_2 \|f\|_{H^2(\mathbb{R}^3)}.$$

Using this with the Hartree equation (4) we obtain

$$\|\partial_t u_N(t)\|_{L^\infty(\mathbb{R}^3)} \leq C(1 + C_2) \|u\|_{H^4(\mathbb{R}^3)}.$$

For the particular case $p = 2$, we can take $C_2 = \|\hat{w}\|_{L^\infty(\mathbb{R}^3)}$. Finally, we recall that $d\Gamma(1) = \mathcal{N}$ and that for any $f \in L^2(\mathbb{R}^3)$ we have

$$a^*(f)a(f) \leq \|f\|_{L^2(\mathbb{R}^3)}^2 \mathcal{N}.$$

We will now pursue and estimate separately the terms involving R_j for $j = 0 \dots 4$, where we recall that $\mathcal{E}_N(t) = \frac{1}{2} \sum_{j=0}^4 (R_j + R_j^*)$.

Step 1: Bounds involving R_0

We have

$$\begin{aligned}\pm R_0 &= \pm d\Gamma(Q(t)[w_N * |u_N(t)|^2 + \tilde{K}_1(t) - \mu_N(t)]Q(t)) \frac{1 - \mathcal{N}}{N - 1} \\ &\leq C \frac{\mathcal{N}^2}{N} \left(\|w_N * |u_N(t)|^2\|_{L^\infty(\mathbb{R}^3)} + \|\hat{w}\|_{L^\infty(\mathbb{R}^3)} \|u_N(t)\|_{L^\infty(\mathbb{R}^3)}^2 + \|\hat{w}\|_{L^\infty(\mathbb{R}^3)} \|u_N(t)\|_{L^4(\mathbb{R}^3)}^4 \right) \\ &\leq C_t \frac{\mathcal{N}^2}{N},\end{aligned}$$

which, after noting that $\mathcal{N} \leq d\Gamma(1 - \Delta)$ and projecting on $\mathcal{F}^{\leq m}(\mathcal{H}_+)$, gives (23) for the R_0 part. We turn to the estimate of $\partial_t R_0$ and start by computing

$$\partial_t Q(t) = -|\partial_t u_N(t)\rangle \langle u_N(t)| - |u_N(t)\rangle \langle \partial_t u_N(t)|,$$

from which we have

$$\|\partial_t Q(t)\|_{op} \leq 2 \|u_N(t)\|_{L^2(\mathbb{R}^3)} \|\partial_t u_N(t)\|_{L^2(\mathbb{R}^3)}.$$

Using the Cauchy-Schwarz inequality for operators we obtain

$$\begin{aligned}
\pm \partial_t R_0 &= \pm \frac{1-N}{1-N} d\Gamma \left(\partial_t Q(t) [w_N * |u_N(t)|^2 + \tilde{K}_1(t) - \mu_N(t)] Q(t) + h.c. \right) \\
&\quad + \frac{1-N}{1-N} d\Gamma \left(Q(t) [2w_N * \Re(\partial_t u(t) \overline{u(t)}) + \partial_t \tilde{K}_1(t) - \partial_t \mu_N(t)] Q(t) \right) \\
&\leq C \frac{\mathcal{N}^2}{N} \left(\|\partial_t Q(t)\|_{op}^2 + \|w_N * |u_N(t)|^2\|_{L^\infty(\mathbb{R}^3)}^2 + \|\widehat{K}_1\|_{op}^2 \right. \\
&\quad \left. + \|w_N * \Re(\partial_t u_N(t) \overline{u_N(t)})\|_{L^\infty(\mathbb{R}^3)} + \|\partial_t \tilde{K}_1(t)\|_{op} + C_t \right) \\
&\leq C_t \frac{\mathcal{N}^2}{N}.
\end{aligned}$$

Projecting on $\mathcal{F}^{\leq m}$ and noting that $\mathcal{N} \leq d\Gamma(1 - \Delta)$ gives the result.

Step 2: Bounds involving R_1

Recall that for any $f \in L^2(\mathbb{R}^3)$ we have $a^*(f)a(f) \leq \|f\|_{L^2(\mathbb{R}^3)}^2 \mathcal{N}$. Hence, using the Cauchy-Schwarz inequality we obtain

$$\begin{aligned}
\pm(R_1 + R_1^*) &= \mp 2 \left(\frac{\mathcal{N}\sqrt{N-N}}{N-1} a(Q(t)[w_N * |u_N(t)|^2]u_N(t)) + h.c. \right) \\
&\leq C\eta \frac{\mathcal{N}^2}{N^{1/2}} + \eta^{-1} a^*(Q(t)[w_N * |u_N(t)|^2]u_N(t)) a(Q(t)[w_N * |u_N(t)|^2]u_N(t)) \\
&\leq CN^{-1/2} (\eta\mathcal{N} + \eta^{-1} \| [w_N * |u_N(t)|^2]u_N(t) \|_{L^2(\mathbb{R}^3)}^2) \mathcal{N} \\
&\leq C_t \frac{\eta\mathcal{N} + \eta^{-1}}{N^{1/2}} \mathcal{N}.
\end{aligned}$$

Projecting onto $\mathcal{F}^{\leq m}$ and optimizing over η gives the result. The term $\partial_t R_1$ is dealt with similarly.

Step 3: Bounds involving R_2

Define $\chi(x) = 1 - \sqrt{(N-x)(N-x-1)}/(N-1)$ for $x \leq N$ and note that $0 \leq \chi(x) \leq x/(N-1)$. Writing $Q(t) = 1 - |u_N(t)\rangle \langle u_N(t)|$ in the expression of R_2 and expanding, we obtain after a simple computation that

$$\begin{aligned}
R_2 &= \left(2a^*(u_N(t))a^*([w_N * |u_N(t)|^2]u_N(t)) - 2\mu_N(t)a^*(u_N(t))a^*(u_N(t)) \right. \\
&\quad \left. - \iint u(t, x)w_N(x-y)u(t, y)a_x^*a_y^* dx dy \right) \chi(\mathcal{N}). \quad (27)
\end{aligned}$$

In the expression above, because of the $a^*(u_N(t))$ appearing in normal order, the first two terms vanish when the expectation is taken against an element of $\mathcal{F}(\mathcal{H}_+)$. We therefore focus on the

last term. Applying Lemma 12 we have

$$\begin{aligned}
& \pm \left(\mathbf{1}^{\leq m} \iint u(t, x) w_N(x - y) u(t, y) a_x^* a_y^* dx dy \chi(\mathcal{N}) + h.c. \right) \mathbf{1}^{\leq m} \\
& \leq C \left(\eta \| \mathbf{1}^{\leq m} \chi(\mathcal{N}) \|_{op}^2 \| (1 - \Delta_x)^{-1/2} u_N(t) w_N * (u_N(t) \cdot) \|_{\mathfrak{S}_2}^2 + \eta^{-1} d\Gamma(1 - \Delta) \right) \\
& \leq C_{t, \varepsilon} \left(\eta \frac{m^2}{N^2} N^{\beta + \varepsilon} + \eta^{-1} d\Gamma(1 - \Delta) \right) \\
& \leq C_{t, \varepsilon} \sqrt{\frac{m}{N^{1 - \beta - \varepsilon}}} d\Gamma(1 - \Delta).
\end{aligned}$$

We have used that

$$\begin{aligned}
\| (1 - \Delta_x)^{-1/2} u_N(t) w_N * (u_N(t) \cdot) \|_{\mathfrak{S}_2} & \leq \| (1 - \Delta_x)^{-1/2} u_N(t) \|_{\mathfrak{S}_{3 + \varepsilon_3}} \| w_N * (u_N(t) \cdot) \|_{\mathfrak{S}_{6 - \varepsilon_2}} \\
& \leq C \| u_N(t) \|_{L^{3 + \varepsilon_3}} \| w_N \|_{L^{6/5 + \varepsilon_1}(\mathbb{R}^3)} \| u_N(t) \|_{L^{6 - \varepsilon_2}(\mathbb{R}^3)} \\
& \leq C_{t, \varepsilon} N^{\beta/2 + \varepsilon},
\end{aligned}$$

where we used Hölder's inequality in Schatten spaces and the Kato-Seiler-Simon inequality: for any $p \geq 2$ and $f, g \in L^p(\mathbb{R}^3)$

$$\| f(x) g(k) \|_{\mathfrak{S}_p} \leq C_p \| f \|_{L^p(\mathbb{R}^3)} \| g \|_{L^p(\mathbb{R}^3)},$$

for some constant $C_p > 0$ where $f(x)$ and $g(k)$ are respectively the multiplication by f and the multiplication by g in Fourier space. We choose $\varepsilon_3, \varepsilon_2$ and ε_1 such that

$$\frac{1}{2} = \frac{1}{3 + \varepsilon_3} + \frac{1}{6 - \varepsilon_2}, \quad 1 = \frac{1}{6 - \varepsilon_2} + \frac{1}{6/5 + \varepsilon_1}, \quad 3\beta(1 - \frac{1}{6/5 + \varepsilon_1}) = \frac{\beta}{2} + \varepsilon.$$

We continue with the estimation of $\partial_t R_2$. Differentiating (27), we have

$$\begin{aligned}
\partial_t R_2 & = 2 \left(a^*(\partial_t u_N(t)) a^*([w_N * |u_N(t)|^2] u_N(t)) + a^*(u_N(t)) a^*(\partial_t([w_N * |u_N(t)|^2] u_N(t))) \right. \\
& \quad \left. - \partial_t \mu_N(t) a^*(u_N(t)) a^*(u_N(t)) - 2\mu_N(t) a^*(\partial_t u_N(t)) a^*(u_N(t)) \right. \\
& \quad \left. - \iint \partial_t u(t, x) w_N(x - y) u(t, y) a_x^* a_y^* dx dy \right) \chi(\mathcal{N}).
\end{aligned}$$

Again, when taking the expectation with an element of $\mathcal{F}(\mathcal{H}_+)$, all the terms above containing $a^*(u_N(t))$ in normal order vanish. Hence, it remains to estimate

$$\begin{aligned}
& \pm 2 \mathbf{1}^{\leq m} \left(a^*(\partial_t u_N(t)) a^*([w_N * |u_N(t)|^2] u_N(t)) \right. \\
& \quad \left. - \iint \partial_t u(t, x) w_N(x - y) u(t, y) a_x^* a_y^* dx dy \right) \chi(\mathcal{N}) \mathbf{1}^{\leq m} + h.c. \\
& \leq 4 \| \partial_t u_N(t) \|_{L^2(\mathbb{R}^3)} \| [w_N * |u_N(t)|^2] u_N(t) \|_{L^2(\mathbb{R}^3)} \chi(m) \mathcal{N} \\
& \quad + \left(\eta \frac{m^2}{N^2} \| (1 - \Delta_x)^{-1/2} \partial_t u_N(t) w_N * (u_N(t) \cdot) \|_{\mathfrak{S}_2}^2 + \eta^{-1} d\Gamma(1 - \Delta) \right) \\
& \leq C_{t, \varepsilon} \left(\frac{m}{N} \mathcal{N} + \left(\eta \frac{m^2}{N^{2 - \beta + \varepsilon}} + \eta^{-1} d\Gamma(1 - \Delta) \right) \right).
\end{aligned}$$

Here we used again Lemma 12 and a similar argument as for estimating $\|(1 - \Delta_x)^{-1/2} u_N(t) w_N * (u_N(t) \cdot)\|_{\mathfrak{S}_2}$. Projecting on $\mathcal{F}^{\leq m}$ and optimizing over η yields the desired estimate.

Step 4: Bounds involving R_3

Again, a computation shows that

$$\begin{aligned} R_3 = & \frac{\sqrt{N - \mathcal{N}}}{N - 1} \left(\iint w_N(x - y) \overline{u(t, x)} a_y^* a_x a_y dx dy - d\Gamma(T(t)) a(u_N(t)) \right. \\ & - d\Gamma([w_N * |u_N(t)|^2]) a(u_N(t)) + a^*(w * |u_N(t)|^2 u_N(t)) a(u_N(t)) a(u_N(t)) \\ & \left. + a^*(u_N(t)) a(u_N(t)) a(w * |u_N(t)|^2 u_N(t)) - 2\mu_N(t) a^*(u_N(t)) a(u_N(t)) a(u_N(t)) \right), \quad (28) \end{aligned}$$

where $T(t)$ is the operator defined by $T(t)(\varphi) = w_N * (\overline{u_N(t)} \varphi)$ for all $\varphi \in L^2(\mathbb{R}^3)$. It is bounded with norm less than $\|\widehat{w}\|_{L^\infty(\mathbb{R}^3)} \|u_N(t)\|_{L^\infty(\mathbb{R}^3)}$. Dealing with R_3 , and for the same reasons as previously, we only need to estimate the first term, which we do using Lemma 13. We proceed as follows:

$$\begin{aligned} \pm \left(\frac{\sqrt{N - \mathcal{N}}}{N - 1} \iint w_N(x - y) \overline{u(x)} a_y^* a_x a_y dx dy + h.c. \right) \\ \leq CN^{-1/2} \|w_N\|_{L^{6/5}(\mathbb{R}^3)} \|u_N(t)\|_{L^\infty(\mathbb{R}^3)} (\eta \mathcal{N} + \eta^{-1}) d\Gamma(1 - \Delta) \\ \leq C_t \frac{\eta \mathcal{N} + \eta^{-1}}{N^{(1-\beta)/2}} d\Gamma(1 - \Delta), \end{aligned}$$

for all $\eta > 0$. Projecting on $\mathcal{F}^{\leq m}$ and optimizing over η gives the result. We now continue with the estimates involving $\partial_t R_3$. Differentiating (28) we have

$$\begin{aligned} \partial_t R_3 = & \frac{\sqrt{N - \mathcal{N}}}{N - 1} \left(\iint w_N(x - y) \overline{\partial_t u(t, x)} a_y^* a_x a_y dx dy - d\Gamma(\partial_t T(t)) a(u_N(t)) \right. \\ & - d\Gamma(T(t)) a(\partial_t u_N(t)) - d\Gamma(\partial_t([w_N * |u_N(t)|^2]) a(u_N(t)) - d\Gamma([w_N * |u_N(t)|^2]) a(\partial_t u_N(t)) \\ & + a^*(\partial_t(w * |u_N(t)|^2 u_N(t))) a(u_N(t)) a(u_N(t)) + 2a^*(w * |u_N(t)|^2 u_N(t)) a(\partial_t u_N(t)) a(u_N(t)) \\ & + a^*(\partial_t u_N(t)) a(u_N(t)) a(w * |u_N(t)|^2 u_N(t)) + a^*(u_N(t)) a(\partial_t u_N(t)) a(w * |u_N(t)|^2 u_N(t)) \\ & + a^*(u_N(t)) a(u_N(t)) a(\partial_t(w * |u_N(t)|^2 u_N(t))) - 2\partial_t \mu_N(t) a^*(u_N(t)) a(u_N(t)) a(u_N(t)) \\ & \left. - 2\mu_N(t) a^*(\partial_t u_N(t)) a(u_N(t)) a(u_N(t)) - 4\mu_N(t) a^*(u_N(t)) a(\partial_t u_N(t)) a(u_N(t)) \right). \end{aligned}$$

Again, any term containing $a^*(u_N(t))$ or $a(u_N(t))$ in normal order vanishes when taking the expectation with an element of $\mathcal{F}(\mathcal{H}_+)$. It remains to estimate

$$\begin{aligned}
& \pm \frac{\sqrt{N-\mathcal{N}}}{N-1} \left(\iint w_N(x-y) \overline{\partial_t u(t,x)} a_y^* a_x a_y dx dy - d\Gamma(T(t)) a(\partial_t u_N(t)) \right. \\
& \qquad \qquad \qquad \left. - d\Gamma([w_N * |u_N(t)|^2]) a(\partial_t u_N(t)) + h.c. \right) \\
& \leq CN^{-1/2} \left(\|w_N\|_{L^{6/5}(\mathbb{R}^3)} \|\partial_t u_N(t)\|_{L^\infty(\mathbb{R}^3)} (\eta\mathcal{N} + \eta^{-1}) d\Gamma(1-\Delta) + \eta' a^*(\partial_t u_N(t)) a(\partial_t u_N(t)) \right. \\
& \qquad \qquad \qquad \left. + (\eta')^{-1} \left(d\Gamma(T(t)) d\Gamma(T(t)^*) + d\Gamma([w_N * |u_N(t)|^2])^2 \right) \right) \\
& \leq C_t N^{-1/2} \left(N^{\beta/2} (\eta\mathcal{N} + \eta^{-1}) d\Gamma(1-\Delta) + \eta' \|\partial_t u_N(t)\|_{L^2(\mathbb{R}^3)}^2 \mathcal{N} \right. \\
& \qquad \qquad \qquad \left. + (\eta')^{-1} \left(\|T(t)\|_{op}^2 + \|w_N * |u_N(t)|^2\|_{L^\infty(\mathbb{R}^3)}^2 \right) \mathcal{N}^2 \right) \\
& \leq C_t N^{(\beta-1)/2} (\eta\mathcal{N} + \eta^{-1}) d\Gamma(1-\Delta),
\end{aligned}$$

for all $\eta > 0$. We used the Cauchy-Schwarz inequality and Lemma 13 to obtain the second inequality and we took $\eta' = \eta^{-1}$ and used again that $\mathcal{N} \leq d\Gamma(1-\Delta)$ to obtain the last. Projecting on $\mathcal{F}^{\leq m}(\mathcal{H}_+)$ and optimizing with respect to $\eta > 0$, we obtain the desired result.

Step 5: Bounds involving R_4

From $\pm w_N(x-y) \leq N^\beta \|w\|_{L^{3/2}(\mathbb{R}^3)} (1-\Delta_x)$ one has

$$\begin{aligned}
\pm R_4 & \leq CN^{\beta-1} d\Gamma(Q(t)(1-\Delta_x)Q(t)) d\Gamma(Q(t)) \\
& \leq C \frac{\mathcal{N}}{N^{1-\beta}} d\Gamma(Q(t)(1-\Delta_x)Q(t)).
\end{aligned}$$

Next we turn to

$$\begin{aligned}
\partial_t R_4 & = \frac{1}{(N-1)} \iiint (\partial_t Q(t) \otimes Q(t) w_N Q(t) \otimes Q(t))(x, y, x', y') a_x^* a_y^* a_{x'} a_{y'} dx dy dx' dy' + h.c. \\
& = -\frac{1}{(N-1)} \iiint (1 \otimes Q(t) w_N Q(t) \otimes Q(t))(x, y, x', y') \times \\
& \qquad \qquad \qquad \times \left(\overline{\partial_t u(t,x)} a^*(u_N(t)) + \overline{u(t,x)} a^*(\partial_t u_N(t)) \right) a_y^* a_{x'} a_{y'} dx dy dx' dy' + h.c.
\end{aligned}$$

Again, since we are interested in taking the expectation of an element of $\mathcal{F}(\mathcal{H}_+)$, we can ignore the terms containing $a^*(u_N(t))$ or $a(u_N(t))$ and consider the remaining terms where $Q(t)$ is replaced by 1. Then the same computations as in the proof of Lemma 13 but replacing χ_1 by

$a^*(\partial_t u_N(t))$ give

$$\begin{aligned} & \pm \frac{1}{N-1} \left(\iint w_N(x-y)u(t,x)a^*(\partial_t u_N(t))a_y^*a_x \, dx \, dy + h.c. \right) \\ & \leq \frac{1}{N-1} \left(\eta \|\partial_t u_N(t)\|_{L^2(\mathbb{R}^3)}^2 \mathcal{N}^2 + \eta^{-1} N^\beta \|w\|_{L^{6/5}(\mathbb{R}^3)}^2 \|u_N(t)\|_{L^\infty(\mathbb{R}^3)}^2 \mathcal{N} d\Gamma(1-\Delta) \right) \\ & \leq C_t \frac{\mathcal{N}}{N^{1-\beta/2}} d\Gamma(1-\Delta), \end{aligned}$$

where we have optimized over $\eta > 0$. Projecting on $\mathcal{F}^{\leq m}$ concludes the proof of Lemma 11. \square

Bogoliubov stability: proof of Lemma 10

Recall that

$$\begin{aligned} \mathbb{H}(t) + d\Gamma(\Delta) &= d\Gamma(1 + w * |u_N(t)|^2 + Q(t)\tilde{K}_1(t)Q(t) - \mu_N(t)) \\ & \quad + \left(\iint K_2(t,x,y)a_x^*a_y^* \, dx \, dy + \iint \overline{K_2(t,x,y)}a_x a_y \, dx \, dy \right). \end{aligned}$$

For the first term we have

$$\begin{aligned} & \pm d\Gamma(1 + w_N * |u_N(t)|^2 + Q(t)\tilde{K}_1(t)Q(t) - \mu_N(t)) \\ & \leq \left(1 + \|w_N * |u_N(t)|^2\|_{L^\infty(\mathbb{R}^3)} + \|\tilde{K}_1(t)\|_{op} + |\mu_N(t)| \right) \mathcal{N}. \end{aligned}$$

We expand the second term and we use Lemma 12,

$$\begin{aligned} & \pm \left(\iint K_2(t,x,y)a_x^*a_y^* \, dx \, dy + h.c. \right) \\ & = \pm \left(\iint w_N(x-y)u(t,x)u(t,y)a_x^*a_y^* \, dx \, dy \right. \\ & \quad \left. - 2a^*([w_N * |u_N(t)|^2]u_N(t))a^*(u_N(t)) + 2\mu_N(t)a^*(u_N(t))a^*(u_N(t)) + h.c. \right) \quad (29) \\ & \leq C \left(\eta \|(1-\Delta_x)^{-1/2}u_N(t)w_N * (u_N(t) \cdot)\|_{\mathfrak{S}_2}^2 + \eta^{-1} d\Gamma(1-\Delta) \right. \\ & \quad \left. + \|[w_N * |u_N(t)|^2]u_N(t)\|_{L^2(\mathbb{R}^3)} \|u_N(t)\|_{L^2(\mathbb{R}^3)} + \|u_N(t)\|_{L^2(\mathbb{R}^3)}^2 |\mu_N(t)| \mathcal{N} \right) \\ & \leq C_{t,\varepsilon} (\mathcal{N} + \eta N^{\beta+\varepsilon} + \eta^{-1} d\Gamma(1-\Delta)), \end{aligned}$$

for $\eta > 0$. We then evaluate

$$\begin{aligned} \partial_t \mathbb{H}(t) &= d\Gamma \left(2w_N * \Re(\partial_t \overline{u_N(t)} u_N(t)) + \partial_t(Q(t)\tilde{K}_1(t)Q(t)) - \partial_t \mu_N(t) \right) \\ & \quad + \iint \partial_t K_2(t,x,t)a_x^*a_y^* \, dx \, dy + \iint \overline{\partial_t K_2(t,x,t)}a_x a_y \, dx \, dy. \end{aligned}$$

For the first term we have

$$\begin{aligned}
& \pm d\Gamma \left(w_N * \Re(\overline{\partial_t u_N(t)} u_N(t)) + \partial_t(Q(t)\tilde{K}_1(t)Q(t)) - \partial_t \mu_N(t) \right) \\
& \leq \left(\|w_N * \Re(\overline{\partial_t u_N(t)} u_N(t))\|_{L^\infty(\mathbb{R}^3)} + \|\partial_t \tilde{K}_1(t)\|_{op} \right. \\
& \quad \left. + \|\tilde{K}_1(t)\|_{op} \|\partial_t u_N(t)\|_{L^2(\mathbb{R}^3)} + |\partial_t \mu_N(t)| + 1 \right) \mathcal{N} \\
& \leq C_t \mathcal{N}.
\end{aligned}$$

To estimate the second and third terms, we differentiate (29) and obtain that

$$\begin{aligned}
& \pm \left(\iint \partial_t K_2(t, x, y) a_x^* a_y^* dx dy + h.c. \right) \\
& = \pm \left(2 \iint w_N(x-y) (\partial_t u(t, x)) u(t, y) a_x^* a_y^* dx dy - 2a^* (\partial_t([w_N * |u_N(t)|^2]u_N(t))) a^*(u_N(t)) \right. \\
& \quad \left. + a^*([w_N * |u_N(t)|^2]u_N(t)) a^*(\partial_t u_N(t)) + 2\partial_t \mu_N(t) a^*(u_N(t)) a^*(u_N(t)) \right. \\
& \quad \left. + 2\mu_N(t) a^*(\partial_t u_N(t)) a^*(u_N(t)) + h.c. \right) \\
& \leq C \left(\eta \|(1 - \Delta_x)^{-1/2} \partial_t u_N(t) w_N * (u_N(t) \cdot)\|_{\mathfrak{S}_2}^2 + \eta^{-1} d\Gamma(1 - \Delta) \right. \\
& \quad \left. + \left(\|\partial_t([w_N * |u_N(t)|^2]u_N(t))\|_{L^2(\mathbb{R}^3)} \|u_N(t)\|_{L^2(\mathbb{R}^3)} \right. \right. \\
& \quad \left. \left. + \|([w_N * |u_N(t)|^2]u_N(t))\|_{L^2(\mathbb{R}^3)} \|\partial_t u_N(t)\|_{L^2(\mathbb{R}^3)} \right. \right. \\
& \quad \left. \left. + |\partial_t \mu_N(t)| \|u_N(t)\|_{L^2(\mathbb{R}^3)}^2 + \mu_N(t) \|u_N(t)\|_{L^2(\mathbb{R}^3)} \|\partial_t u_N(t)\|_{L^2(\mathbb{R}^3)} \right) \mathcal{N} \right) \\
& \leq C_{t,\varepsilon} (\mathcal{N} + \eta N^{\beta+\varepsilon} + \eta^{-1} d\Gamma(1 - \Delta)),
\end{aligned}$$

where we used the Cauchy-Schwarz inequality and Lemma 12.

Finally, since

$$i[\mathbb{H}, \mathcal{N}] = - \iint \left(iK_2(t, x, y) a_x^* a_y^* + \overline{iK_2(t, x, y)} a_x a_y \right) dx dy,$$

we can estimate this term in a similar manner as before and obtain the desired bound. \square

3.3 Norm approximation

We follow and adapt the arguments in [NN17], we obtain the following lemma.

Lemma 14. *Let $M = N^{1-\delta}$ with $\delta \in (0, 1)$, then we have*

$$\|\Phi_N(t) - \Phi_{N,M}(t)\|_{L^2(\mathbb{R}^{3N})}^2 \leq C_{t,\varepsilon} \left(\frac{1}{M^{1/2}} + (|e_N| + N)^{1/4} \left(\frac{N^{3(\beta+\varepsilon)/4}}{M} + \frac{N^{(\beta+\varepsilon-1)/2}}{M^{1/4}} \right) \right).$$

Proof. The proof follows the one of [NN17], it differs in that it uses Lemma 13 to deal with three

body terms and that one has to be a little bit more careful when estimating the two-body terms.

We have

$$\|\Phi_N(t) - \Phi_{N,M}(t)\|_{L^2(\mathbb{R}^{3N})}^2 = 2(1 - \Re\langle\Phi_N(t), \Phi_{N,M}(t)\rangle).$$

Let $M/2 \leq m \leq M - 3$ and decompose

$$\langle\Phi_N(t), \Phi_{N,M}(t)\rangle = \langle\Phi_N(t), \mathbf{1}^{\leq m}\Phi_{N,M}(t)\rangle + \langle\Phi_N(t), \mathbf{1}^{> m}\Phi_{N,M}(t)\rangle.$$

The second term is estimated using the Cauchy-Schwarz inequality

$$\begin{aligned} |\langle\Phi_N(t), \mathbf{1}^{> m}\Phi_{N,M}(t)\rangle| &\leq \|\Phi_N(t)\|_{L^2(\mathbb{R}^{3N})} \|\mathbf{1}^{> m}\Phi_{N,M}(t)\|_{L^2(\mathbb{R}^{3N})} \\ &\leq \langle\Phi_{N,M}(t), (\mathcal{N}/m)\Phi_{N,M}(t)\rangle^{1/2} \\ &\leq C_t M^{-1/2}. \end{aligned} \tag{30}$$

We now want to prove that the first term remains close to 1. To this aim we compute its time derivative

$$\frac{d}{dt}\langle\Phi_N(t), \mathbf{1}^{\leq m}\Phi_{N,M}(t)\rangle = \langle\Phi_N(t), i[\mathcal{G}_N(t), \mathbf{1}^{\leq m}]\Phi_{N,M}(t)\rangle$$

and consider its average over the parameter $M/2 \leq m \leq M - 3$

$$\frac{1}{M/2 - 2} \sum_{m=M/2}^{M-3} \langle\Phi_N(t), i[\mathcal{G}_N(t), \mathbf{1}^{\leq m}]\Phi_{N,M}(t)\rangle.$$

The gain obtained by averaging comes from the fact that the commutator $[\mathcal{G}_N(t), \mathbf{1}^{\leq m}]$ is localized in $\{m - 2 \leq \mathcal{N} \leq m + 2\}$. As was shown in [NN17] we have

$$\sum_{m=M/2}^{M-3} i[\mathcal{G}_N(t), \mathbf{1}^{\leq m}] = A_1\chi_1(\mathcal{N})^2 + A_2\chi_2(\mathcal{N})^2 + h.c.,$$

where

$$\begin{aligned} A_1 &= \frac{i}{2} \iiint (Q(t) \otimes Q(t) w_N Q(t) \otimes 1)(x, y, x', y') u(t, x) a_x^* a_y^* a_{y'} dx dy dx' dy' \\ &\quad - a^*(Q(t)[w * |u_N(t)u_N(t)|^2]u_N(t))\mathcal{N} \\ &=: A_1^3 + A_1^1, \\ A_2 &= \frac{i}{2} \iint K_2(t, x, y) a_x^* a_y^* dx dy, \end{aligned}$$

and

$$\begin{aligned} \chi_1(\mathcal{N})^2 &= \frac{\sqrt{N - \mathcal{N}}}{N - 1} \mathbf{1}(M/2 \leq \mathcal{N} \leq M - 3), \\ \chi_2(\mathcal{N})^2 &= \frac{\sqrt{(N - \mathcal{N})(N - \mathcal{N} - 1)}}{N - 1} [\mathbf{1}(M/2 - 1 < \mathcal{N} \leq M - 3) + \mathbf{1}(M/2 \leq \mathcal{N} < M - 3)]. \end{aligned}$$

Note that since $\Phi_N(t), \Phi_{N,M}(t) \in \mathcal{F}(\mathcal{H}_+)$, we can replace $Q(t)$ by 1 in the expression of the

quantities $\langle \Phi_N(t), A_i^j \chi_i(\mathcal{N}) \Phi_{N,M}(t) \rangle$. We have

$$\begin{aligned}
& \left| \langle \Phi_N(t), (A_1^3 \chi_1(\mathcal{N})^2 + h.c.) \Phi_{N,M}(t) \rangle \right| \\
&= \frac{1}{2} \left| \langle \Phi_N(t), \left(\int i w_N(x-y) u(t,x) \chi_1(\mathcal{N}-1) a_x^* a_y^* a_y \chi_1(\mathcal{N}) dx dy + h.c. \right) \Phi_{N,M}(t) \rangle \right| \\
&\leq C N^{-1/2} \langle \Phi_N(t), \|w_N\|_{L^{6/5}(\mathbb{R}^3)} \mathbf{1}^{\geq M/2+1} \mathbf{1}^{\leq M-2} (\eta_1 \mathcal{N} + \eta_1^{-1} \mathcal{N} d\Gamma(1-\Delta)) \Phi_N(t) \rangle^{\frac{1}{2}} \\
&\quad \times \langle \Phi_{N,M}(t), \|w_N\|_{L^{6/5}(\mathbb{R}^3)} \mathbf{1}^{\geq M/2+1} \mathbf{1}^{\leq M-2} (\eta_2 \mathcal{N} + \eta_2^{-1} \mathcal{N} d\Gamma(1-\Delta)) \Phi_{N,M}(t) \rangle^{\frac{1}{2}} \\
&\leq C_{t,\varepsilon} N^{-1/2} \|w\|_{L^{6/5}(\mathbb{R}^3)} \left\{ N^{\beta/2} (\eta_1 M + \eta_1^{-1} M(|e_N| + N)) \times \right. \\
&\quad \left. \times N^{\beta/2} (\eta_2 N^{\beta+\varepsilon} + \eta_2^{-1} M N^{\beta+\varepsilon}) \right\}^{\frac{1}{2}} \\
&\leq C_{t,\varepsilon} N^{-1/2} N^{\beta+\varepsilon/2} M^{3/4} (|e_N| + N)^{1/4}.
\end{aligned}$$

We have used that

$$\langle \Phi_{N,M}(t), \mathcal{N} \Phi_{N,M}(t) \rangle \leq \langle \Phi_{N,M}(t), d\Gamma(1-\Delta) \Phi_{N,M}(t) \rangle \leq C_{t,\varepsilon} N^{\beta+\varepsilon}$$

and the estimate (22). Next we have

$$\begin{aligned}
& \left| \langle \Phi_N(t), A_1^1 \chi_1(\mathcal{N})^2 \Phi_{N,M}(t) \rangle \right| \\
&= \left| \langle \Phi_N(t), \chi_1(\mathcal{N}-1) a^*(Q(t)[w * |u_N(t)|^2] u_N(t)) \mathcal{N} \chi_1(\mathcal{N}) \Phi_{N,M}(t) \rangle \right| \\
&\leq C N^{-1/2} \langle \Phi_N(t), \mathbf{1}^{\leq M+1} a^*(Q(t)[w * |u_N(t)|^2] u_N(t)) a(Q(t)[w * |u_N(t)|^2] u_N(t)) \Phi_N(t) \rangle^{1/2} \times \\
&\quad \times \langle \Phi_{N,M}(t), \mathbf{1}^{\leq M} \mathcal{N}^2 \Phi_{N,M}(t) \rangle^{1/2} \\
&\leq C \| |w_N * |u_N(t)|^2 | u_N(t) \|_{L^2(\mathbb{R}^3)} N^{-1/2} \langle \Phi_N(t), \mathbf{1}^{\leq M} \mathcal{N} \Phi_N(t) \rangle^{1/2} \langle \Phi_{N,M}(t), \mathbf{1}^{\leq M} \mathcal{N}^2 \Phi_{N,M}(t) \rangle^{1/2} \\
&\leq C_{t,\varepsilon} N^{-1/2} N^{(\beta+\varepsilon)/2} M.
\end{aligned}$$

The term with $\langle \Phi_N(t), \chi_1(\mathcal{N})^2 (A_1^1)^* \Phi_{N,M}(t) \rangle$ is dealt with similarly. Finally, we apply Lemma 12 as well as the Cauchy-Schwarz inequality to bound the last term,

$$\begin{aligned}
& \left| \langle \Phi_N(t), (A_2 \chi_2(\mathcal{N})^2 + h.c.) \Phi_{N,M}(t) \rangle \right| \\
&= \left| \langle \Phi_N(t), \left(\iint i w_N(x-y) u(x) u(y) a_x^* a_y^* \chi_2(\mathcal{N})^2 dx dy + h.c. \right) \Phi_{N,M}(t) \rangle \right| \\
&\leq \left(\eta \| \chi_2(\mathcal{N}) \|_{op}^2 \| (1-\Delta_x)^{-1/2} u_N(t) w_N * (u_N(t) \cdot) \|_{\mathfrak{S}_2}^2 + \eta^{-1} \langle \Phi_N(t), d\Gamma(1-\Delta) \Phi_N(t) \rangle \right)^{1/2} \times \\
&\quad \times \left(\eta' \| \chi_2(\mathcal{N}) \|_{op}^2 \| (1-\Delta_x)^{-1/2} u_N(t) w_N * (u_N(t) \cdot) \|_{\mathfrak{S}_2}^2 + (\eta')^{-1} \langle \Phi_{N,M}(t), d\Gamma(1-\Delta) \Phi_{N,M}(t) \rangle \right)^{1/2} \\
&\leq (\eta N^{\beta+\varepsilon} + \eta^{-1} \langle \Phi_N(t), d\Gamma(1-\Delta) \Phi_N(t) \rangle)^{1/2} \times \\
&\quad \times (\eta' N^{\beta+\varepsilon} + (\eta')^{-1} \langle \Phi_{N,M}(t), d\Gamma(1-\Delta) \Phi_{N,M}(t) \rangle)^{1/2}. \tag{31}
\end{aligned}$$

Now we use again that $\langle \Phi_{N,M}(t), d\Gamma(1 - \Delta)\Phi_{N,M}(t) \rangle \leq C_{t,\varepsilon} N^{\beta+\varepsilon}$ and that $\langle \Phi_N(t), d\Gamma(1 - \Delta)\Phi_N(t) \rangle \leq C(|e_N| + N)$. After optimizing over η and η' we obtain

$$(31) \leq C_{t,\varepsilon} \frac{(|e_N| + N)^{1/4} N^{3(\beta+\varepsilon)/4}}{M}.$$

Hence we have shown that

$$\left| \frac{d}{dt} \left(\frac{1}{M/2 - 2} \sum_{m=M/2}^{M-3} \langle \Phi_N(t), \mathbf{1}^{\leq m} \Phi_{N,M}(t) \rangle \right) \right| \leq C_{t,\varepsilon} \left(\frac{(|e_N| + N)^{1/4} N^{3(\beta+\varepsilon)/4}}{M} + \frac{(|e_N| + N)^{1/4} N^{(\beta+\varepsilon-1)/2}}{M^{1/4}} + N^{(\beta+\varepsilon-1)/2} \right). \quad (32)$$

On the other hand, recall that $\Phi_{N,M}(0) = \Phi_N(0) = \Phi(0)$, so that for $M/2 \leq m \leq M - 3$,

$$\begin{aligned} \langle \Phi_N(0), \mathbf{1}^{\leq m} \Phi_{N,M}(0) \rangle &= \langle \Phi(0), \mathbf{1}^{\leq m} \Phi(0) \rangle \\ &= 1 - \langle \Phi(0), \mathbf{1}^{> m} \Phi(0) \rangle \\ &\geq 1 - \langle \Phi(0), \mathbf{1}^{> m} (\mathcal{N}/m) \Phi(0) \rangle \\ &\geq 1 - CM^{-1}. \end{aligned} \quad (33)$$

Gathering (30), (32) (33) we obtain

$$\begin{aligned} \|\Phi_N(t) - \Phi_{N,M}(t)\|_{L^2(\mathbb{R}^{3N})}^2 &\leq C_{t,\varepsilon} \left(\frac{1}{M^{1/2}} + \frac{(|e_N| + N)^{1/4} N^{3(\beta+\varepsilon)/4}}{M} + \frac{(|e_N| + N)^{1/4} N^{(\beta+\varepsilon-1)/2}}{M^{1/4}} \right). \end{aligned}$$

□

As in [NN17] we compare the Bogoliubov dynamics and the truncated one.

Lemma 15. *Let $M = N^\alpha$ with $0 < \alpha < 1 - \beta$, let N be large enough, then we have*

$$\|\Phi(t) - \Phi_{N,M}(t)\|_{L^2(\mathbb{R}^{3N})}^2 \leq C_{t,\varepsilon} \left(\frac{1}{M^{1/2}} + \frac{N^{\beta+\varepsilon}}{M} + \frac{M}{N^{1-2\beta-\varepsilon}} + \frac{M}{N^{(1-2\beta-2\varepsilon)/2}} \right).$$

Proof. The proof is similar as the one in [NN17] except that we use the estimates of Lemma 11. As before, we have

$$\|\Phi(t) - \Phi_{N,M}(t)\|_{L^2(\mathbb{R}^{3N})}^2 \leq 2(1 - \Re \langle \Phi_{N,M}(t), \Phi(t) \rangle). \quad (34)$$

We let $M/2 \leq m \leq M - 3$ and decompose

$$\langle \Phi_{N,M}(t), \Phi(t) \rangle = \langle \Phi_{N,M}(t), \mathbf{1}^{\leq m} \Phi(t) \rangle + \langle \Phi_{N,M}(t), \mathbf{1}^{> m} \Phi(t) \rangle.$$

The second term is bounded by the Cauchy-Schwarz inequality

$$\begin{aligned} |\langle \Phi_{N,M}(t), \mathbf{1}^{> m} \Phi(t) \rangle| &\leq \|\mathbf{1}^{> m} \Phi_{N,M}(t)\| \|\mathbf{1}^{> m} \Phi(t)\| \\ &\leq \langle \Phi_{N,M}(t), (\mathcal{N}/m) \Phi_{N,M}(t) \rangle^{1/2} \times \langle \Phi(t), (\mathcal{N}/m) \Phi(t) \rangle^{1/2} \\ &\leq C_t M^{-1}. \end{aligned} \quad (35)$$

As in the proof of Lemma 14, we will show that the first term remains close to 1, we compute its time derivative

$$\frac{d}{dt} \langle \Phi_{N,M}(t), \mathbf{1}^{\leq m} \Phi(t) \rangle = i \langle \Phi_{N,M}(t), ((\mathcal{G}_N(t) - \mathbb{H}) \mathbf{1}^{\leq m} + i[\mathbb{H}, \mathbf{1}^{\leq m}]) \Phi(t) \rangle.$$

The first term is estimated using Lemma 11 and the Cauchy-Schwarz inequality, we obtain

$$\begin{aligned} & \left| \langle \Phi_{N,M}(t), (\mathcal{G}_N(t) - \mathbb{H}) \mathbf{1}^{\leq m} \Phi(t) \rangle \right| \\ &= \left| \langle \Phi_{N,M}(t), \mathbf{1}^{\leq M} (\mathcal{G}_N(t) - \mathbb{H}) \mathbf{1}^{\leq M} \mathbf{1}^{\leq m} \Phi(t) \rangle \right| \\ &\leq C_{t,\varepsilon} \left\langle \Phi(t), \sqrt{\frac{M}{N^{1-\beta-\varepsilon}}} d\Gamma(1-\Delta) \Phi(t) \right\rangle^{1/2} \times \left\langle \Phi_{N,M}(t), \sqrt{\frac{M}{N^{1-\beta-\varepsilon}}} d\Gamma(1-\Delta) \Phi_{N,M}(t) \right\rangle^{1/2} \\ &\leq C_{t,\varepsilon} \sqrt{\frac{M}{N^{1-3\beta-3\varepsilon}}}, \end{aligned} \quad (36)$$

where we used Proposition 8, Proposition 9. For the second term, the same computations as in Lemma 14 show that

$$\left| \frac{1}{M/2-2} \sum_{m=M/2}^{M-3} \langle \Phi_N(t), i[\mathbb{H}(t), \mathbf{1}^{\leq m}] \Phi(t) \rangle \right| \leq C_{t,\varepsilon} \frac{N^{\beta+\varepsilon}}{M} \quad (37)$$

where we have used that $\langle \Phi(t), d\Gamma(1-\Delta) \Phi(t) \rangle \leq C_{t,\varepsilon} N^{\beta+\varepsilon}$. On the other hand, as in Lemma 14 we have

$$\langle \Phi_{N,M}(0), \mathbf{1}^{\leq m} \Phi(0) \rangle = \langle \Phi(0), \mathbf{1}^{\leq m} \Phi(0) \rangle \geq 1 - CM^{-1}. \quad (38)$$

Gathering (36),(37) and (38) we obtain

$$\Re \langle \Phi_{N,M}(t), \mathbf{1}^{\leq m} \Phi(t) \rangle \geq 1 - C_{t,\varepsilon} \left(M^{-1} + \frac{N^{\beta+\varepsilon}}{M} + \sqrt{\frac{M}{N^{1-3\beta-3\varepsilon}}} \right).$$

Together with (34) and (35), this concludes the proof. \square

3.4 Proof of Theorem 3

Proof of 1)

The triangle inequality and Lemmas 14 and 15 give, for all $\varepsilon > 0$

$$\begin{aligned} \|\Phi_N(t) - \Phi(t)\|_{L^2(\mathbb{R}^{3N})} &\leq \|\Phi_N(t) - \Phi_{N,M}(t)\|_{L^2(\mathbb{R}^{3N})} + \|\Phi_{N,M}(t) - \Phi(t)\|_{L^2(\mathbb{R}^{3N})} \\ &\leq C_{t,\varepsilon} \left(\frac{1}{M^{1/2}} + (|e_N| + N)^{1/4} \left(\frac{N^{3(\beta+\varepsilon)/4}}{M} + \frac{N^{\beta+\varepsilon/2-1/2}}{M^{1/4}} \right) \right. \\ &\quad \left. + \frac{N^{\beta+\varepsilon}}{M} + \sqrt{\frac{M}{N^{1-3(\beta+\varepsilon)}}} \right). \end{aligned}$$

Using that $|e_N| \leq N^{3\beta+1}$ and taking $M = N^{1/2}$ we obtain

$$\|\Phi_N(t) - \Phi(t)\|_{L^2(\mathbb{R}^{3N})} \leq C_{t,\varepsilon} \left(N^{-(6\beta-1)/4+\varepsilon} + N^{-(7\beta-2)/4+\varepsilon} \right),$$

for any $\varepsilon > 0$ small enough.

Proof of 2)

Using Lemma 14 and Proposition 8 we have

$$\begin{aligned} \langle \Phi_N(t), \frac{\mathcal{N}}{N} \Phi_N(t) \rangle &= \langle \Phi_N(t), \frac{\mathcal{N}}{N} (\Phi_N(t) - \Phi_{N,M}(t)) \rangle + \langle \Phi_N(t), \frac{\mathcal{N}}{N} \Phi_{N,M}(t) \rangle \\ &\leq \|\Phi_N(t)\|_{L^2(\mathbb{R}^{3N})} \left(\|\Phi_N(t) - \Phi_{N,M}(t)\|_{L^2(\mathbb{R}^{3N})} + \langle \Phi_{N,M}(t), \frac{\mathcal{N}}{N} \Phi_{N,M}(t) \rangle \right) \\ &\leq C_{t,\varepsilon} \left(\frac{1}{M^{1/2}} + (|e_N| + N)^{1/4} \left(\frac{N^{3(\beta+\varepsilon)/4}}{M} + \frac{N^{\beta+\varepsilon/2-1/2}}{M^{1/4}} \right) \right. \\ &\quad \left. + N^{-1} \langle \Phi_{N,M}(t), d\Gamma(1 - \Delta) \Phi_{N,M}(t) \rangle \right) \\ &\leq C_{t,\varepsilon} \left(\frac{1}{M^{1/2}} + \left(\frac{N^{3\beta/2+3\varepsilon/4+1/4}}{M} + \frac{N^{7\beta/4+\varepsilon/2-1/4}}{M^{1/4}} \right) + N^{\beta-1} \right). \end{aligned}$$

Taking $M = N^\alpha$ with $\beta < \alpha < 1 - \beta$ we obtain after optimizing over α

$$\begin{aligned} \|\Gamma_{\Psi_N(t)}^{(1)} - |u_N(t)\rangle \langle u_N(t)|\|_{\mathfrak{S}_1} &\leq \langle \Phi_N(t), \frac{\mathcal{N}}{N} \Phi_N(t) \rangle \\ &\leq C_{t,\varepsilon} \left(N^{-(3-10\beta)/4+\varepsilon} + N^{-(1-4\beta)/4+\varepsilon} \right), \end{aligned}$$

for any $\varepsilon > 0$ small enough.

Proof of 3)

Using that when $\widehat{w} \geq 0$ we have the bound $|e_N| \leq C(N + N^{3\beta})$, the same computation as before with $M = N^{-(1-\beta)/2}$ and assuming $1/6 < \beta < 1/5$ shows that

$$\|\Phi_N(t) - \Phi(t)\|_{L^2(\mathbb{R}^{3N})} \leq C_{t,\varepsilon} N^{-(1-5\beta)/4+\varepsilon},$$

for any $\varepsilon > 0$ small enough. Now take $M = N^\alpha$ with $\beta < \alpha < 1 - \beta$, with the same computation as before, after optimizing over α , we obtain

$$\begin{aligned} \|\Gamma_{\Psi_N(t)}^{(1)} - |u_N(t)\rangle \langle u_N(t)|\|_{\mathfrak{S}_1} &\leq \langle \Phi_N(t), \frac{\mathcal{N}}{N} \Phi_N(t) \rangle \\ &\leq C_{t,\varepsilon} \left(N^{-(1-\beta)/2+\varepsilon} + N^{-(2-5\beta)/2+\varepsilon} + N^{-(3-8\beta)/4+\varepsilon} \right), \end{aligned}$$

for any $\varepsilon > 0$. □

Chapitre 3

Existence of minimizers in generalized Gross-Pitaevskii theory with the Lee-Huang-Yang correction

Ce chapitre reprend l'intégralité de l'article dont le préprint est accessible en ligne sur arXiv / Hal.

Abstract

We study the dipolar Gross-Pitaevskii functional with the Lee-Huang-Yang (LHY) correction term without trapping potential and in the regime where the dipole-dipole interaction dominates the repulsive short-range interaction. We show that, above a critical mass, the functional admits minimizers and we prove their regularity and exponential decay. We also estimate the critical mass in terms of the parameters of the system.

Résumé

Nous étudions la fonctionnelle de Gross-Pitaevskii dipolaire avec correction de Lee-Huang-Yang (LHY) sans confinement et dans le régime où l'interaction dipole-dipole domine l'interaction courte portée répulsive. Nous montrons qu'il existe une masse critique au dessus de laquelle la fonctionnelle admet des minimiseurs et nous montrons qu'ils sont réguliers et décroissent exponentiellement. Nous donnons aussi une estimée de la masse critique en fonction des paramètres du système.

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Recent progress in the realization of Bose-Einstein condensates (BEC) of *dipolar* atoms have exhibited new and complex phenomena as compared with simpler chemical elements [KSWW+16; FKSWP16; CBPM+16; SWBFP16; CBPF+18]. For a survey on the properties of dipolar BEC, see [LMSLP09]. This specificity is due to the long-range nature of the dipolar interaction, which persists in the dilute regime, as opposed to short-range ones which become delta like. The resulting model thus contains two competing interactions, one partly attractive and anisotropic, another one repulsive. The system is stable when the repulsive term compensates the attractiveness of the dipole-dipole interaction (DDI), or when the trapping potential is strongly confining in some well-chosen directions. Otherwise, the condensate experiences collapse and blow up, a phenomenon known as Bose-nova [SSZL00; KLMFGP08; LMFK+08]. Nevertheless, new experiments have revealed that when the scattering length, which controls the scattering length of the repulsive interaction, is lowered sufficiently slowly, the condensate remains in a meta-stable state leading to the formation of stable self-bounded droplets [KSWW+16; FKSWP16; CBPM+16; SWBFP16]. The stabilization mechanism is believed to be caused by the Lee-Huang-Yang corrections [LHY57; Pet15] and is accounted for in the Gross-Pitaevskii framework by a term proportional to $|\psi|^5$ where ψ is the wave function of the condensate. The LHY correction for dipolar gases has been computed in [SUXF06; LP11; LP12]. The phenomenon has also been numerically investigated in [BWBB16b; BWBB16a; WS16]. The generalized Gross-Pitaevskii functional used in the physics literature [WS16; BWBB16a; SWBFP16] is given by the following

$$\mathcal{E}_{\text{dip}}^{GP}(\psi) = \int_{\mathbb{R}^3} |\nabla\psi|^2 + \frac{a_s}{2} \int_{\mathbb{R}^3} |\psi|^4 + \frac{a_{\text{dd}}}{2} \int_{\mathbb{R}^3} K \star |\psi|^2 |\psi|^2 + \frac{2}{5} \gamma_{\text{QF}} \int_{\mathbb{R}^3} |\psi|^5, \quad (1)$$

where $\psi \in H^1(\mathbb{R}^3)$ is normalized as

$$\int_{\mathbb{R}^3} |\psi|^2 = N, \quad (2)$$

with N the number of atoms. The parameter a_s is proportional to the scattering length, the parameter a_{dd} is proportional to the square of the moment of the dipoles and we will always assume $a_{\text{dd}} > 0$. Finally, the coefficient $\gamma_{\text{QF}} > 0$ in front of the LHY corrections physically depends on a_s and a_{dd} but we take it independent of them for the analysis. The acronym QF stands for quantum fluctuation which is the term used in the physics literature to refer to the cause of the LHY corrections. For a dipolar Bose gas, we have $K = K_{\text{dip}}$ with

$$K_{\text{dip}}(x) = \frac{3}{4\pi} \frac{1 - 3 \cos^2(\theta_x)}{|x|^3} =: \frac{\Omega_{\text{dip}}(x/|x|)}{|x|^3},$$

where $\cos(\theta_x) = n \cdot x/|x|$ and where n is a fixed unit vector aligned with all the dipoles. Here we consider a general long-range interaction of the form

$$K(x) = \frac{\Omega(x/|x|)}{|x|^3} \quad \text{with} \quad \int_{\mathbb{S}^2} \Omega(y) d\sigma(y) = 0, \quad (3)$$

where Ω is an even continuous function on the sphere \mathbb{S}^2 and σ is the Haar measure on the sphere. These are the most important properties to keep.

Solitary waves are solutions of the following Gross-Pitaevskii equation

$$-\Delta\psi + a_s |\psi|^2 \psi + a_{\text{dd}} K \star |\psi|^2 \psi + \gamma_{\text{QF}} |\psi|^3 \psi = \mu \psi, \quad (4)$$

for some chemical potential $\mu \in \mathbb{R}$. They can be obtained by looking at critical points of $\mathcal{E}_{\text{dip}}^{GP}$ restricted to the unit sphere in $L^2(\mathbb{R}^3)$. Of course, the easiest way to find critical points is to

minimize the functional and look for the ground state.

Without the LHY correction ($\gamma_{\text{QF}} = 0$) and with a trapping potential V_{ext} , the functional $\mathcal{E}_{\text{dip}}^{GP}$ has been extensively studied [BCW10; AS11; BAC12; CMS08; CH15b]. A necessary and sufficient condition for $\mathcal{E}_{\text{dip}}^{GP}$ to be bounded below on the unit sphere of $L^2(\mathbb{R}^3)$ is, in our units, $a_s \geq a_{\text{dd}}$. This comes from the fact that the kinetic energy term and the interaction term do not have the same scaling properties with respect to dilations. Adding the (positive) LHY term allows to prevent the collapse and to access the previously unstable regime $a_s < a_{\text{dd}}$. Without confining potential, a necessary condition for the minimizing sequences of $\mathcal{E}_{\text{dip}}^{GP}$ to be pre-compact is the negativity of the ground state energy, as we will prove. But because of the stabilization mechanism itself, this condition does not hold for all possible choices of parameters $a_s, a_{\text{dd}}, \gamma_{\text{QF}}$ and N . The case $\gamma_{\text{QF}} < 0$ was analyzed in [LS18] where the authors find solutions to (4) by means of mountain pass arguments.

In this paper, we study the existence and non existence of the minimizers of (1) as well as their regularity. Our main result is Theorem 1 in which we show that the minimum energy is decreasing in N and that there is some critical mass $N_c(a_s, a_{\text{dd}}, \gamma_{\text{QF}})$ below which it is zero and there is no ground state and above which it is negative and there is at least one ground state. We also derive some upper and lower bounds on N_c .

During the preparation of this work a similar result was announced [LS19] in which the authors study the existence of standing waves for the dipolar Gross-Pitaevskii functional with the LHY non-linearity replaced by $|\psi|^p$ for $p \in (4, 6]$. However, the case of a general long-range interaction given by (3) is not dealt with and does not seem to follow from their proof. Their approach uses the particular symmetry of the dipole-dipole potential which allows to reformulate the interaction energy as the sum of a local term and another term involving the Riesz transform.

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1 Main results

We first rescale the functional to get rid of redundant parameters. For $\lambda > 0$ and $\psi \in H^1(\mathbb{R}^3)$ such that $\int_{\mathbb{R}^3} |\psi|^2 = \lambda$, we denote $\psi_{\alpha, \ell} = \alpha^{1/2} \ell^{3/2} \psi(\ell \cdot)$ and compute

$$\mathcal{E}_{\text{dip}}^{GP}(\psi_{\alpha, \ell}) = \alpha \ell^2 \left(\int_{\mathbb{R}^3} |\nabla \psi|^2 + \frac{a_s \alpha \ell}{2} \int_{\mathbb{R}^3} |\psi|^4 + \frac{a_{\text{dd}} \alpha \ell}{2} \int_{\mathbb{R}^3} K \star |\psi|^2 |\psi|^2 + \frac{2}{5} \gamma_{\text{QF}} \alpha^{3/2} \ell^{5/2} \int_{\mathbb{R}^3} |\psi|^5 \right).$$

Note that $N = \alpha \lambda$. Taking $\alpha \ell a_s = 1$ and $\alpha^{3/2} \ell^{5/2} \gamma_{\text{QF}} = 1$, denoting $b = a_{\text{dd}}/a_s$ and dividing by $\alpha \ell^2$ we obtain

$$\mathcal{E}_b(\psi) := \int_{\mathbb{R}^3} |\nabla \psi|^2 + \frac{1}{2} \int_{\mathbb{R}^3} |\psi|^4 + \frac{b}{2} \int_{\mathbb{R}^3} K \star |\psi|^2 |\psi|^2 + \frac{2}{5} \int_{\mathbb{R}^3} |\psi|^5, \quad (5)$$

with the new constraint $\int_{\mathbb{R}^3} |\psi|^2 = \lambda$.

Recall that the third term with K has to be understood in the sense of the principal value, that is $K = \lim_{\varepsilon \rightarrow 0} \mathbb{1}_{|x| > \varepsilon} K$ in \mathcal{D}' . It is classical [Duo01] that when Ω is an even continuous function on the sphere \mathbb{S}^2 satisfying (3), then for $1 < p < \infty$ and any $f \in L^p(\mathbb{R}^3)$, the following limit exists for almost all $x \in \mathbb{R}^3$

$$K * f(x) := \lim_{\varepsilon \rightarrow 0} (\mathbb{1}_{|x| > \varepsilon} K) * f(x).$$

Moreover there exists some constant $C_p > 0$ such that for any $\varepsilon > 0$ and any $f \in L^p(\mathbb{R}^3)$ we have

$$\|(\mathbb{1}_{|x| > \varepsilon} K) * f\|_{L^p(\mathbb{R}^3)} \leq C_p \|f\|_{L^p(\mathbb{R}^3)}, \quad (6)$$

$$\|K * f\|_{L^p(\mathbb{R}^3)} \leq C_p \|f\|_{L^p(\mathbb{R}^3)}. \quad (7)$$

In particular, $\widehat{K} \in L^\infty(\mathbb{R}^3)$ and up to modifying the parameter b , we will assume that

$$\inf \widehat{K} = -1.$$

We now state our main result. We first need some notations and definitions. For $\lambda > 0$, $b > 1$, we denote by

$$E(\lambda, b) = \inf_{\int |\psi|^2 = \lambda} \mathcal{E}_b(\psi) \quad (8)$$

the ground state energy with mass constraint λ .

Theorem 1. *For any fixed $b > 1$, the function*

$$\lambda \in \mathbb{R}_+ \mapsto E(\lambda, b)$$

is non-increasing and there exists $0 < \lambda_c(b) < \infty$ such that the following holds

- *for $0 < \lambda < \lambda_c(b)$, we have $E(\lambda, b) = 0$ and there is no minimizer*
- *the function $\lambda \mapsto E(\lambda, b)$ is strictly decreasing on $[\lambda_c(b), +\infty)$. For every $\lambda \geq \lambda_c(b)$ it admits at least one minimizer. It solves the equation*

$$(-\Delta + |\psi|^2 + bK \star |\psi|^2 + |\psi|^3 - \mu) \psi = 0, \quad (9)$$

with $\mu < 0$. In addition, ψ is C^∞ and decays exponentially.

Finally we have

$$\frac{2^{1/2} 5^{1/2} 3\pi}{(b-1)^{5/2}} \leq \lambda_c(b), \quad (10)$$

and in the dipolar case (2) we have

$$\lambda_c(b) \leq 84.437 \frac{1}{(b-1)^{5/2}}. \quad (11)$$

It is an interesting problem to derive the exact asymptotics of $\lambda_c(b)$ as $b \rightarrow 1$ or as $b \rightarrow \infty$. The rest of the paper is dedicated to the proof of Theorem 1.

2 Proof of Theorem 1

When b is fixed, to simplify notations, we will simply denote by $E(\lambda)$ and \mathcal{E} respectively $E(\lambda, b)$ and \mathcal{E}_b .

2.1 Monotonicity of $\lambda \mapsto E(\lambda, b)$

Let $b > 1$ and show that $\lambda \mapsto E(\lambda)$ is non-increasing. It suffices to prove that for all $\lambda_1, \lambda_2 \geq 0$,

$$E(\lambda_1 + \lambda_2) \leq E(\lambda_1) + E(\lambda_2). \quad (12)$$

and that $E \leq 0$. By density we can take $\psi^{(i)}$, for $i \in \{1, 2\}$, with compact support and such that $\mathcal{E}(\psi^{(i)}) \leq E(\lambda_i) + \varepsilon$, for some $\varepsilon > 0$. We then obtain

$$\begin{aligned} E(\lambda_1 + \lambda_2) &\leq \limsup_{t \rightarrow \infty} \mathcal{E}(\psi^{(1)} + \psi^{(2)}(\cdot - te_1)) = \mathcal{E}(\psi^{(1)}) + \mathcal{E}(\psi^{(2)}) \\ &\leq E(\lambda_1) + E(\lambda_2) + 2\varepsilon, \end{aligned}$$

where $e_1 = (1, 0, 0)$. It remains to take ε to zero to obtain (12). To show that $E(\lambda) \leq 0$ for all $\lambda \geq 0$, we take $\varphi \in C^\infty(\mathbb{R}^3)$ with compact support and such that $\int_{\mathbb{R}^3} |\varphi|^2 = \lambda$, we denote $\varphi_n(x) = n^{-3/2} \varphi(n^{-1}(x - n^2))$ for $n \geq 1$. We have $\int_{\mathbb{R}^3} |\nabla \varphi_n|^2 = n^{-2} \int_{\mathbb{R}^3} |\nabla \varphi|^2$ and $\|\varphi_n\|_{L^p(\mathbb{R}^3)} = n^{3(1/p-1/2)} \|\varphi\|_{L^p(\mathbb{R}^3)}$ for $p \geq 1$. Using (7) with $p = 4$ for the interaction term and $p = 5$ for the LHY term, we obtain $\mathcal{E}(\varphi_n) \rightarrow 0$ as $n \rightarrow \infty$.

2.2 $0 < \lambda_c(b) < \infty$

To prove that $\lambda_c(b) > 0$ it suffices to show the lower bound (10). Let $\psi \in H^1(\mathbb{R}^3)$. By Hölder's inequality we have

$$\begin{aligned} \|\psi\|_{L^6(\mathbb{R}^3)}^2 &\geq \|\psi\|_{L^2(\mathbb{R}^3)}^{-2/9} \|\psi\|_{L^5(\mathbb{R}^3)}^{20/9}, \\ -\|\psi\|_{L^4(\mathbb{R}^3)}^4 &\geq -\|\psi\|_{L^2(\mathbb{R}^3)}^{2/3} \|\psi\|_{L^5(\mathbb{R}^3)}^{10/3}. \end{aligned}$$

On the other hand

$$\int_{\mathbb{R}^3} K * |\psi|^2 |\psi|^2 = \int_{\mathbb{R}^3} \widehat{K} \left| \widehat{|\psi|^2} \right|^2 \geq - \int_{\mathbb{R}^3} |\psi|^4.$$

since we have, by assumption, $\inf \widehat{K} = -1$. Denoting $\lambda = \|\psi\|_{L^2(\mathbb{R}^3)}^2$ and $X = \|\psi\|_{L^5(\mathbb{R}^3)}^5$, we can then bound by below the Gross-Pitaevskii energy in the following way

$$\mathcal{E}(\psi) \geq C_{\text{Sob}} \lambda^{-1/9} X^{4/9} - \frac{b-1}{2} \lambda^{1/3} X^{2/3} + \frac{2}{5} X =: F_1(\lambda, X),$$

where $C_{\text{Sob}} = 3(2\pi)^{2/3}/4$ is the optimal constant in Sobolev's inequality [LL01]. We want to compute

$$\lambda_0 = \sup \{ \lambda > 0 \mid F_1(\lambda, X) \geq 0, \forall X \geq 0 \}.$$

By the form of F_1 , there is a unique such λ_0 , and there is some $X_0 > 0$ such that the following system holds

$$\begin{cases} F_1(\lambda_0, X_0) &= 0, \\ (\partial_X F_1)(\lambda_0, X_0) &= 0. \end{cases}$$

Solving this, we obtain

$$\lambda_0 = \left(\frac{5}{3}\right)^{1/2} 2^{5/2} \frac{C_{\text{Sob}}^{3/2}}{(b-1)^{5/2}} = \frac{2^{1/2} 5^{1/2} 3\pi}{(b-1)^{5/2}}.$$

To prove that $\lambda_c(b) < \infty$, let us take $\psi \in H^1(\mathbb{R}^3)$ such that $\int_{\mathbb{R}^3} |\psi|^2 = 1$ and

$$\int_{\mathbb{R}^3} |\psi|^4 + bK * |\psi|^2 |\psi|^2 < 0$$

which is possible because $b > 1$, see the proof of [Tri18, Theorem 1]. With $\psi_{\lambda,\ell} = \lambda^{1/2} \ell^{3/2} \psi(\ell \cdot)$, we have

$$\mathcal{E}(\psi_{\lambda,\ell}) = \lambda \ell^2 \left(\int_{\mathbb{R}^3} |\nabla \psi|^2 + \frac{\lambda \ell}{2} \left(\int_{\mathbb{R}^3} |\psi|^4 + \frac{b}{2} \int_{\mathbb{R}^3} K * |\psi|^2 |\psi|^2 \right) + \frac{2}{5} \alpha^{3/2} \ell^{5/2} \int_{\mathbb{R}^3} |\psi|^5 \right),$$

taking $\lambda \rightarrow \infty$ and $\ell = \lambda^{-1/2}$, we obtain $\mathcal{E}(\psi_{\lambda,\ell}) \rightarrow -\infty$, which proves that $\lambda_c(b) < \infty$ since $E(\lambda)$ cannot stay equal to 0 on \mathbb{R}_+ .

2.3 Properties of solutions to (9)

If ψ is a stationary point of the functional \mathcal{E} under the mass constraint λ , it solves the Euler-Lagrange equation (9) for some Lagrange multiplier μ . We begin by showing some relations between μ, λ and the different terms in $\mathcal{E}(\psi)$. We define

$$\begin{aligned} T(\psi) &= \int |\nabla \psi|^2 > 0, \\ I(\psi) &= \frac{a_s}{2} \int |\psi|^4 + \frac{a_{\text{dd}}}{2} \int K * |\psi|^2 |\psi|^2, \\ Q(\psi) &= \frac{2}{5} \gamma \int |\psi|^5 > 0. \end{aligned}$$

When there is no ambiguity, we will simply denote them by T, I and Q .

Lemma 2. *Let $\lambda > 0$, $b > 1$ and let ψ be solution to (9) with $\int_{\mathbb{R}^3} |\psi|^2 = \lambda$. Let μ be the associated Lagrange multiplier in (9), then following equalities hold:*

$$T = \frac{3}{2} (E - \mu\lambda), \tag{13}$$

$$I = \frac{E + 5\lambda\mu}{2}, \tag{14}$$

$$Q = -(\mu\lambda + E). \tag{15}$$

In particular, if $E \leq 0$ then $\mu < 0$.

Proof. We have

$$T + I + Q = E(\lambda), \tag{16}$$

$$I + \frac{3}{2}Q = -E(\lambda) + \mu\lambda, \tag{17}$$

$$2T + 3I + \frac{9}{2}Q = 0. \tag{18}$$

The equation (16) is simply the definition of \mathcal{E} . Equation (17) is obtained by integrating the Euler-Lagrange equation (9) against the solution ψ . Finally, (18) is a consequence of the virial theorem: for $\alpha > 0$ we denote $\psi_\alpha = \alpha^{3/2}\psi(\alpha\cdot)$ and since the function $\alpha \mapsto \mathcal{E}(\psi_\alpha)$ is stationary at $\alpha = 1$, its derivative vanishes, this gives (18) (we can also obtain (18) by multiplying (9) by $x \cdot \nabla \psi$). It remains to solve the linear system (16),(17),(18) which gives the result. The negativity of μ comes from (13), indeed we have $\lambda\mu = E - 2T/3 < 0$, if $E \leq 0$. \square

We then state some lemma about the regularity of the solutions of the Euler-Lagrange equation (9). We give its proof in Appendix A.

Lemma 3. *Let $\psi \in H^1(\mathbb{R}^3)$ be a solution of the Euler-Lagrange equation (9) for some $\mu < 0$. Then $\psi \in C^\infty(\mathbb{R}^3)$ and there exists some constants $C, t > 0$ such that for all $x \in \mathbb{R}^3$*

$$0 < |\psi(x)| \leq Ce^{-t|x|}.$$

2.4 Existence of a minimizer, case $\lambda > \lambda_c$

We begin with the case $\lambda > \lambda_c(b)$. We use the concentration-compactness method [Lio84a; Lio84b; Lie83]. In particular, we follow [Lew10] and use the following lemma.

Lemma 4. *Let $\{\psi_n\}$ be any bounded sequence in $H^1(\mathbb{R}^3)$, define*

$$\mathbf{m}(\{\psi_n\}) = \sup \left\{ \int |\psi|^2 \mid \exists \{x_{n_k}\} \subset \mathbb{R}^3, \psi_{n_k}(\cdot - x_{n_k}) \rightharpoonup \psi \text{ weakly in } H^1(\mathbb{R}^3) \right\}.$$

Then the following assertions are equivalent

- $\mathbf{m}(\{\psi_n\}) = 0$
- $\psi_n \rightarrow 0$ strongly in $L^p(\mathbb{R}^3)$ for all $2 < p < 6$.

We can now show that minimizing sequences are precompact in $H^1(\mathbb{R}^3)$. Let $\{\psi_n\} \subset H^1(\mathbb{R}^3)$, $\int_{\mathbb{R}^3} |\psi_n|^2 = \lambda$, with $\lambda > \lambda_c(b)$ so that $E(\lambda) < 0$, be a minimizing sequence for \mathcal{E} . By (7) we verify that $\{\psi_n\}$ is bounded in $H^1(\mathbb{R}^3)$ so that we can apply the above lemma. If $\mathbf{m}(\{\psi_n\}) = 0$ then it follows that $\mathcal{E}(\psi_n) \rightarrow 0$ which contradicts $E(\lambda) < 0$. We can therefore find $Q_1 \in H^1(\mathbb{R}^3)$, $Q_1 \neq 0$, such that, up to translations, $\psi_n \rightharpoonup Q_1$ weakly in $H^1(\mathbb{R}^3)$. We denote

$$\psi_n = Q_1 + r_n, \quad r_n \rightharpoonup 0 \quad \text{in } H^1(\mathbb{R}^3).$$

Because of the weak convergence in $H^1(\mathbb{R}^3)$, we have

$$\int_{\mathbb{R}^3} |\nabla \psi_n|^2 = \int_{\mathbb{R}^3} |\nabla Q_1|^2 + \int_{\mathbb{R}^3} |\nabla r_n|^2 + o(1).$$

Moreover, up to extracting a subsequence, we can assume strong local convergence in $L^2(\mathbb{R}^3)$ and convergence. By [LL01, Theorem 1.9], we obtain

$$\lim_{n \rightarrow \infty} \int_{\mathbb{R}^3} |\psi_n|^p - |r_n|^p = \int_{\mathbb{R}^3} |Q_1|^p,$$

for all $2 \leq p \leq 6$. To deal with the non-local term, we note that $\|r_n Q_1\|_{L^2(\mathbb{R}^3)} \rightarrow 0$ as $n \rightarrow \infty$ since $r_n^2 \rightharpoonup 0$ in $L^2(\mathbb{R}^3)$. Hence by (7) we conclude that

$$\int_{\mathbb{R}^3} K * |\psi_n|^2 |\psi_n|^2 = \int_{\mathbb{R}^3} K * |Q_1|^2 |Q_1|^2 + \int_{\mathbb{R}^3} K * |r_n|^2 |r_n|^2 + o(1).$$

Denoting $\lambda_1 = \|Q_1\|_{L^2(\mathbb{R}^3)}^2$ and $\tilde{r}_n = (\lambda - \lambda_1)r_n/\|r_n\|_{L^2(\mathbb{R}^3)}$, so that $\|\tilde{r}_n - r_n\|_{H^1(\mathbb{R}^3)} \rightarrow 0$, we obtain from the previous estimates

$$\begin{aligned}\mathcal{E}(\psi_n) &= \mathcal{E}(Q_1) + \mathcal{E}(\tilde{r}_n) + o(1) \\ &\geq \mathcal{E}(Q_1) + E(\lambda - \lambda_1) + o(1),\end{aligned}\tag{19}$$

where we used that \mathcal{E} is locally uniformly continuous in $H^1(\mathbb{R}^3)$. From this we obtain that $E(\lambda) = E(\lambda_1) + E(\lambda - \lambda_1)$, that Q_1 is a minimizer of \mathcal{E} for the mass constraint λ_1 and that $\{\tilde{r}_n\}$ is a minimizing sequence for the mass constraint $\lambda - \lambda_1$. If $\lambda_1 = \lambda$ the result is proved since $E(0) = 0$. Let us then assume $\lambda_1 < \lambda$, in this case one must have $\mathbf{m}(\{\tilde{r}_n^{(2)}\}) > 0$, otherwise we obtain by Lemma 4 that $\liminf \mathcal{E}(\tilde{r}_n) \geq 0$ and from (19) that $E(\lambda) = E(\lambda_1)$, since E is non-increasing. But Q_1 is a minimizer of \mathcal{E} and therefore satisfies (9) with some $\mu < 0$ by Lemma 2. Hence for any $\varepsilon > 0$ small enough we have

$$\mathcal{E}((1 + \varepsilon)Q_1) = \mathcal{E}(Q_1) + 2\mu\lambda_1\varepsilon + o(\varepsilon) < \mathcal{E}(Q_1),\tag{20}$$

since $\mu < 0$. For $\varepsilon > 0$ small enough we thus obtain $E(\lambda) \leq E(\lambda_1 + \varepsilon) < E(\lambda_1)$ which contradicts $E(\lambda) = E(\lambda_1)$, hence $\mathbf{m}(\{\tilde{r}_n^{(2)}\}) > 0$. Doing the same procedure for \tilde{r}_n as we did with ψ_n we obtain

$$\tilde{r}_n = Q_2 + q_n, \quad q_n \rightarrow 0 \quad \text{in} \quad H^1(\mathbb{R}^3),$$

and we denote $\lambda_2 = \int_{\mathbb{R}^3} |Q_2|^2$. From (19), the same computations as before lead to

$$E(\lambda) \leq E(\lambda_1) + E(\lambda_2) + E(\lambda - \lambda_1 - \lambda_2),$$

and $\mathcal{E}(Q_2) = E(\lambda_2)$. From this and (12) we deduce that

$$E(\lambda_1 + \lambda_2) = E(\lambda_1) + E(\lambda_2),\tag{21}$$

which we will prove cannot hold. Since $(Q_i)_{i \in \{1,2\}}$ are minimizers, they satisfy the Euler-Lagrange equation (9) and by Lemma 3 they are C^∞ and have exponential decay. Let us write $Q_i = Q_i\chi(\cdot/R) + Q_i(1 - \chi(\cdot/R)) = Q_{(i,1)} + Q_{(i,2)}$ for some $\chi \in C_c^\infty(\mathbb{R}^3)$ with $\chi \equiv 1$ in $B(0, 1)$ and $\chi \equiv 0$ in $\mathbb{R}^3 \setminus B(0, 2)$. We have $\|Q_{(i,2)}\|_{L^p(\mathbb{R}^3)} \leq Ce^{-tR}$, for $2 \leq p \leq 6$, for some constants $C, t > 0$. Taking $u \in \mathbb{S}^2$, we define

$$\psi_R = Q_1 + Q_2(\cdot - R^2u).$$

Since $\|\psi_R\|_{L^2(\mathbb{R}^3)} \rightarrow \lambda_1 + \lambda_2$ when $R \rightarrow \infty$ we can write $\psi_R = \tilde{\psi}_R + \psi_R\tilde{\psi}_R$ with $\|\tilde{\psi}_R\|_{L^2(\mathbb{R}^3)} = \lambda_1 + \lambda_2$ and $\|\psi_R - \tilde{\psi}_R\|_{H^1(\mathbb{R}^3)} = \mathcal{O}(e^{-tR})$ when $R \rightarrow \infty$. We then have

$$\begin{aligned}\mathcal{E}(\psi_R) &= \mathcal{E}(\tilde{\psi}_R) + \mathcal{O}(e^{-tR}) \\ &= \mathcal{E}(Q_1) + \mathcal{E}(Q_2) + b \int_{\mathbb{R}^3} K \star Q_{1,1}^2 Q_{2,1}^2(\cdot - R^2u) + \mathcal{O}(e^{-tR}) + \mathcal{O}(e^{-tR^2}),\end{aligned}\tag{22}$$

as $R \rightarrow \infty$, where we used (7). We will now use the following lemma whose proof is postponed until the end of the argument.

Lemma 5. *Let $\varphi \in C^0(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$. Then for all $u \in \mathbb{S}^2$,*

$$\sup_{v \in B(0,R)} K \star (|\varphi|^2 \mathbf{1}_{B(0,R)})(R^2u + v) \leq \frac{\int_{\mathbb{R}^3} |\varphi|^2}{R^6} (\Omega(u) + o(1)),$$

as $R \rightarrow \infty$

We use the above lemma with u such that $\Omega(u) = \inf \Omega < 0$ and obtain

$$\int_{\mathbb{R}^3} K \star Q_{1,1}^2 Q_{2,1}^2 (\cdot - R^2 u) \leq \frac{1}{R^6} \int_{\mathbb{R}^3} Q_{1,1}^2 \int_{\mathbb{R}^3} Q_{2,1}^2 (\inf \Omega + o(1)).$$

Using this in (22) gives

$$\begin{aligned} E(\lambda_1 + \lambda_2) &\leq \mathcal{E}(Q_1 + Q_2(\cdot - \alpha u)) \\ &\leq \mathcal{E}(Q_1) + \mathcal{E}(Q_2) + \lambda_1 \lambda_2 \frac{\inf \Omega}{R^6} + \mathcal{O}(e^{-tR}) \\ &\leq E(\lambda_1) + E(\lambda_2) + \lambda_1 \lambda_2 \frac{\inf \Omega}{R^6} + \mathcal{O}(e^{-tR}) \\ &< E(\lambda_1) + E(\lambda_2), \end{aligned}$$

which contradicts (21).

We conclude that $\lambda_2 = 0$ and that there exists $\{x_n\} \subset \mathbb{R}^3$ such that $\{\psi_n(\cdot - x_n)\}$ is relatively compact in $L^p(\mathbb{R}^3)$ for $p \in [2, 6)$. We can obtain a minimizer by extracting a converging subsequence. By a classical argument we indeed have strong convergence in $H^1(\mathbb{R}^3)$ [Lio84a].

Proof of Lemma 5. We extend the function Ω to the whole of \mathbb{R}^3 by $\Omega(x) = \Omega(x/|x|)$. Let ω be the modulus of uniform continuity of Ω in $B(0, 2) \setminus B(0, 1/2)$. For $u \in \mathbb{S}^2$ we have

$$\begin{aligned} \alpha^3 \left| \int_{\mathbb{R}^3} \frac{\Omega(R^2 u + v - y)}{|R^2 u + v - y|^3} |\varphi(y)|^2 dy - \Omega(u) \frac{\int_{\mathbb{R}^3} |\varphi|^2}{R^6} \right| \\ \leq \left| \int_{B(0, R)} \frac{\Omega(u + (v - y)/R^2) - \Omega(u)}{|u + (v - y)/R^2|^3} |\varphi(y)|^2 dy \right| \\ \quad + \left| \int_{\mathbb{R}^3} \Omega(u) \left(\frac{1}{|u + (v - y)/R^2|^3} - 1 \right) |\varphi(y)|^2 dy \right| \\ \leq \left(\frac{\omega(2R^{-1})}{(1 - 2R^{-1})^3} + 2\|\Omega\|_{L^\infty(\mathbb{S}^2)} R^{-1} \frac{3}{(1 - 2R^{-1})^4} \right) \int_{\mathbb{R}^3} |\varphi|^2 \rightarrow 0, \end{aligned}$$

as $R \rightarrow \infty$, which concludes the proof. \square

2.5 Non-existence of minimizers for $0 < \lambda < \lambda_c$

Assume there is a solution Q to the minimization problem for $0 < \lambda < \lambda_c$, then by definition of $\lambda_c(b)$ we have $E(\lambda) = 0$. Moreover, Q satisfies the Euler-Lagrange equation (9) with some chemical potential $\mu < 0$. Then, the same computation as in (20) shows that $\lambda' \mapsto E(\lambda', b)$ is decreasing in a neighborhood of λ contradicting the fact that $\lambda < \lambda_c$.

2.6 Existence of minimizer, for $\lambda = \lambda_c$

For the existence in the case $\lambda = \lambda_c$, we take a sequence $\lambda_n \rightarrow \lambda$ as $n \rightarrow \infty$ with $\lambda_n > \lambda$ for all $n \geq 1$ and consider minimizers for the problem with mass constraint λ_n : for all $n \geq 1$ we take some $\psi_n \in H^1(\mathbb{R}^3)$ with $\int_{\mathbb{R}^3} |\psi_n|^2 = \lambda_n$ and $\mathcal{E}(\psi_n) = E(\lambda_n, b)$. For all n , ψ_n verifies the Euler-Lagrange equation (9) for some $\mu_n < 0$. We will use Lemma 4, assume first that

$\mathbf{m}(\{\psi_n\}) = 0$, then, with the notations of Lemma 2, $I(\psi_n) \rightarrow 0$ and $Q(\psi_n) \rightarrow 0$ from which we deduce, by Lemma 2, that $T(\psi_n) \rightarrow 0$. But by the Sobolev inequality we have

$$|I(\psi_n)| \leq C \|\psi_n\|_{L^2(\mathbb{R}^3)} \|\nabla \psi_n\|_{L^2(\mathbb{R}^3)}^3 = C \lambda_n^{1/2} T(\psi_n)^{3/2},$$

hence $I(\psi_n) = o(T(\psi_n))$ and $\mathcal{E}(\psi_n) \geq 0$. This contradicts the fact that $E(\lambda_n, b) < 0$ for all n . This proves that $\mathbf{m}(\{\psi_n\}) > 0$, and we can show as before that there is some $\lambda_1 \leq \liminf\{\lambda_n\} = \lambda_c$ such that there is some solution Q_1 to the minimization problem with constraint λ_1 . But since there is no minimizer on $[0, \lambda_c)$, we necessarily have $\lambda_1 = \lambda_c$.

2.7 Upper bound on $\lambda_c(b)$ in the dipolar case

We now prove the upper bound (11) in the dipolar case. Following the computations done in [BWBB16b], we use a Gaussian ansatz. We take $n = e_z$ in the definition of K_{dip} . For $\lambda, \sigma_\rho, \sigma_z > 0$ define

$$\psi_{\sigma_\rho, \sigma_z}^\lambda = \sqrt{\frac{8\lambda}{\pi^{3/2}\sigma_\rho^2\sigma_z}} e^{-2\left(\frac{\rho^2}{\sigma_\rho^2} + \frac{z^2}{\sigma_z^2}\right)},$$

where (ρ, z) are the cylindrical coordinates. The normalization is such that $\|\psi_{\sigma_\rho, \sigma_z}^\lambda\|_{L^2(\mathbb{R}^3)}^2 = \lambda$. We have

$$\frac{\mathcal{E}(\psi_{\sigma_\rho, \sigma_z}^\lambda)}{2\lambda} = \frac{2}{\sigma_\rho^2} + \frac{1}{\sigma_z^2} - \frac{\lambda}{2^{1/2}\pi^{3/2}\sigma_\rho^2\sigma_z} \left(b f\left(\frac{\sigma_\rho}{\sigma_z}\right) - 1 \right) + \frac{2^6\lambda^{3/2}}{5^{5/2}\pi^{9/4}\sigma_\rho^3\sigma_z^{3/2}},$$

where [BWBB16b]

$$f(x) = \frac{1+2x^2}{1-x^2} - 3x^2 \frac{\tanh^{-1}(\sqrt{1-x^2})}{(1-x^2)^{3/2}}.$$

Denoting $\alpha = \sigma_\rho/\sigma_z$ and $Y = \sigma_\rho^{-2}$ we define

$$F_2(\lambda, Y, \alpha) = (2 + \alpha^2)Y - \lambda Y^{3/2} \frac{\alpha}{2^{1/2}\pi^{3/2}} (bf(\alpha) - 1) + \lambda^{3/2} Y^{9/4} \alpha^{3/2} \frac{2^6}{5^{5/2}\pi^{9/4}}.$$

We define

$$\lambda_1(\alpha) = \sup \{ \lambda > 0 \mid F_2(\lambda, Y, \alpha) \geq 0, \forall Y \geq 0 \}$$

which by the form of F_2 , exists, is unique and satisfies the following system

$$\begin{cases} F_2(\lambda_1(\alpha), Y_0, \alpha) = 0, \\ (\partial_Y F_2)(\lambda_1(\alpha), Y_0, \alpha) = 0, \end{cases}$$

for some $Y_0 > 0$. Solving this system gives

$$\lambda_1(\alpha) = \frac{\pi^{3/2} 2^{19/12}}{3^{3/2}} \frac{(2 + \alpha^2)^{3/2}}{\alpha (bf(\alpha) - 1)^{5/2}}.$$

Optimizing over α one can obtain numerically

$$\inf_{\alpha > 0} \lambda_1(\alpha) \leq 84.437 \frac{1}{(b-1)^{5/2}}.$$

Appendix A Proof of Lemma 3

Let ψ be a minimizer of \mathcal{E} for the mass constraint $\lambda > 0$. By convexity of the gradient [LL01, Theorem 7.8] we have $\mathcal{E}(\psi) \geq \mathcal{E}(|\psi|)$. Hence $|\psi|$ also minimizes \mathcal{E} and satisfies the Euler-Lagrange equation (9), therefore, without loss of generality we can assume $\psi \geq 0$.

Regularity and positivity Following the proof of [LSY00, Lemma A.5], for $t > 0$, we rewrite (9) as

$$(-\Delta + t^2)\psi = -(W - \mu - t^2)\psi, \quad (23)$$

with $W = (\psi^2 + bK \star \psi^2 + \psi^3)$. Solving the equation we find

$$\psi(x) := - \int_{\mathbb{R}^3} Y_t(x-y) (W(y) - \mu - t^2) \psi(y) dy, \quad (24)$$

where $Y_t(x) = (4\pi|x|)^{-1}e^{-t|x|}$ is the Yukawa potential. We want to prove that $-\Delta\psi \in L^2(\mathbb{R}^3)$, by the Euler-Lagrange equation it suffices to show that $\psi \in L^8(\mathbb{R}^3)$. But since $\psi \in H^1(\mathbb{R}^3)$ we have $W\psi \in L^2(\mathbb{R}^3)$ and deduce from the Euler-Lagrange equation that $-\Delta\psi \in L^2(\mathbb{R}^3)$. The usual bootstrapping argument and (7) give $\psi \in H^k(\mathbb{R}^3)$ for all $k \geq 1$ and hence $\psi \in C^\infty(\mathbb{R}^3)$.

In particular we have $-\Delta\psi \in L^\infty(\mathbb{R}^3)$, using that $\psi \geq 0$ and applying Harnack's inequality [GT15, Theorem 8.20] we deduce that if ψ vanishes then $\psi \equiv 0$ which is excluded by assumption ($\mathcal{E}(\psi) < 0$), hence $\psi > 0$.

Exponential decay Let $0 < t^2 < -\mu/2$. Before proving the exponential decay, we first need to show that $K \star |\psi|^2$ vanishes at infinity in the sense that

$$\forall \varepsilon > 0, \exists R_\varepsilon > 0 \text{ s.t. } \sup_{|x| > R_\varepsilon} \{K \star |\psi|^2(x)\} < \varepsilon. \quad (25)$$

Let $\varepsilon > 0$, by the cancellation property (3) we can write

$$\begin{aligned} |K \star \psi^2(x)| &= \left| \int_{\mathbb{R}^3} \frac{\Omega((x-y)/|x-y|)}{|x-y|^3} (\psi(y)^2 - \psi(x)^2) dy \right| \\ &\leq \int_{B(x,\varepsilon)} \frac{|\Omega((x-y)/|x-y|)|}{|x-y|^2} \|\psi\|_{L^\infty(\mathbb{R}^3)} \|\psi\|_{C^{0,\alpha}(\mathbb{R}^3)} + \int_{B(x,\varepsilon)^c} \frac{|\Omega((x-y)/|x-y|)|}{|x-y|^3} \psi(y)^2. \end{aligned}$$

Now using that $\Omega \in L^\infty(\mathbb{S}^2)$ and $\psi^2 \in L^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ we have for all $x \in B(0, R)$, for any $R > 0$,

$$|K \star \psi^2(x)| \leq C\varepsilon \|\Omega\|_{L^\infty(\mathbb{S}^2)} \|\psi\|_{L^\infty(\mathbb{R}^3)} \|\nabla\psi\|_{L^\infty(\mathbb{R}^3)} + \int_{B(x,\varepsilon)^c} \frac{|\Omega((x-y)/|x-y|)|}{|x-y|^3} \psi(y)^2.$$

Note that the second term above tends to zero at infinity at fixed ε because, for instance, $\mathbf{1}_{|x| > \varepsilon} |x|^{-3}, \psi^2 \in L^2(\mathbb{R}^3)$, this proves that $K \star |\psi|^2$ tends to zero at infinity. Hence W vanishes at ∞ and from (23) we deduce that

$$(-\Delta + t^2)(\psi - CY_t) \leq 0, \quad \text{in } B(0, R)^c,$$

for R large enough and $C > 0$. Since ψ is bounded, we can find $C > 0$ so that $\psi - CY_t \leq 0$ in $B(0, R)$ (and in particular on $\partial B(0, R)$), applying the maximum principle shows that $\psi \leq CY_t$, in the whole \mathbb{R}^3 and conclude the proof.

Deuxième partie

Limites semi-classiques de grands
systèmes fermioniques

Chapitre 4

Semi-classical limit of large fermionic systems at positive temperature

Ce chapitre est constitué d'une version étendue d'un article soumis, dont le préprint est disponible en ligne sur arXiv / Hal. Les travaux présentés ont été réalisés en collaboration avec Mathieu Lewin et Peter Madsen. Les appendices A, B et C ne sont pas présents dans l'article [LMT19]. L'Appendice A définit l'ensemble grand-canonique et donne une preuve de l'inégalité (28) sur l'entropie d'un état fermionique. Dans l'Appendice B on étudie la limite thermodynamique pour l'ensemble canonique avec une interaction en champ moyen et on montre l'équivalence avec l'ensemble grand-canonique. Finalement, dans l'Appendice C rappelle quelques définitions sur les états produits fermioniques.

Abstract

We study a system of N interacting fermions at positive temperature in a confining potential. In the regime where the intensity of the interaction scales as $1/N$ and with an effective semi-classical parameter $\hbar = N^{-1/d}$ where d is the space dimension, we prove the convergence to the corresponding Thomas-Fermi model at positive temperature.

Résumé

Nous étudions un système de N fermions en interaction à température positive dans un potentiel confinant. Nous considérons le régime où l'interaction est multipliée par $1/N$ et où le paramètre semi-classique vérifie $\hbar = N^{-1/d}$ avec d la dimension de l'espace. Nous montrons la convergence du système à N corps vers le modèle de Thomas-Fermi à température positive.

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In this article we study mean-field-type limits for a system of N fermions at temperature $T > 0$ in a fixed confining potential. We assume that the interaction has an intensity of the order $1/N$ and that there is an effective semi-classical parameter $\hbar = N^{-1/d}$ where d is the space dimension. In the limit $N \rightarrow \infty$ we obtain the nonlinear Thomas-Fermi problem at the same temperature $T > 0$. This paper is an extension of a recent work [FLS18] by Fournais, Solovej and the first author where the case $T = 0$ was solved.

Physically, the Thomas-Fermi model is a rather crude approximation of quantum many-body systems in normal conditions, and it has to be refined in order to obtain a quantitative description of their equilibrium properties. However, certain physical systems in extreme conditions are rather well described by Thomas-Fermi theory. It then becomes important to take into account the effect of the temperature. For instance, the positive-temperature Thomas-Fermi model has been thoroughly studied for very heavy atoms [FMT49; GP55; Lat55; CA57; NT81]. It has also played an important role in astrophysics, where the very high pressure encountered in the core of neutron stars and white dwarfs makes it valuable for all kinds of elements of the periodic table [MB40; Mar55; BBJL68; BB81]. Finally, the Thomas-Fermi model is also useful for ultracold dilute atomic Fermi gases, but the interaction often becomes negligible due to the Pauli principle, except in the presence of spin or of several interacting species [GPS08].

In the regime considered in this paper, a mean-field scaling is coupled to a semi-classical limit. This creates some mathematical difficulties. Before [FLS18], this limit has been rigorously considered at $T = 0$ for atoms by Lieb and Simon in [LS77b; LS77a] and for pseudo-relativistic stars by Lieb, Thirring and Yau in [LT84; LY87]. Upper and lower bounds on the next order correction have recently been derived in [HPR18; BNPSS18], for particles evolving on the torus. The positive temperature Thomas-Fermi model was derived for confined gravitational systems in [HT71; HNT72; Mes81b; Mes81a; Mes81c] and for atoms in [NT81]. There are several mathematical works on the time-dependent setting [NS81; Spo81; BGGM03; EESY04; AMS08; FK11; BPS14b; BPS14a; BJPSS16; BBPPT15; PP16; BPSS16; GMP16; GP17; DRS18], in which the Schrödinger dynamics has been proved to converge to the time-dependent Vlasov equation in the limit $N \rightarrow \infty$. Finally, the first two terms in the expansion of the (free) energy of a Fermi gas with spin in the limit $\rho \rightarrow 0$ was provided in [LSS05] at $T = 0$ and in [Sei06] at $T > 0$.

The mean-field limit at positive temperature for fermions is completely different from the bosonic case. It was proved in [LNR14] that in the similar mean-field regime for bosons, the leading order is the same at $T > 0$ as when $T = 0$. Only the next (Bogoliubov) correction depends on T [LNSS15]. In order to observe an effect of the temperature at the leading order of the bosonic free energy, one should take $T \sim N$, a completely different limit where nonlinear Gibbs measures arise [Got05; LNR15a; LNR18b; LNR18c; LNR18a; Rou15a]. Without statistics (boltzons), the temperature does affect the leading order of the energy [LNR15c], and the same happens for fermions, as we will demonstrate.

Our method for studying the Fermi gas in the coupled mean-field/semi-classical limit relies on techniques previously introduced in [FLS18]. Assuming that the interaction is positive-type ($\hat{w} \geq 0$), the lower bound follows from using coherent states and inequalities on the entropy. We discuss later in Remark 6 a conjectured inequality on the entropy of large fermionic systems which would imply the result for any interaction potential, not necessarily of positive-type. The upper bound is slightly more tedious. The idea is to construct a trial state with locally constant density in small boxes of side length much larger than \hbar , and to use the equivalence between the canonical and grand-canonical ensembles for the free Fermi gas. Finally, the convergence of states requires the tools recently introduced in [FLS18] based on the classical de Finetti theorem for fermions.

The article is organized as follows. In the next section we introduce both the N -particle quantum Hamiltonian and the positive-temperature Thomas-Fermi theory which is obtained in

the limit. We then state our main theorems, Theorem 2 and Theorem 8. As an intermediate result for the upper bound, we show in Section 2 how to approximate a classical density by an N body quantum state. In Section 3, we use this trial state and some known results about the free Fermi gas at positive temperature to prove our main result in the non-interacting case. The interacting case is dealt with in Section 4. Finally, in Section 5 we study the Gibbs state and the minimizers of the Thomas-Fermi functional at positive temperature (Theorem 1).

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1 Models and main results

1.1 The Vlasov and Thomas-Fermi functionals at $T > 0$

For a given density $\rho > 0$ and an inverse temperature $\beta > 0$, the Vlasov functional at positive temperature is given by

$$\begin{aligned} \mathcal{E}_{\text{Vla}}^{\beta, \rho}(m) &= \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} (|p + A(x)|^2 + V(x)) m(x, p) \, dx \, dp \\ &\quad + \frac{1}{2\rho} \iint_{\mathbb{R}^{2d}} w(x - y) \rho_m(x) \rho_m(y) \, dx \, dy \\ &\quad + \frac{1}{(2\pi)^d \beta} \iint_{\mathbb{R}^{2d}} s(m(x, p)) \, dx \, dp, \end{aligned} \tag{1}$$

where $s(t) = t \log t + (1 - t) \log(1 - t)$ is the fermionic entropy, and

$$\rho_m(x) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} m(x, p) \, dp$$

is the spatial density of particles. Here m is a positive measure on the phase space $\mathbb{R}^d \times \mathbb{R}^d$, with the convention

$$\frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} m(x, p) \, dx \, dp = \int_{\mathbb{R}^d} \rho_m(x) \, dx = \rho,$$

and which is assumed to satisfy Pauli's principle $0 \leq m \leq 1$. For convenience we have added the factor $1/\rho$ in front of the interaction energy, because it will naturally arise in the mean-field limit. This dependence of the Vlasov functional is emphasized by adding the index ρ on $\mathcal{E}_{\text{Vla}}^{\beta, \rho}$, this density coincides with the mass constraint we impose on the semi-classical measures even though it could be considered as independent. We denote the Vlasov minimum free energy by

$$\boxed{e_{\text{Vla}}^{\beta}(\rho) = \inf_{\substack{0 \leq m \leq 1 \\ (2\pi)^{-d} \iint_{\mathbb{R}^{2d}} m = \rho}} \mathcal{E}_{\text{Vla}}^{\beta, \rho}(m).} \tag{2}$$

Precise assumptions on A, V and w will be given later.

Similarly as in the case $T = 0$, we can rewrite the minimum as a two-step procedure where we first choose a density $\nu \in L^1(\mathbb{R}^d, \mathbb{R}_+)$ with $\int_{\mathbb{R}^d} \nu = \rho$ and minimize over all m such that $\rho_m = \nu$, before minimizing over ν . For any fixed constants $\nu \in \mathbb{R}_+$ and $A \in \mathbb{R}^d$ we can solve the problem at fixed x and obtain

$$\begin{aligned} \min_{\substack{0 \leq m(p) \leq 1 \\ (2\pi)^{-d} \int_{\mathbb{R}^d} m(p) dp = \nu}} & \left(\frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} |p + A|^2 m(p) dp + \frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^d} s(m(p)) dp \right) \\ & = -\frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^d} \log \left(1 + e^{-\beta(p^2 - \mu_{\text{FG}}(\beta, \nu))} \right) dp + \mu_{\text{FG}}(\beta, \nu) \nu \end{aligned}$$

where $\mu_{\text{FG}}(\beta, \nu)$ is the unique solution to the implicit equation

$$\frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{1}{1 + e^{\beta(p^2 - \mu_{\text{FG}}(\beta, \nu))}} dp = \nu$$

and with the unique corresponding minimizer

$$m_{\nu, A}(p) = \frac{1}{1 + e^{\beta(|p+A|^2 - \mu_{\text{FG}}(\beta, \nu))}}.$$

This is the uniform Fermi gas at density $\nu > 0$. For later purposes we introduce the free energy of the Fermi gas

$$F_\beta(\nu) := -\frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^d} \log \left(1 + e^{-\beta(p^2 - \mu_{\text{FG}}(\beta, \nu))} \right) dp + \mu_{\text{FG}}(\beta, \nu) \nu. \quad (3)$$

Note that A only appears in the formula of the minimizer. It does not affect the value of the minimum $F_\beta(\nu)$.

All this allows us to reformulate the Vlasov minimization problem using only the density, leading to the Thomas-Fermi type minimization problem

$$\begin{aligned} e_{\text{Vla}}^\beta(\rho) = \min_{\substack{\nu \in L^1(\mathbb{R}^d, \mathbb{R}_+) \\ \int_{\mathbb{R}^d} \nu(x) dx = \rho}} & \left\{ \int_{\mathbb{R}^d} F_\beta(\nu(x)) dx + \int_{\mathbb{R}^d} V(x) \nu(x) dx \right. \\ & \left. + \frac{1}{2\rho} \iint_{\mathbb{R}^{2d}} w(x-y) \nu(x) \nu(y) dx dy \right\}. \quad (4) \end{aligned}$$

The Vlasov minimization (2) on phase space will be more tractable and we will almost never use the Thomas-Fermi formulation (4) of the problem.

Now we discuss the existence of a unique Vlasov minimizer for (2), under appropriate assumptions on V, A, w . We use everywhere the notation $V_\pm = \max(\pm V, 0)$ for the positive and negative parts of V , which are both positive functions by definition.

Theorem 1 (Minimizers of the Vlasov functional). *Fix $\rho, \beta_0 > 0$. Suppose that $V_- \in L^{d/2}(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$, $A \in L^1_{\text{loc}}(\mathbb{R}^d)$ and that $V_+ \in L^1_{\text{loc}}(\mathbb{R}^d)$ satisfies $\int_{\mathbb{R}^d} e^{-\beta_0 V_+(x)} dx < \infty$. Let*

$$w \in L^{1+\frac{d}{2}}(\mathbb{R}^d) + L^\infty_\varepsilon(\mathbb{R}^d) + \mathbb{R}_+ \delta_0.$$

Then, for all $\beta > \beta_0$, there are minimizers for the Vlasov problem (2). Any minimizer m_0 solves

the nonlinear equation

$$m_0(x, p) = \frac{1}{1 + \exp\left(\beta(|p + A(x)|^2 + V(x) + \rho^{-1}w * \rho_{m_0}(x) - \mu)\right)}, \quad (5)$$

for some Lagrange multiplier μ . The minimum can be expressed in terms of m_0 and μ as

$$\begin{aligned} e_{\text{Vla}}^\beta(\rho) &= -\frac{1}{(2\pi)^d \beta} \iint_{\mathbb{R}^{2d}} \log\left(1 + e^{-\beta(|p|^2 + V(x) + \rho^{-1}w * \rho_{m_0}(x) - \mu)}\right) dx dp \\ &\quad + \mu\rho - \frac{1}{2\rho} \iint_{\mathbb{R}^{2d}} w(x-y) \rho_{m_0}(x) \rho_{m_0}(y) dx dy. \end{aligned} \quad (6)$$

Furthermore, if $\widehat{w} \geq 0$, then $\mathcal{E}_{\text{Vla}}^{\beta, \rho}$ is strictly convex and therefore has a unique minimizer. In this case, for $\rho' > 0$ define

$$F_{\text{Vla}}^\beta(\rho, \rho') := \inf_{\substack{0 \leq m \leq 1 \\ (2\pi)^{-d} \iint_{\mathbb{R}^{2d}} m = \rho}} \mathcal{E}_{\text{Vla}}^{\beta, \rho'}(m). \quad (7)$$

Then, for any $\rho' > 0$, $F_{\text{Vla}}^\beta(\cdot, \rho')$ is C^1 on \mathbb{R}_+ and the multiplier appearing in (5) is given by

$$\mu = \frac{\partial F_{\text{Vla}}^\beta}{\partial \rho}(\rho, \rho') \Big|_{\rho' = \rho}. \quad (8)$$

We recall that, for $p \geq 1$, $f \in L^p(\mathbb{R}^3) + L_\varepsilon^\infty(\mathbb{R}^3)$ if and only if for all $\varepsilon > 0$ we can write $f = f_1 + f_2$ with $f_1 \in L^p(\mathbb{R}^3)$ and $\|f_2\|_{L^\infty(\mathbb{R}^3)} \leq \varepsilon$. The proof of Theorem 1 is classical and given for completeness in Section 5. Note that the magnetic potential A has only a trivial effect on the minimization problem. The minimizers for a given A are exactly equal to the $m_0(x, p + A)$ with m_0 a minimizer for $A \equiv 0$. The value of the minimal energy, the density ρ_{m_0} and the Lagrange multiplier μ are unchanged under this transformation.

The two conditions $e^{-\beta V_+} \in L^1(\mathbb{R}^d)$ and $V_- \in L^{d/2}(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ have been chosen to ensure that the minimizer has a finite total mass and a finite total energy. This is because

$$\begin{aligned} &\iint_{\mathbb{R}^{2d}} \frac{1}{1 + e^{\beta(p^2 + V_+(x) - V_-(x))}} dx dp \\ &\leq \iint_{\mathbb{R}^{2d}} \left(e^{-\beta(p^2/2 + V_+(x))} + |\{p^2 \leq 2V_-(x)\}| \right) dx dp \\ &\leq C \int_{\mathbb{R}^d} \left(\beta^{-\frac{d}{2}} e^{-\beta V_+(x)} + V_-(x)^{\frac{d}{2}} \right) dx \end{aligned} \quad (9)$$

and, similarly,

$$\begin{aligned} &\iint_{\mathbb{R}^{2d}} \log\left(1 + e^{-\beta(p^2 + V_+(x) - V_-(x))}\right) dx dp \\ &\leq \iint_{\mathbb{R}^{2d}} e^{-\beta(p^2/2 + V_+(x))} dx dp + C \iint_{\{p^2 \leq 2V_-(x)\}} (1 + \beta V_-(x)) dx dp \\ &\leq C \int_{\mathbb{R}^d} \left(\beta^{-\frac{d}{2}} e^{-\beta V_+(x)} + V_-(x)^{\frac{d}{2}} + \beta V_-(x)^{1+\frac{d}{2}} \right) dx. \end{aligned}$$

1.2 The N -body Gibbs state and its limit

The mean-field limit

Here we analyze the ‘mean-field’ limit where the interaction has a fixed range and a small intensity. We consider the following Hamiltonian

$$H_{N,\hbar} = \sum_{j=1}^N |i\hbar\nabla_{x_j} + A(x_j)|^2 + V(x_j) + \frac{1}{N} \sum_{1 \leq j < k \leq N} w(x_j - x_k) \quad (10)$$

acting on the Hilbert space $\bigwedge_1^N L^2(\mathbb{R}^d)$ of anti-symmetric functions. For simplicity we neglect the spin variable. In the mean-field regime, which is dealt with by Theorem 2, it could be easily added. However, as previously mentioned, it would have non-trivial consequences for the (very) dilute regime covered by Theorem 8, where only particles with different spins interact. We suppose that

$$|A|^2, w \in L^{1+\frac{d}{2}}(\mathbb{R}^d) + L_\varepsilon^\infty(\mathbb{R}^d)$$

and that w is an even function. We also assume that the potential $V \in L_{\text{loc}}^{1+d/2}(\mathbb{R}^d)$ is confining, that is, $V(x) \rightarrow \infty$ when $|x| \rightarrow \infty$, and that the divergence is so fast that $\int e^{-\beta_0 V_+(x)} dx < \infty$ for some $\beta_0 > 0$. Note that this implies that V_- has a compact support, hence in particular $V_- \in L^{d/2}(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$. At inverse temperature $\beta > \beta_0$, the canonical free energy is given by the functional

$$\mathcal{E}_{\text{Can}}^{N,\hbar}(\Gamma) = \text{Tr}(H_{N,\hbar}\Gamma) + \frac{1}{\beta} \text{Tr}(\Gamma \log \Gamma), \quad (11)$$

defined for all fermionic quantum states $\Gamma = \Gamma^* \geq 0$ with $\text{Tr}(\Gamma) = 1$. The minimum over all Γ is uniquely attained at the Gibbs state

$$\Gamma_{N,\hbar,\beta} = Z^{-1} e^{-\beta H_{N,\hbar}},$$

where $Z = \text{Tr} e^{-\beta H_{N,\hbar}}$, which leads to the minimum free energy

$$e_{\text{Can}}^\beta(\hbar, N) := \min_{\Gamma} \mathcal{E}_{\text{Can}}^{N,\hbar}(\Gamma) = -\frac{1}{\beta} \log \text{Tr} e^{-\beta H_{N,\hbar}}.$$

Our main result is the following.

Theorem 2 (Mean-field limit). *Let $\beta_0, \rho > 0$. Assume that $V \in L_{\text{loc}}^{1+d/2}(\mathbb{R}^d)$ is such that $V(x) \rightarrow \infty$ at infinity and that $\int e^{-\beta_0 V_+(x)} dx < \infty$. Furthermore, assume $|A|^2, w \in L^{1+d/2}(\mathbb{R}^d) + L_\varepsilon^\infty(\mathbb{R}^d)$ with w even and satisfying $\widehat{w} \geq 0$. Then, for all $\beta > \beta_0$ we have the convergence*

$$\lim_{\substack{N \rightarrow \infty \\ \hbar^d N \rightarrow \rho}} \hbar^d e_{\text{Can}}^\beta(\hbar, N) = e_{\text{Vla}}^\beta(\rho). \quad (12)$$

Moreover, if (Γ_N) is a sequence of approximate Gibbs states, that is, satisfying

$$\mathcal{E}_{\text{Can}}^{N,\hbar}(\Gamma_N) = e_{\text{Can}}^\beta(\hbar, N) + o(1), \quad (13)$$

then the one-particle density of Γ_N satisfies the following convergence

$$\hbar^d \rho_{\Gamma_N}^{(1)} \rightharpoonup \rho_{m_0} \text{ weakly in } L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d),$$

and

$$m_{f,\Gamma_N}^{(1)} \longrightarrow m_0 \text{ strongly in } L^1(\mathbb{R}^{2d}), \quad (14)$$

$$\rho_{m_{f,\Gamma_N}^{(1)}} \longrightarrow \rho_{m_0} \text{ strongly in } L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d), \quad (15)$$

where $m_{f,\Gamma_N}^{(k)}$ is the k -particle Husimi function of Γ_N and m_0 is the unique minimizer of the Vlasov functional in Eq. (5). The k -particle Husimi functions converge weakly in the sense that

$$\int_{\mathbb{R}^{2dk}} m_{f,\Gamma_N}^{(k)} \varphi \rightarrow \int_{\mathbb{R}^{2dk}} m_0^{\otimes k} \varphi \quad (16)$$

for all $\varphi \in L^1(\mathbb{R}^{2dk}) + L^\infty(\mathbb{R}^{2dk})$. Similarly, if we denote by $\mathcal{W}_{\Gamma_N}^{(k)}$ the k -particle Wigner measure of Γ_N , we also have,

$$\int_{\mathbb{R}^{2dk}} \mathcal{W}_{\Gamma_N}^{(k)} \varphi \rightarrow \int_{\mathbb{R}^{2dk}} m_0^{\otimes k} \varphi, \quad (17)$$

for all φ satisfying $\partial_{x_1}^{\alpha_1} \dots \partial_{x_k}^{\alpha_k} \partial_{p_1}^{\beta_1} \dots \partial_{p_k}^{\beta_k} \varphi \in L^\infty(\mathbb{R}^{2dk})$, where $\alpha_j, \beta_j \leq 1$ for all $1 \leq j \leq k$.

We have denoted by $\rho_\Gamma^{(1)}$ the one-particle density of the state Γ , which is the unique function such that

$$\text{Tr} \left(\sum_{j=1}^N F(x_j) \right) \Gamma = \int_{\mathbb{R}^3} F(x) \rho_\Gamma^{(1)}(x) dx.$$

for all bounded functions $F \in L^\infty(\mathbb{R}^3)$.

The Husimi function $m_{f,\Gamma_N}^{(k)}$ (based on a given shape function f) and the Wigner measure $\mathcal{W}_{\Gamma_N}^{(k)}$ are defined and studied at length in [FLS18]. These are some natural semiclassical measures that can be associated with Γ_N in the k -particle phase space \mathbb{R}^{2dk} . We will recall their definition in the proof later in Section 4.3.

Remark 3. For simplicity we work with a confining potential V but Theorems 1 and 2 hold the same when \mathbb{R}^d is replaced by a bounded domain Ω with any boundary conditions.

Remark 4. Our lower bound relies on the strong assumption that $\widehat{w} \geq 0$, but the upper bound does not. It is classical that a positive Fourier transform allows to easily bound the interaction from below by a one-body potential, see Eq. (43) below.

Remark 5. As mentioned in (13), we can handle approximate Gibbs states with a free energy close to the minimum with an error $o(1)$, although the energy is itself of order N . Our proof actually applies to the one-particle Husimi function under the weaker condition that $\mathcal{E}_{\text{Can}}^{N,\hbar}(\Gamma_N) = e_{\text{Can}}^\beta(\hbar, N) + o(N)$ but our argument does not easily generalize to higher order Husimi functions. Of course, for the exact quantum Gibbs state we have equality $\mathcal{E}_{\text{Can}}^{N,\hbar}(\Gamma_{N,\hbar,\beta}) = e_{\text{Can}}^\beta(\hbar, N)$.

Remark 6. Without the assumption $\widehat{w} \geq 0$, the Vlasov functional $\mathcal{E}_{\text{Vla}}^{\beta,\rho}$ can have several minimizers and the limit in Eq. (16) is believed to be an average over the set of minimizers of $\mathcal{E}_{\text{Vla}}^{\beta,\rho}$. Namely there exists a so called de Finetti measure \mathcal{P} [FLS18], concentrated on the set \mathcal{M} of

minimizers for e_{Vla}^β , such that

$$m_{f, \Gamma_N}^{(k)} \rightharpoonup \int_{\mathcal{M}} m^{\otimes k} d\mathcal{P}(m),$$

in the sense defined in Theorem 2. We conjecture the following Fatou-type inequality on the entropy

$$\liminf_{\substack{N \rightarrow \infty \\ \hbar^d N \rightarrow \rho}} \hbar^d \text{Tr } \Gamma_N \log \Gamma_N \geq \int_{\mathcal{M}} \left(\int_{\mathbb{R}^{2d}} s(m) \right) d\mathcal{P}(m) \quad (18)$$

for general sequences (Γ_N) with de Finetti measure \mathcal{P} . Should this inequality be true, we could remove the assumption $\widehat{w} \geq 0$ in Theorem 2. In fact, in our proof we show that the above inequality holds when the right-hand side is replaced by

$$\int_{\mathbb{R}^{2d}} s \left(\int_{\mathcal{M}} m d\mathcal{P}(m) \right).$$

When there is a unique minimizer, the two coincide.

A completely different route for handling non positive-definite potentials would be to extend the method in [HT71; HNT72] where the (attractive) Newton potential was covered, using an approximation by a finite sum of rank-one interactions.

Example 7 (Large atoms in a strong harmonic potential). The Hamiltonian in Eq. (10) can describe a large atom in a strong harmonic potential. Indeed, consider N electrons in a harmonic trap and interacting with a nucleus of charge Z . In the Born-Oppenheimer approximation, the N electrons are described by the Hamiltonian

$$\sum_{j=1}^N -\Delta_{x_j} + \omega^2 |x_j|^2 - \frac{Z}{|x_j|} + \sum_{j < k} \frac{1}{|x_j - x_k|}.$$

Scaling length in the manner $x_j = N^{-1/3} x'_j$ we see that this Hamiltonian is unitarily equivalent to

$$N^{4/3} \left(\sum_{j=1}^N -N^{-\frac{2}{3}} \Delta_{x_j} + (\omega N^{-1})^2 |x_j|^2 - \frac{ZN^{-1}}{|x_j|} + \frac{1}{N} \sum_{j < k} \frac{1}{|x_j - x_k|} \right).$$

Hence taking Z proportional to N and ω proportional to N , we obtain the Hamiltonian of Eq. (10) with $d = 3$, $A = 0$, $V(x) = |x|^2$ and $w(x) = |x|^{-1}$. In the limit we find the positive-temperature Thomas-Fermi model for an atom in a harmonic trap, which has stimulated many works in the Physics literature [FMT49; GP55; Lat55; CA57]. This convergence has been proved for the first time by Narnhofer and Thirring in [NT81], but starting from the grand-canonical model instead of the canonical ensemble as we do here. This was generalized to strong magnetic fields in [HY04].

The dilute limit

In this section we deal with the case where the interaction potential has a range depending on N and tending to zero in our limit $N \rightarrow \infty$ with $\hbar^d N \rightarrow \rho$. This is classically taken into account by choosing the interaction in the form

$$w_N(x) := N^{dn} w(N^\eta x) \quad (19)$$

for a fixed w and a fixed parameter $\eta > 0$. In our confined system, the average distance between the particles is of order $N^{-1/d} \simeq \rho^{-1/d} \hbar$. The system is dilute when the particles interact rarely, that is, $\eta > 1/d$. For bosons in 3D, the limit involves the finite-range interaction $4\pi a \delta_0$ where $a = \int_{\mathbb{R}^d} w / (4\pi)$ for $\eta < 1$ and $a = a_s$, the s -wave scattering length a_s when $\eta = 1$. Due to the anti-symmetry the s -wave scattering length does not appear for fermions, except if there are several different species, e.g. with spin. This regime has been studied in [LSS05] for the ground state and [Sei06] at positive temperature, for the infinite translation-invariant gas. Here we extend these results to the confined case but do not consider any spin for shortness, hence we obtain a trivial limit. Our main result for dilute systems is the following.

Theorem 8 (Dilute limit). *Let $\beta_0, \rho > 0$. We assume that $V \in L_{\text{loc}}^{1+d/2}(\mathbb{R}^d)$ is such that $V(x) \rightarrow \infty$ at infinity and that $\int e^{-\beta_0 V_+(x)} dx < \infty$. Furthermore, assume that $|A|^2 \in L^{1+d/2}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ and $w \in L^1(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ is even.*

- If $0 < \eta < 1/d$ and $\widehat{w} \geq 0$ then, for all $\beta > \beta_0$ we have

$$\lim_{\substack{N \rightarrow \infty \\ \hbar^d N \rightarrow \rho}} \hbar^d e_{\text{Can}}^\beta(\hbar, N) = e_{\text{Vla}}^{\beta, (\int_{\mathbb{R}^d} w) \delta_0}(\rho)$$

where $e_{\text{Vla}}^{\beta, (\int_{\mathbb{R}^d} w) \delta_0}(\rho)$ is the minimum of the Vlasov energy with interaction potential $(\int_{\mathbb{R}^d} w) \delta_0$.

- If $\eta > 1/d$, $d \geq 3$ and $w \geq 0$ is compactly supported, then for all $\beta > \beta_0$ we have

$$\lim_{\substack{N \rightarrow \infty \\ \hbar^d N \rightarrow \rho}} \hbar^d e_{\text{Can}}^\beta(\hbar, N) = e_{\text{Vla}}^{\beta, 0}(\rho)$$

where $e_{\text{Vla}}^{\beta, 0}(\rho)$ is the minimum of the Vlasov energy without interaction potential.

In both cases, we have the same convergence of approximate Gibbs states as in Theorem 2.

The proof of Theorem 8 is given in Section 4.

2 Construction of trial states

In this section we construct a trial state for the proof of the upper bound. In the dilute case this construction is similar to the one in [Sei06] where the thermodynamic limit of non-zero spin interacting fermions were studied in the grand-canonical picture. This construction allows us to prove the following proposition.

Proposition 9 (Trial states). *Let $\rho_0 \in C_c^\infty(\mathbb{R}^d)$ be such that $\int_{\mathbb{R}^d} \rho_0 = 1$. Assume $|A|^2 \in L^{1+d/2}(\mathbb{R}^d)$, $w \in L^1(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$. If $\eta d > 1$, we assume w to be compactly supported. Then, there is a sequence of states Γ_N on $\bigwedge_{i=1}^N L^2(\mathbb{R}^d)$ satisfying*

$$\hbar^d \left(\text{Tr} \sum_{i=1}^N (i\hbar \nabla + A)^2 \Gamma_N + \text{Tr} \Gamma_N \log \Gamma_N \right) \xrightarrow[\hbar^d N \rightarrow 1]{N \rightarrow \infty} \int_{\mathbb{R}^d} F_\beta(\rho_0), \quad (20)$$

$$\left\| \frac{1}{N} \rho_{\Gamma_N}^{(1)} - \rho_0 \right\|_{L^1(\mathbb{R}^d)} \xrightarrow[\hbar^d N \rightarrow 1]{N \rightarrow \infty} 0 \quad (21)$$

and

$$\frac{\hbar^d}{N} \int_{\mathbb{R}^{2d}} w_N(x-y) \rho_{\Gamma_N}^{(2)}(x,y) dx dy \xrightarrow[\hbar^d N \rightarrow 1]{N \rightarrow \infty} \begin{cases} \int_{\mathbb{R}^d} (w * \rho_0) \rho_0 & \text{if } \eta = 0 \\ \left(\int_{\mathbb{R}^d} w \right) \int_{\mathbb{R}^d} \rho_0^2 & \text{if } 0 < d\eta < 1 \\ 0 & \text{if } d\eta > 1, d \geq 3. \end{cases} \quad (22)$$

Furthermore, we can take $\rho_{\Gamma_N}^{(1)}$ to be supported in a compact set which is independent of N and uniformly bounded in $L^\infty(\mathbb{R}^d)$ so that the convergence (21) holds in fact in all $L^p(\mathbb{R}^d)$ for $1 \leq p < \infty$.

Proof. The proof consists in dividing the space into small cubes in which we take a correlated version of the minimizer for the free case (correlations are only needed for the case $d\eta > 1$) and then do the thermodynamic limit in these cubes (or equivalently the limit where the effective Planck constant in front of the Laplacian tends to zero). This choice allows us to control the one-body density, which will be almost constant in these boxes. Without loss of generality, we will write the proof for $A = 0$. The proof is the same for $A \neq 0$.

Step 1. Definition of the trial state

Let $\rho_0 \in C_c^\infty(\mathbb{R}^d)$ and take $R > 0$ such that $\text{supp } \rho_0 \subset [-R/2, R/2]^d =: C_R$. Divide C_R in small cubes of size $\ell > 0$, $C_R \subset \bigcup_{z \in B(R\ell^{-1}) \cap \mathbb{Z}^d} \Lambda_z$ with $\Lambda_z := z\ell + [-\ell/2, \ell/2]^d$ and $B(R\ell^{-1})$ the ball centered at the origin with radius $R\ell^{-1}$. We will take later $1 \gg \ell \gg \hbar$. For all z define $N_z := \lfloor \hbar^d \ell^d \min_{x \in \Lambda_z} \rho_0(x) \rfloor$ so that $\sum_z N_z \leq N$. For $0 < \varepsilon < \ell/4$ and for all z , define the box

$$\tilde{\Lambda}_z := z\ell + \left[-\frac{\ell - \varepsilon}{2}, \frac{\ell - \varepsilon}{2} \right]^d \subset \Lambda_z$$

and denote by

$$\tilde{\Gamma}_z = \frac{e^{-\beta(\sum_{i=1}^{N_z} -\hbar^2 \Delta_i^{\text{per}})}}{Z_z} = \sum_{k \in \mathcal{P}_{N_z}(\mathbb{Z}^d)} \lambda_k |e_{k_1} \wedge \dots \wedge e_{k_{N_z}}\rangle \langle e_{k_1} \wedge \dots \wedge e_{k_{N_z}}|$$

the canonical minimizer of the free energy at inverse temperature β of N_z free fermions in the box $\tilde{\Lambda}_z$ with periodic boundary conditions, where $\mathcal{P}_n(E)$ denotes the set of all subsets of E with n elements. For $j \in \mathbb{Z}^d$,

$$e_j(x) = (\ell - \varepsilon)^{-d/2} e^{i \frac{2\pi}{\ell - \varepsilon} j \cdot x}$$

are the eigenfunctions of the periodic Laplacian in $\tilde{\Lambda}_z$ and λ_k the eigenvalues of $\tilde{\Gamma}_z$ associated with $e_k = e_{k_1} \wedge \dots \wedge e_{k_{N_z}}$. Note that we omit the z dependence of λ_k and e_k . We now regularize these functions and construct a state in the slightly larger cube Λ_z with Dirichlet boundary condition. Let $\chi \in C^\infty(\mathbb{R}^d)$ such that $\chi \equiv 0$ in $\mathbb{R}^d \setminus B(0,1)$, $\chi \geq 0$ and $\int_{\mathbb{R}^d} \chi = 1$, denote $\chi_\varepsilon = \varepsilon^{-d} \chi(\varepsilon^{-1} \cdot)$ and define for $j \in \mathbb{Z}^d$

$$f_j := e_j \sqrt{\mathbb{1}_{\tilde{\Lambda}_z} * \chi_\varepsilon}.$$

Note that

$$\begin{aligned} \int_{\Lambda_z} f_j \bar{f}_k &= \int e_j \bar{e}_k (\mathbb{1}_{\tilde{\Lambda}_z} * \chi_\varepsilon) = \int \int_{\tilde{\Lambda}_z} e_j(x) \bar{e}_k(x) \chi_\varepsilon(y-x) dy dx \\ &= \int_{\tilde{\Lambda}_z} e_j \bar{e}_k \int_{\mathbb{R}^d} \chi = \delta_{j,k}. \end{aligned}$$

Hence the family $(f_j)_j$ is still orthonormal and one can check that it satisfies $f_j \equiv e_j$ in $[-(\ell - 2\varepsilon)/2, (\ell - 2\varepsilon)/2]^d$ and as well as the Dirichlet boundary condition on Λ_z . Besides from having a state satisfying the Dirichlet boundary condition, we also want to add correlations in order to deal with the $d\eta > 1$ case. Let $\varphi \in C_c^\infty(\mathbb{R}^d)$ such that $\varphi \equiv 0$ in $B(0,1)$, $\varphi \equiv 1$ in $B(0,2)^c$ and $\varphi \leq 1$ almost everywhere and for $s > 0$ denote $\varphi_s = \varphi(s^{-1}\cdot)$. Following [Sei06], we define the correlation function $F(x_1, \dots, x_{N_z}) = \prod_{i < j} \varphi_s(x_i - x_j)$ and the state

$$\Gamma_z = \sum_{k \in \mathcal{P}_{N_z}(\mathbb{Z}^d)} \lambda_k Z_k^{-1} |F f_{k_1} \wedge \dots \wedge f_{k_{N_z}}\rangle \langle F f_{k_1} \wedge \dots \wedge f_{k_{N_z}}|,$$

where $Z_k = \|F f_{k_1} \wedge \dots \wedge f_{k_{N_z}}\|_{L^2(\Lambda_z^{N_z})}^2$ are normalization factors. Now consider the state

$$\Gamma := \bigwedge_z \Gamma_z.$$

We will show that Γ satisfies the three limits Eq. (20), (21) and (22). This state does not have the exact number of particle N but satisfies $\sum_z N_z = N - \mathcal{O}(\ell N)$. Hence we will only have to correct the particle number by adding $\mathcal{O}(\ell N)$ uncorrelated particles of low energy, for instance outside the support of ρ_0 . This will not modify the validity of the three limits. Now we focus on Γ and compute its free energy.

In the case $\eta d < 1$, we choose the following regime for the parameters introduced above.

$$s \ll \hbar \ll \varepsilon \ll \ell \ll N^{-\eta} \text{ and } s\ell \ll \hbar^2.$$

One could in fact take $\Gamma_{F=1}$ (removing the factor F , see below) and remove the dependence in s . In the case $\eta d > 1$, the convergence holds in the regime

$$N^{-\eta} \ll s \ll \hbar \ll \varepsilon \ll \ell \text{ and } s\ell \ll \hbar^2.$$

Step 2. Verification of (20)

We fix z and work in the cube Λ_z . Let us first compute the kinetic energy of the correlated Slater determinants appearing in the definition of Γ_z (note that this is not an eigenfunction decomposition due of the lack of orthogonality). Let us denote $X = (\sqrt{\mathbb{1}_{\tilde{\Lambda}_z} * \chi_\varepsilon})^{\otimes N_z}$ so that $\Psi_k^z := f_{k_1} \wedge \dots \wedge f_{k_{N_z}} = X e_{k_1} \wedge \dots \wedge e_{k_{N_z}}$ (we will omit the superscript z when there is no ambiguity) and denote $\nabla, -\Delta$ the gradient and the Laplacian for all coordinates x_1, \dots, x_{N_z} in the box Λ_z with Dirichlet boundary condition, we can check that

$$\nabla (F X e_{k_1} \wedge \dots \wedge e_{k_{N_z}}) = \left(X \nabla F + F \nabla X + i F X \sum_{j=1}^{N_z} \frac{2\pi k_j}{\ell - \varepsilon} \right) e_{k_1} \wedge \dots \wedge e_{k_{N_z}}.$$

Hence,

$$\overline{\text{Tr}}(-\Delta)\Gamma_z = \sum_{k \in \mathcal{P}_{N_z}(\mathbb{Z}^d)} \frac{\lambda_k}{Z_k} \left(\varepsilon_k + \|(X\nabla F + F\nabla X)e_{k_1} \wedge \dots \wedge e_{k_{N_z}}\|_{L^2(\Lambda_z^{N_z})}^2 \right)$$

where

$$\varepsilon_k := \left| 2\pi(\ell - \varepsilon)^{-1} \sum_{j=1}^{N_z} k_j \right|^2$$

is the eigenvalue of $-\Delta^{\text{per}}$ associated with the eigenfunction e_k . Note that $\lambda_k \propto e^{-\beta\hbar^2\varepsilon_k}$. We will show that $\sum_k \lambda_k Z_k^{-1} \varepsilon_k \simeq \sum_k \lambda_k \varepsilon_k = \text{Tr}(-\Delta^{\text{per}})\tilde{\Gamma}$ and that the second summand above is an error term. For that we first need to estimate the normalization factors Z_k and then bound the factor with the ∇F and ∇X . We will use several times that for any sequence $0 < a_1, \dots, a_p \leq 1$ we have

$$1 \geq \prod_{n=1}^p (1 - a_n) \geq 1 - \sum_{n=1}^p a_n. \quad (23)$$

Hence,

$$\begin{aligned} Z_k &= \int_{\Lambda_z^{N_z}} \prod_{1 \leq n < m \leq N_z} \varphi_s(x_n - x_m)^2 |\Psi_k|^2 dX \\ &\geq 1 - \int_{\Lambda_z^{N_z}} \sum_{1 \leq n < m \leq N_z} (1 - \varphi_s(x_n - x_m)^2) |\Psi_k|^2 dX \\ &\geq 1 - \int_{\Lambda_z^2} (1 - \varphi_s(x_1 - x_2)^2) \rho_{\Psi_k}^{(1)}(x_1) \rho_{\Psi_k}^{(1)}(x_2) dx_1 dx_2 \\ &\geq 1 - C s^d \ell^d \hbar^{-2d}, \end{aligned} \quad (24)$$

where we used that $\rho_{\Psi_k}^{(2)}(x, y) \leq \rho_{\Psi_k}^{(1)}(x) \rho_{\Psi_k}^{(1)}(y)$ because Ψ_k is a Slater determinant, and that $\rho_{\Psi_k}^{(1)} = N_z \ell^{-d} \mathbb{1}_{\tilde{\Lambda}_z} * \chi_\varepsilon \leq C \hbar^{-d}$.

Then we compute

$$|\nabla_{x_1} F|^2 = \sum_{\substack{m \neq n \\ m, n \geq 2}}^{N_z} \frac{\nabla \varphi_s(x_1 - x_m) \cdot \nabla \varphi_s(x_1 - x_n)}{\varphi_s(x_1 - x_m) \varphi_s(x_1 - x_n)} F^2 + \sum_{m \geq 2}^{N_z} \frac{|\nabla \varphi_s(x_1 - x_m)|^2}{\varphi_s(x_1 - x_m)^2} F^2$$

and obtain

$$\begin{aligned} \|\nabla F \Psi_k\|_{L^2(\Lambda_z^{N_z})}^2 &\leq C \int_{\Lambda_z^{3d}} |\nabla \varphi_s(x_1 - x_2)| |\nabla \varphi_s(x_1 - x_3)| \times \\ &\quad \times \rho_{\Psi_k}^{(1)}(x_1) \rho_{\Psi_k}^{(1)}(x_2) \rho_{\Psi_k}^{(1)}(x_3) dx_1 dx_2 dx_3 \\ &\quad + C \int_{\Lambda_z^{2d}} |\nabla \varphi_s(x_1 - x_2)|^2 \rho_{\Psi_k}^{(1)}(x_1) \rho_{\Psi_k}^{(1)}(x_2) dx_1 dx_2 \\ &\leq C s^{-2} (s^{2d} \ell^d \hbar^{-3d} + s^d \ell^d \hbar^{-2d}). \end{aligned}$$

Now we turn to the ∇X part. We have

$$\nabla_{x_1} X(x_1, \dots, x_{N_z}) = \frac{\nabla \sqrt{\mathbb{1}_{\tilde{\Lambda}_z} * \chi_\varepsilon(x_1)}}{\sqrt{\mathbb{1}_{\tilde{\Lambda}_z} * \chi_\varepsilon(x_1)}} X(x_1, \dots, x_{N_z})$$

and

$$\begin{aligned} \int_{\Lambda_z^{N_z}} |\nabla X|^2 |e_{k_1} \wedge \dots \wedge e_{k_{N_z}}|^2 &= \int_{\Lambda_z^{N_z}} \sum_{j=1}^{N_z} \left| \frac{\nabla \sqrt{\mathbb{1}_{\tilde{\Lambda}_z} * \chi_\varepsilon(x_1)}}{\sqrt{\mathbb{1}_{\tilde{\Lambda}_z} * \chi_\varepsilon(x_1)}} \right|^2 |\Psi_k|^2 \\ &= \int_{\Lambda_z} \left| \frac{\nabla \sqrt{\mathbb{1}_{\tilde{\Lambda}_z} * \chi_\varepsilon(x_1)}}{\sqrt{\mathbb{1}_{\tilde{\Lambda}_z} * \chi_\varepsilon(x_1)}} \right|^2 \rho_{\Psi_k}^{(1)} \\ &\leq C \int_{\Lambda_z} \left| \nabla \sqrt{\mathbb{1}_{\tilde{\Lambda}_z} * \chi_\varepsilon(x_1)} \right|^2 N_z \ell^{-d} \\ &\leq C N_z \ell^{-d} \int_{\Lambda_z} \int |\nabla \sqrt{\chi_\varepsilon}|^2 \leq C \ell^d \hbar^{-d} \varepsilon^{-2}, \end{aligned}$$

where we used the pointwise bound $\left| \nabla \sqrt{\mathbb{1}_{\tilde{\Lambda}_z} * \chi_\varepsilon(x_1)} \right|^2 \leq \int |\nabla \sqrt{\chi_\varepsilon}|^2$. Since X and F are both bounded by 1 we obtain

$$\begin{aligned} \mathrm{Tr}(-\Delta)\Gamma_z &= \mathrm{Tr}(-\Delta^{\mathrm{per}})\tilde{\Gamma}_z + \mathcal{O}\left(\frac{s^{2(d-1)}\ell^d\hbar^{-3d} + s^{d-2}\ell^d\hbar^{-2d} + \ell^d\hbar^{-d}\varepsilon^{-2}}{1 - C s^d \ell^d \hbar^{-2d}}\right. \\ &\quad \left. + N_z^{1+2/d} s^d \ell^d \hbar^{-2d}\right). \end{aligned}$$

We proceed with estimating the entropy of Γ_z . Thanks to [Sei06, Lemma 2] we have

$$\begin{aligned} \mathrm{Tr} \Gamma_z \log \Gamma_z &\leq \mathrm{Tr} \tilde{\Gamma}_z \log \tilde{\Gamma}_z - \log \min_k Z_k \\ &= \mathrm{Tr} \tilde{\Gamma}_z \log \tilde{\Gamma}_z + \mathcal{O}(s^d \ell^d \hbar^{-2d}), \end{aligned}$$

where we used the estimate (24) on Z_k . Combining the last two estimates gives

$$\begin{aligned} &\mathrm{Tr}(-\hbar^2 \Delta)\Gamma + \mathrm{Tr} \Gamma \log \Gamma \\ &= \sum_z \mathrm{Tr}(-\hbar^2 \Delta)\Gamma_z + \mathrm{Tr} \Gamma \log \Gamma_z \\ &\leq \sum_z e_{\mathrm{Can}}^{\beta, \mathrm{per}}(\tilde{\Lambda}_z, \hbar, N_z) + \ell^{-d} \mathcal{O}(s^d \ell^d \hbar^{-2d}) + \mathcal{O}\left((\hbar^{-d} \ell^d)^{1+2/d} s^d \ell^d \hbar^{-2d}\right) \\ &\quad + \hbar^2 \ell^{-d} \mathcal{O}\left(\frac{s^{2(d-1)}\ell^d\hbar^{-3d} + s^{d-2}\ell^d\hbar^{-2d} + \ell^d\hbar^{-d}\varepsilon^{-2}}{1 - C s^d \ell^d \hbar^{-2d}}\right), \end{aligned}$$

where we used that $N_z \leq \|\rho_0\|_{L^\infty(\mathbb{R}^d)} \hbar^{-d} \ell^d$. It is a known fact [Rob71, Proposition 2.1.3], [Rue99, Part 3.4] (see also [Mad19] for more details) that

$$e_{\mathrm{Can}}^{\beta, \mathrm{per}}(\tilde{\Lambda}_z, \hbar, N_z) = \hbar^{-d} \ell^d F_\beta(N_z / (\hbar^{-d} \ell^d)) + o(\hbar^{-d} \ell^d) \quad (25)$$

locally uniformly in $\rho_z := N_z \hbar^d \ell^{-d}$ as $\hbar \rightarrow 0$ under the condition $\hbar \ll \ell$. This is the thermodynamic limit of the free Fermi gas. By the continuity of F_β and the estimate $N_z / (\hbar^{-d} (\ell - \varepsilon)^d) = \rho(z) + \mathcal{O}(\varepsilon \ell^{-1})$ we obtain

$$\begin{aligned} \hbar^d (\text{Tr}(-\hbar^2 \Delta) \Gamma + \text{Tr} \Gamma \log \Gamma) &\leq \ell^d \sum_{z \in \mathbb{Z}^d} F_\beta(\rho(z)) + o(1) + \mathcal{O}(\varepsilon/\ell) \\ &+ \mathcal{O}((s\ell/\hbar^2)^d \ell^2) + \mathcal{O}(s/\hbar)^d + \mathcal{O}\left(\frac{(s/\hbar)^{2(d-1)} + (s/\hbar)^{d-2} + (\hbar/\varepsilon)^2}{1 - C(s\ell/\hbar^2)^d}\right). \end{aligned}$$

If $s \ll \hbar \ll \varepsilon \ll \ell$ with the extra condition that $s\ell \ll \hbar^2$ we obtain the upper bound in (20) by passing to the limit and by identifying the first term above as a Riemann sum. The lower bound is obtained in the same fashion by seeing Γ_z as a trial state for the periodic case.

Step 3. Verification of (21)

Let us recall that $\Gamma_{F=1}$ is the uncorrelated version of the trial state (which corresponds to taking $\varphi \equiv 1$) and that we denote by $\rho_{F=1}^{(k)}$ its k -particle density, for $k \geq 1$. From (23) and using that $\Gamma_{F=1}$ is a sum of Slater determinants we have

$$\begin{aligned} N^{-1} \|\rho_\Gamma^{(1)} - \rho_{F=1}^{(1)}\|_{L^1(\mathbb{R}^d)} &\leq N^{-1} \sum_{z \in \mathbb{Z}^d} \sum_{k \in \mathcal{P}_{N_z}(\mathbb{Z}^d)} \lambda_k^z \iint_{\mathbb{R}^{2d}} (1 - \varphi_s(x_1 - x_2)^2) \rho_{\Psi_k^z}^{(2)}(x_1, x_2) dx_1 dx_2 \\ &\leq CN^{-1} \sum_{z \in \mathbb{Z}^d} \iint_{\Lambda_z^2} (1 - \varphi_s(x_1 - x_2)^2) N_z^2 \ell^{-2d} dx_1 dx_2 \\ &\leq CN^{-1} \sum_{z \in \mathbb{Z}^d} s^d \ell^d N_z^2 \ell^{-2d} \\ &\leq C(s/\hbar)^d. \end{aligned}$$

We also used that $\rho_{\Psi_k^z}^{(2)} \leq \rho_{\Psi_k^z}^{(1)} \otimes \rho_{\Psi_k^z}^{(1)} \leq \|\rho_0\|_{L^\infty(\mathbb{R}^d)} N_z^2 \ell^{-2d}$. Finally, denoting by $\Gamma_{z,F=1}$ the uncorrelated version of Γ_z and by $\rho_{z,F=1}^{(1)}$ its one-body density we have

$$\begin{aligned} \|N^{-1} \rho_{F=1}^{(1)} - \rho_0\|_{L^1(\mathbb{R}^d)} &\leq \sum_z \|N^{-1} \rho_{z,F=1}^{(1)} - \rho_0 \mathbf{1}_{\Lambda_z}\|_{L^1(\mathbb{R}^d)} \\ &\leq C \sum_z (\|\nabla \rho_0\|_{L^\infty(\mathbb{R}^d)} \ell^{d+1} + \|\rho_0\|_{L^\infty(\mathbb{R}^d)} \ell^{d-1} \varepsilon) \\ &\leq C(\ell + \varepsilon/\ell). \end{aligned}$$

We have used that in $z\ell + [-(\ell - 2\varepsilon)/2, (\ell - 2\varepsilon)/2]^d$,

$$N^{-1} \rho_{z,F=1}^{(1)} = N^{-1} \ell^{-d} [\hbar^{-d} \ell^d \min_{\Lambda_z} \rho_0] = \rho_0 + \mathcal{O}(\hbar^d \ell^d) + \mathcal{O}(\|\nabla \rho_0\|_{L^\infty(\mathbb{R}^d)} \ell)$$

and that

$$\|N^{-1} \rho_{z,F=1}^{(1)} - \rho_0 \mathbf{1}_{\Lambda_z}\|_{L^\infty(\Lambda_z)} \leq C \|\rho_0\|_{L^\infty(\mathbb{R}^d)}.$$

Under the stated conditions on \hbar, ℓ, s and ε we have $N^{-1} \rho_\Gamma^{(1)} \rightarrow \rho_0$ in $L^1(\mathbb{R}^d)$.

Step 4. Verification of (22)

Let us first turn to the case $0 \leq \eta d < 1$. Note that the two-particle density matrices satisfy

$$\begin{aligned} \Gamma^{(2)} &= \sum_{z \in \mathbb{Z}^d} \Gamma_z^{(2)} + \sum_{z \neq z'} \Gamma_z^{(1)} \otimes \Gamma_{z'}^{(1)} \\ &= \Gamma^{(1)} \otimes \Gamma^{(1)} + \sum_{z \in \mathbb{Z}^d} \Gamma_z^{(2)} - \Gamma_z^{(1)} \otimes \Gamma_z^{(1)}. \end{aligned} \quad (26)$$

In particular we obtain for the two-particle reduced density

$$\rho_\Gamma^{(2)} = \rho_\Gamma^{(1)} \otimes \rho_\Gamma^{(1)} + \sum_{z \in \mathbb{Z}^d} \rho_{\Gamma_z}^{(2)} - \rho_{\Gamma_z}^{(1)} \otimes \rho_{\Gamma_z}^{(1)}. \quad (27)$$

The second term above is negligible in our regime. Indeed, using the triangle inequality, the Lieb-Thirring inequality [LT75; LT76] (the reader can refer to [FLS18, Lem. 3.4] for the exact version of the LT inequality we use) and Young's inequality we obtain

$$\begin{aligned} & N^{-2} \left| \sum_{z \in \mathbb{Z}^d} \int_{\mathbb{R}^d} w_N(x-y) \left(\rho_{\Gamma_z}^{(2)} - \rho_{\Gamma_z}^{(1)} \otimes \rho_{\Gamma_z}^{(1)} \right) \right| \\ & \leq CN^{-2} \|w_N\|_{L^{1+d/2}(\mathbb{R}^d)} \sum_{z \in \mathbb{Z}^d} \left\{ \|\rho_{\Gamma_z}^{(1)}\|_{L^{1+2/d}(\mathbb{R}^d)} \|\rho_{\Gamma_z}^{(1)}\|_{L^1(\mathbb{R}^d)} \right. \\ & \quad \left. + N_z^2 \left(\frac{\text{Tr} \Gamma_z \left(\sum_{j=1}^{N_z} -\Delta_{z_j} \right)}{N_z^{1+2/d}} \right)^{\frac{1}{1+2/d}} \right\} \\ & \leq CN^{-2} N^{d\eta \frac{d}{d+2}} \sum_{z \in \mathbb{Z}^d} N_z^2 \ell^{-\frac{2}{1+2/d}} \\ & \leq C(N^\eta \ell)^d \ell^{d(1-\frac{1}{d+2})} \end{aligned}$$

where we used that $\rho_{\Gamma_z}^{(1)} \leq CN_z \ell^{-d} \leq C \|\rho_0\|_{L^\infty(\mathbb{R}^d)} \hbar^{-d}$ almost everywhere and the estimate on the kinetic energy of Γ_z computed before. Hence, if $N^{-1} \rho_\Gamma^{(1)} \rightarrow \rho_0$ in $L^1(\mathbb{R}^d)$ and if $\ell = o(N^{-\eta})$, since both $N^{-1} \rho_\Gamma^{(1)}$ and ρ_0 are bounded (uniformly in N) in $L^\infty(\mathbb{R}^d)$, by (27) and the use of Young's inequality we obtain (22) for $0 \leq \eta d < 1$.

The case $\eta d > 1$ is easier to handle since in this case $N^{-\eta} = o(s)$. Indeed, due to the correlation factor F and because w is compactly supported we will have $\text{Tr} w_N(x-y)\Gamma = 0$ for N sufficiently large. \square

3 Proof of Theorem 2 in the non-interacting case $w \equiv 0$

In this section we prove the convergence (12) of the free energy in Theorem 2 in the case where the interaction is dropped, that is $w \equiv 0$. We study the interacting case later in Section 4. The convergence of states will be discussed in Section 4.3.

The non-interacting case is well understood since the Hamiltonian is quadratic in creation and annihilation operators in the grand canonical picture. The minimizers are known to be the so-called quasi-free states [BLS94]. For those we have an explicit formula and the argument of the proof is reduced to a usual semi-classical limit. The upper bound on the free energy is a

consequence of Proposition 9 from the previous section. The proof of the lower bound relies on localization and the use of coherent states.

We start with the following well-known lemma, the proof of which can for instance rely on Klein's inequality and the convexity of the fermionic entropy s [Thi02].

Lemma 10 (The minimal free energy of quasi-free states). *Let $\beta > 0$, and let H be a self-adjoint operator on a Hilbert space \mathfrak{H} such that $\text{Tr } e^{-\beta H} < \infty$. Then*

$$\min_{\substack{0 \leq \gamma \leq 1 \\ \gamma \in \mathfrak{S}_1(\mathfrak{H})}} \left(\text{Tr } H \gamma + \frac{1}{\beta} \text{Tr } s(\gamma) \right) = -\frac{1}{\beta} \text{Tr } \log (1 + e^{-\beta H}),$$

with the unique minimizer being $\gamma_0 = \frac{1}{1 + e^{\beta H}}$.

With Lemma 10 at hand we are able to provide the

Proof of Theorem 2 in the non-interacting case. Suppose that $w = 0$. We start out by proving the upper bound on the energy, using the trial states constructed in the previous section. Let $\rho > 0$ and $0 \leq \nu \in C_c^\infty(\mathbb{R}^d)$ with $\int_{\mathbb{R}^d} \nu(x) dx = \rho$. By Proposition 9 we then have a sequence (Γ_N) of canonical N -particle states satisfying

$$\hbar^d \text{Tr} \left(\sum_{j=1}^N |i\hbar \nabla_{x_j} + A(x_j)|^2 \Gamma_N \right) + \frac{\hbar^d}{\beta} \text{Tr} \Gamma_N \log \Gamma_N \rightarrow \int_{\mathbb{R}^d} F_\beta(\nu(x)) dx.$$

The one-particle densities $\hbar^d \rho_{\Gamma_N}^{(1)}$ converge to ν strongly in $L^1(\mathbb{R}^d)$ and are uniformly bounded in $L^\infty(\mathbb{R}^d)$. Hence they converge strongly in all $L^p(\mathbb{R}^d)$ for $p \in [1, \infty)$. Since $V \in L_{\text{loc}}^{1+d/2}(\mathbb{R}^d)$ and $\rho_{\Gamma_N}^{(1)}$ are, by construction, supported in a fixed compact set, we have

$$\hbar^d \text{Tr} V(x) \Gamma_N^{(1)} = \hbar^d \int_{\mathbb{R}^d} V(x) \rho_{\Gamma_N}^{(1)}(x) dx \rightarrow \int_{\mathbb{R}^d} V(x) \nu(x) dx.$$

This means that

$$\hbar^d e_{\text{Can}}^\beta(\hbar, N) \leq \hbar^d \mathcal{E}_{\text{Can}}^{N, \hbar}(\Gamma_N) \rightarrow \int_{\mathbb{R}^d} F_\beta(\nu(x)) dx + \int_{\mathbb{R}^d} V(x) \nu(x) dx,$$

and, since ν is arbitrary, we have shown that

$$\limsup_{\substack{N \rightarrow \infty \\ \hbar^d N \rightarrow \rho}} \hbar^d e_{\text{Can}}^\beta(\hbar, N) \leq e_{\text{Vla}}^\beta(\rho).$$

To prove the lower bound, we use the following bound [BLS94; Thi02] on the entropy

$$\text{Tr} \Gamma \log \Gamma \geq \text{Tr} \left(\Gamma^{(1)} \log \Gamma^{(1)} + \left(1 - \Gamma^{(1)}\right) \log \left(1 - \Gamma^{(1)}\right) \right) = \text{Tr } s \left(\Gamma^{(1)} \right) \quad (28)$$

which follows from the fact that quasi-free states maximize the entropy at given one-particle density matrix $\Gamma^{(1)}$. The bound applies to any N -particle state Γ whose one-particle density is

$\Gamma^{(1)}$. Applying Lemma 10 above, we have for any $\mu \in \mathbb{R}$ and any N -body state Γ

$$\begin{aligned} \mathcal{E}_{\text{Can}}^{N, \hbar}(\Gamma) &\geq \text{Tr}(|i\hbar\nabla + A(x)|^2 + V(x) - \mu) \Gamma^{(1)} + \frac{1}{\beta} \text{Tr} s(\Gamma^{(1)}) + \mu N \\ &\geq -\frac{1}{\beta} \text{Tr} \log \left(1 + e^{-\beta(|i\hbar\nabla + A(x)|^2 + V(x) - \mu)} \right) + \mu N. \end{aligned}$$

Thus, we are left to using the known semi-classical convergence (whose proof is recalled below in Proposition 11)

$$\begin{aligned} \liminf_{\hbar \rightarrow 0} -\frac{\hbar^d}{\beta} \text{Tr} \log \left(1 + e^{-\beta(|i\hbar\nabla + A(x)|^2 + V(x) - \mu)} \right) \\ \geq -\frac{1}{(2\pi)^d \beta} \iint_{\mathbb{R}^{2d}} \log \left(1 + e^{-\beta(p^2 + V(x) - \mu)} \right) dx dp, \end{aligned} \quad (29)$$

and to take $\mu = \mu_{\text{Vla}}(\rho)$. Recognizing the expression of the Vlasov free energy on the right-hand side we appeal to Theorem 1 and immediately obtain

$$\liminf_{\substack{N \rightarrow \infty \\ \hbar^d N \rightarrow \rho}} \hbar^d e_{\text{Can}}^\beta(\hbar, N) \geq e_{\text{Vla}}^\beta(\rho),$$

concluding the proof of (12) in the non-interacting case. \square

In (29) we have used the following well-known fact, which we prove for completeness.

Proposition 11 (Semi-classical limit). *Let $\beta_0 > 0$, we assume that $|A|^2 \in L^{1+d/2}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$, $V \in L_{\text{loc}}^{1+d/2}(\mathbb{R}^d)$ is such that $V(x) \rightarrow \infty$ at infinity and that $\int e^{-\beta_0 V_+(x)} dx < \infty$. Then for any chemical potential $\mu \in \mathbb{R}$ and all $\beta > \beta_0$,*

$$\begin{aligned} \limsup_{\hbar \rightarrow 0} \frac{\hbar^d}{\beta} \text{Tr} \log \left(1 + e^{-\beta(|i\hbar\nabla + A|^2 + V - \mu)} \right) \\ \leq \frac{1}{(2\pi)^d \beta} \iint_{\mathbb{R}^{2d}} \log \left(1 + e^{-\beta(p^2 + V(x) - \mu)} \right) dx dp. \end{aligned} \quad (30)$$

This result is known [Thi02] and the proof we provide here is essentially the one in [Sim80], where however the von Neumann entropy $x \log(x)$ was used instead of the Fermi-Dirac entropy $x \log(x) + (1-x) \log(1-x)$. In fact, Theorem 2 shows that the inequality (30) is indeed an equality.

Proof of Proposition 11. Without loss of generality we may assume that $\mu = 0$. We also assume in a first step that $V_- \in L^\infty(\mathbb{R}^d)$ and then remove this assumption at the end of the proof. Due to technical issues involving the potential V , we need to localize the minimization problem on some bounded set. Let $\chi, \eta \in C^\infty(\mathbb{R}^d)$ satisfy $\chi^2 + \eta^2 = 1$, $\text{supp } \chi \subseteq B(0, 1)$ and $\text{supp } \eta \subseteq B(0, \frac{1}{2})^c$. For $R > 0$, denote $\chi_R = \chi(\frac{\cdot}{R})$ and $\eta_R = \eta(\frac{\cdot}{R})$. Let $H_\hbar = |i\hbar\nabla + A|^2 + V$ and take $\gamma^\hbar = \frac{1}{1 + e^{\beta H_\hbar}}$ as in Lemma 10. By the IMS localization formula [Sim83] we have

$$\text{Tr} H_\hbar \gamma^\hbar = \text{Tr} (H_\hbar \chi_R \gamma^\hbar \chi_R) + \text{Tr} (H_\hbar \eta_R \gamma^\hbar \eta_R) - \hbar^2 \text{Tr} \left(|\nabla \chi_R|^2 + |\nabla \eta_R|^2 \right) \gamma^\hbar, \quad (31)$$

and using the convexity of s and [BK90, Theorem 14],

$$\begin{aligned} \operatorname{Tr} s(\gamma^{\hbar}) &= \operatorname{Tr} \chi_R s(\gamma^{\hbar}) \chi_R + \operatorname{Tr} \eta_R s(\gamma^{\hbar}) \eta_R \\ &\geq \operatorname{Tr} s(\chi_R \gamma^{\hbar} \chi_R) + \operatorname{Tr} s(\eta_R \gamma^{\hbar} \eta_R). \end{aligned} \quad (32)$$

We first deal with the localization outside the ball. The operators we consider in $B(0, \frac{R}{2})^c$ are the ones with Dirichlet boundary condition. We obtain by Lemma 10 that the remainder terms are bounded by

$$\begin{aligned} &\operatorname{Tr}(H_{\hbar} \eta_R \gamma^{\hbar} \eta_R) + \frac{1}{\beta} \operatorname{Tr} s(\eta_R \gamma^{\hbar} \eta_R) \\ &\geq -\frac{1}{\beta} \operatorname{Tr}_{L^2(B(0, \frac{R}{2})^c)} \log(1 + e^{-\beta(|i\hbar\nabla + A|^2 + V - C)}) \\ &\geq -\frac{C}{\beta} \operatorname{Tr}_{L^2(B(0, \frac{R}{2})^c)} e^{-\beta(|i\hbar\nabla + A|^2 + V)} \\ &\geq -\frac{C}{\beta} \operatorname{Tr}_{L^2(B(0, \frac{R}{2})^c)} e^{-\beta(-\hbar^2 \Delta^D + V)} \end{aligned} \quad (33)$$

$$\geq -\frac{C}{\beta} \operatorname{Tr}_{L^2(\mathbb{R}^d)} e^{-\beta(-\hbar^2 \Delta + (1-\alpha)V + \alpha \inf_{B(0, R)^c} V)} \quad (34)$$

$$\geq -\frac{C e^{-\beta \alpha \inf_{B(0, R)^c} V}}{(2\pi\hbar)^d} \iint_{\mathbb{R}^{2d}} e^{-\beta(p^2 + (1-\alpha)V(x))} dx dp, \quad (35)$$

where $\alpha > 0$ is such that $\beta(1 - \alpha) > \beta_0$. The inequality (33) comes from the diamagnetic inequality [CFKS87] and (34) is obtained by the min-max characterization of the eigenvalues. The last inequality follows from Golden-Thompson's formula [RS72, Theorem VIII.30].

The error term in the IMS formula can be estimated by

$$\begin{aligned} -\operatorname{Tr} \left(|\nabla \chi_R|^2 + |\nabla \eta_R|^2 \right) \gamma^{\hbar} &\geq -\frac{C}{R} \operatorname{Tr} \gamma^{\hbar} \\ &\geq -\frac{C}{R} \operatorname{Tr} e^{-\beta H_{\hbar}} \\ &\geq -\frac{C}{R (2\pi\hbar)^d} \iint_{\mathbb{R}^{2d}} e^{-\beta(p^2 + V(x))} dx dp, \end{aligned} \quad (36)$$

where we used again the diamagnetic and Golden-Thompson inequalities.

Next we derive a bound on the densities $\rho_{\gamma_R^{\hbar}}$, where $\gamma_R^{\hbar} = \chi_R \gamma^{\hbar} \chi_R$, using the Lieb-Thirring inequality [LT75; LT76]. Combining (31), (32), (35) and (36) we have shown

$$\begin{aligned} \operatorname{Tr} H_{\hbar} \gamma_R^{\hbar} + \frac{1}{\beta} \operatorname{Tr} s(\gamma_R^{\hbar}) - \frac{\varepsilon(R)}{\hbar^d} &\leq \operatorname{Tr} H_{\hbar} \gamma^{\hbar} + \frac{1}{\beta} \operatorname{Tr} s(\gamma^{\hbar}) \\ &= -\frac{1}{\beta} \operatorname{Tr} \log(1 + e^{-\beta H_{\hbar}}) \leq 0 \end{aligned} \quad (37)$$

where $\varepsilon(R) \rightarrow 0$ when $R \rightarrow \infty$. By Lemma 10 we have

$$\begin{aligned} \operatorname{Tr} H_h \gamma_R^h + \frac{1}{\beta} \operatorname{Tr} s(\gamma_R^h) &\geq \frac{1}{2} \operatorname{Tr} (-\hbar^2 \Delta) \gamma_R^h \\ &\quad - \frac{1}{\beta} \operatorname{Tr} \log \left(1 + e^{-\beta(i\hbar \nabla + A)^2/2 + V} \right) - \frac{C}{\hbar^d} \end{aligned}$$

where, as in (35),

$$\operatorname{Tr} \log \left(1 + e^{-\beta(i\hbar \nabla + A)^2/2 + V} \right) \leq \frac{C e^{-\alpha\beta \inf V}}{(2\pi\hbar)^d} \iint_{\mathbb{R}^{2d}} e^{-\beta(p^2/2 + (1-\alpha)V(x))} dx dp.$$

This implies the following bound on the kinetic energy

$$\operatorname{Tr} (-\hbar^2 \Delta) \gamma_R^h \leq \frac{C}{\hbar^d}. \quad (38)$$

By the Lieb-Thirring inequality [FLS18, Lem. 3.4], we obtain

$$\int_{\mathbb{R}^d} \rho_{\gamma_R^h}(x)^{1+\frac{2}{d}} dx \leq C \operatorname{Tr} (-\Delta \gamma_R^h) \leq \frac{1}{\hbar^{d+2}} C. \quad (39)$$

We return to the estimate on the localized terms in (31) and (32), using coherent states. Let $f \in C_c^\infty(\mathbb{R}^d)$ be a real-valued and even function, and consider the coherent state $f_{x,p}^h(y) = \hbar^{-\frac{d}{4}} f(\hbar^{-\frac{1}{2}}(y-x)) e^{i\frac{p \cdot y}{\hbar}}$. The projections $|f_{x,p}^h\rangle \langle f_{x,p}^h|$ give rise to a resolution of the identity on $L^2(\mathbb{R}^d)$:

$$\frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^{2d}} |f_{x,p}^h\rangle \langle f_{x,p}^h| = \operatorname{Id}_{L^2(\mathbb{R}^d)}. \quad (40)$$

Using this in combination with Jensen's inequality and the spectral theorem, we obtain

$$\begin{aligned} \operatorname{Tr} s(\chi_R \gamma^h \chi_R) &= \frac{1}{(2\pi\hbar)^d} \iint_{\mathbb{R}^{2d}} \langle f_{x,p}^h, s(\gamma_R^h) f_{x,p}^h \rangle dx dp \\ &\geq \frac{1}{(2\pi\hbar)^d} \iint_{\mathbb{R}^{2d}} s(\langle f_{x,p}^h, \gamma_R^h f_{x,p}^h \rangle) dx dp. \end{aligned} \quad (41)$$

On the other hand, applying [FLS18, Corollary 2.5] we have

$$\begin{aligned} \operatorname{Tr} H_h \chi_R \gamma^h \chi_R &= \frac{1}{(2\pi\hbar)^d} \iint_{\mathbb{R}^{2d}} \langle f_{x,p}^h, H_h \gamma_R^h f_{x,p}^h \rangle dx dp \\ &= \frac{1}{(2\pi\hbar)^d} \iint_{\mathbb{R}^{2d}} (|p+A|^2 + V(x)) \langle f_{x,p}^h, \gamma_R^h f_{x,p}^h \rangle dx dp \\ &\quad + \int_{\mathbb{R}^d} \rho_{\gamma_R^h} (A^2 - A^2 * |f^h|^2) - 2\Re \operatorname{Tr} (A - A * |f^h|^2) \cdot i\hbar \nabla \gamma_R^h \\ &\quad - \hbar \int_{\mathbb{R}^d} |\nabla f|^2 + \int_{\mathbb{R}^d} \rho_{\gamma_R^h} (V - V * |f^h|^2) \end{aligned} \quad (42)$$

Since $\hbar^d \rho_{\gamma_R^h}$ is supported in $B(0, R)$ and is uniformly bounded in $L^{1+2/d}(\mathbb{R}^d)$ by (39), and $V *$

$|f^\hbar|^2$ converges to V locally in $L^{1+d/2}(\mathbb{R}^d)$. The same argument applied to A and $|A|^2$ combined with Hölder's inequality, the Lieb-Thirring inequality and (38) shows that the remainder terms above are $o(\hbar^{-d})$. At last, combining (37), (41) and (42) as well as a simple adaptation of Proposition 16 to finite domains (Remark 17) yields

$$\begin{aligned} \limsup_{\hbar \rightarrow 0} \hbar^d \operatorname{Tr} \log \left(1 + e^{-\beta(|i\hbar\nabla + A|^2 + V)} \right) \\ \leq \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} \log \left(1 + e^{-\beta(p^2 + V(x))} \right) dx dp + \varepsilon(R), \end{aligned}$$

where $\varepsilon(R) \rightarrow 0$ when $R \rightarrow \infty$. This concludes the proof in the case $V_- \in L^\infty(\mathbb{R}^d)$. We now remove this unnecessary assumption: let us consider a potential V satisfying the assumptions of Proposition 11 (possibly unbounded below). For $K > 0$, we take the cut off potential $V_K = V \mathbb{1}_{\{V \geq -K\}}$ and for any $0 < \varepsilon < 1$ we obtain using Lemma 10

$$\begin{aligned} -\frac{1}{\beta} \operatorname{Tr} \log \left(1 + e^{-\beta(|i\hbar\nabla + A|^2 + V)} \right) \\ \geq \min_{0 \leq \gamma \leq 1} \left(\operatorname{Tr} \left((1 - \varepsilon) |i\hbar\nabla + A|^2 + V_K \right) \gamma + \frac{1}{\beta} \operatorname{Tr} s(\gamma) \right) \\ \quad + \min_{0 \leq \gamma \leq 1} \operatorname{Tr} \left(\varepsilon |i\hbar\nabla + A|^2 + V - V_K \right) \gamma \\ = -\frac{1}{\beta} \operatorname{Tr} \log \left(1 + e^{-\beta((1-\varepsilon)|i\hbar\nabla + A|^2 + V_K)} \right) \\ \quad - \operatorname{Tr} \left(\varepsilon |i\hbar\nabla + A|^2 + V - V_K \right)_-. \end{aligned}$$

Applying the Lieb-Thirring inequality, we obtain

$$\operatorname{Tr} \left(\varepsilon |i\hbar\nabla + A|^2 + V - V_K \right)_- \leq C \hbar^{-d} \varepsilon^{-d/2} \int_{\mathbb{R}^d} (V - V_K)_-^{1+d/2} dx.$$

This means that for any K and ε

$$\begin{aligned} \limsup_{\hbar \rightarrow 0} \hbar^d \operatorname{Tr} \log \left(1 + e^{-\beta(|i\hbar\nabla + A|^2 + V)} \right) \\ \leq \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} \log \left(1 + e^{-\beta((1-\varepsilon)p^2 + V_K(x))} \right) dx dp \\ \quad + \varepsilon^{-d/2} C \int_{\mathbb{R}^d} (V - V_K)_-^{1+d/2} dx. \end{aligned}$$

First taking $K \rightarrow \infty$ and afterwards $\varepsilon \rightarrow 0$, the result follows using the monotone convergence theorem. \square

4 Proof of Theorem 2 in the general case

In this section we deal with the interacting case $w \neq 0$. We first focus on the proof of Theorem 2 (mean-field limit) before proving Theorem 8 (dilute limit).

4.1 Convergence of the energy in the mean-field limit $\eta = 0$

Here we prove (12) in the case of general $w \in L^{1+d/2}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$. The upper bound on the canonical energy follows immediately from the trial states constructed in Proposition 9, so we concentrate on proving the lower bound. This is the content of the following proposition.

Proposition 12. *Let $\beta_0, \rho > 0$, $V \in L^{1+d/2}_{\text{loc}}(\mathbb{R}^d)$ such that $V(x) \rightarrow \infty$ when $|x| \rightarrow \infty$ and $\int e^{-\beta_0 V_+(x)} dx < \infty$. Furthermore, let $|A|^2, w \in L^{1+d/2}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$, w be even and satisfy $\widehat{w} \geq 0$. Then we have*

$$\liminf_{\substack{N \rightarrow \infty \\ \hbar^d N \rightarrow \rho}} \hbar^d e_{\text{Can}}^\beta(\hbar, N) \geq e_{\text{Vla}}^\beta(\rho).$$

Proof. The main idea of the proof is to replace w by an effective one-body potential, and then use the lower bound in the non-interacting case.

We begin by regularizing the interaction potential: let $\varphi \in C_c^\infty(\mathbb{R}^d)$ even and real-valued, define $\chi = \varphi * \varphi$ and $w_\varepsilon = w * \chi_\varepsilon$ with $\chi_\varepsilon = \varepsilon^{-d} \chi(\varepsilon^{-1} \cdot)$ for $\varepsilon > 0$. Note that $\widehat{w}_\varepsilon \geq 0$. Moreover, if $\alpha > 0$ and $w = w_1 + w_2$ with $w_1 \in L^{1+d/2}(\mathbb{R}^d)$ and $\|w_2\|_{L^\infty(\mathbb{R}^d)} \leq \alpha$ then $w_{1,\varepsilon} := w_1 * \chi_\varepsilon$ satisfies $\widehat{w_{1,\varepsilon}} \in L^1(\mathbb{R}^d)$ and $w_{2,\varepsilon} := w_2 * \chi_\varepsilon$ satisfies $\|w_{2,\varepsilon}\|_{L^\infty(\mathbb{R}^d)} \leq \alpha$. Then, using the Lieb-Thirring inequality, we can replace w by w_ε up to an error of order $\|w_1 - w_{1,\varepsilon}\|_{L^{1+d/2}(\mathbb{R}^d)} + C\alpha$, see for instance [FLS18, Lem. 3.4]. It remains to let ε tend to zero and then let α tend to zero. We therefore assume for the rest of the proof that w satisfies $\widehat{w} \in L^1(\mathbb{R}^d)$.

Now, with $0 \leq \widehat{w} \in L^1(\mathbb{R}^d)$, it is classical that we can bound w from below by a one-body potential, see, e.g., [FLS18, Lem. 3.6]. More precisely, we have for all $x_1, \dots, x_N \in \mathbb{R}^d$ and $\varphi \in C_c^\infty(\mathbb{R}^d)$

$$\int_{\mathbb{R}^d} \widehat{w} \left| \widehat{\sum_{i=1}^N \delta_{x_i}} - \varphi \right|^2 \geq 0,$$

which after expanding is the same as

$$\sum_{1 \leq i < j \leq N} w(x_i - x_j) \geq \sum_{i=1}^N w * \varphi(x_i) - \frac{1}{2} \int_{\mathbb{R}^d} (\varphi * w) \varphi - \frac{N}{2} w(0). \quad (43)$$

Let m_0 be the minimizer of the semiclassical problem with density ρ , whose existence is guaranteed by Theorem 1. For any N -body trial state Γ we obtain from (43)

$$\begin{aligned} \text{Tr } H_{N,\hbar} \Gamma &\geq \text{Tr} \left((i\hbar \nabla + A(x))^2 + V(x) + \rho^{-1} w * \rho_{m_0}(x) \right) \Gamma^{(1)} \\ &\quad - \frac{N}{2\rho^2} \int_{\mathbb{R}^d} (\rho_{m_0} * w) \rho_{m_0} - \frac{1}{2} w(0), \end{aligned}$$

where $\Gamma^{(1)}$ is the 1-particle reduced density matrix of Γ . Let $\mu_{\text{Vla}}(\rho)$ be the chemical potential corresponding to the minimizer m_0 and define $V^{\text{eff}} = V + \rho^{-1} w * \rho_{m_0}(x) - \mu_{\text{Vla}}(\rho)$. Denoting by $e_{\text{Can}}^{\beta, \text{eff}}(\hbar, N)$ the minimum of the canonical energy with potential V^{eff} and with no interaction,

we obtain using the convergence shown for the non-interacting case in Section 3,

$$\begin{aligned} \hbar^d e_{\text{Can}}^\beta(\hbar, N) &\geq \hbar^d e_{\text{Can}}^{\beta, \text{eff}}(\hbar, N) - \frac{\hbar^d N}{2\rho^2} \int_{\mathbb{R}^d} (\rho_{m_0} * w) \rho_{m_0} + \mu_{\text{Vla}}(\rho) \hbar^d N \\ &\xrightarrow[\hbar^d N \rightarrow \rho]{N \rightarrow \infty} -\frac{1}{\beta(2\pi)^d} \iint_{\mathbb{R}^{2d}} \log(1 + e^{-\beta(p^2 + V^{\text{eff}}(x))}) dx dp \\ &\quad - \frac{1}{2\rho} \int_{\mathbb{R}^d} (\rho_{m_0} * w) \rho_{m_0} + \mu_{\text{Vla}}(\rho) \rho \\ &= e_{\text{Vla}}^\beta(\rho), \end{aligned}$$

where the last equality is due to Theorem 1. This concludes the proof of the convergence of energy in Theorem 2. \square

4.2 Convergence of the energy in the dilute limit $\eta > 0$

Here we prove the convergence of the energy in Theorem 8 where $\eta > 0$. We first state a lemma about the regularity of the minimizers of (4) when the interaction has a Dirac component. It will be needed in the proof of the convergence of the energy in Theorem 8 below.

Lemma 13. *Let $\beta, a, \rho > 0$, let A, V satisfy the assumptions of Theorem 1, let $w = a\delta_0$ for some $a > 0$. If $m \in L^1(\mathbb{R}^{2d})$ satisfies the non-linear equation (5), then $\rho_m \in L^{1+d/2}(\mathbb{R}^d)$.*

Proof. For simplicity and without loss of generality, we assume that $a = \rho = 1$, $\mu = 0$ and we take $w = \delta_0$ and $A = 0$. Since $\rho_m \in L^1(\mathbb{R}^d)$, it is sufficient to show that $\rho_m \mathbf{1}_{\{\rho_m(x) \geq 1\}}$ is in $L^{1+d/2}(\mathbb{R}^d)$. Recalling that m satisfies the equation

$$m(x, p) = \frac{1}{1 + e^{\beta(p^2 + V(x) + \rho_m(x))}}, \quad (44)$$

we immediately have

$$\rho_m(x) \leq \frac{e^{-\beta(V(x) + \rho_m(x))}}{(2\pi)^d} \int_{\mathbb{R}^d} e^{-\beta p^2} dp = C_{d, \beta} e^{-\beta(V(x) + \rho_m(x))},$$

where $C_{d, \beta} = (\pi/(4\beta))^{3/2}$, implying that

$$\rho_m(x) e^{\beta \rho_m(x)} \leq C_{d, \beta} e^{\beta V_-(x)}.$$

Hence

$$\rho_m \mathbf{1}_{\{\rho_m \geq 1\}} \leq (V_- + \log C_{d, \beta}) \mathbf{1}_{\{\rho_m \geq 1\}} \in L^{1+\frac{d}{2}}(\mathbb{R}^d),$$

since $V_- \in L^{1+\frac{d}{2}}(\mathbb{R}^d)$ and $\{\rho_m \geq 1\}$ has finite measure by Markov's inequality. \square

Case $0 < \eta < 1/d$

In this case, we take $w \in L^1(\mathbb{R}^d)$ with $0 \leq \widehat{w} \in L^1(\mathbb{R}^d)$. Take $w_N = N^{d\eta} w(N^\eta \cdot)$ and consider the canonical model with this interaction. Denoting $a = \int_{\mathbb{R}^d} w(x) dx$, Proposition 9 implies that

$$\limsup_{\substack{N \rightarrow \infty \\ \hbar^d N \rightarrow \rho}} \hbar^d e_{\text{Can}}^\beta(N, \hbar) \leq e_{\text{Vla}}^{\beta, a\delta_0}(\rho).$$

To show the lower bound, we follow the argument of Proposition 12. Denote by m_0 the minimizer of the Vlasov functional with the delta interaction $a\delta_0$, and let Γ_N be the Gibbs state minimizing the canonical free energy functional. Applying (43) with $\varphi = \frac{N}{\rho}\rho_{m_0}$, we obtain

$$\begin{aligned} \mathrm{Tr} H_{N,\hbar}\Gamma_N &\geq \mathrm{Tr} \left((i\hbar\nabla + A)^2 + V^{\mathrm{eff}} \right) \Gamma_N^{(1)} + \frac{1}{\rho} \mathrm{Tr} (w_N * \rho_{m_0} - a\rho_{m_0}) \Gamma_N^{(1)} \\ &\quad - \frac{N}{2\rho^2} \int_{\mathbb{R}^d} (\rho_{m_0} * w_N) \rho_{m_0} + \mu_{\mathrm{Vla}}^{a\delta_0}(\rho) N + o(\hbar^{-d}), \end{aligned} \quad (45)$$

where $V^{\mathrm{eff}} = V + \frac{a}{\rho}\rho_{m_0} - \mu_{\mathrm{Vla}}^{a\delta_0}(\rho)$. Here, by Hölder's inequality, we have

$$\begin{aligned} \hbar^d \mathrm{Tr}(w_N * \rho_{m_0} - a\rho_{m_0})\Gamma_N^{(1)} &= \hbar^d \int_{\mathbb{R}^d} (w_N * \rho_{m_0} - a\rho_{m_0}) \rho_{\Gamma_N^{(1)}} \\ &\leq \left\| \hbar^d \rho_{\Gamma_N^{(1)}} \right\|_{L^{1+2/d}(\mathbb{R}^d)} \|w_N * \rho_{m_0} - a\rho_{m_0}\|_{L^{1+d/2}(\mathbb{R}^d)}, \end{aligned}$$

which tends to 0 since $\|\hbar^d \rho_{\Gamma_N^{(1)}}\|_{L^{1+2/d}(\mathbb{R}^d)}$ is bounded, by the Lieb-Thirring inequality, and since $\rho_{m_0} \in L^{1+\frac{d}{2}}(\mathbb{R}^d)$ by Lemma 13. Finally we have,

$$\int_{\mathbb{R}^d} (\rho_{m_0} * w_N) \rho_{m_0} \longrightarrow a \int_{\mathbb{R}^d} \rho_{m_0}^2.$$

Hence, continuing from (45), we conclude that

$$\begin{aligned} \liminf_{\substack{N \rightarrow \infty \\ \hbar^d N \rightarrow \rho}} \hbar^d e_{\mathrm{Can}}^\beta(N, \hbar) &\geq -\frac{1}{(2\pi)^d \beta} \iint_{\mathbb{R}^{2d}} \log \left(1 + e^{-\beta(p^2 + V^{\mathrm{eff}}(x))} \right) dx dp \\ &\quad + \mu_{\mathrm{Vla}}^{a\delta_0}(\rho) \rho - \frac{a}{2\rho} \int_{\mathbb{R}^d} \rho_{m_0}^2 \\ &= e_{\mathrm{Vla}}^{\beta, a\delta_0}(\rho). \end{aligned}$$

Case $\eta > 1/d$

Here we treat the dilute limit. Assume that $d \geq 3$, $0 \leq w \in L^1(\mathbb{R}^d)$, and that w is compactly supported. Then, since $w \geq 0$, we have the immediate lower bound

$$\liminf_{\substack{N \rightarrow \infty \\ \hbar^d N \rightarrow \rho}} \hbar^d e_{\mathrm{Can}}^\beta(N, \hbar) \geq \liminf_{\substack{N \rightarrow \infty \\ \hbar^d N \rightarrow \rho}} \hbar^d e_{\mathrm{Can}}^{\beta, 0}(N, \hbar) = e_{\mathrm{Vla}}^{\beta, 0}(\rho).$$

On the other hand, it follows from Proposition 9 that we also have the corresponding upper bound, so

$$\lim_{\substack{N \rightarrow \infty \\ \hbar^d N \rightarrow \rho}} \hbar^d e_{\mathrm{Can}}^\beta(N, \hbar) = e_{\mathrm{Vla}}^{\beta, 0}(\rho).$$

This finishes the proof of the convergence of the energy in the dilute limit.

4.3 Convergence of states

Strong convergence of the one-particle Husimi and Wigner measures

Here we concentrate on proving the limits (14) and (15) for the one-particle Husimi measure and the associated density. We start by briefly recalling the definitions.

For $f \in L^2(\mathbb{R}^d)$ a normalized, real-valued function and $(x, p) \in \mathbb{R}^{2d}$, $\hbar > 0$, we define $f_{x,p}^{\hbar}(y) = \hbar^{-d/4} f((x-y)/\hbar^{1/2}) e^{ip \cdot y/\hbar}$ and denote by $P_{x,p}^{\hbar} = |f_{x,p}^{\hbar}\rangle \langle f_{x,p}^{\hbar}|$ the orthogonal projection onto $f_{x,p}^{\hbar}$. For $k \geq 1$, we introduce the k -particle Husimi measure of a state Γ

$$m_{f,\Gamma}^{(k)}(x_1, p_1, \dots, x_k, p_k) = \frac{N!}{(N-k)!} \text{Tr} \left(P_{x_1, p_1}^{\hbar} \otimes \dots \otimes P_{x_k, p_k}^{\hbar} \otimes \mathbb{1}_{N-k} \Gamma \right),$$

for $x_1, p_1, \dots, x_k, p_k \in \mathbb{R}^{2dk}$. See [FLS18] for alternative formulas of $m_{f,\Gamma}^{(k)}$. We also recall the definition of the Wigner measure,

$$\begin{aligned} \mathcal{W}_{\Gamma}^{(k)}(x_1, \dots, p_k) &= \int_{\mathbb{R}^{dk}} \int_{\mathbb{R}^{d(N-k)}} e^{-i \sum_{\ell=1}^k p_{\ell} \cdot y_{\ell}} \times \\ &\times \Gamma(x_1 + \hbar y_1/2, \dots, x_k + \hbar y_k/2, z_{k+1}, \dots, z_N) dy_1 \dots dy_k dz_{k+1} \dots dz_N, \end{aligned}$$

for $x_1, p_1, \dots, x_k, p_k \in \mathbb{R}^{2dk}$, where $\Gamma(\cdot, \cdot)$ is the kernel of the operator Γ .

Using [FLS18, Theorem 2.7] and the fact that the Husimi measures are bounded both in the x and p variables, we obtain the existence of a Borel probability measure \mathcal{P} on

$$\mathcal{S} = \left\{ \mu \in L^1(\mathbb{R}^{2d}), \quad 0 \leq \mu \leq 1, \quad \int_{\mathbb{R}^{2d}} \mu = \rho \right\}$$

such that, up to a subsequence, we have

$$\int_{\mathbb{R}^{2dk}} m_{f,\Gamma_N}^{(k)} \varphi \rightarrow \int_{\mathcal{S}} \left(\int_{\mathbb{R}^{2dk}} m^{\otimes k} \varphi \right) d\mathcal{P}(m),$$

for any $\varphi \in L^1(\mathbb{R}^{2dk}) + L^{\infty}(\mathbb{R}^{2dk})$ and similarly for the Wigner measures. There is no loss of mass in the limit due to the confining potential V . Our goal is to show that $\mathcal{P} = \delta_{m_0}$, where m_0 is the Vlasov minimizer from Theorem 1.

We begin with the case $\eta = 0$. Using coherent states, the tightness of $(m_{f,\Gamma_N}^{(1)})_N$ and a finite volume approximation we obtain

$$\begin{aligned} \lim_{\substack{N_j \rightarrow \infty \\ \hbar^d N_j \rightarrow \rho}} \hbar^d e^{\beta} \mathcal{E}_{\text{Can}}(\hbar, N_j) &\geq \frac{1}{(2\pi)^d} \int_{\mathcal{S}} \left(\int_{\mathbb{R}^{2dk}} (p^2 + V(x)) m(x, p) \right) d\mathcal{P}(m) \\ &+ \frac{1}{2\rho} \int_{\mathcal{S}} \left(\int_{\mathbb{R}^{2dk}} (w * \rho_m) \rho_m \right) d\mathcal{P}(m) + \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} s \left(\int_{\mathcal{S}} m d\mathcal{P}(m) \right). \end{aligned} \quad (46)$$

The lower semi-continuity of the entropy term can be justified as in the proof of Lemma 19. The case $0 < \eta < 1/d$ can be adapted using (43) with $\varphi = N\rho_{m_0}$ and the case $\eta > 1/d$ is even easier since the interaction is assumed non-negative and can therefore be dropped.

If we denote $\bar{m} = \int_{\mathcal{S}} m d\mathcal{P}(m)$, the right side of (46) is not exactly $\mathcal{E}_{\text{Can}}(\bar{m})$ because of the interaction term. In the case $0 \leq \eta < 1/d$ we assumed $\widehat{w} \geq 0$, hence the following inequality

follows from convexity:

$$\int_{\mathcal{S}} \left(\int_{\mathbb{R}^{2dk}} w * \rho_m \rho_m \right) d\mathcal{P}(m) \geq \int_{\mathbb{R}^{2d}} w * \rho_{\bar{m}} \rho_{\bar{m}}. \quad (47)$$

The case $1/d < \eta$ is immediate since we assumed $w \geq 0$ and the limiting energy has no interaction term. Gathering the above inequalities we have

$$\lim_{\substack{N_j \rightarrow \infty \\ \hbar^d N_j \rightarrow \rho}} \hbar^d e_{\text{Can}}^\beta(\hbar, N_j) \geq \mathcal{E}_{\text{Vla}}^{\beta, \rho, \bullet}(\bar{m}) \geq e_{\text{Vla}}^{\beta, \bullet}(\rho),$$

where $\mathcal{E}_{\text{Vla}}^{\beta, \rho, \bullet}$ and $e_{\text{Vla}}^{\beta, \bullet}(\rho)$ are the appropriate limiting functional and energy: i.e. $\bullet = w$ if $\eta = 0$, $\bullet = (\int_{\mathbb{R}^d} w) \delta_0$ if $0 < d\eta < 1$ and $\bullet = 0$ if $d\eta \geq 1$ and $d \geq 3$. Now, by Theorem 2 and Theorem 8 the above inequalities are in fact equalities and \bar{m} is therefore the unique minimizer of $\mathcal{E}_{\text{Vla}}^{\beta, \rho, \bullet}$ that is m_0 . Since this limit does not depend on the subsequence we have taken, we conclude that the whole sequence $m_{f, \Gamma_N}^{(1)}$ converges weakly to m_0 , and similarly for the Wigner measure.

Note that, when $\hat{w} > 0$ and $0 < d\eta < 1$, the equality in (47) gives that \mathcal{P} is concentrated on functions m which all share the same density ρ_{m_0} , by strict convexity. But this is the only information that we have obtained so far on \mathcal{P} . If the conjectured entropy inequality (18) was valid, then we would conclude immediately that $\mathcal{P} = \delta_{m_0}$. Since we do not have this inequality, we will have to go back later to the proof that $\mathcal{P} = \delta_{m_0}$.

So far the convergence of $m_{f, \Gamma_N}^{(1)}$ is only weak but it can be improved using the (one-particle) entropy. Going back to the previous estimates we now have

$$\hbar^d e_{\text{Can}}^\beta(\hbar, N) = e_{\text{Vla}}^{\beta, \bullet}(\rho) + \frac{1}{(2\pi)^d \beta} \iint_{\mathbb{R}^{2d}} (s(m_{f, \Gamma_N}^{(1)}) - s(m_0)) + o(1). \quad (48)$$

As before we denote by $e_{\text{Vla}}^{\beta, \bullet}(\rho)$ the appropriate limiting energy, depending on the choice of η . Recall that in the case $\eta > 1/d$, the interaction potential is assumed to be non negative, so the interaction term is just dropped. We now focus on the second term in (48). Let us remark that

$$\begin{aligned} & s(m_{f, \Gamma_N}^{(1)}) - s(m_0) \\ &= m_{f, \Gamma_N}^{(1)} \log \left(\frac{m_{f, \Gamma_N}^{(1)}}{m_0} \right) + (1 - m_{f, \Gamma_N}^{(1)}) \log \left(\frac{1 - m_{f, \Gamma_N}^{(1)}}{1 - m_0} \right) \\ & \quad + (m_0 - m_{f, \Gamma_N}^{(1)}) \log \left(\frac{1 - m_0}{m_0} \right) \\ & \geq m_0 \log \left(\frac{m_{f, \Gamma_N}^{(1)}}{m_0} \right) + \beta(m_0 - m_{f, \Gamma_N}^{(1)}) \left(p^2 + V + \frac{1}{\rho} w_N * \rho_{m_0} - \mu + \beta^{-1} \right), \end{aligned}$$

where we used the expression of m_0 (5) and the pointwise inequality $x \log(x/y) + (y-x) \geq 0$ for any $x, y > 0$. Integrating over x and p , we obtain on the right side the sum of the relative von Neumann entropy of $m_{f, \Gamma_N}^{(1)}$ and m_0 , and a term which tends to zero, due to the weak convergence we have proven. By Pinsker's inequality and (48) we obtain

$$\hbar^d e_{\text{Can}}^\beta(\hbar, N) - e_{\text{Vla}}^{\beta, \bullet}(\rho) \geq \frac{1}{2(2\pi)^d \beta} \left(\int_{\mathbb{R}^{2d}} |m_{f, \Gamma_N}^{(1)} - m_0| \right)^2 + o(1).$$

The convergence of the energies gives the strong convergence in $L^1(\mathbb{R}^{2d})$ of $m_{f,\Gamma_N}^{(1)}$ towards the Vlasov minimizer m_0 , hence in $L^p(\mathbb{R}^{2d})$ for all $1 \leq p < \infty$ since the Husimi measures are bounded by 1. This automatically gives that $\rho_{m_{f,\Gamma_N}^{(1)}} \rightarrow \rho_{m_0}$ strongly in $L^1(\mathbb{R}^d)$. The weak convergence in $L^{1+2/d}(\mathbb{R}^d)$ follows from the (classical) Lieb-Thirring inequality

$$\|\rho_m\|_{L^{1+d/2}(\mathbb{R}^d)} \leq C \|m\|_{L^1(\mathbb{R}^{2d}, p^2 dx dp)}^{\frac{d}{d+2}} \|m\|_{L^\infty(\mathbb{R}^{2d})}^{\frac{2}{d+2}}$$

for any m in $L^1(\mathbb{R}^{2d})$.

Finally, by the Lieb-Thirring inequality $\hbar^d \rho_{\Gamma_N}^{(1)}$ is bounded in $L^1(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$, hence this sequence is weakly precompact in those spaces. On the other hand, for any $\varphi \in C_c^\infty(\mathbb{R}^d)$ we have by [FLS18, Lemma 2.4]

$$\int_{\mathbb{R}^d} \rho_{m_{f,\Gamma_N}^{(1)}} \varphi = \int_{\mathbb{R}^d} \hbar^d \rho_{\Gamma_N}^{(1)} \varphi * |f^\hbar|^2.$$

Let $\tilde{\rho}$ be an accumulation point for $\hbar^d \rho_{\Gamma_N}^{(1)}$. By passing to the limit in both sides we obtain

$$\int_{\mathbb{R}^d} \rho_{m_0} \varphi = \int_{\mathbb{R}^d} \tilde{\rho} \varphi.$$

The test function φ being arbitrary, we conclude that $\hbar^d \rho_{\Gamma_N}^{(1)}$ has a single accumulation point and therefore converges weakly in $L^1(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ towards ρ_{m_0} .

Weak convergence of the k -particle Husimi and Wigner measures

At this point we have proved the strong convergence of $m_{f,\Gamma_N}^{(1)}$ towards m_0 in $L^p(\mathbb{R}^{2d})$ for all $1 \leq p < \infty$. Our argument works for any sequence of approximate Gibbs states (Γ_N) in the sense that

$$\mathcal{E}_{\text{Can}}^{N,\hbar}(\Gamma_N) = e_{\text{Can}}^\beta(\hbar, N) + o(N).$$

Here we discuss the weak convergence of the higher order Husimi functions. This is not an easy fact in the canonical ensemble case. For instance, when $w \equiv 0$ one can use Wick's formula in the grand canonical case but there is no such formula in the canonical ensemble [Sch17; GMST18]. Here we will use a Feynman-Hellmann-type argument, which forces us to consider the exact Gibbs state, and not only an approximate equilibrium state. We will come back to approximate Gibbs states at the end of the proof but our argument will require that they approach the right energy with an error of order $o(1)$ instead of $o(N)$.

In order to access the two-particle Husimi function, the usual Feynman-Hellmann argument is to perturb the N -body Hamiltonian by a positive two-body term of order N , multiplied by a small (possibly negative) parameter ε . This modifies the effective Vlasov energy and, after taking the limit, one then looks at the derivative at $\varepsilon = 0$. The problem here is to control negative values of ε . For atoms one can use the strong repulsion at the origin of the Coulomb interaction to control a negative two-body term, as was done in [NT81].¹ For a general interaction or even when $w \equiv 0$, such an argument fails. Another difficulty is the need to re-prove the existence of the limit with the perturbation, since in the canonical ensemble trial states are not so easy to construct.

We follow a different route and use instead an argument inspired of a new technique recently introduced in [LNR18a]. The idea is to perturb the energy by a one body term of order 1. This

1. After inspection one sees that the argument used in [NT81] works under the condition that $\hat{w}(p) \geq a|p|^{-a}$ for some $a > 0$ for large p . Not all interaction potentials can therefore be covered.

will not modify the leading order in the limit and will force us to look at the next order. Since we are only interested in deviations in ε , the existence of the limit for the one-particle Husimi measure will help us to identify the deviation. Then, in order to access the two-body Husimi measure, we look at the second derivative at $\varepsilon = 0$ instead of the first derivative.

Let us detail the argument. Let $b \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{R}_+)$ be a non-negative function on the phase space and introduce its coherent state quantization

$$B_{\hbar} := \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} b(x, p) P_{x,p}^{\hbar} dx dp,$$

where we recall that $P_{x,p}^{\hbar} = |f_{x,p}^{\hbar}\rangle \langle f_{x,p}^{\hbar}|$ is the orthogonal projection onto $f_{x,p}^{\hbar}$. We then consider the operator

$$B_{N,\hbar} := \sum_{j=1}^N (B_{\hbar})_j \quad (49)$$

in the N -particle space. Note that B_{\hbar} is a bounded self-adjoint operator with

$$0 \leq B_{\hbar} \leq \|b\|_{L^\infty(\mathbb{R}^{2d})} \hbar^d \quad (50)$$

due to the coherent state representation (40) and that it is trace-class with

$$\mathrm{Tr}(B_{\hbar}) \leq \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} b(x, p) dx dp. \quad (51)$$

In particular $B_{N,\hbar}$ is bounded uniformly in N , with

$$\|B_{N,\hbar}\| \leq \min \left(N \hbar^d \|b\|_{L^\infty(\mathbb{R}^{2d})}, (2\pi)^{-d} \|b\|_{L^1(\mathbb{R}^{2d})} \right).$$

This is because

$$\left\| \sum_{j=1}^N C_j \right\|_{\mathcal{B}(\wedge^N L^2(\mathbb{R}^3))} \leq \|C\|_{\mathfrak{S}^1(L^2(\mathbb{R}^3))} \quad (52)$$

for any trace class operator C . We introduce the perturbed Hamiltonian

$$H_{N,\hbar}(\varepsilon) := H_{N,\hbar} + \varepsilon B_{N,\hbar},$$

for $\varepsilon \in \mathbb{R}$. The perturbation is uniformly bounded, hence will not affect the limit $N \rightarrow \infty$ for fixed ε . More precisely, let us call

$$\Gamma_{N,\hbar,\beta}(\varepsilon) := \frac{e^{-\beta H_{N,\hbar}(\varepsilon)}}{\mathrm{Tr} e^{-\beta H_{N,\hbar}(\varepsilon)}}$$

the associated Gibbs state and

$$F_{N,\hbar,\beta}(\varepsilon) := -\frac{\log \mathrm{Tr}(e^{-\beta H_{N,\hbar}(\varepsilon)})}{\beta}$$

the corresponding free energy. Everywhere we assume that $\hbar N^{1/d} \rightarrow \rho$ and $\beta > 0$ is fixed. By plugging $\Gamma_{N,\hbar,\beta}(\varepsilon)$ into the variational principle at $\varepsilon = 0$ and conversely, we obtain immediately

that

$$F_{N,\hbar,\beta}(0) + \frac{\varepsilon}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} b m_{f,\Gamma_{N,\hbar,\beta}(\varepsilon)}^{(1)} \leq F_{N,\hbar,\beta}(\varepsilon) \leq F_{N,\hbar,\beta}(0) + \frac{\varepsilon}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} b m_{f,\Gamma_{N,\hbar,\beta}(0)}^{(1)}. \quad (53)$$

We have used here that $\text{Tr}(B_{\hbar}\Gamma^{(1)}) = (2\pi)^{-d} \iint_{\mathbb{R}^{2d}} b m_{f,\Gamma}^{(1)}$ for all states Γ . Since $0 \leq m_{f,\Gamma}^{(1)} \leq 1$, this proves that

$$F_{N,\hbar,\beta}(\varepsilon) = \mathcal{E}_{\text{Can}}^{N,\hbar}(\Gamma_{N,\hbar,\beta}(\varepsilon)) = e_{\text{Can}}^{\beta}(\hbar, N) + \mathcal{O}(\varepsilon)$$

where $\mathcal{O}(\varepsilon)$ is even uniform in N . Hence from the analysis in the previous section, we deduce immediately that

$$m_{\Gamma_{N,\hbar,\beta}(\varepsilon)}^{(1)} \longrightarrow m_0$$

strongly in $L^1(\mathbb{R}^{2d})$ for any fixed ε . Going back to (53) we infer that

$$F_{N,\hbar,\beta}(\varepsilon) = F_{N,\hbar,\beta}(0) + \frac{\varepsilon}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} b m_0 + o(1).$$

A different way to state the same limit is

$$f_N(\varepsilon) := \frac{\text{Tr} e^{-\beta H_{N,\hbar} - \beta \varepsilon B_{N,\hbar}}}{\text{Tr} e^{-\beta H_{N,\hbar}}} \longrightarrow \exp\left(-\frac{\varepsilon \beta}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} b m_0\right). \quad (54)$$

It turns out that the so-defined function f_N is C^∞ on \mathbb{R} with all its derivatives locally uniformly bounded in N . This follows from the following general fact.

Lemma 14. *Let A be a self-adjoint operator such that $\text{Tr}(e^A) < \infty$ and let B be a bounded self-adjoint operator, on a Hilbert space \mathfrak{H} . Then the function*

$$\varepsilon \in \mathbb{R} \mapsto \frac{\text{Tr}(e^{A+\varepsilon B})}{\text{Tr}(e^A)}$$

is C^∞ and its derivatives are bounded by

$$\left| \frac{d^k}{d\varepsilon^k} \frac{\text{Tr}(e^{A+\varepsilon B})}{\text{Tr}(e^A)} \right| \leq \|B\|^k \frac{\text{Tr}(e^{A+\varepsilon B})}{\text{Tr}(e^A)} \leq \|B\|^k e^{|\varepsilon| \|B\|}$$

for $k \geq 0$.

Proof. Note that $\text{Tr}(e^{A+\varepsilon B}) \leq e^{|\varepsilon| \|B\|} \text{Tr}(e^A)$ since $A + \varepsilon B \leq A + |\varepsilon| \|B\|$. We have for the first derivative

$$\frac{d}{d\varepsilon} \frac{\text{Tr}(e^{A+\varepsilon B})}{\text{Tr}(e^A)} = \frac{\text{Tr}(B e^{A+\varepsilon B})}{\text{Tr}(e^A)}$$

which is then clearly bounded by $\|B\| e^{|\varepsilon| \|B\|}$. The second derivative is given by Duhamel's formula

$$\frac{d^2}{d\varepsilon^2} \frac{\text{Tr}(e^{A+\varepsilon B})}{\text{Tr}(e^A)} = \int_0^1 \frac{\text{Tr}(B e^{t(A+\varepsilon B)} B e^{(1-t)(A+\varepsilon B)})}{\text{Tr}(e^A)} dt \quad (55)$$

and we have by Hölder's inequality in Schatten spaces

$$\begin{aligned} \left| \text{Tr}(B e^{t(A+\varepsilon B)} B e^{(1-t)(A+\varepsilon B)}) \right| &\leq \|B\|^2 \left\| e^{t(A+\varepsilon B)} \right\|_{\mathfrak{S}^{\frac{1}{t}}} \left\| e^{(1-t)(A+\varepsilon B)} \right\|_{\mathfrak{S}^{\frac{1}{1-t}}} \\ &= \|B\|^2 \text{Tr}(e^{A+\varepsilon B}) \leq \|B\|^2 e^{|\varepsilon| \|B\|} \text{Tr}(e^A), \end{aligned}$$

as claimed. The argument is the same for the higher order derivatives. The function is indeed real-analytic on \mathbb{R} but this fact is not needed in our argument. \square

Since $B_{N,\hbar}$ is bounded uniformly in N and \hbar , we conclude from the lemma that f_N is bounded in $W_{\text{loc}}^{k,\infty}$ for all k . This implies that $f_N^{(k)}$ converges locally uniformly to the k th derivative of the right side of (54) for all k . In particular, we have

$$f_N''(0) \longrightarrow \left(\frac{\beta}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} b m_0 \right)^2. \quad (56)$$

On the other hand, we can compute the second derivative $f_N''(0)$ explicitly, using (55):

$$f_N''(0) = \beta^2 \int_0^1 \frac{\text{Tr}(B_{N,\hbar} e^{-t\beta H_{N,\hbar}} B_{N,\hbar} e^{-(1-t)\beta H_{N,\hbar}})}{\text{Tr}(e^{-\beta H_{N,\hbar}})} dt. \quad (57)$$

We claim that this indeed behaves as

$$f_N''(0) = \frac{\beta^2}{(2\pi)^{2d}} \iint_{\mathbb{R}^{4d}} b \otimes b m_{f,\Gamma_{N,\hbar,\beta}}^{(2)} + o(1) \quad (58)$$

and first explain why this is useful before justifying (58). From the weak convergence of $m_{f,\Gamma_{N,\hbar,\beta}}^{(2)}$ mentioned in the previous section, we obtain

$$\lim_{\substack{N \rightarrow \infty \\ N\hbar^d \rightarrow \rho}} f_N''(0) = \frac{\beta^2}{(2\pi)^{2d}} \int_{\mathcal{S}} \left(\int_{\mathbb{R}^{2d}} b m \right)^2 d\mathcal{P} \quad (59)$$

with the de Finetti measure \mathcal{P} . Comparing (56) with (59) and using $m_0 = \int_{\mathcal{S}} m d\mathcal{P}$, we conclude that

$$\int_{\mathcal{S}} \left(\int_{\mathbb{R}^{2d}} b m \right)^2 d\mathcal{P}(m) = \left(\int_{\mathcal{S}} \int_{\mathbb{R}^{2d}} b m d\mathcal{P}(m) \right)^2$$

for every non-negative $b \in C_c^\infty(\mathbb{R}^{2d})$. This proves that $\mathcal{P} = \delta_{m_0}$ as desired. The limits (16) and (17) then follow for all $k \geq 2$. Therefore, it only remains to prove (58).

The idea of the proof of (58) is simple. Since we are in a semi-classical regime, the order of the operators in the trace (57) should not matter. If we put the two $B_{N,\hbar}$ together, we obtain after a calculation

$$\text{Tr} \left((B_{N,\hbar})^2 \Gamma_{N,\hbar,\beta} \right) = \text{Tr} \left((B_\hbar)^2 \Gamma_{N,\hbar}^{(1)} \right) + \frac{1}{(2\pi)^{2d}} \iint_{\mathbb{R}^{4d}} b \otimes b m_{f,\Gamma_{N,\hbar,\beta}}^{(2)}.$$

The first term tends to zero since

$$\text{Tr} \left((B_\hbar)^2 \Gamma_{N,\hbar}^{(1)} \right) \leq N \|B_\hbar\|^2 \leq \|b\|_{L^\infty(\mathbb{R}^{2d})}^2 N \hbar^{2d},$$

whereas the second term converges to $(2\pi)^{-2d} \int_{\mathcal{S}} \left(\iint_{\mathbb{R}^{2d}} b m \right)^2 d\mathcal{P}(m)$ due to the weak convergence

of $m_{f,\Gamma_{N,\hbar,\beta}}^{(2)}$. Therefore we have to compare $f_N''(0)$ with $\text{Tr}(B_{N,\hbar})^2\Gamma_{N,\hbar,\beta}$.

In [LNR18a], it is proven that the function

$$t \mapsto \text{Tr} \left(B_{N,\hbar} e^{-t\beta H_{N,\hbar}} B_{N,\hbar} e^{-(1-t)\beta H_{N,\hbar}} \right)$$

is convex on $[0, 1]$, non-increasing on $[0, 1/2]$ and non-decreasing on $[1/2, 1]$. Using that the function is minimal at $t = 1/2$ and above its tangent at $t = 0$ provides the bound

$$\begin{aligned} & \text{Tr} \left(B_{N,\hbar} e^{-t\beta H_{N,\hbar}} B_{N,\hbar} e^{-(1-t)\beta H_{N,\hbar}} \right) \\ & \geq \text{Tr} \left(B_{N,\hbar} e^{-\frac{\beta}{2} H_{N,\hbar}} B_{N,\hbar} e^{-\frac{\beta}{2} H_{N,\hbar}} \right) \\ & \geq \text{Tr} \left((B_{N,\hbar})^2 e^{-\beta H_{N,\hbar}} \right) + \frac{\beta}{4} \text{Tr} \left(\left[[H_{N,\hbar}, B_{N,\hbar}], B_{N,\hbar} \right] e^{-\beta H_{N,\hbar}} \right) \end{aligned}$$

for all $t \in [0, 1]$, see [LNR18a]. Inserting in (57), we find that

$$f_N''(0) \geq \beta^2 \text{Tr} \left((B_{N,\hbar})^2 \Gamma_{N,\hbar,\beta} \right) + \frac{\beta^3}{4} \text{Tr} \left(\left[[H_{N,\hbar}, B_{N,\hbar}], B_{N,\hbar} \right] \Gamma_{N,\hbar,\beta} \right). \quad (60)$$

Hence (58) readily follows from the following result.

Lemma 15 (Convergence of the double commutator). *With $B_{N,\hbar}$ as in (49), we have*

$$\lim_{\substack{N \rightarrow \infty \\ N\hbar^d \rightarrow \rho}} \text{Tr} \left(\left[[H_{N,\hbar}, B_{N,\hbar}], B_{N,\hbar} \right] \Gamma_{N,\hbar,\beta} \right) = 0. \quad (61)$$

Proof. We have

$$\begin{aligned} \left[[H_{N,\hbar}, B_{N,\hbar}], B_{N,\hbar} \right] &= \sum_{j=1}^N \left[[H_{1,\hbar}, B_{\hbar}], B_{\hbar} \right]_j \\ &+ \frac{1}{N} \sum_{1 \leq j \neq k \leq N} \left[[w_{jk}, (B_{\hbar})_j], (B_{\hbar})_j + (B_{\hbar})_k \right] \end{aligned} \quad (62)$$

with $H_{1,\hbar} = |i\hbar\nabla + A|^2 + V$ the one-particle operator and w_{jk} the multiplication operator by $w_N(x_j - x_k)$. The commutators have been used to dramatically reduce the number of terms, but will not play any role anymore. We will estimate separately the terms $(B_{\hbar}H_{1,\hbar}B_{\hbar})_j$, $(H_{1,\hbar}B_{\hbar}^2)_j$, $w_{jk}(B_{\hbar})_j(B_{\hbar})_{j'}$ and $(B_{\hbar})_jw_{jk}(B_{\hbar})_{j'}$ with $j' \in \{k, j\}$.

First we deal with the kinetic energy. For instance we can bound, by Hölder's inequality in Schatten spaces,

$$\begin{aligned} & \|B_{\hbar}(-\hbar^2\Delta)B_{\hbar}\|_{\mathfrak{S}^1} + \|(-\hbar^2\Delta)(B_{\hbar})^2\|_{\mathfrak{S}^1} \\ & \leq 2 \|B_{\hbar}\| \|B_{\hbar}\|_{\mathfrak{S}^1}^{\frac{1}{2}} \|(-\hbar^2\Delta)B_{\hbar}^{\frac{1}{2}}\|_{\mathfrak{S}^2} \leq \frac{C}{N} \|(-\hbar^2\Delta)B_{\hbar}^{\frac{1}{2}}\|_{\mathfrak{S}^2}. \end{aligned}$$

We have used here our estimates (50) and (51) on the norm and trace of the non-negative operator

B_{\hbar} . The last Hilbert-Schmidt norm is equal to

$$\begin{aligned} \left\| (-\hbar^2 \Delta) B_{\hbar}^{\frac{1}{2}} \right\|_{\mathfrak{S}^2}^2 &= \text{Tr} \left((-\hbar^2 \Delta) B_{\hbar} (-\hbar^2 \Delta) \right) \\ &= \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} b(x, p) \left\| \hbar^2 \Delta f_{x,p}^{\hbar} \right\|^2 dx dp. \end{aligned}$$

Using that

$$\begin{aligned} \hbar^2 \Delta f_{x,p}^{\hbar}(y) &= \hbar \hbar^{-d/4} (\Delta f) \left(\frac{x-y}{\sqrt{\hbar}} \right) e^{ip \cdot y / \hbar} - |p|^2 f_{x,p}^{\hbar}(y) \\ &\quad + 2i\sqrt{\hbar} \hbar^{-d/4} p \cdot (\nabla f) \left(\frac{x-y}{\sqrt{\hbar}} \right) e^{ip \cdot y / \hbar}, \end{aligned}$$

we find that

$$\left\| (-\hbar^2 \Delta) B_{\hbar}^{\frac{1}{2}} \right\|_{\mathfrak{S}^2} \leq C \iint_{\mathbb{R}^{2d}} (|p|^4 + \hbar|p|^2 + \hbar^2) b(x, p) dx dp.$$

This is uniformly bounded since b has a compact support in the phase space. Using (52), we conclude as we wanted that

$$\text{Tr} \left(\Gamma_{N,\hbar,\beta} \sum_{j=1}^N [[-\hbar^2 \Delta, B_{\hbar}], B_{\hbar}]_j \right) = \mathcal{O}(N^{-1}).$$

For the potential term we have to use more information on the state $\Gamma_{N,\hbar,\beta}$. We first estimate

$$\text{Tr} \left(\Gamma_{N,\hbar,\beta}^{(1)} V B_{\hbar}^2 \right) \leq \|B_{\hbar}\|^{\frac{3}{2}} \left\| (\Gamma_{N,\hbar,\beta}^{(1)})^{\frac{1}{2}} |V|^{\frac{1}{2}} \right\|_{\mathfrak{S}^2} \left\| |V|^{\frac{1}{2}} B_{\hbar}^{\frac{1}{2}} \right\|_{\mathfrak{S}^2}.$$

Using the Lieb-Thirring inequality for $V_- \in L^{1+d/2}(\mathbb{R}^3)$ as in (39) and that the energy is $\mathcal{O}(N)$ for V_+ , we see that

$$\left\| (\Gamma_{N,\hbar,\beta}^{(1)})^{1/2} |V|^{1/2} \right\|_{\mathfrak{S}^2}^2 = \text{Tr} \Gamma_{N,\hbar,\beta}^{(1)} |V| = \mathcal{O}(N).$$

Hence we can deduce that

$$\text{Tr} \left(\Gamma_{N,\hbar,\beta}^{(1)} V B_{\hbar}^2 \right) \leq \frac{C}{N} \left\| |V|^{\frac{1}{2}} B_{\hbar}^{\frac{1}{2}} \right\|.$$

Like for the kinetic energy, we compute the Hilbert-Schmidt norm

$$\begin{aligned} \left\| |V|^{\frac{1}{2}} B_{\hbar}^{\frac{1}{2}} \right\|_{\mathfrak{S}^2}^2 &= \text{Tr} |V|^{\frac{1}{2}} B_{\hbar} |V|^{\frac{1}{2}} \\ &= \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} b(x, p) \left\| |V|^{\frac{1}{2}} f_{x,p}^{\hbar} \right\|_{L^2(\mathbb{R}^d)}^2 dx dp \\ &= \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} b(x, p) |V| * |f_{0,0}^{\hbar}|^2(x) dx dp \\ &\leq C \int_{B_R} |V(x)| dx \end{aligned} \tag{63}$$

where B_R is a fixed large ball, chosen large enough such that $\text{supp}(b) \subset B_{R-1}$. We are using here that $f_{0,0}^{\hbar}$ has compact support, hence $\text{supp}(f_{0,0}^{\hbar}) \subset B_1$, for \hbar small enough. Since $V \in L_{\text{loc}}^1(\mathbb{R}^d)$

by assumption, this proves that

$$\mathrm{Tr} \left(\Gamma_{N,\hbar,\beta}^{(1)} V B_{\hbar}^2 \right) = \mathcal{O}(N^{-1}).$$

The argument is similar for $\mathrm{Tr} \left(\Gamma_{N,\hbar,\beta}^{(1)} B_{\hbar}^2 V \right)$. Finally, we also have

$$\mathrm{Tr} \left(\Gamma_{N,\hbar,\beta}^{(1)} B_{\hbar} V B_{\hbar} \right) \leq \|B_{\hbar}\| \left\| B_{\hbar}^{\frac{1}{2}} |V|^{\frac{1}{2}} \right\|_{\mathfrak{S}^2}^2 = \mathcal{O}(N^{-1}) \quad (64)$$

by (63). This concludes the proof that the potential terms tend to 0. The argument is exactly the same for $|A|^2$. For $i\hbar\nabla \cdot A + A \cdot i\hbar\nabla$, we argue similarly, using that

$$\left\| |A| B_{\hbar}^{\frac{1}{2}} \right\|_{\mathfrak{S}^2} + \left\| A \cdot (i\hbar\nabla) B_{\hbar}^{\frac{1}{2}} \right\|_{\mathfrak{S}^2} \leq C \int_{B_R} |A|$$

and

$$\left\| |i\hbar\nabla| \sqrt{\Gamma_{N,\hbar,\beta}^{(1)}} \right\|_{\mathfrak{S}^2}^2 = \mathrm{Tr}(-\hbar^2 \Delta) \Gamma_{N,\hbar,\beta}^{(1)} = \mathcal{O}(N).$$

Let us finally turn to the interaction. First we look at

$$\mathrm{Tr} \left(\Gamma_{N,\hbar,\beta} \frac{1}{N} \sum_{1 \leq j \neq k \leq N} (B_{\hbar})_j w_{jk} (B_{\hbar})_k \right) = (N-1) \mathrm{Tr} \left(\Gamma_{N,\hbar,\beta} (B_{\hbar})_1 w_{12} (B_{\hbar})_2 \right)$$

and use the Cauchy-Schwarz inequality to estimate

$$\pm (B_{\hbar})_1 w_{12} (B_{\hbar})_2 \leq (B_{\hbar})_1 |w_{12}| (B_{\hbar})_1 + (B_{\hbar})_2 |w_{12}| (B_{\hbar})_2.$$

We look for instance at

$$(N-1) \mathrm{Tr} \left(\Gamma_{N,\hbar,\beta} (B_{\hbar})_2 w_{12} (B_{\hbar})_2 \right) = \mathrm{Tr} \left(\Gamma_{N,\hbar,\beta} \sum_{j=2}^N (B_{\hbar})_j w_{1j} (B_{\hbar})_j \right).$$

For fixed x_1 , the operator $\sum_{j=2}^N (B_{\hbar})_j w_{1j} (B_{\hbar})_j$ (acting on the remaining $N-1$ variables) is estimated as in (52) by

$$\left\| \sum_{j=2}^N (B_{\hbar})_j w_{1j} (B_{\hbar})_j \right\| \leq \left\| |B_{\hbar}| w_N(x_1 - \cdot) |B_{\hbar}| \right\|_{\mathfrak{S}^1} \leq \frac{C}{N} \sup_{x_1 \in \mathbb{R}^d} \int_{B(x_1, R)} |w_N|.$$

When $\eta > 0$ the supremum can be bounded by $\int_{\mathbb{R}^d} |w_N| = \int_{\mathbb{R}^d} |w|$, since we assume that $w \in L^1(\mathbb{R}^d)$ in this case. When $\eta = 0$ (hence $w_N = w$) this can be controlled by

$$\sup_{x_1 \in \mathbb{R}^d} \int_{B(x_1, R)} |w| \leq |B_R| \|w_2\|_{L^\infty(\mathbb{R}^d)} + |B_R|^{1+\frac{2}{d}} \|w_1\|_{L^{1+\frac{d}{2}}(\mathbb{R}^d)}$$

since $w = w_1 + w_2 \in L^{1+d/2} + L^\infty(\mathbb{R}^d)$. In all cases, we have proved that

$$\mathrm{Tr} \left(\Gamma_{N,\hbar,\beta} \frac{1}{N} \sum_{1 \leq j \neq k \leq N} (B_{\hbar})_j w_{jk} ((B_{\hbar})_j + (B_{\hbar})_k) \right) = \mathcal{O}(N^{-1}).$$

It then remains to look at

$$\begin{aligned} & \left| (N-1) \operatorname{Tr} \left(\Gamma_{N,\hbar,\beta}(B_{\hbar})_{j'}(B_{\hbar})_2 w_{12} \right) \right| \\ & \leq (N-1) \sqrt{\operatorname{Tr} \left(\Gamma_{N,\hbar,\beta}(B_{\hbar})_{j'}(B_{\hbar})_2 |w_{12}|(B_{\hbar})_2(B_{\hbar})_{j'} \right)} \sqrt{\operatorname{Tr}(\Gamma_{N,\hbar,\beta}|w_{12}|)}, \end{aligned}$$

where $j' \in \{1, 2\}$. The first term is estimated as before by

$$\operatorname{Tr} \left(\Gamma_{N,\hbar,\beta}(B_{\hbar})_{j'}(B_{\hbar})_2 |w_{12}|(B_{\hbar})_2(B_{\hbar})_{j'} \right) \leq \frac{C}{N^3} \sup_{x \in \mathbb{R}^d} \int_{B(x,R)} |w_N|.$$

The supremum is uniformly bounded. Hence

$$\left| (N-1) \operatorname{Tr} \left(\Gamma_{N,\hbar,\beta}(B_{\hbar})_{j'}(B_{\hbar})_2 w_{12} \right) \right| \leq \frac{C}{N^{1/2}} \sqrt{\operatorname{Tr}(\Gamma_{N,\hbar,\beta}|w_{12}|)}. \quad (65)$$

The estimate on $\operatorname{Tr}(\Gamma_{N,\hbar,\beta}|w_{12}|)$ depends on the value of η . If $\eta = 0$, then $w_N = w$ and we have $\operatorname{Tr}(\Gamma_{N,\hbar,\beta}|w_{12}|) = \mathcal{O}(1)$ by the Lieb-Thirring inequality. If $\eta > 1/d$, we have assumed that $w \geq 0$, hence $\operatorname{Tr}(\Gamma_{N,\hbar,\beta}|w_{12}|) = \operatorname{Tr}(\Gamma_{N,\hbar,\beta} w_{12})$ is uniformly bounded since this term appears in the energy. Finally, when $0 < \eta < 1/d$, the Lieb-Thirring inequality implies

$$\operatorname{Tr}(\Gamma_{N,\hbar,\beta}|w_{12}|) \leq C \|w_N\|_{L^{1+d/2}(\mathbb{R}^d)} = CN^{d\eta \frac{d/2}{1+d/2}} \|w\|_{L^{1+d/2}(\mathbb{R}^d)}.$$

When inserted in (65), we obtain an error of the order $N^{-\frac{1}{2} + \frac{d\eta}{2} \frac{1}{1+d/2}} \rightarrow 0$. This concludes the proof of Lemma 15. \square

At this point we have finished the proof of Theorems 2 and 8 for the exact N -particle Gibbs states $\Gamma_{N,\hbar,\beta}$. It is possible to handle approximate Gibbs states using the relative entropy and Pinsker's inequality as we did for the one-particle Husimi functions. Indeed, consider a sequence of states Γ_N such that

$$\mathcal{E}_{\text{Can}}^{N,\hbar}(\Gamma_N) = e_{\text{Can}}^{\beta}(\hbar, N) + o(1).$$

We can write

$$\mathcal{E}_{\text{Can}}^{N,\hbar}(\Gamma_N) - e_{\text{Can}}^{\beta}(\hbar, N) = \frac{1}{\beta} \mathcal{H}(\Gamma_N, \Gamma_{N,\hbar,\beta})$$

where $\mathcal{H}(A, B) = \operatorname{Tr}(A(\log A - \log B))$ if the relative entropy. From the quantum Pinsker inequality $\mathcal{H}(A, B) \geq \|A - B\|_{\mathfrak{S}^1}^2 / 2$ we infer that

$$\operatorname{Tr} |\Gamma_N - \Gamma_{N,\hbar,\beta}| \longrightarrow 0$$

in trace norm. Since $\|m_{f,\Gamma}^{(k)}\|_{L^\infty(\mathbb{R}^{2dk})} \leq \operatorname{Tr} |\Gamma|$ by [FLS18, Eq. (1.15)], we conclude that

$$\left\| m_{f,\Gamma_N}^{(k)} - m_{f,\Gamma_{N,\hbar,\beta}}^{(k)} \right\|_{L^\infty(\mathbb{R}^{2dk})} \longrightarrow 0.$$

Therefore $m_{f,\Gamma_N}^{(k)}$ has the same weak limit as the exact Gibbs state. The proof of Theorems 2 and 8 is now complete.

5 Proof of Theorem 1: study of the semiclassical functional

This section is devoted to the proof of Theorem 1 and some auxiliary results on the semiclassical functional. We begin our analysis with the free particle case ($w = 0$) and then generalize to systems with pair interaction. We recall that the magnetic potential does not affect the energy, only the minimizer, and can be removed by a change of variables so we do not consider it here. For this section and for $\rho > 0$ we denote by

$$S_{\text{Vla}}(\rho) = \left\{ m \in L^1(\mathbb{R}^{2d}) \mid 0 \leq m \leq 1, \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} m = \rho \right\}.$$

the set of admissible semi-classical measures.

5.1 The free gas

Proposition 16 (Minimizing the free semi-classical energy). *Suppose that $w = 0$, and that $V_+ \in L^1_{\text{loc}}(\mathbb{R}^d)$ satisfies $\int_{\mathbb{R}^d} e^{-\beta V_+(x)} dx < \infty$ for some $\beta > 0$ and $V_- \in L^{d/2}(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$. Fix $\rho > 0$ and define $m_0 \in S_{\text{Vla}}(\rho)$ by*

$$m_0(x, p) := \frac{1}{1 + e^{\beta(p^2 + V(x) - \mu)}},$$

where μ is the unique chemical potential such that

$$\frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} m_0(x, p) dx dp = \rho.$$

Then

$$\begin{aligned} e_{\text{Vla}}^{\beta, 0}(\rho) &= \mathcal{E}_{\text{Vla}}^{\beta, \rho, 0}(m_0) \\ &= -\frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^{2d}} \log\left(1 + e^{-\beta(p^2 + V(x) - \mu)}\right) dx dp + \mu \rho. \end{aligned} \quad (66)$$

Proof. The map

$$\begin{aligned} R : \mathbb{R} &\longrightarrow \mathbb{R} \\ \mu &\longmapsto (2\pi)^{-d} \iint_{\mathbb{R}^{2d}} m_0(x, p) dx dp \end{aligned}$$

is well-defined on \mathbb{R} , using that

$$\frac{1}{1 + e^{\beta(p^2 + V(x) - \mu)}} \leq \frac{\max(1, e^{\beta\mu})}{1 + e^{\beta(p^2 + V(x))}}$$

which is integrable under our conditions on V , by the remarks after Theorem 1. In addition, R is increasing and continuous with

$$\lim_{\mu \rightarrow -\infty} R(\mu) = 0, \quad \lim_{\mu \rightarrow +\infty} R(\mu) = +\infty.$$

Therefore we can always find μ so that the density of m_0 equals the given ρ . Note then that

$$1 - m_0(x, p) = e^{\beta(p^2 + V(x) - \mu)} m_0(x, p) = \frac{1}{1 + e^{-\beta(p^2 + V(x) - \mu)}},$$

so that

$$\begin{aligned} \mathcal{E}_{\text{Vla}}^{\beta,\rho,0}(m_0) &= \frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^{2d}} \left\{ \beta (p^2 + V(x) - \mu) m_0 + m_0 \log m_0 \right. \\ &\quad \left. - m_0 \log \left(e^{\beta(p^2 + V(x) - \mu)} m_0 \right) \right\} dx dp \\ &\quad + \frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^{2d}} (\log(1 - m_0) + \beta \mu m_0) dx dp \\ &= -\frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^{2d}} \log \left(1 + e^{-\beta(p^2 + V(x) - \mu)} \right) dx dp + \mu \rho, \end{aligned}$$

showing the second equality in (66). That m_0 is the minimizer follows from the fact that the free energy is strictly convex. For instance, for any other $m \in S_{\text{Vla}}(\rho)$, since the function $s(t) = t \log t + (1 - t) \log(1 - t)$ is convex on $(0, 1)$ with derivative $s'(t) = \log\left(\frac{t}{1-t}\right)$, we have pointwise

$$\begin{aligned} s(m) &\geq s(m_0) + s'(m_0)(m - m_0) \\ &= -\beta(p^2 + V(x) - \mu)m + \beta(p^2 + V(x) - \mu)m_0 + s(m_0), \end{aligned} \quad (67)$$

replacing m_0 by its expression implies that $\mathcal{E}_{\text{Vla}}^{\beta,\rho,0}(m) \geq \mathcal{E}_{\text{Vla}}^{\beta,\rho,0}(m_0)$. That m_0 is the unique minimizer follows from the fact that $\mathcal{E}_{\text{Vla}}^{\beta,\rho,0}$ is a strictly convex functional. \square

Remark 17. For an arbitrary domain $\Omega \subseteq \mathbb{R}^{2d}$, we have by the very same arguments that

$$\begin{aligned} \min_{\substack{m \in L^1(\Omega) \\ 0 \leq m \leq 1}} \left\{ \frac{1}{(2\pi)^d} \int_{\Omega} \left((p^2 + V(x)) m(x, p) dx + \frac{1}{\beta} s(m(x, p)) \right) dx dp \right\} \\ = -\frac{1}{(2\pi)^d \beta} \int_{\Omega} \log \left(1 + e^{-\beta(p^2 + V(x))} \right) dx dp. \end{aligned}$$

with the unique minimizer $\widetilde{m}_0(x, p) = (1 + e^{\beta(p^2 + V(x))})^{-1}$ and no chemical potential since we have dropped the mass constraint.

5.2 The interacting gas

We now deal with the interacting case. When $w \neq 0$, to retrieve the existence of minimizers as well as their expression, we need to use compactness techniques and compute the Euler-Lagrange equation. We divide the proof in several lemmas. We start by proving the semi-continuity of the functional in Lemma 18 and then prove the existence of minimizers on $S_{\text{Vla}}(\rho)$ in Lemma 19. To obtain the form of the minimizers we compute the Euler-Lagrange equation but because the entropy s is not differentiable in 0 and 1 we first need to prove in Lemma 20 that minimizers cannot be equal to 0 nor 1 in sets of non zero measure. The proof of Theorem 1 is given at the end of this subsection.

Lemma 18. Fix $\rho, \beta_0 > 0$. Suppose that $w = 0$, and that $V_+ \in L_{\text{loc}}^1(\mathbb{R}^d)$, $V_- \in L^{d/2}(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ satisfies $\int_{\mathbb{R}^d} e^{-\beta_0 V_+(x)} dx < \infty$. Then for all $\beta > \beta_0$, $\mathcal{E}_{\text{Vla}}^{\beta,\rho,0}$ is L^1 -strongly lower semi-continuous on $S_{\text{Vla}}(\rho)$.

Proof. We have to show that for any $C_0 \in \mathbb{R}$

$$\mathcal{L}(C_0) := \left\{ m \in S_{\text{Vla}}(\rho) \mid \mathcal{E}_{\text{Vla}}^{\beta, \rho, 0}(m) \leq C_0 \right\}$$

is closed with respect to the L^1 -norm on $S_{\text{Vla}}(\rho)$. Let $(m_n) \subseteq \mathcal{L}(C_0)$ be a sequence converging towards some $m \in L^1(\mathbb{R}^d)$ with respect to the L^1 -norm. By the L^1 convergence we immediately have $\frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} m = \rho$, we can also extract a subsequence converging almost everywhere and obtain $0 \leq m \leq 1$. Applying Remark 17 with $\Omega = \{|x| + |y| \geq R\}$, we have for any $R > 0$ that

$$\begin{aligned} & \frac{1}{(2\pi)^d} \iint_{|x|+|p| \geq R} (p^2 + V(x)) m_n(x, p) + \frac{1}{\beta} s(m_n(x, p)) \, dx dp \\ & \geq -\frac{1}{\beta} \iint_{|x|+|p| \geq R} \log\left(1 + e^{-\beta(p^2 + V(x))}\right) \, dx dp = o_R(1). \end{aligned} \quad (68)$$

Now we use that (m_n) is bounded in $L^\infty(\mathbb{R}^{2d})$ to obtain that $m_n \rightarrow m$ in $L^p(\mathbb{R}^{2d})$ for all $1 \leq p < \infty$. By Fatou's lemma and dominated convergence we obtain

$$\begin{aligned} & \liminf_{n \rightarrow \infty} \iint_{|x|+|p| \leq R} (p^2 + V_+(x)) m_n(x, p) \, dx dp \\ & \geq \iint_{|x|+|p| \leq R} (p^2 + V_+(x)) m(x, p) \, dx dp, \\ & \iint_{|x|+|p| \leq R} V_-(x) m_n(x, p) \, dx dp \xrightarrow{n \rightarrow \infty} \iint_{|x|+|p| \leq R} V_-(x) m(x, p) \, dx dp. \end{aligned}$$

It remains to deal with the entropy term: by continuity of s and by dominated convergence we have

$$\iint_{|x|+|p| \leq R} s(m_n(x, p)) \, dx dp \xrightarrow{n \rightarrow \infty} \iint_{|x|+|p| \leq R} s(m(x, p)) \, dx dp.$$

All in all we obtain

$$\begin{aligned} C_0 & \geq \liminf_{n \rightarrow \infty} \mathcal{E}_{\text{Vla}}^{\beta, \rho, 0}(m_n) \\ & \geq \frac{1}{(2\pi)^d} \iint_{|x|+|p| \leq R} (p^2 + V(x)) m(x, p) \, dx dp \\ & \quad + \frac{1}{\beta} \iint_{|x|+|p| \leq R} s(m(x, p)) \, dx dp + o(R) \\ & \geq \frac{1}{(2\pi)^d} \iint_{|x|+|p| \leq R} (p^2 + V_+(x)) m(x, p) \, dx dp + o(R) \\ & \quad - \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} V_-(x) m(x, p) \, dx dp + \frac{1}{\beta} \iint_{\mathbb{R}^{2d}} s(m(x, p)) \, dx dp. \end{aligned}$$

Finally, we use the monotone convergence theorem and let R tend to ∞ to obtain $\mathcal{E}_{\text{Vla}}^{\beta, \rho, 0}(m) \leq C_0$. \square

Lemma 19. Fix $\rho, \beta_0 > 0$. Suppose that $w \in L^{1+d/2}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d) + \mathbb{R}_+\delta_0$, $V_+ \in L^1_{\text{loc}}(\mathbb{R}^d)$, $V_- \in L^{1+d/2}(\mathbb{R}^d)$ satisfies $\int_{\mathbb{R}^d} e^{-\beta_0 V_+(x)} \, dx < \infty$ and $V_+(x) \rightarrow \infty$ as $|x| \rightarrow \infty$. Then for all $\beta > \beta_0$, $\mathcal{E}_{\text{Vla}}^{\beta, \rho}$ is bounded below and has a minimizer m_0 in $S_{\text{Vla}}(\rho)$.

Proof. Let $(m_n) \subseteq S_{\text{Vla}}(\rho)$ be a minimizing sequence, i.e. $\mathcal{E}_{\text{Vla}}^{\beta, \rho}(m_n) \rightarrow e_{\text{Vla}}^{\beta}(\rho)$ as $n \rightarrow \infty$. Since (m_n) is bounded in both $L^1(\mathbb{R}^{2d})$ and $L^\infty(\mathbb{R}^{2d})$, one can verify that up to extraction the sequence has a weak limit $m_0 \in L^1(\mathbb{R}^{2d}) \cap L^\infty(\mathbb{R}^{2d})$ satisfying

$$\int_{\mathbb{R}^{2d}} m_n(x, p) \varphi(x, p) dx dp \rightarrow \int_{\mathbb{R}^{2d}} m_0(x, p) \varphi(x, p) dx dp \quad (69)$$

for any $\varphi \in L^1(\mathbb{R}^{2d}) + L^\infty(\mathbb{R}^{2d})$. Moreover, the weak limit m_0 satisfies $0 \leq m_0 \leq 1$ and $\int_{\mathbb{R}^{2d}} m_0 \leq \rho(2\pi)^d$. Note that we do not have pointwise convergence a priori. Let us prove that m_0 is a minimizer of $\mathcal{E}_{\text{Vla}}^{\beta, \rho}$ in $S_{\text{Vla}}(\rho)$. Our first step is to show the tightness of the sequence of probability measures (m_n) to obtain $\int_{\mathbb{R}^{2d}} m_0 = (2\pi)^d \rho$, then we argue that $m_0 \in S_{\text{Vla}}(\rho)$ and minimizes $\mathcal{E}_{\text{Vla}}^{\beta, \rho}$ using weak lower-semicontinuity.

We start out by bounding the interaction term using some of the kinetic energy. Let $\varepsilon > 0$ and let us write $w = w_1 + w_2 + a\delta_0$ with $w_1 \in L^{1+d/2}(\mathbb{R}^d)$, $\|w_2\|_{L^\infty(\mathbb{R}^d)} < \varepsilon$ and $a \geq 0$. We use Young's inequality to bound the interaction term

$$\begin{aligned} \int_{\mathbb{R}^d} w * \rho_{m_n} \rho_{m_n} &\geq \|w_1\|_{L^{1+d/2}(\mathbb{R}^d)} \|\rho_{m_n}\|_{L^{1+2/d}(\mathbb{R}^d)} \|\rho_{m_n}\|_{L^1(\mathbb{R}^d)} \\ &\quad + \|w_2\|_{L^\infty(\mathbb{R}^d)} \|\rho_{m_n}\|_{L^1(\mathbb{R}^d)}^2 \\ &\geq C\varepsilon \iint_{\mathbb{R}^{2d}} p^2 m_n(x, p) dx dp - C. \end{aligned} \quad (70)$$

In the last inequality we have used the well-known fact [LL01] that

$$\begin{aligned} \int_{\mathbb{R}^d} p^2 m(x, p) dp &\geq \inf_{\substack{0 \leq \tilde{m} \leq 1 \\ \int \tilde{m} = (2\pi)^d \rho_m(x)}} \int_{\mathbb{R}^d} p^2 \tilde{m}(p) dp \\ &= (2\pi)^d c_{\text{TF}} \frac{d}{d+2} \rho_m(x)^{1+2/d}, \end{aligned} \quad (71)$$

which gives the Lieb-Thirring inequality for classical measures on phase space. Similarly we have

$$\int_{\mathbb{R}^d} V_-(x) \rho_{m_n}(x) dx \leq C \left(\varepsilon^{-d/2} \|V_-\|_{L^{1+d/2}(\mathbb{R}^d)}^{1+d/2} + \varepsilon \|\rho_{m_n}\|_{L^{1+2/d}(\mathbb{R}^d)}^{1+2/d} \right). \quad (72)$$

Now using Proposition 16, (71), (70) and (72), denoting $\alpha = (\beta - \beta_0)/(2\beta)$ we have

$$\begin{aligned} C \geq \mathcal{E}_{\text{Vla}}^{\beta, \rho}(m_n) &\geq \frac{\alpha}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} (p^2 + V(x)) m_n + \frac{1}{2\rho} \int_{\mathbb{R}^d} (w * \rho_{m_n}) \rho_{m_n} \\ &\quad + \frac{1}{2} e_{\text{Vla}}^{\beta(1-\alpha), 0}(\rho) \\ &\geq \frac{\alpha - C\varepsilon}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} (p^2 + V_+(x)) m_n - C \end{aligned} \quad (73)$$

Note that by construction, $\beta(1-\alpha) > \beta_0$. Taking $\varepsilon > 0$ sufficiently small but positive, the above inequality shows the tightness condition

$$\iint_{\mathbb{R}^{2d}} (p^2 + V_+(x)) m_n(x, p) dx dp \leq C. \quad (74)$$

Therefore $\iint_{\mathbb{R}^{2d}} m_0 = (2\pi)^d \rho$.

Now we prove that $\liminf_{n \rightarrow \infty} \mathcal{E}_{\text{Vla}}^{\beta, \rho}(m_n) \geq \mathcal{E}_{\text{Vla}}^{\beta, \rho}(m_0)$. From the tightness condition it is easy to verify that $\rho_{m_n} \rightharpoonup \rho_{m_0}$ and that

$$\int_{\mathbb{R}^d} (w - a\delta_0) * \rho_{m_n} \rho_{m_n} \rightarrow \int_{\mathbb{R}^d} (w - a\delta_0) * \rho_{m_0} \rho_{m_0}.$$

To finish, we deal with the delta part of the interaction as well as the entropy part. We use that a continuous convex function is always weakly lower semi-continuous. We obtain

$$\begin{aligned} a \int_{\mathbb{R}^d} \rho_{m_0}^2 &= \int_{\mathbb{R}^d} \lim_{n \rightarrow \infty} \rho_{m_n}^2 \leq \lim_{n \rightarrow \infty} \int_{\mathbb{R}^d} \rho_{m_n}^2, \\ \int_{\mathbb{R}^d} s(m_0) &= \int_{\mathbb{R}^d} \lim_{n \rightarrow \infty} s(m_n) \leq \liminf_{n \rightarrow \infty} \int_{\mathbb{R}^d} s(m_n). \end{aligned}$$

□

Lemma 20. Fix $\rho, \beta_0 > 0$. Suppose that $w \in L^{1+d/2}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d) + \mathbb{R}_+ \delta_0$, $V_+ \in L^1_{\text{loc}}(\mathbb{R}^d)$, $V_- \in L^{1+d/2}(\mathbb{R}^d)$ satisfies $\int_{\mathbb{R}^d} e^{-\beta_0 V_+(x)} dx < \infty$ and $V_+(x) \rightarrow \infty$ as $|x| \rightarrow \infty$. Then any minimizer $m_0 \in S_{\text{Vla}}(\rho)$ of $\mathcal{E}_{\text{Vla}}^{\beta, \rho}$ satisfies

$$0 < m(x, p) < 1 \quad \text{for } (x, p) \in \mathbb{R}^{2d} \text{ almost everywhere.}$$

Proof. Define $\Omega_1 := \{m_0 = 1\}$ and $\Omega_0 := \{m_0 = 0\}$. Our goal is to prove that Ω_1 and Ω_0 have 0 measure. To this end, we will first show that $|\Omega_1| |\Omega_0| = 0$. Then we use that at least one of them is a null set to prove that so is the other one. Let us first assume neither of them are null sets. Let $r > 0$, $0 < \lambda < \frac{1}{2}$ and for almost every $(\xi_1, \xi_2) \in \Omega_1 \times \Omega_0$ define

$$\varphi_1 = \lambda \mathbf{1}_{B(\xi_1, r) \cap \Omega_1}, \quad \varphi_2 = \lambda \mathbf{1}_{B(\xi_2, r') \cap \Omega_0},$$

where $r' := \min \{s \geq 0 \mid |B(\xi_2, s) \cap \Omega_0| = |B(\xi_1, r) \cap \Omega_1|\}$. We will use the notation $v(r) = |B(\xi_1, r) \cap \Omega_1|$. Note that by Lebesgue's density theorem, for almost every $(\xi_1, \xi_2) \in \Omega_1 \times \Omega_0$ we have $v(r) > 0$ and $r' < \infty$. In order to obtain a contradiction, we will use $m_0 - \varphi_1 + \varphi_2 \in S_{\text{Vla}}(\rho)$ as a trial state and that m_0 is a minimizer of $\mathcal{E}_{\text{Vla}}^{\beta, \rho}$. Let us estimate the entropy, using that $s(0) = s(1) = 0$ and $s(t) = s(1-t)$, we obtain

$$\begin{aligned} \iint_{\mathbb{R}^{2d}} s(m_0 - \varphi_1 + \varphi_2) &= \iint_{\mathbb{R}^{2d}} s(m_0) + s(\varphi_1) + s(\varphi_2) \\ &= 2s(\lambda) v(r) + \iint_{\mathbb{R}^{2d}} s(m_0). \end{aligned}$$

It remains to estimate the contribution to the interaction energy, we have

$$\begin{aligned} \int_{\mathbb{R}^d} \rho_{m_0 - \varphi_1 + \varphi_2} w * \rho_{m_0 - \varphi_1 + \varphi_2} &= \int_{\mathbb{R}^d} \rho_{m_0} w * \rho_{m_0} + 2 \int_{\mathbb{R}^d} \rho_{\varphi_2 - \varphi_1} w * \rho_{m_0} \\ &\quad + \int_{\mathbb{R}^d} \rho_{\varphi_2 - \varphi_1} w * \rho_{\varphi_2 - \varphi_1}. \end{aligned}$$

Let $\varepsilon > 0$ and let us write $w = w_1 + w_2 + a\delta_0$ with $w_1 \in L^{1+d/2}(\mathbb{R}^d)$, $\|w_2\|_{L^\infty(\mathbb{R}^d)} < \varepsilon$ and $a \geq 0$.

We first use Young's inequality to bound the last term

$$\begin{aligned} & \int_{\mathbb{R}^d} w * (\rho_{\varphi_2} - \rho_{\varphi_1}) (\rho_{\varphi_2} - \rho_{\varphi_1}) \\ & \leq \|w_1\|_{L^{1+d/2}(\mathbb{R}^d)} \|\rho_{\varphi_2} - \rho_{\varphi_1}\|_{L^1(\mathbb{R}^d)} \|\rho_{\varphi_2} - \rho_{\varphi_1}\|_{L^{1+2/d}(\mathbb{R}^d)} \\ & \quad + \|w_2\|_{L^\infty(\mathbb{R}^d)} \|\rho_{\varphi_2} - \rho_{\varphi_1}\|_{L^1(\mathbb{R}^d)}^2 + a \|\rho_{\varphi_2} - \rho_{\varphi_1}\|_{L^2(\mathbb{R}^d)}^2 \\ & \leq C\lambda^2 \left(\|w\|_{L^{1+d/2}(\mathbb{R}^d)} v(r)^{1+\frac{d}{d+2}} + \|w_2\|_{L^\infty(\mathbb{R}^d)} v(r)^2 + av(r) \right). \end{aligned}$$

Next and similarly we estimate the second term (minus the delta interaction)

$$\begin{aligned} & \int_{\mathbb{R}^d} (w_1 + w_2) * \rho_{m_0} (\rho_{\varphi_2} - \rho_{\varphi_1}) \\ & \leq \|w_1\|_{L^{1+d/2}(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^{1+2/d}(\mathbb{R}^d)} \|\rho_{\varphi_2} - \rho_{\varphi_1}\|_{L^1(\mathbb{R}^d)} \\ & \quad + \|w_2\|_{L^\infty(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^1(\mathbb{R}^d)} \|\rho_{\varphi_2} - \rho_{\varphi_1}\|_{L^1(\mathbb{R}^d)} \\ & \leq C\lambda (\|w_1\|_{L^{1+d/2}(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^{1+2/d}(\mathbb{R}^d)} + \|w_2\|_{L^\infty(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^1(\mathbb{R}^d)}) v(r). \end{aligned}$$

Since m_0 is a minimizer, these estimates imply that

$$\begin{aligned} \mathcal{E}_{\text{Vla}}^{\beta,\rho}(m_0) & \leq \mathcal{E}_{\text{Vla}}^{\beta,\rho}(m_0 - \varphi_1 + \varphi_2) \\ & \leq \mathcal{E}_{\text{Vla}}^{\beta,\rho}(m_0) + \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} (p^2 + V(x) + a\rho_{m_0})(\varphi_2 - \varphi_1) \\ & \quad + C\lambda^2 \left(\|w\|_{L^{1+d/2}(\mathbb{R}^d)} v(r)^{1+\frac{d}{d+2}} + \|w_2\|_{L^\infty(\mathbb{R}^d)} v(r)^2 + av(r) \right) \\ & \quad + C\lambda \left(\|w_1\|_{L^{1+d/2}(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^{1+2/d}(\mathbb{R}^d)} \right. \\ & \quad \left. + \|w_2\|_{L^\infty(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^1(\mathbb{R}^d)} \right) v(r) + \frac{2s(\lambda)}{(2\pi)^d \beta} v(r). \end{aligned}$$

Now we divide the last inequality by $v(r)$ and we let r tend to zero and use the Lebesgue differentiation theorem (and the Lebesgue density theorem), to obtain that for almost all $(\xi_1, \xi_2) \in \Omega_1 \times \Omega_0$

$$\begin{aligned} -\frac{2s(\lambda)}{\lambda\beta} & \leq -p_1^2 - V(x_1) - a\rho_{m_0}(x_1) + p_2^2 + V(x_2) + a\rho_{m_0}(x_2) \\ & \quad + C \|w\|_{L^{1+d/2}(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^{1+2/d}(\mathbb{R}^d)}. \end{aligned}$$

Now letting λ tend to zero, we have that for almost all $(\xi_1, \xi_2) \in \Omega_1 \times \Omega_0$, $p_2^2 + V(x_2) + a\rho_{m_0}(x_2) - p_1^2 - V(x_1) - a\rho_{m_0}(x_1) = \infty$ which, since $V \in L_{\text{loc}}^{1+d/2}(\mathbb{R}^d)$ and $\rho_{m_0} \in L_{\text{loc}}^{1+2/d}(\mathbb{R}^d)$, implies that $|\Omega_1 \times \Omega_0| = 0$. Therefore, at least one of them is a null set, we will treat the case where $|\Omega_0| = 0$ and $|\Omega_1| \neq 0$, the other one can be dealt with similarly. Because m has finite mass we can find $\varepsilon > 0$ such that $\Omega_{2,\varepsilon} := \{1 - \varepsilon \leq m(x, p) \leq 1 - \varepsilon/2\}$ is not a null set. Defining φ_1 and φ_2 (replacing Ω_0 by $\Omega_{2,\varepsilon}$) as before and doing the same computations we obtain that for almost all

$$(\xi_1, \xi_2) \in \Omega_1 \times \Omega_{2,\varepsilon}$$

$$-\frac{s(\lambda)}{\lambda\beta} \leq -p_1^2 - V(x_1) - a\rho_{m_0}(x_1) + p_2^2 + V(x_2) + a\rho_{m_0}(x_2) + \frac{s(m(\xi_2) - \lambda) - s(m(\xi_2))}{\lambda} + C \|w\|_{L^{1+d/2}(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^{1+2/d}(\mathbb{R}^d)}.$$

Because s is continuously differentiable on $[1 - 2\varepsilon, 1 - \varepsilon/2]$, the difference quotient above is bounded uniformly in $\xi_2 \in \Omega_{2,\varepsilon}$ and $\lambda > 0$ small enough. Letting λ tend to zero, we end up with the same contradiction as before showing that Ω_1 is a null set. \square

Proof of Theorem 1. We assume $A = 0$ without loss of generality, since it can be removed by a change of variable.

We will first show that the expression (5) of the minimizers is correct by computing the Euler-Lagrange equation associated with any such minimizer m_0 . This gives automatically the expression of the minimum energy (6). We conclude, in the case $\widehat{w} \geq 0$, by showing that the chemical potential μ is given by (8).

Let $\varepsilon > 0$ small enough and $\varphi \in L^1 \cap L^\infty(\{\varepsilon < m_0 < 1 - \varepsilon\})$ such that $\iint_{\mathbb{R}^{2d}} \varphi(x, p) \, dx \, dp = (2\pi)^d \rho$. For $\delta = \frac{\varepsilon}{1 + \|\varphi\|_\infty}$ we have

$$m_t := \frac{m_0 + t\varphi}{1 + t} \in S_{V_{1a}}(\rho)$$

for all $t \in (-\delta, \delta)$. Since m_0 is a minimizer, we must have $\frac{d}{dt} \mathcal{E}_{V_{1a}}^\beta(m_t)|_{t=0} = 0$. Using that $\frac{d}{dt} m_t = (\varphi - m_0)(1 + t)^{-2}$ and $s'(t) = \log\left(\frac{t}{1-t}\right)$ we obtain

$$\begin{aligned} & \iint_{\mathbb{R}^{2d}} \left(p^2 + V(x) + \frac{1}{\rho} w * \rho_{m_0}(x) + \frac{1}{\beta} \log\left(\frac{m_0(x, p)}{1 - m_0(x, p)}\right) \right) \varphi(x, p) \, dx \, dp \\ &= \iint_{\mathbb{R}^{2d}} \left(p^2 + V(x) + \frac{1}{\rho} w * \rho_{m_0}(x) + \frac{1}{\beta} \log\left(\frac{m_0(x, p)}{1 - m_0(x, p)}\right) \right) m_0(x, p) \, dx \, dp. \end{aligned} \tag{75}$$

Denoting the right hand side by $(2\pi)^d \mu_{V_{1a}}(\rho) \rho$, we have shown for any φ verifying the above conditions that

$$\begin{aligned} & \iint_{\{\varepsilon < m < 1 - \varepsilon\}} \left(p^2 + V(x) + \frac{1}{\rho} w * \rho_{m_0}(x) + \frac{1}{\beta} \log\left(\frac{m_0(x, p)}{1 - m_0(x, p)}\right) - \mu_{V_{1a}}(\rho) \right) \varphi(x, p) \, dx \, dp = 0. \end{aligned}$$

This is enough for the left factor in the integrand above to be zero almost everywhere on $\{\varepsilon < m < 1 - \varepsilon\}$. But ε can be taken arbitrary small and by Lemma 20 we have $\bigcup_{\varepsilon > 0} \{\varepsilon < m < 1 - \varepsilon\} = \{0 < m < 1\} = \mathbb{R}^{2d}$ almost everywhere, from which we obtain (5).

That $\rho_{m_0} \in L^2(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ follows from Lemma 13 and the fact that m_0 satisfies (5).

It remains to prove (8) when it is assumed that $\widehat{w} \geq 0$. This is a classical argument and we only sketch it, we refer to [LS77b] for further details. First note that the assumption $\widehat{w} \geq 0$ ensures the convexity of $\mathcal{E}_{V_{1a}}^{\beta, \rho}$, hence for $\rho' > 0$, $F_{V_{1a}}^\beta(\rho', \rho)$ is the minimum of a convex function under a

linear constraint, it is therefore convex. This implies that, for $\rho' > 0$, the function $F_{\text{Vla}}^\beta(\cdot, \rho')$ is continuous on \mathbb{R}_+ and continuously differentiable except maybe in a countable number of values of ρ . We first show that

$$\mathbb{R}_+^* \ni \rho \mapsto \mu(\rho) \in \mathbb{R}$$

defines a bijection, where $\mu(\rho)$, defined in (5), is the Lagrange multiplier associated to the constraint ρ . Consider, for $\mu \in \mathbb{R}$, the unconstrained minimization problem

$$\inf_{0 \leq m \leq 1} \mathcal{E}_{\text{Vla}}^{\beta, \rho'}(m) - \frac{\mu}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} m = \inf_{\rho \geq 0} F_{\text{Vla}}^\beta(\rho, \rho') - \mu\rho. \quad (76)$$

This yields a minimizer m^μ and hence a density $\rho(\mu) := (2\pi)^{-d} \iint m^\mu$, see Remark 17. The expression of m^μ can be computed through the Euler-Lagrange equation,

$$m^\mu = \frac{1}{1 + e^{\beta(p^2 + V + \rho'^{-1} \rho_{m^\mu} * w - \mu)}}$$

From (76), the density m^μ must also satisfy $\mathcal{E}_{\text{Vla}}^{\beta, \rho'}(m^\mu) = F_{\text{Vla}}^\beta(\rho(\mu), \rho')$ and since $\widehat{w} \geq 0$, we conclude that m^μ is also the unique solution of this equation and must satisfy (5) where $\mu(\rho)$ appears. By identification, $\mu = \mu(\rho)$ is the Lagrange multiplier associated to the minimization problem at density ρ . This proves the bijective correspondance between $\mu(\rho)$ and ρ .

Finally, if $F_{\text{Vla}}^\beta(\cdot, \rho')$ is differentiable in some ρ_0 , the above discussion shows (8) for $\rho = \rho_0$. But because of the one-to-one correspondance between μ and ρ , $\partial_\rho F_{\text{Vla}}^\beta$ cannot be discontinuous, this concludes the proof. \square

Appendix A Grand canonical ensemble

This section is devoted to the study of the grand canonical ensemble where the conservation of the number of particle is broken. The thermodynamic limit of this ensemble is often easier to study than the canonical ensemble, we will use it as middle step for the proof of our main result. This section makes use of the formalism of the second quantization, we follow [Lew11] and refer to it for further details.

Let \mathfrak{H} be a separable Hilbert space, for $N \geq 1$ we denote by $\mathfrak{H}^N := \bigwedge^N \mathfrak{H}$ the antisymmetric tensor product of N copies of \mathfrak{H} . Define the fermionic Fock space over \mathfrak{H}

$$\mathcal{F} = \mathcal{F}_a(\mathfrak{H}) := \bigoplus_{n \geq 0} \mathfrak{H}^n$$

where $\bigwedge^0 \mathfrak{H} = \mathbb{C}$ by convention. For $N_1, N_2 \geq 1$ and $\psi_1 \in \mathfrak{H}^{N_1}$, $\psi_2 \in \mathfrak{H}^{N_2}$ define the antisymmetric tensor product $\psi_1 \wedge \psi_2 \in \mathfrak{H}^{N_1+N_2}$ by

$$\psi_1 \wedge \psi_2 = \frac{1}{\sqrt{N_1! N_2! (N_1 + N_2)!}} \sum_{\sigma \in \mathcal{S}_{N_1+N_2}} (-1)^\sigma P_\sigma(\psi_1 \otimes \psi_2),$$

where $(-1)^\sigma$ is the signature of the permutation σ and P_σ is the operator satisfying

$$P_\sigma \bigotimes_{i=1}^{N_1+N_2} u_i = \bigotimes_{i=1}^{N_1+N_2} u_{\sigma^{-1}(i)}$$

for any $(u_i) \subset \mathfrak{H}$. For any $f \in \mathfrak{H}$, the creation operator $a^\dagger(f)$ satisfies $a^\dagger(f)\mathfrak{H}^N \subset \mathfrak{H}^{N+1}$ for all $N \geq 0$ and

$$a^\dagger(f)\psi = f \wedge \psi$$

for all $N \geq 0$, $\psi \in \mathfrak{H}^N$. The annihilation operator $a(f)$ satisfies $a(f)\mathfrak{H}^N \subset \mathfrak{H}^{N-1}$ for all $N \geq 1$, $a(f)\mathbb{C} = \{0\}$ and

$$\langle \psi_{N-1}, a(f)\psi_N \rangle = \langle a^\dagger(f)\psi_{N-1}, \psi_N \rangle$$

for all $N \geq 1$, $\psi_{N-1} \in \mathfrak{H}^{N-1}$ and $\psi_N \in \mathfrak{H}^N$. These two operators are adjoints from one another. They verify the Canonical Anticommutation Relations

$$\begin{cases} a(f)a^\dagger(g) + a^\dagger(g)a(f) = \langle f, g \rangle \mathbb{1} \\ a^\dagger(f)a^\dagger(g) + a^\dagger(g)a^\dagger(f) = 0 \\ a(f)a(g) + a(g)a(f) = 0. \end{cases}$$

Let H be a self-adjoint operator on \mathfrak{H} such that e^{-H} is trace class. The second quantization of H , acting on \mathcal{F} , is defined as

$$\mathbb{H} := 0 \oplus \bigoplus_{n \geq 1} \sum_{j=1}^n H_j, \quad (77)$$

where H_j is the operator acting as H on the j^{th} variable. At inverse temperature $\beta > 0$ and chemical potential $\mu \in \mathbb{R}$, the grand canonical functional is defined by

$$\mathcal{E}_{\text{GC}}^{\beta, \mu}(\Gamma) := \text{Tr } \mathbb{H} - \mu \mathcal{N} \Gamma + \frac{1}{\beta} \text{Tr } \Gamma \log \Gamma$$

where $\mathcal{N} = d\Gamma(1)$ is the number operator. The free energy functional is defined on the set of grand canonical states

$$\mathcal{S}_{\text{GC}} = \{\Gamma \in \mathfrak{S}_1(\mathcal{F}) \mid 0 \leq \Gamma, \text{Tr } \Gamma = 1\}. \quad (78)$$

The minimization of the free energy is obtained from Gibbs' variational principle.

Lemma 21 (Gibb's variational principle). *Let $\beta > 0$ and \mathfrak{H} be a Hilbert space. Let H be a self-adjoint operator on \mathfrak{H} such that $\text{Tr } e^{-\beta H} < \infty$. Then for all states $\Gamma \in \mathcal{S}(\mathfrak{H}) = \{\Gamma \in \mathfrak{B}(\mathfrak{H}) \mid 0 \leq \Gamma, \text{Tr } \Gamma = 1\}$ we have*

$$\text{Tr } H \Gamma + \frac{1}{\beta} \text{Tr } \Gamma \log \Gamma \geq -\frac{1}{\beta} \ln \text{Tr } e^{-\beta H},$$

with equality if and only if $\Gamma = e^{-\beta H} / \text{Tr } e^{-\beta H}$.

Proof. The function $S : x \mapsto x \log x$ is convex so that we can apply Klein's inequality [Rue99, Theorem 2.5.2]: for any $\Gamma \in \mathcal{S}(\mathfrak{H})$ such that $\text{Tr } H \Gamma < \infty$ we have

$$\text{Tr} \left(S(\Gamma) - S(e^{-\beta H} / \text{Tr } e^{-\beta H}) - (\Gamma - e^{-\beta H} / \text{Tr } e^{-\beta H}) S'(e^{-\beta H} / \text{Tr } e^{-\beta H}) \right) \geq 0$$

with equality if and only if $\Gamma = e^{-\beta H} / \text{Tr } e^{-\beta H}$. Here $S'(x) = \log x + 1$ and the last term above makes sense because the range of Γ is contained in the domain of H . Rearranging the inequality gives the result. \square

Applying Gibbs' variational principle we obtain that $\mathcal{E}_{\text{GC}}^{\beta, \mu}(\Gamma)$ is minimized by

$$\Gamma_0 := e^{-\beta(\mathbb{H} - \mu \mathcal{N})} Z^{-1}, \quad (79)$$

where we denote by $Z = \text{Tr} e^{-\beta(\mathbb{H}-\mu\mathcal{N})}$ the partition function. The minimum energy is

$$e_{\text{GC}}^\beta(\mu) := \inf_{\Gamma \in S_{\text{GC}}} \mathcal{E}_{\text{GC}}^{\beta,\mu}(\Gamma) = -\frac{1}{\beta} \log \text{Tr} e^{-\beta(\mathbb{H}-\mu\mathcal{N})}. \quad (80)$$

Minimizers of free systems such as the one defined above belong to a class of operators called quasi-free states. These operators satisfy useful properties, we will review some of them we are interested in. These are known results (see e.g. [BLS94; Sol07]) but for the sake of completeness we recall them.

Proposition 22 (1-body reduced density matrix of quasi-free states). *Let $\Gamma_0 = \frac{1}{Z} e^{-\beta\mathbb{H}}$ the quasi-free state (79) associated the the Hamiltonian H . Then*

— the 1-body reduced density matrix $\Gamma_0^{(1)}$ of Γ_0 is given by

$$\Gamma_0^{(1)} = \frac{1}{1 + e^{\beta H}}, \quad (81)$$

— the entropy of Γ_0 satisfies

$$S(\Gamma_0) := \text{Tr}_{\mathcal{F}} \Gamma_0 \log \Gamma_0 = \text{Tr}_{\mathfrak{H}} \left(\Gamma_0^{(1)} \log \Gamma_0^{(1)} + \left(1 - \Gamma_0^{(1)}\right) \log \left(1 - \Gamma_0^{(1)}\right) \right), \quad (82)$$

— for all $\Gamma \in S_{\text{GC}}$ such that $\Gamma^{(1)} = \Gamma_0^{(1)}$ we have

$$S(\Gamma) \geq S(\Gamma_0). \quad (83)$$

Proposition 23. *Let $\Gamma \in S_{\text{GC}}$ be any grand canonical fermionic state with $\text{Tr}(\Gamma\mathcal{N}) = \text{Tr}(\Gamma^{(1)}) < \infty$, then there exists $p \geq 0$, $(\varphi_i)_{1 \leq i \leq p} \subset \mathfrak{H}$ an orthonormal family (possibly empty) and Γ_{QF} a quasi-free state on $\mathcal{F} \left((\text{span}\{\varphi_i\}_{1 \leq i \leq p})^\perp \right)$ such that*

$$\begin{aligned} \Gamma^{(1)} &= (|\varphi_1 \wedge \dots \wedge \varphi_p\rangle \langle \varphi_1 \wedge \dots \wedge \varphi_p| \wedge \Gamma_{QF})^{(1)} \\ &= \sum_{i=1}^p |\varphi_i\rangle \langle \varphi_i| + \Gamma_{QF}^{(1)}, \end{aligned}$$

where the antisymmetric product of operators is stated in Definition 32.

An immediate application of Proposition 22 and Proposition 23 are the following corollaries.

Corollary 24 (Entropy bound). *For all $\Gamma \in S_{\text{GC}}$ with $\text{Tr}(\Gamma\mathcal{N}) = \text{Tr}(\Gamma^{(1)}) < \infty$ we have*

$$\text{Tr}_{\mathcal{F}} \Gamma \log \Gamma \geq \text{Tr}_{\mathfrak{H}} \left(\Gamma^{(1)} \log \Gamma^{(1)} + \left(1 - \Gamma^{(1)}\right) \log \left(1 - \Gamma^{(1)}\right) \right).$$

Corollary 25. *Let $\beta > 0$, $\mu \in \mathbb{R}$ and H be a self-adjoint operator on \mathfrak{H} such that $\text{Tr} e^{-\beta H} < \infty$ then*

$$e_{\text{GC}}^\beta(\mu) = -\frac{1}{\beta} \text{Tr}(\log(1 + e^{-\beta(H-\mu)})).$$

Proof of Proposition 22. Without loss of generality we can assume $\beta = 1$. Since e^{-H} is trace class, we may write $H = \sum_i h_i |u_i\rangle \langle u_i|$, where (u_i) is an orthonormal basis of \mathfrak{H} and $(h_i) \subset \mathbb{R}$

with $h_i \rightarrow \infty$ as $i \rightarrow \infty$. Then its second quantization is [Lew11]

$$d\Gamma(H) = \sum_{i \geq 1} h_i a_i^\dagger a_i,$$

where $a_i := a(\varphi_i)$ and $a_i^\dagger := a^\dagger(\varphi_i)$. Since $(u_i)_i$ is orthonormal one can verify that $(a_i^\dagger a_i)_i$ is a family of commuting projections which allows us to write

$$e^{-d\Gamma(H)} = \prod_{i \geq 1} e^{-h_i a_i^\dagger a_i} = \prod_{i \geq 1} \left((1 - a_i^\dagger a_i) + e^{-h_i} a_i^\dagger a_i \right).$$

Note that the antisymmetric Fock space generated by a single normalized vector u satisfies $\mathcal{F}_a(\mathbb{C}u) = (\mathbb{C} \oplus \mathbb{C}u)$. We will use that $\mathcal{F}_a\left(\bigoplus_{i \geq 1} \mathbb{C}u_i\right) \simeq \bigotimes_{i \geq 1} \mathcal{F}_a(\mathbb{C}u_i)$ via the unitary operator defined on the canonical basis of $\mathcal{F}_a\left(\bigoplus_{i \geq 1} \mathbb{C}u_i\right)$ by

$$\begin{aligned} \mathcal{U} : \mathcal{F}_a\left(\bigoplus_{i \geq 1} \mathbb{C}u_i\right) &\longrightarrow \bigotimes_{i \geq 1} \mathcal{F}_a(\mathbb{C}u_i) = \bigotimes_{i \geq 1} \mathbb{C}^2 \\ u_{i_1} \wedge \dots \wedge u_{i_k} &\longmapsto \bigotimes_{i \geq 1} \left(\prod_{p=1}^k (1 - \delta_{i,i_p}) \right) \end{aligned}$$

for all $k \geq 1$. Here $\bigotimes_{i \geq 1} \mathbb{C}^2$ is defined by considering the linear span of all elements of the form $\bigotimes_{i \geq 1} u_i$ with $u_i \in \mathbb{C}^2$ and $u_i = (1, 0)^\top$ except for finitely many i , and then taking the completion with respect to the canonical scalar product $\langle \bigotimes_i u_i, \bigotimes_i v_i \rangle = \prod_i \langle u_i, v_i \rangle_{\mathbb{C}^2}$. For more details on infinite tensor products of Hilbert space and von Neumann algebras, see for instance [BR02; Gui66]. The image of the canonical basis by \mathcal{U} is clearly orthonormal, one can check its completeness using the one-to-one correspondance $\mathcal{P}_{fin}(\mathbb{Z}_+) \simeq L^1(\mathbb{Z}_+, \{0, 1\})$, where $\mathcal{P}_{fin}(\mathbb{Z}_+)$ is the set of all finite subsets of \mathbb{Z}_+ . One verifies that

$$\mathcal{U}^* a_k^\dagger a_k \mathcal{U} = \bigotimes_{i \geq 1} \begin{pmatrix} 1 - \delta_{i,k} & 0 \\ 0 & 1 \end{pmatrix},$$

so that, in this representation of the Fock space, the Gibbs state Γ_0 becomes

$$\mathcal{U}^* \Gamma_0 \mathcal{U} = \bigotimes_{i \geq 1} \frac{1}{Z_i} \begin{pmatrix} 1 & 0 \\ 0 & e^{-h_i} \end{pmatrix}, \quad (84)$$

where $Z_i = 1 + e^{-h_i}$. From here, using the additivity of the logarithm we have

$$\begin{aligned} \langle u_i, \Gamma_0^{(1)} u_j \rangle &= \text{Tr}(\Gamma_0 a^*(u_i) a(u_j)) = \frac{e^{-h_i}}{1 + e^{-h_i}} \delta_{ij}, \\ \text{Tr} \Gamma_0 \log \Gamma_0 &= \sum_{i \geq 1} S(Z_i^{-1}) + S((1 + e^{-h_i}) Z_i^{-1}) \end{aligned}$$

implying that

$$\begin{aligned}\Gamma_0^{(1)} &= (1 + e^H)^{-1}, \\ S(\Gamma_0) &= \text{Tr} \Gamma_0^{(1)} \log \Gamma_0^{(1)} + (1 - \Gamma_0^{(1)}) \log(1 - \Gamma_0^{(1)}).\end{aligned}$$

To obtain Eq. (83) we use that Γ_0 minimizes the grand canonical functional. Indeed, for all Γ such that $\Gamma^{(1)} = \Gamma_0^{(1)}$ we have

$$\mathcal{E}_{\text{GC}}(\Gamma) = \text{Tr}(H\Gamma_0^{(1)}) + S(\Gamma) \geq \mathcal{E}_{\text{GC}}(\Gamma_0) = \text{Tr}(H\Gamma_0^{(1)}) + S(\Gamma)$$

and hence $S(\Gamma) \geq S(\Gamma_0)$. \square

Proof of Proposition 23. Using the canonical anti-commutation relations or the unitary transform \mathcal{U} of the proof of Proposition 22, it can be checked that we have $\|a(f)\| = \|a^\dagger(f)\| = \|f\|$ for all $f \in \mathfrak{H}$, hence for any state $\Gamma \in S_{\text{GC}}$ and for all $f \in \mathfrak{H}$,

$$\langle f, \Gamma^{(1)} f \rangle = \text{Tr}(\Gamma a^\dagger(f) a(f)) \leq \|f\|^2$$

so that $0 \leq \Gamma^{(1)} \leq \mathbb{1}$. Thus we may write $\Gamma^{(1)} = \sum_j \mu_j |\varphi_j\rangle \langle \varphi_j|$ with $0 \leq \mu_j \leq 1$ and $\sum_j \mu_j = N$, where $(\varphi_j)_j$ is an orthonormal basis of \mathfrak{H} . We want to define a quasi-free state having $\Gamma^{(1)}$ as one-body density matrix. In order to do that we want to define a self-adjoint operator H on \mathfrak{H} by

$$H := \log \frac{1 - \Gamma^{(1)}}{\Gamma^{(1)}} = \sum_j \log \frac{1 - \mu_j}{\mu_j} |\varphi_j\rangle \langle \varphi_j|$$

and consider the quasi-free state $\Gamma_{QF} := e^{-d\Gamma(H)} / \text{Tr} e^{-d\Gamma(H)}$. We need to take care of the eigenvalues $\mu_j \in \{0, 1\}$. The zero eigenvalues are not a problem since we can set $H = +\infty$ (i.e. take the kernel of $\Gamma^{(1)}$ out of the domain of H) so we assume without loss of generality that $\mu_j > 0$ for all $j \geq 1$. But we cannot do the same of the eigenvalues which are equal to 1 since we want to recover them when we compute the 1-pdm. Let j_0 such that $\mu_{j_0} = 1$, this would mean that

$$\langle \varphi_{j_0}, \Gamma^{(1)} \varphi_{j_0} \rangle = \text{Tr} \Gamma a_{j_0}^\dagger a_{j_0} = 1.$$

Let us write spectral decomposition of $\Gamma = \sum_j \lambda_j |\Psi_j\rangle \langle \Psi_j|$, from the equality above, and because $\text{Tr} \Gamma = 1$, we obtain that for all $j \geq 1$, $\langle \Psi_j, a_{j_0}^\dagger a_{j_0} \Psi_j \rangle = 1$. This implies that for all $j \geq 1$ we have $\Psi_j = a_{j_0}^\dagger a_{j_0} \Psi_j = a_{j_0}^\dagger \widetilde{\Psi}_j = \varphi_{j_0} \wedge \widetilde{\Psi}_j$ with $\widetilde{\Psi}_j = a_{j_0} \Psi_j$. We recognize the anti-symmetrization of states defined in Eq. (102), we have: $\Gamma = |\varphi_{j_0}\rangle \langle \varphi_{j_0}| \wedge \widetilde{\Gamma}$ with $\widetilde{\Gamma} = \sum_j \lambda_j |\widetilde{\Psi}_j\rangle \langle \widetilde{\Psi}_j|$. Repeating the procedure as many times as necessary, we can assume that $\Gamma = |\varphi_1 \wedge \dots \wedge \varphi_p\rangle \langle \varphi_1 \wedge \dots \wedge \varphi_p| \wedge \widetilde{\Gamma}$ with $\widetilde{\Gamma}$ a state on $\mathcal{F} \left((\text{span}\{\varphi_i\}_{1 \leq i \leq p})^\perp \right)$ satisfying $\widetilde{\Gamma}^{(1)} < 1$. We can now define the Hamiltonian H on

$$D(H) := \left\{ \psi \in (\text{span}\{\varphi_i\}_{1 \leq i \leq p})^\perp \mid \sum_{j > p} (\log \frac{1 - \mu_j}{\mu_j})^2 |\langle \psi, \varphi_j \rangle|^2 < \infty \right\}$$

as above and consider the corresponding quasifree state Γ_{QF} . Now using Proposition 22 to compute the 1-body reduced density matrix of Γ_{QF} we obtain

$$\Gamma_{QF}^{(1)} = (1 + \exp(\log \frac{1 - \widetilde{\Gamma}^{(1)}}{\widetilde{\Gamma}^{(1)}}))^{-1} = \widetilde{\Gamma}^{(1)}.$$

Applying Lemma 33 ends the proof. \square

Proof of Corollary 25. Since Γ_0 minimizes $\mathcal{E}_{GC}^{\beta,\mu}$ on S_{GC} and thanks to Proposition 22 we can compute $e_{GC}^\beta(\mu) = \beta^{-1} \text{Tr} \log(\Gamma_0^{(1)})$ hence the result. \square

Appendix B The free Fermi gas in the canonical ensemble

This section is devoted to the study of the free gas. We prove the existence of thermodynamic limit for the canonical ensemble in Section B.1 and conclude by proving the equivalence of the canonical ensemble and the grand-canonical ensemble in Section B.2. Of course, the existence of the thermodynamic limit is well known but we deal with a mean-field interaction therefore we wanted to state the whole proof for completeness.

B.1 Thermodynamic limit of the canonical ensemble

Here we follow the method used in [Rue99], i.e. the subadditivity of the energy, to prove the thermodynamic limit directly for the canonical ensemble. But unlike in [Rue99] and because we only consider free particles we do not use the micro-canonical ensemble as a starting point. We deal with the interacting case separately to take into account the mean-field regime.

Let $L > 0$, $\Lambda_L := [0, L]^d$ and $-\Delta_L$ be the Laplacian with Dirichlet boundary condition in Λ_L . Define the free energy of a N particle state $\gamma \in S_{\text{Can}}$ at inverse temperature $\beta > 0$

$$\mathcal{E}_{\text{Can},0}^{N,L}(\gamma) = \text{Tr} \left(\sum_{i=1}^N (-\Delta_L)_i \gamma \right) + \frac{1}{\beta} \text{Tr}(\gamma \ln \gamma).$$

Define the minimum free energy

$$e_{\text{Can}}^0(L, N) = \inf_{\Gamma \in S_{\text{Can}}} \mathcal{E}_{\text{Can},0}^{N,L}(\Gamma).$$

Let Λ be an open subset of \mathbb{R}^3 , we denote $\delta(\Lambda)$ the diameter of Λ , $\partial\Lambda = \bar{\Lambda} \setminus \Lambda$ its boundary, and for $h \geq 0$, $\partial\Lambda_h := \{x \in \mathbb{R}^d, \text{dist}(x, \Lambda) \leq h\}$. Following [Rue99; Fis64] we make the following definition.

Definition 26. Let $(\Lambda_N)_N$ be a sequence of open connected subsets of \mathbb{R}^d . We say that this sequence of sets tends to infinity in the sense of Fisher if

$$\lim_{N \rightarrow \infty} |\Lambda_N| = +\infty \tag{85}$$

and there exists a shape function $\pi : \mathbb{R}_+^* \rightarrow \mathbb{R}_+^*$ such that

$$\lim_{\alpha \rightarrow 0} \pi(\alpha) = 0 \tag{86}$$

and for sufficiently small α and all N

$$|\partial(\Lambda_N)_{\alpha\delta(\Lambda)}| \leq |\Lambda_N| \pi(\alpha). \tag{87}$$

Theorem 27 (Thermodynamic limit for the canonical ensemble without interaction). *There exists a function $f_{\text{Can}}^0 : \mathbb{R}_+ \rightarrow \mathbb{R}$ such that for any $\rho > 0$ and any sequence of sets $(\Lambda_N)_N$ tending*

to infinity in the sense of Fisher and such that

$$\lim_{N \rightarrow \infty} \frac{N}{|\Lambda_N|} = \rho > 0 \quad (88)$$

we have

$$\lim_{N \rightarrow \infty} \frac{e_{\text{Can}}^0(\Lambda_N, N)}{|\Lambda_N|} = f_{\text{Can}}^0(\rho). \quad (89)$$

The proof goes as follows, we first prove the result in the case of a fixed density $N/|\Lambda_N| = \rho$ for a particular sequence of cubes and then for arbitrary cubes. In a second step, we prove it for cubes with $N/|\Lambda_N| \rightarrow \rho$ as $N \rightarrow \infty$. And in a last step, we show it for an arbitrary sequence using approximation of cubes.

For simplicity, when $\rho = N/|\Lambda_N|$ is assumed to be constant we take it equal to 1.

We begin with a simple Lemma.

Lemma 28. (*Upper bound on the free energy in a box*) For all $L, N > 0$ we have

$$e_{\text{Can}}^0(N, L) \leq \frac{\pi^2 d}{2} \times \frac{N^{1+2/d}}{L^2}.$$

Proof. For $\ell > 0$, define $u^\ell(x) = \prod_{i=1}^d \sin(\frac{\pi x_i}{\ell})$ for $x = (x_1, \dots, x_d) \in [0, \ell]^d$ and 0 elsewhere. For $k \in \mathbb{Z}^d$ let $u_k^\ell(x) = u^\ell(x - k\ell)$. Take $\ell = LN^{-1/d}$ and define

$$\psi := \bigwedge_{k \in \mathbb{Z}^d \cap \Lambda_{L/\ell}} u_k^\ell.$$

We have

$$\mathcal{E}_{\text{Can},0}^{N,L}(|\psi\rangle \langle \psi|) = N\ell^{-2} \int_{\mathbb{R}^d} |\nabla u^1|^2 \quad (90)$$

which proves the result. \square

Proof of Theorem 27.

• *A special sequence of cubes at $\rho = 1$.*

For $k \geq 0$, define $N_k = 2^{dk}$ and $\Lambda_{N_k} = [0, 2^k]^d$. For $u \in \{0, 2^k\}^d$, let γ_k^u be the unique minimizer of the canonical free energy $e_{\text{Can}}^0(u + \Lambda_{N_k}, N_k)$. Notice that $\Lambda_{N_{k+1}} = \bigcup_u (u + \Lambda_{N_k})$. Using Lemma 35 and the sequence $(\gamma_k^u)_u$ we can define $\tilde{\gamma}_{k+1}$, a state of $\bigwedge^{2^d} \left(\bigwedge^{N_k} L^2(\Lambda_{N_{k+1}}) \right) = \bigwedge^{N_{k+1}} L^2(\Lambda_{N_{k+1}})$ such that Eq. (106) and Eq. (107) are verified. Therefore

$$\frac{e_{\text{Can}}^0(\Lambda_{N_{k+1}}, N_{k+1})}{N_{k+1}} \leq \frac{\mathcal{E}_{\text{Can},0}(\tilde{\gamma}_{k+1})}{N_{k+1}} = \frac{1}{N_{k+1}} \sum_{u \in \{0, 2^k\}^d} \mathcal{E}_{\text{Can},0}(\gamma_k^u) = \frac{e_{\text{Can}}^0(\Lambda_{N_k}, N_k)}{N_k}. \quad (91)$$

The sequence $\left(\frac{e_{\text{Can}}^0(\Lambda_{N_k}, N_k)}{N_k} \right)_k$ is decreasing and therefore has a limit when $k \rightarrow \infty$. This limit is finite since the sequence is bounded, see for instance Proposition 12. We denote by $f_{\text{Can}}^0(\rho)$ this limit.

• *Cubes at $\rho = 1$.*

Define $C_N = C(N^{1/d}) := [0, N^{1/d}]$, we will show that there is $k_1(N), k_2(N) \rightarrow \infty$ as $N \rightarrow \infty$

such that

$$\frac{e_{\text{Can}}^0(\Lambda_{N_{k_2}}, N_{k_2})}{N_{k_2}} + o(1) \leq \frac{e_{\text{Can}}^0(C_N, N)}{N} \leq \frac{e_{\text{Can}}^0(\Lambda_{N_{k_1}}, N_{k_1})}{N_{k_1}} + o(1) \quad (92)$$

First let us find the upper bound by dividing the box C_N in boxes of side length 2^{k_0} , for some $k_0 \geq 1$, plus a remaining part which will have a negligible impact. We will make an ansatz out of this decomposition. Let N be sufficiently large, then there is a unique couple $q_N \in \mathbb{N}$ and $2^{k_0} \leq r_N < 2^{k_0+1}$ such that

$$N^{1/d} = q_N 2^{k_0} + r_N. \quad (93)$$

Putting 2^{dk_0} of the N particles in each box, it remains

$$N^- = N - 2^{dk_0} q_N^d = \mathcal{O}(N^{1-\frac{1}{d}})$$

particles which we place in the remaining part of the box C_N . More precisely, for $u \in [0, q_N - 1]^d$ and $v \in [0, q_N - 1]^{d-1}$, let γ_u^+ be the minimizer of $\mathcal{E}_{\text{Can}}^0$ in the box $2^{k_0}u + \Lambda_{N_{k_0}}$ with N_{k_0} particles and let γ_v^- be the minimizer in the box $(q_N, v) + C(r_N)$ with 1 particle. Note that

$$\left(\bigcup_{u \in [0, q_N - 1]^d} (2^{k_0}u + \Lambda_{N_{k_0}}) \right) \cup \left(\bigcup_{v \in [0, q_N - 1]^{d-1}} ((q_N, v) + C(r_N)) \right) \subset C_N.$$

Because $N^- = o(q_N^{d-1})$ we can find $(v_i)_{1 \leq i \leq N^-} \subset [0, q_N - 1]^{d-1}$, with $v_i \neq v_j$ if $i \neq j$, we can construct by Lemma 35 a state γ of $\bigwedge^N L^2(C_N)$ out of $(\gamma_u^+)_u \cup (\gamma_{v_i}^-)_i$ such that

$$\mathcal{E}_{\text{Can}}^0(\gamma) = q_N^d e_{\text{Can}}^0(\Lambda_{N_{k_0}}, N_{k_0}) + N^- e_{\text{Can}}^0(C(r_N), 1).$$

By Lemma 28

$$e_{\text{Can}}^0(C(r_N), 1) \leq C \frac{1}{r_N^2} = \mathcal{O}(1)$$

so that

$$\frac{e_{\text{Can}}^0(C_N)}{N} \leq \frac{e_{\text{Can}}^0(\Lambda_{N_{k_0}}, N_{k_0})}{2^{k_0}} + \mathcal{O}(N^{-1/d}).$$

This proves the upper bound since k_0 was taken arbitrarily large. For the lower bound we will do the opposite: we will divide $\Lambda_{N_{2k}}$ in cubes C_N plus a remaining term having a negligible impact. Take $k = \lfloor \log_2(N)/d \rfloor$ and consider $\Lambda_{N_{2k}}$. There exists a unique couple $(q_N, r_N) \in \mathbb{N}^2$ with $N^{1/d} \leq r_N \leq 2N^{1/d}$ such that

$$2^{2k} = q_N N^{1/d} + r_N.$$

Putting N of the 2^{2kd} particles in each of the q_N copies of C_N , it remains

$$N^- = 2^{2kd} - q_N^d N = q_N^d N \left(\left(1 + \frac{r_N}{q_N N^{1/d}} \right)^d - 1 \right) = \mathcal{O}(N^{2-1/d})$$

particles which we will place in the remaining part of the box $\Lambda_{N_{2k}}$. As previously, for $u \in [0, q_N - 1]^d$ and $v \in [0, q_N - 1]^{d-1}$, let γ_u^+ be the minimizer of $\mathcal{E}_{\text{Can}}^0$ in the box $N^{1/d}u + C_N$ with N particles and let γ_v^- be the minimizer in the box $(q_N, v) + C(r_N)$ with N_v particles such that $N_v \leq CN$ (for some constant C independent of N) and $\sum_v N_v = N^-$ (which is possible to do, cf. table below). Now by Lemma 35 we can construct as before a state γ on $\bigwedge^{N_{2k}} L^2(\Lambda_{N_{2k}})$

having free energy

$$\mathcal{E}_{\text{Can}}^0(\gamma) = q_N^d e_{\text{Can}}^0(C_N, N) + N^- e_{\text{Can}}^0(C(r_N), CN).$$

Using Lemma 28 to bound the second term in the right hand side above, we obtain

$$\frac{e_{\text{Can}}^0(\Lambda_{N_{2k}})}{N_{2k}} \leq \frac{e_{\text{Can}}^0(C_N, N)}{N} + \mathcal{O}(N^{-1/d}).$$

For the sake of clarity we summarize the more relevant quantities in this table. We say that $f = \Theta(g)$ if $f = \mathcal{O}(g)$ and $g = \mathcal{O}(f)$.

Total number of particles	2^{2kd}	$\Theta(N^2)$
Nb of waste particles N^-	$2^{2kd} - q_N^d N$	$\mathcal{O}(N^{2-1/d})$
Side length of a waste box	r_N	$\Theta(N^{1/d})$
Nb of waste boxes	$(2^{2k}/r_N)^{d-1}$	$\Theta(N^{1-1/d})$
Nb of part. per waste box	$\mathcal{O}(N^{2-1/d})/\Theta(N^{1-1/d})$	$\mathcal{O}(N)$
Free energy per waste box	$\mathcal{O}(N^{1+2/d}/r_N^2)$	$\mathcal{O}(N)$
Total contribution of the waste energy	$\Theta(N^{1-1/d}) \times \mathcal{O}(N)$	$\mathcal{O}(N^{2-1/d})$

• *Cubes with $\rho_N \rightarrow \rho$.*

Let $C_N := [0, L_N]^d$ a sequence of cubes of $\rho_N = N/|C_N| \rightarrow \rho$ as $N \rightarrow \infty$. Let $\varepsilon > 0$ and N_0 such that for $N \geq N_0$ we have $\rho - \varepsilon \leq \rho_N \leq \rho + \varepsilon$. Let $L_N^\pm = N^{1/d}/(\rho \pm \varepsilon)^{1/d}$ and define $C_N^\pm = [0, L_N^\pm]^d$ then we have $C_N^+ \subset C_N \subset C_N^-$. Let γ^\pm, γ the minimizers in C_N^\pm and C_N . Clearly γ^+ is a state on $\bigwedge^N L^2(C_N)$ and γ is a state on $\bigwedge^N L^2(C_N^-)$, so we obtain

$$\frac{e_{\text{Can}}^0(C_N^+, N)}{|C_N^+|} \leq (1 + \frac{\varepsilon}{\rho}) \frac{e_{\text{Can}}^0(C_N, N)}{|C_N|} \leq (1 + \frac{\varepsilon}{\rho})(1 - \frac{\varepsilon}{\rho})^{-1} \frac{e_{\text{Can}}^0(C_N^-, N)}{|C_N^-|}$$

so that

$$f_{\text{Can}}^0(\rho - \varepsilon) + \mathcal{O}(\varepsilon/\rho) \leq \frac{e_{\text{Can}}^0(C_N, N)}{|C_N|} \leq f_{\text{Can}}^0(\rho + \varepsilon) + \mathcal{O}(\varepsilon/\rho).$$

Now it remains to notice that $-\Delta_{L_N^+}$ is unitarily equivalent to $(L_0^+/L_0^-)^2 (-\Delta_{L_0^-})$ which easily gives that $f_{\text{Can}}^0(\rho - \varepsilon) = \mathcal{O}(\varepsilon/\rho) + f_{\text{Can}}^0(\rho + \varepsilon)$ and shows that

$$\lim_{N \rightarrow \infty} \frac{e_{\text{Can}}^0(C_N, N)}{|C_N|} = f_{\text{Can}}^0(\rho).$$

• *Arbitrary sets with $\rho_N \rightarrow \rho$*

Let (Λ) a sequence of sets going to infinity in the sense of Fisher (this sequence depends on N but we omit it for clarity). We first prove an upper bound of the free energy in the boxes Λ with density ρ_N . Let $\ell > 0$ and define

$$C_{\text{in}}(\ell) := \bigcup_{\substack{k \in \mathbb{Z}^d \\ k\ell + \Lambda_\ell \subset \Lambda}} k\ell + \Lambda_\ell.$$

We have

$$\Lambda \setminus C_{\text{in}}(\ell) \subset \left\{ x \in \Lambda, d(x, \partial\Lambda) \leq 2\sqrt{d}\ell \right\} \subset \partial\Lambda_{2\sqrt{d}\ell}$$

and therefore

$$|C_{\text{in}}(\ell)| = |\Lambda| + o(|\Lambda|)$$

as soon as $\ell = o(\delta(\Lambda))$ and we will take $1 \ll \ell \ll \delta(\Lambda)$. We can find integers $(n_k)_k$ such that

$$\begin{aligned} \sum_{\substack{k \in \mathbb{Z}^d \\ k\ell + \Lambda_\ell \subset \Lambda}} n_k &= N \\ n_k &= \lfloor \rho_N \ell^d \rfloor + o(\ell^{-d}) \end{aligned}$$

and thus define γ_k the minimizer of the free energy in the box $k\ell + \Lambda_\ell$ with n_k particles. By Lemma 35 we construct a state γ in Λ with N particles with free energy

$$\mathcal{E}_{\text{Can}}^0(\gamma) = \sum_{\substack{k \in \mathbb{Z}^d \\ k\ell + \Lambda_\ell \subset \Lambda}} e_{\text{Can}}^0(\Lambda_\ell, n_k)$$

so that

$$\frac{e_{\text{Can}}^0(\Lambda, N)}{|\Lambda|} \leq \left(\frac{\ell^d}{|C_{\text{in}}(\ell)|} + o\left(\frac{\ell^d}{|C_{\text{in}}(\ell)|}\right) \right) \sum_{\substack{k \in \mathbb{Z}^d \\ k\ell + \Lambda_\ell \subset \Lambda}} (f(\rho) + o(1)).$$

This gives the upper bound. We summarize the most relevant quantities in this table.

Total number of particles	N	N
Nb of boxes	$ C_{\text{in}}(\ell) \ell^{-d}$	$ \Lambda \ell^{-d} + o(\Lambda \ell^{-d})$
Nb of waste particles	$N - C_{\text{in}}(\ell) \ell^{-d}$	$o(N)$
Nb of part. per box n_k	$\simeq N/(C_{\text{in}}(\ell) \ell^{-d})$	$\lfloor \rho_N \ell^d \rfloor + o(\ell^{-d})$

Let us now prove the lower bound. The idea is to put Λ in a box and to take as ansatz for the free energy in the box the minimizer in Λ and in a volume $C_{\text{out}}(\ell)$ which will consist in cubes of side length ℓ outside Λ but in the box. More precisely, up to translation we can assume that $\Lambda \subset C_{2\sqrt{d}\delta\Lambda}$ and define

$$C_{\text{out}}(\ell) := \bigcup_{\substack{k \in \mathbb{Z}^d \\ k\ell + \Lambda_\ell \subset C_{2\sqrt{d}\delta\Lambda} \\ k\ell + \Lambda_\ell \cap \Lambda = \emptyset}} k\ell + \Lambda_\ell.$$

By construction we obtain $C_{2\sqrt{d}\delta\Lambda} \setminus (C_{\text{out}}(\ell) \cup \Lambda) \subset \partial\Lambda_{2\sqrt{d}\ell}$ so that

$$|C_{2\sqrt{d}\delta\Lambda}| = |C_{\text{out}}(\ell)| + |\Lambda| + o(|\Lambda|). \quad (94)$$

As before let γ_k be the minimizer in the box $k\ell + \Lambda_\ell$ with $\lfloor \rho_N \ell^d \rfloor$ particles, let γ be the minimizer in Λ , by Lemma 35 we can construct a state in $C_{2\sqrt{d}\delta\Lambda}$ with $N' := N + \lfloor \rho_N \ell^d \rfloor |C_{\text{out}}(\ell)|\ell^{-d}$ particles verifying Eq. (107) and Eq. (106). We obtain

$$\frac{e_{\text{Can}}^0(C_{2\sqrt{d}\delta\Lambda}, N')}{|C_{2\sqrt{d}\delta\Lambda}|} \leq \frac{|\Lambda|}{|C_{2\sqrt{d}\delta\Lambda}|} \frac{e^0(\Lambda, N)}{N} + \frac{|C_{\text{out}}(\ell)|}{|C_{2\sqrt{d}\delta\Lambda}|} \frac{e^0(\Lambda_\ell, \lfloor \rho_N \ell^d \rfloor)}{N}$$

which gives, using (94) the desired lower bound. \square

B.2 Proof of Proposition 29: Equivalence of ensembles for the free gas in a box

In this section we show the equivalence of the canonical ensemble and the grand canonical ensemble for free fermions in a box. More precisely, let $L > 0$ and consider the cube $C_L = (-\frac{L}{2}, \frac{L}{2})^d$. With Δ^L denoting the Dirichlet Laplacian in the box C_L , we know by Theorem 27 that the semi-classical limit

$$f_{\text{Can}}^L(\beta, \rho) := \lim_{\substack{N \rightarrow \infty \\ N\hbar^d \rightarrow \rho}} \hbar^d e_{\text{Can}}^{\beta, L}(\hbar, N) = \lim_{\substack{N \rightarrow \infty \\ N\hbar^d \rightarrow \rho}} -\frac{\hbar^d}{\beta} \log \text{Tr} e^{-\beta \sum_{i=1}^N -\hbar^2 \Delta_i^L} \quad (95)$$

exists, where $e_{\text{Can}}^{\beta, L}(\hbar, N)$ is the minimum free energy of N fermions with Hamiltonian $H_{N, \hbar} := \sum_{i=1}^N -\hbar^2 \Delta_i^L$. Similarly, we define

$$\begin{aligned} f_{\text{GC}}^L(\beta, \mu) &:= \lim_{\substack{N \rightarrow \infty \\ N\hbar^d \rightarrow \rho}} \hbar^d e_{\text{GC}}^{\beta, L}(\hbar, \mu) \\ &= -\frac{L^d}{(2\pi)^d \beta} \int_{\mathbb{R}^d} \log \left(1 + e^{-\beta(p^2 - \mu)} \right) dp. \end{aligned}$$

An immediate consequence of the identification of a canonical N -particle states as a grand canonical state on Fock space is the following inequality that holds for any $\mu \in \mathbb{R}$

$$e_{\text{Can}}^{\beta, L}(\hbar, N) = \min_{\Gamma \in S_{\text{Can}}^N} \left(\text{Tr} (H_{N, \hbar} - \mu N) \Gamma + \frac{1}{\beta} \text{Tr} \Gamma \log \Gamma \right) + \mu N \geq e_{\text{GC}}^{\beta, L}(\mu, \hbar) + \mu N.$$

Multiplying by \hbar^d and passing to the limit we obtain that for any $\rho > 0, \mu \in \mathbb{R}$

$$f_{\text{Can}}^L(\beta, \rho) \geq f_{\text{GC}}^L(\beta, \mu) + \mu \rho. \quad (96)$$

The next proposition states that for fixed $\rho > 0$ the opposite inequality holds for a unique chemical potential $\mu(\rho)$.

Proposition 29 (Equivalence of ensembles). *For all $\rho > 0$, we have*

$$\begin{aligned} f_{\text{Can}}^L(\beta, \rho) &= \lim_{\substack{N \rightarrow \infty \\ N\hbar^d \rightarrow \rho}} \hbar^d e_{\text{GC}}^{\beta, L}(\hbar, \mu(\rho)) + \hbar^d N \mu(\rho) \\ &= -\frac{L^d}{(2\pi)^d \beta} \int_{\mathbb{R}^d} \log \left(1 + e^{-\beta(p^2 - \mu(\rho))} \right) dp + \mu(\rho) \rho, \end{aligned}$$

where $\mu(\rho)$ satisfies

$$\rho = \frac{L^d}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{1}{1 + e^{\beta(p^2 - \mu(\rho))}} dp. \quad (97)$$

Remark 30. *As explained in Section B.1 the thermodynamic limit does not depend on the sequence of domains we take. Nevertheless the L dependance above is correct because the volume of $\hbar^{-1}C_L$ is $(L\hbar^{-1})^d$ and we are interested in $\hbar^d e_{\text{GC}}^{\beta, L}$.*

To prove the latter Proposition we first need some technical lemma.

Lemma 31 (Properties of $f_{\text{Can}}^L(\beta, \rho)$). *For any $\beta > 0$,*

1. the function $f_{\text{Can}}^L(\beta, \rho)$ is continuous at $\rho = 0$ and $f_{\text{Can}}^L(\beta, 0) = 0$,
2. $f_{\text{Can}}(\beta, \rho)$ is convex in ρ and hence also continuous in $\rho \in \mathbb{R}_+$,
3. the convergence in (95) is locally uniform in ρ .

Proof. Proof of (1).

For $\rho > 0$, combining (96) with Proposition 11, we have for any $\mu \in \mathbb{R}$,

$$\begin{aligned} f_{\text{Can}}^L(\beta, \rho) &\geq -\frac{L^d}{(2\pi)^d \beta} \int_{\mathbb{R}^d} \log(1 + e^{-\beta(p^2 - \mu)}) \, dp + \mu\rho \\ &\geq -\frac{L^d}{(2\pi)^d \beta} \int_{\mathbb{R}^d} e^{-\beta(p^2 - \mu)} \, dp + \mu\rho = -C_{\beta, L} e^{\beta\mu} + \mu\rho. \end{aligned}$$

Choosing for instance $\mu = \frac{1}{\beta} \log \rho$ yields

$$f_{\text{Can}}^L(\beta, \rho) \geq -C_{\beta, L} \rho + \frac{1}{\beta} \rho \log \rho,$$

implying that $\liminf_{\rho \rightarrow 0} f_{\text{Can}}^L(\beta, \rho) \geq 0$. If $\hbar^d N \rightarrow 0$ then the same argument shows that for any $\mu \in \mathbb{R}$

$$\liminf \hbar^d e_{\text{Can}}^{\beta, L}(\hbar, N) \geq -C_{\beta, L} e^{\beta\mu}.$$

Taking $\mu \rightarrow -\infty$ shows $\liminf \hbar^d e_{\text{Can}}^{\beta, L}(\hbar, N) \geq 0$.

For the upper bound, let u_1, \dots, u_N be the eigenvectors corresponding to the N first eigenvalues $\lambda_1, \dots, \lambda_N$ of the Dirichlet Laplacian $-\Delta^L$, and consider $\Gamma = |\wedge_i u_i\rangle \langle \wedge_i u_i|$. Then we have

$$\begin{aligned} -\frac{\hbar^d}{\beta} \log \text{Tr} e^{-\beta H_{N, \hbar}} &\leq \hbar^d \left(\text{Tr} H_{N, \hbar} \Gamma + \frac{1}{\beta} \text{Tr} \Gamma \log \Gamma \right) = \hbar^d \langle \wedge_i u_i, H_{N, \hbar} \wedge_i u_i \rangle \\ &= \hbar^d \sum_{i=1}^N \hbar^2 \lambda_i \leq C_d \hbar^{d+2} N^{1+\frac{2}{d}}, \end{aligned}$$

implying that $f_{\text{Can}}^L(\beta, \rho) \leq C_d \rho^{1+\frac{2}{d}}$. Hence $f_{\text{Can}}^L(\beta, 0) = 0$ and $\limsup_{\rho \rightarrow 0} f_{\text{Can}}^L(\beta, \rho) \leq 0$, so we conclude that $f_{\text{Can}}^L(\beta, \rho)$ is continuous at $\rho = 0$.

Proof of (2).

Let $\rho_1, \rho_2 > 0$, $t \in (0, 1)$ and put $\rho = t\rho_1 + (1-t)\rho_2$. Suppose that Λ_N is a sequence of boxes such that $N|\Lambda_N|^{-1} \rightarrow \rho$ and $\Lambda_N \rightarrow \infty$ in the sense of Fischer. We cut each box Λ_N in two pieces $\Lambda_N^{(1)}$ and $\Lambda_N^{(2)}$ such that $|\Lambda_N^{(1)}| = t|\Lambda_N|$ and $|\Lambda_N^{(2)}| = (1-t)|\Lambda_N|$, and put $N_1 = \lfloor t|\Lambda_N| \rho_1 \rfloor$, $N_2 = \lfloor (1-t)|\Lambda_N| \rho_2 \rfloor$. Then $\Lambda_N^{(i)} \rightarrow \infty$ in the sense of Fischer and $N_i |\Lambda_N^{(i)}|^{-1} \rightarrow \rho_i$ as $N \rightarrow \infty$. Using the anti-symmetrization of the minimizers of the free energy in $\Lambda_N^{(1)}$ and $\Lambda_N^{(2)}$ as a trial state, we have by (106) and (107) that

$$e_{\text{Can}}^\beta(\Lambda_N, N_1 + N_2) = e_{\text{Can}}^\beta(\Lambda_N^{(1)}, N_1) + e_{\text{Can}}^\beta(\Lambda_N^{(2)}, N_2).$$

Thus we obtain, using that the thermodynamic limit is independent of the sequence of sets,

$$\begin{aligned} f_{\text{Can}}(\beta, \rho) &= \lim_{N \rightarrow \infty} \frac{e^{\beta_{\text{Can}}(\Lambda_N, N_1 + N_2)}}{|\Lambda_N|} \leq \lim_{N \rightarrow \infty} t \frac{e^{\beta_{\text{Can}}(\Lambda_N^{(1)}, N_1)}}{|\Lambda_N^{(1)}|} + (1-t) \frac{e^{\beta_{\text{Can}}(\Lambda_N^{(2)}, N_2)}}{|\Lambda_N^{(2)}|} \\ &= t f_{\text{Can}}(\beta, \rho_1) + (1-t) f_{\text{Can}}(\beta, \rho_2), \end{aligned}$$

showing convexity.

Proof of (3).

The local uniform convergence is a consequence of the following elementary general fact which is easily shown by contradiction. Let X be a locally compact metric space and let (g_n) be a sequence of functions on X . If there is some $g \in C^0(X)$ such that $g_n(x_n) \rightarrow g(x)$ for any convergent sequence (x_n) in X with limit x , then $g_n \rightarrow g$ locally uniformly in X . Supposing that $N\hbar^d \rightarrow \rho$, we define a new quantity $\rho_N = N\hbar^d$ and do a simple change of variables

$$f_{\text{Can}}^L(\beta, \rho) = \lim_{\substack{N \rightarrow \infty \\ \rho_N \rightarrow \rho}} -\frac{\rho_N}{N\beta} \log \text{Tr} e^{-\beta \sum_{i=1}^N -(\frac{\rho_N}{N})^{\frac{2}{d}} \Delta_i^L} = \lim_{N \rightarrow \infty} g_N(\beta, \rho_N),$$

and then apply the fact to conclude the proof. \square

Proof of Proposition 29. By Eq. (96) we only need to prove the converse inequality. We will bound the grand canonical free energy from below by the Legendre transform of the canonical energy. The same approach is used in [Rue99], but we spell it out here for the sake of completeness. Let $\mu \in \mathbb{R}$ and define

$$f_{\text{Can}}^{L,*}(\beta, \mu) := \sup_{0 \leq \rho < \infty} (\mu\rho - f_{\text{Can}}^L(\beta, \rho))$$

which is a finite number by Eq. (96). It is easy to see that $f_{\text{Can}}(\beta, \rho) \geq C\rho^{1+2/d} - C$, therefore we can choose $C > 0$ such that the supremum above is attained in the interval $[0, C]$ (f_{Can}^L is continuous in ρ), i.e. $f_{\text{Can}}^{L,*}(\beta, \mu) = \sup_{0 \leq \rho \leq C} (\mu\rho - f_{\text{Can}}^L(\beta, \rho))$. Since f_{Can}^L is continuous in ρ and because the convergence Eq. (95) is locally uniform in ρ , we have for any $\varepsilon > 0$ that

$$-\frac{\hbar^d}{\beta} \log \text{Tr} e^{-\beta H_{n,\hbar}} \geq f_{\text{Can}}^L(\beta, n\hbar^d) - \varepsilon,$$

as long as $n\hbar^d \leq C$ and \hbar is sufficiently small. This implies that

$$\begin{aligned} \sum_{n \leq C\hbar^{-d}} \text{Tr} e^{-\beta(H_{n,\hbar} - \mu n)} &\leq \sum_{n \leq C\hbar^{-d}} e^{\beta\hbar^{-d}(\mu n\hbar^d - f_{\text{Can}}^L(\beta, n\hbar^d) + \varepsilon)} \leq \sum_{n \leq C\hbar^{-d}} e^{\varepsilon\beta\hbar^{-d}} e^{\beta\hbar^{-d} f_{\text{Can}}^{L,*}(\beta, \mu)} \\ &\leq C\hbar^{-d} e^{\varepsilon\beta\hbar^{-d}} e^{\beta\hbar^{-d} f_{\text{Can}}^{L,*}(\beta, \mu)}. \end{aligned} \quad (98)$$

We now estimate the terms with $n > C\hbar^{-d}$. Note for any n that

$$\begin{aligned} -\frac{1}{\beta} \log \text{Tr} e^{-\beta H_{n,\hbar}} &= \min_{\Gamma \in \mathcal{S}_{\text{Can}}^n} \left(\text{Tr} H_{n,\hbar} \Gamma + \frac{1}{\beta} \text{Tr} \Gamma \log \Gamma \right) \\ &\geq \frac{1}{2} \min_{\Gamma \in \mathcal{S}_{\text{Can}}^n} \text{Tr} H_{n,\hbar} \Gamma + \frac{1}{2} \min_{\Gamma \in \mathcal{S}_{\text{Can}}^n} \left(\text{Tr} H_{n,\hbar} \Gamma + \frac{2}{\beta} \text{Tr} \Gamma \log \Gamma \right), \end{aligned} \quad (99)$$

where by the Lieb-Thirring inequality

$$H_{n,\hbar} \geq C_{LT} \frac{\hbar^2 n^{1+\frac{2}{d}}}{L^2}.$$

Furthermore, we have by (96) for any $\tilde{\mu} \in \mathbb{R}$ and \hbar sufficiently small that

$$\min_{\Gamma \in S_{\text{Can}}^n} \left(\text{Tr } H_{n,\hbar} \Gamma + \frac{2}{\beta} \text{Tr } \Gamma \log \Gamma \right) \geq \hbar^{-d} \left(f_{\text{GC}}^L \left(\frac{\beta}{2}, \tilde{\mu} \right) - \varepsilon \right) + \tilde{\mu} n.$$

Thus, continuing from (99), we find for any $n > C\hbar^{-d}$

$$\begin{aligned} \text{Tr } e^{-\beta H_{n,\hbar}} &\leq e^{-\frac{\beta}{2} C_{LT} L^{-2} \hbar^2 n^{1+\frac{2}{d}} - \frac{\beta}{2\hbar^d} (f_{\text{GC}}^L(\frac{\beta}{2}, \tilde{\mu}) - \varepsilon)} e^{-\frac{\beta}{2} \tilde{\mu} n} \\ &\leq e^{-\frac{\beta}{2} n (C_{LT} L^{-2} C^{\frac{2}{d}} + C^{-1} (f_{\text{GC}}^L(\frac{\beta}{2}, \tilde{\mu}) - \varepsilon))} e^{-\frac{\beta}{2} \tilde{\mu} n}, \end{aligned}$$

where the second inequality follows from $n > C\hbar^{-d}$ and the fact that f_{GC}^L is negative. We settle on the choice $\tilde{\mu} = 2\mu$ and note that by possibly choosing C larger we can make the exponent $C_{LT} L^{-2} C^{\frac{2}{d}} + \frac{1}{C} (f_{\text{GC}}^L(\frac{\beta}{2}, \tilde{\mu}) - \varepsilon)$ as large as we like. Hence we obtain the bound

$$\sum_{n > C\hbar^{-d}} e^{\beta \mu n} \text{Tr } e^{-\beta H_{n,\hbar}} \leq \sum_{n > C\hbar^{-d}} \left(\frac{1}{2} \right)^n \quad (100)$$

for some sufficiently large C .

Now, combining (98) and (100) we obtain the bound

$$\begin{aligned} \hbar^d e_{\text{GC}}^\beta(\mu, \hbar) &= -\frac{\hbar^d}{\beta} \log \sum_{n \geq 0} e^{\beta \mu n} \text{Tr } e^{-\beta H_{N,\hbar}} \\ &\geq -\frac{\hbar^d}{\beta} \log \left(C\hbar^{-d} e^{\varepsilon \beta \hbar^{-d}} e^{\beta \hbar^{-d} f_{\text{Can}}^*(\beta, \mu)} + o(1) \right) \\ &= -f_{\text{Can}}^*(\beta, \mu) + \varepsilon + o(1), \end{aligned}$$

showing that $f_{\text{GC}}^L(\beta, \mu) \geq -f_{\text{Can}}^*(\beta, \mu)$. Now, since f_{Can}^L is convex in ρ , it is its own double Legendre transform, $f_{\text{Can}}^L(\beta, \rho) = \sup_{\mu} (\mu \rho - f_{\text{Can}}^*(\beta, \mu))$. Thus, in light of (96) we have shown

$$f_{\text{Can}}^L(\beta, \rho) \geq \sup_{\mu} (f_{\text{GC}}^L(\beta, \mu) + \mu \rho) \geq \sup_{\mu} (\mu \rho - f_{\text{Can}}^*(\beta, \mu)) = f_{\text{Can}}^L(\beta, \rho),$$

so we must have equality everywhere, concluding the proof. \square

Appendix C On the anti-symmetrization of states

In the following section, we recall the anti-symmetrization of states living in orthogonal subspaces of the same Hilbert space, as well as some properties of this anti-symmetrization procedure we need. Let \mathfrak{H} be a separable Hilbert space. For $N \geq 1$, and for $\sigma \in S(N)$ we consider the permutation operator P_σ acting as

$$P_\sigma \varphi_1 \otimes \dots \otimes \varphi_N = \varphi_{\sigma(1)} \otimes \dots \otimes \varphi_{\sigma(N)}$$

on product states for any $\varphi_1, \dots, \varphi_N \in \mathfrak{H}$. This allows us to define the projection $\Pi : \otimes^N \mathfrak{H} \rightarrow \wedge^N \mathfrak{H}$ onto the fermionic subspace by

$$\Pi = \frac{1}{N!} \sum_{\sigma \in S_N} (-1)^\sigma P_\sigma.$$

Let $N = N_1 + N_2$ and $\Psi_i \in \wedge^{N_i} \mathfrak{H}$ for $i \in \{1, 2\}$, we define the anti-symmetrization of the two wave functions Ψ_1 and Ψ_2 to be

$$\Psi_1 \wedge \Psi_2 = \left(\frac{(N_1 + N_2)!}{N_1! N_2!} \right)^{\frac{1}{2}} \Pi(\Psi_1 \otimes \Psi_2).$$

We want to carry this anti-symmetrization procedure over to general fermionic states. We begin with pure states, notice that

$$\Pi |\Psi_1 \otimes \Psi_2\rangle \langle \Psi_1 \otimes \Psi_2| \Pi = \frac{N_1! N_2!}{(N_1 + N_2)!} |\Psi_1 \wedge \Psi_2\rangle \langle \Psi_1 \wedge \Psi_2|.$$

Based on this we make the following definition.

Definition 32. For $i \in \{1, 2\}$, let $N_i \geq 1$ and Γ_i be a fermionic state on $\wedge^{N_i} \mathfrak{H}$. We define the anti-symmetrization of the two states to be

$$\Gamma_1 \wedge \Gamma_2 := \frac{(N_1 + N_2)!}{N_1! N_2!} \Pi(\Gamma_1 \otimes \Gamma_2) \Pi. \quad (101)$$

We may write $\Gamma_1 = \sum_k \mu_k |\psi_k\rangle \langle \psi_k|$ with $\psi_k \in \wedge^{N_1} \mathfrak{H}$ being an orthonormal basis of $\wedge^{N_1} \mathfrak{H}$, and similarly $\Gamma_2 = \sum_j \lambda_j |\varphi_j\rangle \langle \varphi_j|$. The preceding calculations show that

$$\Gamma_1 \wedge \Gamma_2 = \sum_{k,j} \mu_k \lambda_j |\psi_k \wedge \varphi_j\rangle \langle \psi_k \wedge \varphi_j|. \quad (102)$$

Of course, this procedure generalizes easily to an arbitrary number states.

Lemma 33 (One- and two-body densities). For $i \in \{1, 2\}$, let $N_i \geq 1$ and Γ_i be a fermionic state on $\wedge^{N_i} \mathfrak{H}$. Assume there are orthogonal projectors P_1, P_2 such that $P_1 P_2 = 0$ and $\Gamma_i P_i = \Gamma_i$ for $i \in \{1, 2\}$. Then the one-body reduced density matrix of $\Gamma_1 \wedge \Gamma_2$ is

$$(\Gamma_1 \wedge \Gamma_2)^{(1)} = \Gamma_1^{(1)} + \Gamma_2^{(1)}. \quad (103)$$

In particular, $\Gamma_1 \wedge \Gamma_2$ is a state on $\wedge^{N_1 + N_2} \mathfrak{H}$. Moreover, for any $W \in \mathcal{B}(\mathfrak{H}^{\otimes 2})$ such that $[W, P_i] = 0$ for all $i \in \{1, 2\}$ we have

$$\text{Tr } W (\Gamma_1 \wedge \Gamma_2)^{(2)} = \text{Tr } W \left(\Gamma_1^{(2)} + \Gamma_2^{(2)} + \Gamma_1^{(1)} \otimes \Gamma_2^{(1)} + \Gamma_2^{(1)} \otimes \Gamma_1^{(1)} \right). \quad (104)$$

Corollary 34. In particular, if $\mathfrak{H} = L^2(\mathbb{R}^d)$ we have

$$\rho_{\Gamma_1 \wedge \Gamma_2}^{(2)}(x, y) = \rho_{\Gamma_1}^{(2)}(x, y) + \rho_{\Gamma_2}^{(2)}(x, y) + \rho_{\Gamma_1}^{(1)}(x) \rho_{\Gamma_2}^{(1)}(y) + \rho_{\Gamma_2}^{(1)}(x) \rho_{\Gamma_1}^{(1)}(y). \quad (105)$$

Proof. In view of (102) it is enough to check these properties for pure states. Let $N = N_1 + N_2$

and $\Psi_i \in \bigwedge^{N_i} \mathfrak{H}$ for $i \in \{1, 2\}$. Let $\Gamma_i = |\Psi_i\rangle \langle \Psi_i|$ for $i \in \{1, 2\}$ and $A \in \mathcal{B}(\mathfrak{H})$ we have

$$\mathrm{Tr} A (\Gamma_1 \wedge \Gamma_2)^{(1)} = \frac{N \times N!}{N_1! N_2!} \langle \Psi_1 \otimes \Psi_2 | \left(P_1^{\otimes N_1} \otimes P_2^{\otimes N_2} \Pi A \Pi P_1^{\otimes N_1} \otimes P_2^{\otimes N_2} \right) | \Psi_1 \otimes \Psi_2 \rangle.$$

We have

$$P_1^{\otimes N_1} \otimes P_2^{\otimes N_2} \Pi A \Pi P_1^{\otimes N_1} \otimes P_2^{\otimes N_2} = \frac{1}{(N!)^2} \sum_{\sigma, \sigma' \in S(N)} (-1)^{\sigma \sigma'} P_1^{\otimes N_1} \otimes P_2^{\otimes N_2} P_\sigma A P_{\sigma'} P_1^{\otimes N_1} \otimes P_2^{\otimes N_2}.$$

Because $P_1 P_2 = 0$, the terms in the sum above are non null only if $\sigma'([1, N_1]) \subset \sigma^{-1}([1, N_1]) \cup \{1\}$ and $\sigma'([N_1 + 1, N]) \subset \sigma^{-1}([N_1 + 1, N]) \cup \{1\}$. We change variable $\sigma' := \sigma^{-1} \alpha$ and notice that the latter condition is equivalent to $\alpha([1, N_1]) \subset [1, N_1]$ and $\alpha([N_1 + 1, N]) \subset [N_1 + 1, N]$. Now note that

$$\sum_{\alpha \in S(N_1, N_2)} (-1)^\alpha P_\alpha \Psi_1 \otimes \Psi_2 = N_1! N_2! \Psi_1 \otimes \Psi_2$$

where $S(N_1, N_2)$ denotes the bijections of $[1, N]$ preserving $[1, N_1]$. Note also that

$$\sum_{\sigma \in S(N)} P_\sigma A_1 P_{\sigma^{-1}} = (N-1)! \sum_{i=1}^N A_i.$$

It remains to compute

$$\langle \Psi_1 \otimes \Psi_2 | \sum_{i=1}^N A_i | \Psi_1 \otimes \Psi_2 \rangle = N_1 \langle \Psi_1 | A_1 | \Psi_1 \rangle + N_2 \langle \Psi_2 | A_1 | \Psi_2 \rangle,$$

hence

$$\mathrm{Tr} A (\Gamma_1 \wedge \Gamma_2)^{(1)} = \mathrm{Tr} A \Gamma_1^{(1)} + \mathrm{Tr} A \Gamma_2^{(1)}.$$

Now let $W \in \mathcal{B}(\mathfrak{H}^{\otimes 2})$ such that $[W, P_i] = 0$ for all $i \in \{1, 2\}$. Doing the same computation as before, we find that we need to estimate

$$\frac{1}{(N!)^2} \sum_{\sigma, \sigma' \in S(N)} (-1)^{\sigma \sigma'} P_1^{\otimes N_1} \otimes P_2^{\otimes N_2} P_\sigma W P_{\sigma'} P_1^{\otimes N_1} \otimes P_2^{\otimes N_2}.$$

But now since W commutes with the P_i 's, we obtain the same condition as before for the terms in the sum to be non zero. It remains to notice that

$$\sum_{\sigma \in S(N)} P_\sigma W_{1,2} P_{\sigma^{-1}} = \frac{N!}{N(N-1)} \sum_{i \neq j}^N W_{i,j}$$

and compute

$$\langle \Psi_1 \otimes \Psi_2 | \frac{1}{2} \sum_{i \neq j}^N W_{i,j} | \Psi_1 \otimes \Psi_2 \rangle = \mathrm{Tr} W_{1,2} \left(\Gamma_1^{(2)} + \Gamma_2^{(2)} + \Gamma_1^{(1)} \otimes \Gamma_2^{(1)} + \Gamma_2^{(1)} \otimes \Gamma_1^{(1)} \right).$$

□

Lemma 35 (Additivity of entropy and kinetic energy). *Denoting by $H_{N,\Lambda} = \sum_{i=1}^N -\Delta_i^\Lambda$ the*

N-body Laplacian on Λ (with Dirichlet boundary conditions), then the anti-symmetrization of two fermionic states satisfies

$$\mathrm{Tr}(\Gamma_1 \wedge \Gamma_2) \log(\Gamma_1 \wedge \Gamma_2) = \mathrm{Tr} \Gamma_1 \log \Gamma_1 + \mathrm{Tr} \Gamma_2 \log \Gamma_2, \quad (106)$$

and

$$\mathrm{Tr} H_{N_1+N_2, \Lambda} \Gamma_1 \wedge \Gamma_2 = \mathrm{Tr} H_{N_1, \Lambda_1} \Gamma_1 + \mathrm{Tr} H_{N_2, \Lambda_2} \Gamma_2. \quad (107)$$

Proof. Using (102) along with the spectral theorem it is obvious that (106) holds, and (107) follows directly from (103). \square

Chapitre 5

The Scott correction in Dirac-Fock theory

Ce chapitre présente des travaux réalisés en collaboration avec Søren Fournais et Mathieu Lewin. Ces travaux feront l'objet d'un article qui est en cours de rédaction.

Abstract

We give the first derivation of the Scott correction in the large- Z expansion of the energy of an atom in Dirac-Fock theory.

Résumé

Nous donnons la première dérivation de la correction de Scott dans le développement de l'énergie d'un atome pour Z grand dans la théorie de Dirac-Fock.

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1 Introduction

An impressive success of the many-particle Schrödinger equation is its theoretical ability to describe all the atoms of the periodic table. This model has no other parameter than the integer $N = Z$, where N is the number of electrons which is equal to the number of protons Z in a neutral atom. Unfortunately, the exponentially increasing complexity of the problem in N makes any precise computation of the N -particle wavefunction impossible in practice. It is therefore important to rely on approximate models and to know whether the true equation simplifies in some limits.

The most famous result in this direction is the Lieb-Simon proof [LS73; LS77b; LS77a; Lie81a] of the leading asymptotics of the ground state energy of a non-relativistic atom with N quantum electrons and a pointwise nucleus of charge $Z = N$,

$$E_{\text{NR}}(N, Z = N) = Z^{\frac{7}{3}} e_{\text{TF}} + o(Z^{\frac{7}{3}}) \quad (1)$$

where

$$e_{\text{TF}} = \min_{\substack{\rho \geq 0 \\ \int_{\mathbb{R}^3} \rho = 1}} \left\{ \frac{3}{10} (3\pi^2)^{\frac{2}{3}} \int_{\mathbb{R}^3} \rho(x)^{\frac{5}{3}} dx - \int_{\mathbb{R}^3} \frac{\rho(x)}{|x|} dx + \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho(x)\rho(y)}{|x-y|} dx dy \right\}$$

is the minimum Thomas-Fermi energy [Tho27; Fer27]. Thomas-Fermi theory does not only provide the leading order of the energy. It also describes the precise behavior of the density of electrons at the distance $Z^{-1/3}$ to the nucleus and it is believed to provide a surprisingly accurate estimate on the size of alkali atoms [Sol16].

The expansion (1) has been continued in many works. The best known result at the moment is

$$E_{\text{NR}}(N, Z = N) = Z^{\frac{7}{3}} e_{\text{TF}} + \frac{Z^2}{2} + Z^{\frac{5}{3}} c_{\text{DS}} + o(Z^{\frac{5}{3}}). \quad (2)$$

The Z^2 term is the *Scott correction* [Sco52; Sch80] which is the main subject of this article and was rigorously derived in [SW87a; SW87b; SW89; Hug90; IS93; ILS96]. This was then generalized in several directions [Bac89; SS03], including for magnetic fields [Ivr96; Ivr97; Sob96]. The next order $Z^{5/3}$ contains both an exchange term predicted by Dirac [Dir30] and a semi-classical correction derived by Schwinger [Sch81; ES84a; ES84c; ES84b]. It was rigorously established in an impressive series of works by Fefferman and Seco [FS89; FS90; FS92; FS93; FS94c; FS94a; FS94b; FS95]. It should be mentioned that although the leading $Z^{7/3}$ Thomas-Fermi term and the $Z^{5/3}$ Dirac exchange term are somewhat universal (that is, arise for other types of interactions in mean-field limits [FLS18; Bac92; GS94; BNPSS18]), the Z^2 Scott correction and the $Z^{5/3}$ Schwinger term are specific to the Coulomb potential. More precisely, these are semi-classical corrections due to the singularity of the Coulomb potential at the origin. It should also be noted that the three leading terms in (1) are already correctly described in Hartree-Fock theory [Bac92; Bac93; GS94]. The exchange term only participate to the $Z^{5/3}$ term and it can be dropped for the first two terms [LS77a], leading to the so-called *reduced* Hartree-Fock model [Sol91].

It is well known in Physics and Chemistry that, in heavy atoms, relativistic effects start to play an important role, even for not so large values of Z . Without relativity, gold would have the same color as silver [GA10], mercury would not be liquid at room temperature [CPWS13] and cars would not start [ZP11]. The reason why relativistic effects become important is because, in an atom, most of the electrons live at a distance $Z^{-1/3}$ to the nucleus, hence they experiment very strong Coulomb forces leading to very high velocities, of the order of the speed of light. This is even more dramatic for the Scott correction which is due to the few electrons living at

the very short distance Z^{-1} to the nucleus. Indeed, Schwinger has predicted [Sch80] that small relativistic effects should not affect the leading Thomas-Fermi energy in the large- Z expansion, but should modify the Scott correction.

A truly relativistic model should involve the Dirac operator [Tha92; ELS08]. Unfortunately, there is no well-defined N -particle Dirac Hamiltonian at the moment [Der12], except for $N = 2$ [DO18], and even if there was one it would probably have no bound state. In the very unlikely case of the existence of bound states, it would anyway be impossible to identify a ground state. The one-particle Dirac operator is unbounded both from above and below and any N -particle Dirac Hamiltonian would have the whole line as its spectrum. A better theory should probably involve bound states in Quantum Electrodynamics [Sha02], but this is far from being understood mathematically.

Several authors have instead studied the expansion of the ground state for simplified relativistic models. Sørensen studied a pseudo-relativistic Hamiltonian where the Laplacian is replaced by a non-local fractional Laplacian (the "Chandrasekhar" operator), and proved that the leading Thomas-Fermi term is unchanged in this case [Øst05]. The Scott correction for this model was then derived in [Øst98; SSS10; FSW08], but it does not coincide with Schwinger's original prediction [Sch80], since the spectral properties of the Dirac operator and of the fractional Laplacian are different. Siedentop and co-workers [CS06; FSW09; HS15] have then considered *projected Dirac operators* in order to suppress its negative spectrum, in the spirit of Brown-Ravenhall [BR51] and Mittleman [Mit81]. However, the Scott correction depends in a non trivial way on the chosen projector, which is somewhat arbitrary. The expected relativistic Scott correction has been obtained in the recent work [HS15] which covers the larger class of projectors and in particular includes the positive spectral projection of the non-interacting Dirac-Coulomb operator, which happens to give the correct Scott term. However, discrepancies could re-appear in the next order term for this projector.

In this paper we provide the first rigorous derivation of the relativistic Scott correction for a truly relativistic model without projectors. As we have said, we cannot start with the ill-defined N -body Dirac theory. However, let us recall that the Scott correction is already fully included in Hartree-Fock theory, even without exchange term. In all the previous works on the Scott correction, the reduction from the N -particle Schrödinger Hamiltonian to the (reduced) Hartree-Fock ground state is usually an easy step. In the non-relativistic case, it for instance immediately follows from the Lieb-Oxford inequality [Lie79; LO80]. For this reason, we directly start with (reduced) Dirac-Fock theory and prove the Scott correction within this theory. In order to simplify our exposition we discard the exchange term completely but we expect the same results when it is included. The exchange term is a lower order correction.

Dirac-Fock theory is the relativistic counterpart of the Hartree-Fock model and it has the advantage of having well-defined solutions which can be interpreted as ground states, even though the corresponding energy functional is unbounded from below [ES99; Pat00; ES01; ES02; HS07; ELS08; Sér09]. Those correspond to electronic states in the positive spectral subspace of their own mean-field Dirac operator. Hence this theory does rely on a projector but it is unknown *a priori* and depends in a nonlinear way on the solution itself. Previous results, in particular from [HS15], can therefore not be directly applied in this context. Our main task will be to estimate this nonlinear projector and to compare it with the non-interacting Dirac-Coulomb operator, in order to reduce the problem to a fixed projector as recently treated in [HS15]. Note that the predictions of Dirac-Fock theory for the Scott correction agree quite well with experimental data for $Z = 1, \dots, 120$, according to [Des73] and as was discussed in [HS15, Sec. 6].

The paper is organized as follows. In the next section we first state some spectral properties of Dirac operators with Coulomb potentials before we are able to properly introduce the Dirac-Fock minimization principle and finally give its large- Z expansion. The rest of the paper is devoted

to the proof of our main result on the Scott correction.

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2 Main result

2.1 Gaps in Dirac-Coulomb operators

In this section we discuss some important properties of Dirac operators with Coulomb potentials that will be important in our situation. Throughout the whole section we will be looking at operators in the form

$$D_0 + \rho * \frac{1}{|x|} \tag{3}$$

where ρ is a signed bounded measure in \mathbb{R}^3 . We are typically interested in the case where $\rho = \alpha\rho_+ - \kappa\delta_0$, with $\kappa\delta_0$ the density of the point nucleus and $\rho_+ \in (L^1 \cap L^{3/2})(\mathbb{R}^3)$ a more regular measure describing the quantum electrons. Here and everywhere, we work in a system of units such that $\hbar = m = c = 1$. Then we have $\kappa = \alpha Z$ where Z is the number of protons and $\alpha = e^2 \simeq 1/137.04$ is the Sommerfeld fine structure constant, which is the square of the charge of the electron. We recall that the free Dirac operator D_0 in 3d is given by

$$D_0 = -i \boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + \beta = -i \sum_{k=1}^3 \alpha_k \partial_k + \beta, \tag{4}$$

where $\alpha_1, \alpha_2, \alpha_3$ and β are 4×4 Hermitian matrices satisfying the anticommutation relations

$$\begin{cases} \alpha_k \alpha_\ell + \alpha_\ell \alpha_k &= 2 \delta_{k\ell} \mathbf{1}_{\mathbb{C}^4}, \\ \alpha_k \beta + \beta \alpha_k &= 0, \\ \beta^2 &= \mathbf{1}_{\mathbb{C}^4}. \end{cases} \tag{5}$$

The usual representation in 2×2 blocks is given by

$$\beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \quad \alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}, \quad k = 1, 2, 3,$$

with 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 is self-adjoint in $L^2(\mathbb{R}^3, \mathbb{C}^4)$ with domain $H^1(\mathbb{R}^3, \mathbb{C}^4)$ and its spectrum is $\sigma(D_0) = (-\infty, -1] \cup [1, \infty)$, see [Tha92; ELS08].

If $|\rho|^{1/2} \in H^{1/2}(\mathbb{R}^3)$, then the Coulomb potential is in $L^\infty(\mathbb{R}^3)$ and by the Hardy-Kato inequality

$$\frac{1}{|x|} \leq \frac{\pi}{2} \sqrt{-\Delta}, \tag{6}$$

we deduce the pointwise bound

$$\left| \rho * \frac{1}{|x|} \right| \leq \frac{\pi}{2} \left\langle \sqrt{|\rho|}, \sqrt{-\Delta} \sqrt{|\rho|} \right\rangle. \quad (7)$$

Hence $D_0 + \rho * |x|^{-1}$ is self-adjoint on the same domain $H^1(\mathbb{R}^3, \mathbb{C}^4)$.

When

$$\rho = \rho_+ - \kappa \delta_0$$

with $\rho_+ \geq 0$, $\rho_+^{1/2} \in H^{1/2}(\mathbb{R}^3)$ and $0 \leq \kappa < 1$, then it immediately follows that $D_0 + \rho * |x|^{-1} - \kappa |x|^{-1}$ is self-adjoint on the same domain as $D_0 - \kappa |x|^{-1}$. The latter operator has a unique distinguished self-adjoint extension on $H^1(\mathbb{R}^3, \mathbb{C}^4)$, whose domain is always included in $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$. We refer for instance to [ELS19b, Section 1] for a review of important properties of such operators.

The condition that $\kappa = \alpha Z < 1$ means that in principle we cannot consider atoms with nuclear charge higher than 137. In order to relate the Dirac-Coulomb model to its non-relativistic counterpart, we will however take $\alpha \rightarrow 0$ (non-relativistic limit) at the same time as $Z \rightarrow \infty$, while keeping $\kappa = \alpha Z$ fixed. This is the natural limit for the large- Z expansion of relativistic systems.

The following well-known result is a more quantitative expression of the fact that the domain of $D_0 + \rho * |x|^{-1}$ contains $H^1(\mathbb{R}^3, \mathbb{C}^4)$.

Lemma 1 (Upper bound on $(D_\rho)^2$). *Let ρ be a signed, bounded measure on \mathbb{R}^3 . For every $\Psi \in H^1(\mathbb{R}^3, \mathbb{C}^4)$, we have*

$$\left\| \left(D_0 + \rho * \frac{1}{|x|} \right) \Psi \right\|_{L^2(\mathbb{R}^3, \mathbb{C}^4)} \leq (1 + 2|\rho|(\mathbb{R}^3)) \|D_0 \Psi\|_{L^2(\mathbb{R}^3, \mathbb{C}^4)}. \quad (8)$$

Hence, in the situations recalled above where $D_0 + \rho * |x|^{-1}$ has a distinguished self-adjoint extension on $H^1(\mathbb{R}^3, \mathbb{C}^4)$, we have

$$\left(D_0 + \rho * \frac{1}{|x|} \right)^2 \leq (1 + 2|\rho|(\mathbb{R}^3))^2 |D_0|^2 \quad (9)$$

and

$$\left| D_0 + \rho * \frac{1}{|x|} \right| \leq (1 + 2|\rho|(\mathbb{R}^3)) |D_0|. \quad (10)$$

Proof. The estimate (8) follows from Hardy's inequality $|x|^{-2} \leq 4(-\Delta) \leq 4|D_0|^2$. The last inequality (10) is a consequence of (9) since the square root is operator monotone. \square

The purpose of the section is to discuss lower bounds similar to (10). From now on, we use the shorthand notation

$$D_\kappa := D_0 - \frac{\kappa}{|x|}$$

for the usual Dirac-Coulomb operator, with $0 \leq \kappa < 1$, and

$$D_{\kappa, \rho} := D_0 - \frac{\kappa}{|x|} + \rho * \frac{1}{|x|}$$

when it is perturbed by a density ρ (typically positive and regular enough in our context).

We recall that the lowest eigenvalue of D_κ in the gap $[-1; 1]$ is $\sqrt{1 - \kappa^2}$ and that the operator has an increasing sequence of eigenvalues tending to the upper threshold 1 [Tha92]. In addition, it was proved in [MM17] that for all $0 \leq \kappa < 1$, there exists a constant $c_\kappa > 0$ so that

$$c_\kappa |D_0| \leq |D_\kappa|. \tag{11}$$

When $\kappa \geq \sqrt{3}/2$, $(D_\kappa)^2$ cannot be lower bounded by $(D_0)^2$, otherwise the domain would be equal to $H^1(\mathbb{R}^3, \mathbb{C}^4)$. However, due to the explicit form of the domain of D_κ as explained in [ELS19b], we indeed have

$$c_\kappa(s) |D_0|^{2s} \leq |D_\kappa|^2 \tag{12}$$

for all $0 \leq s < \min(1, 1/2 + \sqrt{1 - \kappa^2})$. By interpolation, this gives

$$c'_\kappa(s) |D_0|^{1+\eta(2s-1)} \leq |D_\kappa|^{1+\eta}, \quad \forall \eta \in [0, 1]. \tag{13}$$

A natural question, which will play an important role later in our study, is to ask how the eigenvalues of $D_{\kappa,\rho}$ behave for a *general* positive density ρ . For which ρ can one guarantee that the gap around the origin is preserved? First we introduce a critical value ν_c that works for $\kappa \equiv 0$, before looking at the case $\kappa > 0$.

Let ρ be a non-negative density such that $\sqrt{\rho} \in H^{1/2}(\mathbb{R}^3)$ and $\int_{\mathbb{R}^3} \rho = 1$. Since the associated Coulomb potential is bounded uniformly by (7), the eigenvalues of $D_{0,\nu\rho} = D_0 + \nu\rho * |x|^{-1}$ are all confined to an interval of size proportional to ν at the edges of the gap $[-1, 1]$, for ν small enough. Actually, the min-max characterization of the eigenvalues from [DES00] implies that there is no eigenvalue close to 1 and that there are infinitely many close to -1 , since the potential is repulsive. In addition, these eigenvalues are monotonically increasing with ν . Let then $\nu_c(\rho)$ be the first value of the coupling constant ν , for which the largest negative eigenvalue vanishes:

$$\nu_c(\rho) := \min \{ \nu > 0 : 0 \in \sigma(D_{0,\nu\rho}) \}.$$

Let finally

$$\boxed{\nu_c := \inf_{\substack{\rho \geq 0 \\ \int_{\mathbb{R}^3} \rho = 1 \\ \sqrt{\rho} \in H^{1/2}(\mathbb{R}^3)}} \nu_c(\rho)} \tag{14}$$

be the lowest possible critical value among all probability densities. Loosely speaking, ν_c is the largest possible repulsive charge that we can add while guaranteeing that the eigenvalues will stay in $[-1, 0]$, independently of the shape of the density ρ . By charge conjugation, we get the reverse picture if we place an arbitrary attractive charge, that is, we allow negative ν 's.

All our next results will be stated in terms of this critical ν_c . Following [ELS19b], we conjecture that $\nu_c = 1$, that is, the worse case is when the density is a Dirac delta. We can only prove the following

Lemma 2 (Estimates on ν_c). *We have*

$$0.91 \simeq \frac{2}{\frac{\pi}{2} + \frac{2}{\pi}} \leq \nu_c \leq 1. \tag{15}$$

Proof. The upper bound is obtained by concentrating ρ at the origin to make it converge to δ_0

and by using the exact Coulomb value. The lower bound follows from Tix's inequality [Tix98]

$$P_0^+ \left(D_0 - \frac{\kappa}{|x|} \right) P_0^+ \geq (1 - \kappa) P_0^+, \quad \forall 0 \leq \kappa \leq \frac{2}{\frac{\pi}{2} + \frac{2}{\pi}}, \quad (16)$$

where $P_0^+ = \mathbf{1}(D_0 \geq 0)$ is the positive spectral projector of the free Dirac operator. By translation invariance we deduce that

$$P_0^+ \left(D_0 - \nu \rho * \frac{1}{|x|} \right) P_0^+ \geq (1 - \nu) P_0^+ \quad (17)$$

for every probability measure ρ . Let us now explain how to derive the lower bound in (15) using (17). We can use the min-max characterization from [DES00], as described also in [ELS19b]. For simplicity we work with $D_{0,-\nu\rho} = D_0 - \nu\rho * |x|^{-1}$ instead of $D_{0,\nu\rho} = D_0 + \nu\rho * |x|^{-1}$, which is the same by charge conjugation. We define

$$a_- := \max_{\substack{\Psi \in P_0^- L^2 \\ \|\Psi\|=1}} \langle \Psi, (D_0 - \nu\rho * |x|^{-1}) \Psi \rangle$$

which satisfies $a_- = -1$ due to the negative sign of the potential $-\rho * |x|^{-1}$. Then we look at the min-max value

$$\lambda_1(\nu) := \inf_{\Psi_+ \in P_0^+ L^2} \sup_{\Psi_- \in P_0^- L^2} \frac{\langle \Psi_+ + \Psi_-, (D_0 - \nu\rho * |x|^{-1}) (\Psi_+ + \Psi_-) \rangle}{\|\Psi_+ + \Psi_-\|^2}.$$

Taking $\Psi_- \equiv 0$ and using Tix's inequality (17), we obtain

$$\lambda_1(\nu) \geq (1 - \nu).$$

In particular $\lambda_1(\nu) > a_-$, hence $\lambda_1(\nu)$ is the lowest eigenvalue of $D_{-\nu\rho}$ above -1 , by [DES00]. This proves as we wanted that $\lambda_1(\nu) > 0$ for $\nu < 2/(\pi/2 + 2/\pi)$. In other words, we have $\nu_c(\rho) \geq 2/(\pi/2 + 2/\pi)$. \square

We now investigate the case of a negative point charge together with a smoother positive charge, $\rho_+ - \kappa\delta_0$. Similarly as before, we introduce

$$\nu_c(\kappa, \rho_+) := \min \{ \nu > 0 : 0 \in \sigma(D_{\kappa, \nu\rho_+}) \}$$

and

$$\nu_c(\kappa) := \inf_{\substack{\rho_+ \geq 0 \\ \rho_+(\mathbb{R}^3)=1}} \nu_c(\kappa, \rho_+).$$

This critical charge is actually equal to the one at $\kappa = 0$.

Lemma 3. *For every $\kappa \in [0, 1)$, we have*

$$\nu_c(\kappa) = \nu_c.$$

Proof. By the min-max principle of [DES00] one can see that the negative eigenvalues of $D_{\kappa, \nu\rho_+}$ are decreasing with respect to κ and increasing with respect to ν (a different proof of this will be given in the proof of Theorem 4 in Section 3 below). In particular, we have $\nu_c(\kappa, \rho_+) \geq \nu_c(0, \rho_+) = \nu_c(\rho_+)$. After minimizing over ρ_+ , this gives $\nu_c(\kappa) \geq \nu_c$. However, by placing

ρ_+ very far away from the origin, we also see that $\nu_c(\kappa) \leq \nu_c$ and there must therefore be equality. \square

Our main result in this section is that the gap implies a universal operator bound.

Theorem 4 (Gap of general sub-critical Dirac-Coulomb operators). *For every $0 \leq \kappa < 1$ and every $0 \leq \nu < \nu_c$, there exists a universal constant $c_{\kappa,\nu} > 0$ so that*

$$c_{\kappa,\nu} |D_0| \leq |D_{\kappa,\rho}| \tag{18}$$

for every non-negative ρ so that $\sqrt{\rho} \in H^{1/2}(\mathbb{R}^3)$ and $\int_{\mathbb{R}^3} \rho = \nu$. One can for instance take

$$c_{\kappa,\nu} = \frac{c_\kappa^2}{1 + 2(\nu + \kappa)} \left(1 + \frac{\pi}{2c_\kappa} \frac{\nu \nu_c}{\nu_c - \nu} \right)^{-2} \tag{19}$$

where c_κ is the best constant in (11).

The proof is provided in Section 3. Theorem 4 gives a lower bound, similar to the upper bound (10), which is completely independent of the shape of the negative charge ρ and this will play a decisive role in the study of our nonlinear problem, where ρ is unknown. The constant in (19) is not at all optimal and it is only displayed for concreteness.

Remark 5 (More general negative densities). *The theorem applies to all positive Borel measures ρ . It is not at all necessary that $\sqrt{\rho} \in H^{1/2}(\mathbb{R}^3)$. But we have stated it in this context since this is what we will need later, and because working with a bounded repulsive Coulomb potential simplifies some technical arguments.*

Remark 6 (A better estimate on the gap of $D_{\kappa,\rho}$). *The estimate (18) implies the following estimate on the gap around the origin:*

$$\sigma(D_{\kappa,\rho}) \cap (-c_{\kappa,\nu}; c_{\kappa,\nu}) = \emptyset.$$

However, we indeed have

$$\sigma(D_{\kappa,\rho}) \cap (\lambda_c(\nu); \sqrt{1 - \kappa^2}) = \emptyset,$$

where

$$\lambda_c(\nu) := \sup_{\substack{\rho \geq 0 \\ \int_{\mathbb{R}^3} \rho = \nu}} \lambda_1(D_{0,\rho}) < 0.$$

is the largest possible value of the last negative eigenvalue, when optimized over all densities ρ with subcritical mass $\int_{\mathbb{R}^3} \rho = \nu < \nu_c$. This is due to the min-max principle of [DES00], which implies that the negative eigenvalues are decreasing in κ at fixed ρ and that the positive eigenvalues are increasing in ν at fixed κ , as we have already mentioned. The existence of an optimizer ρ for this problem is established in [ELS19a].

Remark 7 (More general positive densities). *We have considered an attractive Dirac charge because this is what will be needed later. It is also possible to show that for any $\rho_\pm \geq 0$ with $\int_{\mathbb{R}^3} \rho_\pm = \nu_\pm < \nu_c$, we have with $\rho = \rho_+ - \rho_-$*

$$c_{\nu_+,\nu_-} |D_0| \leq \left| D_0 + \rho * \frac{1}{|x|} \right|$$

for some $c_{\nu_+, \nu_-} > 0$ and

$$\sigma \left(D_0 + \rho * \frac{1}{|x|} \right) \cap (-\lambda_c(\nu_+); \lambda_c(\nu_-)) = \emptyset.$$

2.2 A minimization principle in Dirac-Fock theory

The Dirac-Fock energy functional is obtained from the Hartree-Fock model by replacing $-\Delta/2$ by $D_0 - 1$. In the spirit of [Lie81b; BLS94], we consider mixed quasi-free states and express everything in terms of the one particle density matrix γ , which is a bounded self-adjoint operator on $L^2(\mathbb{R}^3, \mathbb{C}^4)$ such that $0 \leq \gamma \leq 1$ and $\text{Tr} \gamma = N$ for N electrons. The (reduced) Dirac-Fock energy reads

$$\mathcal{E}_{\kappa, \alpha}^{\text{DF}}(\gamma) = \text{Tr}(D_\kappa - 1)\gamma + \frac{\alpha}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\gamma(x)\rho_\gamma(y)}{|x-y|} dx dy \quad (20)$$

where

$$\rho_\gamma(x) = \text{Tr}_{\mathbb{C}^4} \gamma(x, x)$$

is the associated density. The functional $\mathcal{E}_{\kappa, \alpha}^{\text{DF}}$ is unbounded from below, due to the fact that D_κ is itself unbounded. Critical points satisfy the self-consistent equation

$$[\gamma, D_{\kappa, \alpha \rho_\gamma}] = 0$$

where $D_{\kappa, \alpha \rho_\gamma} = D_\kappa + \alpha \rho_\gamma * |x|^{-1}$ is called the *mean-field* or *Fock operator*. We are interested in the stationary states satisfying the more precise equation

$$\gamma = \mathbb{1}(0 \leq D_{\kappa, \alpha \rho_\gamma} \leq \mu), \quad (21)$$

that is, γ is the orthogonal projection corresponding to the N first *positive* eigenvalues of its Fock operator. Re-expressed in terms of the N first eigenfunctions, this gives a system of N coupled nonlinear Dirac equations

$$\left(D_\kappa + \alpha \sum_{j=1}^N |\varphi_j|^2 * \frac{1}{|x|} \right) \varphi_j = \mu_j \varphi_j, \quad (22)$$

with $0 < \mu_1 \leq \dots \leq \mu_N = \mu$ the N first positive eigenvalues. States satisfying (21) can be interpreted as *ground states* since they solve the same kind of equation as for Hartree-Fock minimizers. It will be useful to introduce the projector

$$P_{\kappa, \gamma}^+ := \mathbb{1}(D_{\kappa, \alpha \rho_\gamma} \geq 0)$$

on the positive spectral subspace of the mean-field operator and to note that $\gamma P_{\kappa, \gamma}^+ = \gamma$, or equivalently $0 \leq \gamma \leq P_{\kappa, \gamma}^+$.

The existence of infinitely many solutions to (22) was proved for the first time by Esteban-Séré in [ES99] (with exchange term, but the argument works the same without exchange) for all

$$\max(\kappa, 3\alpha N) < \frac{2}{\pi/2 + 2/\pi}, \quad N \leq Z = \kappa/\alpha,$$

using a concavity argument in the negative directions. Although in this work the μ_j are known to be positive, they are however not necessarily the N first eigenvalues. The result of [ES99] was then generalized to the range

$$\max(\kappa, \alpha N) < \frac{2}{\pi/2 + 2/\pi}, \quad N \leq Z = \kappa/\alpha,$$

by Paturel in [Pat00]. That is, the unphysical factor 3 was removed, using a Lyapounov-Schmidt reduction and a linking argument. In [ES01], Esteban and Séré have shown that their first solution indeed converges to the (non-relativistic) Hartree-Fock minimizer in the limit $\alpha \rightarrow 0$ at fixed Z and N , after a proper rescaling. Furthermore, the μ_j are the first eigenvalues of $D_{\kappa, \alpha \rho_\gamma}$ for α small enough. This is the justification that (21) is the natural equation for a Dirac-Fock ground state. Finally, they proved in the same article [ES01] that for α small enough, their solution solves the following minimization problem

$$E^{\text{DF}}(\kappa, \alpha, N) = \min_{\substack{0 \leq \gamma \leq P_{\kappa, \gamma}^+ \\ \text{Tr}(\gamma) \leq N}} \mathcal{E}_{\kappa, \alpha}^{\text{DF}}(\gamma). \quad (23)$$

In words, the Dirac-Fock ground state minimizes the Dirac-Fock energy among all the states which live in the positive spectral subspace of their own mean-field operator $P_{\kappa, \gamma}^+$. This is a very nonlinear constraint but it is physically meaningful. Using a simpler fixed point technique, Huber and Siedentop have later obtained a similar result in [HS07] for α small enough at fixed $\kappa = \alpha Z$ and N , that is, for large atoms but small interactions. Finally, in the unpublished work [Sér09], Séré has directly studied the minimization problem (23) for κ and αN fixed but small enough, with quantitative estimates. His argument is based on the function

$$\theta(\gamma) = \lim_{n \rightarrow \infty} \gamma_n$$

where the sequence γ_n is recursively defined by

$$\begin{cases} \gamma_{n+1} = P_{\kappa, \gamma_n}^+ \gamma_n P_{\kappa, \gamma_n}^+ \\ \gamma_0 = \gamma. \end{cases}$$

The function θ is used to project any γ sufficiently close to satisfying the constraint $P_{\kappa, \gamma}^- \gamma = 0$ to a new state $\theta(\gamma)$ which does satisfy this constraint. This allows to show that the set of states $\{\gamma : P_{\kappa, \gamma}^- \gamma = 0\}$ is a smooth manifold on which one can use variational techniques.

To summarize the situation, there are solutions to the Dirac-Fock equations (21) for $\max(\alpha Z, \alpha N) < 2/(\pi/2 + 2/\pi)$. One of these solutions is known to solve the minimization problem (23), but only in a limiting regime of small α (either with N and Z fixed, or κ and N fixed or κ and αN small but fixed). In this paper we will study the limit of (23) in the whole range

$$0 \leq \kappa < 1, \quad 0 \leq \alpha N < \nu_c$$

where ν_c is the critical number defined in the previous section, although minimizers are not necessarily known to exist in all cases. Note that we have required $\text{Tr}(\gamma) \leq N$ instead of $\text{Tr} \gamma = N$ in (20). We believe that minimizers always exist in (20), that they satisfy $\text{Tr} \gamma = N$ and the nonlinear equation (21). The question of whether $E^{\text{DF}}(\kappa, \alpha, N)$ is a well-defined number arises immediately, but this turns out to be a simple consequence of the analysis in the previous

section.

Lemma 8 ($\mathcal{E}_{\kappa,\alpha}^{\text{DF}}$ is bounded from below on positive energy states). *Let $0 \leq \kappa < 1$ and $0 \leq \nu < \nu_c$. There exists a constant $\alpha_c = \alpha_c(\kappa, \nu)$ so that*

$$\mathcal{E}_{\kappa,\alpha}^{\text{DF}}(\gamma) \geq \frac{c_{\kappa,\nu}}{2} \text{Tr}(\sqrt{-\Delta}\gamma) - \text{Tr}(\gamma) \quad (24)$$

for all $0 \leq \alpha \leq \alpha_c$ and every density matrix $0 \leq \gamma = \gamma^* \leq 1$ satisfying the nonlinear constraint $\gamma P_{\kappa,\gamma}^- = 0$ and such that $\alpha \text{Tr}(\gamma) \leq \nu$ and $\text{Tr}(\sqrt{-\Delta}\gamma) < \infty$. In particular, $E^{\text{DF}}(\kappa, \alpha, N)$ is well defined in (20).

Proof. Since $D_{\kappa,\alpha\rho_\gamma}\gamma = |D_{\kappa,\alpha\rho_\gamma}|\gamma$ since $0 \leq \gamma \leq P_{\kappa,\gamma}^+$, we have by (18) and $|D_0|^2 = 1 - \Delta$

$$\begin{aligned} \mathcal{E}_{\kappa,\alpha}^{\text{DF}}(\gamma) &= \text{Tr} D_{\kappa,\alpha\rho_\gamma}\gamma - \frac{\alpha}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\gamma(x)\rho_\gamma(y)}{|x-y|} dx dy - \text{Tr}(\gamma) \\ &\geq c_{\kappa,\nu} \text{Tr} \sqrt{1-\Delta}\gamma - \frac{\alpha}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\gamma(x)\rho_\gamma(y)}{|x-y|} dx dy - \text{Tr}(\gamma). \end{aligned}$$

The Lieb-Thirring inequality [LS10, Theorem 4.3] states that

$$\text{Tr} \sqrt{1-\Delta}\gamma \geq \text{Tr} \sqrt{-\Delta}\gamma \geq c_{\text{LT}} \int_{\mathbb{R}^3} \rho_\gamma^{4/3}. \quad (25)$$

On the other hand, the Hardy-Littlewood-Sobolev [LL01, Theorem 4.3] and Hölder inequalities give

$$\iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\gamma(x)\rho_\gamma(y)}{|x-y|} dx dy \leq c_{\text{HLS}} \|\rho_\gamma\|_{L^{6/5}(\mathbb{R}^3)}^2 \leq c_{\text{HLS}} (\text{Tr} \gamma)^{2/3} \int_{\mathbb{R}^3} \rho_\gamma^{4/3} \quad (26)$$

hence we conclude that

$$\mathcal{E}_{\kappa,\alpha}^{\text{DF}}(\gamma) \geq \frac{c_{\kappa,\nu}}{2} \text{Tr}(\sqrt{-\Delta}\gamma) - \text{Tr}(\gamma) + \frac{1}{2} \left(c_{\kappa,\nu} c_{\text{LT}} - c_{\text{HLS}} \alpha^{1/3} \nu^{2/3} \right) \int_{\mathbb{R}^3} \rho_\gamma^{4/3}$$

where the last term is non-negative for

$$\alpha \leq \alpha_c := \left(\frac{c_{\kappa,\nu} c_{\text{LT}}}{c_{\text{HLS}} \nu^{2/3}} \right)^3.$$

Note that $0 \leq \gamma \leq P_{\kappa,\gamma}^+$ trivially implies $\gamma P_{\kappa,\gamma}^- = 0$. □

2.3 The Scott correction

We are finally able to state the main theorem of this article. For a given constant $\lambda > 0$, we define the Thomas-Fermi energy

$$e_{\text{TF}}(\lambda) = \min_{\substack{\rho \geq 0 \\ \int_{\mathbb{R}^3} \rho = 1}} \left\{ \frac{3}{10} (3\pi^2)^{2/3} \int_{\mathbb{R}^3} \rho(x)^{5/3} dx - \lambda \int_{\mathbb{R}^3} \frac{\rho(x)}{|x|} dx + \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho(x)\rho(y)}{|x-y|} dx dy \right\}. \quad (27)$$

We note that $e_{\text{TF}}(\lambda)$ is non-increasing and concave in λ . It is constant, equal to $e_{\text{TF}}(1) < 0$ for $\lambda \in (0; 1]$. On the other hand, the Scott correction was defined in [HS15] to be

$$c_{\text{Scott}}(\kappa) := \frac{\kappa^2}{2} + \sum_{n \geq 1} \left\{ \lambda_n \left(D_0 - \frac{\kappa}{|x|} - 1 \right) - \lambda_n \left(-\frac{\Delta}{2} - \frac{\kappa}{|x|} \right) \right\}, \tag{28}$$

where λ_n are the eigenvalues in $[-2, 0]$ of the operator in the parenthesis, repeated in case of multiplicity and arranged in increasing order.

Our main result concerns the case of neutral atoms, as is classically considered for the Scott correction. This forces us to take $\nu = \kappa < \nu_c$. However, several parts of our approach apply to the case of general $\kappa < 1$ and $\nu < \nu_c$, as we will see.

Theorem 9 (Scott correction in Dirac-Fock theory). *Let $0 < \kappa < \nu_c$. Then we have*

$$\lim_{\substack{N \rightarrow \infty \\ \alpha N \rightarrow \kappa}} \left| E^{\text{DF}}(\kappa, \alpha, N) - e_{\text{TF}}(1) \alpha^2 N^{\frac{7}{3}} - c_{\text{Scott}}(\kappa) \right| = 0. \tag{29}$$

Note that our energy is multiplied by α^2 compared to [HS15] and several other works on the subject. We have

$$\alpha^2 N^{\frac{7}{3}} = \kappa^2 N^{\frac{1}{3}}$$

hence the energy is of order $N^{1/3}$ in our regime, whereas the Scott correction is of order 1.

Remark 10. *It is only because we rely on existing results, in particular from [HS15], that we need to impose $\kappa = \nu$ (neutral atoms). We believe that for all $0 < \kappa < 1$ and $0 < \nu < \nu_c$, we have*

$$\lim_{\substack{N \rightarrow \infty \\ \alpha N \rightarrow \nu}} \left| E^{\text{DF}}(\kappa, \alpha, N) - e_{\text{TF}}(\kappa/\nu) \alpha^2 N^{\frac{7}{3}} - c_{\text{Scott}}(\kappa) \right| = 0.$$

That is, the result should apply to ions, as first considered by Bach in [Bac89]. Several of our intermediate steps will actually be valid in this regime.

The rest of the paper is devoted to the proof of Theorems 4 and 9.

3 Proof of Theorem 4

In this section we provide the proof of Theorem 4 which states that

$$|D_{\kappa, \rho}| \geq c_{\kappa, \nu} |D_0|$$

as soon as $\int_{\mathbb{R}^3} \rho = \nu < \nu_c$ and $0 \leq \kappa < 1$. Our argument uses the Birman-Schwinger principle as in Nenciu’s work [Nen76] on the distinguished self-adjoint extensions of D_κ .

Lemma 11. *Let A be a self-adjoint operator such that $0 \notin \sigma(A)$ and let B be a positive, A -bounded operator, on a Hilbert space \mathfrak{H} . If $-1 \notin \sigma(\sqrt{B}A^{-1}\sqrt{B})$ then $0 \notin \sigma(A + B)$ and the resolvent of $A + B$ is given by*

$$\frac{1}{A + B} = \frac{1}{A} - \frac{1}{A} \sqrt{B} \frac{1}{1 + \sqrt{B}A^{-1}\sqrt{B}} \sqrt{B} \frac{1}{A}. \tag{30}$$

Proof. First note that since B is A -bounded, the operator $A + B$ is well defined on $D(A)$. If

$-1 \notin \sigma(\sqrt{B}A^{-1}\sqrt{B})$ then we can define the bounded operator

$$R := \frac{1}{A} - \frac{1}{A}\sqrt{B}\frac{1}{1 + \sqrt{B}A^{-1}\sqrt{B}}\sqrt{B}\frac{1}{A}.$$

It remains to verify that

$$\begin{aligned} (A + B)R &= 1 - \sqrt{B}\frac{1}{1 + \sqrt{B}A^{-1}\sqrt{B}}\sqrt{B}\frac{1}{A} \\ &\quad + B\frac{1}{A} - \sqrt{B}\sqrt{B}\frac{1}{A}\sqrt{B}\frac{1}{1 + \sqrt{B}A^{-1}\sqrt{B}}\sqrt{B}\frac{1}{A} \\ &= 1 - B\frac{1}{A} - \sqrt{B}\frac{1 + \sqrt{B}A^{-1}\sqrt{B}}{1 + \sqrt{B}A^{-1}\sqrt{B}}\sqrt{B}\frac{1}{A} = 1, \end{aligned}$$

which proves that $0 \notin \sigma(A + B)$ and (30). \square

The formula (30) was used by Nenciu with $A = D_0$ and $B = \kappa/|x|$ to prove the existence of the unique distinguished self-adjoint extension for D_κ . The critical value $\kappa = 1$ arises from the fact that

$$\left\| \frac{1}{|x|^{1/2}} \frac{1}{D_0} \frac{1}{|x|^{1/2}} \right\| = 1.$$

This relation has been conjectured by Nenciu [Nen76] and was later proved by Wüst [Wüs77] and Kato [Kat83]. It has recently been rediscovered in [ADV13, Thm. 1.3].

The lemma implies the following.

Corollary 12. *Let A be a self-adjoint operator such that $0 \notin \sigma(A)$ and let B be a positive bounded operator, on a Hilbert space \mathfrak{H} . Denote by*

$$\lambda_c(B) := \min \sigma \left(\sqrt{B}\frac{1}{A}\sqrt{B} \right)$$

the minimum of the spectrum of $\sqrt{B}A^{-1}\sqrt{B}$ and

$$\nu_c(B) = \begin{cases} -\frac{1}{\lambda_c(B)} & \text{if } \lambda_c(B) < 0 \\ +\infty & \text{otherwise.} \end{cases}$$

Then

$$0 \notin \sigma(A + \nu B)$$

for all $0 \leq \nu < \nu_c(B)$ whereas $0 \in \sigma(A + \nu_c(B)B)$ if $\nu_c(B) < \infty$.

Proof. For $\nu > 0$ we have $1 + \nu\sqrt{B}A^{-1}\sqrt{B} \geq 1 + \nu\lambda_c(B)$ hence the result follows from Lemma 11. \square

Now we go back to our Dirac operator. Note that by charge conjugation invariance, the spectrum of the operator

$$M_\rho = \sqrt{\rho * |x|^{-1}} \frac{1}{D_0} \sqrt{\rho * |x|^{-1}}$$

is symmetric with respect to the origin. When $\sqrt{\rho} \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$, M_ρ is a compact operator. Corollary 12 implies that the critical value $\nu_c(\rho)$ at which the largest eigenvalue of $D_0 + \nu\rho * |x|^{-1}$

crosses the origin is given by

$$-\frac{1}{\nu_c(\rho)} = -\|M_\rho\| = \min_{\Psi \in L^2(\mathbb{R}^3, \mathbb{C}^4)} \frac{\langle \Psi, M_\rho \Psi \rangle}{\|\Psi\|^2}.$$

In particular,

$$-\frac{1}{\nu_c} = \inf_{\rho} \min_{\Psi \in L^2(\mathbb{R}^3, \mathbb{C}^4)} \frac{\langle \Psi, M_\rho \Psi \rangle}{\|\Psi\|^2}.$$

Now we look at the operator

$$D_{\kappa, \rho} = D_\kappa + \nu \rho * \frac{1}{|x|}$$

and recall that D_κ is invertible for $0 \leq \kappa < 1$. The previous theory tells us that for a probability density ρ with $\sqrt{\rho} \in H^{1/2}(\mathbb{R}^3)$, no eigenvalue will cross 0 for $\nu < \nu_c(\kappa, \rho)$ given by

$$-\frac{1}{\nu_c(\kappa, \rho)} = \min_{\Psi \in L^2(\mathbb{R}^3, \mathbb{C}^4)} \frac{\langle \sqrt{\rho} * |x|^{-1} \Psi, \frac{1}{D_\kappa} \sqrt{\rho} * |x|^{-1} \Psi \rangle}{\|\Psi\|^2}.$$

In order to prove a lower bound on $|D_{\kappa, \rho}|$, we use Formula (30). We write

$$\begin{aligned} |D_0|^{1/2} \frac{1}{|D_{\kappa, \rho}|^{1/2}} &= |D_0|^{1/2} \frac{1}{D_{\kappa, \rho}} |D_{\kappa, \rho}|^{1/2} U_{\kappa, \rho} \\ &= \left(|D_0|^{1/2} \frac{1}{D_\kappa} |D_{\kappa, \rho}|^{1/2} \right. \\ &\quad \left. + |D_0|^{1/2} \frac{1}{D_\kappa} \sqrt{V_\rho} \frac{1}{1 + M_{\kappa, \rho}} \sqrt{V_\rho} \frac{1}{D_\kappa} |D_{\kappa, \rho}|^{1/2} \right) U_{\kappa, \rho}, \end{aligned}$$

where $U_{\kappa, \rho} = \text{sgn}(D_{\kappa, \rho})$ is a unitary operator, $V_\rho = \rho * |x|^{-1}$ and $M_{\kappa, \rho} = \sqrt{V_\rho} D_\kappa^{-1} \sqrt{V_\rho}$. We have

$$\|(1 + M_{\kappa, \rho})^{-1}\| \leq \frac{\nu_c}{\nu_c - \nu}.$$

This gives

$$\begin{aligned} \left\| |D_0|^{1/2} \frac{1}{|D_{\kappa, \rho}|^{1/2}} \right\| &\leq \left\| |D_0|^{1/2} \frac{1}{|D_\kappa|^{1/2}} \right\| \left\| \frac{1}{|D_\kappa|^{1/2}} |D_{\kappa, \rho}|^{1/2} \right\| \times \\ &\quad \times \left(1 + \frac{\nu_c}{\nu_c - \nu} \left\| \sqrt{V_\rho} \frac{1}{|D_\kappa|^{1/2}} \right\|^2 \right). \end{aligned} \quad (31)$$

The best constant c_κ such that $c_\kappa |D_0| \leq |D_\kappa|$ is exactly given by

$$\frac{1}{c_\kappa} = \left\| \frac{1}{|D_\kappa|^{1/2}} |D_0| \frac{1}{|D_\kappa|^{1/2}} \right\| = \left\| |D_0|^{1/2} \frac{1}{|D_\kappa|^{1/2}} \right\|^2.$$

From the Hardy-Kato inequality (6), we have

$$\left\| \sqrt{V_\rho} \frac{1}{|D_\kappa|^{1/2}} \right\|^2 = \left\| \frac{1}{|D_\kappa|^{1/2}} V_\rho \frac{1}{|D_\kappa|^{1/2}} \right\| \leq \frac{\pi \nu}{2} \left\| \frac{1}{|D_\kappa|^{1/2}} |D_0| \frac{1}{|D_\kappa|^{1/2}} \right\| = \frac{\pi \nu}{2 c_\kappa}.$$

On the other hand we have by (10)

$$\begin{aligned} \left\| \frac{1}{|D_\kappa|^{1/2}} |D_{\kappa,\rho}|^{1/2} \right\| &\leq \left\| \frac{1}{|D_\kappa|^{1/2}} |D_0|^{1/2} \right\| \left\| \frac{1}{|D_0|^{1/2}} |D_{\kappa,\rho}|^{1/2} \right\| \\ &\leq \sqrt{\frac{1+2(\kappa+\nu)}{c_\kappa}}. \end{aligned} \quad (32)$$

Inserting in (31), we obtain

$$\left\| |D_0|^{1/2} \frac{1}{|D_{\kappa,\rho}|^{1/2}} \right\|^2 \leq \frac{1+2(\nu+\kappa)}{c_\kappa^2} \left(1 + \frac{\pi}{2c_\kappa} \frac{\nu_c \nu}{\nu_c - \nu} \right)^2,$$

which concludes the proof of Theorem 4. \square

Remark 13. *Our bound (32) is far from optimal, in particular when $\nu = 0$. This is why we obtain $c_{\kappa,0} \neq c_\kappa$.*

4 A bound on differences of spectral projections

In this section we prove the following estimate on the difference of two spectral projectors, when the electric field has a small energy, first in Hilbert-Schmidt norm and then in the Schatten space \mathfrak{S}^6 .

Proposition 14 (Schatten class estimates on differences of projections). *Let $0 \leq \kappa < 1$ and $\varepsilon > 0$. There exists a constant $B = B(\kappa)$ and a constant $C = C(\kappa, \varepsilon)$ such that*

$$\left\| |D_\kappa|^{1/2} \left(\mathbf{1}(D_\kappa + V \leq 0) - \mathbf{1}(D_\kappa \leq 0) \right) |D_\kappa|^{-1/2} \right\|_{\mathfrak{S}^2} \leq B \left(1 + \|\nabla V\|_{L^3(\mathbb{R}^3)} \right) \|\nabla V\|_{L^2(\mathbb{R}^3)} \quad (33)$$

and

$$\left\| |D_\kappa|^{1/2} \left(\mathbf{1}(D_\kappa + V \leq 0) - \mathbf{1}(D_\kappa \leq 0) \right) |D_\kappa|^{-\varepsilon} \right\|_{\mathfrak{S}^6} \leq C \|\nabla V\|_{L^2(\mathbb{R}^3)} \quad (34)$$

for every $V \in L^6(\mathbb{R}^3)$ such that $\|V\|_{L^6(\mathbb{R}^3)} \leq 1/B$. This implies

$$\begin{aligned} \left\| |D_\kappa|^{1/2} \left(\mathbf{1}(D_\kappa + V \leq 0) - \mathbf{1}(D_\kappa \leq 0) \right) |D_\kappa|^{-\frac{6-p}{8}-\varepsilon} \right\|_{\mathfrak{S}^p} \\ \leq C^{\frac{3p-6}{2p}} B^{\frac{6-p}{2p}} \left(1 + \|\nabla V\|_{L^3(\mathbb{R}^3)} \right)^{\frac{6-p}{2p}} \|\nabla V\|_{L^2(\mathbb{R}^3)} \end{aligned} \quad (35)$$

for all $2 \leq p \leq 6$.

We have the convention that if $f \notin X$ then $\|f\|_X = \infty$. In the lemma we can replace $|D_\kappa|^{1/2}$ by $|D_0|^{1/2}$ everywhere since those are comparable.

Proof. In the whole proof we denote by C a generic constant whose value can change from line to line, but which only depends on κ and ε . For $0 \leq \kappa < 1$ we have by (11)

$$\left\| V \frac{1}{D_\kappa} \right\|_{\mathfrak{S}^6} \leq C \left\| V \frac{1}{|D_0|^{1/2+\varepsilon}} \right\|_{\mathfrak{S}^6} \leq C \|V\|_{L^6(\mathbb{R}^3)} \quad (36)$$

for every $\varepsilon < \sqrt{1 - \kappa^2}$, where in the last inequality we have used the Kato-Seiler-Simon inequality [Sim79]

$$\|f(x)g(-i\nabla)\|_{\mathfrak{S}^p} \leq (2\pi)^{-\frac{d}{p}} \|f\|_{L^p(\mathbb{R}^d)} \|g\|_{L^p(\mathbb{R}^d)}, \quad \forall p \geq 2. \tag{37}$$

By the Rellich-Kato theorem, this proves that when $\|V\|_{L^6}$ is small enough, $D_\kappa + V$ is self-adjoint on the same domain as D_κ , with

$$\frac{1}{C}(D_\kappa + V)^2 \leq (D_\kappa)^2 \leq C(D_\kappa + V)^2 \tag{38}$$

for some constant C depending only on the maximal allowed value of $\|V\|_{L^6}$. In particular, $D_\kappa + V$ has a gap around the origin. In the rest of the proof we always assume that $\|V\|_{L^6}$ is small enough.

Throughout the proof we denote for simplicity $P_{\kappa,V}^\pm := \mathbb{1}_{\mathbb{R}^\pm}(D_0 + V)$.

• **Proof of the \mathfrak{S}^6 estimate (34)**

We use Stone’s formula for spectral projections and the resolvent formula to express the difference as

$$P_{\kappa,V}^+ - P_\kappa^+ = -\frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D_\kappa + i\eta} V \frac{1}{D_\kappa + V + i\eta} d\eta.$$

Hence

$$\left\| |D_\kappa|^{\frac{1}{2}} (P_{\kappa,V}^+ - P_\kappa^+) |D_\kappa|^{-\varepsilon} \right\|_{\mathfrak{S}^6} \leq \frac{1}{2\pi} \int_{\mathbb{R}} \left\| \frac{|D_\kappa|^{\frac{1}{2}}}{D_\kappa + i\eta} V \frac{1}{D_\kappa + V + i\eta} \frac{1}{|D_\kappa|^\varepsilon} \right\|_{\mathfrak{S}^6} d\eta.$$

Writing

$$\frac{1}{D_\kappa + V + i\eta} \frac{1}{|D_\kappa|^\varepsilon} = \frac{1}{|D_\kappa|^\varepsilon} \left(|D_\kappa|^\varepsilon \frac{1}{|D_{\kappa,V}|^\varepsilon} \right) \frac{1}{D_\kappa + V + i\eta} \left(|D_{\kappa,V}|^\varepsilon \frac{1}{|D_\kappa|^\varepsilon} \right)$$

and using (38), we find

$$\begin{aligned} & \left\| \frac{|D_\kappa|^{\frac{1}{2}}}{D_\kappa + i\eta} V \frac{1}{D_\kappa + V + i\eta} \frac{1}{|D_\kappa|^\varepsilon} \right\|_{\mathfrak{S}^6} \\ & \leq \frac{C}{\langle \eta \rangle} \left\| \frac{1}{|D_\kappa|^{\frac{1}{2}} + \langle \eta \rangle^{\frac{1}{2}}} V \frac{1}{|D_\kappa|^\varepsilon} \right\|_{\mathfrak{S}^6} \\ & \leq \frac{C}{\langle \eta \rangle} \left\| \frac{1}{|D_0|^{\frac{1}{2}} + \langle \eta \rangle^{\frac{1}{2}}} V \frac{1}{|D_0|^\varepsilon} \right\|_{\mathfrak{S}^6} \leq \frac{C \|V\|_{L^6}}{\langle \eta \rangle^{1+\varepsilon}}, \end{aligned}$$

by the Kato-Seiler-Simon inequality (37) and the fact that $|D_\kappa|$ is comparable to $|D_0|$ in the quadratic form sense. Here $\langle \eta \rangle = \sqrt{1 + \eta^2}$ is the Japanese bracket. We obtain (34) after integrating over η .

• **Proof of the Hilbert-Schmidt estimate (33)**

The proof of (33) is much more involved. We start by iterating the resolvent formula twice to obtain

$$\begin{aligned} P_{\kappa,V}^+ - P_{\kappa}^+ &= -\frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D_{\kappa} + i\eta} V \frac{1}{D_{\kappa} + i\eta} d\eta \\ &\quad + \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D_{\kappa} + i\eta} V \frac{1}{D_{\kappa} + i\eta} V \frac{1}{D_{\kappa} + i\eta} d\eta \\ &\quad - \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{D_{\kappa} + i\eta} V \frac{1}{D_{\kappa} + i\eta} V \frac{1}{D_{\kappa} + i\eta} V \frac{1}{D_{\kappa} + V + i\eta} d\eta. \end{aligned} \quad (39)$$

Since $D_{\kappa} + V$ is comparable to D_{κ} by (38) and $|D_{\kappa}|^{1/2}$ is comparable to $|D_0|^{1/2}$, the last term can be bounded by Hölder's inequality in Schatten spaces by

$$\begin{aligned} &\left\| |D_{\kappa}|^{\frac{1}{2}} \int_{\mathbb{R}} \frac{1}{D_{\kappa} + i\eta} V \frac{1}{D_{\kappa} + i\eta} V \frac{1}{D_{\kappa} + i\eta} V \frac{1}{D_{\kappa} + V + i\eta} d\eta \right\|_{\mathfrak{S}^2} \\ &\leq C \int_{\mathbb{R}} \frac{d\eta}{\langle \eta \rangle^{\frac{1}{2}}} \left\| \frac{1}{|D_0|^{\frac{1}{2}} + \langle \eta \rangle^{\frac{1}{2}}} V \frac{1}{|D_0|^{\frac{1}{2}} + \langle \eta \rangle^{\frac{1}{2}}} \right\|_{\mathfrak{S}^6}^3 \\ &\leq C \|V\|_{L^6}^3 \int_{\mathbb{R}} \frac{d\eta}{\langle \eta \rangle^2}. \end{aligned}$$

It is here not necessary to use the operator $|D_{\kappa}|^{-1/2}$ on the right side. It therefore remains to estimate the first two terms in (39).

We start with the second term in (39). Using that

$$\int_{\mathbb{R}} \frac{1}{(D_{\kappa} + i\eta)^3} d\eta = 0$$

by Cauchy's formula, we have

$$\begin{aligned} &\int_{\mathbb{R}} \frac{1}{D_{\kappa} + i\eta} V \frac{1}{D_{\kappa} + i\eta} V \frac{1}{D_{\kappa} + i\eta} d\eta \\ &= \int_{\mathbb{R}} \frac{1}{D_{\kappa} + i\eta} V \frac{1}{D_{\kappa} + i\eta} \left[V, \frac{1}{D_{\kappa} + i\eta} \right] d\eta + \int_{\mathbb{R}} \left[\frac{1}{D_{\kappa} + i\eta}, V \right] \frac{1}{(D_{\kappa} + i\eta)^2} V d\eta. \end{aligned}$$

Inserting then

$$\left[V, \frac{1}{D_{\kappa} + i\eta} \right] = \frac{1}{D_{\kappa} + i\eta} [D_{\kappa}, V] \frac{1}{D_{\kappa} + i\eta} = -i \frac{1}{D_{\kappa} + i\eta} \boldsymbol{\alpha} \cdot \nabla V \frac{1}{D_{\kappa} + i\eta}$$

we obtain

$$\begin{aligned} &\int_{\mathbb{R}} \frac{1}{D_{\kappa} + i\eta} V \frac{1}{D_{\kappa} + i\eta} V \frac{1}{D_{\kappa} + i\eta} d\eta \\ &= -i \int_{\mathbb{R}} \frac{1}{D_{\kappa} + i\eta} V \frac{1}{(D_{\kappa} + i\eta)^2} \boldsymbol{\alpha} \cdot \nabla V \frac{1}{D_{\kappa} + i\eta} d\eta \\ &\quad + i \int_{\mathbb{R}} \frac{1}{D_{\kappa} + i\eta} \boldsymbol{\alpha} \cdot \nabla V \frac{1}{(D_{\kappa} + i\eta)^3} V d\eta. \end{aligned}$$

We estimate this term using that $|D_\kappa|^{1+\varepsilon} \geq c|D_0|^{1+\varepsilon'}$ where $\varepsilon' < \min(\varepsilon, 2\varepsilon\sqrt{1-\kappa^2})$, see (13). This gives

$$\begin{aligned} & \left\| |D_\kappa|^{\frac{1}{2}} \int_{\mathbb{R}} \frac{1}{D_\kappa + i\eta} V \frac{1}{D_\kappa + i\eta} V \frac{1}{D_\kappa + i\eta} d\eta |D_\kappa|^{-\frac{1}{2}} \right\|_{\mathfrak{S}^2} \\ & \leq C \int_{\mathbb{R}} \left\| \frac{1}{|D_0|^{\frac{1}{2}}} V \frac{1}{|D_0|^{\frac{1}{2}}} \right\|_{\mathfrak{S}^6} \left\| \frac{1}{|D_0|^{\frac{1}{2}}} \alpha \cdot \nabla V \frac{1}{|D_0|^{\frac{1}{2}+\varepsilon'}} \right\|_{\mathfrak{S}^3} \frac{d\eta}{\langle \eta \rangle^{2-\varepsilon}} \\ & \leq C \|V\|_{L^6} \|\nabla V\|_{L^3}. \end{aligned}$$

This gives rise to the term $\|V\|_{L^6} \|\nabla V\|_{L^3}$ in our estimate (33).

Finally, we deal with the first term in (39). If we had D_0 in place of D_κ , the result would follow directly from the Kato-Seiler-Simon inequality. The difficulty here is that high powers of D_κ are not comparable with D_0 when κ is close to 1. So we express the difference exactly. We insert the resolvent formula

$$\begin{aligned} \frac{1}{D_\kappa + i\eta} &= \frac{1}{D_0 + i\eta} - \kappa \frac{1}{D_0 + i\eta} \frac{1}{|x|} \frac{1}{D_\kappa + i\eta} \\ &= \frac{1}{D_0 + i\eta} - \kappa \frac{1}{D_\kappa + i\eta} \frac{1}{|x|} \frac{1}{D_0 + i\eta} \end{aligned}$$

in the first term in (39) and we obtain the rather lengthy formula

$$\begin{aligned} & \int_{\mathbb{R}} |D_\kappa|^{\frac{1}{2}} \frac{1}{D_\kappa + i\eta} V \frac{1}{D_\kappa + i\eta} |D_\kappa|^{-\frac{1}{2}} d\eta \\ &= \int_{\mathbb{R}} |D_\kappa|^{\frac{1}{2}} \frac{1}{D_0 + i\eta} V \frac{1}{D_0 + i\eta} |D_\kappa|^{-\frac{1}{2}} d\eta \\ & \quad - \kappa \int_{\mathbb{R}} |D_\kappa|^{\frac{1}{2}} \left(\frac{1}{D_0 + i\eta} \frac{1}{|x|} \frac{1}{D_0 + i\eta} V \frac{1}{D_0 + i\eta} + \text{h.c.} \right) |D_\kappa|^{-\frac{1}{2}} d\eta \\ & \quad + \kappa^2 \int_{\mathbb{R}} |D_\kappa|^{\frac{1}{2}} \left(\frac{1}{D_\kappa + i\eta} \frac{1}{|x|} \frac{1}{D_0 + i\eta} \frac{1}{|x|} \frac{1}{D_0 + i\eta} V \frac{1}{D_0 + i\eta} + \text{h.c.} \right) |D_\kappa|^{-\frac{1}{2}} d\eta \\ & \quad + \kappa^2 \int_{\mathbb{R}} |D_\kappa|^{\frac{1}{2}} \frac{1}{D_\kappa + i\eta} \frac{1}{|x|} \frac{1}{D_0 + i\eta} V \frac{1}{D_0 + i\eta} \frac{1}{|x|} \frac{1}{D_\kappa + i\eta} |D_\kappa|^{-\frac{1}{2}} d\eta. \end{aligned} \tag{40}$$

In order to estimate the last two terms we can use that for $s > 0$, we have

$$\frac{1}{|D_0|^{\frac{1}{2}}} \frac{1}{|x|} \frac{1}{|D_0|^{\frac{1}{2}+s}} \in \mathfrak{S}_w^3$$

by Cwikel's inequality [Sim79]. In particular, we deduce that

$$\frac{1}{|D_0|^{\frac{1}{2}}} \frac{1}{|x|} \frac{1}{|D_0|^{\frac{1}{2}+s}} \in \mathfrak{S}^p$$

for all $p > 3$ and all $s > 0$. For instance we can control the last term by

$$\begin{aligned} & \left\| |D_\kappa|^{\frac{1}{2}} \frac{1}{D_\kappa + i\eta} \frac{1}{|x|} \frac{1}{D_0 + i\eta} V \frac{1}{D_0 + i\eta} \frac{1}{|x|} \frac{1}{D_\kappa + i\eta} |D_\kappa|^{-\frac{1}{2}} \right\|_{\mathfrak{S}^2} \\ & \leq \frac{C}{\langle \eta \rangle} \left\| \frac{1}{|D_0|^{\frac{1}{2}}} \frac{1}{|x|} \frac{1}{|D_0|^{\frac{1}{2}+s}} \right\|_{\mathfrak{S}^4}^2 \left\| \frac{1}{(|D_0| + \langle \eta \rangle)^{\frac{1}{2}-s}} V \frac{1}{(|D_0| + \langle \eta \rangle)^{\frac{1}{2}-s}} \right\|_{\mathfrak{S}^6} \\ & \leq \frac{C}{\langle \eta \rangle^{\frac{3}{2}-6s}} \|V\|_{L^6} \end{aligned}$$

which is integrable over η for $s > 0$ small enough. The argument is the same for the other term of order κ^2 . On the other hand, for the first term in (40), we use that

$$\int_{\mathbb{R}} \frac{1}{(D_0 + i\eta)^2} d\eta = 0$$

and insert one commutator, which yields

$$\begin{aligned} & \left\| \int_{\mathbb{R}} |D_\kappa|^{\frac{1}{2}} \frac{1}{D_0 + i\eta} V \frac{1}{D_0 + i\eta} |D_\kappa|^{-\frac{1}{2}} d\eta \right\|_{\mathfrak{S}^2} \\ & = \left\| \int_{\mathbb{R}} |D_\kappa|^{\frac{1}{2}} \frac{1}{(D_0 + i\eta)^2} \alpha \cdot \nabla V \frac{1}{D_0 + i\eta} |D_\kappa|^{-\frac{1}{2}} d\eta \right\|_{\mathfrak{S}^2} \leq C \|\nabla V\|_{L^2}. \end{aligned}$$

It remains to estimate the second term in (40)

$$\int_{\mathbb{R}} |D_\kappa|^{\frac{1}{2}} \frac{1}{D_0 + i\eta} \frac{1}{|x|} \frac{1}{D_0 + i\eta} V \frac{1}{D_0 + i\eta} |D_\kappa|^{-\frac{1}{2}} d\eta.$$

This is the most difficult since $V \in L^6$ and $1/|x|$ only yields an operator in \mathfrak{S}_w^3 , by Cwikel's inequality. The idea here is to split

$$\frac{1}{|x|} = \frac{\chi(x)}{|x|} + \frac{1 - \chi(x)}{|x|}$$

where $\chi \in C_c^\infty$ is equal to 1 in a neighborhood of the origin. The term involving $\chi/|x|$ is easily handled using that $\chi/|x| \in L^p$ for all $p < 3$, hence

$$\frac{1}{|D_0|^{\frac{1}{2}}} \frac{\chi}{|x|} \frac{1}{|D_0|^{\frac{1}{2}+s}} \in \mathfrak{S}^p \subset \mathfrak{S}^3$$

for $s > 0$. We can then write

$$\begin{aligned} & \int_{\mathbb{R}} \left\| |D_\kappa|^{\frac{1}{2}} \frac{1}{D_0 + i\eta} \frac{\chi}{|x|} \frac{1}{D_0 + i\eta} V \frac{1}{D_0 + i\eta} |D_\kappa|^{-\frac{1}{2}} \right\|_{\mathfrak{S}^2} d\eta \\ & \leq \int_{\mathbb{R}} \frac{C}{\langle \eta \rangle} \left\| \frac{1}{|D_0|^{\frac{1}{2}}} \frac{\chi}{|x|} \frac{1}{|D_0|^{\frac{1}{2}+s}} \right\|_{\mathfrak{S}^3} \left\| \frac{1}{(|D_0| + \langle \eta \rangle)^{\frac{1}{2}-s}} V \frac{1}{|D_0|^{\frac{1}{2}}} \right\|_{\mathfrak{S}^6} d\eta \leq C \|V\|_{L^6}. \end{aligned}$$

The term with $(1 - \chi)/|x|$ is treated exactly as we did before for the quadratic term in V .

Namely, we write

$$\begin{aligned} & |D_\kappa|^{\frac{1}{2}} \int_{\mathbb{R}} \frac{1}{D_0 + i\eta} \frac{1-\chi}{|x|} \frac{1}{D_0 + i\eta} V \frac{1}{D_0 + i\eta} d\eta |D_\kappa|^{-\frac{1}{2}} \\ &= -i |D_\kappa|^{\frac{1}{2}} \int_{\mathbb{R}} \frac{1}{D_0 + i\eta} \frac{1-\chi}{|x|} \frac{1}{(D_0 + i\eta)^2} \boldsymbol{\alpha} \cdot \nabla V \frac{1}{D_0 + i\eta} d\eta |D_\kappa|^{-\frac{1}{2}} \\ &\quad + i |D_\kappa|^{\frac{1}{2}} \int_{\mathbb{R}} \frac{1}{D_0 + i\eta} \boldsymbol{\alpha} \cdot \nabla \left(\frac{1-\chi}{|x|} \right) \frac{1}{(D_0 + i\eta)^3} V d\eta |D_\kappa|^{-\frac{1}{2}} \end{aligned}$$

Now it suffices to use that $(1-\chi)/|x|$ is bounded and that its gradient is in L^3 to conclude.

Our final estimate takes the form

$$C(1 + \|\nabla V\|_{L^3}) \|V\|_{L^6} + \|\nabla V\|_{L^2}$$

for $\|V\|_{L^6}$ small enough. We obtain the stated inequality (33) by the Sobolev inequality $\|V\|_{L^6} \leq C\|\nabla V\|_{L^2}$. Finally, the last inequality (35) follows by complex interpolation. This concludes the proof of Proposition 14. \square

5 Proof of Theorem 9

In the whole argument we fix $0 < \kappa < 1$ and $0 < \nu < \nu_c$ and we assume that α is small enough. Only when required we will impose $\kappa = \nu$. In order to simplify our writing we change notation and denote by

$$D_{\kappa,\gamma} := D_0 - \frac{\kappa}{|x|} + \alpha \rho_\gamma * \frac{1}{|x|}$$

the mean-field operator and by

$$V_\gamma := \alpha \rho_\gamma * \frac{1}{|x|}$$

the corresponding mean-field operator. We recall that

$$P_{\kappa,\gamma}^\pm = \mathbb{1}_{\mathbb{R}^\pm}(D_{\kappa,\gamma})$$

are the associated spectral projector. Finally, we denote by

$$D(f, f) := \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{f(x)f(y)}{|x-y|} dx dy = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{|\widehat{f}(k)|^2}{|k|^2} dk$$

the Coulomb energy.

5.1 Lower bound

In this section we prove the following result.

Proposition 15 (Lower bound in terms of the Dirac-Coulomb projected Dirac-Fock). *Let $0 < \kappa < 1$ and $0 < \nu < \nu_c$. Then we have for a constant C depending on κ and ν*

$$E^{\text{DF}}(\kappa, \alpha, N) \geq \inf_{\substack{0 \leq \gamma \leq 1 \\ P_{\kappa,\gamma}^- \gamma = 0 \\ \text{Tr}(\gamma) \leq N}} \left\{ \text{Tr}(D_\kappa - 1)\gamma + \frac{\alpha}{2} D(\rho_\gamma, \rho_\gamma) \right\} - \frac{C}{N^{\frac{1}{15}}} \quad (41)$$

for all $\alpha N \leq \nu$ and α small enough.

Proof. From Lemma 8 we have

$$0 \geq E^{\text{DF}}(\kappa, \alpha, N) \geq -CN.$$

Note that $E^{\text{DF}}(\kappa, \alpha, N) \leq 0$, since one can take $\gamma = 0$ in the variational principle (20). We use a kind of boot-strap argument, showing first a lower bound of the order $-CN^{1/3}$ before getting lower order errors.

• **Proof that $E^{\text{DF}}(\kappa, \alpha, N) \geq -CN^{1/3}$**

Let γ_N be an approximate minimizer for $E^{\text{DF}}(\kappa, \alpha, N)$. Then by (24)

$$\text{Tr} \sqrt{-\Delta} \gamma_N \leq CN.$$

By (26) and the Lieb-Thirring inequality (25), we have for all density matrices γ

$$\iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\gamma(x) \rho_\gamma(y)}{|x-y|} dx dy \leq C (\text{Tr} \gamma)^{2/3} \text{Tr}(\sqrt{-\Delta} \gamma). \quad (42)$$

In particular, the direct term in the Dirac-Fock energy satisfies

$$\alpha \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_{\gamma_N}(x) \rho_{\gamma_N}(y)}{|x-y|} dx dy \leq CN^{2/3}. \quad (43)$$

Going back to the Dirac-Fock energy and using that $E^{\text{DF}}(\kappa, \alpha, N) \leq 0$, we find

$$\text{Tr}(D_{\kappa, \gamma_N} - 1) \gamma_N = \text{Tr}(|D_{\kappa, \gamma_N}| - 1) \gamma_N \leq CN^{2/3}.$$

Now we replace D_{κ, γ_N} by D_κ . We have

$$\begin{aligned} \text{Tr} D_{\kappa, \gamma_N} \gamma_N &= \text{Tr} P_{\kappa, \gamma_N}^+ (D_\kappa + V_{\gamma_N}) P_{\kappa, \gamma_N}^+ \gamma_N \\ &= \text{Tr} P_\kappa^+ D_\kappa P_\kappa^+ \gamma_N + \alpha D(\rho_{\gamma_N}, \rho_{\gamma_N}) \\ &\quad + \text{Tr}(P_{\kappa, \gamma_N}^+ - P_\kappa^+) D_\kappa (P_{\kappa, \gamma_N}^+ - P_\kappa^+) \gamma_N \end{aligned} \quad (44)$$

since

$$\text{Tr} P_\kappa^+ D_\kappa (P_{\kappa, \gamma_N}^+ - P_\kappa^+) \gamma_N = -\text{Tr} P_\kappa^+ D_\kappa (P_{\kappa, \gamma_N}^- - P_\kappa^-) \gamma_N = 0.$$

Note that by (43)

$$\left\| \alpha \rho_{\gamma_N} * \frac{1}{|x|} \right\|_{L^6} \leq C \alpha D(\rho_{\gamma_N}, \rho_{\gamma_N})^{1/2} \leq C \sqrt{\alpha} N^{1/3} \leq C \frac{\sqrt{\nu}}{N^{1/6}} \rightarrow 0.$$

Hence we may apply Proposition 14. In addition, we have

$$\left\| \alpha \nabla \left(\rho_{\gamma_N} * \frac{1}{|x|} \right) \right\|_{L^3} \leq \alpha \left\| \rho_{\gamma_N} * \frac{1}{|x|^2} \right\|_{L^3} \leq C \alpha \|\rho_{\gamma_N}\|_{L^{3/2}}$$

by the Hardy-Littlewood-Sobolev inequality. By the Sobolev and Hoffmann-Ostenhof inequalities we have

$$\|\rho_{\gamma_N}\|_{L^{3/2}} \leq C \left\langle \sqrt{\rho_{\gamma_N}}, \sqrt{-\Delta} \sqrt{\rho_{\gamma_N}} \right\rangle \leq C \text{Tr} \sqrt{-\Delta} \gamma_N \leq CN.$$

Hence

$$\left\| \alpha \nabla \left(\rho_{\gamma_N} * \frac{1}{|x|} \right) \right\|_{L^3} \leq C \alpha N \leq C \nu$$

is uniformly bounded. By Hölder's inequality in Schatten spaces and Proposition 14 with $3/10 > 1/8$ we can now bound

$$\begin{aligned} & \left| \operatorname{Tr}(P_{\kappa, \gamma_N}^+ - P_{\kappa}^+) D_{\kappa} (P_{\kappa, \gamma_N}^+ - P_{\kappa}^+) \gamma_N \right| \\ & \leq \left\| |D_{\kappa}|^{\frac{1}{2}} (P_{\kappa, \gamma_N}^+ - P_{\kappa}^+) |D_{\kappa}|^{-\frac{3}{10}} \right\|_{\mathfrak{S}^5}^2 \left\| |D_{\kappa}|^{\frac{3}{10}} \gamma_N |D_{\kappa}|^{\frac{3}{10}} \right\|_{\mathfrak{S}^{5/3}} \\ & \leq C N^{\frac{3}{5}} \alpha^2 D(\rho_{\gamma_N}, \rho_{\gamma_N}). \end{aligned} \quad (45)$$

We have used here that

$$\begin{aligned} \left\| |D_{\kappa}|^{\frac{3}{10}} \gamma_N |D_{\kappa}|^{\frac{3}{10}} \right\|_{\mathfrak{S}^{5/3}}^{\frac{5}{3}} &= \operatorname{Tr} \left(|D_{\kappa}|^{\frac{3}{10}} \gamma_N |D_{\kappa}|^{\frac{3}{10}} \right)^{\frac{5}{3}} \\ &\leq \operatorname{Tr} |D_{\kappa}|^{\frac{1}{2}} \gamma_N^{\frac{5}{3}} |D_{\kappa}|^{\frac{1}{2}} \leq \operatorname{Tr} |D_{\kappa}|^{\frac{1}{2}} \gamma_N |D_{\kappa}|^{\frac{1}{2}} \leq C N \end{aligned}$$

since $0 \leq \gamma_N \leq 1$, and by the Araki-Lieb-Thirring inequality [LT76; LS10]. The same argument as for (45) implies also that

$$\left| \operatorname{Tr}(P_{\kappa, \gamma_N}^+ - P_{\kappa}^+) (P_{\kappa, \gamma_N}^+ - P_{\kappa}^+) \gamma_N \right| \leq C N^{\frac{3}{5}} \alpha^2 D(\rho_{\gamma_N}, \rho_{\gamma_N}).$$

As a conclusion we have proved the lower bound

$$\mathcal{E}_{\kappa, \alpha}^{\text{DF}}(\gamma_N) \geq \operatorname{Tr} P_{\kappa}^+ (D_{\kappa} - 1) P_{\kappa}^+ \gamma_N + \frac{\alpha}{2} \left(1 - C \alpha N^{\frac{3}{5}} \right) D(\rho_{\gamma_N}, \rho_{\gamma_N}) \quad (46)$$

where C depends on ν . Noticing that $\operatorname{Tr} P_{\kappa}^+ \gamma_N P_{\kappa}^+ \leq \operatorname{Tr} \gamma_N \leq N$, we conclude that

$$E^{\text{DF}}(\kappa, \alpha, N) \geq \min_{\substack{0 \leq \gamma \leq 1 \\ P_{\kappa}^+ \gamma = 0 \\ \operatorname{Tr}(\gamma) \leq N}} \operatorname{Tr}(D_{\kappa} - 1) \gamma = \sum_{n=1}^N (\lambda_n(D_{\kappa}) - 1).$$

The sum of the N first eigenvalues of the Dirac-Coulomb operator on the right is explicit, since those eigenvalues are known analytically. It behaves like $N^{1/3}$. Hence we have proved, as we wanted, that

$$E^{\text{DF}}(\kappa, \alpha, N) \geq -C N^{\frac{1}{3}},$$

that

$$\operatorname{Tr}(|D_{\kappa}| - 1) P_{\kappa}^+ \gamma_N P_{\kappa}^+ \leq C N^{\frac{1}{3}}$$

and that

$$\alpha D(\rho_{\gamma_N}, \rho_{\gamma_N}) \leq C N^{\frac{1}{3}}. \quad (47)$$

Inserting (47) in the error term in (45) we find

$$\left| \operatorname{Tr}(P_{\kappa, \gamma_N}^+ - P_{\kappa}^+)^2 \gamma_N \right| + \left| \operatorname{Tr}(P_{\kappa, \gamma_N}^+ - P_{\kappa}^+) D_{\kappa} (P_{\kappa, \gamma_N}^+ - P_{\kappa}^+) \gamma_N \right| \leq \frac{C}{N^{\frac{1}{15}}}. \quad (48)$$

This term can therefore be neglected in the expansion of the energy up to the order $O(N^{-1/15})$.

We now prove that

$$\alpha D(\rho_{\gamma_N}, \rho_{\gamma_N}) = \alpha D(\rho_{P_{\kappa}^+ \gamma_N P_{\kappa}^+}, \rho_{P_{\kappa}^+ \gamma_N P_{\kappa}^+}) + O(N^{-1/6}).$$

To simplify our argument we introduce the densities

$$\rho_N^{\sigma, \sigma'} := \rho_{P_{\kappa}^{\sigma} \gamma_N P_{\kappa}^{\sigma'}}, \quad \sigma, \sigma' \in \{\pm\}.$$

We then write

$$D(\rho_{\gamma_N}, \rho_{\gamma_N}) = D(\rho_N^{++}, \rho_N^{++}) + 2D(\rho_{\gamma_N}, r_N) - D(r_N, r_N)$$

with $r_N := \rho_N^{+-} + \rho_N^{-+} + \rho_N^{--}$. We claim that

$$D(r_N, r_N) \leq CN^{\frac{1}{3}}, \quad (49)$$

the proof of which we postpone until the end of the argument. Using that $\alpha D(\rho_{\gamma_N}, \rho_{\gamma_N}) = O(N^{1/3})$, we deduce from the Cauchy-Schwarz inequality for the scalar product $D(\cdot, \cdot)$ that

$$\left| \alpha D(\rho_{\gamma_N}, \rho_{\gamma_N}) - \alpha D(\rho_N^{++}, \rho_N^{++}) \right| \leq \frac{C}{N^{\frac{1}{6}}}.$$

In order to prove (49), we show that $\|r_N\|_{L^{6/5}(\mathbb{R}^3)} = O(N^{1/6})$ by duality. Let F be any function in $L^6(\mathbb{R}^3)$. Then we have

$$\begin{aligned} \left| \int_{\mathbb{R}^3} F \rho_N^{-+} \right| &= \left| \text{Tr} (F P_{\kappa}^- \gamma_N P_{\kappa}^+) \right| \\ &\leq \|F |D_0|^{-\frac{1}{2}}\| \left\| |D_0|^{\frac{1}{2}} (P_{\kappa}^- - P_{\kappa, \gamma}^-) |D_0|^{-\frac{1}{2}} \right\|_{\mathfrak{S}^2} \left\| |D_0|^{\frac{1}{2}} \gamma_N \right\|_{\mathfrak{S}^2}. \end{aligned}$$

From the Hardy-Littlewood-Sobolev inequality, we have

$$\left\| |D_0|^{-\frac{1}{2}} \right\| \leq C \|F\|_{L^6(\mathbb{R}^3)}.$$

On the other hand

$$\left\| |D_0|^{\frac{1}{2}} \gamma_N \right\|_{\mathfrak{S}^2}^2 = \text{Tr} |D_0|^{\frac{1}{2}} \gamma_N^2 |D_0|^{\frac{1}{2}} \leq \text{Tr} |D_0|^{\frac{1}{2}} \gamma_N |D_0|^{\frac{1}{2}} \leq CN$$

and

$$\left\| |D_0|^{\frac{1}{2}} (P_{\kappa}^- - P_{\kappa, \gamma}^-) |D_0|^{-\frac{1}{2}} \right\|_{\mathfrak{S}^2} \leq C \alpha D(\rho_{\gamma_N}, \rho_{\gamma_N})^{\frac{1}{2}} \leq \frac{C}{N^{\frac{1}{3}}}$$

by Proposition 14 and (47). This gives

$$\left| \int_{\mathbb{R}^3} F \rho_N^{-+} \right| \leq CN^{\frac{1}{6}} \|F\|_{L^6(\mathbb{R}^3)}$$

and by duality we conclude that

$$\left\| \rho_N^{-+} \right\|_{L^{6/5}(\mathbb{R}^3)} \leq CN^{\frac{1}{6}}.$$

The argument is the same for ρ_N^{-+} and ρ_N^{--} , which leads to (49), by the Hardy-Littlewood-Sobolev

inequality.

As a conclusion we have shown the desired lower bound

$$E^{\text{DF}}(\kappa, \nu, \alpha) \geq \inf_{\substack{0 \leq \gamma \leq 1 \\ P_{\kappa}^{-} \gamma = 0 \\ \alpha \text{Tr}(\gamma) \leq \nu}} \left\{ \text{Tr}(D_{\kappa} - 1)\gamma + \frac{\alpha}{2} D(\rho_{\gamma}, \rho_{\gamma}) \right\} - \frac{C}{N^{1/5}} \quad (50)$$

in terms of the reduced Dirac-Fock problem projected to the positive spectral subspace of the Dirac-Coulomb operator D_{κ} . This concludes the proof of Proposition 15. \square

5.2 Upper bound

In this section we prove the following result.

Proposition 16. *Let $0 < \kappa < 1$ and $0 < \nu < \nu_c$ and let d_N a sequence of self-adjoint operators such that*

$$0 \leq d_N \leq 1, \quad \text{Tr} \sqrt{-\Delta} d_N \leq CN, \quad \text{Tr} d_N \leq N$$

and

$$P_{\kappa}^{-} d_N = 0.$$

Then there is a sequence γ_N of self-adjoint operators satisfying the nonlinear constraint

$$P_{\kappa, \gamma_N}^{-} \gamma_N = 0$$

such that

$$0 \leq \gamma_N \leq 1, \quad \text{Tr} \sqrt{-\Delta} \gamma_N \leq CN, \quad \text{Tr} \gamma_N \leq N$$

and and

$$\mathcal{E}_{\kappa, \alpha}^{\text{DF}}(\gamma_N) = \mathcal{E}_{\kappa, \alpha}^{\text{DF}}(d_N) + \mathcal{O}(N^{-1/15}).$$

Proof. We split the proof into several steps.

• Séré's retraction θ

We will use the following result of Séré [Sér09].

Theorem 17. *Let $(X, \|\cdot\|_X)$ be a Banach space and \mathcal{U} an open subset of X . Let $T : \mathcal{U} \rightarrow X$ a continuous map. We assume :*

- \mathcal{U} has a nonempty subset F which is closed in X and such that $T(F) \subset F$;
- $\exists k \in (0, 1), \forall x \in T^{-1}(\mathcal{U}), \|T^2(x) - T(x)\|_X \leq k\|T(x) - x\|_X$.

Then there exists an open neighborhood \mathcal{V} of F in X with $\text{Fix}(T) \subset \mathcal{V} \subset \mathcal{U}, T(\mathcal{V}) \subset \mathcal{V}$ and such that for any $x \in \mathcal{V}$, the sequence $(T^p(x))_p$ has a limit $\theta(x) \in \mathcal{V}$ for the norm $\|\cdot\|_X$, with the estimate

$$\forall x \in \mathcal{V}, \|\theta(x) - T^p(x)\|_X \leq \frac{k^p}{1-k} \|T(x) - x\|_X. \quad (51)$$

In this way we obtain a retraction θ of \mathcal{V} onto $\text{Fix}(T) \subset \mathcal{V}$ whose restriction to F is a retraction of F onto $F \cap \text{Fix}(T)$.

Here we have denoted by $\text{Fix}(T)$ the fixed points of T . To apply Séré's result we define, for $\kappa \in (0, 1)$,

$$X = \left\{ \gamma \in \mathcal{B}(\mathcal{H}), \gamma^* = \gamma, |D_{\kappa}|^{1/2} \gamma |D_{\kappa}|^{1/2} \in \mathfrak{S}_1 \right\},$$

and

$$\begin{aligned} T : X &\longrightarrow \mathcal{B}(\mathcal{H}) \\ \gamma &\mapsto P_\gamma^+ \gamma P_\gamma^+. \end{aligned}$$

Let us take some fixed $\nu < \nu_c$ and define

$$F = \{0 \leq \gamma \leq 1, \|\gamma\|_X + \lambda \|T(\gamma) - \gamma\|_X \leq MN, \quad \alpha \operatorname{Tr} \gamma \leq \nu\}$$

for some $\lambda, M > 0$ that we will choose later. For $r > 0$, we define $\mathcal{U} = F + B_X(r)$. Note that $F \neq \emptyset$ since $0 \in F$.

We will first check that the assumptions of Theorem 17 are satisfied in our regime, and then we will apply it to prove Proposition 16.

• **Verifying the stability (Assumption 1)**

Here, we assume that the retraction property holds for some k . Let us check that $T(F) \subset F$. That $T\gamma \in X$ is a consequence of Hardy's inequality and Theorem 4. By definition of T we also have directly that $0 \leq T(\gamma) \leq 1$ and $\alpha \operatorname{Tr} T(\gamma) \leq \alpha \operatorname{Tr} \gamma \leq \nu$. It remains to verify the norm condition in the definition of F . Using the triangle inequality we obtain

$$\|T(\gamma)\|_X + \lambda \|T^2(\gamma) - T(\gamma)\|_X \leq \|\gamma\|_X + (1 + \lambda k) \|X - T(\gamma)\|_X.$$

Choosing $\lambda > 1/(1 - k)$ in the above inequality implies $T\gamma \in F$.

• **Verifying the retraction property (Assumption 2)**

Let $\gamma \in \mathcal{U}$, we have

$$\begin{aligned} T^2\gamma &= P_{\kappa, T\gamma}^+ T\gamma P_{\kappa, T\gamma}^+ \\ &= P_{\kappa, \gamma}^+ T\gamma P_{\kappa, \gamma}^+ + \left(P_{\kappa, T\gamma}^+ - P_{\kappa, \gamma}^+\right) T\gamma P_{\kappa, T\gamma}^+ + P_{\kappa, \gamma}^+ T\gamma \left(P_{\kappa, T\gamma}^+ - P_{\kappa, \gamma}^+\right). \end{aligned}$$

Note that $\alpha \operatorname{Tr} T(\gamma) \leq \alpha \operatorname{Tr}(\gamma) < \nu$ so that $|D_{\kappa, T(\gamma)}|^{1/2}$, $|D_{\kappa, \gamma}|^{1/2}$ and $|D_\kappa|^{1/2}$ are comparable as a consequence of Hardy's inequality (10) and Theorem 4.

At this step we need two technical lemmas whose proofs are postponed to the end of the argument.

Lemma 18 (Hölder inequality in weighted Schatten space). *Let $\gamma \in X$ such that $0 \leq \gamma \leq 1$. Let $0 \leq a, b \leq 1/2$ and define $q = 1/a + 1/b$, then*

$$\| |D_\kappa|^a \gamma |D_\kappa|^b \|_{\mathfrak{S}^q} \leq \|\gamma\|_X^{a+b}$$

Lemma 19 (Estimate on differences of projectors in X). *Let $0 < \nu < \nu_c$ and $0 < \kappa < 1$, then for all $\gamma_1, \gamma_2 \in \{\gamma \in X, \|\gamma\|_X \leq M, \alpha \operatorname{Tr}(\gamma) \leq \nu\}$, we have*

$$\| |D_\kappa|^{1/2} (P_{\kappa, \gamma_1}^+ - P_{\kappa, \gamma_2}^+) |D_\kappa|^{-\varepsilon} \|_{\mathfrak{S}^6} \leq C_{\nu, \kappa, \varepsilon} \alpha \|\gamma_1 - \gamma_2\|_X.$$

Now, using that $P_{\kappa,\gamma}^+ T(\gamma) P_{\kappa,\gamma}^+ = T(\gamma)$, we obtain by Hölder's inequality and Lemma 19, that

$$\begin{aligned} & \|T^2(\gamma) - T(\gamma)\|_X \\ & \leq C_{\kappa,\nu} \left\| |D_\kappa|^{\frac{1}{2}} (P_{\kappa,T(\gamma)}^+ - P_{\kappa,\gamma}^+) |D_\kappa|^{-\frac{1}{3}} \right\|_{\mathfrak{S}^6} \left\| |D_\kappa|^{\frac{1}{3}} T(\gamma) |D_\kappa|^{\frac{1}{2}} \right\|_{\mathfrak{S}^{6/5}} \\ & \leq C_{\kappa,\nu} \alpha \left\| |D_\kappa|^{\frac{1}{3}} T(\gamma) |D_\kappa|^{\frac{1}{2}} \right\|_{\mathfrak{S}^{6/5}} \|T(\gamma) - \gamma\|_X, \end{aligned}$$

where $C_{\kappa,\nu}$ is a constant depending only on κ and ν . Using that $\gamma \in \mathcal{U}$ and Lemma 18 we obtain

$$\left\| |D_\kappa|^{\frac{1}{3}} T(\gamma) |D_\kappa|^{\frac{1}{2}} \right\|_{\mathfrak{S}^{6/5}} \leq \|\gamma\|_X^{5/6} \leq C_{\kappa,\nu} (MN + r)^{5/6}.$$

Hence

$$\|T^2(\gamma) - T(\gamma)\|_X \leq C_{\kappa,\nu} \alpha^{1/6} (\nu M + \alpha r) \|T(\gamma) - \gamma\|_X.$$

This shows that for any $M, r > 0$ fixed, taking N sufficiently large is enough for the retraction property to hold with a retraction factor

$$k \leq C_{\kappa,\nu} \alpha^{1/6}. \quad (52)$$

• Conclusion of the proof of Proposition 16

The same proof as for the lower bound, starting from (44), but with γ_N replaced by d_N , shows that

$$\mathcal{E}_{\kappa,\alpha}^{\text{DF}}(T(d_N)) = \mathcal{E}_{\kappa,\alpha}^{\text{DF}}(d_N) + \mathcal{O}(N^{-1/15}).$$

Note that this does not hold for any trial state as we use intensively that $P_\kappa^- d_N = P_{\kappa,d_N}^- T(d_N) = 0$. In fact, the same argument applied n times leads to

$$\mathcal{E}_{\kappa,\alpha}^{\text{DF}}(T^n(d_N)) = \mathcal{E}_{\kappa,\alpha}^{\text{DF}}(d_N) + \mathcal{O}(N^{-1/15}).$$

We now use the retraction θ , for which we have from Theorem 17 that

$$\|\theta(d_N) - T^n(d_N)\|_X \leq \frac{k^n}{1-k} \|T(d_N) - d_N\|_X.$$

In view of (52) it is sufficient for our purpose to show

$$\alpha^{n/6} \|T d_N - d_N\|_X = o(N^{-1/15})$$

for a certain n . This is clearly the case for $n = 3$ although this is not optimal since it only uses that $\|T(d_N)\|_X + \|d_N\|_X \leq CN$. We therefore obtain

$$\begin{aligned} \mathcal{E}_{\kappa,\alpha}^{\text{DF}}(\theta(d_N)) &= \mathcal{E}_{\kappa,\alpha}^{\text{DF}}(T^3(d_N)) + \text{Tr}(D_\kappa - 1)(\theta(d_N) - T^3(d_N)) \\ &\quad + \frac{\alpha}{2} (D(\rho_{T^3(d_N)} - \rho_{\theta(d_N)}, \rho_{T^3(d_N)}) + D(\rho_{T^3(d_N)} - \rho_{\theta(d_N)}, \rho_{\theta(d_N)})) \\ &= \mathcal{E}_{\kappa,\alpha}^{\text{DF}}(T^3(d_N)) + \mathcal{O}(\|\theta(d_N) - T^3(d_N)\|_X) \end{aligned}$$

where we used that,

$$\alpha D(\rho_{T^3(d_N)} - \rho_{\theta(d_N)}, \rho_{T^3(d_N)}) \leq C\alpha \|\theta(d_N) - T^3(d_N)\|_X \|T^3(d_N)\|_X$$

and that $\alpha \|T^3(d_N)\|_X = \mathcal{O}(1)$. The last error term is dealt with similarly. Finally, we obtain as we wanted

$$\mathcal{E}_{\kappa,\alpha}^{\text{DF}}(\theta(d_N)) = \mathcal{E}_{\kappa,\alpha}^{\text{DF}}(d_N) + \mathcal{O}(N^{-1/15}),$$

which concludes the proof of Proposition 16. \square

It remains to provide the

Proof of Lemma 18. Define $p_a = 1/a$ and $p_b = 1/b$. By Hölder inequality we have

$$\| |D_\kappa|^a \gamma |D_\kappa|^b \|_{\mathfrak{S}_q} \leq \| |D_\kappa|^a \gamma^{1/2} \|_{\mathfrak{S}_{p_a}} \| \gamma^{1/2} |D_\kappa|^b \|_{\mathfrak{S}_{p_b}}.$$

We bound each of the factors above using the Araki-Lieb-Thirring inequality together with the fact that $0 \leq \gamma \leq 1$. We have

$$\begin{aligned} \| |D_\kappa|^a \gamma^{1/2} \|_{\mathfrak{S}_{p_a}} &= \left(\text{Tr} (|D_\kappa|^a \gamma |D_\kappa|^a)^{p_a/2} \right)^{1/p_a} \\ &\leq \left(\text{Tr} |D_\kappa|^{1/2} \gamma^{p_a/2} |D_\kappa|^{1/2} \right)^{1/p_a} \\ &\leq \left(\text{Tr} |D_\kappa|^{1/2} \gamma |D_\kappa|^{1/2} \right)^{1/p_a} \\ &\leq \| \gamma \|_X^a. \end{aligned}$$

The same proof holds for the other term and gives the desired result. \square

Proof of Lemma 19. We use Stone's formula and the resolvent identity to express the difference as

$$\begin{aligned} &|D_\kappa|^{1/2} (P_{\kappa,\gamma_1} - P_{\kappa,\gamma_2}) |D_\kappa|^{-\varepsilon} \\ &= \frac{1}{2\pi} \int_{\mathbb{R}} |D_\kappa|^{1/2} \frac{1}{D_{\kappa,\gamma_1} + i\eta} \alpha \left((\rho_{\gamma_2} - \rho_{\gamma_1}) * \frac{1}{|x|} \right) \frac{1}{D_{\kappa,\gamma_2} + i\eta} |D_\kappa|^{-\varepsilon} d\eta. \end{aligned}$$

The argument is now exactly the same as for (34). \square

5.3 Conclusion of the proof of Theorem 9

At this point we have not used that $\kappa = \nu$. Handrek and Siedentop [HS15] have shown that the projected Dirac-Fock problem behaves as

$$\begin{aligned} &\inf_{\substack{0 \leq \gamma \leq 1 \\ P_\kappa^- \gamma = 0 \\ \text{Tr}(\gamma) \leq N}} \left\{ \text{Tr}(D_\kappa - 1)\gamma + \frac{\alpha}{2} D(\rho_\gamma, \rho_\gamma) \right\} \\ &= e_{\text{TF}}(1) \alpha^2 N^{7/3} + c_{\text{Scott}}(\kappa) + \mathcal{O}(\alpha^2 N^{47/24}), \end{aligned} \quad (53)$$

only for $\kappa = \nu$. To obtain the upper bound they have constructed a state d_N which satisfies the assumptions of Proposition 16 and is such that

$$\text{Tr}(D_\kappa - 1)d_N + \frac{\alpha}{2} D(\rho_{d_N}, \rho_{d_N}) = e_{\text{TF}}(1) \alpha^2 N^{7/3} + c_{\text{Scott}}(\kappa) + \mathcal{O}(\alpha^2 N^{47/24}). \quad (54)$$

Hence the final result follows, for $\kappa = \nu$ from our lower bound in Proposition 15 and from the construction of the trial state γ_N from d_N in Proposition 16. This concludes the proof of Theorem 9. \square

Remark 20. *Should the limit be proven for the Dirac-Fock projected energy with P_κ^+ for $\nu \neq \kappa$, our result would immediately apply to the unprojected Dirac-Fock theory, with the same value of κ and ν .*

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Mean-field limits in quantum mechanics

Résumé

Cette thèse est consacrée à la dérivation et à l'étude de différents modèles non-linéaires en mécanique quantique. Ces modèles décrivent des systèmes à grand nombre de particules dans l'approximation de champ moyen. Dans une première partie, nous étudions la validité de modèles effectifs décrivant un gaz de bosons dipolaires. Nous montrons que les minimiseurs ainsi que les solutions de l'équation dépendante du temps sont correctement décrits au premier ordre par la théorie de Gross-Pitaevskii. Pour la dynamique, nous montrons également que le second ordre est donné par la théorie de Bogoliubov. Nous étudions aussi la fonctionnelle de Gross-Pitaevskii dipolaire avec un terme de correction quintique prenant en compte les corrections de Lee-Huang-Yang. La seconde partie de la thèse est consacrée à l'étude de limites semi-classiques pour les grands systèmes fermioniques. Nous nous intéressons d'abord à un gaz de fermions à température positive dans la limite semi-classique et nous montrons que l'énergie libre, ainsi que les états de Gibbs approchés, sont donnés par la théorie de Vlasov. Nous étudions ensuite l'énergie d'un atome lourd dans la limite non-relativiste où nous calculons le second ordre de son développement, la correction de Scott, pour le modèle de Dirac-Fock.

Mots clés : variational methods, partial differential equations, spectral theory, mathematical physics, quantum mechanics, quantum gases

Abstract

This thesis is devoted to the derivation and the study of several non-linear models in quantum mechanics. These models describe systems consisting of a large number of particles in the mean-field approximation. In the first part we study the validity of some effective models describing a gas of dipolar bosons. We show that the ground state as well as the time-evolved solutions are correctly described by the Gross-Pitaevskii theory, at first order. For the dynamics, we also show that the second order is given by Bogoliubov's theory. Moreover, we study a modified Gross-Pitaevskii functional including a quintic term accounting for the Lee-Huang-Yan corrections. The second part of this thesis is devoted to the study of large fermionic systems. We first analyse a fermionic gas at positive temperature in the semi-classical limit and we show that the latter and the approximate Gibbs states are given by Vlasov's theory. Then, we study the energy of heavy atoms in the non-relativistic limit where we compute the second term of its expansion, the Scott correction, for the Dirac-Fock model.

Keywords: méthodes variationnelles, équations aux dérivées partielles, théorie spectrale, physique mathématique, mécanique quantique, gaz quantique

RÉSUMÉ

Cette thèse est consacrée à la dérivation et à l'étude de différents modèles non-linéaires en mécanique quantique. Ces modèles décrivent des systèmes à grand nombre de particules dans l'approximation de champ moyen. Entre autres nous étudions la théorie de Gross-Pitaevskii, la théorie de Bogoliubov, la théorie de Vlasov, la théorie de Thomas-Fermi et le modèle de Dirac-Fock.

MOTS CLÉS

Méthodes variationnelles, équations aux dérivées partielles, théorie spectrale, physique mathématique, mécanique quantique, gaz quantiques

ABSTRACT

This thesis is devoted to the derivation and the study of several non-linear models in quantum mechanics. These models describe systems consisting of a large number of particles in the mean-field approximation. For instance, we study the Gross-Pitaevskii theory, the Bogoliubov theory, the Vlasov Theory, the Thomas-Fermi theory and the Dirac-Fock model.

KEYWORDS

Variational methods, partial differential equations, spectral theory, mathematical physics, quantum mechanics, quantum gases

