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Particules fermioniques et opérateurs de Schrödinger dans la limite semiclassique

Ngoc Nhi Nguyen

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Fermionic particles and Schrödinger
operators in the semiclassical limit
*Particules fermioniques et opérateurs de Schrödinger dans
la limite semiclassique*

Thèse de doctorat de l'université Paris-Saclay

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Spécialité de doctorat : Mathématiques fondamentales
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d'Orsay** (Université Paris-Saclay, CNRS), sous la direction de **Julien SABIN**,
Maître de conférences, HDR

Thèse soutenue à Paris-Saclay, le 13 décembre 2022, par

Ngoc Nhi NGUYEN

Composition du jury

Membres du jury avec voix délibérative

Nicolas Burq Professeur, Université Paris-Saclay, LMO	Président
Phan Thành Nam Professeur, University of Munich	Rapporteur & Examineur
Melissa Tacy Maîtresse de conférences, University of Auckland	Rapportrice
Rupert Frank Professeur, University of Munich	Examineur
Katya Krupchyk Professeure, University of California, Irvine	Examinatrice
Maciej Zworski Professeur, University of California, Berkeley	Examineur

Titre : Particules fermioniques et opérateurs de Schrödinger dans la limite semiclassique

Mots clés : Opérateurs de Schrödinger, fermions, analyse semiclassique, familles orthonormées de fonctions propres, Hartree-Fock.

Cette thèse est consacrée à l'étude mathématique de la concentration spatiale de systèmes de fermions piégés. En mécanique quantique, les différents états possibles d'une particule correspondent aux fonctions propres des opérateurs de Schrödinger. Une description fine de ces fonctions propres permet donc de déterminer des propriétés physiques pertinentes comme la position de la particule. Nous nous plaçons pour cela dans la limite semiclassique. Dans le chapitre 1, nous considérons

le cas sans interaction : nous étendons les estimées semiclassiques L^p de Koch-Tataru-Zworski d'une fonction individuelle au cadre de familles orthonormées de fonctions propres et discutons de leur optimalité. Dans le chapitre 2, nous étudions le cas avec interaction d'un système grand-canonique de particules fermioniques en prouvant des asymptotiques semiclassiques sur l'état fondamental dans l'approximation d'Hartree-Fock. Nous en déduisons en particulier une loi de Weyl intégrée.

Title : Fermionic particles and Schrödinger operators in the semiclassical limit

Keywords : Schrödinger operators, fermions, semiclassical analysis, orthonormal families of eigenfunctions, Hartree-Fock.

Abstract : This thesis is devoted to the mathematical study of the spatial concentration of trapped fermion systems. In quantum mechanics, the different possible states of a particle correspond to the eigenfunctions of the Schrödinger operators. A fine description of these eigenfunctions allows to determine relevant physical properties such as the position of the particle. To do so, we place ourselves in the semiclassical limit. In chapter 1,

we consider the case without interaction : we extend the semiclassical L^p Koch-Tataru-Zworski estimates of an individual function to the framework of orthonormal families of eigenfunctions and discuss their optimality. In chapter 2, we study the interacting case of a fermionic grand-canonical system by proving semiclassical asymptotics on the ground state in the Hartree-Fock approximation. In particular, we deduce an integrated Weyl law.

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Figure 1 – Des poules pendant le confinement 2020.

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⁶apparemment juste le directeur, le jury, les personnes qui ont contribué à améliorer le manuscrit. Cependant dans les implications logiques, comment peut-on rencontrer de nouvelles personnes sans contexte d'activités scientifiques ? De même, il est difficile de rédiger \LaTeX sur une machine défaillante.

⁷qui apparaissent dans cette dernière version,

⁸collègues, amis, proches et poules

⁹I would probably be dead from overheating.

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¹⁰en dehors du superbe encadrement scientifique avec Julien.

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¹¹qui ne s'étendent pas qu'au LMO

¹²déjà cités plus ou moins

Notation

\mathbb{N}	set of positive integers $\{0, 1, 2, \dots\}$	
\mathbb{N}^*	set of non-negative integers $\{1, 2, \dots\}$	
x'	last coordinates $(x_2, \dots, x_d) \in \mathbb{R}^{d-1}$ of $x \in \mathbb{R}^d$	
$ x $	Euclidian norm on \mathbb{R}^n	
$x \cdot \xi$ or $\langle x, \xi \rangle$	Euclidian inner-product for $x, \xi \in \mathbb{R}^n$	
$\langle x \rangle$	Japanese bracket $\sqrt{1 + x ^2}$	
$ \nu _{\ell^\alpha}$	ℓ^α norm on \mathbb{R}^n	
	or on the sequences $\nu = \{\nu_j\}_{j \in \mathbb{N}} \subset \mathbb{C}$	
$\langle \cdot, \cdot \rangle$	scalar product on a Hilbert space	
\mathbb{S}^n	n -dimensional unitary sphere	
\lesssim	means \leq up to a positive multiplicative constant	
\gtrsim	means \geq up to a positive multiplicative constant	
\sim	means \sim up to a positive multiplicative constant	
Δ	usual Laplacian on $L^2(\mathbb{R}^d)$	
Δ_g	Laplace-Beltrami operator associated to a metric g	
$\hbar > 0$	Planck reduced constant	in Chapt. 0, Sect. I.1
$h > 0$	semiclassical parameter, Planck reduced constant	
$\lambda \in \mathbb{R}$	can refer to an eigenvalue	in Chapt. 0, Sect. I.1
	the coupling constant of (I.5)	
	the high frequency parameter	in Chapt. 0, Sect. I.2
m	order function on $\mathbb{R}^n \times \mathbb{R}^n$	in Chapt. 1 (Def. II.1)
	probability density on $\mathbb{R}^n \times \mathbb{R}^n$	in Chapt. 2
$\mathcal{O}(h^\infty)$	$\mathcal{O}(h^N)$ for all $N \geq 0$	
$\mathcal{S}(\mathbb{R}^n)$	class of Schwartz functions on \mathbb{R}^n	
$\mathcal{S}'(\mathbb{R}^n)$	tempered distributions on \mathbb{R}^n	
$S(m)$	the class of symbols associated to an order function m	c.f. Chapt. 1 (Def. II.2)
$\ f\ _{S(m)}$	seminorm on $S(m)$	
$a^w, a^w(x, hD)$	Weyl quantization of a symbol a	c.f. Chapt. 1 (Def. II.4)
$ u\rangle \langle v $	operator $f \in \mathcal{H} \mapsto \langle v, f \rangle_{\mathcal{H}} u$	
γ^*	adjoint of an operator γ in \mathcal{H}	
$\mathcal{B}(\mathcal{H})$	set of bounded linear operators on \mathcal{H}	
ρ_γ	density of the operator γ	
$\gamma(x, y)$	integral kernel of the operator γ	
$\text{Tr}_{\mathcal{H}}(\gamma)$	trace of the operator γ in \mathcal{H}	
$\mathfrak{S}^\alpha(\mathcal{H}, \mathcal{H}')$	\mathfrak{S}^α Schatten space on the Hilbert spaces $\mathcal{H} \rightarrow \mathcal{H}'$	c.f. Chapt. 1 (Def. II.19)
$\ \gamma\ _{\mathfrak{S}^\alpha(\mathcal{H}, \mathcal{H}')}$	\mathfrak{S}^α Schatten norm of operators	
(r or g)-HF	(reduced or generalized)-Hartree-Fock	in Chapter 2
TF	Thomas-Fermi	
Vlas	Vlaslov	

Chapitre 0

Introduction (en français)

L'objectif de cette thèse est d'étudier les systèmes de particules fermioniques, et en particulier leurs propriétés de concentration spatiale, dans le régime semi-classique.

Le chapitre 1 est consacré à l'étude des densités pour les systèmes de particules sans interaction. Dans le chapitre 2, nous abordons le problème de l'asymptotique ponctuelle dans ce cas plus difficile des systèmes en interaction.

Dans cette introduction, nous présentons d'abord dans la Section I les motivations physiques, le formalisme mathématique que nous utiliserons pour décrire ces systèmes fermioniques et un état de l'art. Mes contributions sont ensuite présentées dans la section II.

I CADRE GÉNÉRAL

Quelques références Le lecteur ou la lectrice intéressée par les bases de la mécanique quantique peut consulter par exemple les livres [CTDL21, BDJ02]. Nous recommandons aux lecteurs généraux les livres de vulgarisation [BL14, Nav15, CC14a, CC14b] qui contiennent également des biographies des grandes figures de la physique et des anecdotes croustillantes mentionnées dans les notes de bas de page de cette introduction. Pour les références sur la théorie spectrale, nous renvoyons aux livres suivants : [Dav95, LS10, Lew22]. De même, nous nous référons aux livres [DS99, Zwo12] pour une introduction sur l'analyse semi-classique.

I.1 Motivation physique et objets étudiés

L'étude spectrale des opérateurs de Schrödinger dans la limite semi-classique peut être motivée par leur interprétation physique.

On s'intéresse à des particules quantiques de masse $m > 0$ dans l'espace euclidien de dimension $d \geq 1$, confinées dans un champ de force externe qui dérive d'un potentiel scalaire $V : \mathbb{R}^d \rightarrow \mathbb{R}$. Nous considérons des *potentiels confinants*, ce qui signifie que $V(x) \rightarrow \infty$ lorsque $|x| \rightarrow \infty$. Un exemple bien connu de potentiel confinant est l'oscillateur harmonique $V(x) = |x|^2$. Il existe deux types différents de particules quantiques : les *bosons* et les *fermions*, qui obéissent à des statistiques différentes.

- Les bosons sont les particules responsables des interactions. Ils s'agrègent dans un même état quantique pour former des condensats selon la statistique de *Bose-Einstein*. Les bosons élémentaires connus sont les photons, les gluons, les bosons de Higgs et les bosons Z, W .
- Les fermions sont des particules qui composent la matière. Ils obéissent notamment au *principe d'exclusion de Pauli*¹ qui stipule que deux fermions ne peuvent pas occuper le même

¹énoncé en 1925 par Wolfgang Pauli (1900-1958) [Pau25] lui-même.

état quantique. Il existe des fermions élémentaires, qui comprennent les quarks et les leptons (les principaux exemples sont les électrons, les muons, les neutrinos, les tauons) et aussi des fermions composites, les hadrons (comme les protons et les neutrons, qui composent les noyaux avec une interaction forte).

Nous nous concentrerons sur les particules fermioniques. et nous les considérerons comme non relativistes et sans spin. Les statistiques des particules fermioniques sont encore un sujet de recherche actif en physique théorique, en citant ne serait-ce que les articles de Dean, Le Doursal, Majumbar, Schehr et Smith [DLDS15, DLDMS18, DLDMS19, DLDS⁺21, SDLD⁺20].

Le formalisme de la mécanique quantique À la fin du XIXe siècle, des expériences remirent en cause la physique classique, dont les concepts étaient insuffisants pour décrire les objets à l'échelle atomique ou subatomique, et firent émerger de nouvelles idées, avec lesquelles s'est construite la physique quantique que nous connaissons aujourd'hui. Par exemple, Max Planck (1858-1957) [Pla01] déduisit la loi dite de Planck en 1900 du spectre de rayonnement du corps noir et Albert Einstein (1879-1955) [Ein05] comprit l'effet photoélectrique en 1905. Cela conduisit à l'hypothèse de l'énergie *quantifiée*, mot donné par Einstein pour désigner la fragmentation de l'énergie en morceaux discrets qu'il appelait « *quanta* », considérées comme des particules. Ces fragments doivent être des multiples de la *constante de Planck*² $h \simeq 6,62 \times 10^{-34}$ J.s. Rappelons dans ce paragraphe quelques postulats de la mécanique quantique non relativiste et leurs implications.

Contrairement à la mécanique classique, où la position-impulsion $(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d$ de la particule est régie par l'équation de Hamilton

$$\begin{cases} \dot{x}(t) &= \frac{1}{m}\xi(t), \\ \dot{\xi}(t) &= -\nabla V(x(t)), \end{cases} \quad (\text{I.1})$$

une particule quantique est décrite par un système d'états dans l'espace de Hilbert $L^2(\mathbb{R}^d, \mathbb{C})$ et peut être interprétée comme *fonctions d'onde*³. Lorsqu'un état $\psi(t)$, à l'instant $t \geq 0$, est normalisé sur $L^2(\mathbb{R}^d)$, le nombre $|\psi(t, x)|^2$ peut être interprété comme la densité de la probabilité de présence⁴ à la position $x \in \mathbb{R}^d$. On s'attendrait à trouver la particule aux positions où les valeurs de $|\psi(t)|^2$ sont maximales. De même, la densité de probabilité des moments $\xi \in \mathbb{R}^d$ est donnée par $|\hat{\psi}(t, \xi)|^2$. Nous définissons ici la transformée de Fourier comme

$$\forall \xi \in \mathbb{R}^d, \quad \hat{\psi}(t, \xi) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{-i\xi \cdot x} \psi(t, x) dx.$$

Expliquons pourquoi nous allons nous concentrer sur l'étude spectrale d'une observable quantique, appelée opérateur de Schrödinger. L'évolution temporelle de ces états $\psi_h \in L^2(\mathbb{R}^d)$,

²Paradoxalement, Planck était perturbé par le principe de quantification et défendait la continuité de la matière. Il ne pouvait admettre que sa loi du rayonnement conduise à une rupture avec la mécanique classique. La tragédie de sa vie est qu'il est devenu, malgré lui, une grande figure de la révolution quantique.

³Louis De Broglie (1892-1987) a émis l'hypothèse de la dualité onde-corpuscule de la matière dans sa thèse de 1923 sur le mouvement des électrons libres [dB24]. Cette correspondance constitue un premier type de limite semi-classique.

⁴Cette interprétation probabiliste, parfois appelée « *interprétation de Copenhague* » est due à Max Born (1882-1970) dans un article [Bor26] intitulé *Mécanique quantique des processus de collision* en 1926.

par exemple égale à $\psi^0 \in L^2(\mathbb{R}^d)$ au temps $t = 0$, est décrite par la dite *équation de Schrödinger*⁵

$$\begin{cases} i\hbar\partial_t\psi_h(t, x) &= -\frac{\hbar^2}{2m}\Delta\psi_h(t, x) + V(x)\psi_h(t, x) & \text{au temps } t > 0, \\ \psi_h(t = 0, x) &= \psi^0(x), \end{cases} \quad (\text{I.2})$$

où $\hbar := h/(2\pi)$ est la *constante de Planck réduite* et Δ est l'opérateur laplacien $\Delta := \sum_{j=1}^d \partial_{x_j}^2$. Les parties respectives $-\frac{\hbar^2}{2m}\Delta$ et la multiplication par $V(x)$ correspondent aux énergies cinétique et potentielle de la particule. L'étude de ces états ψ_h se réduit à l'étude spectrale de l'hamiltonien quantique $P := -\frac{\hbar^2}{2m}\Delta + V(x)$ sur $L^2(\mathbb{R}^d)$, appelé *opérateur de Schrödinger*. Il suffit de connaître son spectre discret (quand il existe, c'est le cas lorsque V est confinant : l'opérateur auto-adjoint P sur $L^2(\mathbb{R}^d)$ a une résolvante compacte et admet une suite de valeurs propres qui tend vers $+\infty$), composé de ses *valeurs propres* $\lambda_h^j \in \mathbb{R}$: c'est un nombre pour lequel il existe $\psi_h^j \neq 0$ tel que $P\psi_h^j = \lambda_h^j\psi_h^j$ et

$$\lambda_h^1 \leq \lambda_h^2 \leq \dots \leq \lambda_h^j \xrightarrow{j \rightarrow +\infty} +\infty,$$

et une base orthonormale associée de *fonctions propres* $\{\psi_h^j\}_{j \in \mathbb{N}} \subset L^2(\mathbb{R}^d)$. En effet, connaissant une solution u_h^j de l'équation de Schrödinger stationnaire au niveau d'énergie λ_h^j , on peut déduire les solutions de (I.2) comme combinaison linéaire des fonctions

$$\psi_h^j(t, x) = e^{-i\lambda_h^j t/\hbar} u_h^j(x).$$

Remarquons que le module $|\psi_h^j(t, x)|$ reste constant : $|\psi_h^j(t, x)|^2 = |u_h^j(x)|^2$ pour tout $t \geq 0$. Ainsi, on peut se concentrer sur les solutions stationnaires de l'équation de Schrödinger. De plus, comme on peut le voir dans la notation, les fonctions propres et les valeurs propres de P dépendent de la constante \hbar . En particulier, la distance entre les valeurs propres dépend de \hbar (par exemple, celle-ci est proportionnelle à \hbar lorsque P est l'oscillateur harmonique, c'est-à-dire $V(x) = |x|^2$).

La question est de comprendre plus finement les propriétés spectrales de P . L'astuce consiste à passer à la *limite semi-classique*⁶, c'est-à-dire à faire en sorte que la constante de Planck réduite \hbar s'approche de 0. Dans cette limite, le système se comporte comme en régime classique. Cette stratégie permet de déduire des informations de l'observable classique $p : \mathbb{R}_x^d \times \mathbb{R}_\xi^d \rightarrow \mathbb{R}$ qui est l'analogue de P . La relation de continuité classique-quantique est appelée « *principe de correspondance* »⁷. En mathématiques, on l'appelle analyse semi-classique ou microlocale. Une opération cruciale (mais non unique), que l'on appelle *quantification*⁸, est la correspondance d'une fonction très régulière de l'espace des phases à un opérateur linéaire auto-adjoint dans $L^2(\mathbb{R}^d)$.

Exemple. La position $(x, \xi) \mapsto x$ correspond à l'opérateur de multiplication par x . De même, l'impulsion $(x, \xi) \mapsto \xi$ est associée à l'opérateur d'impulsion $\frac{\hbar}{i}\nabla_x$. Comme ci-dessous, les opérateurs

⁵Erwin Schrödinger (1887-1961) généralisa l'approche de De Broglie quelques années plus tard aux particules confinées dans un potentiel externe à l'aide des outils mathématiques des équations d'onde. Sa célèbre équation, qui devint son œuvre maîtresse, apparut pour la première fois en 1926 dans l'article [Sch26], dont le titre traduit est *La quantification comme un problème de valeur propre*. Selon [BL14], malgré sa vie sentimentale tumultueuse et des relations polyamoureuses aussi nombreuses que ses articles, il aurait accompli son œuvre cruciale dans une période d'exubérance amoureuse. Cependant, avant de mourir de la tuberculose, Schrödinger fut obsédé par donner une signification physique aux états ψ_h . Il insistait en particulier d'interpréter $|\psi_h|^2$ comme la densité de la charge électrique de la particule et rejetait l'interprétation probabiliste de Born.

⁶A l'origine, dans le but de déduire le spectre du rayonnement des corps noirs en 1900, Planck considérait comme discret le four qui contenait les corps noirs, délimité par des grilles d'une certaine longueur h qu'il faisait tendre vers 0 afin de retrouver un espace continu. La valeur limite est celle qui porte son nom $h \simeq 6,62 \times 10^{-34}$ J.s.

⁷énoncé par Niels Bohr (1885-1962) [Boh24] en 1923. Il calcula notamment les propriétés subatomiques en se basant sur les postulats de la mécanique classique.

⁸Nous renvoyons à [DS99, Chap.7] ou [Zwo12, Chap.4] pour plus de détails.

de Schrödinger $P = -\frac{\hbar^2}{2m}\Delta + V(x)$ sont associés à l'énergie hamiltonienne classique $p(x, \xi) = \frac{1}{2m}|\xi|^2 + V(x)$, qui est l'énergie totale d'une particule classique piégée dans un potentiel V , décrite par l'équation de Hamilton (I.1).

Un exemple frappant du principe de correspondance est la *loi de Weyl intégrée* (voir par exemple [Zwo12, Thm. 6.8]), qui donne des asymptotiques du nombre $N_\hbar(I)$ de valeurs propres de P dans un intervalle fixe $I \subset \mathbb{R}$ dépendant de l'hamiltonien classique $p(x, \xi) = \frac{1}{2m}|\xi|^2 + V(x)$

$$N_\hbar(I) = (2\pi\hbar)^{-d} \left| \{(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d : p(x, \xi) \in I\} \right| + \mathcal{O}_{\hbar \rightarrow 0}(\hbar^{-(d-1)}). \quad (\text{I.3})$$

Systèmes quantiques à plusieurs particules Jusqu'à présent, nous n'avons pas vu la différence entre la nature bosonique ou fermionique des particules. Elle n'entre en jeu que lorsque nous nous intéressons à des systèmes de plusieurs particules indiscernables. Un système de N particules fermioniques indiscernables est décrit par des fonctions d'onde antisymétriques⁹ du sous-espace $L_a^2(\mathbb{R}^{dN}) = L_a^2((\mathbb{R}^d)^N)$ de $L^2(\mathbb{R}^{dN})$

$$L_a^2(\mathbb{R}^{dN}) := \{\Psi_N \in L^2(\mathbb{R}^{dN}) : \Psi_N(x^1, \dots, x^N) = \varepsilon(\sigma)\Psi_N(x^{\sigma(1)}, \dots, x^{\sigma(N)}) \quad \forall \sigma \in \mathfrak{S}_N\}.$$

Dans la définition ci-dessus, $\varepsilon(\sigma)$ désigne la signature d'une permutation $\sigma \in \mathfrak{S}_N$. Le principe d'exclusion de Pauli impose que deux fermions ne peuvent pas occuper le même état quantique. Cela conduit à l'espace ci-dessus d'états antisymétriques par rapport aux permutations des variables de position. Pour tout état Ψ_N normalisé dans $L^2(\mathbb{R}^{dN})$, la quantité $|\Psi_N(x^1, \dots, x^N)|^2$ (resp. $|\hat{\Psi}_N(\xi^1, \dots, \xi^N)|^2$) peut être interprétée comme la densité de probabilité que la $j^{\text{ème}}$ particule se trouve à la position $x^j \in \mathbb{R}^d$ (resp. a la quantité de mouvement $\xi^j \in \mathbb{R}^d$) pour tout $1 \leq j \leq N$. De plus, en fixant

$$\rho_{\gamma_{\Psi_N^{(1)}}}(x) := N \int_{\mathbb{R}^{(N-1)d}} |\Psi_N(x, x^2, \dots, x^N)|^2 dx^2 \cdots dx^N,$$

sa normalisation $N^{-1}\rho_{\gamma_{\Psi_N^{(1)}}}(x)$ correspond à la densité de probabilité de toute particule du système dans l'état Ψ_N de se trouver à une position $x \in \mathbb{R}^d$. Nous expliquerons plus tard d'où vient cette notation $\gamma_{\Psi_N^{(1)}}$. De plus, la dynamique des états quantiques $\Psi_{N,\hbar}$ est donnée par l'équation de Schrödinger dans $L_a^2(\mathbb{R}^{dN})$ pour un état initial $\psi_N^0 \in L_a^2(\mathbb{R}^{dN})$

$$\begin{cases} i\hbar\partial_t \Psi_{N,\hbar}(t) = P_N \Psi_{N,\hbar}(t) & \forall t > 0 \\ \Psi_{N,\hbar}(t=0) = \psi_N^0. \end{cases} \quad (\text{I.4})$$

Ici P_N désigne l'hamiltonien quantique des N particules de même masse m , piégées dans un potentiel externe $V : \mathbb{R}^d \rightarrow \mathbb{R}$ avec un potentiel d'interaction $w : \mathbb{R}^d \rightarrow \mathbb{R}$ entre deux particules, qui est une fonction paire,

$$P_N = \sum_{j=1}^N \left(-\frac{1}{2m}\hbar^2\Delta_{x^j} + V(x^j) \right) + \lambda \sum_{1 \leq i < j \leq N} w(x^i - x^j). \quad (\text{I.5})$$

L'interaction entre les particules est répulsive lorsque $w \geq 0$ et est attractive lorsque $w \leq 0$. Le facteur λ devant le terme d'interaction est la constante de couplage. Afin de simplifier ces formules,

⁹ce qui les distingue des particules bosoniques pour lesquelles les états sont symétriques et appartiennent à

$$L_s^2(\mathbb{R}^{dN}) := \{\Psi_N \in L^2(\mathbb{R}^{dN}) : \Psi_N(x^1, \dots, x^N) = \Psi_N(x^{\sigma(1)}, \dots, x^{\sigma(N)}) \quad \forall \sigma \in \mathfrak{S}_N\}.$$

nous supposons dans la suite de cette thèse que la masse $m = 1/2$. L'énergie totale du système dans un état Ψ_N est la valeur moyenne $\mathcal{E}_N(\Psi_N) = \langle \Psi_N, P_N \Psi_N \rangle_{L^2}$ de l'énergie quantique P_N . L'énergie fondamentale de P_N (lorsqu'elle existe) est définie par sa valeur propre minimale et peut être obtenue par la minimisation du problème variationnel

$$e_N = \inf\{\langle \Psi, P_N \Psi \rangle_{L^2} : \Psi \in L^2_a(\mathbb{R}^{dN}) \text{ et } \|\Psi\|_{L^2(\mathbb{R}^{dN})} = 1\}. \quad (\text{I.6})$$

Il s'avère que ce problème de minimisation n'est pas facile à résoudre en général.

Systèmes de fermions libres Lorsqu'il n'y a pas d'interaction, c'est-à-dire lorsque $w = 0$, l'avantage est la réduction de la dimension du problème : au lieu de travailler avec une fonction d'onde dans $L^2(\mathbb{R}^{dN})$, il suffit de considérer N fonctions d'onde de $L^2(\mathbb{R}^d)$. En effet, une fonction propre naturelle $\Psi_{N,\hbar}$ de P_N , non corrélée, normalisée dans $L^2(\mathbb{R}^{dN})$, est un *déterminant de Slater*¹⁰ notée $u_{\hbar}^1 \wedge \cdots \wedge u_{\hbar}^N$

$$\Psi_{N,\hbar}(x^1, \dots, x^N) = \frac{1}{\sqrt{N!}} \sum_{\sigma \in \mathfrak{S}_N} \varepsilon(\sigma) \prod_{i=1}^N u_{\hbar}^j(x^{\sigma(i)}) = \det \left((u_{\hbar}^i(x^j))_{1 \leq i, j \leq N} \right), \quad (\text{I.7})$$

associé à une famille orthonormée de fonctions $\{u_{\hbar}^j\}_{1 \leq j \leq N}$ de $L^2(\mathbb{R}^d)$. Lorsque les particules fermioniques sont libres, les fonctions propres de P_N sont exactement des déterminants de Slater. Par conséquent, c'est également le cas de l'état fondamental. Ainsi, le problème de minimisation (I.6) peut être restreint sur l'espace des déterminants de Slater associés aux fonctions propres orthonormales de l'opérateur de Schrödinger à un corps $P = P_1$. De plus, étant donnée une famille orthonormale $\{u_{\hbar}^j\}_{1 \leq j \leq N} \subset L^2(\mathbb{R}^d)$, la densité de l'état $u_{\hbar}^1 \wedge \cdots \wedge u_{\hbar}^N$ est donnée par

$$\rho_{u_{\hbar}^1 \wedge \cdots \wedge u_{\hbar}^N}(x) = \sum_{j=1}^N |u_{\hbar}^j(x)|^2.$$

La quantité normalisée $N^{-1} \rho_{u_{\hbar}^1 \wedge \cdots \wedge u_{\hbar}^N}(x)$ représente la densité de probabilité de N particules fermioniques libres en un point $x \in \mathbb{R}^d$. Chaque état, à un ensemble de niveaux d'énergie λ_{\hbar}^j associé à une particule indexée par j , est une fonction propre normalisée u_{\hbar}^j ($(\lambda_{\hbar}^j, u_{\hbar}^j)$ sont ici des paires valeur propre-fonction propre de P). On remarque que lorsque l'on intègre $\rho_{u_{\hbar}^1 \wedge \cdots \wedge u_{\hbar}^N}$ sur l'espace entier \mathbb{R}^d , on obtient le nombre N de particules.

Notation. Rappelons la notation de Dirac $|u\rangle \langle v|$, qui désigne l'opérateur sur $L^2(\mathbb{R}^d)$, associé aux fonctions $u, v \in L^2(\mathbb{R}^d)$

$$f \in L^2(\mathbb{R}^d) \mapsto \langle v, f \rangle_{L^2(\mathbb{R}^d)} u.$$

Lorsque $u = v$ et u est normalisée dans L^2 , l'opérateur $|u\rangle \langle u|$ est le projecteur orthogonal sur l'espace $\text{Vect}\{u\}$.

Il convient également de noter que $\rho_{u_{\hbar}^1 \wedge \cdots \wedge u_{\hbar}^N}$ est le noyau intégral, évalué sur la diagonale, du projecteur orthogonal de rang N de la famille orthonormale $\text{Vect}\{u_{\hbar}^j\}_{1 \leq j \leq N} \subset L^2(\mathbb{R}^d)$.

$$\gamma_{u_{\hbar}^1 \wedge \cdots \wedge u_{\hbar}^N} := \sum_{j=1}^N |u_{\hbar}^j\rangle \langle u_{\hbar}^j|.$$

¹⁰Ce nom est dû à John Clarke Slater (1900-1976) du fait de sa formulation dans [Sla29], bien qu'il ait également été introduit indépendamment par Dirac [Dir26].

Cet opérateur $\gamma_{u_{\hbar}^1 \wedge \dots \wedge u_{\hbar}^N}$ est appelé la *matrice densité à un corps* du système et $\rho_{u_{\hbar}^1 \wedge \dots \wedge u_{\hbar}^N}$ sa *densité* associée. Il s'avère que $\gamma_{u_{\hbar}^1 \wedge \dots \wedge u_{\hbar}^N}$ est très utile pour obtenir des informations sur le système. Nous reviendrons sur l'interprétation de ce cas dans la section I.3.

En outre, on peut considérer, pour un niveau d'énergie $E \in \mathbb{R}$ fixée, une famille de fonctions propres $\{u_{\hbar}^j\}_{1 \leq j \leq N_{E,\hbar}}$ associées aux valeurs propres λ_{\hbar}^j de P inférieures ou égales à E . La taille de ce système $N_{E,\hbar}$ dépend de E et de la constante de Planck réduite \hbar . Notamment, $N_{E,\hbar} \rightarrow \infty$ lorsque $\hbar \rightarrow 0$. L'asymptotique de $\rho_{u_{\hbar}^1 \wedge \dots \wedge u_{\hbar}^{N_{E,\hbar}}}$ est connue en théorie spectrale sous le nom de *loi de Weyl ponctuelle*. Lorsque l'on peut intégrer cette formule sur l'espace entier \mathbb{R}^d , cela donne l'asymptotique du nombre $N_{E,\hbar}$, qui est la loi de Weyl intégrée (I.3) pour $I = (-\infty, E]$. Nous discuterons plus profondément de l'état de l'art des lois de Weyl dans les sections I.2 et I.3.

Motivons maintenant ce travail de thèse en posant des questions plus spécifiques et naïves.

Question 1. Quel type de phénomène de concentration spatiale peut-il se produire pour les fonctions propres lorsque $\hbar \rightarrow 0$?

Question 2. Comment mesurer mathématiquement la concentration ou la délocalisation des fonctions propres ?

Question 3. Quelle est l'influence de l'interaction sur ces propriétés de concentration ?

I.2 État de l'art sur la concentration des quasimodes et des fonctions propres

Motivés par les questions 1 et 2, nous donnons maintenant un aperçu des résultats mathématiques sur les fonctions propres.

La concentration des fonctions propres nécessite un paramètre mesurable. Il existe deux régimes différents dans lesquels elle peut être observée. D'une part, il y a le point de vue *semi-classique*, qui est historiquement le plus ancien, comme en témoigne l'approximation Brillouin-Kramers-Wentzel (BKW)¹¹ des fonctions d'onde en dimension 1, connue aussi sous le nom de méthode Liouville-Green (LG)¹² (voir par exemple [Olv97, Chap.6]). L'idée est de considérer $P = -\hbar^2 \Delta + V$ à une énergie fixe lorsque le paramètre semi-classique $\hbar \rightarrow 0$. D'autre part, on peut se placer dans un cadre *haute fréquence*, ce qui signifie de regarder les fonctions propres de $P = -\Delta + V$ associées à une valeur propre $\lambda \rightarrow \infty$. Nous avons fait le choix de commencer par ce régime qui est techniquement plus simple.

Le problème de la concentration des fonctions propres de haute fréquence sur les variétés riemanniennes compactes lisses et sans bords est un sujet de recherche actif depuis les années 1980 et s'étend aux sous-variétés (comme décrit dans [Sog15]). Nous commençons donc par présenter une littérature partielle de certains problèmes connexes. Cela permettra de faire le lien avec notre cas euclidien avec un potentiel confinant dans un régime semi-classique. Nous verrons pourquoi, la plupart du temps, il faut revoir nos ambitions à la baisse et restreindre nos estimations à des généralisations de fonctions propres appelées quasimodes ou fonctions dans des agrégats spectraux.

Variétés riemanniennes compactes sans bords On considère des variétés riemanniennes lisses et compactes M sans frontière de dimension $n \geq 2$ que l'on dote d'une métrique g . On désigne par Δ_g l'opérateur de Laplace-Beltrami sur (M, g) . On se place dans le cas sans potentiel.

¹¹due à Léon Brillouin (1889-1969) [Bri26], Hendrik Anthony Kramers (1894-1952) [Kra26] et Gregor Wentzel (1898-1978) [Wen26] dans les années 1920

¹²Joseph Liouville (1809-1882) [Lio36] et George Green (1793-1841) [Gre37] introduisirent cette méthode un siècle auparavant pour les solutions d'équations différentielles du second ordre de la forme $y''(x) = f(x)y(x)$ mais elle passa relativement inaperçue. Les solutions y sont exprimées sous la forme $y(x) \sim f(x)^{-1/4} \exp\left(\pm \int_{x_0}^x \sqrt{f(t)} dt\right)$.

	Point de vue haute fréquence	Point de vue semi-classique
Variétés	[Sog85, Sog88, FS17b]	
Sous-variétés	[Hu09]	[BZ16, BGT07, Tac10]
Cas euclidien	[KT05]	[KTZ07, Ngu22]

TABLE 1 – Un aperçu non exhaustif de la littérature sur les estimées L^q sur les variétés.

L'exemple de la sphère ronde standard Commençons par nous concentrer sur la sphère de dimension n pour $n \geq 2$

$$\mathbb{S}^n := \{(x_1, x_2, \dots, x_{n+1}) \in \mathbb{R}^{n+1} : x_1^2 + x_2^2 + \dots + x_{n+1}^2 = 1\},$$

qui a le mérite de donner des résultats explicites sur les fonctions propres exactes et une réponse à la question 1. Nous désignons par $\Delta_{\mathbb{S}^n}$ l'opérateur de Laplace-Beltrami par rapport à la métrique induite par la métrique euclidienne sur \mathbb{R}^{n+1} . Ce dernier admet comme spectre discret $\{\ell(\ell+n-1)\}_{\ell \in \mathbb{N}}$. Pour chaque $\ell \in \mathbb{N}$, chaque fonction propre associée à la valeur propre $\ell(\ell+n-1)$ de multiplicité $\binom{n+\ell}{\ell} - \binom{n+\ell-2}{\ell-2}$, est une restriction de polynômes harmoniques de degré ℓ , appelés *harmoniques sphériques* de degré ℓ . L'espace vectoriel engendré par les harmoniques sphériques forme une base hilbertienne de $L^2(\mathbb{S}^n)$. Nous orientons le lecteur vers les références suivantes : [DX13, Sog85] pour les asymptotiques sur les harmoniques sphériques.

Considérons d'abord la sphère à deux dimensions, qui est la plus intuitive et la plus facile à représenter géométriquement. Il existe une concentration de fonctions propres de $-\Delta_{\mathbb{S}^2}$ aux deux pôles et autour de l'équateur (voir la figure 1). Notons $\{Y_\ell^m\}_{\ell \in \mathbb{N}, -\ell \leq m \leq \ell}$ la base standard des harmoniques sphériques normalisées de $L^2(\mathbb{S}^2)$

$$-\Delta_{\mathbb{S}^2} Y_\ell^m = \ell(\ell+1) Y_\ell^m.$$

D'une part, l'harmonique sphérique *zonale* Y_ℓ^0 se concentre autour du pôle nord $\mathbf{1} := (0, 0, 1)$ et du pôle sud $-\mathbf{1}$. Plus précisément, sa densité de probabilité $|Y_\ell^0|^2$ se concentre en ces deux points extrêmes avec une hauteur ℓ dans une région de taille ℓ^{-1} (voir figure 2a). D'autre part, les harmoniques sphériques d'ordre le plus élevé $Y_\ell^{\pm\ell}$, généralement appelées *faisceaux gaussiens*, se concentrent autour de l'équateur $\gamma_{\text{equat}} := \{x \in \mathbb{S}^2 : x_3 = 0\}$: les densités de probabilité satisfont $|Y_\ell^{\pm\ell}|^2 \gtrsim \ell$ dans une région de taille $\ell^{-1/2}$ (voir figure 2b). Le terme « faisceau gaussien » (*gaussian beams*) provient du profil gaussien centré sur les points de la courbe γ_{equat} . Il est de la forme $Y_\ell^{\pm\ell}(x) = c\ell^{1/4}(x_1 \pm ix_2)^\ell$, qui se comporte comme une exponentielle. On peut d'ailleurs parler de concentration tubulaire de rayon $\ell^{-1/2}$ autour de l'équateur de ces fonctions $\{Y_\ell^{\pm\ell}\}_{\ell \in \mathbb{N}}$.

Rappelons que les points de la sphère \mathbb{S}^2 sont paramétrables par des coordonnées angulaires $(\theta, \varphi) \in [0, \pi] \times [0, 2\pi]$ (c.f. à la figure 1), par la relation

$$(x_1, x_2, x_3) \in \mathbb{R}^3 \iff (\theta, \varphi) \in [0, \pi] \times [0, 2\pi] \text{ avec } \begin{cases} x_1 &= \sin \theta \cos \varphi, \\ x_2 &= \sin \theta \sin \varphi, \\ x_3 &= \cos \theta. \end{cases}$$

Ces phénomènes de saturation sont visibles à travers les asymptotiques locales des harmoniques sphériques

$$Y_\ell^m(\theta, \varphi) = e^{im\varphi} f_\ell^m(\theta)$$

avec f_ℓ^m des fonctions associées aux polynômes de Legendre. Elle provient en effet de l'expression explicite (mais douloureuse à écrire) de Y_ℓ^m

$$\forall (\theta, \varphi) \in [0, \pi] \times [0, 2\pi], \quad Y_\ell^m(\theta, \varphi) = c_{\ell,m} e^{im\varphi} P_\ell^m(\cos \theta)$$

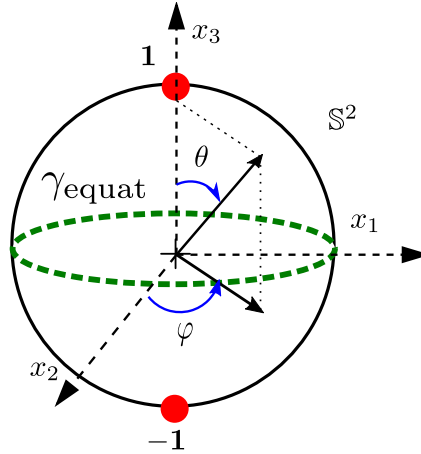


FIGURE 1 – Les régions de concentration sur la sphère bidimensionnelle sont les pôles ± 1 et l'équateur γ_{equat} .

en fonction des fonctions associées aux polynômes de Legendre

$$\forall x \in [-1, 1], \quad P_\ell^m(x) := \begin{cases} \frac{1}{2^\ell \ell!} (1-x^2)^{m/2} \frac{d^{\ell+m}}{dx^{\ell+m}} (x^2-1)^\ell & \text{for } 0 \leq m \leq \ell, \\ (-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_\ell^{-m}(x) & \text{for } -\ell \leq m \leq 0, \end{cases}$$

et des

$$c_{\ell,m} = (-1)^m \sqrt{\frac{4\pi}{2\ell+1} \frac{(\ell+m)!}{(\ell-1)!}}.$$

S'en déduit la borne pour une fonction u , concentrée dans un volume V avec une hauteur L

$$\forall 2 \leq q \leq \infty, \quad \|u\|_{L^q} \gtrsim L \times V^{1/q}.$$

Il en résulte les estimées L^q , valables pour tout $2 \leq q \leq \infty$

$$\| |Y_\ell^0|^2 \|_{L^{q/2}(\mathbb{S}^2)} \gtrsim \ell \times (\ell^{-2})^{2/q} = \ell^{1-\frac{4}{q}}. \quad (\text{I.8})$$

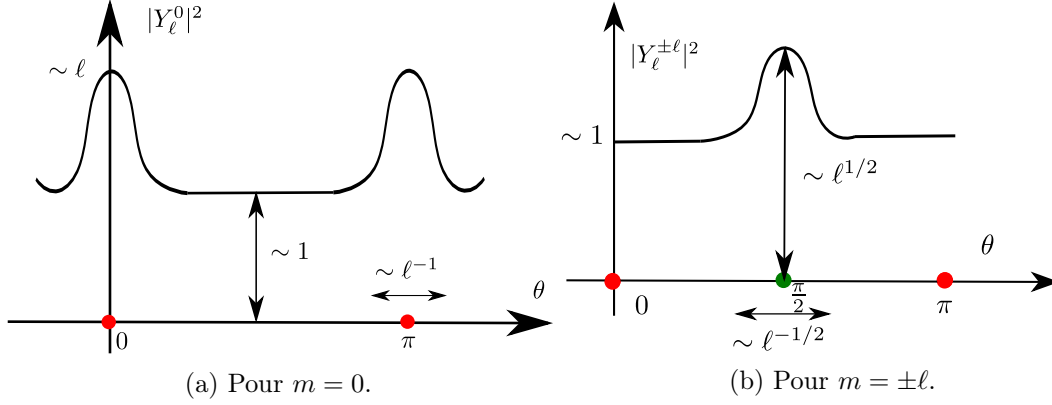
et

$$\| |Y_\ell^{\pm \ell}|^2 \|_{L^{q/2}(\mathbb{S}^2)} \gtrsim \ell^{1/2} \times (\ell^{-1/2})^{2/q} = \ell^{\frac{1}{2}-\frac{1}{q}}. \quad (\text{I.9})$$

Ces estimations ne sont pas très précises, mais donnent une mesure de la concentration de la fonction propre. En effet, la localisation d'une fonction u_ℓ se mesure informellement par l'explosion du quotient $\| |u_\ell|^2 \|_{L^{q/2}(\mathbb{S}^2)} / \| |u_\ell|^2 \|_{L^1(\mathbb{S}^2)} \rightarrow \infty$ lorsque $\ell \rightarrow \infty$ pour q différent de 2. De même, sa non-concentration est tangible lorsque toutes les normes L^q sont du même ordre.

- Existe-t-il une limite supérieure correspondante de (I.8) et (I.9) pour toute harmonique sphérique Y_ℓ^m ?
- De plus, ces phénomènes de concentration sont-ils valables de nouveau pour les sphères de dimension supérieure, et s'étendent-ils à des variétés compactes plus générales ?

Nous pouvons commencer par donner une réponse positive à la question sur la généralisation des phénomènes de concentration en dimension supérieure. En fait restent valides, pour toute dimension $n \geq 2$, la concentration à haute fréquence aux pôles $\pm \mathbf{1} = (0, \dots, 0, \pm 1)$, autour de la courbe équatoriale $\gamma_{\text{equat}} := \{x \in \mathbb{S}^n : (x_3, \dots, x_{n+1}) = 0\}$ et les estimations L^q des harmoniques

FIGURE 2 – Représentation grossière de la densité $|Y_\ell^m|^2$ dans \mathbb{S}^2 en fonction de l'angle polaire θ .

sphériques. Comme dans le cas de la 2-sphère, il existe une harmonique sphérique, qui se concentre aux pôles $\pm \mathbf{1}$ avec un module de hauteur $\ell^{\frac{n-1}{2}}$ dans une région de largeur ℓ^{-1} (voir Figure 4a), et une autre dont le module se concentre autour de l'équateur γ_{equat} avec une longueur $\ell^{\frac{n-1}{4}}$ dans une région de rayon $\ell^{-1/2}$ (voir figure 4b).

La réponse à la question concernant la limite supérieure de (I.8) et (I.9) demeure également positive. Sogge a fourni, dans sa thèse de doctorat [Sog85], des estimées L^q sur les fonctions propres de $-\Delta_{\mathbb{S}^n}$. L'énoncé est le suivant : pour toute dimension $n \geq 2$, il existe $C > 0$ tel que pour tout $\ell \in \mathbb{N}$, toute fonction propre u_ℓ associée à $\ell(\ell + n - 1)$ et tout $2 \leq q \leq \infty$,

$$\| |u_\ell|^2 \|_{L^{q/2}(\mathbb{S}^n)} \leq C \ell^{2s_{\text{Sogge}}(q,n)} \| |u_\ell|^2 \|_{L^1(\mathbb{S}^n)}, \quad (\text{I.10})$$

où

$$s_{\text{Sogge}}(q, n) = \begin{cases} \frac{n-1}{2} \left(\frac{1}{2} - \frac{1}{q} \right) & \text{si } 2 \leq q \leq \frac{2(n+1)}{n-1} := q_c, \\ n \left(\frac{1}{2} - \frac{1}{q} \right) - \frac{1}{2} & \text{si } \frac{2(n+1)}{n-1} \leq q \leq \infty. \end{cases} \quad (\text{I.11})$$

Inversement, l'exposant s_{Sogge} est optimal puisque (I.10) est saturée par les faisceaux gaussiens en faible régime $2 \leq q \leq q_c$ (ce qui correspond à Y_ℓ^m tel $m = \pm \ell$ avec les estimées L^q (I.9))

$$\| |u_\ell|^2 \|_{L^{q/2}(\mathbb{S}^n)} \gtrsim \ell^{n-1} \times (\ell^{-1 \times n})^{2/q}$$

et par les harmoniques sphériques zonales en haut régime $q_c \leq q \leq \infty$ (qui correspond à Y_ℓ^m pour $m = 0$ lorsque $n = 2$, avec les estimées L^q (I.8))

$$\| |u_\ell|^2 \|_{L^{q/2}(\mathbb{S}^n)} \gtrsim \ell^{\frac{n-1}{2}} \times (\ell^{-1/2 \times (n-1)})^{2/q}.$$

Cela montre en particulier deux types de concentration : dans une boule autour des points (ici de rayon $\sim \ell^{-2}$) et dans un tube autour des géodésiques (de largeur $\sim \ell^{-1/2}$).

Variétés compactes plus générales Il se trouve que les estimations L^q de Sogge (I.10) s'étendent à toutes les variétés (M, g) compactes lisses sans bords de dimension n (voir les travaux ultérieurs de Sogge [Sog88, Thm. 2.2]) pour toute fonction propre u_λ de $-\Delta_g$ associée à la valeur propre $\lambda^2 > 0$

$$-\Delta_g u_\lambda = \lambda^2 u_\lambda. \quad (\text{I.12})$$

L'énoncé est le suivant : il existe une constante multiplicative $C > 0$ indépendante de u_λ et $\lambda > 0$ telle que pour tout $2 \leq q \leq \infty$

$$\| u_\lambda \|_{L^q(M)} \leq C \lambda^{s_{\text{Sogge}}(q,n)} \| u_\lambda \|_{L^2(M)}, \quad (\text{I.13})$$

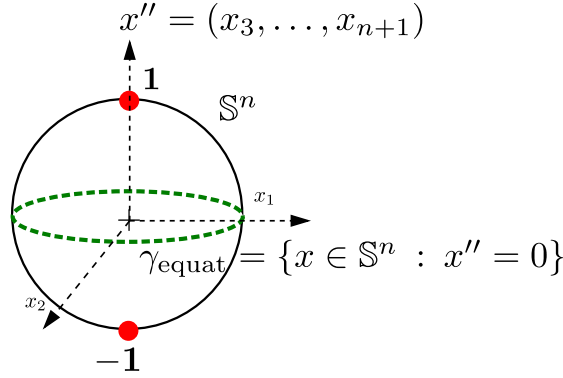


FIGURE 3 – Régions de concentration dans la sphère n : aux pôles ± 1 et autour de l'équateur γ_{equat} .

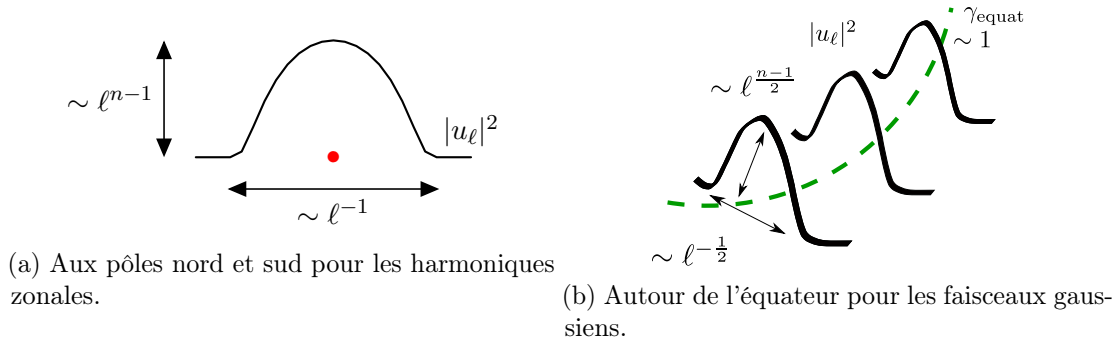


FIGURE 4 – Profils de concentration des harmoniques sphériques sur \mathbb{S}^n .

où s_{Sogge} est défini par (I.11). Comme nous l'avons vu précédemment, ces bornes sont optimales et saturées lorsque M est une sphère (puisque $\ell \sim \lambda$).

Que peut-on dire de l'optimalité des estimations de Sogge pour les fonctions propres (I.13) dans d'autres variétés compactes lisses ? En fait, il existe plusieurs variétés compactes avec des géométries particulières où l'exposant de Sogge n'est pas optimal et peut être amélioré dans certains régimes de q . Il existe notamment des fonctions propres qui saturent des meilleures bornes.

- Un premier exemple, dû à Zygmund [Zyg74] en 1974, pour le tore bidimensionnel $\mathbb{T}^2 := \mathbb{R}^2/\mathbb{Z}^2$ pour l'exposant $q = 4$.

$$\|u_\lambda\|_{L^4(\mathbb{T}^2)} \leq C \|u_\lambda\|_{L^2(\mathbb{T}^2)}.$$

Elle fut ensuite généralisée en dimension supérieure $n \geq 3$ par la fonction propre par Bourgain [Bou93] pour tout $2 \leq q \leq 2n/(n-1)$ et tout $\varepsilon > 0$

$$\|u_\lambda\|_{L^q(\mathbb{T}^n)} \leq C \lambda^\varepsilon \|u_\lambda\|_{L^2(\mathbb{T}^n)}.$$

- Nous mentionnons également les variétés à courbure négative, sur lesquelles nous y reviendrons plus tard.

Par conséquent, un défi consiste à trouver l'exposant s optimal pour une variété M donnée. Les estimations de Sogge restent cependant vraies pour les généralisations des fonctions propres, qui sont

- des *quasimodes* de $-\Delta_g - \lambda^2$: qui sont des fonctions L^2 -normalisées u_λ telles que

$$\|-\Delta_g u_\lambda - \lambda^2 u_\lambda\|_{L^2(M)} \lesssim \lambda \|u_\lambda\|_{L^2(M)}, \quad (\text{I.14})$$

- ou des fonctions des *agrégats spectraux*¹³ de $-\Delta_g$ pour tout $\lambda > 0$: c'est-à-dire des fonctions telles que

$$\mathbf{1}(-\Delta_g \in [\lambda^2, (\lambda + 1)^2]) u_\lambda = u_\lambda, \quad (\text{I.15})$$

i.e. combinaisons linéaires de fonctions propres de $-\Delta_g$ associées aux valeurs propres dans les intervalles $[\lambda^2, (\lambda + 1)^2]$.

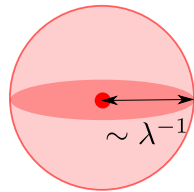
Dans ces cas, nous devons ajouter un autre terme de contrôle $\lambda \|(-\Delta_g - \lambda^2)u_\lambda\|_{L^2(M)}$ à la partie droite de (I.14) :

$$\|u_\lambda\|_{L^q(M)} \leq C \lambda^{s_{\text{Sogge}}(q,n)} (\|u_\lambda\|_{L^2(M)} + \lambda \|(-\Delta_g - \lambda^2)u_\lambda\|_{L^2(M)}). \quad (\text{I.16})$$

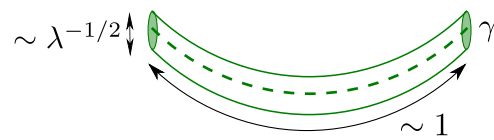
Sogge lui-même [Sog88] avait en fait prouvé (I.16) et avait construit des quasimodes qui la saturaient pour toute variété compacte M . Par conséquent, la puissance s_{Sogge} demeure optimale pour toute variété compacte M . En outre, se produit à nouveau le phénomène de concentration autour des points et des géodésiques pour n'importe quelle variétés compacte pour des fonctions normalisées (voir la figure 5). Pour l'explicitier, il s'agit de généraliser, comme dans [Sog17a, Thm. 5.1.1], les faisceaux sphériques zonaux et gaussiens harmoniques

- Les quasimodes de type zonal, qui se concentrent en un point (voir par exemple la figure 5a). Ils peuvent être utilisés pour saturer les bornes à haut régime $q \geq q_c := 2(n + 1)/(n - 1)$.
- Les quasimodes de type faisceaux gaussiens, qui se concentrent le long d'une courbe avec un profil transversal gaussien (voir par exemple la figure 5b). Ils sont principalement utilisés pour saturer les bornes à bas régime $q \leq q_c$. Ces types de construction ont été développés pour la première fois par Ralston [Ral76, Ral77].

La pertinence des constructions n'est plus à vérifier. En effet, Canzani et Galkowski [CG21] ont prouvé que les fonctions propres qui saturent (I.14) se comportent comme des quasimodes zonaux pour $q \geq q_c$, et Blair et Sogge [BS15, BS17] ont montré que les fonctions propres saturatrices sont similaires à des faisceaux gaussiens pour $q \leq q_c$. Soulignons que les quasimodes de type faisceaux gaussiens sont plus récemment généralisés sous le nom de méthodes de *faisceaux géodésiques* (*geodesic beams*) dans plusieurs travaux de Canzani et Galkowski (en citant uniquement [CG21, CG20a]).



(a) Boule centrée en un point.



(b) Cylindre autour d'une géodésique γ .

FIGURE 5 – Deux différents voisinages de concentration.

De plus, les améliorations des estimations de Sogge [Sog88] ont fait l'objet de nombreux travaux sous certaines hypothèses géométriques. Énumérons une sélection non exhaustive d'améliorations pour les variétés à courbure négative

¹³*spectral clusters* dans les articles

- à haut régime $q > q_c$: [HT15, HR16, SZ02, Sog17b, BS19],
- à bas régime $q < q_c$: [BS17, BS18],
- au point critique $q = q_c$: [Sog16].

Généralisation aux familles orthonormales de fonctions propres et aux lois de Weyl Frank et Sabin [FS17b] ont plus récemment généralisé les estimations de Sogge L^q dans les variétés compactes M aux systèmes orthonormaux de fonctions dans les agrégats spectraux $\Pi_\lambda(L^2(M))$, où l'on note Π_λ le projecteur spectral $\mathbf{1}(-\Delta_g \in [\lambda^2, (\lambda+1)^2])$. Ils ont fourni, pour toute famille orthonormale $\{u_j\}_{1 \leq j \leq N}$ dans $\Pi_\lambda(L^2(M))$, tous $\{\nu_j\}_{1 \leq j \leq N} \subset \mathbb{C}$ et tout $2 \leq q \leq \infty$, des bornes $L^{q/2}$ de la densité

$$\rho_\lambda(x) = \sum_{j=1}^N \nu_j |u_j(x)|^2.$$

Une première approche naïve se déduit des estimées à une fonction (I.16) et de l'inégalité triangulaire

$$\|\rho_\lambda\|_{L^{q/2}(M)} \leq C \lambda^{2s_{\text{Sogge}}(q,n)} \left(\sum_{j=1}^N |\nu_j| \right).$$

On remarque que ρ_λ peut s'écrire sous la forme de densité de l'opérateur borné auto-adjoint de rang N

$$\gamma_\lambda = \sum_{j=1}^N \nu_j |u_j\rangle \langle u_j|.$$

De plus, en défissant par $\|\cdot\|_{\mathfrak{S}^\alpha(L^2(M))}$ la norme de Schatten donnée par la formule (voir la définition II.19 dans le chapitre 1) pour $\alpha \geq 1$)

$$\|\gamma\|_{\mathfrak{S}^\alpha(L^2(M))} = \text{Tr}_{L^2(M)}[(\gamma^* \gamma)^{\alpha/2}]^{1/\alpha},$$

l'estimée déduite de l'inégalité triangulaire s'écrit

$$\|\rho_\lambda\|_{L^{q/2}(M)} \leq C \lambda^{2s_{\text{Sogge}}(q,n)} \|\gamma_\lambda\|_{\mathfrak{S}^1(L^2(M))}.$$

L'exposant $\alpha = 1$ de la norme de Schatten de γ_λ peut en fait être amélioré : c'est-à-dire $\alpha > 1$ dans certains régimes de q . C'est ce qu'ont démontré Frank et Sabin, dont le résultat principal s'énonce sous la forme suivante.

Théorème ([FS17b, Thm.2]). *Il existe $C > 0$ et un exposant $\alpha_{\text{Sogge}} \in [1, \infty]$ défini par la formule (qui est (V.3) dans le chapitre 1)*

$$\alpha_{\text{Sogge}}(q, n) := \begin{cases} \frac{2q}{q+2} & \text{si } 2 \leq q \leq \frac{2(n+1)}{n-1}, \\ \frac{q(n-1)}{2n} & \text{si } \frac{2(n+1)}{n-1} \leq q \leq \infty. \end{cases}$$

tels que pour tout opérateur auto-adjoint γ_λ dans $L^2(M)$ vérifiant $\gamma_\lambda = \gamma_\lambda \Pi_\lambda = \Pi_\lambda \gamma_\lambda$ et pour tout $2 \leq q \leq \infty$

$$\|\rho_\lambda\|_{L^{q/2}(M)} \leq C \lambda^{2s_{\text{Sogge}}(q,n)} \|\gamma_\lambda\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,n)}(L^2(M))}. \quad (\text{I.17})$$

Soulignons que la présence de plusieurs fonctions ajoute à l'exposant de concentration s un nouveau paramètre $\alpha \geq 1$, qui prend en compte les constantes complexes ν_j et la taille de la famille $N = \text{rang } \gamma_\lambda$. Cette dernière dépend parfois du paramètre λ (par exemple lorsque l'on considère une base orthonormée de l'ensemble du groupe spectral). On remarque que

- Les estimations ci-dessus coïncident avec les estimations de Sogge (I.16) lorsque la famille est réduite à une seule fonction $u_\lambda \in L^2(M)$ de l'agrégat spectral $\Pi_\lambda(L^2(M))$. Elles se déduisent en injectant $\gamma_\lambda = |u_\lambda\rangle \langle u_\lambda|$ dans (I.17).
- L'autre cas extrême traité concerne l'ensemble de l'agrégat spectral : $N = \dim \Pi_\lambda(L^2(\mathbb{R}^d)) = \text{rang } \Pi_\lambda$, par exemple avec $\gamma_\lambda = \Pi_\lambda$.
- De plus, ils prennent également en compte le cas intermédiaire : tous les $\gamma_\lambda = \gamma_\lambda \Pi_\lambda = \Pi_\lambda \gamma_\lambda$ avec $1 \leq \text{rang } \gamma_\lambda \leq \text{rang } \Pi_\lambda$.

Une question naturelle concerne l'optimalité des bornes (I.17). Qu'en est-il de l'optimalité du nouvel exposant α_{Sogge} ? Existe-t-il des opérateurs γ_λ qui saturent les estimées (I.17) ?

De plus, en gardant à l'esprit notre motivation initiale sur la concentration des particules, on soulève naturellement la question ci-dessous.

Question 4. L'ajout de plusieurs fonctions modifie-t-il les phénomènes de concentration d'une fonction individuelle ?

Cette question reste pertinente puisque nous rappelons que les fermions ne peuvent pas occuper le même état quantique. On pourrait donc s'attendre à observer un phénomène de non-concentration pour l'ensemble de l'agrégat spectral.

Avant de répondre à ces questions dans le cadre des variétés compactes, expliquons leur lien naturel avec les lois de Weyl. Considérons le cas extrême de l'agrégat spectral entier $\Pi_\lambda(L^2(M))$ avec $\gamma_\lambda = \Pi_\lambda$. La loi de Weyl ponctuelle donne l'asymptotique ponctuelle de la densité ρ_{Π_λ} . Le projecteur Π_λ peut en fait être décrit par une base orthonormée des fonctions propres $\{u_\lambda^j\}_{1 \leq j \leq \dim(E_\lambda(L^2(M)))}$ de Δ_g associées aux valeurs propres dans $[\lambda^2, (\lambda+1)^2]$

$$\Pi_\lambda = \sum_{j=1}^{N_\lambda = \dim(E_\lambda(L^2(M)))} |u_\lambda^j\rangle \langle u_\lambda^j|,$$

Rappelons la formule de la loi de Weyl ponctuelle dans les variétés riemanniennes compactes (M, g) à n dimensions, pour les fonctions propres u_λ^j associées aux valeurs propres E_λ^j dans un intervalle $I = (-\infty, \lambda^2]$. On a uniformément sur M

$$\sum_{j: E_\lambda^j \in I} |u_\lambda^j(x)|^2 = (2\pi)^{-n} \lambda^n |\{\xi \in T_x M^* : |\xi|^2 \leq 1\}| + \mathcal{O}(\lambda^{n-1}). \quad (\text{I.18})$$

Ensuite, comme M est compacte, cette expression intégrée sur M donne la loi de Weyl intégrée, qui procure asymptotiquement le nombre de fonctions propres en I . Historiquement, (I.18) fut conjecturée par Hilbert avec un terme d'erreur $o(\lambda^n)$. Son nom « loi de Weyl » vient du fait que Weyl fut le premier à la prouver (sous sa forme intégrée). Cette loi de Weyl ponctuelle (I.18) fut néanmoins à l'origine démontrée par Avakumović [Ava56], Levitan [Lev52] et fut généralisée par Hörmander [Hor68, Thm. 1.1] aux opérateurs pseudo-différentiels elliptiques auto-adjoints. Sogge et Zelditch [Sog01] étudièrent plus tard les conditions sur M sous lesquelles le reste $\mathcal{O}(\lambda^{n-1})$ est optimal. De plus, on améliora le terme de reste sous des conditions géométriques dans de multiples travaux : citons par exemple l'amélioration logarithmique par Bérard, Bonthonneau et Keeler [Bér77, Bon17, KT98] sous des conditions de courbure négative, et les techniques de faisceaux géodésiques développées par Canzani et Galkowski [CG20b, CG22].

Revenons maintenant aux bornes de Frank-Sabin mentionnées précédemment. Expliquons comment répondre à la question 4, en considérant une fois encore le rang maximal, avec $\gamma_\lambda = \Pi_\lambda$. En effet, d'une part, la limite de L^∞ est déduite par la loi de Weyl ponctuelle

$$\|\rho_{\Pi_\lambda}\|_{L^\infty(M)} \leq C\lambda^{n-1}.$$

D'autre part, en désignant $N(I)$ le nombre de valeurs propres de $-\Delta_g$ dans un intervalle I , en utilisant la relation

$$\|\rho_{\Pi_\lambda}\|_{L^1(M)} = \text{Tr}(\mathbf{1}(-\Delta \in [\lambda^2, (\lambda+1)^2])) = N((-\infty, (\lambda+1)^2]) - N((-\infty, \lambda^2])$$

et la version intégrée de la loi asymptotique de Weyl (I.18), qui dépend du paramètre $\lambda > 0$, pour les intervalles $(-\infty, (\lambda+1)^2]$ et $(-\infty, \lambda^2]$, on peut prouver qu'il existe $C > 0$ et une sous-suite $\lambda_k \rightarrow \infty$ selon lesquelles

$$\forall k \in \mathbb{N}, \quad \|\rho_{\Pi_{\lambda_k}}\|_{L^1(M)} \geq C\lambda_k^{n-1}.$$

Ainsi, pour tout $2 < q < \infty$

$$\underbrace{C\lambda^{-(n-1)}\|\rho_{\Pi_\lambda}\|_{L^1(M)}}_{\limsup_{\lambda \rightarrow \infty} \dots > 0} \leq \dots \leq \lambda^{-(n-1)}\|\rho_{\Pi_\lambda}\|_{L^{q/2}(M)} \leq \dots \leq C'\lambda^{-(n-1)}\|\rho_{\Pi_\lambda}\|_{L^\infty(M)} \underbrace{\lesssim 1}.$$

Il en résulte que toutes les normes L^p sont du même ordre

$$\forall 2 \leq q \leq \infty \quad \|\rho_{\Pi_\lambda}\|_{L^{q/2}(M)} \sim \lambda^{n-1},$$

ce qui reflète le phénomène de non-concentration dans l'ensemble de l'agrégat spectral. Il apparaît donc un changement de comportement entre la concentration pour une fonction et un phénomène de non-concentration pour l'ensemble de l'agrégat spectral. Cette concentration assure par ailleurs l'optimalité de l'exposant α_{Sogge} .

Lien entre le régime haute fréquence et le régime semi-classique De plus, l'équivalence entre ce problème de haute fréquence $\lambda \rightarrow \infty$ et le problème semi-classique s'obtient en écrivant $h = \lambda^{-1}$ (le grand paramètre devient un petit) et $u_h = u_\lambda$. Les définitions (I.12), (I.14), (I.15) et (I.16) deviennent

$$-h^2\Delta_g u_h = u_h, \quad \begin{cases} \|-h^2\Delta_g u_h - u_h\|_{L^2(M)} \lesssim h\|u_h\|_{L^2(M)}, \\ \mathbf{1}(-h^2\Delta_g \in [1, (1+h)^2]) u_h = u_h, \end{cases}$$

et dans le terme de droite

$$\|u_h\|_{L^q(M)} \leq Ch^{-s_{\text{Sogge}}(q,n)} \left(\|u_h\|_{L^2(M)} + \frac{1}{h} \|(-h^2\Delta_g - 1)u_h\|_{L^2(M)} \right),$$

qui est la formulation considérée en rajoutant des potentiels.

Cas euclidien avec un potentiel confinant Nous revenons à notre cadre de départ des opérateurs de Schrödinger $-h^2\Delta + V$ avec un potentiel confinant dans l'espace euclidien \mathbb{R}^d et nous considérons la localisation des fonctions propres « près » d'un niveau d'énergie $E \sim 1$, généralement appelé le *potentiel chimique*.

Question 5. Quel rôle joue le potentiel confinant, et qu'est-ce qui diffère des résultats sur les variétés compactes ?

Il est maintenant nécessaire de prendre en compte la présence d'une zone appelée *région classiquement interdite* :

$$\{x \in \mathbb{R}^d : V(x) > E\}.$$

Ce nom vient de l'illégalité pour une particule classique d'énergie totale $|\xi|^2 + V(x) = E$ de se trouver dans cette région puisque l'énergie cinétique $|\xi|^2$ est positive. Une particule quantique

possède cependant une probabilité non nulle de se trouver dans la région classiquement interdite, mais le comportement classique se produit à la limite semi-classique $h \rightarrow 0$. L'existence d'une zone interdite entraîne bien sûr une zone autorisée, appelée *région classiquement autorisée*, désignée parfois *cœur*¹⁴ dans la suite.

$$\{x \in \mathbb{R}^d : V(x) < E\},$$

où la particule a le plus de chances de se trouver. L'existence d'une région de transition entre les régions classiquement permises et interdites soulève une difficulté supplémentaire, qui n'existe pas dans le cadre précédent des variétés compactes. Les points $\{x \in \mathbb{R}^d : V(x) = E\}$ sont souvent appelés *points tournants*¹⁵.

Littérature pour les systèmes à un seul corps Afin de se faire une idée du comportement des fonctions propres, examinons un modèle jouet classique, l'oscillateur harmonique $V(x) = |x|^2$ en dimension 1. Les relations de récurrence entre les polynômes d'Hermite et les approximations BKW (voir par exemple [Tao12] et [Olv97]) permettent d'écrire des asymptotiques ponctuelles des fonctions propres, qui sont exprimées en termes de fonctions d'Airy.

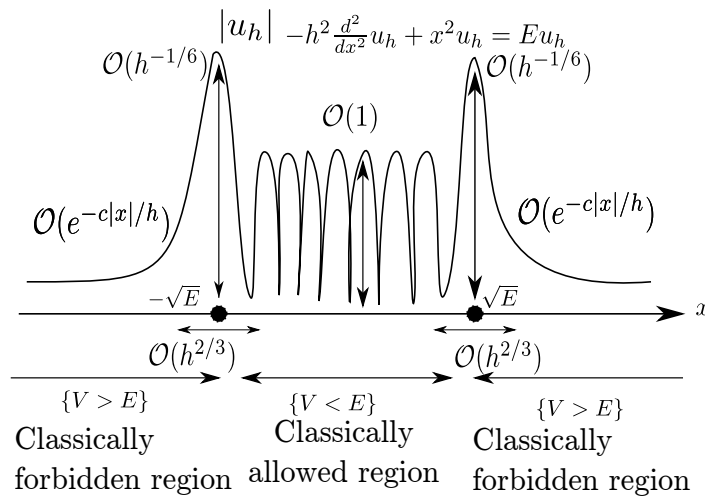


FIGURE 6 – Profil de la fonction propre de l'oscillateur harmonique scalaire associé à la valeur propre E .

Cet exemple met en évidence les différences de comportement de la fonction dans les trois régions différentes et le phénomène de concentration aux points de transition $\{x \in \mathbb{R} : x^2 = E\}$, qui n'existent pas dans le cas d'une variété compacte. Comme le montre la figure 6, la fonction propre u_h oscille avec une hauteur d'ordre ~ 1 dans le volume, décroît exponentiellement en $|x|$ et h dans la région interdite classique et se concentre aux deux bords $\pm\sqrt{E}$ avec une hauteur $\sim h^{-1/6}$ dans un voisinage de longueur $\sim h^{2/3}$. Ceci implique les estimées L^q suivantes :

$$\|u_h\|_{L^q(\mathbb{R})} \lesssim \begin{cases} 1 & \text{for } 2 \leq q \leq 4, \\ h^{-\frac{1}{6} + \frac{3}{2q}} & \text{for } 4 \leq q \leq \infty. \end{cases}$$

On voit tout l'intérêt de considérer toute la plage de valeurs de q puisque la concentration autour des points tournants n'est visible que pour de grandes valeurs de q ($q \geq 4$). De plus, on remarque que la norme L^q n'est pas sensible aux oscillations dans le cœur.

¹⁴traduction française pour *bulk*, suggérée par Julien Sabin. Frédéric Paulin par ailleurs m'a proposé la traduction adorable de *partie ventrue*.

¹⁵bien que cela soit un peu mal interprétable, puisque dans cette thèse nous ajoutons à cette définition une autre hypothèse sur les dérivées d'ordre un de V .

Il serait raisonnable de s'attendre à retrouver les mêmes estimées que celles de Sogge dans le cœur. Cette décroissance exponentielle des fonctions propres dans la région classiquement interdite est connue sous le nom de *estimées d'Agmon*. Celles-ci sont également appelées *estimées de Lithner-Agmon*. Lithner fournit en effet des bornes supérieures pour les potentiels confinants en 1964, et Agmon les prouva indépendamment à la fin des années soixante-dix, avec la décroissance exponentielle des fonctions propres de l'opérateur Schrödinger à N corps [Agm14].

On peut s'attendre à un comportement similaire en dimension supérieure et pour des potentiels confinants plus généraux. La même analogie n'est cependant pas possible afin d'obtenir des expressions exactes des fonctions propres dans le cadre de potentiels plus généraux. Il est néanmoins envisageable d'étudier les estimées L^q , de la forme (I.2) avec \mathbb{R}^d au lieu de M et $P - E$ à la place de $-h^2\Delta_g - 1$. Koch et Tataru [KT05] prouvèrent dans cette optique des estimations de L^q pour l'oscillateur harmonique en dimensions supérieures. Quelques années plus tard, les deux mêmes avec Zworski [KTZ07] les étendirent aux quasimodes microlocalisés d'opérateurs plus généraux, dans un cadre semi-classique. Dire qu'une fonction u_h est microlocalisée signifie que u_h est microlocalement négligeable en dehors d'un certain compact de l'espace des phases $\mathbb{R}_x^d \times \mathbb{R}_\xi^d$. Les propriétés de localisation dépendent du comportement du symbole p où la fonction u_h est microlocalisée. Ils proposent trois conditions sur les points (x_0, ξ_0) des ensembles de niveaux de l'hamiltonien classique $p_E(x, \xi) := p(x, \xi) - E$:

- ⊗ une condition assez générale (*gene*), énoncée dans l'hypothèse 2 :
qui demande seulement que la hessienne $\partial_\xi^2 p_E(x_0, \xi_0) = \partial_\xi^2 p(x_0, \xi_0)$ soit non dégénérée,
- ⊗ une condition de courbure (*Sogge*), énoncée dans l'hypothèse 3 :
qui nécessite en plus de la non-dégénérescence de $\partial_\xi^2 p(x_0, \xi_0)$, que $\nabla_\xi p_E(x_0, \xi_0) = \nabla_\xi p(x_0, \xi_0) \neq 0$ et que la deuxième forme fondamentale de $\{\xi \in \mathbb{R}^d : p_E(x_0, \xi) = 0\}$ soit non-dégénérée en $\xi = \xi_0$,
- ⊗ ou de points tournants (*TP*), énoncée dans l'hypothèse 4 :
outre la non-singularité de $\partial_\xi^2 p(x_0, \xi_0)$, elle demande la condition de non-dégénérescence $\nabla_x p_E(x_0, \xi_0) = \nabla_x p(x_0, \xi_0) \neq 0$.

Exemple. Commentons la signification de ces conditions lorsque $p(x, \xi) = |\xi|^2 + V(x)$ (une représentation intuitive de ces conditions en dimension $d = 1$ pour un potentiel de double puits V est décrite dans la figure 7) :

- ⊗ l'hypothèse (*gene*) est toujours satisfaite (en tout point de $\{(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d : |\xi|^2 + V(x) = E\}$),
- ⊗ l'hypothèse (*Sogge*) est toujours vérifiée pour les points tels que $p(x_0, \xi_0) = E$ et $V(x_0) < E$. La condition de courbure locale est toujours vraie car

$$\{\xi \in \mathbb{R}^d : p_E(x_0, \xi) = 0\} = \{\xi \in \mathbb{R}^d : |\xi|^2 = E - V(x_0)\}$$

est la sphère $(d - 1)$ -dimensionnelle de rayon $\sqrt{E - V(x_0)} > 0$. Celle-ci a bien une courbure positive.

- ⊗ l'hypothèse (*TP*) impose que $V(x_0) = E$, $\xi_0 = 0$ et $\nabla_x V(x_0) \neq 0$.

Rappelons la forme des estimations de Koch-Tataru-Zworski ci-dessous dans (I.19). Tous leurs énoncés sont résumés dans le tableau 2. Ces estimées se présentent comme suit.

Théorème ([KTZ07]). *Pour tout point $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ satisfaisant l'une des conditions ci-dessus : (cond) = (gene), (Sogge) ou (TP), il existe des exposants $s_{\text{cond}} \geq 0$ et $t_{\text{cond}} \geq 0$ associés à (cond) (représentés plus loin dans la figure 1.3 du chapitre 1)*

- un voisinage ouvert et borné $\mathcal{U} \times \mathcal{V}$ of (x_0, ξ_0) ,
- $h_0 > 0$,

tels qu'il existe, pour toute fonction $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ supportée dans $\mathcal{U} \times \mathcal{V}$,

- une constante multiplicative $C = C(d, \chi, h_0) > 0$,

telle que pour tous $2 \leq q \leq \infty$ et $u \in L^2(\mathbb{R}^d)$

$$\|\chi^w(x, hD)u\|_{L^q(\mathbb{R}^d)} \leq Ch^{-s_{\text{cond}}(q,d)} \left(\|u\|_{L^2(\mathbb{R}^d)} + \frac{1}{h} \|(P - E)u\|_{L^2(\mathbb{R}^d)} \right). \quad (\text{I.19})$$

Ici $\chi^w(x, hD)$ désigne la quantification de Weyl de χ .

Notons que les bornes ci-dessus restent vraies pour toutes quantifications de p et de χ . Cela ne fait varier que la constante multiplicative $C > 0$, pour laquelle, comme pour $h_0 > 0$, l'expression explicite n'est jamais donnée.

Condition	sur le symbole $p_E := p(x, \xi) - E$	Énoncés au chapitre 1
<i>générale</i>	(gene)=(Condition 2)	théorème IV.1
<i>de Sogge</i>	(Sogge)=(Condition 3)	théorème V.1
<i>de points tournants</i>	(TP)=(Condition 4)	théorème VI.1

TABLE 2 – Principaux énoncés des estimées de Koch-Tataru-Zworski.

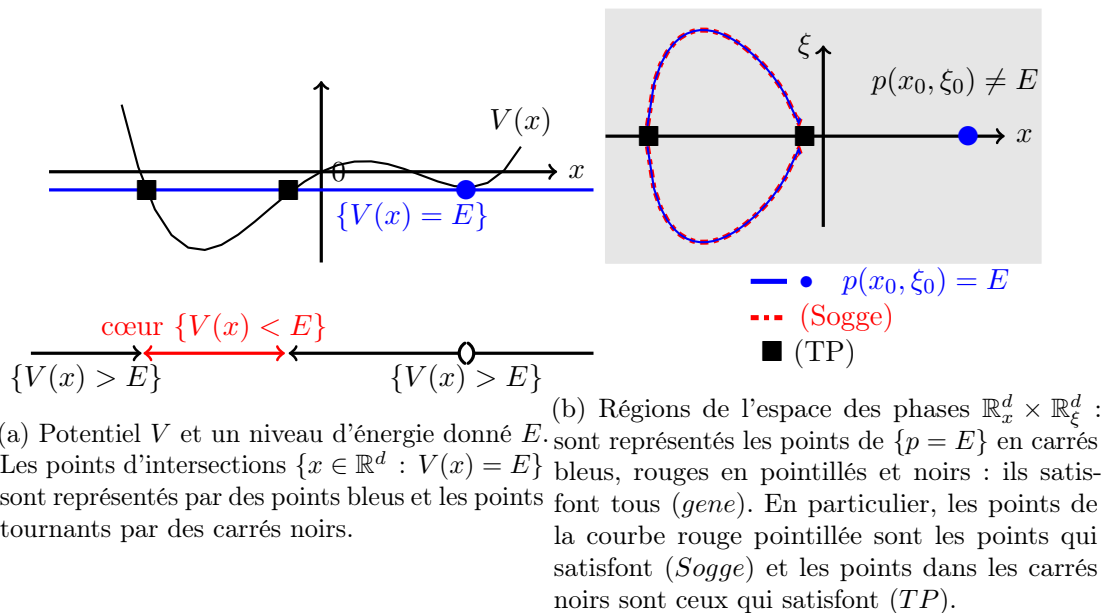


FIGURE 7 – Représentation des points (x_0, ξ_0) de l'espace des phases selon les différentes hypothèses (cond), pour $d = 1$, $p(x, \xi) = |\xi|^2 + V(x)$, une énergie $E > \min V$ et V le potentiel à double puits de la figure 7a.

Généralisation aux familles orthonormales de fonctions propres On considère à nouveau la question 4 dans le cadre euclidien avec un potentiel confinant. Il serait donc raisonnable

de s'attendre à ce que le phénomène de délocalisation apparaisse au niveau d'un certain nombre de particules confinées ensemble.

En reprenant l'exemple de l'oscillateur harmonique scalaire (représenté dans la figure 8), en fixant $\{u_h^j\}_{1 \leq j \leq N_h}$ une famille orthonormée de fonctions propres associées à des valeurs propres inférieures ou égales à E , la densité $\rho_h = \sum_{j=1}^{N_h} |u_h^j|^2$ peut être à nouveau exprimée asymptotiquement avec des fonctions spéciales grâce aux méthodes BKW. À normalisation près, nous trouvons asymptotiquement la densité de la loi du demi-cercle $\frac{1}{2\pi} \sqrt{(E-x^2)_+}$. Comme dans le cas d'un seul corps, ρ_h décroît exponentiellement dans la région classiquement interdite et une concentration de hauteur $\sim h^{-2/3}$ dans le voisinage de $h^{2/3}$ des points tournants. Cependant, la concentration autour de ces points est négligeable par rapport à la concentration dans le cœur qui se produit avec une hauteur de l'ordre de h^{-1} . Cela implique que toutes ses normes L^q sont du même ordre h^{-1} , ce qui traduit un phénomène de délocalisation du système des fonctions propres.

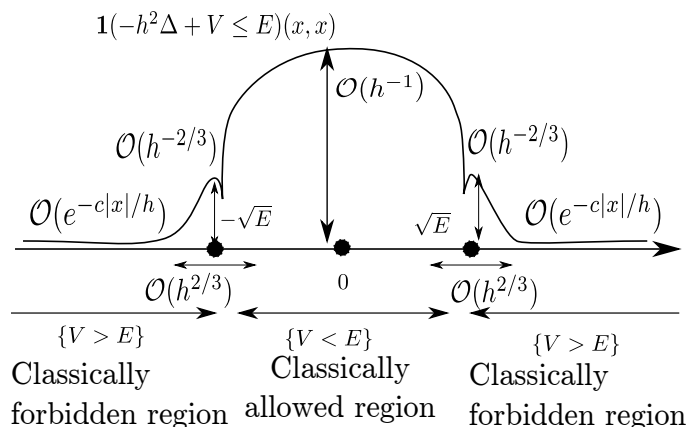


FIGURE 8 – Profil de ρ_h de l'oscillateur harmonique scalaire associé aux valeurs propres inférieures ou égales à E .

Le même comportement peut s'étendre dans les dimensions supérieures. Bien que Karadzhov [Kar89] ait fourni des asymptotiques ponctuelles du projecteur spectral pour les valeurs propres inférieures ou égales à E , les lois de Weyl ponctuelles pour les potentiels confinants généraux sont assez récentes et n'ont été obtenues jusqu'à présent que dans l'article de Deleporte et Lambert [DL21]. Ces derniers ont prouvé des estimations ponctuelles dans la diagonale (et hors diagonales) avec un reste optimal dans une échelle h dans le cœur et de $h^{2/3}$ autour de ses bords¹⁶. Notons la cohérence des asymptotiques exprimées en fonction des fonctions d'Airy et de ces échelles avec celles énoncées dans les articles de physique [DLDMS19].

I.3 Loi de Weyl avec des interactions

Nous nous sommes d'abord limités au cas sans interaction. Revenons maintenant au cas $w \neq 0$. Afin de traiter (partiellement) la question 3, nous introduisons dans cette section le cadre et les approximations mathématiques des systèmes quantiques en interaction. Nous commençons par écrire l'état de l'art pour les systèmes finis canoniques et, nous posons ensuite le problème dans le cadre grand-canonique.

Systèmes finis à N -corps Comme promis, revenons à notre système fermionique N avec le hamiltonien quantique P_N donné par la formule (I.5). Le modèle n'est pas toujours facile à

¹⁶aux points tournants, ce qui correspond aux carrés noirs dans la figure 7. La question des estimations autour des points dégénérés, comme les points critiques qui ne sont pas l'énergie de l'état fondamental (balle en bleu dans la figure), reste encore ouverte.

manipuler directement, en particulier pour calculer l'état fondamental et excité de P_N . C'est donc également le cas pour la question de la concentration. C'est la raison pour lesquelles diverses approximations (qui sont malheureusement non linéaires) sont employées pour traiter ce problème. Nous nous concentrerons sur l'approximation d'Hartree-Fock et l'approximation de Thomas-Fermi, qui ont fait l'objet de plusieurs travaux mathématiques : comme Lieb et Simon [LS77a, LS77b], Bach [Bac92] et Lions [Lio87]. La première est très utilisée en chimie quantique et la seconde moins, mais elle reste intéressante à étudier d'un point de vue théorique. Pour une introduction plus approfondie aux méthodes d'Hartree-Fock et Thomas-Fermi, nous renvoyons aux ouvrages suivants [CLBM06] et [LS10].

Le régime de champ moyen Nous considérons notre système fermionique dans un *régime à champ moyen*, où il y a beaucoup d'interactions entre les particules mais à une faible intensité. Dans cette approximation, avec laquelle nous espérons approcher les propriétés macroscopiques du système, l'interaction entre les particules se voit comme un potentiel effectif dépendant de la densité moyenne du champ généré par toutes les autres particules du système. Cela signifie que pour n'importe quel état $\Psi_N \in L_a^2(\mathbb{R}^{dN})$ avec des corrélations de faible intensité entre chaque particule

$$\left\langle \Psi_N, \sum_{1 \leq i < j \leq N} w(x^i - x^j) \Psi_N \right\rangle_{L^2(\mathbb{R}^{dN})} \simeq \frac{1}{2} \left\langle \Psi_N, \sum_{j=1}^N (w * \rho_{\Psi_N}(x^j)) \Psi_N \right\rangle_{L^2(\mathbb{R}^{dN})}.$$

La notation $w * \rho_{\Psi_N}(x^j)$ désigne ici l'opérateur de multiplication par

$$w * \rho_{\Psi_N}(x^j) := \int_{\mathbb{R}^d} w(x^j - y) \rho_{\Psi_N}(y) dy.$$

Remarque (Échelle de champ moyen et lien entre le système de fermions N et \hbar). On peut prendre $\lambda = 1/N$ pour équilibrer le terme avec l'énergie cinétique et potentielle. De plus, on aimerait également que le nombre de particules $N \rightarrow \infty$ lorsque $\hbar \rightarrow 0$. Pour être sûr d'avoir à nouveau tous les termes du même ordre à la limite semi-classique $\hbar \rightarrow 0$, il est pertinent de relier N et \hbar par la relation $\hbar = N^{-1/d}$. Le hamiltonien quantique P_N , défini dans (I.5), peut être réécrit

$$\begin{aligned} P_N &= \sum_{j=1}^N \left(-N^{-2/d} \Delta_{x^j} + V(x^j) \right) + \frac{1}{N} \sum_{1 \leq i < j \leq N} w(x^i - x^j) \\ &= \sum_{j=1}^N \left(-\hbar^2 \Delta_{x^j} + V(x^j) \right) + \hbar^d \sum_{1 \leq i < j \leq N} w(x^i - x^j). \end{aligned} \tag{I.20}$$

Matrices densité associées à une fonction d'onde Nous commençons par expliquer les avantages de l'adoption du formalisme des matrices densité. Nous rappelons pour tout état $\Psi_N \in L^2(\mathbb{R}^{dN})$, ses *matrices densité à un corps* et *deux corps*, respectivement désignées par $\gamma_{\Psi_N}^{(1)}$ et $\gamma_{\Psi_N}^{(2)}$, sont les opérateurs sur $L^2(\mathbb{R}^d)$ et $L^2(\mathbb{R}^{2d})$ associés aux noyaux intégraux

$$\forall x, y \in \mathbb{R}^d, \quad \gamma_{\Psi_N}^{(1)}(x, y) := N \int_{\mathbb{R}^{d(N-1)}} \overline{\Psi_N(y, x^2, \dots, x^N)} \Psi_N(x, x^2, \dots, x^N) dx^2 \dots dx^N$$

et

$$\begin{aligned} \forall x^1, x^2, y^1, y^2 \in \mathbb{R}^d, \quad \gamma_{\Psi_N}^{(2)}(x^1, x^2, y^1, y^2) &:= \frac{N(N-1)}{2} \int_{\mathbb{R}^{d(N-2)}} \overline{\Psi_N(y^1, y^2, x^3, \dots, x^N)} \times \\ &\quad \times \Psi_N(x^1, x^2, x^3, \dots, x^N) dx^3 \dots dx^N. \end{aligned}$$

Il existe également des *matrices densité à k corps* $\Psi_N^{(k)}$ de Ψ_N , agissant sur $L^2(\mathbb{R}^{kd})$, pour tout $k \in \{1, \dots, N\}$. La matrice densité à k corps $\Psi_N^{(k)}$ correspond à la distribution marginale de la particule k et est obtenue en intégrant les degrés de liberté des autres particules $N - k$.

Dans le cas avec interaction, on remarque d'abord que la valeur moyenne du système à un état $\Psi_N \in L_a^2(\mathbb{R}^{dN})$ est entièrement déterminée par ses matrices densité à un et deux corps du fait de la relation

$$\langle \Psi_N, P_N \Psi_N \rangle_{L^2} = \text{Tr}_{L^2(\mathbb{R}^d)} \left((-\hbar^2 \Delta + V) \gamma_{\Psi_N}^{(1)} \right) + \frac{1}{N} \text{Tr}_{L^2(\mathbb{R}^{2d})} \left(w \gamma_{\Psi_N}^{(2)} \right). \quad (\text{I.21})$$

Approximation effective d'Hartree-Fock Une approche variationnelle, l'approximation *Hartree-Fock*, consiste à manipuler uniquement les déterminants de Slater, que l'on appelle aussi *états d'Hartree-Fock*. L'idée de cette approximation est d'étudier, au lieu de $\langle \Psi_N, P_N \Psi_N \rangle$, la *fonctionnelle d'énergie d'Hartree-Fock*

$$\begin{aligned} \mathcal{E}_N^{\text{HF}}(\gamma) &:= \text{Tr}_{L^2(\mathbb{R}^d)} \left((-\hbar^2 \Delta + V) \gamma \right) \\ &+ \frac{1}{2N} \left(\iint_{\mathbb{R}^d \times \mathbb{R}^d} \rho_\gamma(x) \rho_\gamma(y) w(x-y) dx dy - \iint_{\mathbb{R}^d \times \mathbb{R}^d} |\gamma(x,y)|^2 w(x-y) dx dy \right), \end{aligned}$$

définie pour les opérateurs (suffisamment gentils) bornés γ sur $L^2(\mathbb{R}^d)$, où ρ_γ est la densité de γ . Ici, la partie cinétique de l'énergie est définie par

$$\begin{aligned} &\text{Tr}_{L^2(\mathbb{R}^d)} \left((-\hbar^2 \Delta + V) \gamma \right) \\ &:= \text{Tr}_{L^2(\mathbb{R}^d)} \left(\sqrt{-\hbar^2 \Delta + V + E} \gamma \sqrt{-\hbar^2 \Delta + V + E} \right) - E \int_{\mathbb{R}^d} \rho_\gamma(x) dx, \end{aligned}$$

pour $E > 0$ tel que $V + E$ est positif dans \mathbb{R}^d . Le second terme est appelé le *terme direct*

$$\iint_{\mathbb{R}^d \times \mathbb{R}^d} \rho_\gamma(x) \rho_\gamma(y) w(x-y) dx =: D_w(\rho_\gamma, \rho_\gamma)$$

et le dernier terme est appelé le *terme d'échange*

$$\iint_{\mathbb{R}^d \times \mathbb{R}^d} |\gamma(x,y)|^2 w(x-y) dx dy =: \text{Ex}_w(\gamma).$$

Son origine est entièrement quantique, c'est ce qui se produit lorsque deux particules de même nature sont permutées. Pour les fermions, elle prend en compte l'antisymétrie générée par le principe d'exclusion de Pauli.

La fonction d'onde Ψ_N est en effet un déterminant de Slater, associé à une base orthonormale $\{u_j\}_{1 \leq j \leq N}$ et est défini dans l'espace

$$\mathcal{S}_N := \{u_1 \wedge \dots \wedge u_N : u_j \in H^1(\mathbb{R}^d), \langle u_i, u_j \rangle_{L^2} = \delta_{ij} \quad \forall 1 \leq i, j \leq N\}.$$

On peut montrer que la valeur moyenne du système à un état $\Psi_N \in L_a^2(\mathbb{R}^{dN})$ est exprimée avec la matrice densité à un corps $\gamma_{\Psi_N}^{(1)}$.

$$\langle \Psi_N, P_N \Psi_N \rangle_{L^2} = \mathcal{E}_N^{\text{HF}}(\gamma_{\Psi_N}^{(1)}). \quad (\text{I.22})$$

De plus, $\gamma_{\Psi_N}^{(1)}$ est le projecteur orthogonal sur l'espace généré par $\{u_j\}_{1 \leq j \leq N}$

$$\gamma_{\Psi_N}^{(1)} = \sum_{j=1}^N |u_j\rangle \langle u_j|.$$

Il est plus exactement associé au noyau intégral

$$\gamma_{\Psi_N}^{(1)}(x, y) := \sum_{j=1}^N \overline{u_j(y)} u_j(x) \quad \text{et} \quad \rho_{\gamma_{\Psi_N}^{(1)}}(x) = \sum_{j=1}^N |u_j(x)|^2.$$

Soit e_N^{HF} l'énergie de l'état fondamental d'Hartree-Fock, donnée par le problème de minimisation sur les espaces des déterminants de Slater

$$e_N^{\text{HF}} := \inf \{ \langle \Psi, P_N \Psi \rangle_{L^2} : \Psi \in \mathcal{S}_N \}. \quad (\text{I.23})$$

D'une part, l'énergie fondamentale e_N est toujours bornée supérieurement par e_N^{HF} . La borne inférieure est plus délicate, mais s'obtient sous certaines conditions. En particulier, elle fut traitée par Lieb-Simon [LS77a], Bach [Bac92], Graf-Solovej [GS94] pour les systèmes coulombiens : $V(x) = -|x|^{-1}$ et $w(x) = |x|^{-1}$. Plus récemment, Fournais-Lewin-Solovej [FLS18] l'ont prouvé pour des potentiels plus généraux. Nous allons détailler cela ci-dessous. Dans ces cas, la méthode Hartree-Fock peut donner une bonne approximation de l'énergie fondamentale e_N .

Des résultats similaires existent quant à l'évolution des solutions de l'équation dépendante du temps (I.4), en supposant que la valeur initiale soit égale à un déterminant de Slater. De nombreux travaux [BGGM03, EESY04, RS09, BPS14, BJP⁺16] montrent que sa dynamique¹⁷ est fortement liée à celle de l'équation d'Hartree-Fock à la limite $N \rightarrow \infty$.

Remarque (Problème de minimisation généralisé d'Hartree-Fock). Le problème de minimisation de l'ensemble (I.23) peut être étendu à la dite *énergie Hartree-Fock généralisée*

$$e_N^{\text{gHF}} := \inf \{ \mathcal{E}_N^{\text{HF}}(\gamma) : \gamma \in \mathcal{K}_N \text{ et } \text{Tr}((-\Delta)\gamma) < \infty \},$$

sur l'ensemble des matrices densité des systèmes à N particules

$$\mathcal{K}_N := \{ \gamma \in \mathcal{B}(L^2(\mathbb{R}^d)) : \gamma = \gamma^*, \quad 0 \leq \gamma \leq 1, \quad \text{Tr}(\gamma) = N \}.$$

La condition $\gamma \leq 1$ vient exclusivement du principe d'exclusion de Pauli.

Dans certains cas, $e_N^{\text{HF}} = e_N^{\text{gHF}}$. C'est le cas par exemple lorsque l'interaction est répulsive $w \geq 0$ [Lie81].

Approximation effective de Thomas-Fermi L'approximation de Thomas-Fermi appartient aux modèles de la *Density Functional Theory* (DFT), qui ne dépendent que de la densité d'une particule et n'impliquent plus la fonction d'onde. L'idée est d'approcher l'état fondamental de l'hamiltonien à plusieurs corps (I.20) par la solution d'un problème de minimisation sur les densités $x \mapsto \rho(x)$

$$\inf \left\{ \mathcal{E}(\rho) : \rho \in L^1(\mathbb{R}^d, \mathbb{R}_+), \quad \int_{\mathbb{R}^d} \rho(x) dx = N \right\},$$

où \mathcal{E} est composé d'une fonctionnelle de densité cinétique F , de l'énergie potentielle externe $\rho \mapsto \int_{\mathbb{R}^d} \rho V$ et d'un terme d'interaction $\rho \mapsto \frac{1}{2} D_w(\rho, \rho)$:

$$\mathcal{E}(\rho) = F(\rho) + \int_{\mathbb{R}^d} V(x) \rho(x) dx + \frac{1}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} w(x-y) \rho(x) \rho(y) dx dy.$$

Historiquement, la plus simple et la plus ancienne DFT est l'approximation de Thomas-Fermi¹⁸, qui est apparue dans les années trente pour approcher la distribution d'un gaz électronique

¹⁷plus particulièrement celle de la matrice densité à un corps de l'état fondamental de P_N

¹⁸dont le nom provient des contributions indépendantes de Llewellyn Hilleth Thomas (1903-1992) [Tho27] et d'Enrico Fermi (1901-1954) [Fer27]

uniforme. Hohenberg et Kohn [HK64] justifèrent pour la première fois la validité de la DFT en 1964. Levy [Lev79] et Lieb [Lie02] posèrent plus tard sa formulation (nous nous référons à la revue de Lewin, Lieb et Seiringer [LLS19] pour plus d'exhaustivité sur le sujet).

L'approximation de Thomas-Fermi est associée à l'énergie de Thomas-Fermi \mathcal{E}^{TF} et définie par la fonctionnelle

$$F^{\text{TF}}(\rho) = \frac{d}{d+2} c_{\text{TF}} \int_{\mathbb{R}^d} \rho(x)^{1+2/d} dx,$$

où la constante c_{TF} est définie par

$$c_{\text{TF}} := 4\pi^2 \left(\frac{d}{|\mathbb{S}^{d-1}|} \right)^{2/d}.$$

Expliquons maintenant comment l'énergie de Thomas-Fermi apparaît dans l'approximation du problème de l'état fondamental de l'hamiltonien P_N (comme prouvé par Lieb et Simon [LS77b]). À la limite $N \rightarrow \infty$, la matrice densité à un corps de l'état fondamental de P_N peut se conduire comme la quantification de Weyl de la fonction d'espace de phase

$$m(x, \xi) = \mathbb{1} \left(|\xi|^2 \leq c_{\text{TF}} \rho(x)^{2/d} \right) \quad (\text{I.24})$$

où ρ_{TF} désigne un minimiseur de la fonctionnelle de Thomas-Fermi \mathcal{E}^{TF} . Remarquons que ce type de densités sur l'espace des phases sont en fait des minimiseurs de la *fonctionnelle d'énergie de Vlasov*

$$\mathcal{E}^{\text{Vlas}}(m) := \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |\xi|^2 m(x, \xi) dx d\xi + \int_{\mathbb{R}^d} \rho_m(x) V(x) dx + \frac{1}{2} D_w(\rho_m, \rho_m),$$

définie sur l'ensemble des fonctions intégrable sur l'espace des des phases¹⁹ $m : \mathbb{R}^d \times \mathbb{R}^d \rightarrow [0, 1]$ avec ρ_m définissant la densité spatiale

$$\rho_m(x) := \int_{\mathbb{R}^d} m(x, \xi) d\xi.$$

Pour une densité $\rho \geq 0$ donnée, les fonctionnelles \mathcal{E}^{TF} et $\mathcal{E}^{\text{Vlas}}$ sont reliées par la formule

$$\mathcal{E}^{\text{TF}}(\rho) = \mathcal{E}^{\text{Vlas}} \left(\mathbb{1} \left(|\xi|^2 \leq c_{\text{TF}} \rho(x)^{2/d} \right) \right).$$

Il est utile de mentionner une remarque équivalente au sujet de la dynamique temporelle comme pour l'approximation d'Hartree-Fock. Pour la même condition initiale de la forme (I.24), la solution²⁰ de (I.4) (via la transformation de Wigner) peut être approchée par la solution de l'équation classique, dite de Vlasov, lorsque $N \rightarrow \infty$ [NS81]. Nous pouvons donc également observer une sorte d'équivalence entre les dynamiques d'Hartree et de Vlasov. [APPP11, BPSS16].

En revenant au cadre du temps indépendant, les problèmes de minimisation d'Hartree-Fock et de Thomas-Fermi sont de plus profondément liés. En particulier, il est raisonnable d'approcher l'état fondamental d'Hartree-Fock par celui de Thomas-Fermi aux limites couplées de champ moyen et semi-classique $N \rightarrow \infty$ et $h \rightarrow 0$ ($h = N^{-1/d}$). C'est ce qu'ont réalisé Fournais, Lewin, Solovej [FLS18, Thm 1.1, 1.2, 1.3] en fournissant un lien entre le modèle d'Hartree-Fock N et l'énergie de Thomas-Fermi pour un potentiel V confinant ou non et un potentiel d'interaction w ,

¹⁹Une fois encore, la contrainte $m \leq 1$ provient du principe de Pauli.

²⁰la matrice densité à un corps de l'état fondamental dépendant du temps

avec des conditions appropriées. En particulier, ils ont déduit l'ordre principal de l'énergie de l'état fondamental e_N de P_N à la limite

$$\lim_{N \rightarrow \infty} \frac{e_N}{N} = e^{\text{TF}}(1),$$

avec $e^{\text{TF}}(1)$ désignant l'énergie fondamentale de Thomas-Fermi

$$\inf \left\{ \mathcal{E}^{\text{TF}}(\rho) : \rho \geq 0, \quad \rho \in L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d), \quad \int_{\mathbb{R}^d} V(x)\rho(x)dx < \infty, \quad \int_{\mathbb{R}^d} \rho(x)dx = 1 \right\}.$$

Ils ont également prouvé la convergence faible des matrices densité à k corps de l'état fondamental vers une valeur moyenne sur l'ensemble des minimiseurs de la fonctionnelle de Thomas-Fermi.

Systèmes grand-canoniques de particules On aimerait étudier à nouveau de grands systèmes de fermions en interaction dans un régime de champ moyen. D'une certaine manière, on souhaiterait avoir une description macroscopique de son état, qui permette la fluctuation du nombre de particules et de l'énergie du système. Le cadre canonique avec un nombre fixe de particules comme ci-dessous n'est plus approprié, puisque l'on fixe plutôt dans la loi de Weyl le potentiel chimique E , et on considère des intervalles d'énergie autour de ce paramètre fixe. C'est pourquoi nous adopterons le cadre *grand-canonique*.

Un ensemble grand-canonique est composé de \mathbb{N} systèmes finis identiques de particules avec un potentiel chimique fixe E , qui partage avec les autres les particules et l'énergie. Le système d'états grand-canoniques est décrit par l'*espace de Fock fermionique*

$$\mathcal{F} := \mathbb{C} \oplus \bigoplus_{N=1}^{\infty} L_a^2(\mathbb{R}^{dN}),$$

composé par des suites $\Psi = (\Psi_0, \Psi_1, \dots, \Psi_N, \dots)$ telles que $\Psi_N \in L_a^2(\mathbb{R}^{dN})$ pour tout $N \in \mathbb{N}^*$. L'espace \mathcal{F} est doté du produit scalaire

$$\langle \Psi, \Phi \rangle_{\mathcal{F}} = \sum_{N \in \mathbb{N}} \langle \Psi_N, \Phi_N \rangle_{L^2(\mathbb{R}^{dN})}.$$

De plus, l'hamiltonien à N corps devient

$$\mathbf{P} = \bigoplus_{N=1}^{\infty} P_N,$$

où P_N est le hamiltonien sur $L_a^2(\mathbb{R}^{dN})$ défini par

$$P_N := \sum_{j=1}^N (-\hbar^2 \Delta_{x^j} + V(x^j)) + \hbar^d \sum_{1 \leq i < j \leq N} w(x^i - x^j).$$

En définissant \mathcal{N} comme étant le nombre de particules

$$\mathcal{N} = \bigoplus_{N \in \mathbb{N}} N \mathbf{1}_{L_a^2(\mathbb{R}^{dN})},$$

l'énergie fondamentale $e_{\hbar, V, w}(E)$ de $\mathbf{P} - E\mathcal{N}$ associée à une énergie donnée E

$$e_{\hbar, V, w}(E) := \inf \text{Spec}(\mathbf{P} - E\mathcal{N})$$

se définit également en fonction des énergies de l'état fondamental des hamiltoniens canoniques $P_N - EN$.

$$e_{\hbar,V,w}(E) = \inf_{N \geq 0} e_{N,V,w}(E) =: \inf_{N \geq 0} \text{Spec}(P_N - EN).$$

Définissons par $e_{\hbar,V-E,w}^{\text{gHF}}$ l'énergie fondamentale grand-canonique de la fonctionnelle d'Hartree-Fock généralisée de \hbar associée au potentiel extérieur $V - E$ et au potentiel d'interaction w

$$\begin{aligned} e_{\hbar,V-E,w}^{\text{gHF}} &:= \inf_{\gamma \in \mathcal{K}} \left\{ \text{Tr}((-\hbar^2 \Delta + V - E)\gamma) + \frac{\hbar^d}{2} [D_w(\rho_\gamma, \rho_\gamma) - \text{Ex}_w(\gamma)] \right\} \\ &=: \inf_{\gamma \in \mathcal{K}} \mathcal{E}_{\hbar,V-E,w}^{\text{gHF}}(\gamma). \end{aligned} \quad (\text{I.25})$$

sur l'ensemble

$$\mathcal{K} := \left\{ \gamma \in \mathfrak{S}^1(L^2(\mathbb{R}^d)) : \gamma = \gamma^*, \quad 0 \leq \gamma \leq 1, \quad \text{Tr}((-\Delta)\gamma) < \infty \right\}.$$

Nous observons que lorsque $w \geq 0$, si $e_{\hbar,V-E,w}^{\text{gHF}}$ n'est pas borné inférieurement, l'énergie fondamentale $e_{\hbar,V,w}(E)$ ne peut pas l'être non plus, étant donné la relation

$$e_{\hbar,V,w}(E) \leq e_{\hbar,V-E,w}^{\text{gHF}}.$$

Dans le cas sans interaction $w = 0$, l'énergie fondamentale du système grand-canonique coïncide avec celle de la fonctionnelle \hbar -Hartree-Fock (c.f. (I.21) où n'intervient que le terme cinétique évalué dans la matrice densité à un corps de l'état fondamental)

$$\begin{aligned} e_{\hbar,V-E,w=0}^{\text{gHF}} &= \inf_{\gamma_h \in \mathcal{K}} \text{Tr}((-\hbar^2 \Delta + V - E)\gamma_h) = \text{Tr}((-\hbar^2 \Delta + V - E)_-) \\ &= \frac{|B_{\mathbb{R}^d}(0, 1)|}{(2\pi\hbar)^d(1 + d/2)} \int_{\mathbb{R}^d} [(E - V(x))_+]^{1+d/2} dx + o(\hbar^{-d}). \end{aligned}$$

En outre, la loi de Weyl intégrée (voir par exemple [Zwo12, Chap.6]) donne le premier terme de l'asymptotique semi-classique de la trace du minimiseur \hbar -Hartree-Fock $\gamma_h = \mathbb{1}(-\hbar^2 \Delta + V \leq E)$

$$\text{Tr}_{L^2(\mathbb{R}^d)}(\gamma_h) = \frac{|B_{\mathbb{R}^d}(0, 1)|}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} [(E - V(x))_+]^{d/2} dx + o(\hbar^{-d}).$$

Nous en déduisons alors les mêmes limites pour l'énergie et la matrice densité à un corps de l'état fondamental du système entier

$$\lim_{\hbar \rightarrow 0} \hbar^d e_{\hbar,V,w=0}(E) = \frac{|B_{\mathbb{R}^d}(0, 1)|}{(2\pi)^d(1 + d/2)} \int_{\mathbb{R}^d} [(E - V(x))_+]^{1+d/2} dx \quad (\text{I.26})$$

et

$$\lim_{\hbar \rightarrow 0} \hbar^d \text{Tr}_{L^2(\mathbb{R}^d)}(\gamma_{\Psi_h^{(1)}}) = \frac{|B_{\mathbb{R}^d}(0, 1)|}{(2\pi)^d} \int_{\mathbb{R}^d} [(E - V(x))_+]^{d/2} dx.$$

Question 6. Quel type d'asymptotique peut-on avoir en présence d'une interaction ?

II CONTRIBUTIONS ET ORGANISATION DE CETTE THÈSE

Nous présentons dans cette section nos principales contributions.

II.1 Résultats du chapitre 1 : asymptotiques pour le cas sans interaction

Le chapitre 1, qui fait l'objet de la prépublication [Ngu22], est consacré à la généralisation des estimations L^q microlocalisées de Koch-Tataru-Zworski [KTZ07] (sous la forme (I.19)) aux agrégats spectraux, de manière similaire aux bornes de Frank-Sabin [FS17b] (de la forme (I.17)) mais dans un cadre semi-classique. Nous commençons par exprimer ces estimations de densités sous deux points de vue complémentaires : le cadre semi-classique, qui implique la localisation dans l'espace des phases par rapport au paramètre semi-classique h (sections III, IV, V et VI) et le cadre spectral, où nous considérons les matrices densité dans les clusters spectraux, et nous étudions leurs estimées dans différentes régions de l'espace \mathbb{R}_x^d (Section VII). Dans la dernière section de ce chapitre (Section VIII), nous discutons de l'optimalité à un corps et à plusieurs corps des estimées L^q . Nous détaillons tout d'abord la construction de certains quasimodes spécifiques, qui saturent les bornes L^q à un corps dont la forme est bien connue dans la littérature. Ensuite, nous fournissons l'optimalité des estimations Sogge à plusieurs corps dans la zone classiquement autorisée.

Nous référençons nos résultats dans les tableaux 3 et 4.

Estimées microlocalisées (référéncées dans le tableau 3) En se donnant d'abord pour $d \geq 2$

- une observable classique p , qui peut être $p(x, \xi) = |\xi|^2 + V(x)$ et plus généralement dans la classe de symboles appropriée,
- et un niveau d'énergie $E \in \mathbb{R}$,

l'idée consiste à regarder la densité des opérateurs microlocalisés dans l'espace des phases près des points $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$, qui satisfont certaines hypothèses géométriques (*cond*) par rapport aux ensembles de niveaux d'énergie de $p_E(x, \xi) = p(x, \xi) - E$. Ils peuvent être des points hors de $\{p_E = 0\}$ ou dans l'ensemble de niveaux $\{p_E = 0\}$ sous l'une des trois conditions énoncées dans [KTZ07]. Soit $P := p^w(x, hD)$ la quantification de Weyl de p . Nous avons démontré le théorème suivant.

Théorème 1 (Théorèmes IV.2, V.2 et VI.2). *Pour tout point $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ qui satisfait l'une des conditions (*cond*) = (*gene*), (*Sogge*) ou (*TP*), il existe des exposants $s_{\text{cond}} \geq 0$, $t_{\text{cond}} \geq 0$ et $\alpha_{\text{cond}} \in [1, \infty]$ fixes associés à (*cond*) (résumés dans les figures 1.3, 1.10 et 1.4 du chapitre 1), et*

- un voisinage ouvert borné $\mathcal{U} \times \mathcal{V}$ de (x_0, ξ_0) ,
- $h_0 > 0$,

tels que pour tout $\chi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ supporté dans $\mathcal{U} \times \mathcal{V}$, il existe

- une constante multiplicative $C = C(d, \chi, h_0) > 0$,

pour laquelle on a pour tout $2 \leq q \leq \infty$, tout $h \in (0, h_0]$ et tout opérateur auto-adjoint positif γ sur $L^2(\mathbb{R}^d)$

$$\boxed{\begin{aligned} \|\rho_{\chi^w(x, hD)} \gamma \chi^w(x, hD)\|_{L^{q/2}(\mathbb{R}^d)} &\leq Ch^{-2s_{\text{cond}}(q, d)} \log(1/h)^{2t_{\text{cond}}(q, d)} \times \\ &\times \left(\|\gamma\|_{\mathfrak{S}^{\alpha_{\text{cond}}(q, d)}(L^2(\mathbb{R}^d))} + \frac{1}{h^2} \|(P - E)\gamma(P - E)\|_{\mathfrak{S}^{\alpha_{\text{cond}}(q, d)}(L^2(\mathbb{R}^d))} \right). \end{aligned}} \quad (\text{II.1})$$

Remarque. Une première remarque sur ce théorème est que les exposants satisfont à la condition $\alpha_{\text{cond}}(q, d) > 1$ pour tout $q \in (2, \infty]$ sauf $q = 2d/(d-2)$ pour $\text{cond} = \text{gene}$.

Comparons maintenant nos résultats par rapport aux estimations à un seul corps de Koch, Tataru et Zworski [KTZ07].

- À l'exception des valeurs de $t_{\text{cond}}(q, d)$ dans le cas où $\text{cond} = \text{gene}$ et $2(d+1)/(d-1) \leq q < 2d/(d-2)$ (voir figure 1.5), les exposants s_{cond} et t_{cond} sont les mêmes que dans [KTZ07]. On peut déduire les estimations à un corps (I.19) de (II.1), en prenant $\gamma = |u| \langle u \rangle$.
- Nous avons également prouvé des bornes microlocalisées pour la condition elliptique (*ellip*) : $p(x_0, \xi_0) \neq E$ (voir le théorème III.1) mais nous ne le mettons pas en évidence car ce résultat est plus trivial. Dans ce cas

$$\forall 2 \leq q \leq \infty, \quad (s_{\text{ellip}}(q, d), t_{\text{ellip}}(q, d), \alpha_{\text{ellip}}(q, d)) = \left(d \left(\frac{1}{2} - \frac{1}{q} \right) - 1, 0, \frac{q}{2} \right).$$

- On a seulement traité le cas (*TP*) sur les opérateurs de Schrödinger.

La preuve du théorème ci-dessus, prouvée dans une version duale, repose sur des estimées de Strichartz semi-classiques à plusieurs corps [Ngu22] que nous appliquons à un propagateur microlocalisé $U(t, r)$ dans un petit voisinage de (x_0, ξ_0) . En effet, comme dans le cas à un corps dans [KTZ07], l'esprit est de traiter un problème dépendant du temps

$$[hD_t - A_t(\mathbf{x}, hD_{\mathbf{x}})]u(t, \mathbf{x}) = hf(\mathbf{x}),$$

avec $n = n(d) \geq 1$ et $A_t = a_t(\mathbf{x}, hD_{\mathbf{x}})$ la quantification de Weyl de $a_t : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ qui dépend du symbole p . Ceci fait intervenir un propagateur, qui, lorsqu'il est microlocalisé dans un petit voisinage du point (x_0, ξ_0) , est approché grâce aux techniques de BKW de façon à satisfaire les bornes abstraites

$$\begin{cases} \sup_{r \in J} \|U(t, r)U(s, r)^*\|_{L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n)} & \lesssim 1, \\ \sup_{r \in J} \|U(t, r)U(s, r)^*\|_{L^1(\mathbb{R}^n) \rightarrow L^\infty(\mathbb{R}^n)} & \lesssim h^{-n/2}(h + |t - s|)^{-n/2}, \end{cases} \quad (\text{II.2})$$

Alors, pour tout intervalle compact $J \subset \mathbb{R}$, il reste à contrôler chaque terme de la formule de Duhamel associée (composée avec la microlocalisation)

$$u(t, \mathbf{x}) = U(t, 0)u(0, \mathbf{x}) + \int_0^t U(t, s)f(\mathbf{x})ds + \mathcal{O}(h^\infty)$$

grâce aux estimations de Strichartz. Comme leur nom l'indique, elles font intervenir le paramètre semi-classique h , mais au lieu de déduire des estimées en norme mixte $L_t^p L_{\mathbf{x}}^q$ à partir des bornes $L_{\mathbf{x}}^2 \rightarrow L_{\mathbf{x}}^2$ et $L_{\mathbf{x}}^1 \rightarrow L_{\mathbf{x}}^\infty$, l'esprit est de faire de même en tenant compte du cadre à plusieurs corps. Cela se traduit par la présence de normes de Schatten de $U(t, s)$.

Théorème 2 (Estimées de Strichartz sur les espaces de Schatten, théorème II.23). *Soient $n \geq 2$, un intervalle borné $J \subset \mathbb{R}$ et un propagateur $U(t, r)$ sur $L^2(\mathbb{R}^n)$ satisfaisant les estimées (II.2) pour tous $t, s \in \mathbb{R}$, il existe $C = C(n, J) > 0$ et des exposants $p = p(q, n) \geq 1$, $s = s(q, n) \geq 0$ et $t = t(q, n) \geq 0$ ²¹ tels que pour tout $2 \leq q \leq 2(n+1)/(n-1)$ et tout $W \in L_t^{p(q, n)} L_x^2(\mathbb{R}^{n+1})$*

$$\sup_{r \in J} \|WU(t, r)\|_{\mathfrak{S}^2(\frac{2q}{q+2})'(L_x^2(\mathbb{R}^n) \rightarrow L_{t,x}^2(\mathbb{R}^{n+1}))} \leq Ch^{-s(q, n)} \log^{t(q, n)}(1/h) \|W\|_{L_t^{p(q, n)} L_x^2(\mathbb{R}^{n+1})}.$$

On remarque que la preuve du théorème 2 est très générale puisqu'elle ne nécessite pas plus d'hypothèses que les estimations de l'énergie et de la désintégration TT^* (II.2). Elle s'appuie sur une interpolation complexe dans les espaces de Schatten, dans le même esprit que dans l'article de Frank-Sabin [FS17a].

²¹Nous ne détaillons pas leur expression pour le confort du lecteur.

Estimées des agrégats spectraux (référéncées dans le tableau 3) En se donnant,

- l'hamiltonien classique $p(x, \xi) = |\xi|^2 + V(x)$ avec un potentiel confinant $V : \mathbb{R}^d \rightarrow \mathbb{R}$,
- un niveau d'énergie $E \in \mathbb{R}$,

nous avons déduit des estimations microlocalisées ci-dessus, des bornes qui suivent un autre point de vue, spectral. Il consiste à considérer les fonctions propres associées aux valeurs propres dans des intervalles autour de E . De plus, au lieu d'examiner les objets situés dans l'espace des phases $\mathbb{R}_x^d \times \mathbb{R}_\xi^d$, nous les avons étudiés dans l'espace des positions au niveau de certaines régions $\Omega = \Omega_{V,E,\varepsilon} \subset \mathbb{R}_x^d$, qui ne dépendent que du potentiel V , de l'énergie E et d'une petite erreur $\varepsilon > 0$:

- ⊗ $\Omega = \mathbb{R}^d$,
- ⊗ dans la région classiquement interdite $\Omega = \{V > E + \varepsilon\}$,
- ⊗ dans la région classiquement autorisée $\Omega = \{V < E - \varepsilon\}$,
- ⊗ ou dans un voisinage des points tournants $\Omega = \{|V - E| < \varepsilon\}$ sous la condition supplémentaire²² que tous les points $x \in \mathbb{R}^d$ de $\{V = E\}$ doivent respecter la condition $\nabla_x V(x) \neq 0$.

En notant P la quantification de Weyl de p et par $\Pi_{E,h}$ le projecteur spectral sur la fenêtre spectrale $[E - h, E + h]$

$$\Pi_{E,h} := \mathbf{1}(P \in [E - h, E + h]),$$

nous avons montré les estimées suivantes dans les agrégats spectraux $\Pi_{E,h}(L^2(\mathbb{R}^d))$.

Théorème 3 (Théorème VII.2). *Pour l'une des régions Ω données ci-dessus, il existe*

- $h_0 = h_0(E, \varepsilon) > 0$,
- des exposants fixés $s \in [-\infty, \infty)$, $t \geq 0$ et $\alpha \in [1, \infty]$ (à définir ci-dessous),
- une constante multiplicative $C = C(\Omega, V, E, \varepsilon) > 0$,

telle que pour tout $2 \leq q \leq \infty$, tout $h \in (0, h_0]$ et tout opérateur γ_h tel que $\gamma_h = \Pi_{E,h}\gamma_h = \gamma_h\Pi_{E,h}$

$$\boxed{\|\rho_{\gamma_h}\|_{L^{q/2}(\Omega)} \leq Ch^{-2s(q,d)} \log(1/h)^{2t(q,d)} \|\gamma_h\|_{\mathfrak{S}^{\alpha(q,d)}(L^2(\mathbb{R}^d))},} \quad (\text{II.3})$$

avec

$$(s(q, d), t(q, d), \alpha(q, d)) = \begin{cases} (s_{\text{gene}}(q, d), t_{\text{gene}}(q, d), \alpha_{\text{gene}}(q, d)) & \text{pour tout } \Omega \subset \mathbb{R}_x^d, \\ (-\infty, 0, \infty) & \text{si } \Omega = \{V > E + \varepsilon\}, \\ (s_{\text{Sogge}}(q, d), t_{\text{Sogge}}(q, d), \alpha_{\text{Sogge}}(q, d)) & \text{si } \Omega = \{V < E - \varepsilon\}, \\ (s_{\text{TP}}(q, d), t_{\text{TP}}(q, d), \alpha_{\text{TP}}(q, d)) & \text{si } \Omega = \{|V - E| < \varepsilon\}. \end{cases}$$

Remarque. Comme on peut le voir sur la figure 7, les régions considérées $\Omega \subset \mathbb{R}_x^d$ sont des voisinages des points $x_0 \in \mathbb{R}^d$ tels que $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ obéissent à l'hypothèse (*cond*). Il est donc raisonnable de retrouver les exposants associés $s = s_{\text{cond}}$, $t = t_{\text{cond}}$ et $\alpha = \alpha_{\text{cond}}$.

Bien que nous ne sommes pas parvenus à obtenir des estimations de décroissance exponentielle équivalentes à celles d'Agmon dans la région classiquement interdite $\{V > E + \varepsilon\}$, notons que l'exposant $\alpha = \infty$ est le meilleur possible et que nous avons toujours une décroissance de la concentration en $\mathcal{O}(h^\infty)$. De plus, le théorème donne l'information que les pires concentrations sont *a priori* autour des points tournants, ce qui est cohérent avec la discussion sur l'exemple de l'oscillateur harmonique scalaire et ses estimées ponctuelles.

²²Nous excluons ici les points critiques $x_0 \in \mathbb{R}^d : V(x_0) = E$ tels que $\nabla_x V(x_0) = 0$, c'est-à-dire comme le point bleu de la figure 7.

Optimalité des estimées L^q à plusieurs corps (référéncées dans le tableau 4) Il reste la question de l'optimalité des bornes de Koch-Tataru-Zworski (et de nos bornes L^q) dans un certain régime de q . Les bornes saturées peuvent être reformulées dans l'énoncé suivant.

Théorème. *Pour un potentiel confinant donné $V : \mathbb{R}^d \rightarrow \mathbb{R}$ et une énergie fixée E avec des hypothèses à préciser, il existe*

- une erreur $\varepsilon > 0$,
- une suite d'énergies E_h , qui dépendent de V et E ,
- un quasimode $u_h \in L^2(\mathbb{R}^d)$ de $P - E_h$ ou une matrice densité γ_h de l'agrégat spectral $\mathbb{1}(P \in [E_h - h, E_h + h]) (L^2(\mathbb{R}^d))$,
- des exposants $s = s(q, d) \geq 0$ et $\alpha = \alpha(q, d) \geq 1$, qui sont égaux à s_{cond} et α_{cond} , apparaissant dans les théorèmes 1 et 3, à certains régimes de q (malheureusement pas pour tout q dans $[2, \infty]$),
- un ensemble $\Omega \subset \mathbb{R}_x^d$, qui peut dépendre de V , E_h , ε ,

et

- $h_0 > 0$ (resp. une sous-suite $\{h_n\}_{n \in \mathbb{N}} \subset \mathbb{R}_+^*$ avec $h_n \rightarrow 0$),
- $C = C(d, h_0, V, E, \varepsilon) > 0$,

tels que pour tout $h \in (0, h_0]$ (resp. le long de la sous-suite $h_n \rightarrow 0$) et pour tout $2 \leq q \leq \infty$

$$\boxed{\frac{\|u_h\|_{L^q(\Omega)}}{\|u_h\|_{L^2(\mathbb{R}^d)}} \geq Ch^{-s(d,q)}} \quad (\text{II.4})$$

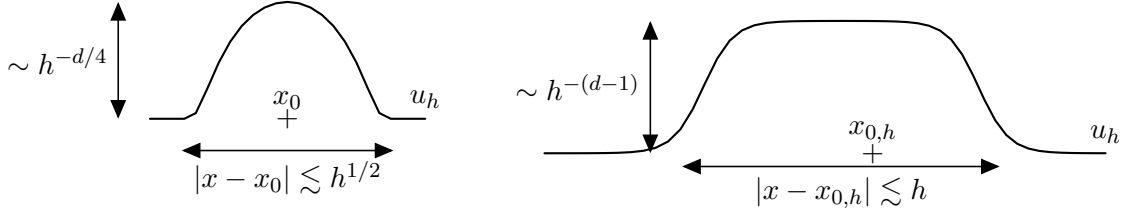
ou

$$\boxed{\|\rho_{\gamma_h}\|_{L^{q/2}(\Omega)} \geq Ch^{-2s(d,q)} \text{rank } \gamma_h^{1/\alpha(q,d)}}. \quad (\text{II.5})$$

Avant d'entrer dans les détails de ces résultats, donnons quelques commentaires sur le théorème ci-dessus.

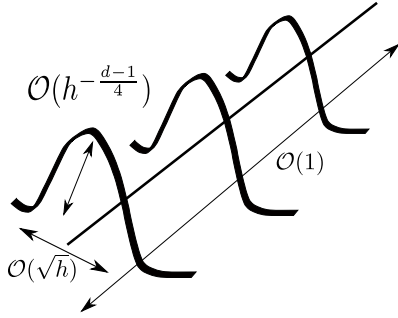
- Le paramètre $\varepsilon > 0$ sert ici à spécifier un rayon minimal, comme dans le théorème 3, afin de définir Ω comme un sous-ensemble du cœur $\{V < E_h - \varepsilon\}$ dépendant de h ou de prendre en compte les points tournants $\{V < E_h + \varepsilon\}$.
- Nous n'avons pas toujours l'expression exacte des suites E_h (nous prouvons seulement leur existence dans certains cas).

Optimalité one-body On construit dans la section VIII.1 du chapitre 1 des quasimodes de type zonal, des quasimodes de type faisceau gaussien et des quasimodes de type état fondamental gaussien, qui saturent les estimations de Koch-Tataru-Zworski dans certains régimes de q . Leur profil de concentration est représenté dans la figure 9 et les exposants optimaux dans la figure 1.16 du chapitre 1.

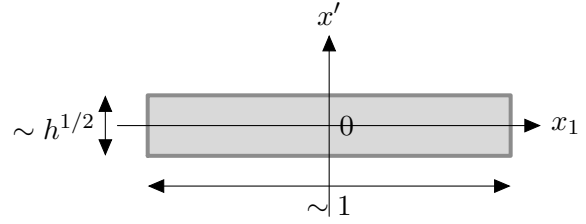


(a) De type état fondamental gaussien (c.f. figure 1.13).

(b) De type zonal (c.f. Figure 1.14).



(c) De type faisceau gaussien (Figure 1.15).



(d) Voisinage de concentration d'un quasimode de type faisceau gaussien.

FIGURE 9 – Concentration des quasimodes saturateurs.

Leur énoncé est le suivant.

Théorème 4 (Propositions VIII.1, VIII.2 and VIII.4). *En se donnant un potentiel confinant $V : \mathbb{R}^d \rightarrow \mathbb{R}$, un niveau d'énergie fixée E , et une erreur $\varepsilon > 0$ avec des hypothèses à préciser, il existe*

- une suite d'énergie E_h qui dépend de V et de E ,
- un quasimode $u_h \in L^2(\mathbb{R}^d)$ de $P - E_h$,
- des exposants $s_{\text{mass}} = s_{\text{mass}}(q, d) \geq 0$ et $s_{\text{conc}} = s_{\text{conc}}(q, d) \geq 0$,
- un ensemble $\Omega \subset \mathbb{R}_x^d$ qui peut dépendre de V , E_h , ε ,

et

- $h_0 > 0$ (resp. une sous-suite $\{h_n\}_{n \in \mathbb{N}} \subset \mathbb{R}_+^*$ avec $h_n \rightarrow 0$),
- $C_{\text{mass}} = C_{\text{mass}}(d, h_0, V, E, \varepsilon) > 0$ et $C_{\text{conc}} = C_{\text{conc}}(d, h_0, V, E, \varepsilon) > 0$,

telle que pour tout $h \in (0, h_0]$ (resp. le long de la sous-suite $h_n \rightarrow 0$) et pour tout $2 \leq q \leq \infty$

$$\boxed{\|u_h\|_{L^2(\mathbb{R}^d)} \leq C_{\text{mass}} h^{s_{\text{mass}}(q,d)}, \quad \|u_h\|_{L^q(\Omega)} \geq C_{\text{conc}} h^{-s_{\text{conc}}(q,d)}} \quad (\text{II.6})$$

Détaillons davantage nos résultats pour chaque cas. Dans les deux premiers cas, nous construisons des fonctions qui se concentrent à des points spécifiques que nous devons déterminer, à savoir $x_0 = x_0(h)$ (voir les figures 9a et 9b). Dans le dernier cas, la concentration se fait autour d'un segment selon une coordonnée euclidienne (voir les figures 9c et 9d).

- (a) *Quasimode de type état fondamental gaussien* (proposition VIII.1) : on impose la condition que E soit un minimum local de V et on fixe $x_0 \in \mathbb{R}^d$ un point où le minimum est atteint. Alors,

- on prend $\Omega = \mathbb{R}^d$,
- on définit u_h comme un oscillateur harmonique translaté à l'énergie fondamentale, normalisé dans L^2 et centré en x_0 avec une échelle de $h^{1/2}$, qui est alors un quasimode de $P - E$,

de sorte que $s_{\text{mass}}(q, d) = 0$ et $s_{\text{conc}}(q, d) = \frac{d}{2}(\frac{1}{2} - \frac{1}{q})$. Cette construction est bien connue (voir [Hel06, Chap.2] et [DS99, Chap.4]).

(b) *Quasimode de type zonal* (proposition VIII.2) : pour un V donné et une énergie $E > \min V$ avec une condition de non-platitude de V dans un voisinage de $\{V = E\}$, nous prouvons l'existence de suites

- $\{E_h\}_{h>0} \subset \mathbb{R}_+^*$ au voisinage E ,
- $\{x_{0,h}\}_{h>0} \subset \mathbb{R}^d$ dans le cœur $\{V < E_h - \varepsilon\}$,

de sorte que nous construisons u_h dans le cluster spectral de P associé à l'intervalle spectral $[E_h - E, E_h + h]$ qui est concentré en $x_{0,h}$

- $u_h(x) := \mathbb{1}(P \in [E_h - E, E_h + h])(x_{0,h}, x)$,
- et on considère le cœur $\Omega = \{V < E_h - \varepsilon\}$ dépendant de h .

Cela donne $s_{\text{mass}}(q, d) = (d - 1)/2$ et $s_{\text{conc}}(q, d) = d - 1 - d/q$. Cette construction est l'analogie de celle de [Sog17a, Chap.5].

(c) *Quasimode de type faisceau gaussien* (proposition VIII.4) : nous considérons $V(x) = |x|^2$, et nous définissons E comme un état excité de l'oscillateur harmonique scalaire de sorte qu'on a

- une fonction propre normalisée u_h dans L^2 , qui est un produit tensoriel d'un état excité associé à E et de $d - 1$ états fondamentaux gaussiens de l'oscillateur harmonique scalaire,
- la valeur propre $E_h = E + (d - 1)h$ de P associée à u_h ,
- et $\Omega = \{V(x) \leq E_h + \varepsilon\}$,

tels que $s_{\text{mass}}(q, d) = 0$ et $s_{\text{conc}}(q, d) = d(\frac{1}{2} - \frac{1}{q}) - \frac{1}{2}$. Cette construction est une version détaillée de [KT05, Sec.5.1].

On en déduit donc, sous les hypothèses précédentes, les bornes inférieures (II.4) sur le quotient de la norme L^q et L^2 à partir du théorème 4. Il suffit de prendre $C = C_{\text{conc}}/C_{\text{mass}}$ et $s = s_{\text{conc}} - s_{\text{mass}}$. En particulier, nous avons montré que dans les trois exemples ci-dessus (voir Figure 1.16 du chapitre 1)

- les quasimodes gaussiens de l'état fondamental (remarque 30 du chapitre 1) : l'exposant $s = s_{\text{gene}}$ pour $2 \leq q \leq 2d/(d - 2)$ est optimal,
- les quasimodes de type zonal (Remarque 32 du chapitre 1) : l'exposant $s = s_{\text{Sogge}} = s_{\text{gene}}$ pour le grand régime $2(d + 1)/(d - 1) \leq q \leq \infty$ est optimal,
- les quasimodes de type faisceau gaussien (remarque 37 du chapitre 1) : l'exposant $s = s_{\text{Sogge}}$ pour le bas régime $2 \leq q \leq 2(d + 1)/(d - 1)$ est optimal.

Il n'est pas certain que les estimations des points tournants dans le régime intermédiaire $q \in [2(d + 3)/(d + 1), 2d/(d - 2)]$ soient optimales et cela reste une question ouverte (voir [KT05, Sec. 5.3] pour un résultat intermédiaire).

Optimalité many-body Comme pour le cas à un corps, nous fournissons dans la section VIII.2 du chapitre 1 une matrice densité qui sature les estimations de Sogge dans la zone classiquement autorisée.

Théorème 5 (Optimalité à plusieurs corps dans le cœur, proposition VIII.5). *Soit un potentiel confinant $V : \mathbb{R}^d \rightarrow \mathbb{R}$ donné et une énergie fixe $E > \min V$ avec la condition de non aplatissement²³ autour de $\{V = E\}$. En notant par $\Pi_{E_h, h} := \mathbb{1}(P \in [E_h - h, E_h + h])$ le projecteur spectral, il existe*

- une erreur $\varepsilon > 0$,
- une suite E_h dans un voisinage de E ,
- $h_0 > 0$ (resp. une sous-suite $\{h_n\}_{n \in \mathbb{N}} \subset \mathbb{R}_+^*$ avec $h_n \rightarrow 0$),
- $C = C(d, h_0, V, E, \varepsilon) > 0$,

pour lesquels on a, pour tout $h \in (0, h_0]$ (resp. le long de la sous-suite $h_n \rightarrow 0$) et pour tout $2 \leq q \leq \infty$

$$\|\rho_{\Pi_{E_h, h}}\|_{L^q(\{V < E_h - \varepsilon\})} \geq Ch^{-(d-1)}.$$

Ce résultat implique la saturation des bornes (II.3) dans la région classiquement autorisée au rang maximal $\text{rank } \gamma_h = \text{rank } \Pi_{E_h, h}$ (voir la remarque 39 du chapitre 1).

Remarque. Pour l’instant, l’optimalité des estimées dans l’ensemble n’est pas connue pour les régimes intermédiaires ($1 < \text{rang } \gamma_h < \text{rang } \Pi_{E_h, h}$). Elle n’a pas encore été faite non plus pour les autres estimées des théorèmes 1 et 3. Ce serait une direction intéressante à explorer.

Estimées L^p microlocalisées (de la forme (II.1))		
Condition	sur le symbole $p_E := p(x, \xi) - E$	Résultat
<i>General</i>	(gene)=(Hypothèse 2)	Théorème IV.2
<i>Sogge</i>	(Sogge)=(Hypothèse 3)	Théorème V.2
<i>Points tournants</i>	(TP)=(Hypothèse 4)	Théorème VI.2
Estimées L^p des agrégats spectraux (de la forme (II.3))		
Région $\Omega_{V, E} \subset \mathbb{R}^d$		Exposant
	$\Omega_{V, E} = \mathbb{R}^d$	(gene)
Classiquement autorisée	$\Omega_{V, E} = \{V > E + \varepsilon\}$	Théorème VII.2
Classiquement interdite	$\Omega_{V, E} = \{V < E - \varepsilon\}$	
Au voisinage des points tournants	$\Omega_{V, E} = \{ V - E < \varepsilon\}$	

TABLE 3 – Résultats principaux des estimées L^p des matrices densité.

Un aperçu des principaux résultats du chapitre 1

²³la même hypothèse que pour la construction du quasimode de type zonal

Optimalité à un corps (de la forme (II.4))				
Type de concentration	Quasimodes saturateurs	Exposant	Régime de q	Résultats Fig. 1.16
<i>Autour de points</i> $x_0 = x_{0,h} \in \mathbb{R}^d$	État fondamental gaussien x_0 loc. min. of $V - E$	s_{gene}	$q \geq \frac{2d}{d-2}$	Prop. VIII.1 Fig. 1.13
	de type zonal au h -cœur $\{V < E_h - \varepsilon\}$	s_{sogge} $= s_{\text{gene}}$	$q \geq q_c = \frac{2(d+1)}{d-1}$	Prop. VIII.2 Fig. 1.14
<i>Autour d'un segment</i> (c.f. Figure 9d)	de type faisceau gaussien	s_{sogge}	$2 \leq q \leq q_c$	Prop. VIII.4 Fig. 1.15

Optimalité à plusieurs corps (de la forme (II.5))				
Région $\Omega_{V,E} \subset \mathbb{R}_x^d$	Densité saturatrice	Exposant	Régime de q	Résultat
Cœur : $\Omega_{V,E} = \{V < E_h - \varepsilon\}$	$\rho_{\Pi_{E_h,h}}$	(Sogge)	$2 \leq q \leq \infty$	Prop. VIII.5

TABLE 4 – Bornes L^q saturées (dans la section VIII du chapitre 1).

II.2 Résultats du chapitre 2 : asymptotiques pour le cas avec interaction

Le chapitre 2 est consacré à la version grand-canonique des limites fermioniques de Fournais, Lewin et Solovej [FLS18]. Cela permet de donner un élément de réponse à la question 6.

On a montré en particulier la convergence faible de la densité des *presque-minimiseurs*²⁴ de la fonctionnelle d'Hartree-Fock généralisée de \hbar (voir (I.15) dans le chapitre 2), i.e.

$$\mathcal{E}_{V-E,w}^{\text{HF}}(\gamma_{\hbar,\text{gHF}}) = e_{\hbar,V-E,w}^{\text{HF}} + o(\hbar^{-d})$$

vers un minimiseur ρ_{TF} de la fonction d'énergie de Thomas-Fermi.

Théorème 6 (Lois de Weyl faible et intégrée, théorèmes 2 et 3 du chapitre 2). *Soit $d \geq 1$. Soient*

- *un potentiel confinant*²⁵ $V : \mathbb{R}^d \rightarrow \mathbb{R}$,
- *un niveau d'énergie* $E \geq \min V$,
- *un potentiel d'interaction* $w : \mathbb{R}^d \rightarrow \mathbb{R}$ pair tel que $w \in L^{1+d/2}(\mathbb{R}^d) + L_\varepsilon^\infty(\mathbb{R}^d)$ ²⁶ et 'répulsif'²⁷.

Alors, il existe un minimiseur ρ_{TF} de l'énergie de Thomas-Fermi $\mathcal{E}_{V-E,w}^{\text{TF}}$ tel que le long d'une sous-suite décroissante $\{\hbar_n\}_n \subset \mathbb{R}_+^$ telle que $\hbar_n \rightarrow 0$*

$$\hbar^d \rho_{\gamma_{\hbar,\text{gHF}}} \rightarrow \rho_{\text{TF}} \quad \text{in } L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d), \quad (\text{II.7})$$

et alors,

$$\boxed{\hbar^d \int_{\mathbb{R}^d} \rho_{\gamma_{\hbar,\text{gHF}}}(x) dx \rightarrow \int_{\mathbb{R}^d} \rho_{\text{TF}}(x) dx.} \quad (\text{II.8})$$

Remarque. On retrouve dans le cas $w = 0$, pour la limite (II.8), la loi de Weyl intégrée énoncée dans (I.26), puisque

$$\rho_{\text{TF}}(x) = \frac{|B_{\mathbb{R}^d}(0,1)|}{(2\pi)^d} [E - V(x)]_+^{d/2}.$$

De plus, on a un meilleur résultat

²⁴il n'est pas évident que les minimiseurs existent

²⁵voir l'hypothèse 5 du chapitre 2

²⁶c.f. la définition I.1 du chapitre 2

²⁷au sens de l'hypothèse 6 ou de l'hypothèse I.13 pour les dimensions $d \in \{1, 2\}$ du chapitre 2

- puisque toutes les limites sont vraies sans passer par une sous-suite $\hbar_n \rightarrow 0$,
- et on a une limite plus forte que (II.7) avec la convergence ponctuelle $\hbar^d \rho_{\gamma_n}(x) \rightarrow \rho_{\text{TF}}(x)$ lorsque $V(x) < E$ (voir [DL21]).

Le théorème 6 peut être ainsi considéré comme une version de la loi de Weyl lorsque nous introduisons des interactions entre les particules.

Remarque. On pourrait avoir directement une convergence $\hbar \rightarrow 0$ sans passer par une sous-suite si on avait l'unicité de la limite, c'est-à-dire si le minimiseur de Thomas-Fermi est unique. C'est typiquement le cas sous l'hypothèse $\hat{w} \geq 0$, puisque dans ce cas la fonctionnelle $\mathcal{E}_{V-E,w}^{\text{TF}}$ est strictement convexe. Il n'est pas clair que cela soit également le cas avec notre condition (hypothèse 8 du chapitre 2)

$$\forall \rho \geq 0, \quad D_w(\rho, \rho) \geq 0.$$

On a en fait déduit ces convergences sur les densités de la preuve de la limite d'énergie Hartree-Fock grand-canonique généralisée.

Théorème 7 (Théorème 1 du chapitre 2). *Sous les mêmes hypothèses que ci-dessus²⁸, nous avons la convergence de l'énergie de l'état fondamental d'Hartree-Fock grand-canonique (défini dans (I.25))*

$$\boxed{\lim_{\hbar \rightarrow 0} \hbar^d e_{\hbar, V-E, w}^{\text{gHF}} = e_{V-E, w}^{\text{TF}}} \quad (\text{II.9})$$

vers l'énergie fondamentale de Thomas-Fermi

$$e_{V-E, w}^{\text{TF}} := \inf \left\{ \mathcal{E}_{V-E, w}^{\text{TF}}(\rho) : \rho \geq 0, \quad \rho \in L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d), \quad \int_{\mathbb{R}^d} V \rho < \infty \right\}.$$

Remarque. Nous avons prouvé des limites sur Hartree-Fock, mais nous pourrions également étudier l'hamiltonien total \mathbf{P} à plusieurs corps comme Fournais, Lewin, Solovej [FLS18]. On s'attendrait à avoir les limites (II.9) et (II.8) pour l'énergie $e_{\hbar, V, w}(E)$.

Mentionnons également un problème intéressant qui est une version ponctuelle de (II.8) dans le même esprit que [DL21]. Cette question est cependant loin d'être triviale, étant donnée la non-linéarité du modèle d'Hartree-Fock.

Conjecture. *La densité (du presque-optimiseur) de l'optimiseur $\gamma_{\hbar, \text{gHF}}$ de l'énergie \hbar -Hartree-Fock converge de manière ponctuelle vers un minimiseur Thomas-Fermi (toujours le long d'une sous-suite)*

$$\rho_{\gamma_{\hbar, \text{gHF}}}(x) \underset{\hbar \rightarrow 0}{\sim} \hbar^{-d} \rho_{\text{TF}}(x),$$

pour x dans le cœur $\{V_{\hbar}^{\text{eff}} < E\}$ associé au potentiel effectif $V_{\hbar}^{\text{eff}} := V + \hbar^d w * \rho_{\gamma_n}$, dont l'expression n'est pas explicite.

²⁸mais on peut autoriser à avoir $w \in L^p(\mathbb{R}^d) + L_{\varepsilon}^{\infty}(\mathbb{R}^d)$ avec p un peu plus général que $1 + d/2$, c'est-à-dire que $\max(d/2) < p < \infty$.

Chapter 0

Introduction (in English)

The aim of this thesis is to study systems of fermionic particles, and in particular their spatial concentration properties, in the semiclassical regime.

Chapter 1 is devoted to a study of densities for non-interacting particle systems. In Chapter 2 we pose the problem of pointwise asymptotics in this more difficult case of interacting systems.

In this introduction, we first present in Section I the physical motivations, the mathematical formalism that we will use to describe these fermionic systems and a state of the art. Then, my contributions are presented in Section II.

I GENERAL FRAMEWORK

Some references The reader interested in the basis on quantum mechanics can consult for instance the books [CTDL21, BDJ02]. We recommend for general readers the popularization books [BL14, Nav15, CC14a, CC14b] which also contain biographies of great figures in physics and juicy anecdotes mentioned in this introduction's footnotes. For references on spectral theory, we refer to the books [Dav95, LS10, Lew22]. As well, for starting references on semiclassical analysis, we refer to the books [DS99, Zwo12].

I.1 Physical motivations and objects at play

One can motivate the spectral study of Schrödinger operators in the semiclassical limit by their physical interpretation.

We consider quantum particles of mass $m > 0$ in the d -dimensional Euclidean space ($d \geq 1$), which are confined in an external force field that derives of a scalar potential $V : \mathbb{R}^d \rightarrow \mathbb{R}$. We consider *trapping potentials*, which means that $V(x) \rightarrow \infty$ as $|x| \rightarrow \infty$. A well-known example of trapping potential is the harmonic oscillator $V(x) = |x|^2$. There exist two different types of quantum particles: *bosons* and *fermions*, with different statistics.

- Bosons are the particles responsible for the interactions. They aggregate in the same quantum state to form condensates according to the *Bose-Einstein* statistics. Elementary known bosons are photons, gluons, Higgs bosons and bosons Z, W.
- Fermions are particles which make up matter. They obey notably the *Pauli exclusion principle*¹ which states that two fermions cannot occupy the same quantum state. There are elementary fermions, that include quarks and leptons (main examples are electrons, muons, neutrinos, tauons) and also composite fermions, the hadrons (such as protons and neutrons, that compose nucleus with a strong interaction).

¹stated in 1925 by Wolfgang Pauli (1900-1958) [Pau25] himself.

We will focus on fermionic particles. The statistics of fermionic particles are still an active research topic in theoretical physics, by quoting only papers of Dean, Le Doursal, Majumbar, Schehr and Smith [DLDMS15, DLDMS18, DLDMS19, DLDS⁺21, SDDL⁺20].

Quantum mechanical formalism At the end of the nineteenth century, experiments challenged classical physics, for which concepts are insufficient to describe objects at the atomic or subatomic scale, and gave rise to new ideas, with which the quantum physics we know today was built. For instance Max Planck (1858-1957) deduced the so-called Planck's law in 1900 [Pla01] from black body radiation spectrum and Albert Einstein (1879-1955) understood the photoelectric effect in 1905 [Ein05]. That led to the hypothesis of the energy *quantized*, word given by Einstein to name the fragmentation of energy in discrete pieces that he called '*quanta*', that he considered as particles. These fragments must be multiples of the *Planck constant*² $h \simeq 6,62 \times 10^{-34}$ J.s. We recall in this paragraph some postulates of non-relativistic quantum mechanics and their consequences.

Unlike classical mechanics, where the position-impulsion $(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d$ of the particle evolve according to Hamilton equation

$$\begin{cases} \dot{x}(t) &= \frac{1}{m}\xi(t), \\ \dot{\xi}(t) &= -\nabla V(x(t)), \end{cases} \quad (\text{I.1})$$

a quantum particule is described by a system of states in the Hilbert space $L^2(\mathbb{R}^d, \mathbb{C})$ and might be interpreted as *wave-functions*³. When a state $\psi(t)$, at time $t \geq 0$, is normalized on $L^2(\mathbb{R}^d)$, the number $|\psi(t, x)|^2$ can be interpreted as the density of the probability of presence⁴ at the position $x \in \mathbb{R}^d$. One would expect to find the particle at positions where the values of $|\psi(t)|^2$ are at their highest level. As well, the density of momenta probability $\xi \in \mathbb{R}^d$ is given by $|\hat{\psi}(t, \xi)|^2$. Here, we define the Fourier transform as

$$\forall \xi \in \mathbb{R}^d, \quad \hat{\psi}(t, \xi) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{-i\xi \cdot x} \psi(t, x) dx.$$

Let us explain why we will focus on the spectral study of a quantum observable, called Schrödinger operator. The time evolution of these states $\psi_h \in L^2(\mathbb{R}^d)$, for instance equal to $\psi^0 \in L^2(\mathbb{R}^d)$ at time $t = 0$, is described by the so-called *Schrödinger equation*⁵

$$\begin{cases} i\hbar \partial_t \psi_h(t, x) &= -\frac{\hbar^2}{2m} \Delta \psi_h(t, x) + V(x) \psi_h(t, x) \quad \text{at time } t > 0, \\ \psi_h(t = 0, x) &= \psi^0(x), \end{cases} \quad (\text{I.2})$$

where $\hbar := h/(2\pi)$ is the *reduced Planck constant*, and Δ is the Laplace operator $\Delta := \sum_{j=1}^d \partial_{x_j}^2$. The respective parts $-\frac{\hbar^2}{2m} \Delta$ and the multiplication by $V(x)$ correspond to the kinetic and the

²Paradoxically, Planck was disturbed by quantization principle and defended the continuity of matter. He could not admit that his law of radiation would lead to a break with classical mechanics. The tragedy of his life is that he became, in spite of himself, a great figure of the quantum revolution.

³Louis De Broglie (1892-1987) put forward the hypothesis of the wave-corpucle duality of matter in his 1923 thesis on the movement of free electrons [dB24]. This correspondence is a first kind of semiclassical limit.

⁴This probabilistic interpretation, sometimes called '*Copenhagen interpretation*', is due to Max Born (1882-1970) in a paper entitled *Quantum mechanics of collision processes* [Bor26] in 1926.

⁵Erwin Schrödinger (1887-1961) generalized De Broglie's approach a few years later to particles confined in an external potential by using mathematical tools for wave equations. His famous equation, that made his masterwork, first appeared in 1926 in [Sch26], which the translated title is *Quantization as an eigenvalue problem*. According to [BL14], despite his tumultuous romantic life and polyamorous relationships as numerous as its papers, he was said to accomplish his crucial work in a period of love exuberance. However, before dying of tuberculosis, Schrödinger was obsessed by giving a physical meaning to the states ψ_h . In particular he insisted on seeing $|\psi_h|^2$ as the density of the electric charge of the particle and rejected Born's probabilistic interpretation.

potential energies of the particle. The study of these states ψ_{\hbar} is reduced to the spectral study of the quantum Hamiltonian $P := -\frac{\hbar^2}{2m}\Delta + V(x)$ on $L^2(\mathbb{R}^d)$, called *Schrödinger operator*. It is enough to know its discrete spectrum (when it exists, since it is the case when V is confining: the self-adjoint operator P on $L^2(\mathbb{R}^d)$ has a compact resolvent and admits a sequence of eigenvalues that approaches $+\infty$), composed of its *eigenvalues* $\lambda_{\hbar}^j \in \mathbb{R}$: there exists a function $\psi_{\hbar}^j \neq 0$ such that $P\psi_{\hbar}^j = \lambda_{\hbar}^j\psi_{\hbar}^j$ and

$$\lambda_{\hbar}^1 \leq \lambda_{\hbar}^2 \leq \dots \leq \lambda_{\hbar}^j \xrightarrow{j \rightarrow +\infty} +\infty,$$

and an orthonormal basis of associated *eigenfunctions* $\{\psi_{\hbar}^j\}_{j \in \mathbb{N}} \subset L^2(\mathbb{R}^d)$. Indeed, knowing a solution u_{\hbar}^j of stationary Schrödinger equation at the level energy λ_{\hbar}^j , one can deduce solutions of (I.2) as linear combination of

$$\psi_{\hbar}^j(t, x) = e^{-i\lambda_{\hbar}^j t/\hbar} u_{\hbar}^j(x).$$

Notice that the modulus $\psi_{\hbar}^j(t, x)$ remains constant: $|\psi_{\hbar}^j(t, x)|^2 = |u_{\hbar}^j(x)|^2$ for any $t \geq 0$. Therefore, one can focus on the stationary solutions of the Schrödinger equation. Furthermore, as can be seen in the notation, the eigenfunctions and eigenvalues of P depend on the constant \hbar . In particular, the distance between the eigenvalues depends on \hbar (for instance when P is the harmonic oscillator, i.e. $V(x) = |x|^2$, this distance is proportional to \hbar).

The question is to understand more finely the spectral properties of P . The trick is to go to the *semiclassical limit*⁶, i.e. to make the reduced Planck constant \hbar approach 0. In this limit, the system behaves like in classical regime. This strategy allows to deduce information from the classical observable $p : \mathbb{R}_x^d \times \mathbb{R}_{\xi}^d \rightarrow \mathbb{R}$ which is the analogous of P . The classical-quantum continuity relation is called the '*correspondence principle*'⁷. In mathematics, it is called semiclassical or microlocal analysis. A crucial operation (nevertheless not unique), that is called *quantization*⁸, is the association of a smooth phase space function to linear self-adjoint operator in $L^2(\mathbb{R}^d)$.

Example. The position $(x, \xi) \mapsto x$ corresponds to the multiplication operator by x . As well, the impulsion $(x, \xi) \mapsto \xi$ is associated to the impulsion operator $\frac{\hbar}{i}\nabla_x$. As below, Schrödinger operators $P = -\frac{\hbar^2}{2m}\Delta + V(x)$ are associated to the classical Hamiltonian energy $p(x, \xi) = \frac{1}{2m}|\xi|^2 + V(x)$, which is the total energy of a classical particle trapped in a potential V , described by Hamilton equation (I.1).

A striking example of the correspondence principle is the *integrated Weyl law* (see for instance [Zwo12, Thm. 6.8]), which give asymptotics of the number $N_{\hbar}(I)$ of eigenvalues of P in a fixed interval $I \subset \mathbb{R}$ depending on the classical Hamiltonian $p(x, \xi) = \frac{1}{2m}|\xi|^2 + V(x)$

$$N_{\hbar}(I) = (2\pi\hbar)^{-d} \left| \{(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d : p(x, \xi) \in I\} \right| + \mathcal{O}_{\hbar \rightarrow 0}(\hbar^{-(d-1)}). \quad (\text{I.3})$$

Systems of several quantum particles Until now, we have not seen the difference between the bosonic or fermionic nature of particles. It comes into play when we are interested in systems of several indistinguishable particles. A system of N indistinguishable fermionic particles is described by wave-functions in the antisymmetric⁹ Hilbert subspace $L_a^2(\mathbb{R}^{dN}) = L_a^2((\mathbb{R}^d)^N)$ of

⁶Originally, to deduce the spectrum of the black-body radiation in 1900, Planck considered the furnace that contained black-bodies as discrete, bounded by grids of a certain length h that he made it tend to 0 in order to find a continuous space. The limit value is the one that bears his name $h \simeq 6,62 \times 10^{-34}$ J.s.

⁷stated by Niels Bohr (1885-1962) in 1923 [Boh24]. In particular, he calculated subatomic properties based on the postulates of classical mechanics.

⁸we refer to [DS99, Chap.7] or [Zwo12, Chap.4] for more details

⁹which distinguishes them from bosonic particles for which the states are symmetric and belong to

$$L_s^2(\mathbb{R}^{dN}) := \{\Psi_N \in L^2(\mathbb{R}^{dN}) : \Psi_N(x^1, \dots, x^N) = \Psi_N(x^{\sigma(1)}, \dots, x^{\sigma(N)}) \quad \forall \sigma \in \mathfrak{S}_N\}.$$

$L^2(\mathbb{R}^{dN})$

$$L_a^2(\mathbb{R}^{dN}) := \{\Psi_N \in L^2(\mathbb{R}^{dN}) : \Psi_N(x^1, \dots, x^N) = \varepsilon(\sigma) \Psi_N(x^{\sigma(1)}, \dots, x^{\sigma(N)}) \quad \forall \sigma \in \mathfrak{S}_N\}.$$

Here, $\varepsilon(\sigma)$ denotes the signature of a permutation $\sigma \in \mathfrak{S}_N$. The Pauli exclusion principle imposes that two fermions cannot occupy the same quantum state. This leads to the above space of antisymmetric states with respect to permutations of position variables. For any L^2 -normalized state Ψ_N , the quantity $|\Psi_N(x^1, \dots, x^N)|^2$ (resp. $|\hat{\Psi}_N(\xi^1, \dots, \xi^N)|^2$) can be interpreted as the probability density that the j^{th} particle number is at the position $x^j \in \mathbb{R}^d$ (resp. has the momentum $\xi^j \in \mathbb{R}^d$) for all $1 \leq j \leq N$. Moreover, setting

$$\rho_{\gamma_{\Psi_N^{(1)}}}(x) := N \int_{\mathbb{R}^{(N-1)d}} |\Psi_N(x, x^2, \dots, x^N)|^2 dx^2 \cdots dx^N,$$

its normalization $N^{-1} \rho_{\gamma_{\Psi_N^{(1)}}}(x)$ corresponds to the probability density of any particle of the system in the state Ψ_N to be at a position $x \in \mathbb{R}^d$. We will explain later where comes from the notation of the symbol $\gamma_{\Psi_N^{(1)}}$. Moreover, the quantum dynamic of states $\Psi_{N,h}$ is given by the Schrödinger equation in $L_a^2(\mathbb{R}^{dN})$ for an initial state $\psi_N^0 \in L_a^2(\mathbb{R}^{dN})$

$$\begin{cases} i\hbar \partial_t \Psi_{N,h}(t) = P_N \Psi_{N,h}(t) & \forall t > 0 \\ \Psi_{N,h}(t=0) = \psi_N^0, \end{cases} \quad (\text{I.4})$$

where P_N denotes the quantum Hamiltonian of the N particles of a same mass m , trapped in an external potential $V : \mathbb{R}^d \rightarrow \mathbb{R}$ with a pairing interaction potential $w : \mathbb{R}^d \rightarrow \mathbb{R}$, which is an even function,

$$P_N = \sum_{j=1}^N \left(-\frac{1}{2m} \hbar^2 \Delta_{x^j} + V(x^j) \right) + \lambda \sum_{1 \leq i < j \leq N} w(x^i - x^j). \quad (\text{I.5})$$

When $w \geq 0$, the interaction between particles is repulsive and when $w \leq 0$, it is attractive. The factor λ written before the interaction term is the coupling constant. In order to simplify the formulas, we assume in the rest of this thesis that the mass $m = 1/2$. The total energy of the system at a state Ψ_N is the average value $\mathcal{E}_N(\Psi_N) = \langle \Psi_N, P_N \Psi_N \rangle_{L^2}$ of the quantum energy P_N . The *ground state* of P_N (when it exists) corresponds to its minimal eigenvalue and can be obtained by the minimization of the variational problem

$$e_N = \inf \{ \langle \Psi, P_N \Psi \rangle_{L^2} : \Psi \in L_a^2(\mathbb{R}^{dN}) \text{ and } \|\Psi\|_{L^2(\mathbb{R}^{dN})} = 1 \}. \quad (\text{I.6})$$

It turns out that this minimization problem is not easy to solve in general.

Systems of free fermions When there is no interaction, i.e. $w = 0$, the advantage is the reduction of the dimension of the problem: instead of working with a wave function in $L^2(\mathbb{R}^{dN})$, one just has to consider N wave functions of $L^2(\mathbb{R}^d)$. Indeed, a natural uncorrelated L^2 -normalized eigenfunction $\Psi_{N,h}$ of P_N is a *Slater determinant*¹⁰ denoted $u_h^1 \wedge \cdots \wedge u_h^N$

$$\Psi_{N,h}(x^1, \dots, x^N) = \frac{1}{\sqrt{N!}} \sum_{\sigma \in \mathfrak{S}_N} \varepsilon(\sigma) \prod_{i=1}^N u_h^j(x^{\sigma(i)}) = \det \left((u_h^i(x^j))_{1 \leq i, j \leq N} \right), \quad (\text{I.7})$$

associated to an orthonormal family $\{u_h^j\}_{1 \leq j \leq N}$ of $L^2(\mathbb{R}^d)$. When the fermionic particles are free, the eigenfunctions of P_N are exactly Slater determinants. Therefore, it is also the case of

¹⁰This name is due to John Clarke Slater (1900-1976) for its formulation in [Sla29], although it was also introduced independently by Dirac [Dir26].

the ground state. Thus, the minimization problem (I.6) can be restricted on the space of Slater determinants associated to the orthonormal eigenfunctions of the one-body Schrödinger operator $P = P_1$. Moreover, given an orthonormal family $\{u_h^j\}_{1 \leq j \leq N} \subset L^2(\mathbb{R}^d)$, the density of the state $u_h^1 \wedge \cdots \wedge u_h^N$ is given by

$$\rho_{u_h^1 \wedge \cdots \wedge u_h^N}(x) = \sum_{j=1}^N |u_h^j(x)|^2.$$

The normalized quantity $N^{-1} \rho_{u_h^1 \wedge \cdots \wedge u_h^N}(x)$ represents the density of probability of N free fermionic particles at a point $x \in \mathbb{R}^d$. Each state associated to a particle indexed by j , is a normalized eigenfunction u_h^j , at a energy level set λ_h^j (where (λ_h^j, u_h^j) are eigenvalue-eigenfunction pairs of P). Notice that when we integrate $\rho_{u_h^1 \wedge \cdots \wedge u_h^N}$ on the whole space \mathbb{R}^d , it gives the number N of particles.

Notation. We recall here the Dirac notation $|u\rangle \langle v|$, for any $u, v \in L^2(\mathbb{R}^d)$: it denotes the operator on $L^2(\mathbb{R}^d)$

$$f \in L^2(\mathbb{R}^d) \mapsto \langle v, f \rangle_{L^2(\mathbb{R}^d)} u.$$

When $u = v$ and if u is L^2 -normalized, $|u\rangle \langle u|$ is the orthogonal projector on the space $\text{span}\{u\}$.

It should also be noted that $\rho_{u_h^1 \wedge \cdots \wedge u_h^N}$ is the upper-diagonal integral kernel of the orthogonal of the orthogonal projector on the N -dimensional span of the orthonormal family $\text{span}\{u_h^j\}_{1 \leq j \leq N} \subset L^2(\mathbb{R}^d)$

$$\gamma_{u_h^1 \wedge \cdots \wedge u_h^N} := \sum_{j=1}^N |u_h^j\rangle \langle u_h^j|.$$

This operator $\gamma_{u_h^1 \wedge \cdots \wedge u_h^N}$ is called the *one-body density matrix* of the system and $\rho_{u_h^1 \wedge \cdots \wedge u_h^N}$ its associated *density*. Let us mention that $\gamma_{u_h^1 \wedge \cdots \wedge u_h^N}$ is very useful to provide information on the system. We will return to the interpretation of this case in Section I.3.

Furthermore, for a fixed energy level set $E \in \mathbb{R}$, we can consider a family of eigenfunctions $\{u_h^j\}_{1 \leq j \leq N_{E,h}}$ associated to eigenvalues λ_h^j less than or equal to E . The size of this system $N_{E,h}$ depends on E and on the reduced Planck constant \hbar . Notably, $N_{E,h} \rightarrow \infty$ when $\hbar \rightarrow 0$. The asymptotics of $\rho_{u_h^1 \wedge \cdots \wedge u_h^{N_{E,h}}}$ is known in spectral theory under the name of *pointwise Weyl law*.

When we can integrate this formula on the whole space \mathbb{R}^d , it gives the asymptotics of the number $N_{E,h}$, which is the integrated Weyl law (I.3) for $I = (-\infty, E]$. We will discuss more deeply about the state of the art of Weyl laws in Sections I.2 and I.3.

We motivate now this PhD work by stating some more specific and naive questions.

Question 7. What type of spatial concentration phenomena can occur for eigenfunctions as $\hbar \rightarrow 0$?

Question 8. How to measure mathematically concentration or delocalization of eigenfunctions?

Question 9. What is the influence of the interaction on these concentration properties?

I.2 State of the art on concentration of quasimodes and eigenfunctions

Motivated by Questions 7 and 8, we give now an overview of mathematical results on eigenfunctions.

The concentration of eigenfunctions needs a parameter to be measured. There are two different regimes where it can be seen. On the one hand, there is the *semiclassical* point of view, which is

historically the older, as evidenced by with Brillouin-Kramers-Wentzel (BKW) approximation¹¹ of wave functions in dimension 1, know also as Liouville-Green (LG) method¹² (see for instance in [Olv97, Chap.6]). The idea is to look at $P = -\hbar^2\Delta + V$ at a fixed energy when the semiclassical parameter $\hbar \rightarrow 0$. On another hand, we can place ourselves in a *high frequency* frame, which means that we look at eigenfunctions of $P = -\Delta + V$ associated to an eigenvalue $\lambda \rightarrow \infty$. We have chosen to start with this regime which is technically simpler.

The problem of the concentration of high frequency eigenfunctions on smooth boundaryless compact Riemannian manifolds is an active research topic since the 1980s and extends to submanifolds (as described in [Sog15]). We therefore start introducing some partial literature of some related problems. This will allow us to make the link with our Euclidean case with a confining potential in a semiclassical regime. We will see why in most of time we have to lower our ambitions and restrict our estimates to generalizations of eigenfunctions called quasimodes or functions in spectral clusters.

	High frequency setting	Semiclassical setting
Full manifolds	[Sog85, Sog88, FS17b]	
Submanifolds	[Hu09]	[BZ16, BGT07, Tac10]
Euclidean case	[KT05]	[KTZ07, Ngu22]

Table 1 – A non-exhaustive overview of literature on L^q bounds on manifolds

Compact Riemannian manifolds without boundary Let us consider smooth compact Riemannian manifolds M without boundary of dimension $n \geq 2$ that we endow with a metric g . Let us denote by Δ_g the Laplace-Beltrami operator on (M, g) . We put ourselves in the case without potential.

The example of the standard round sphere Let us start focusing on the n -sphere for $n \geq 2$

$$\mathbb{S}^n := \{(x_1, x_2, \dots, x_{n+1}) \in \mathbb{R}^{n+1} : x_1^2 + x_2^2 + \dots + x_{n+1}^2 = 1\},$$

which has the merit of giving direct results on the exact eigenfunctions and an answer Question 7. We denote by $\Delta_{\mathbb{S}^n}$ the Laplace-Beltrami operator with respect to the metric induced by the Euclidean metric on \mathbb{R}^{n+1} . The spectrum of $-\Delta_{\mathbb{S}^n}$ is $\{\ell(\ell + n - 1)\}_{\ell \in \mathbb{N}}$. For each $\ell \in \mathbb{N}$, every associated eigenfunction to the eigenvalue $\ell(\ell + n - 1)$, with multiplicity $\binom{n+\ell}{\ell} - \binom{n+\ell-2}{\ell-2}$, is a restriction of harmonics polynomials of degree ℓ , called *spherical harmonics* of degree ℓ . Furthermore, the vector space spanned by the spherical harmonics is dense into $L^2(\mathbb{S}^n)$. We direct the reader to the following references [DX13, Sog85] for asymptotics on spherical harmonics.

First, let us consider the two-dimensional sphere, which is the more intuitive one and the easiest to represent geometrically. There is concentration of eigenfunctions of $-\Delta_{\mathbb{S}^2}$ in the two poles and around the equator (see Figure 1). We denote by $\{Y_\ell^m\}_{\ell \in \mathbb{N}, -\ell \leq m \leq \ell}$ the standard basis of L^2 -normalized spherical harmonics on \mathbb{S}^n

$$-\Delta_{\mathbb{S}^2} Y_\ell^m = \ell(\ell + 1) Y_\ell^m.$$

¹¹due to Léon Brillouin (1889-1969) [Bri26], Hendrik Anthony Kramers (1894-1952) [Kra26] and Gregor Wentzel (1898-1978) [Wen26] in the 1920s

¹²Joseph Liouville (1809-1882) [Lio36] and George Green (1793-1841) [Gre37] introduced this method one century before in 1837 for solutions of second order differential equations for the form $y''(x) = f(x)y(x)$, that are expressed under the form $y(x) \sim f(x)^{-1/4} \exp\left(\pm \int_{x_0}^x \sqrt{f(t)} dt\right)$, but it was relatively unnoticed.

On the one hand, the *zonal spherical harmonics* Y_ℓ^0 concentrates around the north pole $\mathbf{1} := (0, 0, 1)$ and the south pole $-\mathbf{1}$. More precisely, its density of probability $|Y_\ell^0|^2$ concentrates at these two extreme points with height ℓ in a region of size ℓ^{-1} (see Figure 2a). On the other hand, the highest weight spherical harmonics $Y_\ell^{\pm\ell}$, usually called *Gaussian beams*, concentrated around the equator $\gamma_{\text{equat}} := \{x \in \mathbb{S}^2 : x_3 = 0\}$: the densities of probability satisfy $|Y_\ell^{\pm\ell}|^2 \gtrsim \ell$ in a region of size $\ell^{-1/2}$ (see Figure 2b). The term 'Gaussian beam' comes from the Gaussian profile centered in the points of the curve γ_{equat} . It is of the form $Y_\ell^{\pm\ell}(x) = c\ell^{1/4}(x_1 \pm ix_2)^\ell$, which behave like an exponential. We can moreover speak of $\ell^{-1/2}$ width tubular concentration around the equator of these functions $\{Y_\ell^{\pm\ell}\}_{\ell \in \mathbb{N}}$.

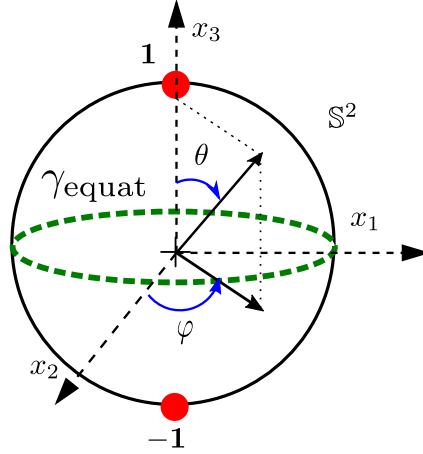


Figure 1 – Concentration regions in the 2-sphere: poles ± 1 and the equator γ_{equat}

Let us recall that the points of the sphere \mathbb{S}^2 can be parametrized by angular coordinates $(\theta, \varphi) \in [0, \pi] \times [0, 2\pi]$ (see Figure 1), through the relation

$$(x_1, x_2, x_3) \in \mathbb{R}^3 \iff (\theta, \varphi) \in [0, \pi] \times [0, 2\pi] \text{ with } \begin{cases} x_1 = \sin \theta \cos \varphi, \\ x_2 = \sin \theta \sin \varphi, \\ x_3 = \cos \theta. \end{cases}$$

We may see these saturation phenomena through the local asymptotics of the spherical harmonics

$$Y_\ell^m(\theta, \varphi) = e^{im\varphi} f_\ell^m(\theta)$$

with f_ℓ^m functions associated to Legendre polynomials. Indeed, it comes from the explicit (but painful to write) expression of Y_ℓ^m

$$\forall (\theta, \varphi) \in [0, \pi] \times [0, 2\pi], \quad Y_\ell^m(\theta, \varphi) = c_{\ell, m} e^{im\varphi} P_\ell^m(\cos \theta)$$

in terms of functions associated to Legendre polynomials

$$\forall x \in [-1, 1], \quad P_\ell^m(x) := \begin{cases} \frac{1}{2^\ell \ell!} (1-x^2)^{m/2} \frac{d^{\ell+m}}{dx^{\ell+m}} (x^2-1)^\ell & \text{for } 0 \leq m \leq \ell, \\ (-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_\ell^{-m}(x) & \text{for } -\ell \leq m \leq 0, \end{cases}$$

and the normalization constants

$$c_{\ell, m} = (-1)^m \sqrt{\frac{4\pi}{2\ell+1} \frac{(\ell+m)!}{(\ell-1)!}}.$$

For a function u which is concentrated in a volume V with a height L , one can deduce the bound for any $2 \leq q \leq \infty$

$$\|u\|_{L^q} \gtrsim L \times V^{1/q}.$$

This results in the L^q estimates, which holds for any $2 \leq q \leq \infty$

$$\| |Y_\ell^0|^2 \|_{L^{q/2}(\mathbb{S}^2)} \gtrsim \ell \times (\ell^{-2})^{2/q} = \ell^{1-\frac{4}{q}}. \quad (\text{I.8})$$

and

$$\| |Y_\ell^{\pm\ell}|^2 \|_{L^{q/2}(\mathbb{S}^2)} \gtrsim \ell^{1/2} \times (\ell^{-1/2})^{2/q} = \ell^{\frac{1}{2}-\frac{1}{q}}. \quad (\text{I.9})$$

These kinds of estimates are not very accurate, but they give a measure of concentration of the eigenfunction. Indeed, localization of a function u_ℓ can be measured informally by the explosion of the quotient $\| |u_\ell|^2 \|_{L^{q/2}(\mathbb{S}^2)} / \| |u_\ell|^2 \|_{L^1(\mathbb{S}^2)} \rightarrow \infty$ as $\ell \rightarrow \infty$ when q differs from 2. As well, its non-concentration can be seen when all L^q -norms are of the same order.

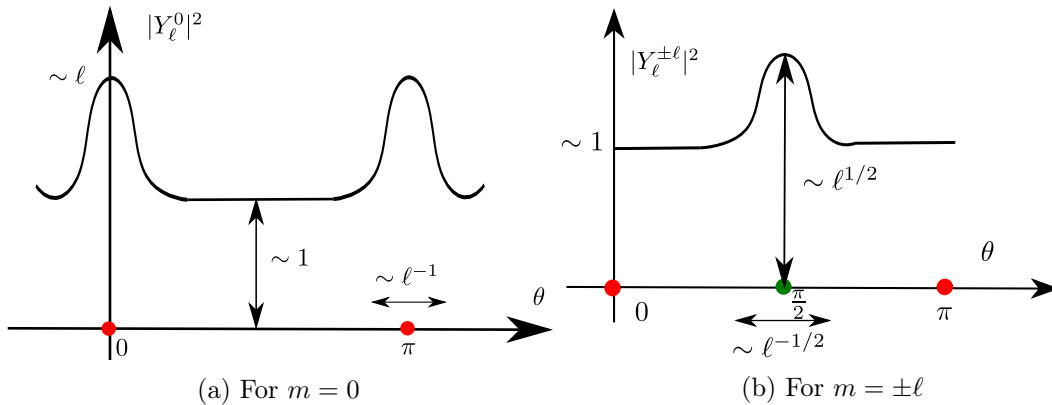


Figure 2 – Rough representation of the density $|Y_\ell^m|^2$ in \mathbb{S}^2 in function of the polar angle θ

- Is there a matching upper bound of (I.8) and (I.9) for any spherical harmonics Y_ℓ^m ?
- Moreover, do these concentration phenomena hold again for sphere in higher dimension, and do they extend to more general compact manifolds?

We can start to give a positive answer of the generalization of the concentration phenomena in higher dimension. Actually, for any dimension $n \geq 2$, the above high frequency concentration at poles $\pm \mathbf{1} = (0, \dots, 0, \pm 1)$ and around the equator curve $\gamma_{\text{equat}} := \{x \in \mathbb{S}^n : (x_3, \dots, x_{n+1}) = 0\}$ and L^q -estimates of spherical harmonics remain valid. As in the 2-sphere case, there exists a spherical harmonic, which concentrates at poles $\pm \mathbf{1}$ with a modulus of height $\ell^{\frac{n-1}{2}}$ in a region of width ℓ^{-1} (see Figure 4a), and another which modulus concentrates around the equator γ_{equat} with length $\ell^{\frac{n-1}{4}}$ in a region of radius $\ell^{-1/2}$ (see Figure 4b).

The answer the question about the upper bound of (I.8) and (I.9) is also yes. In his PhD thesis [Sog85], Sogge provided L^q bounds on eigenfunctions of $-\Delta_{\mathbb{S}^n}$. The statement is the following: for any $n \geq 2$, there exists $C > 0$ such that for any $\ell \in \mathbb{N}$, any eigenfunction u_ℓ associated to $\ell(\ell + n - 1)$ and any $2 \leq q \leq \infty$,

$$\| |u_\ell|^2 \|_{L^{q/2}(\mathbb{S}^n)} \leq C \ell^{2s_{\text{Sogge}}(q,n)} \| |u_\ell|^2 \|_{L^1(\mathbb{S}^n)}, \quad (\text{I.10})$$

where for any $n \geq 1$

$$s_{\text{Sogge}}(q, n) = \begin{cases} \frac{n-1}{2} \left(\frac{1}{2} - \frac{1}{q} \right) & \text{if } 2 \leq q \leq \frac{2(n+1)}{n-1} := q_c, \\ n \left(\frac{1}{2} - \frac{1}{q} \right) - \frac{1}{2} & \text{if } \frac{2(n+1)}{n-1} \leq q \leq \infty. \end{cases} \quad (\text{I.11})$$

Conversely, the exponent s_{Sogge} is sharp, since estimate (I.10) is saturated by Gaussian beams in low range $2 \leq q \leq q_c$ (that corresponds to Y_ℓ^m such $m = \pm\ell$ in dimension $n = 2$, with the L^q estimates (I.9))

$$\| |u_\ell|^2 \|_{L^{q/2}(\mathbb{S}^n)} \gtrsim \ell^{n-1} \times (\ell^{-1 \times n})^{2/q}$$

and by zonal spherical harmonics in large range $q_c \leq q \leq \infty$ (that corresponds to Y_ℓ^m for $m = 0$ when $n = 2$, with the L^q estimates (I.8))

$$\| |u_\ell|^2 \|_{L^{q/2}(\mathbb{S}^n)} \gtrsim \ell^{\frac{n-1}{2}} \times (\ell^{-1/2 \times (n-1)})^{2/q}.$$

That shows in particular two types of concentration: in a ball around points (here of radius $\sim \ell^{-2}$) and in a tube around geodesics (of width $\sim \ell^{-1/2}$).

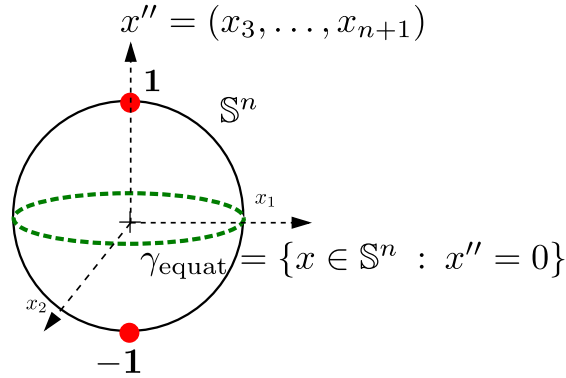


Figure 3 – Concentration regions in the n -sphere: at poles ± 1 and around equator γ_{equat}

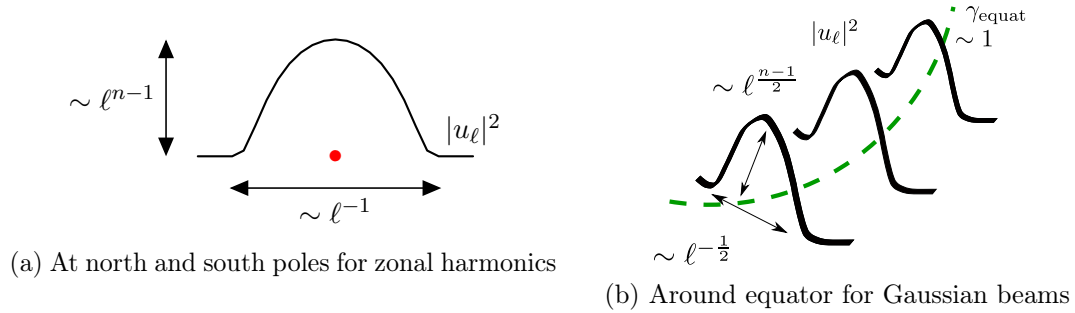


Figure 4 – Profiles of spherical harmonics concentration in \mathbb{S}^n

More general manifolds It turns out that the Sogge L^q -estimates (I.10) extend to all n -dimensional smooth boundaryless compact manifolds (M, g) (see the later Sogge's work [Sog88, Thm. 2.2]) for any eigenfunction u_λ of $-\Delta_g$ associated to the eigenvalue $\lambda > 0$

$$-\Delta_g u_\lambda = \lambda^2 u_\lambda, \quad (\text{I.12})$$

we have

$$\|u_\lambda\|_{L^q(M)} \leq C \lambda^{s_{\text{Sogge}}(q,n)} \|u_\lambda\|_{L^2(M)}, \quad (\text{I.13})$$

with $C > 0$ independent of u_λ and $\lambda > 0$, and all $2 \leq q \leq \infty$, and s_{Sogge} defined by (I.11). As we have seen earlier, these bounds are optimal and saturated when M is a sphere (since $\ell \sim \lambda$).

What can be said about the optimality of Sogge's estimates for eigenfunctions (I.13) in other smooth compact manifolds? Actually, there are several compact manifolds with particular

geometries where the exponent of Sogge is not optimal and can be improved in some regimes of q . Notably, there are eigenfunctions that saturate better bounds.

- A first example, due to Zygmund [Zyg74] in 1974, is the 2-dimensional torus $\mathbb{T}^2 := \mathbb{R}^2/\mathbb{Z}^2$ for the exponent $q = 4$

$$\|u_\lambda\|_{L^4(\mathbb{T}^2)} \leq C \|u_\lambda\|_{L^2(\mathbb{T}^2)}.$$

Then, it is generalized in higher dimension $n \geq 3$ by Bourgain [Bou93] for all $2 \leq q \leq 2n/(n-1)$ and all $\varepsilon > 0$

$$\|u_\lambda\|_{L^q(\mathbb{T}^n)} \leq C \lambda^\varepsilon \|u_\lambda\|_{L^2(\mathbb{T}^n)}.$$

- We mention also manifolds with negative curvature, for which we will come back later.

Therefore, a challenge is to find, for a given M , the optimal exponent s .

However, Sogge estimates remain true for generalizations of eigenfunctions, which are *quasimodes* of $-\Delta_g - \lambda^2$: which are L^2 -normalized functions u_λ such that

$$\|-\Delta_g u_\lambda - \lambda^2 u_\lambda\|_{L^2(M)} \lesssim \lambda \|u_\lambda\|_{L^2(M)}, \quad (\text{I.14})$$

or functions in *spectral clusters* of $-\Delta_g$ for any $\lambda > 0$: that means functions such that

$$\mathbf{1}(-\Delta_g \in [\lambda^2, (\lambda+1)^2]) u_\lambda = u_\lambda, \quad (\text{I.15})$$

i.e. linear combinations of eigenfunctions of $-\Delta_g$ associated with eigenvalues in intervals $[\lambda^2, (\lambda+1)^2]$. In these cases, we must add another control term $\lambda \|(-\Delta_g - \lambda^2)u_\lambda\|_{L^2(M)}$ to the right-hand side of (I.14):

$$\|u_\lambda\|_{L^q(M)} \leq C \lambda^{s_{\text{Sogge}}(q,n)} (\|u_\lambda\|_{L^2(M)} + \lambda \|(-\Delta_g - \lambda^2)u_\lambda\|_{L^2(M)}). \quad (\text{I.16})$$

Actually, Sogge himself [Sog88] proved (I.16) and constructed quasimodes which saturate them for any compact manifold M . Therefore, the power s_{Sogge} is optimal for any compact manifold M . Besides, it is possible to have again the concentration phenomenon around points and geodesics of any compact manifolds of normalized functions (see Figure 5). To do so, the idea is to generalize, as in [Sog17a, Thm. 5.1.1], zonal spherical and Gaussian beams spherical harmonic:

- Zonal-type quasimodes, which concentrate at a point (see for instance Figure 5a). They can be used to saturate the bounds in the large range $q \geq q_c := 2(n+1)/(n-1)$.
- Gaussian beams-type quasimodes, which concentrate along a curve with a gaussian profile transversally (see for instance Figure 5b). They are mostly used to saturate the bounds for low range $q \leq q_c$. These kinds of construction have been first developed by Ralston [Ral76, Ral77].

These approximations are relevant since Canzani and Galkowski [CG21] proved that eigenfunctions that saturate (I.14) behave as zonal quasimodes for $q \geq q_c$, and Blair and Sogge [BS15, BS17] showed that the saturating eigenfunction are similar to Gaussian beams for $q \leq q_c$. We emphasize that Gaussian beams-type quasimodes are more recently generalized under the name of *geodesic beams* methods in several works of Canzani and Galkowski (quoting only [CG21, CG20a]).

Moreover, it is worth mentioning that the improvements of Sogge estimates [Sog88] have been the subject of many works under some geometric assumptions. Here is a non-exhaustive selection of improvements for manifolds with negative curvature

- for large range $q > q_c$: [HT15, HR16, SZ02, Sog17b, BS19],
- for low range $q < q_c$: [BS17, BS18],
- for critical $q = q_c$: [Sog16].

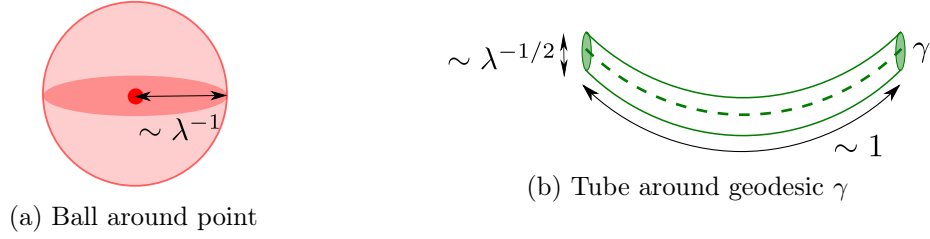


Figure 5 – Two different neighborhoods of concentration

Generalization to orthonormal families of eigenfunctions and Weyl laws More recently, Frank and Sabin [FS17b] generalized Sogge L^q estimates in compact manifolds M to orthonormal systems of functions in spectral clusters $\Pi_\lambda(L^2(M))$, denoting by Π_λ the spectral projector $\mathbb{1}(-\Delta_g \in [\lambda^2, (\lambda+1)^2])$. They provided, for any finite orthonormal family $\{u_j\}_{1 \leq j \leq N}$ of $\Pi_\lambda(L^2(M))$ and for any $\{\nu_j\}_{1 \leq j \leq N} \subset \mathbb{C}$, $L^{q/2}$ bounds of the density for all $2 \leq q \leq \infty$

$$\rho_\lambda(x) = \sum_{j=1}^N \nu_j |u_j(x)|^2.$$

A first naive approach is to deduce from the one-function estimates (I.16) and the triangle inequality

$$\|\rho_\lambda\|_{L^{q/2}(M)} \leq C\lambda^{2s_{\text{Sogge}}(q,n)} \left(\sum_{j=1}^N |\nu_j| \right).$$

Note that ρ_λ can be written as the density of the self-adjoint bounded operator of rank N

$$\gamma_\lambda = \sum_{j=1}^N \nu_j |u_j\rangle \langle u_j|,$$

and denoting by $\|\cdot\|_{\mathfrak{S}^\alpha(L^2(M))}$ the Schatten norm given by the formula (see Definition II.19 in Chapter 1) for $\alpha \geq 1$

$$\|\gamma\|_{\mathfrak{S}^\alpha(L^2(M))} = \text{Tr}_{L^2(M)}[(\gamma^* \gamma)^{\alpha/2}]^{1/\alpha},$$

the bound deduced by triangle inequality becomes

$$\|\rho_\lambda\|_{L^{q/2}(M)} \leq C\lambda^{2s_{\text{Sogge}}(q,n)} \|\gamma_\lambda\|_{\mathfrak{S}^1(L^2(M))}.$$

It turns out that the exponent $\alpha = 1$ of the Schatten norm of γ_λ can be improved: $\alpha > 1$ in some regimes of q . This has been shown by Frank and Sabin, whose main result is stated under the form.

Theorem ([FS17b, Thm.2]). *For any self-adjoint operator γ_λ in $L^2(M)$ such that $\gamma_\lambda = \gamma_\lambda \Pi_\lambda = \Pi_\lambda \gamma_\lambda$ and any $2 \leq q \leq \infty$*

$$\|\rho_\lambda\|_{L^{q/2}(M)} \leq C\lambda^{2s_{\text{Sogge}}(q,n)} \|\gamma_\lambda\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,n)}(L^2(M))}, \quad (\text{I.17})$$

where the exponent $\alpha_{\text{Sogge}} \in [1, \infty]$ is given by the formula (which is (V.3) in Chapter 1)

$$\alpha_{\text{Sogge}}(q, n) := \begin{cases} \frac{2q}{q+2} & \text{if } 2 \leq q \leq \frac{2(n+1)}{n-1}, \\ \frac{q(n-1)}{2n} & \text{if } \frac{2(n+1)}{n-1} \leq q \leq \infty. \end{cases}$$

It is important to underline that dealing with several functions adds to the concentration exponent s a new parameter $\alpha \geq 1$, which takes into account the complex constants ν_j and the family size $N = \text{rank } \gamma_\lambda$, which sometimes depends on the parameter λ (for instance when we consider an orthonormal basis of the whole spectral cluster). Remark that

- The estimates above coincide with the Sogge estimates (I.16) when the family is reduced to a single function $u_\lambda \in L^2(M)$ of the spectral cluster $\Pi_\lambda(L^2(M))$ by injecting $\gamma_\lambda = |u_\lambda\rangle \langle u_\lambda|$ in (I.17).
- The other extreme case covered is the entire spectral cluster: $N = \dim \Pi_\lambda(L^2(\mathbb{R}^d)) = \text{rank } \Pi_\lambda$, for instance with $\gamma_\lambda = \Pi_\lambda$.
- Moreover, they take also in account the intermediary case: all $\gamma_\lambda = \gamma_\lambda \Pi_\lambda = \Pi_\lambda \gamma_\lambda$ with $1 \leq \text{rank } \gamma_\lambda \leq \text{rank } \Pi_\lambda$.

A natural question is the sharpness of the bounds (I.17). What about the optimality of the new exponent α_{Sogge} ? Do exist operators γ_λ that saturate the bounds (I.17)?

Furthermore, keeping in mind our original motivation on particles' concentration, the question below naturally arises.

Question 10. Can adding several functions change the concentration phenomena present in one-body?

This question is relevant since we recall that fermions cannot occupy the same quantum state. One could therefore expect to observe a non-concentration phenomena for the whole spectral cluster.

Before replying to these questions in the setting of compact manifolds, let us explain their natural link with Weyl laws. Let us consider the extremal case of the entire spectral cluster $\Pi_\lambda(L^2(M))$ with $\gamma_\lambda = \Pi_\lambda$. The pointwise asymptotics of the density ρ_{Π_λ} is given by the pointwise Weyl law. Actually, Π_λ can be expressed by an orthonormal basis of $-\Delta_g$'s eigenfunctions $\{u_\lambda^j\}_{1 \leq j \leq \dim(E_\lambda(L^2(M)))}$ with associated eigenvalues contained in $[\lambda^2, (\lambda + 1)^2]$

$$\Pi_\lambda = \sum_{j=1}^{N_\lambda = \dim(E_\lambda(L^2(M)))} |u_\lambda^j\rangle \langle u_\lambda^j|,$$

In n -dimensional compact Riemannian manifolds (M, g) , we recall that the pointwise Weyl law for eigenfunctions u_λ^j associated to eigenvalues E_λ^j in an interval $I = (-\infty, \lambda^2]$ is given by the formula

$$\sum_{j: E_\lambda^j \in I} |u_\lambda^j(x)|^2 = (2\pi)^{-n} \lambda^n |\{\xi \in T_x M^* : |\xi|^2 \leq \lambda^2\}| + \mathcal{O}(\lambda^{n-1}), \quad (\text{I.18})$$

which is uniform in M . Then, using the compactness of M , it is sufficient to integrate this expression on M and we obtain the integrated Weyl law, that provides asymptotics the number of eigenfunctions in I . Historically, it was Hilbert who conjectured (I.18) with an error term $o(\lambda^n)$. Its name 'Weyl law' comes from the fact that Weyl first proved it (under its integrated form) [Wey11]. This pointwise Weyl law (I.18) has been originally proved by Avakumović [Ava56], Levitan [Lev52] and has been generalized by Hörmander [Hor68, Thm. 1.1] to self-adjoint elliptic pseudo-differential operators. Later, Sogge and Zelditch [Sog01] investigated conditions on M under which the remainder $\mathcal{O}(\lambda^{n-1})$ is sharp. Furthermore, the remainder term has been improved under geometric conditions in multiple works: a logarithm improvement by Bérard, Bonthonneau and Keeler [Bér77, Bon17, KT98] under negative curvature conditions, and geodesic beam techniques developed by Canzani and Galkowski [CG20b, CG22].

Let us now go back to Frank-Sabin bounds that we mentioned earlier. Let us explain how to answer Question 10, by considering the maximal rank, once again with $\gamma_\lambda = \Pi_\lambda$. Indeed, on the one hand, L^∞ -bound is deduced by the pointwise Weyl law

$$\|\rho_{\Pi_\lambda}\|_{L^\infty(M)} \leq C\lambda^{n-1}.$$

On the other hand, using the relation

$$\|\rho_{\Pi_\lambda}\|_{L^1(M)} = \text{Tr}(\mathbf{1}(-\Delta \in [\lambda^2, (\lambda+1)^2])) = N((-\infty, (\lambda+1)^2]) - N((-\infty, \lambda^2])$$

where $N(I)$ denotes the number of eigenvalues of $-\Delta_g$ in an interval I , and the integrated version of Weyl law asymptotics (I.18) for the intervals $(-\infty, (\lambda+1)^2]$ and $(-\infty, \lambda^2]$, that depends on the parameter $\lambda > 0$, one can prove that there exists $C > 0$ and a subsequence $\lambda_k \rightarrow \infty$ along that

$$\forall k \in \mathbb{N}, \quad \|\rho_{\Pi_{\lambda_k}}\|_{L^1(M)} \geq C\lambda_k^{n-1}.$$

Thus, for any $2 < q < \infty$

$$\underbrace{C\lambda^{-(n-1)}\|\rho_{\Pi_\lambda}\|_{L^1(M)}}_{\limsup_{\lambda \rightarrow \infty} \dots > 0} \leq \dots \leq \lambda^{-(n-1)}\|\rho_{\Pi_\lambda}\|_{L^{q/2}(M)} \leq \dots \leq \underbrace{C'\lambda^{-(n-1)}\|\rho_{\Pi_\lambda}\|_{L^\infty(M)}}_{\lesssim 1}.$$

Then, one can deduce that all L^p norms are of the same order

$$\forall 2 \leq q \leq \infty \quad \|\rho_{\Pi_\lambda}\|_{L^{q/2}(M)} \sim \lambda^{n-1},$$

that reflects the phenomenon of non-concentration in the whole spectral cluster. As a consequence, there appears a change of behavior between the concentration for a function and a phenomenon of non-concentration for the whole spectral cluster. This concentration provides the optimality of the exponent α_{Sogge} .

Link between high frequency regime and semiclassical regime Furthermore, we can establish the equivalence between this high frequency problem $\lambda \rightarrow \infty$ and a semiclassical problem writing $h = \lambda^{-1}$ (the large parameter becomes a small one) and $u_h = u_\lambda$. Then, (I.12), (I.14), (I.15) and (I.16) become

$$-h^2\Delta_g u_h = u_h, \quad \begin{cases} \|-h^2\Delta_g u_h - u_h\|_{L^2(M)} \lesssim h\|u_h\|_{L^2(M)}, \\ \mathbf{1}(-h^2\Delta_g \in [1, (1+h)^2]) u_h = u_h, \end{cases}$$

and in the right-hand side

$$\|u_h\|_{L^q(M)} \leq Ch^{-s_{\text{Sogge}}(q,n)} \left(\|u_h\|_{L^2(M)} + \frac{1}{h} \|(-h^2\Delta_g - 1)u_h\|_{L^2(M)} \right),$$

which is the formulation we consider when introducing potentials.

Euclidean case with a confining potential We return to our starting setting of the Schrödinger operators $-h^2\Delta + V$ with a confining potential in the Euclidean space \mathbb{R}^d and consider the localization of eigenfunctions 'near' an energy level $E \sim 1$, usually called the *chemical potential*.

Question 11. What role does the confining potential play, and what changes from the results on compact manifolds?

It is now necessary to take into account the presence of a zone known as *classically forbidden region*:

$$\{x \in \mathbb{R}^d : V(x) > E\}.$$

This name comes from the illegality of a classical particle with total energy $|\xi|^2 + V(x) = E$ to be here due to the fact that its kinetic energy ξ^2 is non-negative. A quantum particle has however a non-zero probability to be out in the classically forbidden region, but the classic behaviour occurs at the semiclassical limit $\hbar \rightarrow 0$. The existence of a forbidden zone induces of course an authorized zone, called *classically allowed region* or sometimes *bulk*

$$\{x \in \mathbb{R}^d : V(x) < E\},$$

where the particle is more likely to be. A further difficulty, which does not exist in the previous compact manifold framework, comes from the existence of a transitional region between the classically allowed and forbidden regions. The points $\{x \in \mathbb{R}^d : V(x) = E\}$ are often called *turning points*¹³.

One-body literature To have an intuition of the behavior of eigenfunctions, let us take a look at a classical toy model, which is the harmonic oscillator $V(x) = |x|^2$ in dimension 1. The induction relations between Hermite polynomials and BKW approximations (see for instance [Tao12] and [Olv97]) allow writing pointwise asymptotics of eigenfunctions that are expressed in terms of Airy functions.

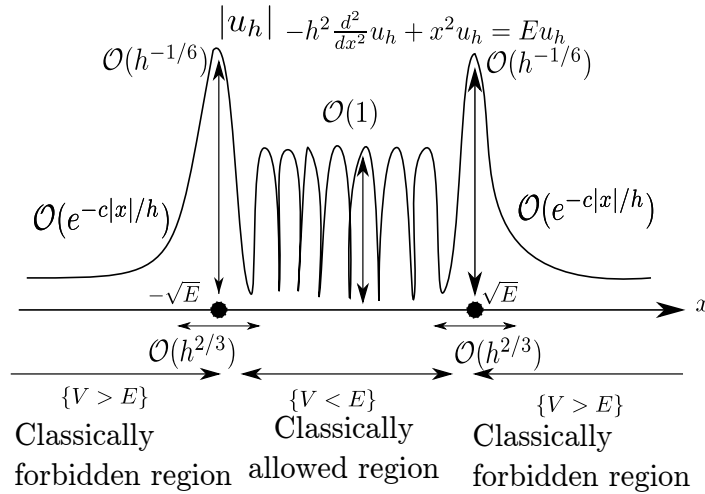


Figure 6 – Eigenfunction’s profile of the scalar harmonic oscillator associated to the eigenvalue E

This example highlights the differences in the behavior of the function in the three different regions and the phenomenon of concentration at the turning points $\{x \in \mathbb{R} : x^2 = E\}$, which does not exist in the compact manifold case. As depicted in Figure 6, the eigenfunction u_h oscillates with height of order ~ 1 in the bulk, decreases exponentially in $|x|$ and \hbar in the classical forbidden region and concentrates at the two edges $\pm\sqrt{E}$ with height $\sim \hbar^{-1/6}$ in neighborhood of length $\sim \hbar^{2/3}$. This implies the following L^q estimates:

$$\|u_h\|_{L^q(\mathbb{R})} \lesssim \begin{cases} 1 & \text{for } 2 \leq q \leq 4, \\ \hbar^{-\frac{1}{6} + \frac{3}{2q}} & \text{for } 4 \leq q \leq \infty. \end{cases}$$

¹³although it is a bit misleading, since in this PhD we add to this definition another assumption on the order one derivatives of V .

We can see the interest of looking at the whole range of q values since the concentration around the turning points is only visible for large q values ($q \geq 4$). Furthermore, notice that the L^q norm are not sensible to the oscillations in the bulk.

It would be reasonable to expect recovering the same estimates as Sogge's into the bulk. This exponential decay of eigenfunctions in the classically forbidden region is known as *Agmon estimates*. These estimates are also called *Lithner-Agmon estimates* because Lithner provided upper bounds for confining potentials in 1964, and Agmon proved them independently in the end of the seventies, with the exponential decay of N -Schrödinger eigenfunctions [Agm14].

We can expect to have a similar behaviour in higher dimensions and for more general confining potentials. However, the same analogy is not possible to have exact expressions of the eigenfunctions for more general potentials. There is still the possibility to investigate the L^q -bounds, of the form (I.2) with \mathbb{R}^d instead of M and $P - E$ instead of $-h^2\Delta_g - 1$. In line with this, Koch and Tataru [KT05] proved L^q estimates for the harmonic oscillator in higher dimensions. A few years later, the same two with Zworski [KTZ07] extended it to microlocalized quasimodes of more general operators in a semiclassical setting. Saying that a function u_h is microlocated means that u_h is negligible microlocally outside the compact of the phase space $\mathbb{R}_x^d \times \mathbb{R}_\xi^d$. The localization properties depend on how behaves the symbol p where the function u_h is microlocalized. They put forward three conditions on the points (x_0, ξ_0) of the level sets of the classical Hamiltonian $p_E(x, \xi) := p(x, \xi) - E$:

- ⊗ a quite general condition (*gene*), stated in Assumption 2:
that only asks that $\partial_\xi^2 p_E(x_0, \xi_0) = \partial_\xi^2 p(x_0, \xi_0)$ to be non-singular,
- ⊗ a curvature condition (*Sogge*), stated in Assumption 3:
that requires, in addition to the non-singularity of $\partial_\xi^2 p(x_0, \xi_0)$, that $\nabla_\xi p_E(x_0, \xi_0) = \nabla_\xi p(x_0, \xi_0) \neq 0$ and that the second fundamental form of $\{\xi \in \mathbb{R}^d : p_E(x_0, \xi) = 0\}$ is non-degenerate at $\xi = \xi_0$,
- ⊗ or turning points (*TP*), stated in Assumption 4:
in addition of the non-singularity of $\partial_\xi^2 p(x_0, \xi_0)$, there is the non-degeneracy condition $\nabla_x p_E(x_0, \xi_0) = \nabla_x p(x_0, \xi_0) \neq 0$.

Example. Let us comment what mean these conditions when $p(x, \xi) = |\xi|^2 + V(x)$ (an intuitive representation of these conditions in dimension $d = 1$ for a double well potential V is depicted in Figure 7):

- ⊗ the assumption (*gene*) is always satisfied,
- ⊗ the assumption (*Sogge*) holds for the points such that $p(x_0, \xi_0) = E$ and $V(x_0) < E$. The local curvature condition is always true because

$$\{\xi \in \mathbb{R}^d : p_E(x_0, \xi) = 0\} = \{\xi \in \mathbb{R}^d : |\xi|^2 = E - V(x_0)\}$$

is the $(d - 1)$ -sphere of radius $\sqrt{E - V(x_0)} > 0$, which has a non-negative curvature.

- ⊗ the assumption (*TP*) imposes that $V(x_0) = E$, $\xi_0 = 0$ and $\nabla_x V(x_0) \neq 0$.

We recall the form of Koch-Tataru-Zworski estimates below in (I.19), and we summarize all their statements in Table 2. These bounds state as the following.

Theorem ([KTZ07]). *For any point $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ that satisfies one of the above conditions: (cond) = (gene), (Sogge) or (TP), there exist fixed $s_{\text{cond}} \geq 0$ and $t_{\text{cond}} \geq 0$ associated to (cond) (represented later in Figure 1.3 on Chapter 1)*

- an open bounded neighborhood $\mathcal{U} \times \mathcal{V}$ of (x_0, ξ_0) ,
- $h_0 > 0$,

such that for any $\chi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ supported into $\mathcal{U} \times \mathcal{V}$, there exists

- a multiplicative constant $C = C(d, \chi, h_0) > 0$,

such that for any $2 \leq q \leq \infty$ and any $u \in L^2(\mathbb{R}^d)$

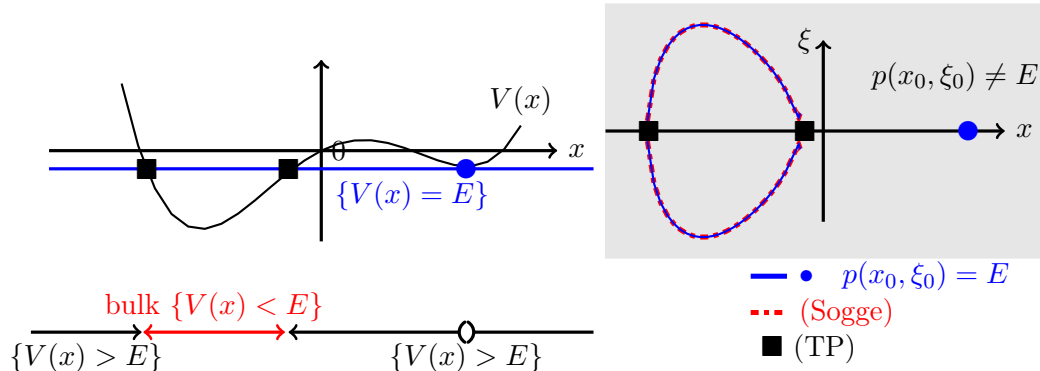
$$\|\chi^w(x, hD)u\|_{L^q(\mathbb{R}^d)} \leq Ch^{-s_{\text{cond}}(q,d)} \left(\|u\|_{L^2(\mathbb{R}^d)} + \frac{1}{h} \|(P - E)u\|_{L^2(\mathbb{R}^d)} \right), \quad (\text{I.19})$$

where $\chi^w(x, hD)$ denotes the Weyl quantization of χ .

Note that the above bounds are true for any quantization of p and χ . It only changes the multiplicative constant $C > 0$, for which, as for $h_0 > 0$, we never give explicit expression.

Condition	on the symbol $p_E := p(x, \xi) - E$	Statements in Chapter 1
<i>General</i>	(gene)=(Assumption 2)	Theorem IV.1
<i>Sogge</i>	(Sogge)=(Assumption 3)	Theorem V.1
<i>Turning points</i>	(TP)=(Assumption 4)	Theorem VI.1

Table 2 – Principal statements of Koch-Tataru-Zworski estimates



(a) Potential V and a given energy level set E . The points of intersections $\{x \in \mathbb{R}^d : V(x) = E\}$ are represented by blue bullets and black squares for turning points.

(b) Regions of the phase-space $\mathbb{R}_x^d \times \mathbb{R}_\xi^d$: are represented the points of $\{p = E\}$ in blue, dashed red and black squares: they all satisfy (gene). In particular, the points of the dashed red curve are the points that satisfy (Sogge) and the points in black squares are the one that satisfy (TP).

Figure 7 – Representation of points (x_0, ξ_0) of the phase-space according to the different assumptions (*cond*), for $d = 1$, $p(x, \xi) = |\xi|^2 + V(x)$, an energy $E > \min V$ and V the double-well potential in Figure 7a.

Generalization to orthonormal families of eigenfunctions We consider again Question 10 in the Euclidean setting with a confining potential. It would therefore be reasonable to expect the phenomenon of delocalization to emerge at a number of particles confined together.

By taking up again the example of the scalar harmonic oscillator (depicted in Figure 8), setting $\{u_h^j\}_{1 \leq j \leq N_h}$ an orthonormal family of eigenfunctions associated to eigenvalues less or equal to E ,

the density $\rho_h = \sum_{j=1}^{N_h} |u_h^j|^2$ can be again expressed asymptotically with special functions thanks to BKW methods. Up to a normalization, we find asymptotically the density of the semicircle law $\frac{1}{2\pi} \sqrt{(E - x^2)_+}$. As in the one-body case, ρ_h has an exponential decay in the classically forbidden region and a concentration with height $\sim h^{-2/3}$ in $h^{2/3}$ -neighborhood of turning points. However, the concentration around turning points is negligible compared to the concentration in the bulk which occurs with a height of order h^{-1} . This implies that all its L^q -norms are of same order h^{-1} , that denotes a phenomenon of non-concentration of the eigenfunctions' system.

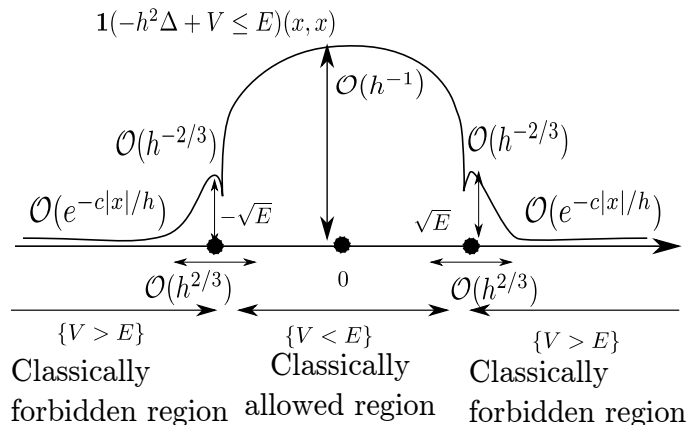


Figure 8 – Profile of ρ_h of the scalar harmonic oscillator associated to the eigenvalues smaller than E

One can extend the same behaviour in higher dimensions. Although Karadzhov [Kar89] provided pointwise asymptotics of the spectral projector on eigenvalues smaller or equal than E , pointwise Weyl laws for general confining potentials are quite recent and have so far only been done in the article of Deleporte and Lambert [DL21]. They proved in-diagonal (and out-diagonal) pointwise estimates with an optimal remainder with a scale h in the bulk and $h^{2/3}$ around its edges¹⁴. Note that the asymptotics expressed with Airy functions and these scales are consistent with those stated in the physics papers [DLDMS19].

I.3 Weyl laws with interaction

At first, we restricted ourselves to the case without interactions. Let us now come back to the case $w \neq 0$. In order to handle (partially) Question 9, we introduce in the section the framework and mathematical approximations of interacting quantum systems. We first begin by writing the state of the art for canonical finite systems. Then, we pose the problem in the non-canonical setting.

Finite N -body systems As promised, let us go back to our N -fermionic system with the quantum Hamiltonian P_N given by the formula (I.5). The model is not always easy to handle directly, in particular to compute the ground and excited states of P_N . It is thus also the case for the question of concentration. That is why various approximations (unfortunately no longer linear) are used to deal with this problem: we will focus on Hartree-Fock approximation and Thomas-Fermi approximation, have been the subject of several mathematical works: as did Lieb and Simon [LS77a, LS77b], Bach [Bac92] and Lions [Lio87]. The first one is very used in quantum chemistry and the second one not so much, but it remains interesting to be studied from a theoretical point

¹⁴for turning points, that corresponds to black squared in Figure 7. The question of estimates around degenerate points as the critical points which are not ground state energy (bullet in blue in the figure) is still open.

of view. For a deeper introduction to Hartree-Fock and Thomas-Fermi methods, we refer to the books [CLBM06] and [LS10].

Mean-field regime We will consider our fermionic system to be in *mean-field regime*, where there are a lot of interactions between the particles but at a low intensity. In this approximation, with which we hope to approach the macroscopic properties of the system, the interaction between particles is seen as an effective potential depending on the average density of the field generated by all other particles in the system. That means that for any state $\Psi_N \in L_a^2(\mathbb{R}^{dN})$ with not so strong correlations between each particle

$$\left\langle \Psi_N, \sum_{1 \leq i < j \leq N} w(x^i - x^j) \Psi_N \right\rangle_{L^2(\mathbb{R}^{dN})} \simeq \frac{1}{2} \left\langle \Psi_N, \sum_{j=1}^N (w * \rho_{\Psi_N}(x^j)) \Psi_N \right\rangle_{L^2(\mathbb{R}^{dN})}.$$

Here, $w * \rho_{\Psi_N}(x^j)$ denote the multiplication operator by

$$w * \rho_{\Psi_N}(x^j) := \int_{\mathbb{R}^d} w(x^j - y) \rho_{\Psi_N}(y) dy.$$

Remark (Mean-field scaling and link between the system of N fermions and \hbar). We can take $\lambda = 1/N$ to balance the term with kinetic and potential energy. Furthermore, one would also like that the number of particles $N \rightarrow \infty$ when $\hbar \rightarrow 0$. To be sure to have again all the terms of the same order at the semiclassical limit $\hbar \rightarrow 0$, it is relevant to link N and \hbar by the relation $\hbar = N^{-1/d}$. The quantum Hamiltonian P_N , defined in (I.5), can be rewritten as

$$\begin{aligned} P_N &= \sum_{j=1}^N \left(-N^{-2/d} \Delta_{x^j} + V(x^j) \right) + \frac{1}{N} \sum_{1 \leq i < j \leq N} w(x^i - x^j) \\ &= \sum_{j=1}^N \left(-\hbar^2 \Delta_{x^j} + V(x^j) \right) + \hbar^d \sum_{1 \leq i < j \leq N} w(x^i - x^j). \end{aligned} \quad (\text{I.20})$$

Density matrices associated to a wave-function We begin by explaining the advantages of adopting the formalism of density matrices. We recall for any state $\Psi_N \in L^2(\mathbb{R}^{dN})$, its *one-particle* and *two-particle density matrices*, respectively denoted by $\gamma_{\Psi_N}^{(1)}$ and $\gamma_{\Psi_N}^{(2)}$, are the operators on $L^2(\mathbb{R}^d)$ and $L^2(\mathbb{R}^{2d})$ associated to the integral kernels

$$\forall x, y \in \mathbb{R}^d, \quad \gamma_{\Psi_N}^{(1)}(x, y) := N \int_{\mathbb{R}^{d(N-1)}} \overline{\Psi_N(y, x^2, \dots, x^N)} \Psi_N(x, x^2, \dots, x^N) dx^2 \dots dx^N$$

and

$$\begin{aligned} \forall x^1, x^2, y^1, y^2 \in \mathbb{R}^d, \quad \gamma_{\Psi_N}^{(2)}(x^1, x^2, y^1, y^2) &:= \frac{N(N-1)}{2} \int_{\mathbb{R}^{d(N-2)}} \overline{\Psi_N(y^1, y^2, x^3, \dots, x^N)} \times \\ &\times \Psi_N(x^1, x^2, x^3, \dots, x^N) dx^3 \dots dx^N. \end{aligned}$$

There are also k -particle density matrices $\Psi_N^{(k)}$ of Ψ_N , that acts on $L^2(\mathbb{R}^{kd})$, for any $k \in \{1, \dots, N\}$. The k -particle density matrix $\Psi_N^{(k)}$ corresponds to the k -particle marginal distribution and is obtained by integrating out the degrees of freedom of the other $N - k$ particles.

In the case with interaction, first notice that the mean-value of the system at a state $\Psi_N \in L_a^2(\mathbb{R}^{dN})$ is entirely determined by its one-particle and two-particle densities matrices

$$\langle \Psi_N, P_N \Psi_N \rangle_{L^2} = \text{Tr}_{L^2(\mathbb{R}^d)} \left((-\hbar^2 \Delta + V) \gamma_{\Psi_N}^{(1)} \right) + \frac{1}{N} \text{Tr}_{L^2(\mathbb{R}^{2d})} \left(w \gamma_{\Psi_N}^{(2)} \right). \quad (\text{I.21})$$

Hartree-Fock effective approximation A variational approach, the *Hartree-Fock* approximation, consists on manipulating only Slater determinants, that are also called *Hartree-Fock states*. The idea of this approximation is to study instead of \mathcal{E}_N , the *Hartree-Fock energy functional*

$$\mathcal{E}_N^{\text{HF}}(\gamma) := \text{Tr}_{L^2(\mathbb{R}^d)} \left((-h^2\Delta + V) \gamma \right) + \frac{1}{2N} \left(\iint_{\mathbb{R}^d \times \mathbb{R}^d} \rho_\gamma(x) \rho_\gamma(y) w(x-y) dx dy - \iint_{\mathbb{R}^d \times \mathbb{R}^d} |\gamma(x,y)|^2 w(x-y) dx dy \right),$$

defined for (nice enough) bounded operator γ on $L^2(\mathbb{R}^d)$, where ρ_γ is the density of γ . Here, the kinetic part of the energy is defined by

$$\text{Tr}_{L^2(\mathbb{R}^d)} \left((-h^2\Delta + V) \gamma \right) := \text{Tr}_{L^2(\mathbb{R}^d)} \left(\sqrt{-h^2\Delta + V + E} \gamma \sqrt{-h^2\Delta + V + E} \right) - E \int_{\mathbb{R}^d} \rho_\gamma(x) dx,$$

for $E > 0$ such that $V + E$ is non-negative in \mathbb{R}^d , the second term is called the *direct term*

$$\iint_{\mathbb{R}^d \times \mathbb{R}^d} \rho_\gamma(x) \rho_\gamma(y) w(x-y) dx =: D_w(\rho_\gamma, \rho_\gamma)$$

and the last term is called the *exchange term*

$$\iint_{\mathbb{R}^d \times \mathbb{R}^d} |\gamma(x,y)|^2 w(x-y) dx dy =: \text{Ex}_w(\gamma),$$

of entirely quantum origin, what happens when two particles of same nature are switched. For fermions, it takes into account the antisymmetry generated by the Pauli exclusion principle.

Indeed, Ψ_N is a Slater determinant, associated to an orthonormal basis $\{u_j\}_{1 \leq j \leq N}$ and in the space

$$\mathcal{S}_N := \{u_1 \wedge \cdots \wedge u_N : u_j \in H^1(\mathbb{R}^d), \langle u_i, u_j \rangle_{L^2} = \delta_{ij} \quad \forall 1 \leq i, j \leq N\},$$

one can show that the mean-value of the system at a state $\Psi_N \in L_a^2(\mathbb{R}^{dN})$ is expressed with the one-particle density matrix $\gamma_{\Psi_N}^{(1)}$

$$\langle \Psi_N, P_N \Psi_N \rangle_{L^2} = \mathcal{E}_N^{\text{HF}}(\gamma_{\Psi_N}^{(1)}). \quad (\text{I.22})$$

Furthermore, $\gamma_{\Psi_N}^{(1)}$ is the orthogonal projector on the space generated by $\{u_j\}_{1 \leq j \leq N}$

$$\gamma_{\Psi_N}^{(1)} = \sum_{j=1}^N |u_j\rangle \langle u_j|.$$

More exactly, γ is associated to the integral kernel

$$\gamma_{\Psi_N}^{(1)}(x, y) := \sum_{j=1}^N \overline{u_j(y)} u_j(x) \quad \text{and} \quad \rho_{\gamma_{\Psi_N}^{(1)}}(x) = \sum_{j=1}^N |u_j(x)|^2.$$

Let the Hartree-Fock ground state energy e_N^{HF} given is by the variational minimization problem on the Slater determinant spaces

$$e_N^{\text{HF}} := \inf \{ \langle \Psi, P_N \Psi \rangle_{L^2} : \Psi \in \mathcal{S}_N \}. \quad (\text{I.23})$$

On the one hand, the ground state energy e_N is always bounded by above by e_N^{HF} . The lower bound is more tricky, but possible under some conditions. In particular, this was treated by Lieb-Simon [LS77a], Bach [Bac92], Graf-Solovej [GS94] for Coulomb systems: $V(x) = -|x|^{-1}$ and $w(x) = |x|^{-1}$. More recently, Fournais-Lewin-Solovej [FLS18] proved it more general potentials. We will detail this below. In these cases, the Hartree-Fock method can give a good approximation of the ground state energy e_N .

Similar results exist concerning the evolution of the solutions of the time dependent equation (I.4), for the initial value to be equal to a Slater determinant. Many works [BGGM03, EESY04, RS09, BPS14, BJP⁺16] show that its dynamics¹⁵ is strongly related to the one of Hartree-Fock equation at the limit $N \rightarrow \infty$.

Remark (Generalized Hartree-Fock minimization problem). The minimization problem (I.23) set can be extended to the so-called *generalized Hartree-Fock energy*

$$e_N^{\text{gHF}} := \inf\{\mathcal{E}_N^{\text{HF}}(\gamma) : \gamma \in \mathcal{K}_N \text{ and } \text{Tr}((-\Delta)\gamma) < \infty\},$$

on the set of density matrices of N particles systems

$$\mathcal{K}_N := \{\gamma \in \mathcal{B}(L^2(\mathbb{R}^d)) : \gamma = \gamma^*, \quad 0 \leq \gamma \leq 1, \quad \text{Tr}(\gamma) = N\}.$$

The condition $\gamma \leq 1$ comes exclusively from the Pauli exclusion principle.

In some cases, $e_N^{\text{HF}} = e_N^{\text{gHF}}$. For instance, when the interaction is repulsive $w \geq 0$ [Lie81].

Thomas-Fermi effective approximation The Thomas-Fermi approximation belongs to *Density Functional Theory* (DFT) models, that only depend on the one-particle density and not involve anymore on the wave-function. The idea is to approach the ground state to the many-body Hamiltonian (I.20) by the solution of a minimization problem on densities $x \mapsto \rho(x)$

$$\inf \left\{ \mathcal{E}(\rho) : \rho \in L^1(\mathbb{R}^d, \mathbb{R}_+), \quad \int_{\mathbb{R}^d} \rho(x) dx = N \right\},$$

where \mathcal{E} is composed by a kinetic density functional F , the external potential energy $\rho \mapsto \int_{\mathbb{R}^d} \rho V$ and an interaction term $\rho \mapsto \frac{1}{2} D_w(\rho, \rho)$:

$$\mathcal{E}(\rho) = F(\rho) + \int_{\mathbb{R}^d} V(x)\rho(x)dx + \frac{1}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} w(x-y)\rho(x)\rho(y)dx dy.$$

Historically, the simplest and oldest DFT was the Thomas-Fermi¹⁶ approximation, that appeared in the thirties to approximate the distribution of uniform electronic gas. Hohenberg and Kohn [HK64] first justified the validity of DFT in 1964. The above formulation of DFT was due later to Levy [Lev79] and Lieb [Lie02] (we refer to the review of Lewin, Lieb and Seiringer [LLS19] for more completeness).

The Thomas-Fermi approximation is associated to the Thomas-Fermi energy \mathcal{E}^{TF} and defined by the functional

$$F^{\text{TF}}(\rho) = \frac{d}{d+2} c_{\text{TF}} \int_{\mathbb{R}^d} \rho(x)^{1+2/d} dx,$$

where the constant c_{TF} is defined by

¹⁵more specifically the one of the one-body density matrix of the ground state of P_N

¹⁶which name is after the independent contributions of Llewellyn Hilleth Thomas (1903-1992) [Tho27] and Enrico Fermi (1901-1954) [Fer27]

We explain now how the Thomas-energy appears in the approximation of the ground state problem of the Hamiltonian P_N (as proved Lieb and Simon [LS77b]). At the limit $N \rightarrow \infty$, the one-particle density matrix of the ground state of P_N may behave like the Weyl quantization of the phase space function

$$m(x, \xi) = \mathbb{1} \left(|\xi|^2 \leq c_{\text{TF}} \rho(x)^{2/d} \right) \quad (\text{I.24})$$

for a minimizer ρ_{TF} of Thomas-Fermi functional \mathcal{E}^{TF} . Notice that this kind of phase space densities are actually minimizers of the *Vlasov energy functional*

$$\mathcal{E}^{\text{Vlas}}(m) := \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |\xi|^2 m(x, \xi) dx d\xi + \int_{\mathbb{R}^d} \rho_m(x) V(x) dx + \frac{1}{2} D_w(\rho_m, \rho_m),$$

defined on the integrable phase space functions¹⁷ $m : \mathbb{R}^d \times \mathbb{R}^d \rightarrow [0, 1]$ with ρ_m denoting the spatial density

$$\rho_m(x) := \int_{\mathbb{R}^d} m(x, \xi) d\xi.$$

For a given $\rho \geq 0$, the functionals \mathcal{E}^{TF} and $\mathcal{E}^{\text{Vlas}}$ are related

$$\mathcal{E}^{\text{TF}}(\rho) = \mathcal{E}^{\text{Vlas}} \left(\mathbb{1} \left(|\xi|^2 \leq c_{\text{TF}} \rho(x)^{2/d} \right) \right).$$

It is worth mentioning an equivalent remark about the time dynamic setting as for the Hartree-Fock approximation. For the same initial condition of the form (I.24), the solution¹⁸ of (I.4) (via the Wigner transformation) can be approached by the solution of the classical equation, called Vlasov, as $N \rightarrow \infty$ [NS81]. We can therefore also see a kind of equivalence between Hartree and Vlasov dynamics [APPP11, BPSS16].

As well, coming back to the independent time setting, the Hartree-Fock and the Thomas-Fermi minimization problems are deeply related. In particular, it is reasonable to approach the Hartree-Fock ground state of by the one of Thomas-Fermi at the coupled mean-field and semiclassical limits $N \rightarrow \infty$ and $h \rightarrow 0$ ($h = N^{-1/d}$). This was what did Fournais, Lewin, Solovej [FLS18, Thm 1.1, 1.2, 1.3] by providing a link between N -Hartree-Fock model and Thomas-Fermi energy for trapping and also non-trapping V and an interaction potential w , under suitable conditions. In particular, they deduced the leading order of the ground state energy e_N of P_N at the limit

$$\lim_{N \rightarrow \infty} \frac{e_N}{N} = e^{\text{TF}}(1),$$

where $e^{\text{TF}}(1)$ denotes the Thomas-Fermi ground state energy

$$\inf \left\{ \mathcal{E}^{\text{TF}}(\rho) : \rho \geq 0, \quad \rho \in L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d), \quad \int_{\mathbb{R}^d} V(x) \rho(x) dx < \infty, \quad \int_{\mathbb{R}^d} \rho(x) dx = 1 \right\}.$$

They proved also the weak convergence of k -particle density matrices of the ground state to a mean-value on all the set of Thomas-Fermi functional's minimizers.

Grand-canonical systems of particles One would like to study large systems of interacting fermions again in a mean-field regime. In a way, we would like to have a macroscopic description of its state, which allows the fluctuation of the number of particles and the energy of the system. The canonical setting with a fixed number of particles as below is no longer appropriate, since in

¹⁷Once again the constraint $m \leq 1$ comes from the Pauli principle.

¹⁸the one-particle density matrix of the time-dependent ground state

the Weyl law we fix rather the chemical potential E , and we consider intervals of energy around this fixed parameter. That is why we will adopt the *grand-canonical* setting.

A grand-canonical ensemble is composed of \mathbb{N} identical systems of finite particles with a fixed chemical potential E , which shares with the other the particles and the energy. The system of grand-canonical states is described by the *fermionic Fock space*

$$\mathcal{F} := \mathbb{C} \oplus \bigoplus_{N=1}^{\infty} L_a^2(\mathbb{R}^{dN}),$$

composed of sequences $\Psi = (\Psi_0, \Psi_1, \dots, \Psi_N, \dots)$ such that $\Psi_N \in L_a^2(\mathbb{R}^{dN})$ for any $N \in \mathbb{N}^*$. We endowed \mathcal{F} by the scalar product

$$\langle \Psi, \Phi \rangle_{\mathcal{F}} = \sum_{N \in \mathbb{N}} \langle \Psi_N, \Phi_N \rangle_{L^2(\mathbb{R}^{dN})}.$$

Moreover, the Hamiltonian becomes

$$\mathbf{P} = \bigoplus_{N=1}^{\infty} P_N,$$

where P_N is the Hamiltonian on $L_a^2(\mathbb{R}^{dN})$ defined by

$$P_N := \sum_{j=1}^N (-\hbar^2 \Delta_{x^j} + V(x^j)) + \hbar^d \sum_{1 \leq i < j \leq N} w(x^i - x^j).$$

Setting \mathcal{N} to be the number of particles

$$\mathcal{N} = \bigoplus_{N \in \mathbb{N}} N \mathbf{1}_{L_a^2(\mathbb{R}^{dN})},$$

for a given energy E , the ground state energy $e_{\hbar, V, w}(E)$ of $\mathbf{P} - E\mathcal{N}$

$$e_{\hbar, V, w}(E) := \inf \text{Spec}(\mathbf{P} - E\mathcal{N})$$

is also defining in function of the ground state energies of the canonical Hamiltonians $P_N - EN$

$$e_{\hbar, V, w}(E) = \inf_{N \geq 0} e_{N, V, w}(E) =: \inf_{N \geq 0} \text{Spec}(P_N - EN).$$

Let us denote by $e_{\hbar, V-E, w}^{\text{gHF}}$ the grand-canonical energy of the \hbar -generalized Hartree-Fock energy associated to the external potential $V - E$ and the potential of interaction w

$$\begin{aligned} e_{\hbar, V-E, w}^{\text{gHF}} &:= \inf_{\gamma \in \mathcal{K}} \left\{ \text{Tr}((-\hbar^2 \Delta + V - E)\gamma) + \frac{\hbar^d}{2} [D_w(\rho_\gamma, \rho_\gamma) - \text{Ex}_w(\gamma)] \right\} \\ &=: \inf_{\gamma \in \mathcal{K}} \mathcal{E}_{\hbar, V-E, w}^{\text{gHF}}(\gamma). \end{aligned} \tag{I.25}$$

on the set

$$\mathcal{K} := \left\{ \gamma \in \mathfrak{S}^1(L^2(\mathbb{R}^d)) : \gamma = \gamma^*, \quad 0 \leq \gamma \leq 1, \quad \text{Tr}((-\Delta)\gamma) < \infty \right\}.$$

We observe that when $w \geq 0$, if $e_{\hbar, V-E, w}^{\text{gHF}}$ is not bounded by below, the energy ground state $e_{\hbar, V, w}(E)$ cannot be either by relation on the grand-canonical energies

$$e_{\hbar, V, w}(E) \leq e_{\hbar, V-E, w}^{\text{gHF}}.$$

In the non-interacting case $w = 0$, the ground state energy of the grand-canonical system coincides with the \hbar -Hartree-Fock energy ground state (see (I.21) where is only involved the kinetic term evaluated in the one-body density matrix of the ground-state)

$$\begin{aligned} e_{\hbar, V-E, w=0}^{\text{gHF}} &= \inf_{\gamma_h \in \mathcal{K}} \text{Tr}((-\hbar^2 \Delta + V - E)\gamma_h) = \text{Tr}((-\hbar^2 \Delta + V - E)_-) \\ &= \frac{|B_{\mathbb{R}^d}(0, 1)|}{(2\pi\hbar)^d(1+d/2)} \int_{\mathbb{R}^d} [(E - V(x))_+]^{1+d/2} dx + o(\hbar^{-d}). \end{aligned}$$

Furthermore, the first semiclassical asymptotic term of the trace of the \hbar -Hartree-Fock minimizer $\gamma_h = \mathbf{1}(-\hbar^2 \Delta + V \leq E)$ is provided by the integrated Weyl law (see for instance [Zwo12, Chap.6])

$$\text{Tr}_{L^2(\mathbb{R}^d)}(\gamma_h) = \frac{|B_{\mathbb{R}^d}(0, 1)|}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} [(E - V(x))_+]^{d/2} dx + o(\hbar^{-d}).$$

As a consequence, we deduce the same limits for the energy and the one-body matrix of the whole system's ground state

$$\lim_{\hbar \rightarrow 0} \hbar^d e_{\hbar, V, w=0}(E) = \frac{|B_{\mathbb{R}^d}(0, 1)|}{(2\pi)^d(1+d/2)} \int_{\mathbb{R}^d} [(E - V(x))_+]^{1+d/2} dx \quad (\text{I.26})$$

and

$$\lim_{\hbar \rightarrow 0} \hbar^d \text{Tr}_{L^2(\mathbb{R}^d)}(\gamma_{\Psi_h^{(1)}}) = \frac{|B_{\mathbb{R}^d}(0, 1)|}{(2\pi)^d} \int_{\mathbb{R}^d} [(E - V(x))_+]^{d/2} dx.$$

Question 12. What kind of asymptotics can we have in the presence of interaction?

II CONTRIBUTIONS AND ORGANIZATION OF THIS THESIS

We present in this section our main contributions.

II.1 Results of Chapter 1: asymptotics for the case without interaction

The Chapter 1, which is the subject of the preprint [Ngu22], is devoted to generalization of microlocalized Koch-Tataru-Zworski L^q estimates [KTZ07] (under the form (I.19)) to spectral clusters, similarly to Frank-Sabin bounds [FS17b] (of the form (I.17)) but in a semiclassical setting. We begin to express these estimates of densities under two complementary point of views: the semiclassical setting, that involves localization in the phase space with respect to the semiclassical parameter \hbar (Sections III, IV, V and VI) and the spectral setting, where we consider density matrices in spectral clusters, and we study their bounds in different regions of the space \mathbb{R}_x^d (Section VII). In the last section of this chapter (Section VIII), we discuss the one-body and many-body optimality of L^q bounds. First, we detail the construction of some specific quasimodes, that saturate one-body L^q bounds for which the form is well known in the literature. Then, we provide the optimality the Sogge many-body estimates in the bulk.

We reference our exact results in Tables 3 and 4.

Microlocalized estimates (referenced in Table 3) First, given $d \geq 2$

- a classical observable p , that can be $p(x, \xi) = |\xi|^2 + V(x)$ and more general one in the suitable symbol class,
- and an energy level set $E \in \mathbb{R}$,

the idea is to look at the density of operators microlocalized in the phase space near point $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$, that satisfy some geometric assumptions (*cond*) with respect to the energy level sets of $p_E(x, \xi) = p(x, \xi) - E$. That can be points out of $\{p_E = 0\}$ or in the level set $\{p_E = 0\}$ under one of the three conditions stated in [KTZ07]. Let $P := p^w(x, hD)$ the Weyl quantization of p . We provide the following theorem.

Theorem 1 (Theorems IV.2, V.2 and VI.2). *For any point $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ that satisfies one of the above conditions: (*cond*) = (*gene*), (*Sogge*) or (*TP*), there exist fixed $s_{\text{cond}} \geq 0$, $t_{\text{cond}} \geq 0$ and $\alpha_{\text{cond}} \in [1, \infty]$ associated to (*cond*) which are summed up in Figures 1.3, 1.10 and 1.4, and*

- an open bounded neighborhood $\mathcal{U} \times \mathcal{V}$ of (x_0, ξ_0) ,
- $h_0 > 0$,

such that for any $\chi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ supported into $\mathcal{U} \times \mathcal{V}$, there exists

- a multiplicative constant $C = C(d, \chi, h_0) > 0$,

such that for any $2 \leq q \leq \infty$, any $h \in (0, h_0]$ and any non-negative self-adjoint operator γ on $L^2(\mathbb{R}^d)$, we have

$$\boxed{\|\rho_{\chi^w(x, hD)\gamma\chi^w(x, hD)}\|_{L^{q/2}(\mathbb{R}^d)} \leq Ch^{-2s_{\text{cond}}(q, d)} \log(1/h)^{2t_{\text{cond}}(q, d)} \times \left(\|\gamma\|_{\mathfrak{S}^{\alpha_{\text{cond}}(q, d)}(L^2(\mathbb{R}^d))} + \frac{1}{h^2} \|(P - E)\gamma(P - E)\|_{\mathfrak{S}^{\alpha_{\text{cond}}(q, d)}(L^2(\mathbb{R}^d))} \right)}. \quad (\text{II.1})$$

Remark. A first remark of this theorem is that, the exponents satisfy $\alpha_{\text{cond}}(q, d) > 1$ for all $q \in (2, \infty]$ except $q = 2d/(d - 2)$ for *cond* = *gene*.

Let us compare now our results with respect to the one-body estimates of Koch, Tataru and Zworski [KTZ07].

- Except for the values of $t_{\text{cond}}(q, d)$ in the case *cond* = *gene* and $2(d + 1)/(d - 1) \leq q < 2d/(d - 2)$ (see Figure 1.5), the exponents s_{cond} and t_{cond} are the same as the one in [KTZ07]. One can deduce the one-body estimates (I.19) from (II.1), by taking $\gamma = |u\rangle\langle u|$.
- We prove also microlocalized bounds for the elliptic condition (*ellip*): $p(x_0, \xi_0) \neq E$ (see Theorem III.1) but we do not highlight it since this result is more trivial. In this case

$$\forall 2 \leq q \leq \infty, \quad (s_{\text{ellip}}(q, d), t_{\text{ellip}}(q, d), \alpha_{\text{ellip}}(q, d)) = \left(d \left(\frac{1}{2} - \frac{1}{q} \right) - 1, 0, \frac{q}{2} \right).$$

- The turning point case (*TP*) is only proved for Schrödinger operators.

The proof of the above theorem, proved into a dual version, relies on many-body semiclassical Strichartz estimates [Ngu22] that we apply to a microlocalized propagator $U(t, r)$ in a small neighborhood of (x_0, ξ_0) . Indeed, as in the one-body case in [KTZ07], the spirit is to deal with a time-dependent problem

$$[hD_t - A_t(\mathbf{x}, hD)]u(t, \mathbf{x}) = hf(\mathbf{x}),$$

with $n = n(d) \geq 1$ and $A_t = a_t(\mathbf{x}, hD_{\mathbf{x}})$ the quantization of $a_t : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ that depends on the symbol p . This involves a propagator, which when microlocalized in a small neighborhood of

the point (x_0, ξ_0) , is approximates thanks to BKW techniques so that it satisfies the abstract bounds

$$\begin{cases} \sup_{r \in J} \|U(t, r)U(s, r)^*\|_{L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n)} & \lesssim 1, \\ \sup_{r \in J} \|U(t, r)U(s, r)^*\|_{L^1(\mathbb{R}^n) \rightarrow L^\infty(\mathbb{R}^n)} & \lesssim h^{-n/2}(h + |t - s|)^{-n/2}, \end{cases} \quad (\text{II.2})$$

Then, for any compact interval $J \subset \mathbb{R}$, it remains bounds the different term of the associated Duhamel formula (composed with the microlocalization)

$$u(t, \mathbf{x}) = U(t, 0)u(0, \mathbf{x}) + \int_0^t U(t, s)f(\mathbf{x})ds + \mathcal{O}(h^\infty)$$

thanks to Strichartz estimates. As the name suggests, they involve the semiclassical parameter h , but instead of deducing mixed $L_t^p L_x^q$ -bounds from the $L_x^2 \rightarrow L_x^2$ and $L_x^1 \rightarrow L_x^\infty$ bounds, the idea is to do the same taking in account the many-body setting. This is reflected in the presence of Schatten norms of $U(t, s)$.

Theorem 2 (Strichartz estimates on Schatten spaces, Theorem II.23). *For $n \geq 2$, a bounded interval $J \subset \mathbb{R}$ and a propagator $U(t, r)$ on $L^2(\mathbb{R}^n)$ that satisfies the estimates (II.2) for all $t, s \in \mathbb{R}$, there exists $C = C(n, J) > 0$ and exponents $p = p(q, n) \geq 1$, $s = s(q, n) \geq 0$ and $t = t(q, n) \geq 0$ ¹⁹ such that for any $2 \leq q \leq 2(n + 1)/(n - 1)$ and any $W \in L_t^{p(q, n)} L_x^2(\mathbb{R}^{n+1})$*

$$\sup_{r \in J} \|WU(t, r)\|_{\mathfrak{S}^{2(\frac{2q}{q+2})'}(L_x^2(\mathbb{R}^n) \rightarrow L_{t,x}^2(\mathbb{R}^{n+1}))} \leq Ch^{-s(q, n)} \log^{t(q, n)}(1/h) \|W\|_{L_t^{p(q, n)} L_x^2(\mathbb{R}^{n+1})}.$$

Notice that the proof of Theorem 2 is very general since requires no more hypothesis that the energy and decay TT^* estimates (II.2). It relies on complex interpolation in the same spirit in Schatten spaces as in the paper of Frank-Sabin [FS17a].

Estimates on spectral clusters (referenced in Table 3) We deduce from the above microlocalized estimates, given

- a classical Hamiltonian $p(x, \xi) = |\xi|^2 + V(x)$ with a confining potential $V : \mathbb{R}^d \rightarrow \mathbb{R}$,
- an energy level set $E \in \mathbb{R}$,

another point of view, a spectral one that consists on considering at eigenfunctions associated to eigenvalues into intervals around E . Furthermore, instead of looking at the objects located in phase space $\mathbb{R}_x^d \times \mathbb{R}_\xi^d$, we study them in position space at some regions $\Omega = \Omega_{V, E, \varepsilon} \subset \mathbb{R}_x^d$, that depend only on the potential V , the energy E and a small error $\varepsilon > 0$

- ⊗ $\Omega = \mathbb{R}^d$,
- ⊗ in the classical forbidden region $\Omega = \{V > E + \varepsilon\}$,
- ⊗ in the bulk $\Omega = \{V < E - \varepsilon\}$,
- ⊗ or in a neighborhood of the turning points $\Omega = \{|V - E| < \varepsilon\}$ under the additional assumption²⁰ that all points $x \in \mathbb{R}^d$ in $\{V = E\}$ must satisfy the condition $\nabla_x V(x) \neq 0$.

Denoting by P the Weyl quantization of p and by $\Pi_{E, h}$ the spectral projector on the window $[E - h, E + h]$

$$\Pi_{E, h} := \mathbf{1}(P \in [E - h, E + h]),$$

we provide the estimates the following in the spectral clusters $\Pi_{E, h}(L^2(\mathbb{R}^d))$.

¹⁹we do not detail their expression for the reader's convenience

²⁰We exclude here critical points $x_0 \in \mathbb{R}^d$: $V(x_0) = E$ such that $\nabla_x V(x_0) = 0$, i.e. the blue point in Figure 7.

Theorem 3 (Theorem VII.2). *For one of the above given regions Ω , there exist*

- $h_0 = h_0(E, \varepsilon) > 0$,
- fixed exponents $s \in [-\infty, \infty)$, $t \geq 0$ and $\alpha \in [1, \infty]$ (to be defined below),
- a multiplicative constant $C = C(\Omega, V, E, \varepsilon) > 0$,

such that for any $2 \leq q \leq \infty$, any $h \in (0, h_0]$ and any γ_h such that $\gamma_h = \Pi_{E,h}\gamma_h = \gamma_h\Pi_{E,h}$

$$\boxed{\|\rho_{\gamma_h}\|_{L^{q/2}(\Omega)} \leq Ch^{-2s(q,d)} \log(1/h)^{2t(q,d)} \|\gamma_h\|_{\mathfrak{S}^{\alpha(q,d)}(L^2(\mathbb{R}^d))} \cdot} \quad (\text{II.3})$$

with

$$(s(q, d), t(q, d), \alpha(q, d)) = \begin{cases} (s_{\text{gene}}(q, d), t_{\text{gene}}(q, d), \alpha_{\text{gene}}(q, d)) & \text{for any } \Omega \subset \mathbb{R}_x^d, \\ (-\infty, 0, \infty) & \text{if } \Omega = \{V > E + \varepsilon\}, \\ (s_{\text{Sogge}}(q, d), t_{\text{Sogge}}(q, d), \alpha_{\text{Sogge}}(q, d)) & \text{if } \Omega = \{V < E - \varepsilon\}, \\ (s_{\text{TP}}(q, d), t_{\text{TP}}(q, d), \alpha_{\text{TP}}(q, d)) & \text{if } \Omega = \{|V - E| < \varepsilon\}. \end{cases}$$

Remark. As we can see in Figure 7, the considered regions $\Omega \subset \mathbb{R}_x^d$ are neighborhood of the points $x_0 \in \mathbb{R}^d$ such that $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ obey Assumption (cond). It is thus reasonable to recover the associated exponents $s = s_{\text{cond}}$, $t = t_{\text{cond}}$ and $\alpha = \alpha_{\text{cond}}$.

Although we do not obtain equivalent exponential decay estimates as the Agmon estimates in the classically forbidden region $\{V > E + \varepsilon\}$, note that the exponent $\alpha = \infty$ is the best possible and that we still have a decrease in $\mathcal{O}(h^\infty)$. Furthermore, the theorem gives the information that the worst concentrations are a priori around the turning points, that is coherent with the discussion on the scalar harmonic oscillator example and the pointwise bounds.

Optimality of the L^q estimates (referenced in Table 4) It remains the question of the sharpness of Koch-Tataru-Zworski (and our) L^q bounds in some regime of q . The saturated bounds can be reformulated into the following statement.

Theorem. *For given a confining potential $V : \mathbb{R}^d \rightarrow \mathbb{R}$, a fixed energy E with assumptions to specify, there exist*

- an error $\varepsilon > 0$,
- a sequence of energy E_h that depends on V and E ,
- a quasimode $u_h \in L^2(\mathbb{R}^d)$ of $P - E_h$ or a density matrix γ_h is the spectral cluster $\mathbb{1}(P \in [E_h - h, E_h + h]) (L^2(\mathbb{R}^d))$,
- exponents $s = s(q, d) \geq 0$ and $\alpha = \alpha(q, d) \geq 1$, which are equal to s_{cond} and α_{cond} , which appear in Theorems 1 and 3, in some regime of q (unfortunately not for all q in $[2, \infty]$),
- a set $\Omega \subset \mathbb{R}_x^d$ that can depend on V , E_h , ε ,

and

- $h_0 > 0$ (resp. a subsequence $\{h_n\}_{n \in \mathbb{N}} \subset \mathbb{R}_+^*$ with $h_n \rightarrow 0$),
- $C = C(d, h_0, V, E, \varepsilon) > 0$,

such that for any $h \in (0, h_0]$ (resp. along the subsequence $h_n \rightarrow 0$) and for any $2 \leq q \leq \infty$

$$\boxed{\frac{\|u_h\|_{L^q(\Omega)}}{\|u_h\|_{L^2(\mathbb{R}^d)}} \geq Ch^{-s(d,q)}} \quad (\text{II.4})$$

or

$$\boxed{\|\rho_{\gamma_h}\|_{L^{q/2}(\Omega)} \geq Ch^{-2s(d,q)} \text{rank } \gamma_h^{1/\alpha(q,d)}}. \quad (\text{II.5})$$

Before going into the details of our results, let us give some comments on the above Theorem.

- The parameter $\varepsilon > 0$ is here to specify a minimal radius, as in Theorem 3, in order to set Ω to be a subset of the h -dependent bulk $\{V < E_h - \varepsilon\}$ or take in account the turning points $\{V < E_h + \varepsilon\}$,
- We do not always have the exact expression of the sequences E_h (in some cases, we only prove their existence).

One-body optimality We construct in Section VIII.1 of Chapter 1: zonal type quasimodes, Gaussian beam type quasimodes and Gaussian ground state type quasimodes, that saturates Koch-Tataru-Zworski estimates in some regimes of q . We depicted their profile of concentration in Figure 9 and the optimal exponents in Figure 1.16 of Chapter 1.

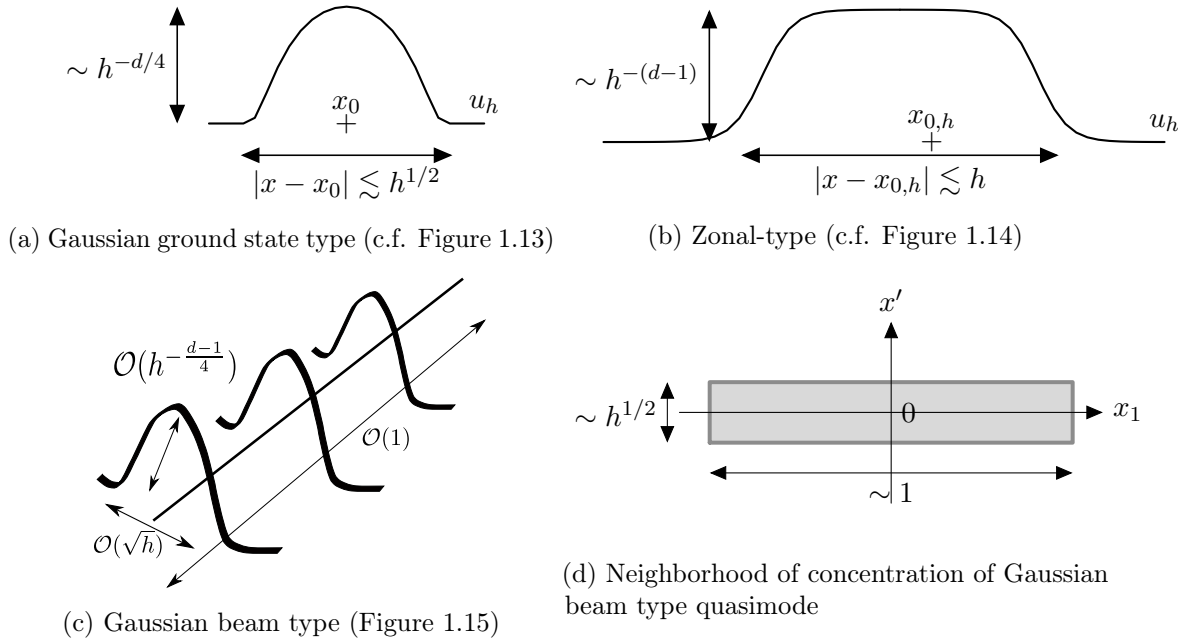


Figure 9 – Concentration of saturating quasimodes

The general statement is the following.

Theorem 4 (Propositions VIII.1, VIII.2 and Proposition VIII.4). *For given a confining potential $V : \mathbb{R}^d \rightarrow \mathbb{R}$, a fixed energy E , and error $\varepsilon > 0$ with assumptions to specify, there exist*

- a sequence of energy E_h that depends on V and E ,
- a quasimode $u_h \in L^2(\mathbb{R}^d)$ of $P - E_h$,
- exponents $s_{\text{mass}} = s_{\text{mass}}(q, d) \geq 0$ and $s_{\text{conc}} = s_{\text{conc}}(q, d) \geq 0$,

- a set $\Omega \subset \mathbb{R}_x^d$ that can depend on V, E_h, ε ,

and

- $h_0 > 0$ (resp. a subsequence $\{h_n\}_{n \in \mathbb{N}} \subset \mathbb{R}_+^*$ with $h_n \rightarrow 0$),
- $C_{\text{mass}} = C_{\text{mass}}(d, h_0, V, E, \varepsilon) > 0$ and $C_{\text{conc}} = C_{\text{conc}}(d, h_0, V, E, \varepsilon) > 0$,

such that for any $h \in (0, h_0]$ (resp. along the subsequence $h_n \rightarrow 0$) and for any $2 \leq q \leq \infty$

$$\boxed{\|u_h\|_{L^2(\mathbb{R}^d)} \leq C_{\text{mass}} h^{s_{\text{mass}}(q,d)}, \quad \|u_h\|_{L^q(\Omega)} \geq C_{\text{conc}} h^{-s_{\text{conc}}(q,d)}} \quad (\text{II.6})$$

Let us detail more our results for each case. In the two first cases, we construct functions, which concentrate at specific points²¹ $x_0 = x_0(h)$ (see Figures 9a and 9b). In the last one, the concentration is around a segment in a direction of one Euclidean coordinate (see Figures 9c and 9d).

- (a) *Gaussian ground state type quasimode* (Proposition VIII.1): we impose the condition that E is a local minimum of V and we set $x_0 \in \mathbb{R}^d$ a point where the minimum is reached. Then,

- we take $\Omega = \mathbb{R}^d$,
- we set u_h to be a L^2 -normalized shifted harmonic oscillator ground state centered in x_0 with an $h^{1/2}$ -scaling, which is then a quasimode of $P - E$,

so that $s_{\text{mass}}(q, d) = 0$ and $s_{\text{conc}}(q, d) = \frac{d}{2}(\frac{1}{2} - \frac{1}{q})$. This construction is well-known (see [Hel06, Chap.2] and [DS99, Chap.4]).

- (b) *Zonal type quasimode* (Proposition VIII.2): for a given V and energy $E > \min V$ with a condition of non-flatness of V in a neighborhood of $\{V = E\}$, we prove the existence of

- $\{E_h\}_{h>0} \subset \mathbb{R}_+^*$ near E ,
- $\{x_{0,h}\}_{h>0} \subset \mathbb{R}^d$ in the bulk $\{V < E_h - \varepsilon\}$,

so that we construct u_h in the spectral cluster of P associated to the spectral interval $[E_h - E, E_h + h]$ which is concentrated in $x_{0,h}$

- $u_h(x) := \mathbb{1}(P \in [E_h - E, E_h + h])(x_{0,h}, x)$,
- and we consider the h -dependent bulk $\Omega = \{V < E_h - \varepsilon\}$.

That gives $s_{\text{mass}}(q, d) = (d - 1)/2$ and $s_{\text{conc}}(q, d) = d - 1 - d/q$. This construction is the analogue of the one in [Sog17a, Chap.5].

- (c) *Gaussian beam type quasimode* (Proposition VIII.4): we consider $V(x) = |x|^2$, and we set E to be an excited state of the scalar harmonic oscillator so that we set

- u_h to be a L^2 -normalized eigenfunction, which is a tensor product of an excited state associated to E and $d - 1$ Gaussian ground states of the scalar harmonic oscillator,
- $E_h = E + (d - 1)h$ to be the eigenvalue of P associated to u_h ,
- and $\Omega = \{V(x) \leq E_h + \varepsilon\}$,

so that $s_{\text{mass}}(q, d) = 0$ and $s_{\text{conc}}(q, d) = d(\frac{1}{2} - \frac{1}{q}) - \frac{1}{2}$. This construction is a detailed version of [KT05, Sec.5.1].

²¹that we have to specify

We deduce the lower bounds (II.4) on the quotient of the L^q and L^2 norm from Theorem 4, under the previous assumptions. Here, it is enough to take $C = C_{\text{conc}}/C_{\text{mass}}$ and $s = s_{\text{conc}} - s_{\text{mass}}$. In particular, we have show that in the above three examples (see Figure 1.16 of Chapter 1)

- (a) the Gaussian ground state quasimodes (Remark 30 of Chapter 1): the exponent $s = s_{\text{gene}}$ for $2 \leq q \leq 2d/(d-2)$ is sharp,
- (b) the zonal type quasimodes (Remark 32 of Chapter 1): the exponent $s = s_{\text{Sogge}} = s_{\text{gene}}$ for large regime $2(d+1)/(d-1) \leq q \leq \infty$ is sharp,
- (c) the Gaussian beam type quasimodes (Remark 37 of Chapter 1): the exponent $s = s_{\text{Sogge}}$ for low regime $2 \leq q \leq 2(d+1)/(d-1)$ is sharp.

It is not clear that the estimates of the turning points in the intermediary regime $q \in [2(d+3)/(d+1), 2d/(d-2)]$ are optimal and this still remains an open question (see [KT05, Sec.5.3] for an intermediar result).

Many-body optimality result Similarly to the one-body case, we provide in Section VIII.2 of Chapter 1 a density matrix that saturates Sogge estimates in the bulk.

Theorem 5 (Many-body optimality in the bulk, Proposition VIII.5). *For given a confining potential $V : \mathbb{R}^d \rightarrow \mathbb{R}$ and a fixed energy $E > \min V$ with the non-flatness condition around $\{V = E\}$ ²² there exist*

- an error $\varepsilon > 0$,
- a sequence of energy E_h in a bounded neighborhood of E ,
- $h_0 > 0$ (resp. a subsequence $\{h_n\}_{n \in \mathbb{N}} \subset \mathbb{R}_+^*$ with $h_n \rightarrow 0$),
- $C = C(d, h_0, V, E, \varepsilon) > 0$,

such that denoting by $\Pi_{E_h, h} := \mathbf{1}(P \in [E_h - h, E_h + h])$ the spectral projector, one has for any $h \in (0, h_0]$ (resp. along the subsequence $h_n \rightarrow 0$) and for any $2 \leq q \leq \infty$

$$\|\rho_{\Pi_{E_h, h}}\|_{L^q(\{V < E_h - \varepsilon\})} \geq Ch^{-(d-1)}.$$

This result implies the saturation of the bounds (II.3) in the classically allowed region at the maximal range $\text{rank } \gamma_h = \text{rank } \Pi_{E_h, h}$ (see Remark 39 in Chapter 1).

Remark. For now, the optimality of the estimates in the bulk is not known for intermediary regimes ($1 < \text{rank } \gamma_h < \text{rank } \Pi_{E_h, h}$). This is not done either for the other estimates of Theorems 1 and 3 have not yet been done. It would be an interesting direction to explore.

An overview of the main results of Chapter 1

²²the same assumption as for the zonal type quasimode construction

Microlocalized L^p estimates (of form (II.1))		
Condition	on the symbol $p_E := p(x, \xi) - E$	Result
<i>General</i>	(gene)=(Assumption 2)	Theorem IV.2
<i>Sogge</i>	(Sogge)=(Assumption 3)	Theorem V.2
<i>Turning points</i>	(TP)=(Assumption 4)	Theorem VI.2
Spectral clusters L^p estimates (of form (II.3))		
Region $\Omega_{V,E} \subset \mathbb{R}^d$		Exponent
	$\Omega_{V,E} = \mathbb{R}^d$	(gene)
Classically forbidden	$\Omega_{V,E} = \{V > E + \varepsilon\}$	
Classically allowed	$\Omega_{V,E} = \{V < E - \varepsilon\}$	(Sogge)
Near turning points	$\Omega_{V,E} = \{ V - E < \varepsilon\}$	(TP)

Table 3 – Main L^p bounds results for density matrices

One-body optimality (of form (II.4))				
Type of concentration	Saturating quasimodes	Exponent	Regime of q	Results Fig. 1.16
<i>Around points</i> $x_0 = x_{0,h} \in \mathbb{R}^d$	Gaussian ground state x_0 loc. min. of $V - E$	s_{gene}	$q \geq \frac{2d}{d-2}$	Prop. VIII.1 Fig. 1.13
	Zonal type in h -bulk $\{V < E_h - \varepsilon\}$	s_{sogge} $= s_{\text{gene}}$	$q \geq q_c = \frac{2(d+1)}{d-1}$	Prop. VIII.2 Fig. 1.14
<i>Around a segment</i> (c.f. Figure 9d)	Gaussian beam type	s_{sogge}	$2 \leq q \leq q_c$	Prop. VIII.4 Fig. 1.15
Many-body optimality (of form (II.5))				
Region $\Omega_{V,E} \subset \mathbb{R}_x^d$	Saturating density	Exponents	Regime of q	Result
Bulk: $\Omega_{V,E} = \{V < E_h - \varepsilon\}$	$\rho_{\Pi_{E_h, h}}$	(Sogge)	$2 \leq q \leq \infty$	Prop. VIII.5

Table 4 – Saturated L^q bounds (in Section VIII of Chapter 1)

II.2 Results of Chapter 2: asymptotics for the case with interaction

Chapter 2 is dedicated to the grand-canonical version of Fournais, Lewin and Solovej fermionic limits [FLS18]. That allows to give an element of answer Question 12.

We provide in particular the weak convergence of the density of the almost-minimizers²³ of \hbar -generalized Hartree-Fock functional (see (I.15) in Chapter 2) i.e.

$$\mathcal{E}_{V-E, w}^{\text{HF}}(\gamma_{\hbar, \text{gHF}}) = e_{\hbar, V-E, w}^{\text{HF}} + o(\hbar^{-d}).$$

towards a minimizer ρ_{TF} of the Thomas-Fermi energy functional.

Theorem 6 (Weak and integrated Weyl law, Theorems 2 and 3 of Chapter 2). *Let $d \geq 1$. Given*

- a confining²⁴ potential $V : \mathbb{R}^d \rightarrow \mathbb{R}$,
- an energy $E \geq \min V$,

²³it is not obvious that minimizers exist

²⁴see Assumption 5 of Chapter 2

- a potential of interaction $w : \mathbb{R}^d \rightarrow \mathbb{R}$ even such that $w \in L^{1+d/2}(\mathbb{R}^d) + L_\varepsilon^\infty(\mathbb{R}^d)$ ²⁵ and 'repulsive'²⁶.

Then, there exists a minimizer ρ_{TF} of the Thomas-Fermi energy $\mathcal{E}_{V-E,w}^{\text{TF}}$ such that along a decreasing subsequence $\{\hbar_n\}_n \subset \mathbb{R}_+^*$ such that $\hbar_n \xrightarrow{n \rightarrow \infty} 0$

$$\hbar^d \rho_{\gamma_{\hbar, \text{gHF}}} \rightharpoonup \rho_{\text{TF}} \quad \text{in } L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d), \quad (\text{II.7})$$

and then,

$$\boxed{\hbar^d \int_{\mathbb{R}^d} \rho_{\gamma_{\hbar, \text{gHF}}}(x) dx \rightarrow \int_{\mathbb{R}^d} \rho_{\text{TF}}(x) dx.} \quad (\text{II.8})$$

Remark. In the case $w = 0$, we recover for the limit (II.8) the integrated Weyl law stated in (I.26), since in this case

$$\rho_{\text{TF}}(x) = \frac{|B_{\mathbb{R}^d}(0, 1)|}{(2\pi)^d} [E - V(x)]_+^{d/2}.$$

Moreover, one has a better result

- since all the limits hold without going along a subsequence $\hbar_n \rightarrow 0$,
- and one has a stronger limit than (II.7) with the pointwise convergence $\hbar^d \rho_{\gamma_{\hbar}}(x) \rightarrow \rho_{\text{TF}}(x)$ when $V(x) < E$ (see [DL21]).

Thus, Theorem 6 can be seen as a version of Weyl's law when we introduce interactions between particles.

Remark. We could have directly a convergence $\hbar \rightarrow 0$ without passing by a sub-sequence if we had uniqueness of the limit, i.e. if the Thomas-Fermi minimizer is unique. This is typically the case under the assumption $\hat{w} \geq 0$, since in this case the functional $\mathcal{E}_{V-E,w}^{\text{TF}}$ is strictly convex. It is not clear whether this is also the case under our condition (Assumption 8 of Chapter 2)

$$\forall \rho \geq 0, \quad D_w(\rho, \rho) \geq 0.$$

Actually, we deduce these convergences on the densities from the proof of the generalized grand-canonical Hartree-Fock energy's limit.

Theorem 7 (Theorem 1 of Chapter 2). *Under the same assumption as above²⁷, we have the convergence of the grand-canonical Hartree-Fock ground state energy (defined in (I.25))*

$$\boxed{\lim_{\hbar \rightarrow 0} \hbar^d e_{\hbar, V-E, w}^{\text{gHF}} = e_{V-E, w}^{\text{TF}},} \quad (\text{II.9})$$

to the Thomas-Fermi ground state energy

$$e_{V-E, w}^{\text{TF}} := \inf \left\{ \mathcal{E}_{V-E, w}^{\text{TF}}(\rho) : \rho \geq 0, \quad \rho \in L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d), \quad \int_{\mathbb{R}^d} V \rho < \infty \right\}.$$

Remark. We have proved limits on Hartree-Fock, but we could also study the full many-body Hamiltonian like Fournais, Lewin, Solovej [FLS18]. One would expect to have the limits (II.9) and (II.8) for the energy $e_{\hbar, V, w}(E)$.

²⁵c.f. Definition I.1 in Chapter 2

²⁶in the sense of Assumption 6 or Assumption I.13 for dimensions $d \in \{1, 2\}$ of Chapter 2

²⁷but we can allow to have in addition $w \in L^p(\mathbb{R}^d) + L_\varepsilon^\infty(\mathbb{R}^d)$ with p in bit more general that $1 + d/2$, i.e. $\max(d/2) < p < \infty$

We mention also an interesting problem which is a pointwise version of (II.8) in the same spirit as [DL21]. Given the Hartree-Fock nonlinearity, this question is far from simple.

Conjecture. *The density of the (almost)-optimizer $\gamma_{\hbar, \text{gHF}}$ of the \hbar -Hartree-Fock energy converges pointwise to a Thomas-Fermi minimizer (always along a subsequence)*

$$\rho_{\gamma_{\hbar, \text{gHF}}}(x) \underset{\hbar \rightarrow 0}{\sim} \hbar^{-d} \rho_{\text{TF}}(x),$$

for x in the bulk $\{V_{\hbar}^{\text{eff}} < E\}$ associated to the effective potential $V_{\hbar}^{\text{eff}} := V + \hbar^d w * \rho_{\gamma_{\hbar}}$, which form is not explicit.

Chapter 1

Non interacting particles: L^p estimates of densities

The contents of this chapter is an extended version of the preprint [Ngu22] (available online, at [hal-03655245](https://arxiv.org/abs/2203.03655)). Sections IV.3, VI.2 (and other surprises) were not present on this online version.

Abstract

We generalize the semiclassical L^p estimates of Koch, Tataru and Zworski in the setting of Schrödinger operators with confining potentials to density matrices. This is motivated by the problem of the concentration of free fermionic particles in a trapping potential. Our proof relies on semiclassical and many-body tools. As an application, we provide bounds on spectral clusters. We also discuss the optimality of the one-body and many-body bounds through explicit examples of quasimodes.

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I INTRODUCTION

This chapter is devoted to estimates related to the spatial concentration of orthonormal families of eigenfunctions of Schrödinger operators

$$P := -h^2\Delta + V$$

in the semiclassical regime $h \rightarrow 0$. Here $V : \mathbb{R}^d \rightarrow \mathbb{R}$ is the potential and $d \geq 1$ is the spatial dimension. We work in the convenient setting where V is smooth and $V(x) \rightarrow \infty$ as $|x| \rightarrow \infty$, so that P is a well-defined self-adjoint, bounded-below operator on $L^2(\mathbb{R}^d)$ with a discrete spectrum going to $+\infty$. This models trapped quantum systems, where particles are confined to live in an essentially bounded region of space. We are interested in the concentration properties of L^2 normalized eigenfunctions $\{u_h\}$ of P associated to an eigenvalue E (we have in mind the case where E is essentially h -independent or bounded in h). More precisely, we aim to determine how “concentrated” such an eigenfunction may be. To do so, we choose to measure concentration through the possible growth of the norms $\|u_h\|_{L^q(\mathbb{R}^d)}$ as $h \rightarrow 0$, for various choices of $q \in [2, \infty]$. Indeed, in the extreme case where u_h is essentially constant (meaning that it is close to an h -independent function), then the norms $\|u_h\|_{L^q(\mathbb{R}^d)}$ do not grow in h . On the contrary, if all the L^2 -mass of u_h is concentrated in a region $\Omega_h \subset \mathbb{R}^d$ with $|\Omega_h| \rightarrow 0$ as $h \rightarrow 0$, then we typically have $\|u_h\|_{L^q(\mathbb{R}^d)} \sim |\Omega_h|^{1/q-1/2} \rightarrow \infty$ as $h \rightarrow 0$, when $q > 2$. In the following, we will consider estimates of the type

$$\|u_h\|_{L^q(\mathbb{R}^d)} \leq Ch^{-s}, \tag{I.1}$$

for some $s > 0$ and $C > 0$ depending only on V and E , which we interpret as a measure of the highest “rate” of concentration of eigenfunctions of P as $h \rightarrow 0$. Notice that Sobolev embeddings imply the previous estimate with $s = d(\frac{1}{2} - \frac{1}{q})$, and we will see several cases where this exponent can be improved. Of particular importance is the determination of the optimal value of the exponent s , which amounts to construct explicit examples of u_h for which the upper bound (I.1) is also a lower bound (with possibly a different value of C).

This strategy to study concentration of functions via L^q norms was invented by Sogge, first in the context of spherical harmonics [Sog85], and then in the context of general compact Riemannian manifolds without boundary (where P is replaced by $-h^2\Delta_g$, the Laplace-Beltrami operator) [Sog88]. He not only considered eigenfunctions but more generally functions u_h in spectral clusters, i.e. that satisfy $u_h = \mathbb{1}(|P - E| \leq h) u_h$. Furthermore, he managed to find the optimal exponent $s = s(q)$ on any manifold, and proved that for high values of q , the highest rate of concentration was attained for specific functions concentrating around a point (generalizing the zonal spherical harmonics) while for low values of q , it was attained for functions concentrating around a curve (generalizing the gaussian beams on spheres). These results were later extended to the case of Schrödinger operators with confining potentials on \mathbb{R}^d (which is the case that we consider here) by Koch and Tataru in [KT05], and their method was revisited from the point of view of semiclassical analysis by Koch, Tataru and Zworski in [KTZ07]. This last article also treats the more general case of quasimodes u_h , i.e. that satisfy $(P - E)u_h = \mathcal{O}_{L^2}(h)$, and we will follow on their approach. Notice that many works were devoted to the improvement of Sogge's estimates for eigenfunctions, in specific geometries (typically with negative curvature, see for instance [HT15, HR16, Sog17b, BS19]). We will not pursue this direction here. The case of confining potentials is more complicated than the one of compact manifolds without potentials, due to the presence of a transition region between the classically allowed region $\{V \leq E\}$ and the classically forbidden region $\{V > E\}$. Indeed, Koch and Tataru discovered specific concentration phenomena in the transition region that did not appear in Sogge's work. This can be first understood in the one dimensional case, as we will explain below.

In this chapter, we investigate the more general situation of concentration of orthonormal families of quasimodes. This is motivated by the study of fermionic systems in quantum mechanics, where a simple way to model N non-interacting fermions is through N orthonormal functions $\{u_h^j\}_{1 \leq j \leq N}$ in $L^2(\mathbb{R}^d)$. The orthonormality is a manifestation of Pauli's exclusion principle, which states that two fermions cannot occupy the same quantum state. Intuitively, it means that two fermions cannot concentrate in the same region in space. Hence, while a single particle may be localized in a small region, many particles will tend to delocalize by this "repulsion" induced by Pauli's principle. To measure quantitatively the concentration of several particles, it is useful to introduce the spatial density of particles

$$\rho_h = \sum_{j=1}^N |u_h^j|^2,$$

and estimate the growth in h of its $L^{q/2}$ -norms, if each of the u_h^j is a quasimode of P . For $N = 1$, we recover the question mentioned above. One can estimate trivially using the triangle inequality and the $N = 1$ estimate (I.1),

$$\|\rho_h\|_{L^{q/2}(\mathbb{R}^d)} \leq \sum_{j=1}^N \|u_h^j\|_{L^q(\mathbb{R}^d)}^2 \leq C^2 h^{-2s} N.$$

Our goal in this work is to prove estimates of the type

$$\|\rho_h\|_{L^{q/2}(\mathbb{R}^d)} \leq C h^{-2s} N^\theta, \tag{I.2}$$

for some $\theta \in [0, 1]$. Notice that this estimate reduces to (I.1) in the case $N = 1$, and that it is a strict improvement of (I.1) only if $\theta < 1$ by the above argument. In the case of the Laplace-Beltrami operator on compact manifolds, it was done in [FS17b], where the sharp exponent $\theta = \theta(q)$ was found. Here, we generalize their work to the case of confining potentials. From the point of view of physics, the statistical properties of systems of non-interacting trapped fermions

and in particular of their possible scales of concentration has attracted some attention recently [DLDMS15, DLDMS18, DLDMS19, DLDS⁺21], and our work goes in a similar direction.

The fact that enough fermions tend to delocalize can be understood by the pointwise Weyl law, which informally states that

$$\rho_h(x) \sim_{h \rightarrow 0} \frac{|B_{\mathbb{R}^d}(0, 1)|}{(2\pi h)^d} (E - V(x))_+^{d/2}, \quad (\text{I.3})$$

when the u_h^j are chosen to be an orthonormal family of eigenfunctions associated to all the eigenvalues less than E of P . For this choice of $\{u_h^j\}_j$, the $L^{q/2}$ -norms of ρ are of the same order Ch^{-d} for all q , which underlines delocalization. Actually, this delocalization also occurs for a much lower number of functions. Indeed, if one does not consider all the eigenvalues less than E of P , but only the eigenvalues between $E - h$ and $E > \min V$, one can show (for $d \geq 2$, see Section VIII.2) that all the $L^{q/2}$ -norms are also of the same order ($Ch^{-(d-1)}$ in this case), so that delocalization is also true for this much smaller spectral window. We will see below that this example is very important to prove the sharpness of the exponent θ that we obtain in our estimates of the type (I.2). This is why (I.2) measures the transition between the localization for small N and the delocalization for N large enough: when $N = 1$, it is saturated by concentrated functions while for N large, it is saturated by a delocalized system of functions. On compact manifolds with $V = 0$, (I.3) was made rigorous by Avakumovic [Ava56], Levitan [Lev52] and Hörmander [Hor68, Thm. 1.1]. For confining potentials, this asymptotic fails close to the transition region $\{V = E\}$ and a pointwise Weyl law was proved for $V(x) = |x|^2$ in [Kar89] and more recently for general potentials in [DL21].

To understand what happens in the transition region $\{V = E\}$, and also to illustrate the transition between localization and delocalization, it is useful to consider the case of the harmonic oscillator $V(x) = x^2$ in $d = 1$, for which many explicit computations are available. For instance, asymptotics as $h \rightarrow 0$ of individual eigenfunctions u_h associated to an eigenvalue $E > 0$ (independent of h) are very well understood using BKW methods (see for instance [Olv97]) as depicted in Figure 1.1: in the classically allowed region $\{V < E\}$, u_h has size 1 (and oscillates, which is not measured by L^q -norms) and in the classically forbidden region $\{V > E\}$, it is exponentially decaying (both in h and $|x|$). An interesting phenomenon appears in the transition region $\{V = E\}$, since u_h has size $h^{-1/6}$ in a neighborhood of size $h^{2/3}$ of this region. One can thus see a concentration phenomenon which does not happen in the absence of a potential. Notice also that the concentration is only visible at the level of L^q -norms for large q because $\|u_h\|_{L^q(\mathbb{R}^d)} = 1$ for $2 \leq q \leq 4$ and $\|u_h\|_{L^q(\mathbb{R}^d)} = h^{-\frac{1}{6} + \frac{2}{3q}}$ for $q \geq 4$. Asymptotics of ρ_h , when u_h^j fill all the energy levels up to E , are also well-known by the same method as depicted in Figure 1.2: in the classically allowed region $\{V < E\}$, ρ_h has size h^{-1} and in the classically forbidden region $\{V > E\}$, it is also exponentially decaying. In the transition region, it displays some concentration, but contrary to the case of individual eigenfunctions, it is too small compared to the bulk $\{V < E\}$, so it is invisible in the $L^{q/2}$ -norms. In this case, all the $L^{q/2}$ -norms are of the same order h^{-1} . Of course, such an accurate pointwise information is very specific to the one-dimensional case and one cannot hope to extend it to higher dimensions. The results of [KT05, KTZ07] cover the higher dimension case using L^q -norms, at the level of eigenfunctions/quasimodes. We extend their results to the case of several functions. These one-dimensional examples also show the different behavior according to the different regions $\{V < E\}$, $\{V > E\}$ and $\{V = E\}$, and the higher dimensional results will also take into account these differences.

Let us now summarize (in a simplified way) our main results, which precise statements are in Theorem VII.2. First, we show that for any $E > \min V$ and for any $\varepsilon \in (0, E - \min V)$, one has

$$\|\rho_h\|_{L^{q/2}(\{V < E - \varepsilon\})} \leq Ch^{-2s} N^\theta,$$

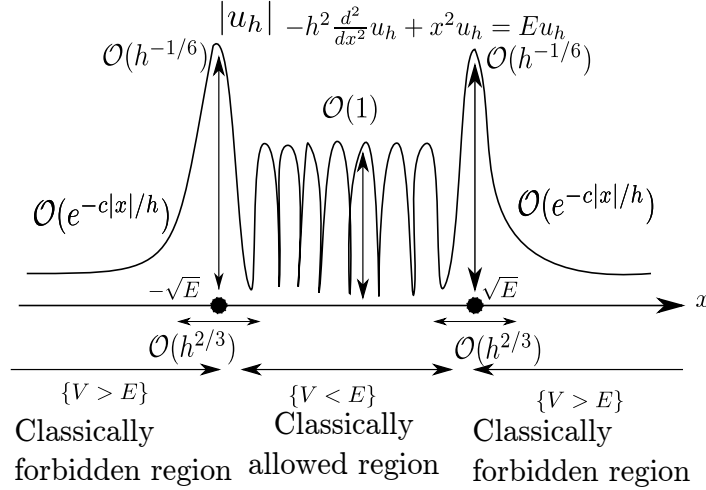


Figure 1.1 – Eigenfunction of the scalar harmonic oscillator associated to the eigenvalue E

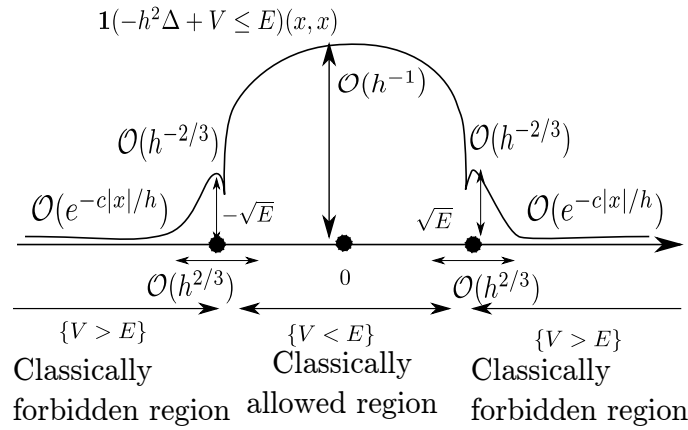


Figure 1.2 – Spectral projector of the scalar harmonic oscillator

for any orthonormal systems $\{u_h^j\}_{1 \leq j \leq N}$ of eigenfunctions associated to eigenvalues in $[E - h, E]$, for any N , with sharp values of s and θ (which are the same as on compact manifolds without potential). The sharp value of s is obtained for $N = 1$, while the sharp value of θ is obtained choosing the maximal number of such $\{u_h^j\}_j$. This case is the same as what happens on compact manifolds since we are far from the transition region. Around the transition region, we obtain a similar estimate

$$\|\rho_h\|_{L^{q/2}(\{|V-E| \leq \varepsilon\})} \leq Ch^{-2s} N^\theta,$$

with different values of exponents s and $\theta < 1$, and under the important assumption that $\nabla_x V \neq 0$ on $\{V = E\}$. These estimates are typically not sharp, even for $N = 1$, as noticed in [KT05], because there are obtained by summing rescaled estimates on multiple scales intermediate between a neighborhood of size $h^{2/3}$ of the transition region and the bulk. It is rather the estimates on each of these individual intermediate scales that are sharp (that is, the value of s is sharp), as proved in [KT05]. The sharpness of the exponent θ in these scales is an open question. Finally, we obtain estimates of the type

$$\|\rho_h\|_{L^{q/2}(\mathbb{R}^d)} \leq Ch^{-2s} N^\theta,$$

without any assumption on E or on the behavior of V on $\{V = E\}$. This is useful for instance in the case where $E = \min V$, in which there is no bulk. The exponent s is also sharp using again

$N = 1$ (the saturation happening for the ground state of P), while the sharpness of the exponent θ is also open.

Let us now comment on the methods of proof and detail the structure of the paper. As we already said, we use the strategy of [KTZ07] based on microlocal analysis, mixed with the many-body tools of [FS17b]. First, we notice (as we will see in Section VII) that it is enough to estimate functions u_h or u_h^j that are microlocalized, meaning that they 'live' in a compact region in the phase space $\mathbb{R}^d \times \mathbb{R}^d$. This is because spectral localization implies microlocalization for elliptic operators (see for instance (VII.8)). By compactness, it is thus enough to treat functions that are microlocalized around a point. Then, the properties of the classical symbol of P ,

$$p_E(x, \xi) = |\xi|^2 + V(x) - E, \quad (x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d,$$

at this point intervene. In Section III, we will treat elliptic points where $p_E \neq 0$. There, the main tools are Sobolev embeddings in the one-body case and the Kato-Seiler-Simon inequalities in the many-body case. In the region where $p_E = 0$, several cases are distinguished:

- In Section IV, we give a general estimate which is valid for any potential V and any energy E . The proof relies on adding an artificial time variable and use many-body Strichartz estimates in the spirit of [FLLS14, FS17a].
- In Section V, we treat the bulk case for which $p_E = 0$ but $V \neq E$. The proof relies on seeing one of the d space variables as a time variable and again use many-body Strichartz estimates.
- In Section VI, we treat the turning point region $p_E = 0$ and $V = E$, under the nondegeneracy assumption that $\nabla_x V \neq 0$ on this set. In a neighborhood of size $h^{2/3}$ of this region, we use a H^1 -estimate of [KTZ07] together with the Kato-Seiler-Simon inequality. The remaining region is split into multiple scales $2^j h^{2/3}$, and each of them is treated using the estimates of Section V by rescaling.

In Section VII, we gather all the previous estimates to obtain our main results on spectral clusters. Finally, we discuss their optimality in Section VIII.

In the following, we will consider a more general description of many-body states than orthonormal functions. Namely, we will consider one-body density matrices (nonnegative compact operators on $L^2(\mathbb{R}^d)$). Such an operator γ can be diagonalized in an orthonormal basis $\{u^j\}_j$ with associated eigenvalues $\{\lambda_j\}_j \subset \mathbb{R}_+$, and each λ_j is interpreted as the average number of particles described by the state γ which have wavefunction u^j . In this formalism, the case described above of N orthonormal functions $\{u^j\}_{1 \leq j \leq N}$ corresponds to $\gamma = P_N$, the orthogonal projection on the space generated by the $\{u^j\}_{1 \leq j \leq N}$. The N^θ factor in the right-side of (I.2) is then interpreted as the Schatten norm $\|P_N\|_{\mathfrak{S}^\alpha}$ where $\alpha = 1/\theta$ (see below for the definition of Schatten spaces). Furthermore, to any one-body density matrix γ , one can associate a density of particles

$$\rho_\gamma = \sum_{j=1}^N \lambda_j |u^j|^2,$$

which measures the spatial distribution of the particles described by γ . We will prove estimates similar to (I.2), where ρ_h in the left-side is replaced by ρ_γ and N^θ in the right-side is replaced by $\|\gamma\|_{\mathfrak{S}^\alpha}$.

As mentioned above, we will consider estimates on microlocalized objects. In the one-body setting, it means that one estimates $\|\chi^w u\|_{L^q}$ instead of $\|u\|_{L^q}$ for a fixed $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$, where χ^w denotes the Weyl quantization of the localization function χ (see below for the

definition). In the many-body setting, it means that one estimates $\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}}$ instead of $\|\rho_\gamma\|_{L^{q/2}}$. Furthermore, we also mentioned that one could more generally estimate quasimodes u_h (meaning that $\|u_h\|_{L^2(\mathbb{R}^d)} = 1$ and $(P - E)u_h = \mathcal{O}_{L^2}(h)$). An equivalent way to consider estimates for microlocalized quasimodes is to replace (I.1) by

$$\|\chi^w u_h\|_{L^q} \leq Ch^{-s} \left(\|u_h\|_{L^2(\mathbb{R}^d)} + \frac{1}{h} \|(P - E)u_h\|_{L^2(\mathbb{R}^d)} \right).$$

The generalization to the many-body setting is given by estimates of the type

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}} \leq Ch^{-2s} \left(\|\gamma\|_{\mathfrak{S}^\alpha} + \frac{1}{h^2} \|(P - E)\gamma(P - E)\|_{\mathfrak{S}^\alpha} \right). \quad (\text{I.4})$$

The advantage of such a formulation is that the microlocalization is imposed by χ^w and the property to be a quasimode is related to the choice of the norm in the right-side. Hence, we may prove (I.4) for general γ , the restriction to be a microlocalized quasimode being included in the form of the inequality. We will prove such estimates in Sections III to VI, with different values of s and α according to the properties of p_E on $\text{supp } \chi$.

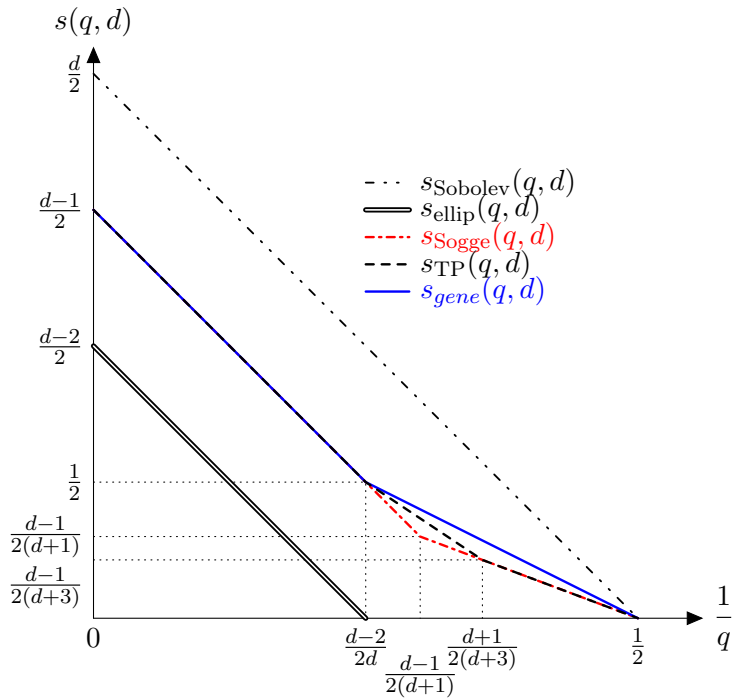


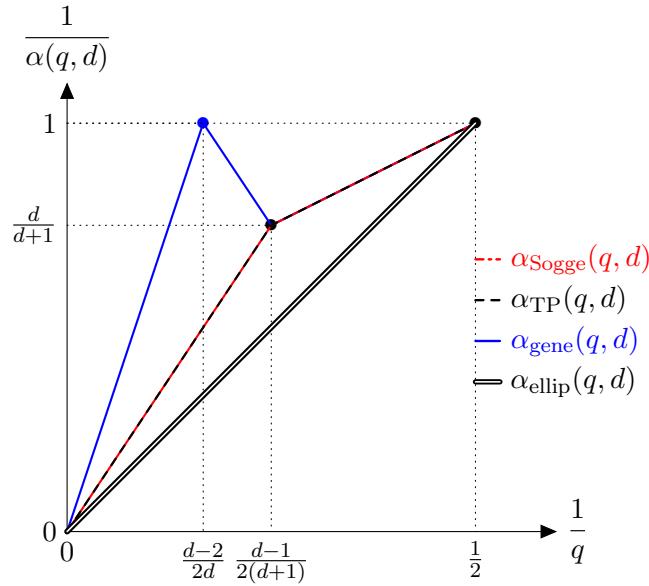
Figure 1.3 – Exponent $s(q, d)$ of microlocalized estimates when $d \geq 2$

II REVIEW OF SEMICLASSICAL ANALYSIS AND DENSITY MATRICES

Before going to the main results and their proofs, we recall the results of semiclassical analysis and density matrix analysis that we will use. We refer to [DS99], [Zwo12] and [Sim05] for further details.

II.1 Symbol classes and quantization

Let us recall the definitions of order functions and symbol classes. In the following, we will fix $d \in \mathbb{N}^*$, and we will use the notation $\langle x \rangle := (1 + |x|^2)^{1/2}$, for $x \in \mathbb{R}^d$.

Figure 1.4 – Schatten exponent $\alpha(q, d)$ when $d \geq 3$

Definition II.1 (Order functions [Zwo12, Sec. 4.4.1]). A function $m \in \mathcal{C}^\infty(\mathbb{R}^d \times \mathbb{R}^d, [0, \infty[)$ is called an *order function* on $\mathbb{R}^d \times \mathbb{R}^d$ if there exist $C, N > 0$ such that

$$\forall (x, \xi), (y, \eta) \in \mathbb{R}^d \times \mathbb{R}^d \quad m(x, \xi) \leq C(1 + |x - y| + |\xi - \eta|)^N m(y, \eta).$$

Remark 1. Relevant examples of order functions are $(x, \xi) \mapsto \langle x \rangle^k \langle \xi \rangle^\ell$ for any $k, \ell \in \mathbb{R}$.

Definition II.2 (Symbols [Zwo12, Sec. 4.4.1]). Let m be an order function on $\mathbb{R}^d \times \mathbb{R}^d$. A function $a \in \mathcal{C}^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ is a *symbol* in the class $S(m)$ if for all $\alpha \in \mathbb{N}^d \times \mathbb{N}^d$, there exists $C_\alpha > 0$ such that

$$\forall (x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d, \quad |\partial_{x, \xi}^\alpha a(x, \xi)| \leq C_\alpha m(x, \xi).$$

Remark 2. In the following, we will consider symbols a which will depend on an external parameter (which can be h). In that case, it will be important that the constants C_α are independent of the parameter.

Remark 3. Below, we will encounter symbols belonging to the Schwartz space $\mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$, which is equivalent to belong to the symbol classes $S(\langle x, \xi \rangle^{-k})$ for all $k \in \mathbb{N}$.

Notation. Let $N \in \mathbb{R}$ and $a \in S(m)$.

- We write $a = \mathcal{O}_{S(m)}(h^N)$ if for any $\alpha \in \mathbb{N}^{2d}$, there exists $C_{\alpha, N} > 0$, independent of h , such that

$$\forall (x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d, \quad |\partial_{x, \xi}^\alpha a(x, \xi)| \leq C_{\alpha, N} h^N m(x, \xi).$$

- We denote $a = \mathcal{O}_{S(m)}(h^\infty)$ if $a = \mathcal{O}_{S(m)}(h^N)$ for any $N \in \mathbb{N}$.

Similarly, for $a \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$, we write $a = \mathcal{O}_{\mathcal{S}}(h^N)$ (resp. $a = \mathcal{O}_{\mathcal{S}}(h^\infty)$) if $a = \mathcal{O}_{S(\langle x, \xi \rangle^{-k})}(h^N)$ (resp. $a = \mathcal{O}_{S(\langle x, \xi \rangle^{-k})}(h^\infty)$) for all $k \in \mathbb{N}$.

It will be essential for us that the classical symbol $p(x, \xi) = |\xi|^2 + V(x)$ is a symbol in the sense of the above definition. This motivates the following definition of the class of potentials that we consider.

Definition II.3. A potential $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$ has *at most polynomial growth* if there exists $k \in \mathbb{N}^*$ such that

$$\forall \alpha \in \mathbb{N}^d, \exists C_\alpha > 0, \forall x \in \mathbb{R}^d, |\partial^\alpha V(x)| \leq C_\alpha \langle x \rangle^k. \quad (\text{II.1})$$

Remark 4. In the above definition, (II.1) implies that $p(x, \xi) = |\xi|^2 + V(x)$ is in the symbol class $S(m)$ for $m(x, \xi) := \langle \xi \rangle^2 \langle x \rangle^k$.

Definition II.4 (Quantization, [Zwo12, Thm. 4.16]). Let m be an order function on $\mathbb{R}^d \times \mathbb{R}^d$ and $a \in S(m)$. Let $h > 0$. Let $\mathfrak{t} \in [0, 1]$. The \mathfrak{t} -quantization of a , denoted by $\text{Op}_h^\mathfrak{t}(a)$, is the linear continuous operator $\mathcal{S}(\mathbb{R}^d) \rightarrow \mathcal{S}(\mathbb{R}^d)$ defined by the formula

$$\text{Op}_h^\mathfrak{t}(a)u(x) = \frac{1}{(2\pi h)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} e^{i\frac{\xi \cdot (x-y)}{h}} a(\mathfrak{t}x + (1-\mathfrak{t})y, \xi) u(y) d\xi dy$$

for any $x \in \mathbb{R}^d$ and any $u \in \mathcal{S}(\mathbb{R}^d)$. For $\mathfrak{t} = 1/2$, $\text{Op}_h^{1/2}(a)$ is called the *Weyl quantization* of a and is also denoted by $a^w(x, hD)$. For $\mathfrak{t} = 1$, $\text{Op}_h^1(a)$ is called the *right quantization* of a and is also denoted by $a^R(x, hD)$.

II.2 Semiclassical pseudodifferential calculus

In the following, we list some standard operations on pseudodifferential operators. We only state them for the Weyl quantization to keep a light notation, but they are still valid for other quantizations.

Proposition II.5 (Composition of pseudodifferential operators [Zwo12, Thm. 4.12 and 4.18]). *Let m_1 and m_2 two order functions on $\mathbb{R}^d \times \mathbb{R}^d$. Let $a \in S(m_1)$ and $b \in S(m_2)$.*

1) *Then, there exists a symbol in $S(m_1 m_2)$, that we denote by $a \# b$, such that*

$$a^w(x, hD)b^w(x, hD) = (a \# b)^w(x, hD).$$

2) *Furthermore, there exists a unique family $\{c_j\}_{j \in \mathbb{N}} \subset S(m_1 m_2)$ supported in $\text{supp } a \cap \text{supp } b$ such that for any $N \in \mathbb{N}^*$, there exists $r_N \in S(m_1 m_2)$ such that*

$$a \# b = \sum_{j=0}^{N-1} h^j c_j + h^N r_N.$$

Moreover, we have $c_0 = ab$.

This result has two important corollaries.

Corollary II.6 (Disjoint supports [Zwo12, Thm. 4.12]). *Let $a \in S(m_1)$ and $b \in S(m_2)$ be such that $\text{supp } a \cap \text{supp } b = \emptyset$. Then,*

$$a \# b = \mathcal{O}_{S(m_1 m_2)}(h^\infty).$$

Corollary II.7 (Commutator). *Let $a \in S(m_1)$ and $b \in S(m_2)$. Then, there exists $r \in S(m_1 m_2)$ such that for any $h > 0$*

$$[a^w(x, hD), b^w(x, hD)] = hr^w(x, hD).$$

The following proposition quantifies the difference between two quantizations of the same symbol.

Proposition II.8 (Change of quantization [Zwo12, Thm. 4.13]). *Let $a \in S(m)$ and $\mathfrak{t}, \mathfrak{s} \in [0, 1]$. Then, there exists $\tilde{a}_{\mathfrak{t}, \mathfrak{s}} \in S(m)$ such that for any $h > 0$*

$$\text{Op}_h^\mathfrak{t}(a) - \text{Op}_h^\mathfrak{s}(a) = h \text{Op}_h^\mathfrak{t}(\tilde{a}_{\mathfrak{t}, \mathfrak{s}}).$$

Let us now recall the definition of locally elliptic symbols.

Definition II.9 (Elliptic symbol). Let m be an order function on $\mathbb{R}^d \times \mathbb{R}^d$. A symbol $a \in S(m)$ is *elliptic* on $U \subset \mathbb{R}^d \times \mathbb{R}^d$ if there exists $C > 0$ such that $|a(x, \xi)| \geq m(x, \xi)/C$ for all $(x, \xi) \in U$.

The following lemma gives local left and right inverses for quantization of locally elliptic symbols. These microlocal equalities will be very useful in the proof of Theorem VI.2.

Lemma II.10 ([KTZ07, Lem. 2.1]). *Let $\chi \in S(1)$, m be an order function and $a \in S(m)$ elliptic on $\text{supp } \chi$. Then, for any $t \in [0, 1]$, there exist $b_t \in S(1/m)$, $r_{1,t}, r_{2,t} \in S(1)$ such that*

$$\begin{aligned} \text{Op}_h^t(b_t) \text{Op}_h^t(a) \text{Op}_h^t(\chi) &= \text{Op}_h^t(\chi) + \text{Op}_h^t(r_{1,t}), \\ \text{Op}_h^t(a) \text{Op}_h^t(b_t) \text{Op}_h^t(\chi) &= \text{Op}_h^t(\chi) + \text{Op}_h^t(r_{2,t}), \end{aligned}$$

where $r_{1,t}, r_{2,t} = \mathcal{O}_{S(1)}(h^\infty)$. If $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ then $r_1, r_2 = \mathcal{O}_{\mathcal{S}}(h^\infty)$.

For any real elliptic $p \in S(m)$ (when $m \geq 1$), the operator $P = p^w(x, hD)$ is self-adjoint on a suitable domain ([Zwo12, Sec. 10.1.2]) so that $f(P)$ is well-defined by functional calculus, for any $f \in \mathcal{C}_c^\infty(\mathbb{R})$. The next theorem states that such $f(P)$ is actually a pseudodifferential operator and provides us information on its associated symbol. This result is crucial for justifying the application of microlocalized estimates (in Sections III, IV, V and VI) to spectral clusters in Section VII.

Theorem II.11 ([DS99, Thm. 8.7]). *Let m be an order function on $\mathbb{R}^d \times \mathbb{R}^d$ such that $m \geq 1$, $p \in S(m)$ be a symbol such that $p + i$ is elliptic on $\mathbb{R}^d \times \mathbb{R}^d$ and $P := p^w(x, hD)$. Let $f \in \mathcal{C}_c^\infty(\mathbb{R})$. Then, there exists $a \in \cap_{k \in \mathbb{N}} S(m^{-k})$ such that $f(P) = a^w(x, hD)$. Moreover, there exist functions $\{a_j\}_{j \in \mathbb{N}} \subset \cap_{k \in \mathbb{N}} S(m^{-k})$ supported in $\text{supp}(f \circ p)$ such that for all $N \geq 1$ there exists $r_N \in \cap_{k \in \mathbb{N}} S(m^{-k})$ such that*

$$a = \sum_{j=0}^{N-1} h^j a_j + h^N r_N.$$

In particular, the principal symbol a_0 is equal to $f \circ p$.

II.3 Semiclassical bounds

When a is in the Schwartz space $\mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$, the operator $a^w(x, hD)$ not only preserves continuously $\mathcal{S}(\mathbb{R}^d)$ (it is still valid for any symbol $a \in S(m)$), but it has the good property of extending to a regularizing operator.

Proposition II.12 ([Zwo12, Thm. 4.1]). *Let $a \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$. Then, for any $h > 0$, the operator $a^w(x, hD)$ maps continuously $\mathcal{S}'(\mathbb{R}^d)$ to $\mathcal{S}(\mathbb{R}^d)$.*

Let us recall the Calderon-Vaillancourt theorem, which implies the L^2 -boundness of the quantizations of symbols in $S(1)$.

Proposition II.13 (Calderon-Vaillancourt [Zwo12, Thm. 4.23]). *Let $a \in S(1)$. Then, for any $h > 0$, the operator $a^w(x, hD)$ extends to a bounded linear operator on $L^2(\mathbb{R}^d)$, with operator norm bounded uniformly in $h \in (0, 1]$.*

Let us state now basic semiclassical L^q estimates, from which one can deduce a semiclassical version of Sobolev embedding for microlocalized functions.

Lemma II.14 (Basic L^q estimates, [KTZ07, Lemma 2.2]). *Let $a \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$. Then, there exists $C > 0$ such that for any $h > 0$ and any $1 \leq p \leq q \leq \infty$*

$$\|a^w(x, hD)u\|_{L^q(\mathbb{R}^d)} \leq Ch^{-d\left(\frac{1}{p} - \frac{1}{q}\right)} \|u\|_{L^p(\mathbb{R}^d)}.$$

The exponent $d(1/p - 1/q)$ on the semiclassical parameter in the previous estimate can be indeed improved in the elliptic setting for $p = 2$.

Lemma II.15 (One-body elliptic estimates, [KTZ07, Thm. 3]). *Let $d \geq 1$. Let m be an order function on $\mathbb{R}^d \times \mathbb{R}^d$, $p \in S(m)$ and $P := p^w(x, hD)$ (or any other quantization). Let $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ such that*

$$p(x_0, \xi_0) \neq 0.$$

Then, there exists a neighborhood \mathcal{V} of (x_0, ξ_0) and $h_0 > 0$, such that for all $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ supported in \mathcal{V} , for any $0 < h \leq h_0$, there exists $C > 0$ such that for all $\mathfrak{t} \in [0, 1]$ and for all $2 \leq q \leq \infty$,

$$\|\text{Op}_h^{\mathfrak{t}}(\chi)u\|_{L^q(\mathbb{R}^d)} \leq Ch^{1-d(\frac{1}{2}-\frac{1}{q})} \left(\|u\|_{L^2(\mathbb{R}^d)} + \frac{1}{h} \|Pu\|_{L^2(\mathbb{R}^d)} \right).$$

Equivalently, for all $2 \leq q \leq \infty$

$$\text{Op}_h^{\mathfrak{t}}(\chi)(1 + P^*P/h^2)^{-1/2} = \mathcal{O} \left(h^{1-d(\frac{1}{2}-\frac{1}{q})} \right) : L^2(\mathbb{R}^d) \rightarrow L^q(\mathbb{R}^d). \quad (\text{II.2})$$

Remark 5. The bound of Lemma II.15 is one power of h better than the one in Lemma II.14 (for $p = 2$, c.f. Figure 1.3), thanks to the term involving the operator P on the right-side. This is particularly relevant for quasimodes u of P , since they satisfy $Pu = \mathcal{O}_{L^2}(h)\|u\|_{L^2}$.

Here, we state the integrated form of Weyl's law, which gives an asymptotics of the number of eigenfunctions of a pseudodifferential operator in a fixed interval as $h \rightarrow 0$.

Proposition II.16 (Integrated Weyl law, [DS99, Chap. 9]). *Let m be an order function such that $m(x, \xi) \rightarrow +\infty$ when $|(x, \xi)| \rightarrow +\infty$ and let $p \in S(m)$ be real valued such that $p + i$ is elliptic on $\mathbb{R}^d \times \mathbb{R}^d$. Let $a < b$ be two real numbers. For any $h > 0$, define $P = p^w(x, hD)$ and denote by $N_h([a, b])$ the number of eigenvalues of P in the interval $[a, b]$. Then, we have*

$$N_h([a, b]) = \frac{1}{(2\pi h)^d} \left[|p^{-1}([a, b])| + o_{h \rightarrow 0}(1) \right].$$

We now review well-known results on quantum dynamics and their propagators.

Lemma II.17 (Properties of the propagator $F(t, t_0)$, [Zwo12, Thm. 10.1]). *Let $n \in \mathbb{N}^*$ and $h > 0$. Let $t_0 \in \mathbb{R}$ and $a \in \mathcal{C}^\infty(\mathbb{R}_t, S_{\mathbb{R}^n \times \mathbb{R}^n}(1))$. The equation*

$$\begin{cases} [hD_t - a^w(t, x, hD_x)]F(t, t_0) = 0, & t \in \mathbb{R}, \\ F(t_0, t_0) = \text{Id}, \end{cases}$$

has a unique solution $\{F(t, t_0)\}_{t \in \mathbb{R}}$ in $\mathcal{C}(\mathbb{R}, \mathcal{B}(L^2(\mathbb{R}^n)))$, which is a family of unitary operators. Furthermore,

(i) *For any compact $J \subset \mathbb{R}$ and any $k, s \in \mathbb{N}$, there exists $C > 0$ (independent of h) such that for any $t, t_0 \in J$,*

$$\left\| (hD_t)^k F(t, t_0) \right\|_{H_h^s(\mathbb{R}^n) \rightarrow H_h^s(\mathbb{R}^n)} \leq C.$$

(ii) *For any $\psi_1 \in \mathcal{C}_c^\infty(\mathbb{R})$, the operator $\psi_1(t)F(t, t_0)$ maps continuously $H_h^s(\mathbb{R}^n)$ into $H_h^s(\mathbb{R}^{n+1})$ for all $s \in \mathbb{N}$ (with an operator norm independent of h).*

(iii) Let us define the operator T_F , which acts on functions on \mathbb{R}^{n+1} , by

$$T_F : u(t, x) \mapsto \psi_1(t) \int_{t_0}^t (F(t, s)u(s))(x) ds.$$

Then, T_F maps continuously $H_h^s(\mathbb{R}^{n+1})$ into $H_h^s(\mathbb{R}^{n+1})$ for all $s \in \mathbb{N}$ (with a bound independent of h).

Remark 6. The proof of (i) is done in [Zwo12, Thm. 10.1] in the case $k = 0$. The bounds for higher values of k can be obtained by induction using the equation satisfied by $F(t, t_0)$. The proofs of (ii) and (iii) follow from (i) by elementary arguments.

Let us now give a statement of semiclassical dispersive estimates, which are crucial ingredients in the proof of our results. The obtention of these dispersive bounds is based on the semiclassical parametrix construction of the propagator $F(t, r)$, using BKW method. The decay estimates then follows from the stationary phase formula. It is done in [Zwo12, Thm. 10.4 and 10.8] or in [DS99, Chapter 10].

Theorem II.18 (Semiclassical dispersive bounds). *Let $n \in \mathbb{N}$ be such that $n \geq 1$. Let $a = a_t(x, \xi) \in \mathcal{C}^\infty(\mathbb{R}_t, S_{\mathbb{R}^n \times \mathbb{R}^n}(1))$. Let $r \in \mathbb{R}$. Let $\{F(t, r)\}_{t \in \mathbb{R}}$ be the propagator of the Schrödinger evolution equation*

$$\begin{cases} [hD_t - a^w(t, x, hD_x)]F(t, r) = 0 & t \in \mathbb{R} \\ F(r, r) = \text{Id}. \end{cases}$$

For any $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$ and $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^n \times \mathbb{R}^n)$, let us define the microlocalized propagator $U(t, r)$ of the previous equation by

$$U(t, r) := \psi(t - r)F(t, r)\chi^w(x, hD).$$

Let $(x_0, \xi_0) \in \mathbb{R}^n \times \mathbb{R}^n$ and $I \subset \mathbb{R}$ a compact interval of \mathbb{R} , such that for all $t \in I$

$$\partial_\xi^2 a_t(x_0, \xi_0) \text{ is non-singular.} \quad (\text{II.3})$$

Then, for every open interval J such that $J \subset I$, there exist $\delta > 0$ independent of h and a neighborhood $U \times V$ of (x_0, ξ_0) such that for every $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$ supported in $(-\delta, \delta)$ and $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^n \times \mathbb{R}^n)$ supported in $U \times V$, we have the uniform bounds for all $t, s \in \mathbb{R}$

$$\begin{cases} \sup_{r \in J} \|U(t, r)U(s, r)^*\|_{L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n)} & \leq C \\ \sup_{r \in J} \|U(t, r)U(s, r)^*\|_{L^1(\mathbb{R}^n) \rightarrow L^\infty(\mathbb{R}^n)} & \leq Ch^{-n/2}(h + |t - s|)^{-n/2}. \end{cases} \quad (\text{II.4})$$

II.4 Density matrices

We finally review some definitions and standard results on Schatten spaces.

Definition II.19 (Schatten spaces). Let $\alpha \geq 1$. For any Hilbert spaces \mathcal{H} and \mathcal{H}' , we define the Schatten space $\mathfrak{S}^\alpha(\mathcal{H}, \mathcal{H}')$ as the set

$$\mathfrak{S}^\alpha(\mathcal{H}, \mathcal{H}') = \{A : \mathcal{H} \rightarrow \mathcal{H}' \text{ compact operator} : \text{Tr}_{\mathcal{H}}((A^*A)^{\alpha/2}) < \infty\}.$$

Endowed with the norm

$$\|A\|_{\mathfrak{S}^\alpha(\mathcal{H}, \mathcal{H}')} := \left(\text{Tr}_{\mathcal{H}}((A^*A)^{\alpha/2}) \right)^{1/\alpha},$$

it is a Banach space.

We can now state the Kato-Seiler-Simon inequalities, which are very useful tools in the many-body setting.

Lemma II.20 (Kato-Seiler-Simon, [Sim05, Thm. 4.1]). *Let $\alpha \geq 2$. Then, for all functions $f, g \in L^\alpha(\mathbb{R}^d)$, the operator $f(x)g(-i\nabla)$ is in $\mathfrak{S}^\alpha(L^2(\mathbb{R}^d))$ and*

$$\|f(x)g(-i\nabla)\|_{\mathfrak{S}^\alpha(L^2(\mathbb{R}^d))} \leq \frac{1}{(2\pi)^{d/2}} \|f\|_{L^\alpha(\mathbb{R}^d)} \|g\|_{L^\alpha(\mathbb{R}^d)}.$$

As a corollary, this implies a version of semiclassical Sobolev embedding estimates $H_h^m \hookrightarrow L^q$ for operators.

Lemma II.21 (Semiclassical Schatten Sobolev estimates). *Let $m \geq 0$ and $q \geq 2$. Then, if $\frac{1}{q} > \frac{1}{2} - \frac{m}{d}$, we have for all $W \in L^{2(q/2)'}(\mathbb{R}^d)$*

$$\left\| W(1 - h^2\Delta)^{-m/2} \right\|_{\mathfrak{S}^{2(q/2)'}(L^2(\mathbb{R}^d))} \leq Ch^{-d(\frac{1}{2} - \frac{1}{q})} \|W\|_{L^{2(q/2)'(\mathbb{R}^d)}}.$$

We will use the following complex interpolation result in Schatten spaces, which can be found in [FS17a, Prop. 1] (see also [Sim05, Thm. 2.9]).

Theorem II.22 (Complex interpolation in Schatten spaces). *Let $n \geq 1$. Let $a_0 < a_1$ be two real numbers. Let T be an application which maps the strip $S = \{z \in \mathbb{C}, a_0 \leq \Re z \leq a_1\}$ into bounded operators on $L^2(\mathbb{R}^{n+1})$. Moreover, let us assume that the family of operators $\{T_z\}_{z \in S}$ is analytic in the sense of Stein i.e.*

$$z \in S \mapsto \langle f, T_z g \rangle_{L^2(\mathbb{R}^{n+1})} \text{ is continuous for all simple functions } f, g.$$

and

$$z \in \overset{\circ}{S} \mapsto \langle f, T_z g \rangle_{L^2(\mathbb{R}^{n+1})} \text{ is analytic for all simple functions } f, g.$$

If there exist $C_0, C_1, b_0, b_1 > 0$ and $1 \leq r_0, r_1, p_0, p_1, q_0, q_1 \leq \infty$ such that for all $\sigma \in \mathbb{R}$, for all simple functions W_1, W_2 on \mathbb{R}^{n+1}

$$\forall j = 0, 1, \quad \|W_1 T_{a_j + i\sigma} W_2\|_{\mathfrak{S}^{r_j}(L^2(\mathbb{R}^{n+1}))} \leq C_j e^{b_j |\sigma|} \|W_1\|_{L_t^{p_j} L_x^{q_j}(\mathbb{R}^{n+1})} \|W_2\|_{L_t^{p_j} L_x^{q_j}(\mathbb{R}^{n+1})}.$$

then, for all $0 \leq \theta \leq 1$

$$\|W_1 T_{a_\theta} W_2\|_{\mathfrak{S}^{r_\theta}(L^2(\mathbb{R}^{n+1}))} \leq C_0^{1-\theta} C_1^\theta \|W_1\|_{L_t^{p_\theta} L_x^{q_\theta}(\mathbb{R}^{n+1})} \|W_2\|_{L_t^{p_\theta} L_x^{q_\theta}(\mathbb{R}^{n+1})},$$

where $a_\theta, r_\theta, p_\theta$ and q_θ are defined by

$$a_\theta = (1 - \theta)a_0 + \theta a_1, \quad \frac{1}{r_\theta} = \frac{1 - \theta}{r_0} + \frac{\theta}{r_1}, \quad \frac{1}{p_\theta} = \frac{1 - \theta}{p_0} + \frac{\theta}{p_1} \text{ and } \frac{1}{q_\theta} = \frac{1 - \theta}{q_0} + \frac{\theta}{q_1}.$$

II.5 Strichartz estimates for density matrices

In this section, we provide Strichartz estimates in Schatten spaces, which will be a key ingredient for our proof. They generalize the one-body Strichartz estimates [KTZ07, Prop. 4.3], which were also the key ingredient of the proof of Koch-Tataru-Zworski. Such many-body Strichartz estimates were discovered in [FLLS14], and later generalized in [FS17a]. Our proof is inspired by the one in [FS17a], and provides a way to obtain the full range of Strichartz estimates in Schatten spaces under the general assumption that the propagator satisfies dispersive estimates such as the one in Theorem II.18. In the one-body case, the fact that Strichartz estimates follow abstractly from dispersive bounds were discovered by Ginibre and Velo [GV92], and we generalize the results to the many-body case. Interestingly, our many-body proof uses complex interpolation in the spirit of the original proof of Strichartz [Str77] rather than the direct approach using the Hardy-Littlewood-Sobolev inequality of [GV92].

Theorem II.23. *Assume the same hypotheses as in Theorem II.18. Let $2 \leq q \leq \frac{2(n+1)}{n-1}$. Then, there exist $C > 0$ and $h_0 > 0$, such that for any $0 < h \leq h_0$, we have*

$$\sup_{r \in J} \|WU(t, r)\|_{\mathfrak{S}^2(\frac{2q}{q+2})'(L^2(\mathbb{R}^n), L^2(\mathbb{R}^{n+1}))} \leq C \|W\|_{L_t^{1+(\frac{2}{q-2}-\frac{n}{2})_-} L_x^{2(q/2)'(\mathbb{R}^{n+1})}} \times \\ \times \begin{cases} h^{-\frac{n}{2}(\frac{1}{2}-\frac{1}{q})} & \text{if } 2 \leq q < \frac{2(n+1)}{n-1}, \\ \log(1/h)^{\frac{1}{n+1}} h^{-\frac{1}{n+1}} & \text{if } q = \frac{2(n+1)}{n-1}, \end{cases}$$

for any $W \in L_t^{\frac{2(\frac{q}{2})'}{1+(\frac{2}{q-2}-\frac{n}{2})_-}} L_x^{2(q/2)'(\mathbb{R}^{n+1})}$.

Proof of Theorem II.23. Fix $r \in J$. Let $z \in \mathbb{C}$. For all $t, s \in \mathbb{R}$, let us define the operator $T_z(t, s, r)$ on $L^2(\mathbb{R}^n)$ by

$$T_z(t, s, r) := (t - s + i0)^z U(t, r) U(s, r)^*.$$

Let the operator $T_z(r)$ acting on functions on \mathbb{R}^{n+1} be defined by

$$\forall (f, g) \quad \langle f, T_z(r)g \rangle_{L^2(\mathbb{R}^{n+1})} = \int_{\mathbb{R} \times \mathbb{R}} \langle f(t), T_z(t, s, r)g(s) \rangle_{L^2(\mathbb{R}^n)} dt ds.$$

Defining $A = WU(t, r) : L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^{n+1})$, we notice that we have $AA^* = WT_0(r)\bar{W}$ so that the bound in the theorem will follow from estimating $WT_0(r)\bar{W}$ in $\mathfrak{S}(\frac{2q}{q+2})'(L^2(\mathbb{R}^{n+1}))$. We will use the following properties of the distribution $m_z(t) = (t + i0)^z$, which can be found in [GS64, Chap. I, Sec. 3.6]:

- ◊ the family $\{m_z\}_{z \in \mathbb{C}} \subset \mathcal{S}'(\mathbb{R})$ is analytic and for any $z \in \mathbb{C}$ each m_z admits a Fourier transform with this expression

$$\mathcal{F}((t + i0)^z)(\omega) = \frac{\sqrt{2\pi} e^{iz\pi/2}}{\Gamma(-z)} \omega_+^{-z-1}. \quad (\text{II.5})$$

- ◊ Let $z = -1 + i\sigma$ with $\sigma \in \mathbb{R}$, then \hat{m}_z is bounded and

$$\|\hat{m}_{-1+i\sigma}\|_{L^\infty(\mathbb{R})} \leq \sqrt{\frac{2}{\pi}} e^{\sigma\pi/2}. \quad (\text{II.6})$$

- ◊ When the real part of z is strictly greater than -1 , m_z is in $L_{\text{loc}}^1(\mathbb{R})$ and

$$|m_z(t)| \leq |t|^{\Re z}.$$

We will obtain bounds on $W_1 T_0(r) W_2$ for all simple functions W_1 and W_2 using Theorem II.22, estimating the operator $W_1 T_z(r) W_2$ in

- \mathfrak{S}^∞ for $\Re z = -1$,
- \mathfrak{S}^2 for $\Re z = \beta \geq \frac{n-1}{2}$.

Step 1. Schatten \mathfrak{S}^∞ -bounds. Let us prove that there exists $C > 0$ such that for any simple functions W_1, W_2 on \mathbb{R}^{n+1} and for any $\sigma \in \mathbb{R}$

$$\sup_{r \in J} \|W_1 T_{-1+i\sigma}(r) W_2\|_{\mathfrak{S}^\infty(L^2(\mathbb{R}^{n+1}))} \leq C e^{\sigma\pi/2} \|W_1\|_{L^\infty(\mathbb{R}^{n+1})} \|W_2\|_{L^\infty(\mathbb{R}^{n+1})}. \quad (\text{II.7})$$

Let $\sigma \in \mathbb{R}$ and F, G be functions $\mathcal{C}_c^\infty(\mathbb{R}^{n+1}) \subset L^2(\mathbb{R}^{n+1})$. We can write

$$\begin{aligned} & \langle F, T_{-1+i\sigma}(r) G \rangle_{L_{t,x}^2} \\ &= \int_{\mathbb{R} \times \mathbb{R}} \langle F(t), T_{-1+i\sigma}(t, s, r) G(s) \rangle_{L_x^2} dt ds \\ &= \int_{\mathbb{R} \times \mathbb{R}} \langle F(t), (t-s+i0)^{-1+i\sigma} U_\chi(t, r) U_\chi(s, r)^* G(s) \rangle_{L_x^2} dt ds \\ &= \int_{\mathbb{R} \times \mathbb{R}} (t-s+i0)^{-1+i\sigma} \langle U_\chi(t, r)^* F(t), U_\chi(s, r)^* G(s) \rangle_{L_x^2} dt ds. \end{aligned}$$

Define the functions f, g by

$$f(t, x; r) := (U_\chi(t, r)^* F(t, \cdot))(x) \quad \text{and} \quad g(t, x; r) := (U_\chi(t, r)^* G(t, \cdot))(x).$$

Given that

$$\sup_{t \in \mathbb{R}} \sup_{r \in J} \|U_\chi(t, r)^*\|_{L_x^2 \rightarrow L_x^2} \lesssim 1,$$

the previous functions satisfy the bounds

$$\begin{aligned} \sup_{r \in J} \|f(t, x; r)\|_{L_{t,x}^2(\mathbb{R}^{n+1})} &\lesssim \|F\|_{L_{t,x}^2(\mathbb{R}^{n+1})}, \\ \sup_{r \in J} \|g(t, x; r)\|_{L_{t,x}^2(\mathbb{R}^{n+1})} &\lesssim \|G\|_{L_{t,x}^2(\mathbb{R}^{n+1})}. \end{aligned}$$

We now write everything with the Fourier transform in the time variable, with $m_z(t) := (t+i0)^z$

$$\begin{aligned} & \langle F, T_{-1+i\sigma}(r) G \rangle_{L_{t,x}^2} \\ &= \int_{\mathbb{R} \times \mathbb{R}} m_{-1+i\sigma}(t-s) \langle f(t; r), g(s; r) \rangle_{L_x^2} dt ds \\ &= \sqrt{2\pi} \int_{\mathbb{R}} \hat{m}_{-1+i\sigma}(\omega) \langle \hat{f}(\omega; r), \hat{g}(\omega; r) \rangle_{L_x^2} d\omega. \end{aligned}$$

Hence, by the Cauchy-Schwarz inequality

$$\begin{aligned} \forall r \in J \quad & \left| \langle F, T_{-1+i\sigma}(r) G \rangle_{L_{t,x}^2} \right| \\ & \leq \sqrt{2\pi} \|\hat{m}_{-1+i\sigma}\|_{L^\infty(\mathbb{R})} \|\mathcal{F}_t(f)\|_{L_{\omega,x}^2(\mathbb{R}^{n+1})} \|\mathcal{F}_t(g)\|_{L_{\omega,x}^2(\mathbb{R}^{n+1})} \\ & \leq \sqrt{2\pi} \|\hat{m}_{-1+i\sigma}\|_{L^\infty(\mathbb{R})} \|f\|_{L_{t,x}^2(\mathbb{R}^{n+1})} \|g\|_{L_{t,x}^2(\mathbb{R}^{n+1})} \\ & \leq C \|\hat{m}_{-1+i\sigma}\|_{L^\infty(\mathbb{R})} \|F\|_{L_{t,x}^2(\mathbb{R}^{n+1})} \|G\|_{L_{t,x}^2(\mathbb{R}^{n+1})}. \end{aligned}$$

Finally, $\hat{m}_{-1+i\sigma} \in L^\infty(\mathbb{R})$ and we have the bound (II.6). Hence, we deduce a bound on $T_{-1+i\sigma} : L^2(\mathbb{R}^{n+1}) \rightarrow L^2(\mathbb{R}^{n+1})$, from which we deduce (II.7).

Step 2. Schatten \mathfrak{S}^2 -bounds. Let $\beta \geq \frac{n-1}{2}$. Let us prove that there exists $C > 0$ such that for any $z \in \mathbb{C}$ with $\Re z = \beta$, and any simple functions W_1, W_2 on \mathbb{R}^{n+1}

$$\begin{aligned} & \sup_{r \in J} \|W_1 T_z(r) W_2\|_{\mathfrak{S}^2(L^2(\mathbb{R}^{n+1}))} \\ & \leq C \|W_1\|_{L_t^{\frac{2}{1+(\beta-\frac{n}{2})}} L_x^2(\mathbb{R}^{n+1})} \|W_2\|_{L_t^{\frac{2}{1+(\beta-\frac{n}{2})}} L_x^2(\mathbb{R}^{n+1})} \times \\ & \quad \times \begin{cases} \log(1/h)^{1/2} h^{-n/2} & \text{if } \beta = \frac{n-1}{2}, \\ h^{-n/2} & \text{if } \frac{n-1}{2} < \beta \leq \infty. \end{cases} \end{aligned} \quad (\text{II.8})$$

By the $L^1 \rightarrow L^\infty$ -bound of (II.4), the integral kernel $T_z(t, s, r)(x, y)$ of $T_z(t, s, r)$ satisfies

$$\begin{aligned} \forall t, s \in \mathbb{R} \quad \sup_{r \in J} \|T_z(t, s, r)(x, y)\|_{L_{x,y}^\infty(\mathbb{R}^n \times \mathbb{R}^n)} &= \sup_{r \in J} \|T_z(t, s, r)\|_{L^1(\mathbb{R}^n) \rightarrow L^\infty(\mathbb{R}^n)} \\ &\lesssim h^{-n/2} |t-s|^{\Re z} (h+|t-s|)^{-n/2}. \end{aligned}$$

Thus, we obtain a bound on the \mathfrak{S}^2 -norm of $W_1 T_z(r) W_2$ for any $\beta := \Re z \geq 0$

$$\begin{aligned} \forall r \in J, \quad & \|W_1 T_z(r) W_2\|_{\mathfrak{S}^2(L^2(\mathbb{R}^{n+1}))}^2 \\ &= \int_{\mathbb{R}^{n+1}} \int_{\mathbb{R}^{n+1}} |W_1(t, x) T_z(t, x, s, y; r) W_2(s, y)|^2 dt dx ds dy \\ &\lesssim h^{-n} \int_{\mathbb{R}} \int_{\mathbb{R}} \mathbb{1}(|t-s| < 2\delta) \frac{|t-s|^{2\beta}}{(h+|t-s|)^n} \|W_1(t)\|_{L^2(\mathbb{R}^n)}^2 \|W_2(s)\|_{L^2(\mathbb{R}^n)}^2 dt ds \\ &\lesssim h^{-n} \begin{cases} \|W_1\|_{L_{t,x}^2(\mathbb{R}^{n+1})}^2 \|W_2\|_{L_{t,x}^2(\mathbb{R}^{n+1})}^2 & \text{if } \beta \geq \frac{n}{2}, \\ \|W_1\|_{L_t^{\frac{2}{1+\beta-\frac{n}{2}}} L_x^2(\mathbb{R}^{n+1})}^2 \|W_2\|_{L_t^{\frac{2}{1+\beta-\frac{n}{2}}} L_x^2(\mathbb{R}^{n+1})}^2 & \text{if } \frac{n-1}{2} < \beta < \frac{n}{2}, \\ \log(1/h) \|W_1\|_{L_t^{\frac{2}{1+\beta-\frac{n}{2}}} L_x^2(\mathbb{R}^{n+1})}^2 \|W_2\|_{L_t^{\frac{2}{1+\beta-\frac{n}{2}}} L_x^{2(\beta+1)}(\mathbb{R}^{n+1})}^2 & \text{if } \beta = \frac{n-1}{2}. \end{cases} \end{aligned}$$

In the first line, we used $|t-s|^{2\beta} (h+|t-s|)^{-n} \lesssim 1$ for $|t-s| < 2\delta$. In the second line, we used $|t-s|^{2\beta} (h+|t-s|)^{-n} \lesssim |t-s|^{2\beta-n}$ and the Hardy-Littlewood-Sobolev inequality. In the third line, we used the Young inequality and

$$\int_{-2\delta}^{2\delta} \frac{|t|^{n-1}}{(h+|t|)^n} dt \lesssim \log(1/h).$$

That ends the proof of (II.8).

Step 3. Conclusion. Interpolating $z = 0$ between $\Re z = -1$ and $\Re z = \beta \geq \frac{n-1}{2}$, by Theorem II.22, we get

$$\begin{aligned} \sup_{r \in J} \|W_1 T_0(r) W_2\|_{\mathfrak{S}^{2(\beta+1)}(L^2(\mathbb{R}^{n+1}))} &\lesssim \|W_1\|_{L_t^{\frac{2(\beta+1)}{1+(\beta-\frac{n}{2})}} L_x^{2(\beta+1)}(\mathbb{R}^{n+1})} \|W_2\|_{L_t^{\frac{2(\beta+1)}{1+(\beta-\frac{n}{2})}} L_x^{2(\beta+1)}(\mathbb{R}^{n+1})} \times \\ &\quad \times \begin{cases} h^{-\frac{n}{2(\beta+1)}} & \text{if } \beta > \frac{n-1}{2}, \\ \log(1/h)^{\frac{1}{n+1}} h^{-\frac{1}{n+1}} & \text{if } \beta = \frac{n-1}{2}. \end{cases} \end{aligned}$$

Defining $q \geq 2$ such that $2(q/2)' = 2(\beta+1)$, we have the desired estimates for all $2 \leq q \leq \frac{2(n+1)}{n-1}$. That ends the proof of Theorem II.23. \square

II.6 Relations between various estimates on quasimodes

Below, we will see several estimates of type (I.4) depending on how the phase space localization is made. Here, we explain how to relate these different estimates.

Let $d \geq 1$. Let m be an order function on $\mathbb{R}^d \times \mathbb{R}^d$, $p \in S(m)$ and $P := p^w(x, hD)$ (or any other quantization). In the following, we will consider parameters $q \in [2, \infty]$, $s, t \geq 0$ and $\alpha \geq 1$ satisfying

$$s \geq d \left(\frac{1}{2} - \frac{1}{q} \right) - 1 \quad \text{and} \quad \alpha \leq \frac{q}{2}. \quad (\text{II.9})$$

Remark 7. The previous assumption states that an estimate with a bound

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}} \leq Ch^{-2s} \log(1/h)^{2t} \left\| (1 + P^*P/h^2)^{1/2} \gamma (1 + P^*P/h^2)^{1/2} \right\|_{\mathfrak{S}^\alpha}$$

with (q, s, t, α) satisfying (II.9), is worse than the elliptic one, i.e. for which there is equality case of (II.9). Such an elliptic estimate is proved in Theorem III.1. Moreover, notice that the norm $\left\| (1 + P^*P/h^2)^{1/2} \gamma (1 + P^*P/h^2)^{1/2} \right\|_{\mathfrak{S}^\alpha}$ is equivalent to the norm $\|\gamma\|_{\mathfrak{S}^\alpha} + \frac{1}{h^2} \|P^* \gamma P\|_{\mathfrak{S}^\alpha}$.

The following is an assumption on $S \subset \mathbb{R}^d \times \mathbb{R}^d$, $q \in [2, \infty]$, $s, t \geq 0$ and $\alpha \geq 1$.

Assumption 1 (Microlocalization around points). The parameters $S \subset \mathbb{R}^d \times \mathbb{R}^d$, $q \in [2, \infty]$, $s, t \geq 0$ and $\alpha \geq 1$ satisfy Assumption 1 if for all $(x_0, \xi_0) \in S$, there exist a neighborhood \mathcal{V} of (x_0, ξ_0) and $h_0 > 0$, such that for all $\chi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ supported in \mathcal{V} , there exists $C > 0$ such that for any $0 < h \leq h_0$ and any bounded non-negative operator γ on $L^2(\mathbb{R}^d)$

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\mathbb{R}^d)} \leq C \log(1/h)^{2t} h^{-2s} \left\| (1 + P^*P/h^2)^{1/2} \gamma (1 + P^*P/h^2)^{1/2} \right\|_{\mathfrak{S}^\alpha}.$$

Theorem II.24 (Microlocalization in a compact). *Let $S \subset \mathbb{R}^d \times \mathbb{R}^d$, $q \in [2, \infty]$, $s, t \geq 0$ and $\alpha \geq 1$ be such that Assumption 1 hold. Then, for all $\chi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ supported in S , there exists $C > 0$ and $h_0 > 0$ such that for any $0 < h \leq h_0$ and any bounded non-negative operator γ on $L^2(\mathbb{R}^d)$*

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\mathbb{R}^d)} \leq C \log(1/h)^{2t} h^{-2s} \left\| (1 + P^*P/h^2)^{1/2} \gamma (1 + P^*P/h^2)^{1/2} \right\|_{\mathfrak{S}^\alpha}.$$

Proof of Theorem II.24. Since $\text{supp } \chi$ is compact and is contained on S , there exist open sets $\{\mathcal{V}_j\}_{j=1}^M$ given by Assumption 1 such that

$$\text{supp } \chi \subset \bigcup_{j=1}^M \mathcal{V}_j.$$

Moreover, one can find a partition of unity $1 = \sum_{j=1}^M \varphi_j$ on $\text{supp } \chi$ with $\text{supp } \varphi_j \subset \mathcal{V}_j$. Then, we have for all $j \in \{1, \dots, M\}$ bounds on $\|W(\chi \varphi_j)^w \sqrt{\gamma}\|_{\mathfrak{S}^2}$

$$\begin{aligned} & \|W(\chi \varphi_j)^w \sqrt{\gamma}\|_{\mathfrak{S}^2} \\ & \leq C \log(1/h)^t h^{-s} \left\| (1 + P^*P/h^2)^{1/2} \gamma (1 + P^*P/h^2)^{1/2} \right\|_{\mathfrak{S}^\alpha}^{1/2} \|W\|_{L^{2(q/2)' }(\mathbb{R}^d)}. \end{aligned}$$

Hence, by the triangle inequality, we deduce the bound on $\|W \chi^w \sqrt{\gamma}\|_{\mathfrak{S}^2}$ and then on $\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\mathbb{R}^d)}$. That ends the proof of Theorem II.24. \square

Theorem II.25 (Microlocalization and localization in space). *Let us impose the same assumptions of the previous Theorem II.24 and (II.9) on (q, s, t, α) . Then, for all $\chi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ and for all set $\Omega \subset \mathbb{R}^d$ such that*

$$\text{supp } \chi \cap \Omega \times \mathbb{R}^d \subset \overset{\circ}{S},$$

there exist $C > 0$ and $h_0 > 0$ such that for any $0 < h \leq h_0$ and any bounded non-negative operator γ on $L^2(\mathbb{R}^d)$

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\Omega)} \leq C \log(1/h)^{2t} h^{-2s} \left\| (1 + P^* P/h^2)^{1/2} \gamma (1 + P^* P/h^2)^{1/2} \right\|_{\mathfrak{S}^\alpha}.$$

Proof of Theorem II.25. Let $\tilde{\Omega} \subset \mathbb{R}^d$ an open bounded set such that $\Omega \subset \bar{\Omega} \subset \tilde{\Omega}$ and such that

$$\{(x, \xi) \in \text{supp } \chi : x \in \tilde{\Omega}\} \subset S.$$

Let $\chi_\Omega \in C_c^\infty(\mathbb{R}^d, [0, 1])$ be a function supported in $\tilde{\Omega}$ such that $\chi_\Omega = 1$ on Ω . We have

$$\begin{aligned} \|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\Omega)} &\leq \|\rho_{\chi_\Omega \chi^w \gamma \chi^w \chi_\Omega}\|_{L^{q/2}(\mathbb{R}^d)} \\ &= \sup_{W \in L^{2(q/2)' }(\mathbb{R}^d)} \frac{\int_{\mathbb{R}^d} \rho_{\chi_\Omega \chi^w \gamma \chi^w \chi_\Omega}(x) W(x)^2 dx}{\|W\|_{L^{2(q/2)' }(\mathbb{R}^d)}^2} \\ &= \sup_{W \in L^{2(q/2)' }(\mathbb{R}^d)} \frac{\text{Tr}_{L^2}(W \chi_\Omega \chi^w \chi_\Omega \gamma \chi^w W)}{\|W\|_{L^{2(q/2)' }(\mathbb{R}^d)}^2} \\ &= \sup_{W \in L^{2(q/2)' }(\mathbb{R}^d)} \frac{\|W \chi_\Omega \chi^w \sqrt{\gamma}\|_{\mathfrak{S}^2}^2}{\|W\|_{L^{2(q/2)' }(\mathbb{R}^d)}^2}. \end{aligned}$$

There exists $r \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$ such that

$$\chi_\Omega \chi^w = (\chi_\Omega \chi)^w + h r^w.$$

On the one hand, by the Hölder and Kato-Seiler-Simon inequalities (Lemma II.21) for $m \in \mathbb{N}$ such that $m > \frac{d}{2(q/2)'}$, for any $N \in \mathbb{N}$

$$\begin{aligned} &h \|W r^w \sqrt{\gamma}\|_{\mathfrak{S}^2} \\ &\leq h \|W \chi_\Omega (1 - h^2 \Delta)^{-m}\|_{\mathfrak{S}^{2(q/2)'}} \|(1 - h^2 \Delta)^m r^w\|_{\mathfrak{S}^\infty} \|\sqrt{\gamma}\|_{\mathfrak{S}^q} \\ &\leq C h^{1-d(\frac{1}{2}-\frac{1}{q})} \|W\|_{L^{2(q/2)' }(\mathbb{R}^d)} \|\gamma\|_{\mathfrak{S}^{q/2}}^{1/2}. \end{aligned}$$

On the other hand, by Theorem II.24 applied to S and (q, s, t, α) , there exist $C > 0$ and h_0 such that for any $0 < h \leq h_0$ and any non-negative operator γ on $L^2(\mathbb{R}^d)$

$$\begin{aligned} \sup_{W \in L^{2(q/2)' }(\mathbb{R}^d)} \frac{\|W (\chi_\Omega \chi)^w \sqrt{\gamma}\|_{\mathfrak{S}^2}^2}{\|W\|_{L^{2(q/2)' }(\mathbb{R}^d)}^2} &= \|\rho_{(\chi_\Omega \chi)^w \gamma (\chi_\Omega \chi)^w}\|_{L^{q/2}(\mathbb{R}^d)} \\ &\leq C \log(1/h)^{2t} h^{-2s} \left\| (1 + P^* P/h^2)^{1/2} \gamma (1 + P^* P/h^2)^{1/2} \right\|_{\mathfrak{S}^\alpha}. \end{aligned}$$

Finally, by the triangle inequality, we get the desired inequality. \square

Remark 8. The above proof shows that the result of Theorem II.25 also holds when $\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\Omega)}$ is replaced by $\|\rho_{\chi^w \chi_\Omega \gamma \chi_\Omega \chi^w}\|_{L^{q/2}(\mathbb{R}^d)}$ or $\|\rho_{\chi_\Omega \chi^w \gamma \chi^w \chi_\Omega}\|_{L^{q/2}(\mathbb{R}^d)}$.

It turns out that one can in fact in a microlocalized estimate change the quantization for the operator P or have the same one by replacing it by another operator having the same symbol to within an error $\mathcal{O}(h)$. We will see the usefulness of this result in Section VI.2.

Lemma II.26. *Let $m : \mathbb{R}^d \times \mathbb{R}^d \rightarrow (0, \infty)$ an order function and let $p, q \in S(m)$ such that $p - q = \mathcal{O}_{S(m)}(h)$. Let $\mathfrak{t} \in [0, 1]$ and let $Q := \text{Op}_h^{\mathfrak{t}}(q)$. Assume also that for given $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$, $(q, s, t, \alpha) \in [0, \infty] \times [0, \infty] \times [2, \infty] \times [1, \infty]$ such that $\alpha \leq q/2$, we have for any bounded positive self-adjoint operator γ on $L^2(\mathbb{R}^d)$*

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\mathbb{R}^d)} \leq Ch^{-2s} \log(1/h)^{2t} \left(\|\gamma\|_{\mathfrak{S}^\alpha} + \frac{1}{h^2} \|Q\gamma Q^*\|_{\mathfrak{S}^\alpha} \right). \quad (\text{II.10})$$

Then, we get up to a different constant $C > 0$ the same estimate with $Q := \text{Op}_h^{\mathfrak{s}}(p)$ instead of P for any $\mathfrak{s} \in [0, 1]$.

Proof of Lemma II.26. We will show that all we need is to write $P = Q + hR$ where R is a quantization of a symbol $r \in S(m)$.

- For more convenience, we can first assume that $\mathfrak{t} = \mathfrak{s}$. In this case, R be the \mathfrak{t} -quantization of the symbol $p - q \in S(m)$.
- Furthermore, the case of the change of quantization is given if we take $P := \text{Op}_h^{\mathfrak{t}}(p)$, $Q := \text{Op}_h^{\mathfrak{s}}(p)$, since (by Proposition II.8) there exists $r_{\mathfrak{t}} \in \mathcal{O}_{\mathcal{S}' \rightarrow \mathcal{S}}(h^\infty)$ such that $P = Q + hR$ for $R = \text{Op}_h^{\mathfrak{t}}(r)$.

Let us prove now (II.10) with Q instead of P . Let $\tilde{\chi} \in \mathcal{C}_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ such that $\tilde{\chi} = 1$ on $\text{supp } \chi$. Let us estimate the norms $\|\rho_{\chi^w \tilde{\chi}^w \gamma \tilde{\chi}^w \chi^w}\|_{L^{q/2}(\mathbb{R}^d)}$ and $\|\rho_{\chi^w (1 - \tilde{\chi}^w) \gamma (1 - \tilde{\chi}^w) \chi^w}\|_{L^{q/2}(\mathbb{R}^d)}$. On the one-hand $Q\tilde{\chi}^w = \tilde{\chi}^w \tilde{P} + [\tilde{P}, \tilde{\chi}^w] + hR\tilde{\chi}^w$. Furthermore, there exists $r_0 \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$ such that $hr_0^w = [\tilde{P}, \tilde{\chi}^w] + hR\tilde{\chi}^w$. We have for any $\alpha \geq 1$ by the Hölder inequality and Calderon-Vaillancourt theorem

$$\begin{aligned} \|Q\gamma Q^*\|_{\mathfrak{S}^\alpha} &= \|Q\sqrt{\gamma}\|_{\mathfrak{S}^{2\alpha}}^2 \leq \|\tilde{\chi}^w\|_{\mathfrak{S}^\infty} \|P\sqrt{\gamma}\|_{\mathfrak{S}^{2\alpha}}^2 + h^2 \|r_0^w\|_{\mathfrak{S}^\infty} \|\sqrt{\gamma}\|_{\mathfrak{S}^{2\alpha}}^2 \\ &\lesssim \|P\sqrt{\gamma}\|_{\mathfrak{S}^{2\alpha}}^2 + h^2 \|\sqrt{\gamma}\|_{\mathfrak{S}^{2\alpha}}^2. \end{aligned}$$

By (II.10) applied $\tilde{\chi}^w \gamma \tilde{\chi}^w$ and the previous inequality

$$\begin{aligned} \|\rho_{\chi^w \tilde{\chi}^w \gamma \tilde{\chi}^w \chi^w}\|_{L^{q/2}(\mathbb{R}^d)} &\lesssim h^{-2s} \log(1/h)^{2t} \left(\|\gamma\|_{\mathfrak{S}^\alpha} + \frac{1}{h^2} \|Q\tilde{\chi}^w \gamma \tilde{\chi}^w Q^*\|_{\mathfrak{S}^\alpha} \right) \\ &\lesssim h^{-2s} \log(1/h)^{2t} \left(\|\gamma\|_{\mathfrak{S}^\alpha} + \frac{1}{h^2} \|P\tilde{\chi}^w \gamma \tilde{\chi}^w P^*\|_{\mathfrak{S}^\alpha} \right). \end{aligned}$$

Besides, since $\chi^w (1 - \tilde{\chi}^w) = \mathcal{O}_{\mathcal{S}' \rightarrow \mathcal{S}}(h^\infty)$, we obtain by the Hölder and Kato-Seiler-Simon inequalities (Lemma II.21 applied to $m > \frac{d}{2(q/2)^\prime}$) so that

$$\begin{aligned} \|W\chi^w (1 - \tilde{\chi}^w) \sqrt{\gamma}\|_{\mathfrak{S}^2} &\leq \|W(1 - h^2\Delta)^{-m}\|_{\mathfrak{S}^{2(q/2)^\prime}} \|(1 - h^2\Delta)^m \chi^w (1 - \tilde{\chi}^w)\|_{\mathfrak{S}^\infty} \|\sqrt{\gamma}\|_{\mathfrak{S}^q} \\ &= \mathcal{O}(h^\infty) \|\gamma\|_{\mathfrak{S}^{q/2}}^{1/2}. \end{aligned}$$

Hence, by duality

$$\|\rho_{\chi^w (1 - \tilde{\chi}^w) \gamma (1 - \tilde{\chi}^w) \chi^w}\|_{L^{q/2}(\mathbb{R}^d)} = \mathcal{O}(h^\infty) \|\gamma\|_{\mathfrak{S}^{q/2}}.$$

Hence, by the triangle inequality

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\mathbb{R}^d)} \leq Ch^{-2s} \log(1/h)^{2t} \left(\|\gamma\|_{\mathfrak{S}^\alpha} + \frac{1}{h^2} \|P\gamma P^*\|_{\mathfrak{S}^\alpha} \right).$$

□

III ELLIPTIC ESTIMATES

In this section, we state and prove estimates in the elliptic region where $p \neq 0$. In the one-body case ($\text{rank } \gamma = 1$), one recovers Lemma II.15.

Theorem III.1 (Many-body elliptic estimates). *Let $d \geq 2$ and $2 \leq q \leq \infty$. Let m be an order function on $\mathbb{R}^d \times \mathbb{R}^d$ and $p \in S(m)$. Let $P := p^w(x, hD)$ (or any other quantization). Let $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ be a point such that*

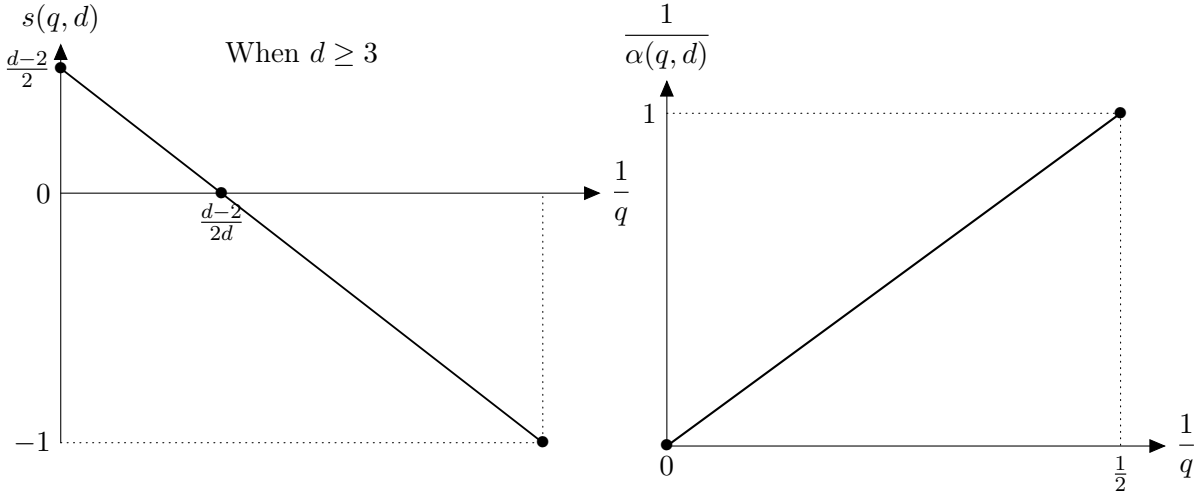
$$p(x_0, \xi_0) \neq 0.$$

Then, there exist a neighborhood \mathcal{V} of (x_0, ξ_0) and $h_0 > 0$, such that for any $\chi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ with support contained in \mathcal{V} , there exists $C > 0$ such that for any $0 < h \leq h_0$, for any bounded non-negative operator γ on $L^2(\mathbb{R}^d)$

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\mathbb{R}^d)} \leq Ch^{-2s(q,d)} \left\| (1 + P^*P/h^2)^{1/2} \gamma (1 + P^*P/h^2)^{1/2} \right\|_{\mathfrak{S}^{\alpha(q,d)}},$$

where the exponents s and α are given by

$$s(q, d) = d \left(\frac{1}{2} - \frac{1}{q} \right) - 1, \quad \alpha(q, d) = \frac{q}{2}.$$



Proof of Theorem III.1. There exists a neighborhood \mathcal{V} of (x_0, ξ_0) where p is non-zero. We have

$$\begin{aligned} & \|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\mathbb{R}^d)} \\ &= \sup_{W \in L^{(q/2)'}(\mathbb{R}^d)} \frac{\int_{\mathbb{R}^d} \rho_{\chi^w \gamma \chi^w}(x) |W(x)|^2 dx}{\|W\|_{L^{2(q/2)' }(\mathbb{R}^d)}^2} \\ &\leq \sup_{W \in L^{(q/2)'}(\mathbb{R}^d)} \frac{\text{Tr}_{L^2}(W \chi^w \gamma \chi^w W)}{\|W\|_{L^{2(q/2)' }(\mathbb{R}^d)}^2} \\ &\leq \sup_{W \in L^{(q/2)'}(\mathbb{R}^d)} \frac{\|W \chi^w (1 + P^*P/h^2)^{-1/2}\|_{\mathfrak{S}^{2(q/2)'}}^2}{\|W\|_{L^{2(q/2)' }(\mathbb{R}^d)}^2} \left\| (1 + P^*P/h^2)^{1/2} \gamma (1 + P^*P/h^2)^{1/2} \right\|_{\mathfrak{S}^{q/2}}. \end{aligned}$$

It remains to prove for any $2 \leq q \leq \infty$

$$\left\| W \chi^w (1 + P^*P/h^2)^{-1/2} \right\|_{\mathfrak{S}^{2(q/2)'}} \lesssim h^{1-d(\frac{1}{2}-\frac{1}{q})} \|W\|_{L^{2(q/2)' }(\mathbb{R}^d)},$$

i.e. for any $2 \leq \alpha \leq \infty$

$$\left\| W\chi^w(1 + P^*P/h^2)^{-1/2} \right\|_{\mathfrak{S}^\alpha} \lesssim h^{1-d/\alpha} \|W\|_{L^\alpha(\mathbb{R}^d)}.$$

Let us show the previous bound with $\alpha = 2$ and $\alpha = \infty$. The proof of Lemma II.15 indeed shows (II.2), that we recall:

$$\forall 2 \leq q \leq \infty, \quad \chi^w(1 + P^*P/h^2)^{-1/2} = \mathcal{O}\left(h^{1-d\left(\frac{1}{2}-\frac{1}{q}\right)}\right) : L^2(\mathbb{R}^d) \rightarrow L^q(\mathbb{R}^d).$$

The case $\alpha = \infty$ is given by the one function's estimate (II.2) applied to $q = 2$

$$\begin{aligned} \left\| W\chi^w(1 + P^*P/h^2)^{-1/2} \right\|_{\mathfrak{S}^\infty} &= \left\| W\chi^w(1 + P^*P/h^2)^{-1/2} \right\|_{L^2 \rightarrow L^2} \\ &\leq \left\| \chi^w(1 + P^*P/h^2)^{-1/2} \right\|_{L^2 \rightarrow L^2} \|W\|_{L^\infty(\mathbb{R}^d)} \\ &\lesssim h \|W\|_{L^\infty(\mathbb{R}^d)}. \end{aligned}$$

Suppose that $\alpha = 2$. We write the \mathfrak{S}^2 norm with respect to the integral kernel and use the one function's estimate (II.2) applied to $q = \infty$

$$\begin{aligned} \left\| W\chi^w(1 + P^*P/h^2)^{-1/2} \right\|_{\mathfrak{S}^2}^2 &= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \left| \left(W\chi^w(1 + P^*P/h^2)^{-1/2} \right) (x, y) \right|^2 dx dy \\ &= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} |W(x)|^2 \left| \left(\chi^w(1 + P^*P/h^2)^{-1/2} \right) (x, y) \right|^2 dx dy \\ &\leq \|W\|_{L^2(\mathbb{R}^d)}^2 \sup_{x \in \mathbb{R}^d} \left\| \left(\chi^w(1 + P^*P/h^2)^{-1/2} \right) (x, \cdot) \right\|_{L^2(\mathbb{R}^d)}^2 \\ &\leq \|W\|_{L^2(\mathbb{R}^d)}^2 \left\| \left(\chi^w(1 + P^*P/h^2)^{-1/2} \right) (x, y) \right\|_{L_x^\infty L_y^2(\mathbb{R}^d \times \mathbb{R}^d)}^2 \\ &\leq \|W\|_{L^2(\mathbb{R}^d)}^2 \left\| \chi^w(1 + P^*P/h^2)^{-1/2} \right\|_{L^2 \rightarrow L^\infty}^2 \\ &\lesssim h^{2-d} \|W\|_{L^2(\mathbb{R}^d)}^2. \end{aligned}$$

We may thus write

$$\left\| W\chi^w(1 + P^*P/h^2)^{-1/2} \right\|_{\mathfrak{S}^2} \lesssim h^{1-d/2} \|W\|_{L^2(\mathbb{R}^d)}.$$

Then, by interpolation between the two previous bounds we get the bounds for all the exponents $2 \leq \alpha \leq \infty$. Finally, for any $2 \leq q \leq \infty$

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\mathbb{R}^d)} \leq Ch^{2-2d\left(\frac{1}{2}-\frac{1}{q}\right)} \left\| (1 + P^*P/h^2)^{1/2} \gamma (1 + P^*P/h^2)^{1/2} \right\|_{\mathfrak{S}^{q/2}}.$$

□

IV MORE GENERAL L^p ESTIMATES

We now turn to the region $p = 0$. We give a general first estimate which holds under the sole assumption that $\partial_\xi^2 p$ is not degenerate. This is particularly useful in the context of Schrödinger operators, because this assumption holds without any hypothesis on the potential V . In the one-body case ($\text{rank } \gamma = 1$), we recover [KTZ07, Thm. 6] (up to logarithmic factors which appear in few cases).

IV.1 Statement of the result

Let $d \geq 1$. Let m be an order function on $\mathbb{R}^d \times \mathbb{R}^d$, $p \in S(m)$ be real-valued and $P := p^w(x, hD)$ (the following theorem are also true for any other quantization P of p).

Assumption 2. A point $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ satisfies the *general nondegeneracy condition* for the symbol p if

$$\partial_{\xi}^2 p(x_0, \xi_0) \text{ is non-degenerate.}$$

Remark 9. For Schrödinger operators $p(x, \xi) = \xi^2 + V(x) - E$ with $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$ satisfying Definition II.3, the previous assumption is satisfied for all $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$.

Recall first the one-body result.

Theorem IV.1 (General one-body estimates, [KTZ07, Thm. 6]). *Let $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ be a point satisfying Assumption 2. Then, there exist a neighborhood \mathcal{V} of (x_0, ξ_0) and $h_0 > 0$, such that for any $\chi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ with support contained in \mathcal{V} , there exists $C > 0$ such that for any $0 < h \leq h_0$, for any $2 \leq q \leq \infty$ and $u \in L^2(\mathbb{R}^d)$,*

$$\|\chi^w u\|_{L^q(\mathbb{R}^d)} \leq C \log(1/h)^{t(q,d)} h^{-s(q,d)} \left(\|u\|_{L^2(\mathbb{R}^d)} + \frac{1}{h} \|Pu\|_{L^2(\mathbb{R}^d)} \right)$$

where $s(q, d)$ and $t(q, d)$ and are given by the formulas

- when $d = 1$:

$$t(q, 1) = 0 \quad \text{and} \quad s(q, 1) = \frac{1}{2} \left(\frac{1}{2} - \frac{1}{q} \right),$$

- when $d = 2$:

$$t(q, 2) = \begin{cases} 0 & \text{if } 2 \leq q < \infty, \\ \frac{1}{2} & \text{if } q = \infty. \end{cases} \quad \text{and} \quad s(q, 2) = \frac{1}{2} - \frac{1}{q},$$

- when $d \geq 3$: $t(q, d) = 0$ and

$$s(q, d) = \begin{cases} \frac{d}{2} \left(\frac{1}{2} - \frac{1}{q} \right) & \text{if } 2 \leq q \leq \frac{2d}{d-2}, \\ d \left(\frac{1}{2} - \frac{1}{q} \right) - \frac{1}{2} & \text{if } \frac{2d}{d-2} \leq q \leq \infty. \end{cases} \quad (\text{IV.1})$$

Equivalently, one has for all $2 \leq q \leq \infty$

$$\chi^w (1 + P^* P / h^2)^{-1/2} = \mathcal{O} \left(\log(1/h)^{t(q,d)} h^{-s(q,d)} \right) : L^2(\mathbb{R}^d) \rightarrow L^q(\mathbb{R}^d).$$

Remark 10. The exponent s_{gene} defined on Theorem IV.1 is larger or equal to the one in Sobolev estimates $s_{\text{Sobolev}}(q, d) = d(1/2 - 1/q)$ ($s_{\text{gene}}(q, d) > s_{\text{Sobolev}}(q, d)$ for $2 < q \leq \infty$, and they are equal for $q = 2$). It is also strictly smaller than the exponent of the elliptic estimates $s_{\text{ellip}}(q, d) = d(1/2 - 1/q) - 1$ (see Figure 1.3).

Theorem IV.2 (General many-body estimates). *Let $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ be a point satisfying Assumption 2. Then, there exist a neighborhood \mathcal{V} of (x_0, ξ_0) and $h_0 > 0$, such that for any $\chi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ with support contained in \mathcal{V} , there exists $C > 0$ such that for any $2 \leq q \leq \infty$, for any $0 < h \leq h_0$, for any bounded non-negative operator γ on $L^2(\mathbb{R}^d)$*

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\mathbb{R}^d)} \leq C \log(1/h)^{2t(q,d)} h^{-2s(q,d)} \left\| (1 + P^2/h^2)^{1/2} \gamma (1 + P^2/h^2)^{1/2} \right\|_{\mathfrak{S}^{\alpha(q,d)}}$$

where $s(q, d)$ is given by the formula (IV.1) and $t(q, d)$, $\alpha(q, d)$ are given by

- when $d = 1$:

$$t(q, 1) = 0 \quad \text{and} \quad \alpha(q, 1) = \frac{q}{2}.$$

- when $d = 2$:

$$t(q, 2) = \begin{cases} 0 & \text{if } 2 \leq q < 6, \\ \frac{1}{2} - \frac{1}{q} & \text{if } 6 \leq q \leq \infty, \end{cases} \quad (\text{IV.2})$$

and

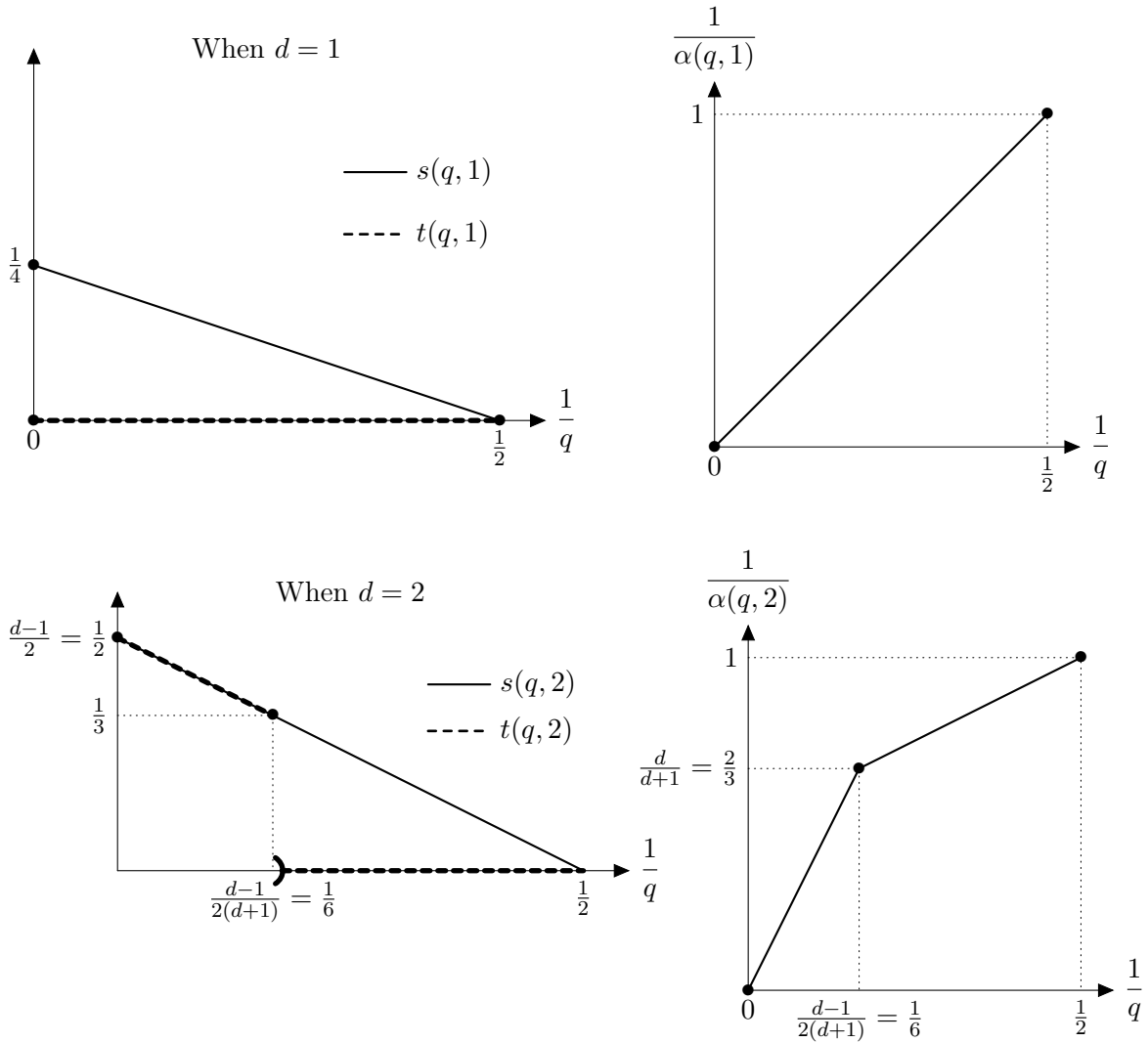
$$\alpha(q, 2) = \begin{cases} \frac{2q}{q+2} & \text{if } 2 \leq q \leq 6, \\ \frac{q}{4} & \text{if } 6 \leq q \leq \infty, \end{cases} \quad (\text{IV.3})$$

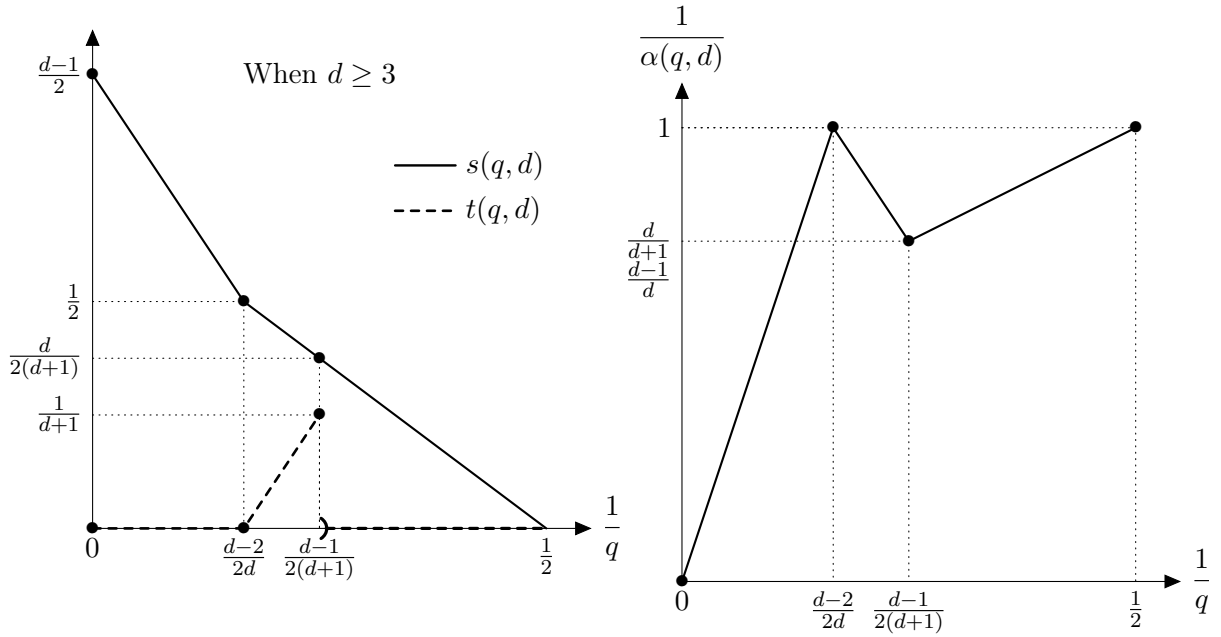
- when $d \geq 3$:

$$t(q, d) = \begin{cases} 0 & \text{if } 2 \leq q < \frac{2(d+1)}{d-1} \\ \frac{d}{q} - \frac{d-2}{2} & \text{if } \frac{2(d+1)}{d-1} \leq q \leq \frac{2d}{d-2} \\ 0 & \text{if } \frac{2d}{d-2} \leq q \leq \infty, \end{cases} \quad (\text{IV.4})$$

and

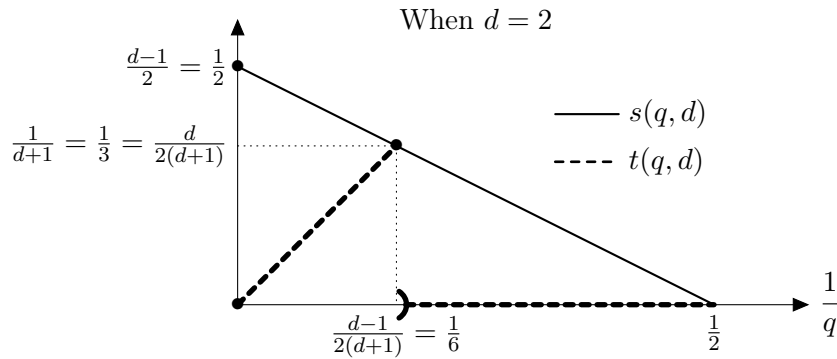
$$\alpha(q, d) = \begin{cases} \frac{2q}{q+2} & \text{if } 2 \leq q \leq \frac{2(d+1)}{d-1} \\ \frac{2q}{d(q-2)} & \text{if } \frac{2(d+1)}{d-1} \leq q \leq \frac{2d}{d-2} \\ \frac{(d-2)}{2d}q & \text{if } \frac{2d}{d-2} \leq q \leq \infty. \end{cases} \quad (\text{IV.5})$$





Some comments on improvement

Remark 11. In dimension 2, in the case of Schrödinger operators for the symbols $p(x, \xi) = |\xi|^2 + V(x)$ satisfying Definition II.3, Smith and Zworski [SZ13] proved that Theorem IV.1 is true with $t(\infty, 2) = 0$ (which means that we can get rid of the logarithm in dimension 2 for $q = \infty$). This implies that we can set $t(\infty, 2) = 0$ in Theorem IV.2 as well, and by interpolation Theorem IV.2 holds for $t(q, 2) = \frac{2}{q}$ for all $q \in [6, \infty]$.



Remark 12. When $d \geq 3$, the Schatten exponent that we obtain in Theorem IV.2 for the Keel-Tao endpoint $q = 2d/(d - 2)$ is $\alpha = 1$. Frank and Sabin [FS17c, Lem. 2] proved that this Schatten exponent is sharp in the related context of the Strichartz estimates associated to the propagator $e^{it\Delta}$. We expect that this result extends to our context, however it is not straightforward to adapt their proof. Indeed, their strategy amounts to showing that the dual operator is not compact, while here the dual operator is compact. Hence, we would rather need to quantify the “loss of compactness“ of our dual operator as $h \rightarrow 0$, which is a very interesting problem. One can quantify the loss of compactness of this operator when h goes to 0

$$\sup_{h>0} \sup_{r \in J} h^{1/2} \|W(x)U_\chi(t, r)\|_{\mathfrak{S}^\beta(L^2(I \times \mathbb{R}^d))} = \infty$$

and find the infimum of $\beta > 1$.

IV.2 Notation for the proof of Theorem IV.1 and Theorem IV.2

- Let $\delta \in]0, 1[$ and $I = [-\delta/2, \delta/2]$.
- Let $J = [-1, 1]$.
- Let $\psi \in C_c^\infty(\mathbb{R})$ such that $\text{supp } \psi \subset \overset{\circ}{I}$ and $\psi \neq 0$.
- Let $\tilde{\psi} \in C_c^\infty(\mathbb{R})$ such that $\tilde{\psi} = 1$ on I and $\text{supp } \tilde{\psi} \subset [-\delta, \delta]$.
- Let $\mathcal{V} = U \times V$ a bounded open neighborhood of (x_0, ξ_0) .
- Let $\chi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ be such that $\text{supp } \chi \subset \mathcal{V}$.
- Let $\tilde{\chi} \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d, [0, 1])$ be such that $\tilde{\chi} = 1$ on $\text{supp } \chi$ and such that $\text{supp } \tilde{\chi} \subset \mathcal{V}$.
- Let $\chi_0 \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ such that $\chi_0 = 1$ on a neighborhood of (x_0, ξ_0) .

We will add constraints on δ and \mathcal{V} along the proof.

IV.3 Proof of the one-body general estimates, Theorem IV.1

We can observe that a transition point in the semiclassical constant $h^{-2s} \log(1/h)^{2t}$ appears in the many-body case at the point $q = 2(d+1)/(d-1)$ for the logarithmic exponent $t(q, d) = 1/(d+1)$ when $d \geq 2$ (the other one $s(q, d)$ remains the same). This is not the case in the one-body case (see Figure 1.5, or Remark 15 which sums up the technical differences of the two proofs).

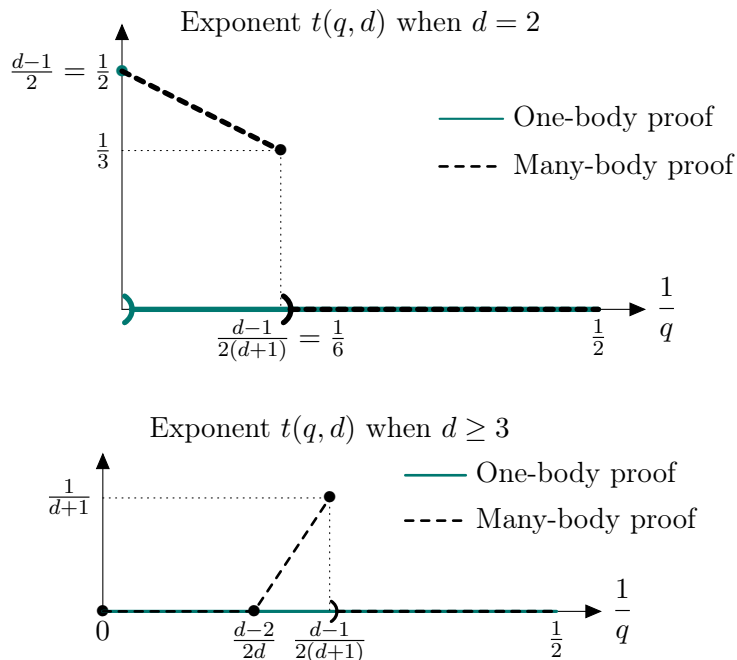


Figure 1.5 – Comparison of the logarithmic exponent $t(q, d)$ for the general estimates

To understand more why this transition point does not appear in the one-body case, let us recall in this section the proof of the one-body estimates. It can be found for instance in Koch-Tataru-Zworski's paper [KTZ07, Thm. 5]. The reader can skip this classical part and go directly to the proof of the many-body estimates (Section IV.4), which can be read independently.

The proof is organized into three steps. We first recall how to introduce the time evolution equation (this step is the same as in the many-body case). Then, we explain why we only need to prove the following dispersive estimates in mixed L^p -norms for a microlocalized propagator $U_\chi(t, r)$ (to be defined later) and we prove them. They rely on Ginibre and Velo spirit [GV92] and Keel-Tao end-point estimates [KT98]. We also recall how we obtain them with complex interpolation, as in the paper of Strichartz [Str77]. This proof has the merit of being comparable with our proof of Strichartz estimates on density matrices (Theorem II.23) since they are based on complex interpolation of the same operator. One can see that the semiclassical constant $h^{-s} \log(1/h)^t$ is actually expressed with respect to integrals of the function $K_{h,\beta}$ (defined by (IV.8)). We will see later precisely in Remark 15 how these expressions differs in the two proofs, and then why the transition point appears only in the many-body proof.

Proposition IV.3 (One-body semiclassical Strichartz estimates). *Suppose that a point $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ satisfies the Assumption 2. Then, there exist $\delta > 0$, a neighborhood $\mathcal{V} = U \times V$ of (x_0, ξ_0) and $h_0 > 0$, such that for any $\chi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ with support contained in \mathcal{V} , there exists $C > 0$ such that for any $0 < h \leq h_0$ and any $2 \leq q \leq \infty$*

$$\sup_{r \in J} \|U_\chi(t, r)\|_{L_x^2(\mathbb{R}^d) \rightarrow L_t^q L_x^q(I \times \mathbb{R}^d)} \leq C \log(1/h)^{t(q,d)} h^{-s(q,d)}$$

with $t(q, d)$ and $s(q, d)$ defined in the statement of Theorem IV.1.

Notice that these bounds correspond to the one-body version of the many-body Strichartz estimates (Theorem II.23). We choose to detail their proof from the energy and decay estimates. We will **admit the end-point Keel-Tao improvement** at $q = 2d/(d-2)$ for dimensions $d \geq 3$, which is technical and already well-explained in the said paper [KT98]:

$$\sup_{r \in J} \|U_\chi(t, r)\|_{L_x^2(\mathbb{R}^d) \rightarrow L_t^q L_x^{\frac{2d}{d-2}}(I \times \mathbb{R}^d)} \leq Ch^{-1/2}.$$

Step 1. Let $u \in L^2(\mathbb{R}^d)$. Defining the operator B_h by $\frac{1}{h}P$, $v(t, x) := u(x)$ satisfies

$$\begin{cases} (hD_t + P)v &= hB_h v, \\ v(0, x) &= u(x). \end{cases}$$

Actually, one would be tempted to work with the evolution propagator $F(t)$ associated to P

$$\begin{cases} (hD_t + P)F(t) = 0, & \forall t \in \mathbb{R}, \\ F(0) = \text{Id}, \end{cases}$$

to write the Duhamel formula to the function $\chi^w v$

$$\chi^w v(t) = F(t)F(0)^* \chi^w v(0) - i \int_0^t F(t)F(r)^* (B_h \chi^w v)(r) dr.$$

Indeed, it does not make sense since the symbol of P is not in the symbol class $S(1)$. This assumption is a crucial condition to get the dispersive semiclassical bounds (Theorem II.18). However, the idea is also the same, we work on another symbol $\chi_0 p$ which is equal to p on a neighborhood of (x_0, ξ_0) , so that we can recover locally the same properties in this neighborhood (here Assumption 2 on p). Let $R_h \in \text{Op}_h^w(\mathcal{S})$ be such that

$$\chi_0^w(x, hD)P = (\chi_0 p)^w(x, hD) - hR_h.$$

Defining the unitary operators $\{F(t)\}_{t \in \mathbb{R}}$ on $L^2(\mathbb{R}^d)$ such that

$$\begin{cases} [hD_t + (\chi_0 p)^w]F(t) = 0, & \forall t \in \mathbb{R}, \\ F(0) = \text{Id}, \end{cases}$$

we have by the Duhamel formula

$$\begin{aligned} \chi^w(x, hD)v(t) &= F(t)\chi^w(x, hD)v(t) - i \int_0^t F(t)F(r)^*(\chi_0^w(x, hD)B_h + R_h)\chi^w(x, hD)v(r)dr \\ &= F(t)F(0)^*\chi^w v(t) - i \int_0^t F(t)F(r)^*\tilde{\chi}^w(x, hD)(\chi_0^w(x, hD)B_h + R_h)\chi^w(x, hD)v(r)dr \\ &\quad - i \int_0^t F(t)F(r)^*(1 - \tilde{\chi})^w(x, hD)(\chi_0^w(x, hD)B_h + R_h)\chi^w(x, hD)v(r)dr, \end{aligned}$$

all $t \in \mathbb{R}$ and for almost all $x \in \mathbb{R}^d$.

Step 2. Let assume temporarily Proposition IV.3. Let $u \in L^2(\mathbb{R}^d)$. For all $\varphi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$, let $U_\varphi(t, r) := U_{\varphi,+}(t, r) + U_{\varphi,-}(t, r)$ where

$$U_{\varphi,+}(t, r) := \mathbf{1}(r \geq 0) \mathbf{1}(t \geq r) \psi(t)F(t)F(r)^*\varphi^w(x, hD)$$

and

$$U_{\varphi,-}(t, r) := \mathbf{1}(r \leq 0) \mathbf{1}(t \leq r) \psi(t)F(t)F(r)^*\varphi^w(x, hD).$$

Let us also define S by

$$S = -i \int_0^t \psi(t)F(t)F(r)^*(1 - \tilde{\chi}^w(x, hD))(\chi_0^w(x, hD)B_h + R_h)\chi^w(x, hD)dr.$$

We obtain with the Duhamel formula

$$\begin{aligned} \psi(t)\chi^w(x, hD)u &= U_\chi(t, 0)u \\ &\quad - \int_I U_{\tilde{\chi}}(t, r)((\chi_0^w(x, hD)B_h + R_h)\chi^w(x, hD)u) dr \\ &\quad + Su. \end{aligned}$$

Let us explain why the term Su is semiclassically negligible. It is due to the following bound.

$$\forall M \in \mathbb{N}, \quad \sup_{r \in J} \|S_r\|_{L^2(\mathbb{R}^d) \rightarrow H_h^M(\mathbb{R}^{d+1})} = \mathcal{O}(h^\infty) \quad (\text{IV.6})$$

Proof. On the one hand, there exists $r \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$ such that $(1 - \tilde{\chi}^w(x, hD))B_h\chi^w(x, hD) = \mathbf{r}^w(x, hD)$. Since $\text{supp}(1 - \tilde{\chi})$ and $\text{supp} \chi$ are disjoint

$$\mathbf{r}^w(x, hD) = \mathcal{O}(h^\infty) : \mathcal{S}'(\mathbb{R}^d) \rightarrow \mathcal{S}(\mathbb{R}^d).$$

On the other hand, by Lemma II.17

$$\forall M \in \mathbb{N}, \exists C > 0 \quad \sup_{r \in J} \|\psi(t)F(t)F(r)^*\|_{H_h^M(\mathbb{R}^d) \rightarrow H_h^M(\mathbb{R}^{d+1})} \leq C.$$

Then, by composition we have for all $M \in \mathbb{N}$

$$\sup_{r \in J} \|\mathbf{1}(r \geq 0) \mathbf{1}(t \geq r) \psi(t)F(t)F(r)^*\mathbf{r}^w\|_{L^2(\mathbb{R}^d) \rightarrow H_h^M(\mathbb{R}^{d+1})} = \mathcal{O}(h^\infty),$$

and

$$\sup_{r \in J} \|\mathbf{1}(r \leq 0) \mathbf{1}(t \leq r) \psi(t)F(t)F(r)^*\mathbf{r}^w\|_{L^2(\mathbb{R}^d) \rightarrow H_h^M(\mathbb{R}^{d+1})} = \mathcal{O}(h^\infty).$$

Finally, we get (IV.6), □

Eventually, by the Hölder inequality and Proposition IV.3

$$\begin{aligned}
\|\psi\|_{L^2(\mathbb{R})} \|\chi^w u\|_{L^q(\mathbb{R}^d)} &= \|\psi(t)\chi^w u\|_{L_t^2 L_x^q(\mathbb{R} \times \mathbb{R}^d)} \\
&\leq \|U_\chi(t, 0)u\|_{L_t^2 L_x^q(\mathbb{R} \times \mathbb{R}^d)} + |I|^{1/2} \sup_{r \in J} \|U_{\tilde{\chi}}(t, r)B_h u\|_{L_t^2 L_x^q(\mathbb{R} \times \mathbb{R}^d)} \\
&\quad + |I|^{1/2} \sup_{r \in J} \|U_r(t, r)u\|_{L_t^2 L_x^q(\mathbb{R} \times \mathbb{R}^d)} + |I|^{1/2} \sup_{r \in J} \|S_r(t)u\|_{L_t^2 L_x^q(\mathbb{R} \times \mathbb{R}^d)} \\
&\lesssim \log(1/h)^{t(q,d)} h^{-s(q,d)} \left(\|u\|_{L^2(\mathbb{R}^d)} + \|B_h u\|_{L^2(\mathbb{R}^d)} \right) + \mathcal{O}(h^\infty) \|u\|_{L^2(\mathbb{R}^d)} \\
&\lesssim \log(1/h)^{t(q,d)} h^{-s(q,d)} \left(\|u\|_{L^2(\mathbb{R}^d)} + \frac{1}{h} \|Pu\|_{L^2(\mathbb{R}^d)} \right).
\end{aligned}$$

Hence

$$\|\chi^w u\|_{L^q(\mathbb{R}^d)} \lesssim \log(1/h)^{t(q,d)} h^{-s(q,d)} \left(\|u\|_{L^2(\mathbb{R}^d)} + \frac{1}{h} \|Pu\|_{L^2(\mathbb{R}^d)} \right).$$

That concludes the proof of Theorem IV.1.

Proofs of Proposition IV.3 (without the Keel-Tao endpoint result).

By a duality argument, it is enough to prove the dual homogeneous estimate

$$\sup_{r \in J} \left\| \int_{\mathbb{R}} U_\chi(t, r)^* W(t) dt \right\|_{L_x^2(\mathbb{R}^d)} \leq C \log(1/h)^{t(q,d)} h^{-s(q,d)} \|W\|_{L_t^2 L_x^{q'}(\mathbb{R}^{d+1})}. \quad (\text{IV.7})$$

By Lemma II.17, we obtain the energy estimates

$$\sup_{r \in J} \|U_\chi(t, r)U_\chi(s, r)^*\|_{L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)} \lesssim 1.$$

Given Assumption 2, we apply Theorem II.18 to $n = d$, $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$, $p = p(x, \xi) \in \mathcal{C}_t^\infty(\mathbb{R}, S_{(x, \xi)}(m))$ and $J = I$. This defines $\delta > 0$ and $\mathcal{V} = U \times V$ a neighborhood of (x_0, ξ_0) such that

$$\sup_{r \in J} \|U_\chi(t, r)U_\chi(s, r)^*\|_{L^1(\mathbb{R}^d) \rightarrow L^\infty(\mathbb{R}^d)} \lesssim h^{-d/2} (h + |t - s|)^{-d/2}.$$

A first proof. Ginibre and Velo proof. Let W be a function on \mathbb{R}^{d+1} and $r \in I$. We can rewrite

$$\begin{aligned}
\left\| \int_{\mathbb{R}} U_\chi(t, r)^* W(t) dt \right\|_{L^2(\mathbb{R}^d)}^2 &= \left\| \int_{\mathbb{R}} U_\chi(t, r)^* W(t) dt \right\|_{L^2(\mathbb{R}^d)}^2 \\
&= \int_I \int_I \langle U_\chi(t, r)^* W(t), U_\chi(s, r)^* W(s) \rangle_{L^2} dt ds \\
&= \int_I \int_I \langle W(t), U_\chi(t, r)U_\chi(s, r)^* W(s) \rangle_{L^2} dt ds.
\end{aligned}$$

By interpolation of the energy and decay estimates, we have uniformly in $t, s \in \mathbb{R}$

$$\forall 1 \leq \mathfrak{r} \leq 2 \quad \sup_{r \in J} \|U_\chi(t, r)U_\chi(s, r)^*\|_{L_x^\mathfrak{r} \rightarrow L_x^{\mathfrak{r}'}} \lesssim \left(h^{-d/2} (h + |t - s|)^{-d/2} \right)^{1-2/\mathfrak{r}}.$$

Let $p, q \geq 2$. By the previous bound for $\tau = q'$ and the Young inequality, there exists $C > 0$ such that for any $r \in J$

$$\begin{aligned} \left\| \int_{\mathbb{R}} U_{\chi}(t, r)^* W(t) dt \right\|_{L^2(\mathbb{R}^d)}^2 &\leq \int_I \int_I \|W(t)\|_{L^{q'}(\mathbb{R}^d)} \|W(s)\|_{L^{q'}(\mathbb{R}^d)} \sup_{r \in J} \|U_{\chi}(t, r) U_{\chi}(s, t)\|_{L_x^{q'} \rightarrow L_x^q} ds dt \\ &\leq C \int_I \int_I \frac{\|W(t)\|_{L^{q'}(\mathbb{R}^d)} \|W(s)\|_{L^{q'}(\mathbb{R}^d)}}{[h^{d/2}(h + |t - s|)^{d/2}]^{1-2/q}} ds dt \\ &\leq C h^{-d(1/2-1/q)} \|W\|_{L_t^{q'} L_x^{q'}(I \times \mathbb{R}^d)}^2 \left\| \frac{1}{(h + |\cdot|)^{d(1/2-1/q)}} \right\|_{L^{p/2}(2I)}. \end{aligned}$$

Since $\frac{\delta}{2} < 1$, we have $2I \subset [-1, 1]$. Let us recall that

$$\int_0^1 \frac{dt}{(h+t)^\alpha} = \begin{cases} C & \text{if } \alpha < 1, \\ \log(1/h) & \text{if } \alpha = 1, \\ Ch^{-(\alpha-1)} & \text{if } \alpha > 1. \end{cases}$$

We apply it with $\alpha = d \left(\frac{1}{2} - \frac{1}{q} \right) \frac{p}{2}$, and we get

$$\left\| \frac{1}{(h + |\cdot|)^{d(1/2-1/q)}} \right\|_{L^{p/2}(2I)} \sim \begin{cases} 1 & \text{if } \frac{2}{p} + \frac{d}{q} > \frac{d}{2}, \\ h^{-1} \log(1/h)^{2/p} & \text{if } \frac{2}{p} + \frac{d}{q} = \frac{d}{2}, \\ h^{\frac{2}{p} - d(\frac{1}{2} - \frac{1}{q})} & \text{if } \frac{2}{p} + \frac{d}{q} < \frac{d}{2}. \end{cases}$$

The better estimates are obtained for $p = 2$. Thus,

$$\sup_{r \in J} \left\| \int_I U_{\chi}(t, r)^* W(t) dt \right\|_{L^2(\mathbb{R}^d)} \lesssim \|W\|_{L_t^2 L_x^{q'}(I \times \mathbb{R}^d)} \begin{cases} h^{-\frac{d}{2}(\frac{1}{2} - \frac{1}{q})} & \text{if } 2 \leq q < \frac{2d}{d-2}, \\ h^{-1/2} \log(1/h)^{1/2} & \text{if } q = \frac{2d}{d-2}, \\ h^{\frac{1}{2} - d(\frac{1}{2} - \frac{1}{q})} & \text{if } q > \frac{2d}{d-2}. \end{cases}$$

In particular,

- when $d = 1$, $2 \leq q \leq 2d/(d-2)_+$ that gives $s(q, 1) = \frac{1}{2} \left(\frac{1}{2} - \frac{1}{q} \right)$,
- when $d = 2$, we have $s(q, 2) = \frac{1}{2} - \frac{1}{q}$ and $t(q, 2) = \begin{cases} 0 & \text{if } 2 \leq q < \infty, \\ \frac{1}{2} & \text{if } q = \infty. \end{cases}$

Furthermore when $d \geq 3$, the proof of Keel-Tao [KT98] at the endpoint $q = 2d/(d-2)$ gives a better estimate without the logarithm term. Finally, we obtain the desired estimates (IV.7).

Proof with complex interpolation. Let us recall the proof of Strichartz's article.

Let $z \in \mathbb{C}$. For all $t, s \in \mathbb{R}$ and $r \in J$, let us define the operator $T_z(t, s, r)$ on $L^2(\mathbb{R}^d)$ by

$$T_z(t, s, r) := (t - s + i0)^z U_{\chi}(t, r) U_{\chi}(s, r)^*.$$

Let the operator $T_z(r)$ acting on functions on \mathbb{R}^{d+1} be defined by

$$\begin{aligned} \forall (f, g) \quad \langle f, T_z(r)g \rangle_{L^2(\mathbb{R}^{d+1})} &= \int_{\mathbb{R} \times \mathbb{R}} \langle f(t), T_z(t, s, r)g(s) \rangle_{L_x^2(\mathbb{R}^d)} dt ds \\ &= \int_{I \times I} \langle f(t), T_z(t, s, r)g(s) \rangle_{L_x^2(\mathbb{R}^d)} dt ds. \end{aligned}$$

The aim is to get a bound $T_0(r) : L_t^2 L_x^{q'} \rightarrow L_t^2 L_x^q$ for $q \geq 2$.

For all $h > 0$ and $\beta \geq 0$, define $K_{h,\beta}$ by

$$\forall t \in \mathbb{R} \quad K_{h,\beta}(t) := h^{-d/2} |t|^\beta (h + |t|)^{-d/2}. \quad (\text{IV.8})$$

First explain how we obtain

- for $\Re z = -1$

$$\sup_{r \in J} \|T_z(r)\|_{L_{t,x}^2(\mathbb{R}^{d+1}) \rightarrow L_{t,x}^2(\mathbb{R}^{d+1})} \lesssim e^{\Im(z)\pi/2}, \quad (\text{IV.9})$$

- for $\Re z = \beta > 0$

$$\sup_{r \in J} \|T_z(r)\|_{L_t^2 L_x^1(\mathbb{R}^{d+1}) \rightarrow L_t^2 L_x^\infty(\mathbb{R}^{d+1})} \lesssim \left(\int_{-1}^1 K_{h,\beta}(t) dt \right). \quad (\text{IV.10})$$

Proof of the bound (IV.9). It is really the same proof as for the bound (II.7), which uses the Fourier transform of the distribution $(t + i0)^z$ for $z \in \mathbb{C}$ such that $\Re z = -1$:

$$\forall F, G \in L_{t,x}^2(\mathbb{R}^{d+1}), \quad \sup_{r \in J} |\langle F, T_z(r)G \rangle| \lesssim \|F\|_{L_{t,x}^2(\mathbb{R}^{d+1})} \|G\|_{L_{t,x}^2(\mathbb{R}^{d+1})}.$$

□

Proof of the bound (IV.10). By the decay estimate on $T_0(r)$, we deduce

$$\sup_{x,y \in \mathbb{R}^d} |T_z(t,s,r)(x,y)| \lesssim h^{-d/2} \frac{|t-s|^\beta}{(h+|t-s|)^{-d/2}}.$$

We have, by the previous bound and the Young inequality, with $\delta > 0$ such that $]-2\delta, 2\delta[\subset [-1, 1]$ there exists $C > 0$ such that for any simple functions f and g on \mathbb{R}^{d+1}

$$\begin{aligned} \left| \langle g, T_z(r)f \rangle_{L_{t,x}^2(\mathbb{R}^{d+1})} \right| &\leq C \int_I \int_I K_{h,\beta}(t-s) \|f(t)\|_{L_x^1(\mathbb{R}^d)} \|g(s)\|_{L_x^1(\mathbb{R}^d)} ds dt \\ &\leq C \|K_{h,\beta}\|_{L^1([-1,1])} \|f\|_{L_t^2 L_x^1(I \times \mathbb{R}^d)} \|g\|_{L_t^2 L_x^1(I \times \mathbb{R}^d)} \end{aligned}$$

That gives us (IV.10). □

Now, let us do the interpolation $z = 0$ between $\Re z = -1$ and $\Re z = \beta$, and $\theta \in [0, 1]$ such that $0 = (1-\theta)(-1) + \theta\beta$ that is $\theta = (\beta+1)^{-1}$.

$$\sup_{r \in J} \|U_\chi(t,r)U_\chi(s,r)^*\|_{L_t^2 L_x^{\left(\frac{2(\beta+1)}{\beta}\right)'(\mathbb{R}^{d+1})} \rightarrow L_t^2 L_x^{\frac{2(\beta+1)}{\beta}(I \times \mathbb{R}^d)}} = \mathcal{O} \left(\left(\int_{-1}^1 K_{h,\beta}(t) dt \right)^{\frac{1}{\beta+1}} \right). \quad (\text{IV.11})$$

Otherwise,

$$\sup_{r \in J} \|U_\chi(t,r)\|_{L_x^2(\mathbb{R}^d) \rightarrow L_t^2 L_x^{\frac{2(\beta+1)}{\beta}(I \times \mathbb{R}^d)}} \lesssim \left(\int_{-1}^1 K_{h,\beta}(t) dt \right)^{\frac{1}{2(\beta+1)}}.$$

We have that

$$\int_{-1}^1 K_{h,\beta}(t) dt = \begin{cases} h^{\beta-d+1} & \text{if } \beta < \frac{d-2}{2}, \\ h^{-d/2} \log(1/h) & \text{if } \beta = \frac{d-2}{2}, \\ h^{-d/2} & \text{if } \beta > \frac{d-2}{2}. \end{cases}$$

Finally with $q = 2(\beta+1)/\beta$ and with Keel-Tao improvement at the end point ($\beta = \frac{d-2}{2}$) for $d \geq 3$, we get the desired estimates. That finishes the proof of IV.3.

Remark 13. Note that $\beta = 0$ gives the one-body L^∞ -bound

$$\sup_{r \in J} \|U_\chi(t,r)\|_{L_x^2(\mathbb{R}^d) \rightarrow L_t^2 L_x^\infty(I \times \mathbb{R}^d)} = \mathcal{O} \left(h^{-\frac{d-1}{2}} \right).$$

IV.4 Proof of Theorem IV.2

We start to give the extremal estimates for $q = 2$ and $q = \infty$.

- By the Calderon-Vaillancourt theorem (Theorem II.13), we have

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^1(\mathbb{R}^d)} = \mathrm{Tr}_{L^2}(\chi^w \gamma \chi^w) \lesssim \|\gamma\|_{\mathfrak{S}^1}.$$

- Furthermore, by the one function L^∞ estimate (c.f. Theorem IV.1)

$$\begin{aligned} & \chi^w \gamma \chi^w \\ &= \chi^w (1 + P^2/h^2)^{-1/2} (1 + P^2/h^2)^{1/2} \gamma (1 + P^2/h^2)^{1/2} \left(\chi^w (1 + P^2/h^2)^{-1/2} \right)^* \\ &\leq \chi^w (1 + P^2/h^2)^{-1/2} \left\| (1 + P^2/h^2)^{1/2} \gamma (1 + P^2/h^2)^{1/2} \right\|_{\mathfrak{S}^\infty} \left(\chi^w (1 + P^2/h^2)^{-1/2} \right)^* \\ &\leq \left\| (1 + P^2/h^2)^{1/2} \gamma (1 + P^2/h^2)^{1/2} \right\|_{\mathfrak{S}^\infty} \chi^w (1 + P^2/h^2)^{-1/2} \left(\chi^w (1 + P^2/h^2)^{-1/2} \right)^*. \end{aligned}$$

Thus,

$$\begin{aligned} \|\rho_{\chi^w \gamma \chi^w}\|_{L^\infty(\mathbb{R}^d)} &\leq \left\| (1 + P^2/h^2)^{1/2} \gamma (1 + P^2/h^2)^{1/2} \right\|_{\mathfrak{S}^\infty} \|\rho_{\chi^w (1 + P^2/h^2)^{-1} \chi^w}\|_{L^\infty(\mathbb{R}^d)} \\ &\lesssim \left\| (1 + P^2/h^2)^{1/2} \gamma (1 + P^2/h^2)^{1/2} \right\|_{\mathfrak{S}^\infty} \begin{cases} h^{-1/2} & \text{if } d = 1, \\ \log(1/h)/h & \text{if } d = 2, \\ h^{-(d-1)} & \text{if } d > 2. \end{cases} \end{aligned}$$

We thus have the bounds for $q = 2$ and $q = \infty$. For $d = 1$, we interpolate between them and get

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\mathbb{R})} \lesssim h^{\frac{1}{q} - \frac{1}{2}} \left\| (1 + P^2/h^2)^{1/2} \gamma (1 + P^2/h^2)^{1/2} \right\|_{\mathfrak{S}^{q/2}(L^2(\mathbb{R}))},$$

which is exactly Theorem IV.2 in the case $d = 1$. For $d \geq 3$, by the triangle inequality at the Keel-Tao endpoint $q = \frac{2d}{d-2}$, we have

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{d/(d-2)}(\mathbb{R}^d)} \lesssim h^{-1/2} \left\| (1 + P^2/h^2)^{1/2} \gamma (1 + P^2/h^2)^{1/2} \right\|_{\mathfrak{S}^1(L^2(\mathbb{R}^d))}.$$

Interpolating this bound with the bound for $q = \infty$ proves Theorem IV.2 in the case $2d/(d-2) \leq q \leq \infty$, $d \geq 3$. The next step is to get estimates for $2 \leq q \leq 2(d+1)/(d-1)$ with $d \geq 2$. The remaining estimates in the range $2(d+1)/(d-1) \leq q \leq 2d/(d-2)$, $d \geq 3$ are then obtained by interpolating the estimates for $q = 2(d+1)/(d-1)$ and $q = 2d/(d-2)$.

We thus now fix $d \geq 2$ and $2 \leq q \leq 2(d+1)/(d-1)$. The idea is to introduce a new variable $t \in \mathbb{R}$. Then, we have

$$\begin{aligned} \|\psi\|_{L^2(I)}^2 \|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\mathbb{R}^d)} &= \sup_{W \in L^{2(q/2)' }(\mathbb{R}^d)} \frac{\|\psi\|_{L^2(I)}^2 \int_{\mathbb{R}^d} \rho_{\chi^w \gamma \chi^w}(x) |W(x)|^2 dx}{\|W\|_{L^{2(q/2)' }(\mathbb{R}^d)}^2} \\ &\leq \sup_{W \in L^{2(q/2)' }(\mathbb{R}^d)} \frac{\|\psi\|_{L^2(I)}^2 \|W(x) \chi^w \sqrt{\gamma}\|_{\mathfrak{S}^2(L^2(\mathbb{R}^d))}^2}{\|W\|_{L^{2(q/2)' }(\mathbb{R}^d)}^2} \\ &\leq \sup_{W \in L^{2(q/2)' }(\mathbb{R}^d)} \frac{\|\psi(t) W(x) \chi^w \sqrt{\gamma}\|_{\mathfrak{S}^2(L^2(\mathbb{R}^d), L^2(\mathbb{R}^{d+1}))}^2}{\|W\|_{L^{2(q/2)' }(\mathbb{R}^d)}^2}. \end{aligned}$$

In the last inequality, we use that for any bounded operator A on $L^2(\mathbb{R}^d)$ and any $\psi \in L^2(\mathbb{R})$, we have (as can be seen by computing $(\psi(t)A)^*\psi(t)A$)

$$\|\psi(t)A\|_{\mathfrak{S}^2(L^2(\mathbb{R}^d), L^2(\mathbb{R}^{d+1}))} = \|\psi\|_{L^2(\mathbb{R})} \|A\|_{\mathfrak{S}^2(L^2(\mathbb{R}^d))}.$$

We define the operator B_h by $\frac{1}{h}P$. Let $u \in L^2(\mathbb{R}^d)$. Then $v(t, x) := u(x)$ satisfies

$$\begin{cases} (hD_t + P)v &= hB_h v, \\ v(0, x) &= u(x). \end{cases}$$

Let $R_h \in \text{Op}_h^w(\mathcal{S})$ be such that

$$\chi_0^w(x, hD)P = (\chi_0 p)^w(x, hD) - hR_h.$$

Defining the unitary operators $\{F(t)\}_{t \in \mathbb{R}}$ on $L^2(\mathbb{R}^d)$ such that

$$\begin{cases} (hD_t + (\chi_0 p)^w)F(t) &= 0, \quad \forall t \in \mathbb{R}, \\ F(0) &= \text{Id}, \end{cases}$$

we have by the Duhamel formula

$$\begin{aligned} \chi^w(x, hD) &= F(t)\chi^w(x, hD) - i \int_0^t F(t)F(r)^*(\chi_0^w(x, hD)B_h + R_h)\chi^w(x, hD)dr \\ &= F(t)F(0)^*\chi^w - i \int_0^t F(t)F(r)^*\tilde{\chi}^w(x, hD)(\chi_0^w(x, hD)B_h + R_h)\chi^w(x, hD)dr \\ &\quad - i \int_0^t F(t)F(r)^*(1 - \tilde{\chi})^w(x, hD)(\chi_0^w(x, hD)B_h + R_h)\chi^w(x, hD)dr, \end{aligned}$$

as an identity between bounded operators on $L^2(\mathbb{R}^d)$ for all $t \in \mathbb{R}$.

Definition IV.4. For all $\varphi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$, let $U_\varphi(t, r) = U_{\varphi, +}(t, r) - U_{\varphi, -}(t, r)$ where

$$U_{\varphi, +}(t, r) := \mathbf{1}(r \geq 0) \mathbf{1}(t \geq r) \psi(t)\tilde{\psi}(t-r)F(t)F(r)^*\varphi^w(x, hD)$$

and

$$U_{\varphi, -}(t, r) := \mathbf{1}(r < 0) \mathbf{1}(t \leq r) \psi(t)\tilde{\psi}(t-r)F(t)F(r)^*\varphi^w(x, hD).$$

Let us also define S by

$$S = -i \int_0^t \psi(t)F(t)F(r)^*(1 - \tilde{\chi}^w(x, hD))(\chi_0^w(x, hD)B_h + R_h)\chi^w(x, hD)dr. \quad (\text{IV.12})$$

By multiplying by ψ on the left of the previous Duhamel formula, we have

$$\psi(t)\chi^w(x, hD) = U_\chi(t, 0) - i \int_J U_{\tilde{\chi}}(t, r)(\chi_0^w B_h \chi^w + R_h \chi^w) dr + S.$$

By the triangle inequality and Hölder inequality, we get for all $\alpha \geq 1$

$$\begin{aligned} &\|\psi(t)W(x)\chi^w\sqrt{\gamma}\|_{\mathfrak{S}^2(L^2(\mathbb{R}^d), L^2(\mathbb{R}^{d+1}))} \\ &\leq \|W(x)U_\chi(t, 0)\|_{\mathfrak{S}^{2\alpha'}(L^2(\mathbb{R}^d), L^2(\mathbb{R}^{d+1}))} \|\sqrt{\gamma}\|_{\mathfrak{S}^{2\alpha}(L^2(\mathbb{R}^d))} \\ &\quad + |J| \sup_{r \in J} \|W(x)U_{\tilde{\chi}}(t, r)\|_{\mathfrak{S}^{2\alpha'}(L^2(\mathbb{R}^d), L^2(\mathbb{R}^{d+1}))} \|(\chi_0^w B_h \chi^w + R_h \chi^w)\sqrt{\gamma}\|_{\mathfrak{S}^{2\alpha}(L^2(\mathbb{R}^d))} \\ &\quad + \|W(x)S\|_{\mathfrak{S}^{2(q/2)'}(L^2(\mathbb{R}^d), L^2(\mathbb{R}^{d+1}))} \|\sqrt{\gamma}\|_{\mathfrak{S}^q(L^2(\mathbb{R}^d))}. \end{aligned}$$

There exists $\mathfrak{r} \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$ such that $[B_h, \chi^w] = \frac{1}{h} [P, \chi^w] = \mathfrak{r}^w$. Thus

$$\begin{aligned} & \|(\chi_0^w B_h \chi^w + R_h \chi^w) \sqrt{\gamma}\|_{\mathfrak{S}^{2\alpha}(L^2(\mathbb{R}^d))} \\ & \leq \|\chi_0^w \chi^w B_h \sqrt{\gamma}\|_{\mathfrak{S}^{2\alpha}(L^2(\mathbb{R}^d))} + \|\chi_0^w [B_h, \chi^w] \sqrt{\gamma}\|_{\mathfrak{S}^{2\alpha}(L^2(\mathbb{R}^d))} + \|R_h \chi^w \sqrt{\gamma}\|_{\mathfrak{S}^{2\alpha}(L^2(\mathbb{R}^d))} \\ & \leq \|\chi_0^w \chi^w\|_{\mathfrak{S}^\infty(L^2(\mathbb{R}^d))} \|B_h \sqrt{\gamma}\|_{\mathfrak{S}^{2\alpha}(L^2(\mathbb{R}^d))} \\ & \quad + \left(\|\chi_0^w [B_h, \chi^w]\|_{\mathfrak{S}^\infty(L^2(\mathbb{R}^d))} + \|R_h \chi^w\|_{\mathfrak{S}^\infty(L^2(\mathbb{R}^d))} \right) \|\sqrt{\gamma}\|_{\mathfrak{S}^{2\alpha}(L^2(\mathbb{R}^d))} \\ & \lesssim \frac{1}{h} \|P\gamma P\|_{\mathfrak{S}^\alpha(L^2(\mathbb{R}^d))}^{1/2} + \|\gamma\|_{\mathfrak{S}^\alpha(L^2(\mathbb{R}^d))}^{1/2}. \end{aligned}$$

We only need to prove the Schatten estimates for the operators $U_\chi(t, r)$, $U_{\bar{\chi}}(t, r)$ and S .

Proposition IV.5. *Recall that S is the operator defined by (IV.12). Let $\beta \geq 2$. Then, we have the bound for all $W \in L^\beta(\mathbb{R}^{d+1})$*

$$\|W(t, x)S\|_{\mathfrak{S}^\beta(L^2(\mathbb{R}^d), L^2(\mathbb{R}^{d+1}))} = \mathcal{O}(h^\infty) \|W\|_{L^\beta(I \times \mathbb{R}^d)}.$$

Before proving this proposition, let us conclude the proof of Theorem IV.2. Given Assumption 2, we apply Theorem II.23 to $n = d$, $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$, $a = \chi_0 p \in \mathcal{C}_t^\infty(\mathbb{R}, \mathcal{S}_{(x, \xi)}(1))$ and $J = [-1, 1]$. Thus, there exist $\delta > 0$ and $\mathcal{V} = U \times V$ neighborhood of (x_0, ξ_0) , so that we have for any $2 \leq q \leq \frac{2(d+1)}{d-1}$

$$\begin{aligned} & \|W(x)U_\chi(t, 0)\|_{\mathfrak{S}^{2\alpha(q, d)'}(L^2(\mathbb{R}^d), L^2(\mathbb{R}^{d+1}))} + \sup_{r \in J} \|W(x)U_{\bar{\chi}}(t, r)\|_{\mathfrak{S}^{2\alpha(q, d)'}(L^2(\mathbb{R}^d), L^2(\mathbb{R}^{d+1}))} \\ & \lesssim \log(1/h)^{t(q, d)} h^{-s(q, d)} \|W\|_{L^{2(q/2)'(\mathbb{R}^d)}} \|\psi\|_{L^\infty(\mathbb{R})}, \end{aligned}$$

for $\alpha(q, d) = \frac{2q}{q+2}$, $s(q, d) = \frac{d}{2}(\frac{1}{2} - \frac{1}{q})$ and $t(q, d) = 0$ for $2 \leq q < \frac{2(d+1)}{d-1}$ and $t(q, d) = \frac{1}{d+1}$ if $q = \frac{2(d+1)}{d-1}$. Hence, for any $2 \leq q \leq \frac{2(d+1)}{d-1}$

$$\begin{aligned} & \|\psi(t)W(x)\chi^w \sqrt{\gamma}\|_{\mathfrak{S}^2(L^2(\mathbb{R}^d), L^2(\mathbb{R}^{d+1}))} \\ & \leq C_I \log(1/h)^{t(q, d)} h^{-s(q, d)} \|W\|_{L^{2(q/2)'(\mathbb{R}^d)}} \times \\ & \quad \times \left(\|\gamma\|_{\mathfrak{S}^{\alpha(q, d)}(L^2(\mathbb{R}^d))}^{1/2} + \frac{1}{h} \|P\gamma P\|_{\mathfrak{S}^{\alpha(q, d)}(L^2(\mathbb{R}^d))}^{1/2} + \|\gamma\|_{\mathfrak{S}^{q/2}(L^2(\mathbb{R}^d))}^{1/2} \right) \\ & \leq C'_I \log(1/h)^{t(q, d)} h^{-s(q, d)} \|W\|_{L^{2(q/2)'(\mathbb{R}^d)}} \left\| (1 + P^2/h^2)^{1/2} \gamma (1 + P^2/h^2)^{1/2} \right\|_{\mathfrak{S}^{\alpha(q, d)}(L^2(\mathbb{R}^d))}^{1/2}, \end{aligned}$$

which finishes the proof of Theorem IV.2. It thus remains to prove Proposition IV.5.

Proof of Proposition IV.5. Let us explain how we deduce the result from the estimates ¹

$$\forall M \in \mathbb{N}, \quad \|S\|_{L^2(\mathbb{R}^d) \rightarrow H_h^M(\mathbb{R}^{d+1})} = \mathcal{O}(h^\infty).$$

Note that $S = \mathbf{1}(t \in I) S$. Then, by Kato-Seiler-Simon (Lemma II.20) applied to $M \in \mathbb{N}$ such that $M\beta > d + 1$

$$\begin{aligned} & \|W(t, x)S\|_{\mathfrak{S}^\beta(L^2(\mathbb{R}^d), L^2(\mathbb{R}^{d+1}))} \\ & \leq \left\| W(t, x) \mathbf{1}(t \in I) (1 - h^2 \Delta_{t, x})^{-M/2} \right\|_{\mathfrak{S}^\beta(L^2(\mathbb{R}^{d+1}))} \left\| (1 - h^2 \Delta_{t, x})^{M/2} S \right\|_{\mathfrak{S}^\infty(L^2(\mathbb{R}^d), L^2(\mathbb{R}^{d+1}))} \\ & = \mathcal{O}(h^\infty) \|W\|_{L^\beta(I \times \mathbb{R}^d)}. \end{aligned}$$

That gives us the desired estimates. □

¹That corresponds to (IV.6) in Section IV.3.

Remark 14. Notice that (II.8) allows to treat the case $\beta \in [0, \frac{d-1}{2})$ leading to better values $\alpha(q, d)$ and $t(q, d)$ but also a worse value of $s(q, d)$ for $d \geq 2$ and $\frac{2(d+1)}{d-1} < q \leq \infty$:

$$s(q, d) = \left(d + \frac{1}{2} - \frac{2}{q-2} \right) \left(\frac{1}{2} - \frac{1}{q} \right), \quad t(q, d) = 0, \quad \alpha(q, d) = \frac{2q}{q+2}.$$

We discard these estimates because we always want to keep the same exponent $s(q, d)$ as in the one-body case (so that our many-body estimates imply the one-body estimates). (c.f. Figure 1.6)

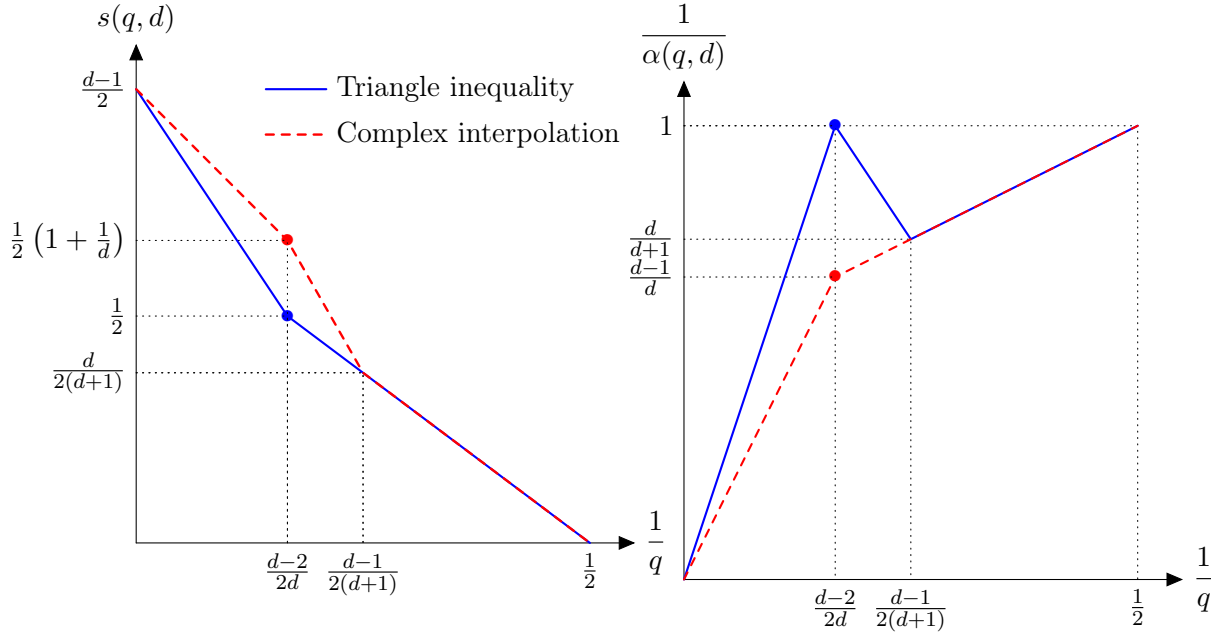


Figure 1.6 – Exponents $s(q, d)$ and $\alpha(q, d)$ for $d \geq 3$, obtained by two different methods at the end-point $q = 2d/(d-2)$

Remark 15. Let us comment on why the many-body case has an additional transition point $q = 2(d+1)/(d-1)$ compared to the one-body case (shown in Figure 1.5). Let $K_{h,\beta}$ be defined by

$$\forall t \in \mathbb{R} \quad K_{h,\beta}(t) := h^{-d/2} |t|^\beta (h + |t|)^{-d/2}.$$

After reminding that q and β are linked by the relation $q = 2(\beta+1)/\beta$ (which is equivalent to $(q/2)' = \beta+1$), we have in the one body case (see for instance the proof by complex interpolation in Section IV.3)

$$\sup_{r \in J} \|T_0(r)\|_{L_t^2 L_x \left(\frac{2(\beta+1)}{\beta} \right)' (\mathbb{R}^{d+1}) \rightarrow L_t^2 L_x \frac{2(\beta+1)}{\beta} (I \times \mathbb{R}^d)} \leq C \left(\int_{-1}^1 K_{h,\beta}(t) dt \right)^{\frac{1}{\beta+1}},$$

while as the above proof (more precisely the proof of Theorem II.23 with $n = d$) shows, we have in the many body case

$$\begin{aligned} & \sup_{r \in J} \|WT_0(r)W\|_{\mathfrak{S}^{2\left(\frac{2(\beta+1)}{2\beta+1}\right)' (L^2(\mathbb{R}^{d+1}))}} \\ & \leq C \|W\|_{L_t \frac{2(\beta+1)}{1+\left(\frac{2(\beta+1)}{\beta}-\frac{d}{2}\right)} - L_x^{2(\beta+1)} (I \times \mathbb{R}^d)}^2 \left(\int_{-1}^1 K_{h,\beta}(t)^2 dt \right)^{\frac{1}{2(\beta+1)}}. \end{aligned}$$

Note that

$$\int_{-1}^1 K_{h,\beta}(t) dt = \begin{cases} h^{\beta-d+1} & \text{if } \beta < \frac{d-2}{2}, \\ h^{-d/2} \log(1/h) & \text{if } \beta = \frac{d-2}{2}, \\ h^{-d/2} & \text{if } \beta > \frac{d-2}{2}. \end{cases}$$

and

$$\left(\int_{-1}^1 K_{h,\beta}(t)^2 dt \right)^{1/2} = \begin{cases} h^{\beta-d+1/2} & \text{if } \beta < \frac{d-1}{2}, \\ h^{-d/2} \log(1/h)^{1/2} & \text{if } \beta = \frac{d-1}{2}, \\ h^{-d/2} & \text{if } \beta > \frac{d-1}{2}, \end{cases}$$

so that the one-body and many-body constants coincide for $\beta > (d-1)/2$ (which corresponds to $2 \leq q < 2(d+1)/(d-1)$) but differ for $\beta \leq (d-1)/2$ (which corresponds to $q > 2(d+1)/(d-1)$). We expect that it is not a technical artifact of the proof, but rather that this transition point does appear in the many-body case. Indeed, a similar phenomenon exists for Strichartz estimates [FLLS14] where the existence of a transition is shown at this point $q = 2(d+1)/(d-1)$. It is a challenging problem to adapt their result to our setting. A related problem would be to get rid of the logarithm in our many-body estimates at $q = 2(d+1)/(d-1)$.

V SOGGE'S L^p ESTIMATES

We now treat the case $p = 0$ and $\nabla_{\xi} p \neq 0$. In the case of Schrödinger operators, it means that we are away from the turning point region $\{V = E\}$. This setting corresponds to the one of Sogge without potential on a compact manifold. In the one-body case ($\text{rank } \gamma = 1$), we recover [KTZ07, Thm. 5].

V.1 Statement of the result

Let $d \geq 2$. For $x \in \mathbb{R}^d$, we denote by x' the $d-1$ last variables of x

$$x' := (x_2, \dots, x_d) \in \mathbb{R}^{d-1}.$$

Let m an order function on $\mathbb{R}^d \times \mathbb{R}^d$, $p \in S(m)$ be real-valued and $P := p^w(x, hD)$ (but the following theorems are true for any other quantization).

Assumption 3. A point $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ satisfies the *Sogge nondegeneracy conditions* for the symbol p if

$$p(x_0, \xi_0) = 0, \quad \nabla_{\xi} p(x_0, \xi_0) \neq 0,$$

and if

$$\begin{aligned} & \text{the second fundamental form of } \{\xi \in \mathbb{R}^d : p(x_0, \xi) = 0\} \\ & \text{is non-degenerate at } \xi_0. \end{aligned} \tag{V.1}$$

First recall the one-body result.

Theorem V.1 (Sogge one-body estimates, [KTZ07, Thm. 5]). *Let $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ be a point satisfying Assumption 3. Then, there exist a neighborhood \mathcal{V} of (x_0, ξ_0) and $h_0 > 0$, such that for any $\chi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ with support contained in \mathcal{V} , there exists $C > 0$ such that for any $0 < h \leq h_0$ and for any $2 \leq q \leq \infty$*

$$\|\chi^w u\|_{L^q(\mathbb{R}^d)} \leq Ch^{-s(q,d)} \left(\|u\|_{L^2(\mathbb{R}^d)} + \frac{1}{h} \|Pu\|_{L^2(\mathbb{R}^d)} \right),$$

where

$$s(q, d) = \begin{cases} \frac{d-1}{2} \left(\frac{1}{2} - \frac{1}{q} \right) & \text{if } 2 \leq q \leq \frac{2(d+1)}{d-1}, \\ d \left(\frac{1}{2} - \frac{1}{q} \right) - \frac{1}{2} & \text{if } \frac{2(d+1)}{d-1} \leq q \leq \infty. \end{cases} \quad (\text{V.2})$$

Equivalently, one has for all $2 \leq q \leq \infty$

$$\chi^w (1 + P^*P/h^2)^{-1/2} = \mathcal{O}(h^{-s(q,d)}) : L^2(\mathbb{R}^d) \rightarrow L^q(\mathbb{R}^d).$$

Remark 16. The exponent s_{Sogge} , defined in (V.2), is always larger than the elliptic one s_{ellip} for any $d \geq 2$ and $2 \in [2, \infty]$. Moreover, it is strictly smaller than s_{gene} for any $q \in (2, 2d/(d-2))$ and they coincide when $q \in \{2\} \cup [2d/(d-2), \infty]$. (c.f. Figure 1.3).

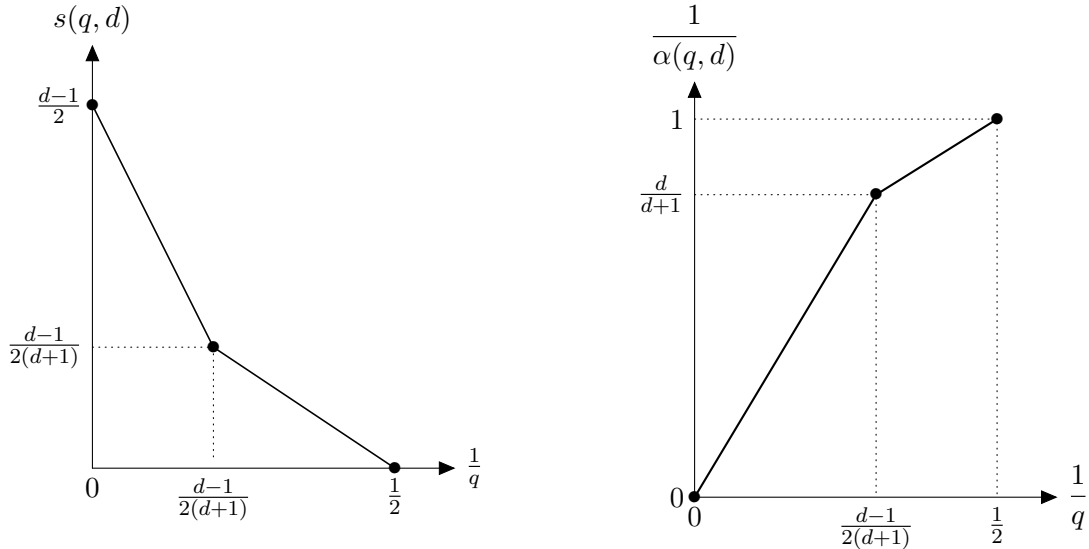
Theorem V.2 (Sogge many-body estimates). *Let $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ be a point satisfying Assumption 3. Then, there exist a neighborhood \mathcal{V} of (x_0, ξ_0) and $h_0 > 0$, such that for any $\chi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ with support contained in \mathcal{V} , there exists $C > 0$ such that for any $0 < h \leq h_0$, for any $2 \leq q \leq \infty$ and for any bounded self-adjoint non-negative operator γ on $L^2(\mathbb{R}^d)$*

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\mathbb{R}^d)} \leq Ch^{-2s(q,d)} \left\| (1 + P^*P/h^2)^{1/2} \gamma (1 + P^*P/h^2)^{1/2} \right\|_{\mathfrak{S}^{\alpha(q,d)}}$$

where $s(q, d)$ is given by the formula (V.2) and $\alpha(q, d)$ is given by

$$\alpha(q, d) = \begin{cases} \frac{2q}{q+2} & \text{if } 2 \leq q \leq \frac{2(d+1)}{d-1}, \\ \frac{q(d-1)}{2d} & \text{if } \frac{2(d+1)}{d-1} \leq q \leq \infty. \end{cases} \quad (\text{V.3})$$

Remark 17. For $d \geq 3$, the exponent $\alpha_{\text{Sogge}} > \alpha_{\text{gene}}$ for $q \in (2d/(d-2), \infty)$ and $\alpha_{\text{Sogge}} = \alpha_{\text{gene}}$ for $q = [2, 2d/d-2]$. It is strictly larger than the one $\alpha_{\text{ellip}}(q, d) = q/2$ in the elliptic estimates for any $q \in (2, \infty)$ and they coincide for $q = 2$ or $q = \infty$ (c.f. Figure 1.4).



V.2 Definitions and notation for the proof of Theorem V.2

- Let $I_0, I \subset \mathbb{R}$ be open intervals which contain $(x_0)_1$ such that

$$I_0 \subset \bar{I}_0 \subset I \subset [(x_0)_1 - 1, (x_0)_1 + 1].$$

- Let $\psi_1 \in C_c^\infty(\mathbb{R}, [0, 1])$ such that $\psi_1 = 1$ on \bar{I}_0 and such that $\text{supp } \psi_1 \subset I$.

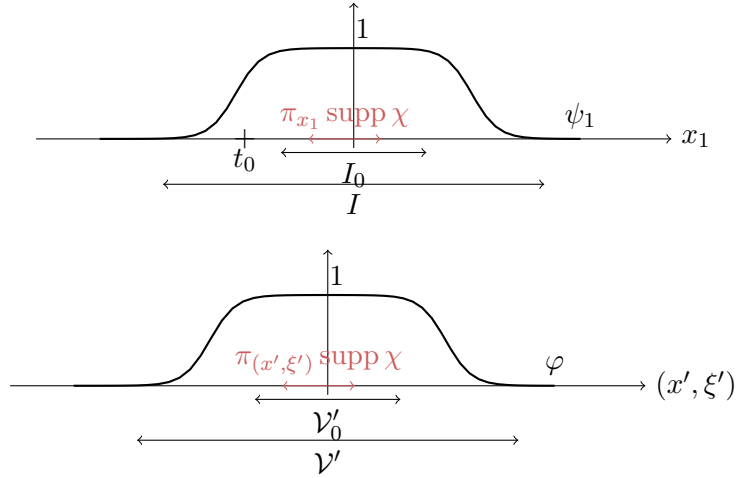
- Let $t_0 \in I \setminus I_0$.
- Let $J \subset \mathbb{R}$ a bounded open interval which contains $(\xi_0)_1$.
- Let $R := |I| > 0$. Note that $R \leq 2$.
- We choose $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$ such that $\psi = 1$ on $[-R, R]$ and $\psi = 0$ outside $[-2R, 2R]$. Note that $\text{supp } \psi \subset [-4, 4]$.
- Let us define $I_r := [(x_0)_1 - 5, (x_0)_1 + 5]$.
- Let $\mathcal{V}'_0 = U'_0 \times V'_0$ and $\mathcal{V}' = U' \times V' \subset \mathbb{R}^{d-1} \times \mathbb{R}^{d-1}$ be bounded open neighborhood of (x'_0, ξ'_0) such that

$$\mathcal{V}'_0 \subset \overline{\mathcal{V}'_0} \subset \mathcal{V}'.$$
- Let $\varphi \in \mathcal{C}_c^\infty(\mathbb{R}^{2(d-1)}, [0, 1])$ such that $\varphi = 1$ on $\overline{\mathcal{V}'_0}$ and $\text{supp } \varphi \subset \mathcal{V}'$.
- We define $\mathcal{V} := I_0 \times J \times \mathcal{V}'_0$ and $\mathcal{W} := I \times J \times \mathcal{V}'$. We will add constraints on the size of \mathcal{W} along the proof.
- Let $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ such that $\text{supp } \chi \subset \mathcal{V}$.

By construction this implies that

$$\pi_{x_1} \text{supp } \chi \subset I_0, \quad \pi_{(x', \xi')} \text{supp } \chi \subset \mathcal{V}'_0,$$

then $\text{supp}(1 - \psi_1) \cap \pi_{x_1} \text{supp } \chi = \emptyset$ and $\text{supp}(1 - \varphi) \cap \pi_{(x', \xi')} \text{supp } \chi = \emptyset$.



V.3 Proof of Theorem V.2

First and foremost, the bounds at the two points $q = 2$ and $q = \infty$ follow from Theorem IV.2. Since we have the bounds for $q = 2$ and $q = \infty$, we now show it for $q = 2(d+1)/(d-1)$, which implies the theorem by interpolation.

Let us first explain why we will focus our proof on $\|\rho_{\psi_1} \chi^w \gamma \chi^w \psi_1\|_{L^{q/2}(\mathbb{R}^d)}$. Recall that

$$\begin{aligned} \|\rho_{\chi^w} \gamma \chi^w\|_{L^{q/2}(\mathbb{R}^d)} &= \sup_{W \in L^{2(q/2)' }(\mathbb{R}^d)} \frac{\int_{\mathbb{R}^d} \rho_{\chi^w} \gamma \chi^w(x) |W(x)|^2 dx}{\|W\|_{L^{2(q/2)' }(\mathbb{R}^d)}^2} \\ &= \sup_{W \in L^{2(q/2)' }(\mathbb{R}^d)} \frac{\|W(x) \chi^w \sqrt{\gamma}\|_{\mathfrak{S}^2(\mathbb{R}^d)}^2}{\|W\|_{L^{2(q/2)' }(\mathbb{R}^d)}^2}. \end{aligned}$$

By the triangle inequality, up to a multiplicative factor, it is bounded by

$$\sup_{W \in L^{2(q/2)' }(\mathbb{R}^d)} \frac{\|W(x)\psi_1(x_1)\chi^w \sqrt{\gamma}\|_{\mathfrak{S}^2(\mathbb{R}^d)}^2}{\|W\|_{L^{2(q/2)' }(\mathbb{R}^d)}^2}$$

and

$$\sup_{W \in L^{2(q/2)' }(\mathbb{R}^d)} \frac{\|W(x)(1 - \psi_1(x_1))\chi^w \sqrt{\gamma}\|_{\mathfrak{S}^2(\mathbb{R}^d)}^2}{\|W\|_{L^{2(q/2)' }(\mathbb{R}^d)}^2}.$$

By construction $\text{supp}(1 - \psi_1)$ and $\pi_{x_1} \text{supp } \chi$ are disjoint. Then

$$(1 - \psi_1(x_1))\chi^w = \mathcal{O}(h^\infty) : \mathcal{S}'(\mathbb{R}^d) \rightarrow \mathcal{S}(\mathbb{R}^d).$$

By the Hölder and Kato-Seiler-Simon inequalities (Lemma II.20), with $M \in \mathbb{N}$ such that $2M(q/2)' > d$

$$\begin{aligned} & \|W(x)(1 - \psi_1(x_1))\chi^w \sqrt{\gamma}\|_{\mathfrak{S}^2(\mathbb{R}^d)} \\ & \leq \|W(x)(1 - h^2\Delta)^{-M}\|_{\mathfrak{S}^{2(q/2)' }(\mathbb{R}^d)} \|(1 - h^2\Delta)^M(1 - \psi_1(x_1))\chi^w\|_{\mathfrak{S}^\infty(\mathbb{R}^d)} \|\sqrt{\gamma}\|_{\mathfrak{S}^q(\mathbb{R}^d)} \\ & = \mathcal{O}(h^{N-d/2}) \|W\|_{L^{2(q/2)' }(\mathbb{R}^d)} \|\gamma\|_{\mathfrak{S}^{q/2}(\mathbb{R}^d)}^{1/2} \quad \forall N \in \mathbb{N}. \end{aligned}$$

Hence, the crucial part of the proof relies on the estimation of

$$\sup_{W \in L^{2(q/2)' }(\mathbb{R}^d)} \frac{\|W(x)\psi_1(x_1)\chi^w \sqrt{\gamma}\|_{\mathfrak{S}^2(\mathbb{R}^d)}^2}{\|W\|_{L^{2(q/2)' }(\mathbb{R}^d)}^2} = \|\rho_{\psi_1 \chi^w \gamma \chi^w \psi_1}\|_{L^{q/2}(\mathbb{R}^d)}.$$

The main idea now is to reduce the problem to an evolution equation in $d - 1$ variables. Up to a permutation of coordinates, by the implicit function theorem, there exist a neighborhood \mathcal{U} of (x_0, ξ_0) , functions $e \in \mathcal{S}(1)$ and $a \in \mathcal{C}_c^\infty(\mathbb{R} \times \mathbb{R}^{d-1} \times \mathbb{R}^{d-1})$, such that

•

$$\partial_{\xi'}^2 a(x_0, \xi'_0) \text{ non-degenerate,} \tag{V.4}$$

• $\inf |e| > 0$,

• for all $(x, \xi) \in \mathcal{U}$

$$p(x, \xi) = e(x, \xi)(\xi_1 - a(x_1, x', \xi')). \tag{V.5}$$

Let us detail² how we get the factorization (V.5) of symbols p near points $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ that satisfy the curvature condition Assumption 3

$$p(x, \xi) = (\xi_1 - a(x, \xi'))e(x, \xi)$$

with e which does not vanish and the non-degeneracy condition (V.4).

²This step is rarely written in papers. The bored reader can go straight to the rest of the proof after the little square.

Proof. Up to a permutation of variables ξ_j , we may assume that $\partial_{\xi_1} p(x_0, \xi_0) > 0$ (the negative case is dealt with in the same way). By the implicit function theorem, there exists a convex open neighborhood $U \times V_1 \times V'$ of $(x_0, (\xi_0)_1, (\xi_0)')$ and a smooth function $\tilde{a} : U \times V' \rightarrow V_1$ such that

$$\begin{aligned} (x, \xi_1, \xi') \in U \times V_1 \times V' \quad p(x, \xi_1, \xi') = 0 \\ \iff (x, \xi') \in U \times V', \quad \xi_1 = \tilde{a}(x, \xi') \end{aligned}$$

and

$$\partial_{\xi_1} p > 0 \text{ on } U \times V_1 \times V'.$$

Moreover, we get by the curvature condition (V.1) of the assumption 3

$$\partial_{\xi'}^2 \tilde{a}(x_0, \xi'_0) \text{ non-degenerate}$$

which is (V.4). The Taylor formula at order 1 gives that

$$\begin{aligned} \forall (x, \xi_1, \xi') \in U \times V_1 \times V' \\ p(x, \xi_1, \xi') = (\xi_1 - \tilde{a}(x, \xi')) \underbrace{\int_0^1 \partial_{\xi_1} p(x, \theta \xi_1 + (1 - \theta)\tilde{a}(x, \xi'), \xi') d\theta}_{:= \tilde{e}(x, \xi)}. \end{aligned}$$

Since $\partial_{\xi_1} p > 0$ on $U \times V_1 \times V'$ which is convex, we deduce that there exists $c > 0$ such that $\tilde{e} \geq c$ on $U \times V_1 \times V'$.

Finally, the symbols \tilde{a} and \tilde{e} can be extended to the full space in such a way that $a \in \mathcal{C}_{x_1}^\infty(\mathbb{R}, S_{(x', \xi)'}(1))$, $e \in S(1)$ and e is elliptic on $\mathbb{R}^d \times \mathbb{R}^d$. Let us now detail this extension.

▷ Let $\tilde{U} \times \tilde{V}_1 \times \tilde{V}'$ be an open neighborhood of $(x_0, (\xi_0)_1, (\xi_0)')$ such that

$$\overline{\tilde{U} \times \tilde{V}_1 \times \tilde{V}'} \subset U \times V_1 \times V'$$

and $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^d \times \mathbb{R} \times \mathbb{R}^{d-1}, [0, 1])$ such that $\chi = 1$ on $\tilde{U} \times \tilde{V}_1 \times \tilde{V}'$ and $\text{supp } \chi \subset U \times V_1 \times V'$. Let us define a and e by

$$a := \tilde{a}\chi \text{ and } e := \tilde{e}\chi + (1 - \chi).$$

Note that on $\mathbb{R}^d \times \mathbb{R}^d$

$$e \geq c\chi + (1 - \chi) \geq \min(1, c) > 0.$$

As desired we get (V.5)

$$\forall (x, \xi) \in \tilde{U} \times \tilde{V}_1 \times \tilde{V}' \quad p(x, \xi) = e(x, \xi) (\xi_1 - a(x, \xi')).$$

□

We thus assume that $\mathcal{W} \subset \mathcal{U}$. Then, since $\text{supp } \chi \subset \mathcal{W}$, we have

$$\forall (x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d, \quad p(x, \xi)\chi(x, \xi) = e(x, \xi)(\xi_1 - a(x, \xi'))\chi(x, \xi).$$

We can write $P\chi^w$ as

$$\begin{aligned} P\chi^w &= (p\chi)^w(x, hD) + hr_1^w(x, hD) \\ &= e^w(hD_{x_1} - a^w(x_1, x', hD_{x'}))\chi^w(x, hD) + hr_2^w(x, hD) + hr_1^w(x, hD) \\ &= e^w(hD_{x_1} - a^w(x_1, x', hD_{x'}))\chi^w(x, hD) + hr^w(x, hD). \end{aligned}$$

By symbolic calculus $r \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$. Let B_h be the following pseudodifferential operator

$$B_h := \frac{1}{h} e^w(x, hD_x)^{-1} (P\chi^w(x, hD_x) - hr^w(x, hD)).$$

By definition B_h satisfies $(hD_{x_1} - a^w)\chi^w = hB_h$. In other terms, we have for all $u \in L^2(\mathbb{R}^d)$

$$[hD_{x_1} - a^w(x, hD_{x'})]\chi^w u = hB_h u.$$

Furthermore, we have

Lemma V.3. *The operator B_h satisfies*

(i) *the localization property*

$$(1 - \varphi^w(x', hD_{x'}))B_h = \mathcal{O}(h^\infty) : \mathcal{S}'(\mathbb{R}^d) \rightarrow \mathcal{S}(\mathbb{R}^d), \quad (\text{V.6})$$

(ii)

$$B_h(1 + P^2/h^2)^{-1/2} = \mathcal{O}(1) : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d). \quad (\text{V.7})$$

Proof of Lemma V.3.

(i) Since B_h satisfies

$$B_h = \frac{1}{h} (hD_{x_1} - a^w(x_1, x', hD_{x'}))\chi^w(x, hD)$$

and $\text{supp}(1 - \varphi)$ and $\pi_{(x', \xi')} \chi$ are disjoint, then

$$(1 - \varphi^w(x', hD_{x'}))B_h = \mathcal{O}(h^\infty) : \mathcal{S}'(\mathbb{R}^d) \rightarrow \mathcal{S}(\mathbb{R}^d).$$

(ii) Besides recalling the definition of B_h , $e \in S(1)$ and $r \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$

$$\begin{aligned} B_h(1 + P^2/h^2)^{-1/2} &= \left(\frac{1}{h} (e^w)^{-1} P - (e^w)^{-1} r^w \right) (1 + P^2/h^2)^{-1/2} \\ &= (e^w)^{-1} \left(\frac{1}{h} P \right) (1 + P^2/h^2)^{-1/2} \\ &\quad - (e^w)^{-1} r^w (1 + P^2/h^2)^{-1/2}. \end{aligned}$$

We obtain (V.7) using that $(e^w)^{-1}$, r^w , $(P/h)(1 + P^2/h^2)^{-1/2}$ and $(1 + P^2/h^2)^{-1/2}$ are $\mathcal{O}(1) : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$. \square

Let $r \in \mathbb{R}$. The following evolution equation

$$\begin{cases} [hD_t - a^w(t, x', hD_{x'})]F(t, r) = 0 & t \in \mathbb{R}, \\ F(r, r) = \text{Id}, \end{cases}$$

is solved by a unique family of unitary operators $\{F(t, r)\}_{t \in \mathbb{R}}$ on $L^2(\mathbb{R}^{d-1})$ (we refer the reader to [Zwo12, Thm. 10.1]). Recall the Duhamel's formula satisfied by all $u \in L^2(\mathbb{R}^d)$ and $t \in \mathbb{R}$

$$\chi^w u(t) = F(t, t_0)(\chi^w u)(t_0) + i \int_{t_0}^t F(t, s)(B_h u)(s) ds \quad \text{in } L^2_{x'}(\mathbb{R}^{d-1}).$$

Defining by $\text{ev}_{x_1=t_0}$ the operator of evaluation in $t_0 \in \mathbb{R}$ of the first variable, which maps functions on \mathbb{R}^d to functions on \mathbb{R}^{d-1}

$$\text{ev}_{x_1=t_0} u(x) = u(t_0, x')$$

and $U(t, r)$ the microlocalized operator on $L^2_{x'}(\mathbb{R}^{d-1})$

$$U(t, r) := \psi(t - r)F(t, r)\varphi^w(x', hD_{x'}),$$

given the support property of ψ_1 and ψ , we get the decomposition

$$\begin{aligned} \psi_1(t)\chi^w(t, x', hD_{t,x'}) &= \psi_1(t) \left(F(t, t_0) \text{ev}_{x_1=t_0} \chi^w + i \left(\int_{t_0}^t F(t, s)(1 - \varphi^w) \text{ev}_{x_1=s} B_h ds \right) \right) \\ &\quad + i\psi_1(t) \left(\int_{t_0}^t U(t, s) \text{ev}_{x_1=s} B_h ds \right). \end{aligned}$$

We notice that each term of this operator maps functions on \mathbb{R}^d into functions on \mathbb{R}^d . Define S by

$$S := \psi_1(t)F(t, t_0) \text{ev}_{x_1=t_0} \chi^w + i\psi_1(t) \left(\int_{t_0}^t F(t, s)(1 - \varphi^w) \text{ev}_{x_1=s} B_h ds \right)$$

We introduce the operator T_U which acts on functions on \mathbb{R}^d

$$T_U f(t) := \psi_1(t) \int_{t_0}^t U(t, s) f(s) ds \quad \text{in } L^2(\mathbb{R}^d).$$

We then have the following results.

Proposition V.4. *Let $\beta \geq 2$. We have the bound*

$$\|WS\|_{\mathfrak{S}^\beta(L^2(\mathbb{R}^d))} = \mathcal{O}(h^\infty) \|W\|_{L^\beta(\mathbb{R}^d)}.$$

Proposition V.5. *If \mathcal{W} is a small enough neighborhood of (x_0, ξ_0) , then the operator T_U satisfies the dual estimates*

$$\|WT_U\|_{\mathfrak{S}^{2\alpha(q,d)}(L^2(\mathbb{R}^d))} \leq Ch^{-s(q,d)} \|W\|_{L^{2(q/2)'(\mathbb{R}^d)}}$$

for all $W \in L^{2(q/2)'(\mathbb{R}^d)}$, where $s(q, d)$ and $\alpha(q, d)$ are defined in the statement of Theorem V.2.

Remark 18. Recall that the operator T_U depends on \mathcal{W} through the functions ψ_1 and φ .

Before proving the previous propositions, we use them to complete the proof of Theorem V.2. By the decomposition of the operator $\psi_1(t)\chi^w$ and by the triangle inequality

$$\|W\psi_1(t)\chi^w \sqrt{\gamma}\|_{\mathfrak{S}^2} \leq \|WS\sqrt{\gamma}\|_{\mathfrak{S}^2} + \|WT_U B_h \sqrt{\gamma}\|_{\mathfrak{S}^2}.$$

Using the Hölder inequality and Proposition V.4, we have

$$\begin{aligned} \|WS\sqrt{\gamma}\|_{\mathfrak{S}^2} &\leq \|WS\|_{\mathfrak{S}^{2(q/2)'}} \|\sqrt{\gamma}\|_{\mathfrak{S}^q} \\ &= \mathcal{O}(h^\infty) \|W\|_{L^{2(q/2)'}} \|\gamma\|_{\mathfrak{S}^{q/2}}^{1/2}. \end{aligned}$$

By the Hölder inequality, Lemma V.3 and Proposition V.5

$$\begin{aligned} &\|WT_U B_h \sqrt{\gamma}\|_{\mathfrak{S}^2} \\ &\leq \|WT_U\|_{\mathfrak{S}^{2\alpha'}} \left\| B_h (1 + P^2/h^2)^{-1/2} \right\|_{\mathfrak{S}^\infty} \left\| (1 + P^2/h^2)^{1/2} \sqrt{\gamma} \right\|_{\mathfrak{S}^{2\alpha}} \\ &\lesssim h^{-s(q,d)} \left\| (1 + P^2/h^2)^{1/2} \gamma (1 + P^2/h^2)^{1/2} \right\|_{\mathfrak{S}^\alpha}^{1/2}. \end{aligned}$$

Then, we have the same bound for the norm $\|W(x)\psi_1(t)\chi^w \sqrt{\gamma}\|_{\mathfrak{S}^2}$.

Finally, we obtain for $q = 2(d+1)/d - 1$

$$\|\rho\chi^w \gamma \chi^w\|_{L^{q/2}(\mathbb{R}^d)} \lesssim h^{-2s(q,d)} \left\| (1 + P^2/h^2)^{1/2} \gamma (1 + P^2/h^2)^{1/2} \right\|_{\mathfrak{S}^{\alpha(q,d)}},$$

which is the desired bound.

Proof of Proposition V.4

Let $\beta \geq 2$ and $W \in L^\beta(\mathbb{R}^d)$. In order to prove the desired inequality, we prove

$$\forall k \in \mathbb{N}, \quad S = \mathcal{O}(h^\infty) : \mathcal{S}'(\mathbb{R}^d) \rightarrow H_h^k(\mathbb{R}^d). \quad (\text{V.8})$$

Assuming this result, we only need to choose $k \in \mathbb{N}$ so that $x \mapsto \langle x \rangle^{-k}$ be $L^\beta(\mathbb{R}^d)$. By the Hölder inequality, the previous inequality (V.8) and Kato-Seiler-Simon inequality (Lemma II.20)

$$\begin{aligned} & \|W(t, x')S\|_{\mathfrak{S}^\beta(L^2(\mathbb{R}^d))} \\ & \leq \left\| W(t, x')(1 - h^2 \Delta_{t, x'})^{-k/2} \right\|_{\mathfrak{S}^\beta(L^2(\mathbb{R}^d))} \left\| (1 - h^2 \Delta_{t, x'})^{k/2} S \right\|_{\mathfrak{S}^\infty(L^2(\mathbb{R}^d))} \\ & \leq C_{d, k, N} h^{N-d/2} \|W\|_{\mathfrak{S}^\beta(L^2(\mathbb{R}^d))} \quad \forall N \in \mathbb{N}. \end{aligned}$$

Hence,

$$\|WS\|_{\mathfrak{S}^\beta(L^2(\mathbb{R}^d))} = \mathcal{O}(h^\infty) \|W\|_{\mathfrak{S}^\beta(L^2(\mathbb{R}^d))}.$$

Let us now prove (V.8).

Since $t_0 \notin \pi_{x_1} \text{supp } \chi$, we have

$$\text{ev}_{x_1=t_0} \chi^w(x, hD) = \mathcal{O}(h^\infty) : \mathcal{S}'_x(\mathbb{R}^d) \rightarrow \mathcal{S}'_{x'}(\mathbb{R}^{d-1}),$$

which together with Lemma II.17, implies that

$$\forall k \in \mathbb{N}, \quad \psi_1(t)F(t, t_0) \text{ev}_{x_1=t_0} \chi^w = \mathcal{O}(h^\infty) : \mathcal{S}'(\mathbb{R}^d) \rightarrow H_h^k(\mathbb{R}^d).$$

Let us prove the same equality for the second term $\psi_1(t) \int_{t_0}^t F(t, s)(1 - \varphi^w(x, hD_{x'})) \text{ev}_{x_1=s} B_h ds$. Recall T_F is the operator which acts on functions in \mathbb{R}^d defined by

$$T_F : u = u(t, x') \mapsto \psi_1(t) \int_{t_0}^t (F(t, s)u(s))(x') ds. \quad (\text{V.9})$$

By Lemma II.17 (to $n = d - 1$, $t = x_1$ and $x = x'$), the operator T_F which maps to $H_h^k(\mathbb{R}^d)$ into $H_h^k(\mathbb{R}^d)$ for all $k \in \mathbb{N}$.

Then, since $1 - \varphi^w$ commutes with $\text{ev}_{x_1=s}$ (because φ^w only acts on the variables (x', ξ')) and given Lemma V.3

$$\begin{aligned} \psi_1(t) \int_{t_0}^t F(t, s)(1 - \varphi^w) \text{ev}_{x_1=s} B_h ds &= \psi_1(t) \int_{t_0}^t F(t, s) \text{ev}_{x_1=s} (1 - \varphi^w) B_h ds \\ &= T_F \circ ((1 - \varphi^w) B_h) \\ &= \mathcal{O}(h^\infty) : \mathcal{S}'(\mathbb{R}^d) \rightarrow H_h^k(\mathbb{R}^d) \quad \forall k \in \mathbb{N}. \end{aligned}$$

Finally, for all $k \in \mathbb{N}$

$$S = \mathcal{O}(h^\infty) : \mathcal{S}'(\mathbb{R}^d) \rightarrow H_h^k(\mathbb{R}^d),$$

what is exactly (V.8).

Proof of Proposition V.5

The operator T_U can be split as $T_U = T_+ - T_-$ with

$$T_+ := \mathbf{1}(t \geq t_0) T_U$$

and

$$T_- := -\mathbf{1}(t \leq t_0) T_U.$$

Their dual operators' expressions are the following

$$T_+^* : \begin{cases} L^2(\mathbb{R}^d) & \rightarrow L^2(\mathbb{R}^d) \\ f & \mapsto \mathbf{1}(r \geq t_0) \int_{\mathbb{R}} \mathbf{1}(s \geq t_0) \mathbf{1}(s \geq r) U(s, r)^* \psi_1(s) f(s) ds \end{cases}$$

and

$$T_-^* : \begin{cases} L^2(\mathbb{R}^d) & \rightarrow L^2(\mathbb{R}^d) \\ f & \mapsto \mathbf{1}(r \leq t_0) \int_{\mathbb{R}} \mathbf{1}(s \leq t_0) \mathbf{1}(t \leq r) U(s, r)^* \psi_1(s) f(s) ds. \end{cases}$$

Then the operators $T_{\pm} T_{\pm}^*$ can be written as

$$\begin{aligned} T_+ T_+^* f(t) &= \int_{r \geq t_0} dr \int_{\mathbb{R}} ds \mathbf{1}(t \geq t_0) \mathbf{1}(t \geq r) \mathbf{1}(s \geq t_0) \mathbf{1}(s \geq r) \times \\ &\quad \times \psi_1(t) U(t, r) U(s, r)^* \psi_1(s) f(s) \end{aligned}$$

and

$$\begin{aligned} T_- T_-^* f(t) &= \int_{r \leq t_0} dr \int_{\mathbb{R}} ds \mathbf{1}(t \leq t_0) \mathbf{1}(t \leq r) \mathbf{1}(s \leq t_0) \mathbf{1}(s \leq r) \times \\ &\quad \times \psi_1(t) U(t, r) U(s, r)^* \psi_1(s) f(s). \end{aligned}$$

Let $r \in \mathbb{R}$. Let us introduce the operators $A_{r, \pm}$

$$A_{r, +} : \begin{cases} L_{x'}^2(\mathbb{R}^{d-1}) & \rightarrow L_{t, x'}^2(\mathbb{R}^d) \\ g & \mapsto \mathbf{1}(t \geq t_0) \psi_1(t) \mathbf{1}(t \geq r) U(t, r) g \end{cases}$$

and

$$A_{r, -} : \begin{cases} L_{x'}^2(\mathbb{R}^{d-1}) & \rightarrow L_{t, x'}^2(\mathbb{R}^d) \\ g & \mapsto \mathbf{1}(t \leq t_0) \psi_1(t) \mathbf{1}(t \leq r) U(t, r) g. \end{cases}$$

Their dual operators can be written as

$$A_{r, +}^* : \begin{cases} L_{t, x'}^2(\mathbb{R}^d) & \rightarrow L_{x'}^2(\mathbb{R}^{d-1}) \\ f & \mapsto \int_{\mathbb{R}} \mathbf{1}(s \geq t_0) \mathbf{1}(s \geq r) U(s, r)^* \psi_1(s) f(s) ds \end{cases}$$

and

$$A_{r, -}^* : \begin{cases} L_{t, x'}^2(\mathbb{R}^d) & \rightarrow L_{x'}^2(\mathbb{R}^{d-1}) \\ f & \mapsto \int_{\mathbb{R}} \mathbf{1}(s \leq t_0) \mathbf{1}(s \leq r) U(s, r)^* \psi_1(s) f(s) ds. \end{cases}$$

The operators $A_{r, \pm} A_{r, \pm}^*$ acts on $L^2(\mathbb{R}^d)$. This gives

$$\begin{aligned} T_+ T_+^* &= \int_{r \geq t_0} A_{r, +} A_{r, +}^* dr = \int_{I_r} A_{r, +} A_{r, +}^* dr, \\ T_- T_-^* &= \int_{r \leq t_0} A_{r, -} A_{r, -}^* dr = \int_{I_r} A_{r, -} A_{r, -}^* dr. \end{aligned}$$

Moreover

$$T_U T_U^* = T_+ T_+^* + T_- T_-^*.$$

Thus, for any $\alpha \geq 1$

$$\begin{aligned} & \|WT_U\|_{\mathfrak{S}^{2\alpha'}(L^2(\mathbb{R}^d))}^2 \\ &= \|WT_U T_U^* \bar{W}\|_{\mathfrak{S}^{\alpha'}(L^2(\mathbb{R}^d))} \\ &\leq |I_r| \left(\sup_{r \in I_r} \|WA_{r,+} A_{r,+}^* \bar{W}\|_{\mathfrak{S}^{\alpha'}(L^2(\mathbb{R}^d))} + \sup_{r \in I_r} \|WA_{r,-} A_{r,-}^* \bar{W}\|_{\mathfrak{S}^{\alpha'}(L^2(\mathbb{R}^d))} \right) \\ &\leq |I_r| \left(\sup_{r \in I_r} \|WA_{r,+}\|_{\mathfrak{S}^{2\alpha'}(L^2(\mathbb{R}^{d-1}), L^2(\mathbb{R}^d))}^2 + \sup_{r \in I_r} \|WA_{r,-}\|_{\mathfrak{S}^{2\alpha'}(L^2(\mathbb{R}^{d-1}), L^2(\mathbb{R}^d))}^2 \right). \end{aligned}$$

Now, notice that

$$\|WA_{r,\pm}\|_{\mathfrak{S}^{2\alpha'}} \leq C \|WU(t, r)\|_{\mathfrak{S}^{2\alpha'}}.$$

Given (V.4), we can apply Theorem II.23 to $n = d - 1$ ³, $(x'_0, \xi'_0) \in \mathbb{R}^{d-1} \times \mathbb{R}^{d-1}$, $a \in \mathcal{C}_{x_1}^\infty(\mathbb{R}, S_{(x', \xi')}(1))$ and $J = I_r$. This defines $\delta > 0$ and $U'_1 \times V'_1$ a neighborhood of (x'_0, ξ'_0) (which corresponds to the neighborhood $U \times V$ in Theorem II.18). Thus, imposing the following constraints on \mathcal{W} :

- $|I| < \frac{\delta}{2}$,
- $\mathcal{V}' \subset U'_1 \times V'_1$.

we obtain

$$\sup_{r \in I_r} \|WU(t, r)\|_{\mathfrak{S}^{d+1}(L^2(\mathbb{R}^{d-1}), L^2(\mathbb{R}^d))} \lesssim h^{-\frac{d-1}{2(d+1)}} \|W\|_{L^{d+1}(\mathbb{R}^d)}.$$

That ends the proof of Proposition V.5.

Bonus : An alternative (happy) ending for the proof of Proposition V.5 An simpler end of proof (Section V.3) for Proposition V.5 is Frank-Lewin-Lieb-Seiringer's method [FLLS14] at $q = 2(d+1)/(d-1)$. This gives the same results as in Theorem II.23 for $n = d - 1$ and $2 \leq q \leq 2(n+2)/n = 2(d+1)/(d-1)$ and this allows to avoid the complex interpolation of the dispersive bounds in the Proof of Theorem II.23. Recall briefly the main steps of this proof. Then, we will explain how to apply it in our case for $n = d - 1$ and $T(t) = U(t, r)$ (we will see that the bounds are uniform in $r \in I$).

Let $n \geq 1$. Let $N > 0$ be an integer. Assume that we have $L^2 \rightarrow L^2$ and $L^1 \rightarrow L^\infty$ bounds

$$\begin{cases} \|T(t)T(s)^*\|_{L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n)} & \lesssim 1, \\ \|T(t)T(s)^*\|_{L^1(\mathbb{R}^n) \rightarrow L^\infty(\mathbb{R}^n)} & \lesssim h^{-n/2} |t-s|^{-n/2}, \quad \forall t, s \in \mathbb{R}. \end{cases}$$

³We also give an alternative proof of the same Strichartz bounds for this special case in the paragraph below. Notice that this method did not appear and was not highlighted in the article for the purpose of generality.

Thus,

$$\begin{aligned}
 & \left\| W(t, x') T(t) \right\|_{\mathfrak{S}^{2N}(L^2(\mathbb{R}^n), L^2(\mathbb{R}^{n+1}))}^{2N} \\
 &= \text{Tr}_{L^2(\mathbb{R}^n)} \left[\left(\int_{\mathbb{R}} T(t) |W(t, x')|^2 T(t)^* dt \right)^N \right] \\
 &= \text{Tr}_{L^2(\mathbb{R}^n)} \left[\int_{\mathbb{R}} \cdots \int_{\mathbb{R}} \prod_{k=1}^N |W(t_k)| T(t_k) T(t_{k+1})^* |W(t_{k+1})| dt_1 \cdots dt_N \right] \\
 &= \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} \text{Tr}_{L^2(\mathbb{R}^n)} \left[\prod_{k=1}^N |W(t_k)| T(t_k) T(t_{k+1})^* |W(t_{k+1})| \right] dt_1 \cdots dt_N \\
 &= \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} \left\| \prod_{k=1}^N |W(t_k)| T(t_k) T(t_{k+1})^* |W(t_{k+1})| \right\|_{\mathfrak{S}^1(L^2(\mathbb{R}^n))} dt_1 \cdots dt_N \\
 &\stackrel{\text{H\"older}}{\leq} \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} \prod_{k=1}^N \left\| |W(t_k)| T(t_k) T(t_{k+1})^* |W(t_{k+1})| \right\|_{\mathfrak{S}^N(L^2(\mathbb{R}^n))} dt_1 \cdots dt_N. \\
 &\stackrel{\text{by interpolation}}{\lesssim} \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} \prod_{k=1}^N h^{-n/N} \frac{\|W(t_k)\|_{L^N(\mathbb{R}^n)} \|W(t_{k+1})\|_{L^N(\mathbb{R}^n)}}{|t_k - t_{k+1}|^{(n+1)/N}} dt_1 \cdots dt_N.
 \end{aligned}$$

The following step is the application of the multilinear Hardy-Littlewood-Sobolev inequality V.6

Theorem V.6 (Multilinear Hardy-Littlewood-Sobolev inequality). *Assume that $(\beta_{ij})_{1 \leq i, j \leq N}$ and $(r_k)_{1 \leq k \leq N}$ be real numbers such that*

$$\forall 1 \leq i, j, k \leq N \quad \beta_{ii} = 0, \quad 0 \leq \beta_{ij} = \beta_{ji} < 1, \quad r_k > 1, \quad \sum_{k=1}^N \frac{1}{r_k} > 1, \quad \sum_{i=1}^N \beta_{ik} = \frac{2(r_k - 1)}{r_k}.$$

Then there exists $C > 0$ such that

$$\left| \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} \frac{f_1(t_1) \cdots f_N(t_N)}{\prod_{i < j} |t_i - t_j|^{\beta_{ij}}} dt_1 \cdots dt_N \right| \leq \prod_{k=1}^N \|f_k\|_{L^{r_k}(\mathbb{R})}$$

for all $1 \leq k \leq N$, $f_k \in L^{r_k}(\mathbb{R})$

Assume that we can use it with $\beta_{k, k+1} = \beta_{k+1, k} = (n+1)/N$ et $r_k = N/2$, then

$$\begin{aligned}
 & \sup_{s \in I} \left\| W(t, x') T(t, s) \right\|_{\mathfrak{S}^{2N}(L^2(\mathbb{R}^n), L^2(\mathbb{R}^{n+1}))}^{2N} \\
 &\lesssim \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} \prod_{k=1}^N h^{-n/N} \frac{\|W(t_k)\|_{L^N(\mathbb{R}^n)} \|W(t_{k+1})\|_{L^N(\mathbb{R}^n)}}{|t_k - t_{k+1}|^{(n+1)/N}} dt_1 \cdots dt_N \\
 &= h^{-n} \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} \prod_{k=1}^N \frac{\|W(t_k)\|_{L^{N/2}(\mathbb{R}^{n+1})}^2}{|t_k - t_{k+1}|^{(n+1)/N}} dt_1 \cdots dt_N.
 \end{aligned}$$

We have

$$\sum_{k=1}^N 1/r_k = 2 > 1.$$

Then, we only have to check that $\beta_{k, k+1} < 1$ and $2(1 - 1/r_k) = \sum_{j=1}^N \beta_{jk}$ for all $k \in \{1, \dots, N\}$.

Actually, it is true when we take $N = 2(q/2)'$ for $q = 2(n+2)/n = 2(d+1)/(d-1)$. Therefore for this q , we have $s(q, d) = 2(d-1)/(d+1)$ and $\alpha(q, d) = 1 + 1/d = (2(q/2)')' = 2q/(q+2)$. That concludes the alternative proof.

VI L^p ESTIMATES AROUND TURNING POINTS

We now treat the turning point region $\{V = E\}$, under the assumption $\nabla_x V \neq 0$ on this set. In the one-body case ($\text{rank } \gamma = 1$), we recover [Zwo12, Thm. 7].

VI.1 Statement of the result

Let $d \geq 2$.

Assumption 4. A point $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ satisfies the following *turning point conditions* for a symbol p if

$$p(x_0, \xi_0) = 0, \quad \nabla_{\xi} p(x_0, \xi_0) = 0, \quad \nabla_x p(x_0, \xi_0) \neq 0, \quad \partial_{\xi}^2 p(x_0, \xi_0) \text{ is positive definite.}$$

Remark 19. For Schrödinger operators $p(x, \xi) = \xi^2 + V(x) - E$ with $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$ satisfying Definition II.3, the previous assumption is equivalent to:

$$\xi_0 = 0, \quad V(x_0) = E, \quad \nabla_x V(x_0) \neq 0.$$

First recall the individual function result.

Theorem VI.1 (Improved one-body estimates, [KTZ07, Thm. 7]). *Let $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$ satisfying Definition II.3, define $p(x, \xi) := |\xi|^2 + V(x)$ and $P := p^w(x, hD)$ (or any other quantization). Let $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ be a point satisfying the Assumption 4 for the symbol p . Then, there exist a neighborhood \mathcal{V} of (x_0, ξ_0) and $h_0 > 0$, such that for any $\chi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ with support contained in \mathcal{V} , there exists $C > 0$ such that for any $0 < h \leq h_0$, for any $2 \leq q \leq \infty$ and for any bounded self-adjoint non-negative operator γ on $L^2(\mathbb{R}^d)$*

$$\|\chi^w u\|_{L^q(\mathbb{R}^d)} \leq C \log(1/h)^{t(q,d)} h^{-s(q,d)} \left(\|u\|_{L^2(\mathbb{R}^d)} + \frac{1}{h} \|Pu\|_{L^2(\mathbb{R}^d)} \right)$$

where $t(q, d)$ and $s(q, d)$ are given by the following formulas

$$t(q, d) = \begin{cases} \frac{d+1}{2(d+3)} & \text{if } q = \frac{2(d+3)}{d+1}, \\ 0 & \text{otherwise,} \end{cases} \quad (\text{VI.1})$$

and

- when $d = 2$:

$$s(q, 2) = \begin{cases} \frac{1}{4} - \frac{1}{2q} & \text{if } 2 \leq q \leq \frac{10}{3}, \\ \frac{1}{2} - \frac{4}{3q} & \text{if } \frac{10}{3} \leq q \leq \infty, \end{cases} \quad (\text{VI.2})$$

- when $d \geq 3$:

$$s(q, d) = \begin{cases} \frac{d-1}{2} \left(\frac{1}{2} - \frac{1}{q} \right) & \text{if } 2 \leq q \leq \frac{2(d+3)}{d+1}, \\ \frac{2d}{3} \left(\frac{1}{2} - \frac{1}{q} \right) - \frac{1}{6} & \text{if } \frac{2(d+3)}{d+1} \leq q \leq \frac{2d}{d-2}, \\ d \left(\frac{1}{2} - \frac{1}{q} \right) - \frac{1}{2} & \text{if } \frac{2d}{d-2} \leq q \leq \infty. \end{cases} \quad (\text{VI.3})$$

Equivalently, one has for all $2 \leq q \leq \infty$

$$\chi^w (1 + P^* P / h^2)^{-1/2} = \mathcal{O}(\log(1/h)^{t(q,d)} h^{-s(q,d)}) : L^2(\mathbb{R}^d) \rightarrow L^q(\mathbb{R}^d).$$

Remark 20. The exponent s_{TP} , defined in Theorem VI.1 satisfies $s_{\text{Sogge}} \leq s_{\text{TP}} \leq s_{\text{gene}}$ for any $d \geq 1$ and $q \in [2, \infty]$. They are all equal for $q = \{2\} \cup [2d/(d-2), \infty]$. Furthermore $s_{\text{TP}} = s_{\text{Sogge}}$ when $q \in [2, 2(d+3)/(d+1)]$. Otherwise, the inequalities are strict. (c.f. Figure 1.3).

Remark 21. Note that the previous result has been proved in [KTZ07, Thm. 7] for slightly more general symbols

$$p(x, \xi) = \sum_{i,j=1}^d a_{ij}(x) \xi_i \xi_j + V(x),$$

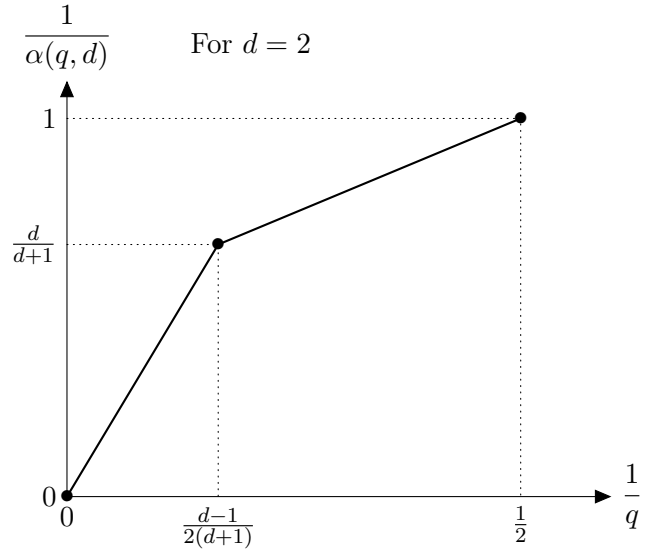
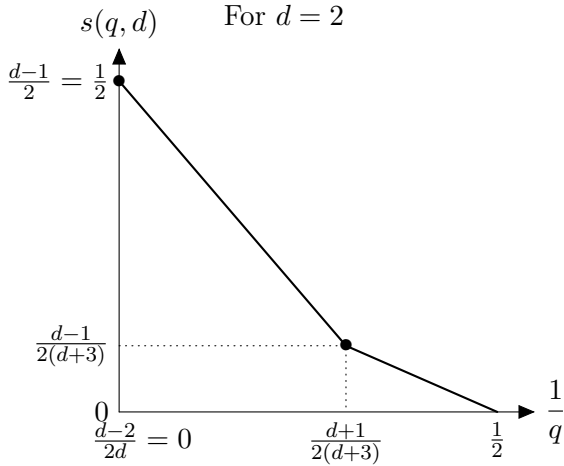
where $\{a_{ij}\}_{1 \leq i,j \leq d} \subset C^\infty(\mathbb{R}^d, \mathbb{R})$ is a positive definite Riemannian metric on \mathbb{R}^d and $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$ satisfy Definition II.3. Our results can also be generalized to this case.

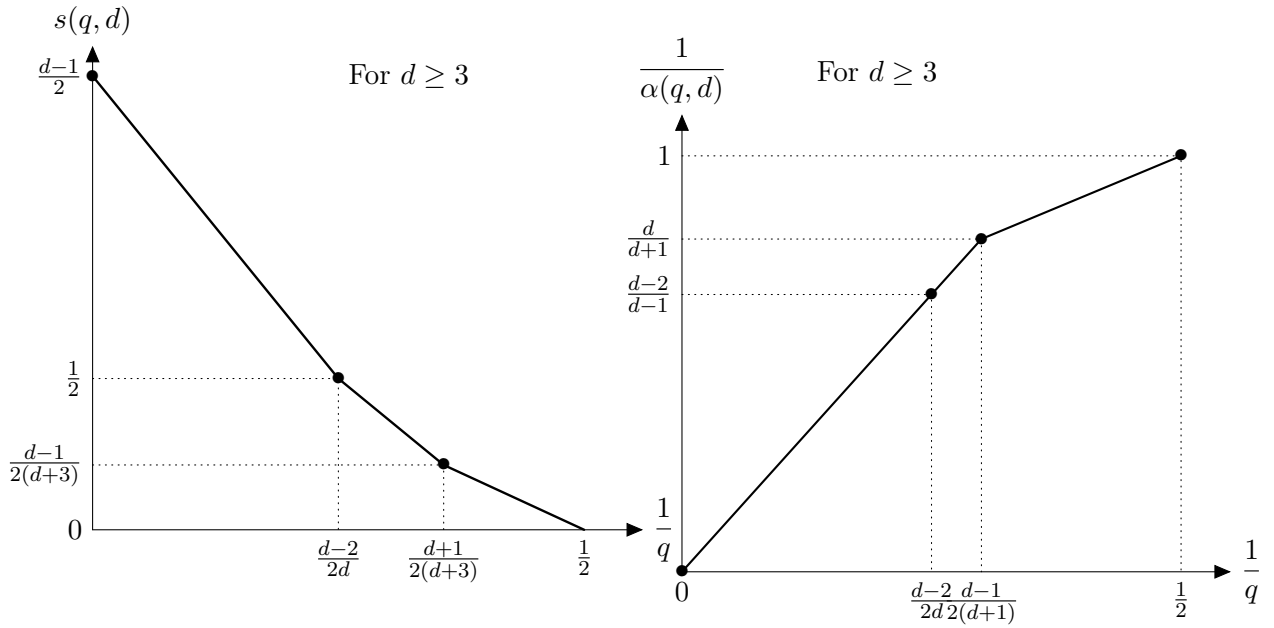
Theorem VI.2 (Improved many-body estimates). *Let $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$ satisfying Definition II.3, define $p(x, \xi) := |\xi|^2 + V(x)$ and $P := p^w(x, hD)$. Let $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ be a point satisfying the Assumption 4 for the symbol p . Then, there exist a neighborhood \mathcal{V} of (x_0, ξ_0) and $h_0 > 0$, such that for any $\chi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ with support contained in \mathcal{V} , there exists $C > 0$ such that for any $0 < h \leq h_0$, for any $2 \leq q \leq \infty$ and for any bounded self-adjoint non-negative operator γ on $L^2(\mathbb{R}^d)$*

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\mathbb{R}^d)} \leq C \log(1/h)^{2t(q,d)} h^{-2s(q,d)} \left\| (1 + P^2/h^2)^{1/2} \gamma (1 + P^2/h^2)^{1/2} \right\|_{\mathfrak{S}^{\alpha(q,d)}}$$

where $t(q, d)$, $s(q, d)$ are given by the formulas (VI.1), (VI.2), (VI.3), and $\alpha(q, d)$ is given by the formula of (V.3).

Remark 22. The proof of [KTZ07] gives the exponent $q = \frac{2d}{d-2}$ as a threshold for the exponent $s(q, d)$. Actually, their proof shows that this threshold can be improved to $q = \frac{2d}{d-4}$ (because they only use a control in H^1 while their proof also provides a control in H^2). We choose to keep this weaker statement because it only applies to functions which are microlocalized around a turning point $(x_0, \xi_0 = 0)$ ($p(x_0, \xi_0) = 0$). In our application to spectral clusters we will also need to deal with points such that $p(x_0, \xi_0) = 0$ and $\xi_0 \neq 0$, where only the Sogge estimates are available.





VI.2 About the change of symbol

In this section, we detail some points which do not appear in [Ngu22] (since nothing is really new). In particular, we start the proof of Theorem VI.2 (and more precisely Lemma VI.8) with replacing the symbol $p(x, \xi) = |\xi|^2 + V(x)$ by the symbol $q(x, \xi) = \xi_1^2 + \sum_{2 \leq i, j \leq d} a_{ij}(x) \xi_i \xi_j - c(x)x_1$ in the neighborhood turning points (points $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ satisfying Assumption (4)). In this section, we explain why this consideration makes sense and how to find the desired estimates with the initial symbol. We did it in the many-body estimates, but it is the same for the one-body estimates. The two main ingredients are Proposition VI.3, that expresses the symbol p in terms of its normal geodesic coordinates, and Lemma II.26.

Proposition VI.3 (Change on geodesic normal coordinates, [LR19]). *Let $p(x, \xi) = |\xi|^2 + V(x)$ with $V \in C^\infty(\mathbb{R}^d)$ satisfying Assumption II.3. Let $x_0 \in \mathbb{R}^d$ such that $V(x_0) = E$ and $\nabla_x V(x_0) \neq 0$.*

1) *Then, there exist $\kappa : \mathbb{R}^d \rightarrow \mathbb{R}^d$ a smooth diffeomorphism and $\delta > 0$ such that for any $(x, \xi) \in B(x_0, \delta) \times \mathbb{R}^d$*

$$p(x, d_x \kappa \cdot \xi) = q(\kappa(x), \xi) \quad (\text{VI.4})$$

where

$$q(x, \xi) = \xi_1^2 + \sum_{2 \leq i, j \leq d} a_{ij}(x) \xi_i \xi_j - c(x)x_1,$$

with $c \in C^\infty(\mathbb{R}^d)$ positive on $B(x_0, \delta)$ and $(a_{ij})_{2 \leq i, j \leq d} \in C^\infty(\mathbb{R}^d)$ positive definite uniformly on \mathbb{R}^d and

$$\forall \alpha \in \mathbb{N}^d, \exists C_\alpha > 0, \forall i, j = \{2, \dots, d\}, \forall x \in \mathbb{R}^d, \quad |\partial^\alpha a_{ij}(x)| + |\partial^\alpha V(x)| \leq C_\alpha.$$

2) *Let $P := p^w(x, hD)$ (or any other quantization). Denote by $d_x \kappa$ the Jacobian matrix of κ at x and $J_\kappa(x) := \det(d_x \kappa)^{1/2}$. Let us define the unitary operator U on $L^2(\mathbb{R}^d)$*

$$U_\kappa v(x) = v(\kappa(x)) J_\kappa(x), \quad (\text{VI.5})$$

and $\tilde{P} := U^* P U$. Then, there exist $r \in C^\infty(\mathbb{R}^d \times \mathbb{R}^d) \cap S(\langle \xi \rangle^2)$ such that

$$\tilde{P} = (hD_{x_1})^2 + \sum_{2 \leq i, j \leq d} a_{ij}(x) (hD_{x_i})(hD_{x_j}) - c(x)x_1 + hr^w(x, hD). \quad (\text{VI.6})$$

Remark 23. Notice that \tilde{P} is the expression of P on normal geodesic coordinates $y = \kappa(x)$. In this new system of coordinates, one has $D_x = d_x \kappa \cdot D_y$. Furthermore, the error term r corresponds to the commutation term.

Let us assume temporarily (or not if the reader is familiar with it) Proposition VI.3 and let us see how the desired microlocalized estimates on p are deduced from the estimates associated to q

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\mathbb{R}^d)} \leq Ch^{-2s} \log(1/h)^{2t} \left(\|\gamma\|_{\mathfrak{S}^\alpha} + \frac{1}{h^2} \|\tilde{P}\gamma\tilde{P}^*\|_{\mathfrak{S}^\alpha} \right)$$

for any quantization \tilde{P} of q . Let q be the symbol defined as in Proposition VI.3. Let κ the smooth diffeomorphism, that links the symbols p and q . Let $P = p^w(x, hD)$ and $\tilde{P} := U_\kappa^* P U_\kappa$. Assume that⁴ there exists a bounded open neighborhood $\mathcal{V} \subset \mathbb{R}^d \times \mathbb{R}^d$ of $(0, 0)$ such that $\pi_x \subset B_{\delta/2}$, such that for any function $\tilde{\chi} \in \mathcal{C}_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ supported on \mathcal{V} and for any non-negative bounded symmetric operator $\tilde{\gamma}$ on $L^2(\mathbb{R}^d)$

$$\|\rho_{\tilde{\chi}^w \tilde{\gamma} \tilde{\chi}^w}\|_{L^{q/2}(\mathbb{R}^d)} \lesssim \log(1/h)^{2t(q,d)} h^{-2s(q,d)} \left(\|\tilde{\gamma}\|_{\mathfrak{S}^{\alpha(q,d)}} + \frac{1}{h^2} \|Q\tilde{\gamma}Q^*\|_{\mathfrak{S}^{\alpha(q,d)}} \right). \quad (\text{VI.7})$$

Lemma II.26 implies the same estimates with \tilde{P} instead of Q . Let us prove the existence of an open bounded neighborhood $\mathcal{V}_{(x_0, \xi_0)} \subset \mathbb{R}^d \times \mathbb{R}^d$ of (x_0, ξ_0) such that for any $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ such that $\text{supp } \chi \subset \mathcal{V}_{(x_0, \xi_0)}$ and for any $\tilde{\gamma}$ for any non-negative bounded symmetric operator $\tilde{\gamma}$ on $L^2(\mathbb{R}^d)$

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\mathbb{R}^d)} \lesssim \log(1/h)^{2t(q,d)} h^{-2s(q,d)} \left(\|\gamma\|_{\mathfrak{S}^{\alpha(q,d)}} + \frac{1}{h^2} \|P\gamma P^*\|_{\mathfrak{S}^{\alpha(q,d)}} \right).$$

By [Zwo12, Thm. 9.3], there exists $r \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$ such that

$$\forall (x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d \quad \tilde{\chi}(\kappa(x), \xi) = \chi(x, {}^T(d_x \kappa) \cdot \xi) + hr(x, {}^T(d_x \kappa) \cdot \xi), \quad U_\kappa^* \chi^w U_\kappa = \tilde{\chi}^w. \quad (\text{VI.8})$$

Let us denote $\mathcal{V}_{(x_0, \xi_0)} := \{(\kappa^{-1}(x), {}^T(d_{\kappa^{-1}(x)} \kappa) \cdot \xi) : (x, \xi) \in \mathcal{V}\}$. Let $\chi \in \mathcal{C}_c^\infty(\mathcal{V}_{(x_0, \xi_0)})$. Let $\tilde{\chi}$ and $r \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$ that satisfy (VI.8). Estimating $\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\mathbb{R}^d)}$ amounts to estimating the norms $h^2 \|\rho_{r^w \gamma r^w}\|_{L^{q/2}(\mathbb{R}^d)}$ and $\|\rho_{U_\kappa \chi^w U_\kappa^* \gamma U_\kappa \chi^w U_\kappa^*}\|_{L^{q/2}(\mathbb{R}^d)}$. On the one hand, since $r \in \mathcal{S}(\mathbb{R}^d)$, by the Kato-Seiler-Simon inequality (Lemma II.21)

$$h^2 \|\rho_{r^w \gamma r^w}\|_{L^{q/2}(\mathbb{R}^d)} \leq h^{2-d(\frac{1}{2}-\frac{1}{q})} \|\gamma\|_{\mathfrak{S}^{q/2}}.$$

On the other hand, denoting $\tilde{\gamma} := U_\kappa^* \gamma U_\kappa$ and noticing that $\text{supp } \tilde{\chi} \subset \mathcal{V}$, one has by (VI.7)

$$\begin{aligned} \|\rho_{U_\kappa \chi^w U_\kappa^* \gamma U_\kappa \chi^w U_\kappa^*}\|_{L^{q/2}(\mathbb{R}^d)} &= \|\rho_{\tilde{\chi}^w \tilde{\gamma} \tilde{\chi}^w}\|_{L^{q/2}(\mathbb{R}^d)} \\ &\lesssim \log(1/h)^{2t(q,d)} h^{-2s(q,d)} \left(\|\tilde{\gamma}\|_{\mathfrak{S}^{\alpha(q,d)}} + \frac{1}{h^2} \|\tilde{P}\tilde{\gamma}\tilde{P}^*\|_{\mathfrak{S}^{\alpha(q,d)}} \right) \\ &= \log(1/h)^{2t(q,d)} h^{-2s(q,d)} \left(\|\gamma\|_{\mathfrak{S}^{\alpha(q,d)}} + \frac{1}{h^2} \|P\gamma P^*\|_{\mathfrak{S}^{\alpha(q,d)}} \right). \end{aligned}$$

Eventually, since (q, s, t, α) satisfy the relation (II.9), one obtains the desired bound by the triangle inequality.

⁴There is what we proved in the proof of Theorem VI.2, more precisely in Lemma VI.8

Proof of Proposition VI.3

The proof is the same as in the notes [LR19] for the local change of coordinates. We nevertheless write more pedestrian constructions and explain in Lemma VI.4 how to get equalities on a local neighborhood of the point x_0 to global objects defined on \mathbb{R}^d .

Extension of a local diffeomorphism. We present first how extending a local diffeomorphism to a global one on the whole Euclidean space.

Lemma VI.4. *Let $\kappa : X \rightarrow \kappa(X)$ be a C^∞ -diffeomorphism of a bounded neighborhood $X \subset \mathbb{R}^d$ of 0 into $\kappa(X)$. Then, there exists $\delta > 0$ and $\tilde{\kappa}$ a C^∞ -diffeomorphism of \mathbb{R}^d such that $\tilde{\kappa} = \kappa$ in the ball \bar{B}_δ .*

To lighten the notations in the proof of Proposition VI.3, we also denote by κ the extension $\tilde{\kappa}$. The parameter δ in notation of Theorem VI.1 and Theorem VI.2 is the same as the one of the previous lemma.

Proof of Lemma VI.4. Let $\chi \in C_c^\infty(\mathbb{R}^d)$ such that $\chi = 1$ in $\{|x| \leq 1\}$ and $\chi = 0$ in $\{|x| \geq 2\}$. Let $\delta > 0$ such that $B_{2\delta} \subset X$ and let

$$\tilde{\kappa}(x) := \chi(x/\delta)\kappa(x) + (1 - \chi(x/\delta))(\kappa(0) + d_0\kappa(x)).$$

Notice that $\tilde{\kappa} \in C^\infty(\mathbb{R}^d)$ is equal to κ on B_δ .

- Let us prove that $\tilde{\kappa}$ is a proper function. Since $J_0\kappa$ is invertible, there exists $c > 0$ such that $|d_0\kappa(x)| \geq c|x|$ for any $x \in \mathbb{R}^d$. Moreover,

$$\tilde{\kappa}(x) = d_0\kappa(x) + \chi(x/\delta)(\kappa(x) - \kappa(0) - d_0\kappa(x)).$$

Thus, $|\kappa(x)| \geq c|x|$ on $\{|x| \geq 2\delta\}$, and we deduce $\kappa(x) \rightarrow +\infty$ as $|x| \rightarrow \infty$.

- Let us show that there exists $\delta > 0$ such that the Jacobian matrix $d_x\kappa$ is invertible for any $x \in \mathbb{R}^d$. For any $x \in \mathbb{R}^d$

$$d_x\kappa = d_0\kappa + \chi(x/\delta)(d_x\kappa - d_0\kappa) + \frac{1}{\delta}\nabla_x\chi(x/\delta) \cdot (\kappa(x) - \kappa(0) - d_0\kappa(x)).$$

On the one hand, $d_0\kappa$ is invertible. On the other hand, we have

$$\forall x \in B_{2\delta}, \quad |d_x\kappa - d_0\kappa| \lesssim \delta, \quad |\kappa(x) - \kappa(0) - d_0\kappa(x)| \lesssim \delta^2.$$

Then, $d_x\kappa = d_0\kappa(\text{Id} + R_\delta(x))$ with $R_\delta(x) \in M_{d \times d}(\mathbb{R})$ such that $\sup_{x \in \mathbb{R}^d} |R_\delta(x)| = \mathcal{O}(\delta)$. Choosing $\delta > 0$ small enough so that $\sup_{x \in \mathbb{R}^d} |R_\delta(x)| < 1$, the matrix $d_x\kappa$ is invertible for any $x \in \mathbb{R}^d$.

Hence, by fixing $\delta > 0$ small enough, it follows from the Hadamard-Levy theorem that $\tilde{\kappa}$ is a global smooth diffeomorphism. \square

Proof of the change to local normal geodesic coordinates. Let us build a smooth diffeomorphism $\kappa : X \rightarrow \kappa(X)$ on an open bounded neighborhood X of x_0 such that we have (VI.4) on $X \times \mathbb{R}^d$.

To do so, it is about composing the local diffeomorphisms κ_j obtained at each step j by restricting their definition domain X_j . Actually, denoting $p_0 := p$, we start at the beginning of each step j with a symbol p_{j-1} (and the smooth diffeomorphism $\kappa_{j-1} : X_{j-2} \rightarrow \kappa_{j-1}(X_{j-1})$ which remains from the previous step). We may assume that p_{j-1} is globally defined on \mathbb{R}^d . Let p_j the

new symbol expected in the new coordinates. With its expression in mind, we prove the existence of the open bounded set X_j and the smooth diffeomorphism $\kappa_j : X_j \rightarrow \kappa_j(X_j)$ such that

$$\forall (x, \xi) \in X_j \times \mathbb{R}^d, \quad p_{j-1}(x, {}^T(d_x \kappa_j) \cdot \xi) = p_j(\kappa_j(x), \xi).$$

Then, we extend p_j to the whole Euclidean space \mathbb{R}^d by extending κ_j with Lemma VI.4. In the end $\kappa = \kappa_3 \circ \kappa_2 \circ \kappa_1$. We will also show that the new expression of the new potential $(U_\kappa^* V U_\kappa)(x) = (V \circ \kappa^{-1})(x)$ is $-x_1 c(x)$ with $c(0) > 0$.

In order to simplify notation, we denote by $\kappa : X \rightarrow \kappa(X)$ the intermediary diffeomorphism and U_κ by the associated transform (defined by (VI.5)) at each step.

Step 0. Without loss of generality (up to a permutation of variables) let us assume that $\partial_{x_1} V(x_0) \neq 0$. We also assume $x_0 = 0$ replacing V by $V(\cdot - x_0)$.

Step 1. Let us write a first diffeomorphism so that the function $x \mapsto -x_1$ replaces V . Denote $\kappa : (x_1, x') \in \mathbb{R} \times \mathbb{R}^{d-1} \mapsto (-V(x), x') \in \mathbb{R} \times \mathbb{R}^{d-1}$. Since ∇V does not vanish at 0 and V is continuous, the local inversion theorem implies that there exists an open neighborhood $X \subset \mathbb{R}^d$ of 0 such that $\kappa : X \rightarrow \kappa(X)$ is a smooth diffeomorphism. Thus, $V(\kappa^{-1}(x)) = -x_1$ on X . At this stage of the proof, the symbol

$$p_1(y, \eta) = \langle \eta, (b_{ij}(y))_{1 \leq i, j \leq d} \eta \rangle - y_1$$

is available with $(b_{ij}(y))_{1 \leq i, j \leq d} \in \mathcal{C}^\infty(\kappa(X))$. Let us verify that the matrix $(b_{ij}(y))_{1 \leq i, j \leq d}$ is symmetric positive definite uniformly on $Y = \kappa(X)$. For this, we express the matrix $(b_{ij}(y))_{1 \leq i, j \leq d}$ in terms of the matrix $(a_{ij}(x))_{1 \leq i, j \leq d}$. Since the identity matrix is symmetric positive definite and $d_x \kappa$ is invertible, for any $y = \kappa(x)$ and any $\eta \in \mathbb{R}^d$

$$\begin{aligned} \langle \eta, (b_{ij}(y))_{i, j} \eta \rangle &= p_1(y, \eta) + y_1 = p(x, {}^T d_x \kappa \cdot \eta) - V(x) = {}^T ({}^T(d_x \kappa) \eta) \text{Id}_d ({}^T(d_x \kappa) \eta) \\ &\geq C |{}^T(d_x \kappa) \eta|^2 \geq \tilde{C} |\eta|^2. \end{aligned}$$

Besides, $(b_{ij}(y))_{1 \leq i, j \leq d} = d_x \kappa {}^T(d_x \kappa) = \text{Id}_d$ is symmetric too.

Step 2. Let us prove that through a smooth change of variable $\kappa : X \rightarrow \kappa(X)$, the symbol p_1 becomes $\kappa : X \rightarrow \kappa(X)$

$$p_2(y, \eta) = \langle \eta, (q_{ij}(y))_{1 \leq i, j \leq d} \eta \rangle + V_2(y), \quad V_2(y) = -y_1 \tilde{c}(y),$$

where $\tilde{c} \in \mathcal{C}^\infty(\kappa(X))$ with $\tilde{c}(0) > 0$ and the symmetric positive definite matrix

$$(q_{ij}(y))_{1 \leq i, j \leq d} = \begin{pmatrix} 1 & q_{12}(y) & \cdots & q_{1d}(y) \\ q_{12}(y) & q_{22}(y) & \cdots & q_{2d}(y) \\ \vdots & \vdots & & \vdots \\ q_{1d}(y) & q_{2d}(y) & \cdots & q_{dd}(y) \end{pmatrix}.$$

Let $e_1 := (1, 0, \dots, 0) \in \mathbb{R}^d$. In this new system of local coordinates $D_x = d_x \kappa \cdot D_y$, the pseudodifferential operator $P_1 + x_1 = \sum_{i, j=1}^d a_{ij}(x) (hD_{x_i}) (hD_{x_j})$ becomes $P_2 := U_\kappa^* (P_1 + x_1) U_\kappa$ and its expression is

$$(hD_{x_1})^2 + 2 \sum_{i=2}^d q_{i1}(x) (hD_{x_i}) (hD_{x_1}) + \sum_{i, j=2}^d q_{ij}(x) (hD_{x_i}) (hD_{x_j}).$$

Since $(b_{ij}(x))_{i,j}$ is symmetric positive definite uniformly on \mathbb{R}^d , by the same argument as in the previous step the matrix $(q_{ij}(y))_{1 \leq i,j \leq d}$ has also these properties for any $y \in \kappa(X)$. Moreover $p_2(y, e_1) = 1$ for any $y \in \mathbb{R}^d$. The idea is to find the smooth diffeomorphism $\kappa_1 : X \rightarrow \kappa_1(X) \subset \mathbb{R}$ (the first coordinate of κ) such that

$$\forall x \in X, \quad 1 = p_2((\kappa_1(x), x'), e_1) = p_1(x, \nabla_x \kappa_1(x)),$$

with the initial condition $\kappa_1(0) = 0$, $\partial_{x_1} \kappa_1(0) = b_{11}(0)^{-1/2}$ and $\partial_{x'} \kappa_1(0) = 0$. There remains to consider

$$\kappa(x) := (\kappa_1(x), x')$$

where κ_1 is a smooth solution of the Eikonale equation on a neighborhood $X \subset \mathbb{R}^d$ of 0

$$\begin{cases} p_1(x, \nabla_x \kappa_1(x)) = 1, \\ \kappa_1(0) = 0, \quad \nabla_x \kappa_1(x) = b_{11}(x)^{-1/2} e_1. \end{cases}$$

The positivity of $(b_{ij}(x))_{1 \leq i,j \leq d}$ implies the existence of a neighborhood $\tilde{X} \subset \mathbb{R}^d$ on which b_{11} is positive. The function

$$\kappa_1(x) := \int_0^{x_1} \frac{dt}{\sqrt{b_{11}(t, x')}},$$

which is $\mathcal{C}^\infty(\tilde{X})$, satisfies the Eikonale equation. Since $\kappa_1 \in \mathcal{C}^\infty(\tilde{X})$ and $\partial_{x_1} \kappa_1(0) \neq 0$, we apply the local inversion theorem so that κ_1 is a smooth diffeomorphism of a smaller neighborhood X of 0 in \mathbb{R}^d which maps \tilde{X} into its image. That gives us the diffeomorphism $\kappa : X \rightarrow \kappa(X)$. From this expression and $\kappa_1^{-1}(0) = 0$, we deduce the new potential

$$\begin{aligned} V_2(y) &= U_\kappa^* y_1 U_\kappa = -(\kappa^{-1}(y)) \cdot e_1 = -(\kappa_1^{-1})(y) \\ &= -y_1 \int_0^1 \partial_{y_1}(\kappa_1^{-1})(\kappa_1^{-1}(ty_1), x') dt = -y_1 \int_0^1 \sqrt{b_{11}(\kappa_1^{-1}(ty_1), x')} dt. \end{aligned}$$

Let us denote $\tilde{c}(y) := \int_0^1 \sqrt{b_{11}(\kappa_1^{-1}(ty_1), x')} dt$, which satisfies as expected $\tilde{c} \in \mathcal{C}^\infty(\kappa(X))$ with $\tilde{c}(0) = \sqrt{b_{11}(0)} > 0$.

Step 3. The idea is now to get rid of the part $2 \sum_{i=1}^d q_{i1}(x) (hD_{x_i})(hD_{x_1})$ in the operator P_2 and to obtain after changing coordinates to this expression $y = \kappa(x)$ the symbol

$$p_3(y, \eta) = \eta_1^2 + \langle \eta', a_{ij}(x) \rangle_{2 \leq i,j \leq d} \eta' \rangle - c(y) y_1$$

with $(a_{ij}(y))_{2 \leq i,j \leq d}$ a symmetric positive definite matrix uniformly on $\kappa(X)$ and $c(0) \neq 0$. We start by writing p_2 into the form

$$p_2(x, \xi) = \left(\xi_1 + \sum_{i=2}^d q_{i1}(x) \xi_i \right)^2 + \sum_{i,j=2}^d \tilde{q}_{ij}(x) \xi_i \xi_j + V_2(x),$$

where $\tilde{q}_{ij}(x) := q_{ij}(x) - q_{i1}(x) q_{j1}(x)$. The symmetry of $(\tilde{q}_{ij})_{2 \leq i,j \leq d}$ comes from the one of $(q_{ij})_{2 \leq i,j \leq d}$. Let us check that $(\tilde{q}_{ij}(x))_{2 \leq i,j \leq d}$ symmetric positive definite matrix uniformly on X .

For any $\xi' \in \mathbb{R}^{d-1}$

$$\begin{aligned} \sum_{2 \leq i, j \leq d} \tilde{q}_{ij}(x) \xi_i \xi_j &= \sum_{2 \leq i, j \leq d} q_{ij}(x) \xi_i \xi_j + \left(\sum_{2 \leq i \leq d} q_{i1}(x) \xi_i \right) \left(\sum_{2 \leq j \leq d} q_{j1}(x) \xi_j \right) \\ &= \langle \xi', (q_{ij}(x))_{2 \leq i, j \leq d} \xi' \rangle + \left(\sum_{2 \leq i \leq d} q_{i1}(x) \xi_i \right)^2 \\ &\geq \langle (0, \xi'), (q_{ij}(x))_{1 \leq i, j \leq d} (0, \xi') \rangle \\ &\geq C |\xi'|^2. \end{aligned}$$

It is now sufficient to construct the change of coordinates $x \mapsto \kappa(x) = y$ for which

$$\begin{aligned} U_\kappa^* D_{x_1} U_\kappa &= D_{x_1} + \sum_{2 \leq i \leq d} q_{i1}(\kappa^{-1}(x)) D_{x_i} = \langle (q_{ij}(\kappa^{-1}(x)))_{1 \leq i, j \leq d} D_x, e_1 \rangle, \\ U_\kappa^* D_{x'} U_\kappa &= (\tilde{b}_{ij}(\kappa^{-1}(x)))_{2 \leq i, j \leq d} D_{x'}, \end{aligned}$$

with $(\tilde{b}_{ij}(y))_{2 \leq i, j \leq d}$ an invertible matrix on $\kappa(X)$. Actually, $U^* D_x U = (d_x \kappa)^{-1} D_x$ on $\kappa(X)$, then

$$(d_x \kappa)^{-1} = \begin{pmatrix} 1 & q_{12}(x) & \cdots & q_{1d}(x) \\ 0 & \tilde{b}_{22}(x) & \cdots & \tilde{b}_{2d}(x) \\ \vdots & \vdots & & \vdots \\ 0 & \tilde{b}_{d2}(x) & \cdots & \tilde{b}_{dd}(x) \end{pmatrix}.$$

One can also assume $(\tilde{b}_{ij}(0, y'))_{2 \leq i, j \leq d} = \text{Id}_{d-1}$ for any $y' \in \pi_{x'} \kappa(X)$. Notice that $(d_x \kappa)^{-1} = d_{\kappa(x)}(\kappa^{-1})$. That involves the relations $\nabla_{y'}(\kappa^{-1})_1(y_1, y') = 0$ for any $y \in \kappa(X)$ and $\partial_{y_j}(\kappa^{-1})_i(0, y') = \delta_{ij}$ for any $i, j \in \llbracket 2, d \rrbracket$. Furthermore, we have for $y \in \kappa(X)$ the invertibility of the matrix

$$d_{(0, y')}(\kappa^{-1}) = \left(\begin{array}{c|ccc} 1 & q_{12}(0, y') & \cdots & q_{1d}(0, y') \\ \hline 0 & & & \\ \vdots & & I_{d-1} & \\ 0 & & & \end{array} \right)$$

The function $\kappa^{-1} = ((\kappa^{-1})_1, \dots, (\kappa^{-1})_d)$ therefore satisfies the differential system

$$\begin{cases} \partial_{y_1}(\kappa^{-1})_1(y_1, y') = 1, & (\kappa^{-1})_1(0, y') = 0, \\ \partial_{y_1}(\kappa^{-1})_j(y_1, y') = q_{j1}((\kappa^{-1})_j(y_1, y')), & (\kappa^{-1})_j(0, y') = y_j \quad \forall j \in \llbracket 2, d \rrbracket. \end{cases}$$

By Cauchy-Lipschitz' theorem (with the initial data $\kappa^{-1}(0) = 0$), this Cauchy problem admits a smooth solution in a neighborhood $Y \subset \mathbb{R}^d$ of 0. (Explicitly $(\kappa^{-1})_1(x_1, x') = x_1$.) By the local inversion theorem, even if it means restricting the neighborhood Y , $\kappa^{-1} : Y \rightarrow \kappa^{-1}(Y)$ is a smooth diffeomorphism. Let us denote $X := \kappa^{-1}(Y)$. Thus, the explicit expression of $P_3 = U_\kappa^* P_2 U_\kappa$ is

$$(hD_{x_1})^2 + \langle (hD_x), {}^T(d_x \kappa)^{-1}(\tilde{q}_{ij}(\kappa^{-1}(x)))_{2 \leq i, j \leq d} (d_x \kappa)^{-1} \cdot (hD_x) \rangle + V_2(\kappa^{-1}(x)).$$

Let us define $(a_{ij}(x))_{1 \leq i, j \leq d}$ by the coefficients of the matrix ${}^T(d_x \kappa)^{-1}(\tilde{q}_{ij}(\kappa^{-1}(x)))_{2 \leq i, j \leq d} (d_x \kappa)^{-1}$, which is symmetric positive definite on $\kappa(X)$ (since $(\tilde{q}_{ij}(x))_{2 \leq i, j \leq d}$ is also that). We thus deduce the ellipticity of the symbol $\lambda(x, \xi') = \sum_{2 \leq i, j \leq d} a_{ij}(x) \xi_i \xi_j$ uniformly in $\kappa(X)$. Eventually, let us check that the potential $x \mapsto V_2(\kappa^{-1}(x))$ is equal to $-c(x)x_1$ with $c(0) > 0$. By definition,

$$V_2(\kappa^{-1}(x)) = -\tilde{c}(\kappa^{-1}(x))(\kappa^{-1}(x) \cdot e_1) = -\tilde{c}(\kappa^{-1}(x)) x_1.$$

Denoting $c := \tilde{c} \circ (\kappa^{-1})$, we obtain the desired relation.

Finally, the principal symbol of P is given by $q(y, \eta) = \eta^2 + \lambda(y, \eta') - c(y)y_1$, in the new basis of local coordinates (by composing all the diffeomorphism of each step).

That ends the proof of Proposition VI.3.

VI.3 Proof of Theorem VI.2

As argued in [KTZ07]⁵, we may reduce the problem to the case

$$p(x, \xi) = \xi_1^2 + \sum_{i,j=2}^d a_{ij}(x) \xi_i \xi_j + V(x), \quad V(x) = -c(x)x_1,$$

where $(a_{ij}(x))_{i,j} \subset \mathcal{C}^\infty(\mathbb{R}^d)$ is positive definite uniformly, $c \in \mathcal{C}^\infty(\mathbb{R}^d)$ with $c(0) > 0$, and

$$\forall \alpha \in \mathbb{N}^d, \exists C_\alpha > 0, \forall i, j = \{2, \dots, d\}, \forall x \in \mathbb{R}^d, \quad |\partial^\alpha a_{ij}(x)| + |\partial^\alpha V(x)| \leq C_\alpha.$$

Notation

- Let $\delta > 0$ such that $\inf_{x \in B_\delta} c(x) > 0$, where $B_\delta := \{x \in \mathbb{R}^d : |x| < \delta\}$.
- Let $\mathcal{V} \subset \mathbb{R}^d \times \mathbb{R}^d$ a bounded open neighborhood of $(x_0, \xi_0) = (0, 0)$ such that $\pi_x \mathcal{V}$ is contained in $B_{\delta/4}$ and such that $\mathcal{V} \subset \mathcal{V}_0$ where \mathcal{V}_0 is given by Corollary VI.6.
- Let $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ such that $\text{supp } \chi \subset \mathcal{V}$.
- Let $M \geq 1$ be larger than $M_0 \geq 1$ given by Corollary VI.6. An other constraint will be given in the proof.
- For all $\varepsilon > 0$, let us define

$$\Omega_\varepsilon := \{x \in \mathbb{R}^d : x_1 < \varepsilon\}.$$

- Let us define $\chi_\varepsilon := \chi_0(\cdot/\varepsilon)$ where $\chi_0 \in \mathcal{C}^\infty(\mathbb{R}, [0, 1])$ is a nonnegative function equal to 1 on $] - \infty, 1]$ and equal to 0 on $[2, \infty[$.
- Let s_{Sogge} and α_{Sogge} be given by the formulas in the statement of Theorem V.2.

As in the proof of Theorem IV.2, we have by the one-body estimates (Theorem VI.1)

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^\infty(\mathbb{R}^d)} \lesssim h^{1-d} \left\| (1 + P^2/h^2)^{1/2} \gamma (1 + P^2/h^2)^{1/2} \right\|_{\mathfrak{S}^\infty(L^2(\mathbb{R}^d))}.$$

We prove the estimates of Theorem VI.2 for low regime $2 \leq q \leq 2d/(d-2)$. The remaining estimates for $2d/(d-2) < q < \infty$ are then obtained by interpolating between $q = 2d/(d-2)$ and $q = \infty$. We now fix $2 \leq q \leq 2d/(d-2)$. The strategy to estimate $\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\mathbb{R}^d)}$ is to estimate $\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\Omega)}$ on various regions Ω that cover \mathbb{R}^d (c.f. Figure 1.7), and then sum the obtained estimates.

Before going into the proof, let us recall some key estimates of Koch-Tataru-Zworski [KTZ07].

Lemma VI.5 ([KTZ07, Lem. 7.3 and Sec. 7]). *Let $d \geq 1$. Then, there exist $M \geq 1$, $h_0 > 0$ and a bounded neighborhood $\mathcal{V} \subset \mathbb{R}^d \times \mathbb{R}^d$ of 0 such that, for any $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ supported in \mathcal{V} , any $h \in (0, h_0]$, and any $\varepsilon \geq Mh^{2/3}$ we have for all $\alpha \in \mathbb{N}^d$ such that $|\alpha| \leq 2$*

$$\|(hD)^\alpha \chi^w u\|_{L^2(\Omega_\varepsilon)} = \mathcal{O}\left(\varepsilon^{\frac{1}{4} + \frac{|\alpha|}{2}}\right) \left(\|u\|_{L^2(\mathbb{R}^d)} + \frac{1}{h} \|Pu\|_{L^2(\mathbb{R}^d)} \right). \quad (\text{VI.9})$$

Remark 24. In [KTZ07], the estimate (VI.9) is proved only for $|\alpha| \leq 1$ and for $|\alpha| = 2$ when $d = 2$ and $\varepsilon = Mh^{2/3}$. Their method allows to treat the case $|\alpha| = 2$ without the restrictions $d = 2$ and $\varepsilon = Mh^{2/3}$.

⁵and as explained in the previous section (Section VI.2),

Remark 25. In the case $\varepsilon = Mh^{2/3}$, the estimate (VI.9) reduces to

$$\sum_{|\alpha| \leq 2} \|(h^{2/3}D)^\alpha \chi^w u\|_{L^2(\Omega_{Mh^{2/3}})} \leq Ch^{1/6} \left(\|u\|_{L^2(\mathbb{R}^d)} + \frac{1}{h} \|Pu\|_{L^2(\mathbb{R}^d)} \right),$$

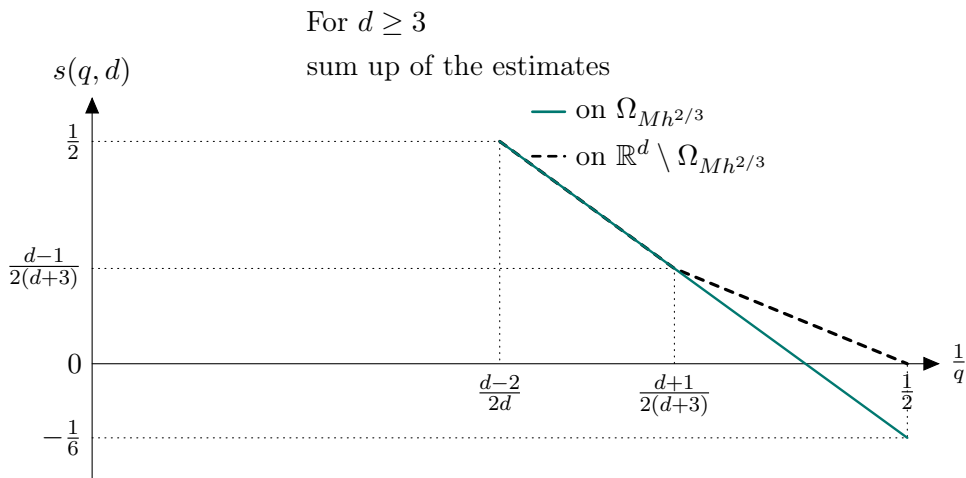
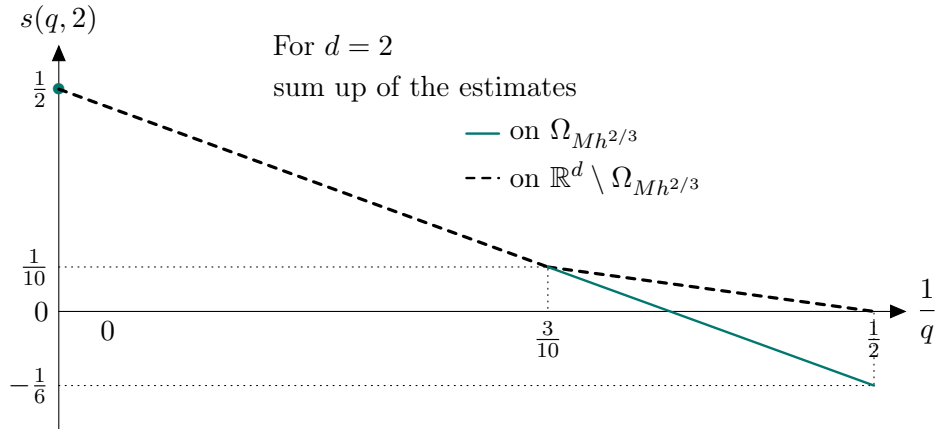
which, by Sobolev embeddings, imply that for all $2 \leq q \leq \frac{2d}{(d-4)_+}$ (excluding $q = \infty$ for $d = 4$)

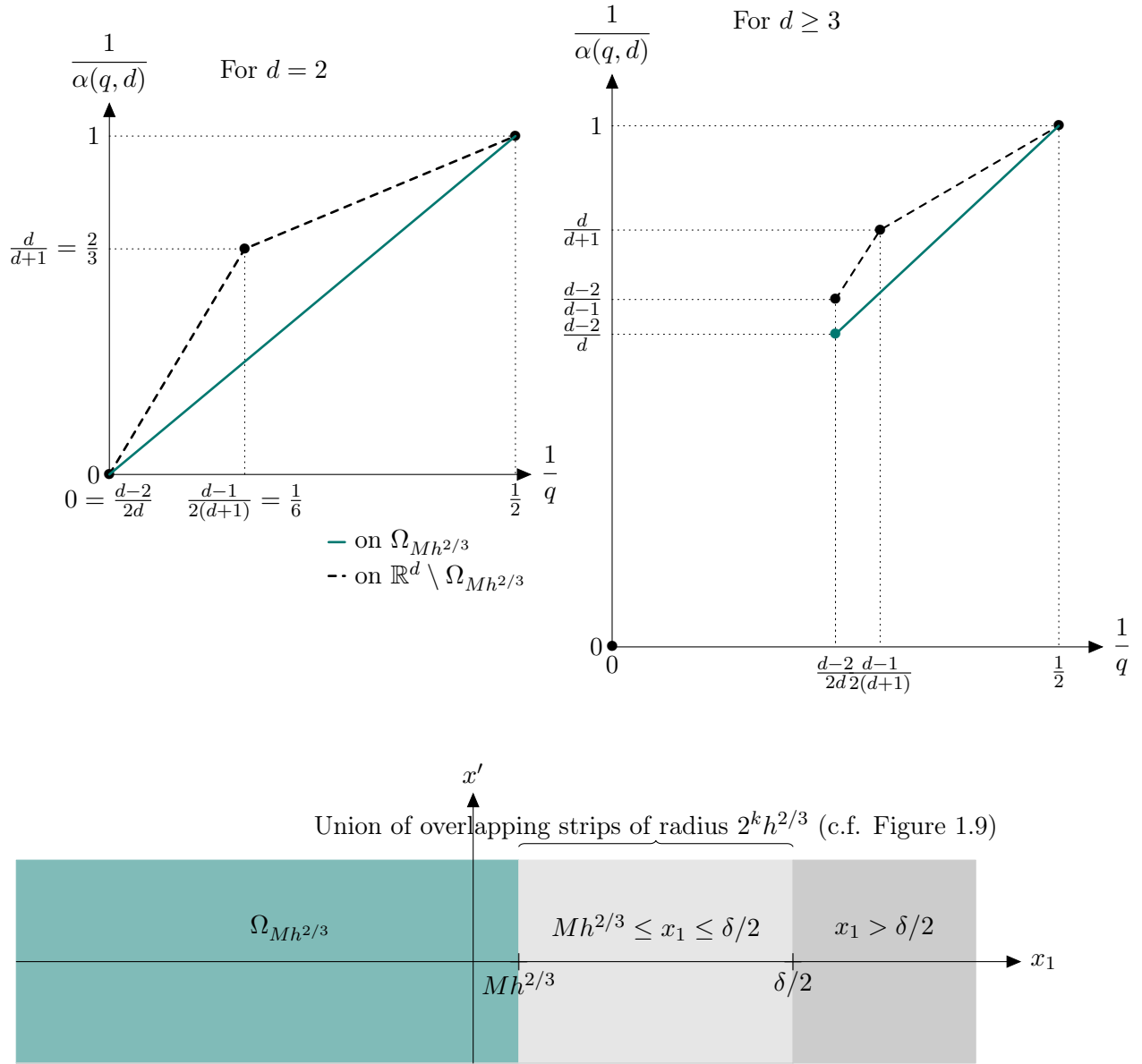
$$\|\chi^w u\|_{L^q(\Omega_{Mh^{2/3}})} \leq Ch^{\frac{1}{6} - \frac{2d}{3}(\frac{1}{2} - \frac{1}{q})} \left(\|u\|_{L^2(\mathbb{R}^d)} + \frac{1}{h} \|Pu\|_{L^2(\mathbb{R}^d)} \right).$$

In dimension $d = 1$, one can even get rid of the microlocalization χ^w in the argument of [KTZ07]. For $\alpha = 0$, this estimate is sharp for $V(x) = x^2 - 1$ and $x_0 = 1$, because Hermite functions behave like $h^{-1/6} \text{Ai}(h^{-2/3}(x-1))$ close to $x = 1$ (c.f. also Figure 1.1 for $E = 1$). The sharpness in higher dimension seems open to us.

Corollary VI.6. *Let $d \geq 1$. Then, there exist $M_0 \geq 1$, $h_0 > 0$ and a bounded neighborhood $\mathcal{V}_0 \subset \mathbb{R}^d \times \mathbb{R}^d$ of 0, such that for any $\chi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ supported in \mathcal{V}_0 , for any $h \in (0, h_0]$ and any $\varepsilon \in [M_0 h^{2/3}, 1]$*

$$(1 - h^2 \Delta) \chi_\varepsilon \chi^w (1 + P^2/h^2)^{-1/2} = \mathcal{O}_{L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)}(\varepsilon^{1/4}).$$



Figure 1.7 – Different regions of \mathbb{R}^d **Estimates on $\Omega_{Mh^{2/3}}$**

Lemma VI.7. Let $d \geq 1$. For $2 \leq q \leq \frac{2d}{(d-2)_+}$ and any bounded self-adjoint operator γ on $L^2(\mathbb{R}^d)$

$$\|\rho \chi^w \gamma \chi^w\|_{L^{q/2}(\Omega_{Mh^{2/3}})} \leq Ch^{\frac{1}{3} - \frac{4d}{3}(\frac{1}{2} - \frac{1}{q})} \left\| \left(1 + \frac{1}{h^2} P^2\right)^{1/2} \gamma \left(1 + \frac{1}{h^2} P^2\right)^{1/2} \right\|_{\mathfrak{S}^{q/2}(L^2(\mathbb{R}^d))}.$$

Remark 26. The previous estimates are also true for all $2 \leq q < \frac{2d}{(d-4)_+}$, but we will not need it (see Remark 22).

Proof of Lemma VI.7. By Corollary VI.6 with $\varepsilon = Mh^{2/3}$

$$(1 - h^{4/3} \Delta) \chi_{Mh^{2/3}} \chi^w (1 + P^2/h^2)^{-1/2} = \mathcal{O}_{L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)}(h^{1/6}),$$

and by the Kato-Seiler-Simon bound applied to $m = 2$, which is true if and only if $q < \frac{2d}{d-4}$ (see Lemma II.21)

$$\left\| W(1 - h^{4/3}\Delta)^{-1} \right\|_{\mathfrak{S}^{2(q/2)'}(L^2(\mathbb{R}^d))} \leq Ch^{-\frac{2d}{3}\left(\frac{1}{2}-\frac{1}{q}\right)} \|W\|_{L^{2(q/2)'}(L^2(\mathbb{R}^d))},$$

we have for $2 \leq q \leq \frac{2d}{(d-2)_+}$ and $W \in L^{2(q/2)'(\mathbb{R}^d)}$

$$\begin{aligned} & \|W\chi_{Mh^{2/3}}\chi^w\sqrt{\gamma}\|_{\mathfrak{S}^2} \\ & \leq \left\| W(1 - h^{4/3}\Delta)^{-1} \right\|_{\mathfrak{S}^{2(q/2)'}} \left\| (1 - h^{4/3}\Delta)\chi_{Mh^{2/3}}\chi^w(1 + P^2/h^2)^{-1/2} \right\|_{\mathfrak{S}^\infty} \times \\ & \quad \times \left\| (1 + P^2/h^2)^{1/2}\sqrt{\gamma} \right\|_{\mathfrak{S}^q} \\ & \lesssim h^{\frac{1}{6}-\frac{2d}{3}\left(\frac{1}{2}-\frac{1}{q}\right)} \|W\|_{L^{2(q/2)'(\mathbb{R}^d)}} \left\| (1 + P^2/h^2)^{1/2}\gamma(1 + P^2/h^2)^{1/2} \right\|_{\mathfrak{S}^{q/2}}^{1/2}, \end{aligned}$$

which by duality ends the proof. \square

Estimates on $\{x \in \mathbb{R}^d : x_1 > \delta/2\}$

Since $\pi_x \text{supp } \chi$ and $\{x \in \mathbb{R}^d : x_1 > \delta/2\}$ are disjoint, we deduce as in the beginning of the proof of Theorem V.2 that for any $2 \leq q \leq \infty$ and any bounded self-adjoint operator γ on $L^2(\mathbb{R}^d)$

$$\|\rho_{\chi^w\gamma\chi^w}\|_{L^{q/2}(\{x \in \mathbb{R}^d : x_1 > \delta/2\})} = \mathcal{O}(h^\infty) \left\| (1 + P^2/h^2)^{1/2}\gamma(1 + P^2/h^2)^{1/2} \right\|_{\mathfrak{S}^{q/2}}.$$

Estimates on $\{x \in \mathbb{R}^d : Mh^{2/3} \leq x_1 \leq \delta/2\}$

In the following, we assume $h_0 < (\delta/(2M))^{3/2}$ to ensure $Mh^{2/3} < \delta/2$ for $M > 0$ be defined later.

Lemma VI.8. *Let $d \geq 2$ and $2 \leq q \leq \frac{2d}{d-2}$. Then, there exists $M > 0$ such that for all bounded self-adjoint non-negative operator γ on $L^2(\mathbb{R}^d)$ we have*

$$\|\rho_{\chi^w\gamma\chi^w}\|_{L^{q/2}(\Omega_{\delta/2} \setminus \Omega_{Mh^{2/3}})} \lesssim C_h^2 \left\| (1 + P^2/h^2)^{1/2} \gamma (1 + P^2/h^2)^{1/2} \right\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}(L^2(\mathbb{R}^d))},$$

where

$$C_h := \begin{cases} h^{-\frac{d-1}{2}\left(\frac{1}{2}-\frac{1}{q}\right)} & \text{if } 2 \leq q < \frac{2(d+3)}{d+1}, \\ \log^{\frac{d+1}{2(d+3)}}(1/h)h^{-\frac{d-1}{2(d+3)}} & \text{if } q = \frac{2(d+3)}{d+1}, \\ h^{\frac{1}{6}-\frac{2d}{3}\left(\frac{1}{2}-\frac{1}{q}\right)} & \text{if } \frac{2(d+3)}{d+1} < q \leq \frac{2d}{d-2}. \end{cases}$$

Remark 27. The previous estimates are also true for all $2 \leq q < \frac{2d}{(d-4)_+}$.

Proof of Lemma VI.8.

We prove the result for P which is the right quantization of the symbol p (so that $P = h^2 D_{x_1}^2 + \sum_{2 \leq i, j \leq d} a_{ij}(x)(hD_{x_i})(hD_{x_j}) - c(x)x_1$ is a differential operator). While the final result does not depend on the choice of quantization, the proof will rely on several space localizations so that it will be useful that the operator P is local. ⁶

Let us now fix some notation. Let $\varepsilon > 0$ and let us define the strips by

$$A_\varepsilon := \{x \in \mathbb{R}^d : |x_1 - \varepsilon| < \varepsilon/2\} \quad \text{and} \quad \tilde{A}_\varepsilon := \{x \in \mathbb{R}^d : |x_1 - \varepsilon| < 3\varepsilon/4\}.$$

⁶This point is explained in details in Section VI.2.

Each strip A_ε or \tilde{A}_ε can be decomposed into a union of boxes of size ε (see for instance Figure 1.8)

$$A_\varepsilon = \bigcup_{k \in \mathbb{Z}^{d-1}} A_\varepsilon^k, \quad \tilde{A}_\varepsilon = \bigcup_{k \in \mathbb{Z}^{d-1}} \tilde{A}_\varepsilon^k$$

defined by

$$\begin{aligned} A_\varepsilon^k &:= \{x \in \mathbb{R}^d : |x_1 - \varepsilon k| < \varepsilon/2, \quad |x' - \varepsilon k|_{\ell^\infty} < \varepsilon/2\} \\ \tilde{A}_\varepsilon^k &:= \{x \in \mathbb{R}^d : |x_1 - \varepsilon k| < 3\varepsilon/4, \quad |x' - \varepsilon k|_{\ell^\infty} < 3\varepsilon/4\}, \\ \tilde{\tilde{A}}_\varepsilon^k &:= \{x \in \mathbb{R}^d : |x_1 - \varepsilon k| < 4\varepsilon/5, \quad |x' - \varepsilon k|_{\ell^\infty} < 4\varepsilon/5\}. \end{aligned}$$

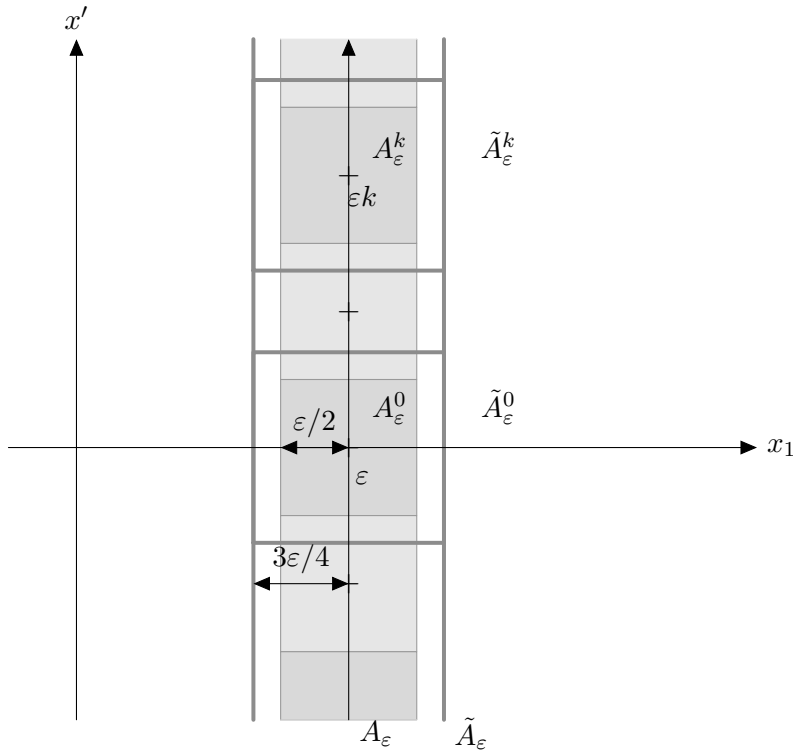
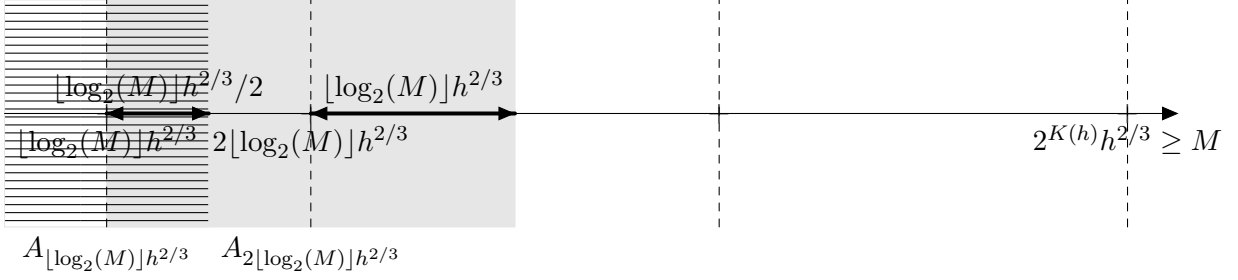


Figure 1.8 – Boxes A_ε^k and \tilde{A}_ε^k

Finally, the set $\Omega_{\delta/2} \setminus \Omega_{Mh^{2/3}} = \{x \in \mathbb{R}^d : Mh^{2/3} \leq x_1 \leq \delta/2\}$ can be covered by a union of $\sim \log(1/h)$ overlapping strips $\bigcup_{k=\lfloor \log_2(M) \rfloor}^{K(h)} A_{2^k h^{2/3}}$ where $K(h) = \lceil \log_2(\delta h^{-2/3}/2) \rceil$ (see for instance Figure 1.9).

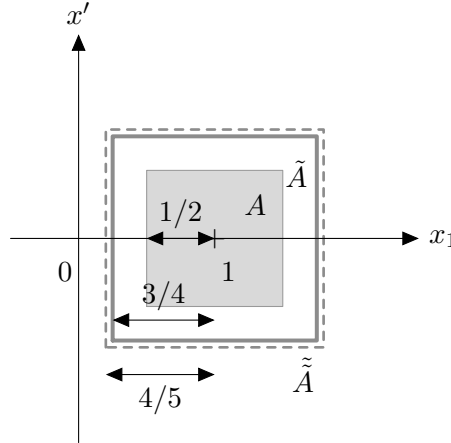
The main steps for the proof of L^q estimates in $\Omega_{\delta/2} \setminus \Omega_{Mh^{2/3}}$ are the following:

0. obtain the estimates on a box A of size 1,
1. obtain the estimates on the boxes A_ε^k of size ε by scaling the previous one,
2. obtain the estimates on the strips A_ε by summing the estimates on the ε -boxes,
3. conclude by summing the estimates on the strips.

Figure 1.9 – Strips A_ε

Step 0. Estimates on a box of size 1. We prove estimates on the boxes

$$\begin{aligned} A &:= \{\tilde{x} \in \mathbb{R}^d : |\tilde{x}_1 - 1| < 1/2, \quad |\tilde{x}'|_{\ell^\infty} < 1/2\}, \\ \tilde{A} &:= \{\tilde{x} \in \mathbb{R}^d : |\tilde{x}_1 - 1| < 3/4, \quad |\tilde{x}'|_{\ell^\infty} < 3/4\}, \\ \tilde{\tilde{A}} &:= \{x \in \mathbb{R}^d : |\tilde{x}_1 - 1| < 4/5, \quad |\tilde{x}'|_{\ell^\infty} < 4/5\}. \end{aligned}$$



Lemma VI.9. Let $d \geq 2$ and $2 \leq q \leq \frac{2d}{d-2}$. Let $\varepsilon_0 > 0$. Let $\tilde{p}_\varepsilon(\tilde{x}, \tilde{\xi}) := \langle \tilde{\xi}, B_\varepsilon(\tilde{x})\tilde{\xi} \rangle + V_\varepsilon(\tilde{x})$ with $\{(B_\varepsilon, V_\varepsilon)\}_{\varepsilon \in [0, \varepsilon_0]} \subset C^\infty(\mathbb{R}^d, \mathbb{R}^{d \times d}_{\text{sym}} \times \mathbb{R})$ and $(\varepsilon, \tilde{x}) \mapsto (B_\varepsilon(\tilde{x}), V_\varepsilon(\tilde{x})) \in \mathcal{C}([0, \varepsilon_0] \times \mathbb{R}^d)$ such that

- for any $\alpha \in \mathbb{N}^d$, there exists $C_\alpha > 0$ such that for any $\varepsilon \in [0, \varepsilon_0]$

$$\forall x \in \mathbb{R}^d \quad |\partial^\alpha B_\varepsilon(\tilde{x})| + |\partial^\alpha V_\varepsilon(\tilde{x})| \leq C_\alpha, \quad (\text{VI.10})$$

- there exists $c > 0$ such that for any $\varepsilon \in [0, \varepsilon_0]$

$$B_\varepsilon \geq c, |V_\varepsilon| \geq c \quad \text{on} \quad \{\tilde{x} \in \mathbb{R}^d : |\tilde{x}_1 - 1| < 9/10, \quad |\tilde{x}'|_{\ell^\infty} < 9/10\}. \quad (\text{VI.11})$$

Let $\tilde{P} := \tilde{p}_\varepsilon^w(\tilde{x}, \tilde{h}D_{\tilde{x}})$ (or any other quantization) and let $\chi_A \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d, [0, 1])$ such that $\chi_A = 1$ on A and $\text{supp } \chi_A \subset \tilde{A}$. Then, there exist $C > 0$ and $\tilde{h}_0 > 0$ such that for all $0 < \tilde{h} \leq \tilde{h}_0$, for all $0 \leq \varepsilon \leq \varepsilon_0$ and all bounded self-adjoint non-negative operator $\tilde{\gamma}$ on $L^2(\mathbb{R}^d)$

$$\|\rho_{\tilde{\gamma}}(\tilde{x})\|_{L^{q/2}(A)} \leq C \tilde{h}^{-2s_{\text{Sogge}}(q,d)} \left\| (1 + \tilde{P}^* \tilde{P} / \tilde{h}^2)^{1/2} \chi_A \tilde{\gamma} \chi_A (1 + \tilde{P}^* \tilde{P} / \tilde{h}^2)^{1/2} \right\|_{\mathfrak{S}^\alpha_{\text{Sogge}}(q,d)}.$$

Proof of Lemma VI.9. Let $\chi_{\tilde{A}} \in \mathcal{C}_c^\infty(\mathbb{R}^d, [0, 1])$ be a cut-off function equal to 1 on \tilde{A} and supported into $\tilde{\tilde{A}}$. It follows from the equality $\chi_{\tilde{A}}^2(\tilde{x})\rho_{\tilde{\gamma}}(\tilde{x}, \tilde{x}) = \rho_{\chi_{\tilde{A}}\tilde{\gamma}\chi_{\tilde{A}}}(\tilde{x}, \tilde{x})$ that

$$\|\rho_{\tilde{\gamma}}\|_{L^{q/2}(A)} \leq \|\chi_{\tilde{A}}^2\rho_{\tilde{\gamma}}\|_{L^{q/2}(\mathbb{R}^d)} = \|\rho_{\chi_{\tilde{A}}\tilde{\gamma}\chi_{\tilde{A}}}\|_{L^{q/2}(\mathbb{R}^d)}.$$

Let

$$\tilde{K} := \bigcup_{0 \leq \varepsilon \leq \varepsilon_0} \left\{ (\tilde{x}, \tilde{\xi}) \in \tilde{\tilde{A}} \times \mathbb{R}^d : \langle \tilde{\xi}, B_\varepsilon(\tilde{x})\tilde{\xi} \rangle + V_\varepsilon(\tilde{x}) \leq \frac{1}{2}(1 + \langle \tilde{\xi}, B_\varepsilon(\tilde{x})\tilde{\xi} \rangle) \right\}.$$

Note that each \tilde{K} is a closed set of \mathbb{R}^d (here we use the continuity of $(B_\varepsilon(\tilde{x}), V_\varepsilon(\tilde{x}))$ in (ε, \tilde{x})). It is also bounded, since it is contained into the bounded set

$$\tilde{\tilde{A}} \times \left\{ \tilde{\xi} \in \mathbb{R}^d : |\tilde{\xi}| \leq c^{-1/2} \sqrt{1 + 2 \sup_{0 \leq \varepsilon \leq \varepsilon_0} \|V_\varepsilon\|_{L^\infty(\mathbb{R}^d)}} \right\}.$$

Let $\tilde{\psi} \in \mathcal{C}_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ be a function $0 \leq \tilde{\psi} \leq 1$, such that $\tilde{\psi} = 1$ in the compact \tilde{K} . The operator is composed of three parts

$$\chi_{\tilde{A}}\tilde{\gamma}\chi_{\tilde{A}} = \tilde{\gamma}_1 + \tilde{\gamma}_2 + \tilde{\gamma}_3,$$

defined by

$$\begin{aligned} \tilde{\gamma}_1 &:= \tilde{\psi}^w \chi_{\tilde{A}} \tilde{\gamma} \chi_{\tilde{A}} \tilde{\psi}^w, \\ \tilde{\gamma}_2 &:= (1 - \tilde{\psi}^w) \chi_{\tilde{A}} \tilde{\gamma} \chi_{\tilde{A}} (1 - \tilde{\psi}^w), \\ \tilde{\gamma}_3 &:= \underbrace{(1 - \tilde{\psi}^w) \chi_{\tilde{A}} \tilde{\gamma} \chi_{\tilde{A}} \tilde{\psi}^w}_{=:\tilde{\gamma}_{3,1}} + \underbrace{\tilde{\psi}^w \chi_{\tilde{A}} \tilde{\gamma} \chi_{\tilde{A}} (1 - \tilde{\psi}^w)}_{=:\tilde{\gamma}_{3,2}}. \end{aligned}$$

Let us prove that for any $i \in \{1, 2, 3\}$

$$\|\rho_{\tilde{\gamma}_i}\|_{L^{q/2}(\mathbb{R}^d)} \lesssim \tilde{h}^{-2s_{\text{Sogge}}(q,d)} \left\| (1 + \tilde{P}^* \tilde{P} / \tilde{h}^2)^{1/2} \chi_{\tilde{A}} \tilde{\gamma} \chi_{\tilde{A}} (1 + \tilde{P}^* \tilde{P} / \tilde{h}^2)^{1/2} \right\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}}.$$

These above bounds together with the triangle inequality prove the lemma.

Estimate of the term $\tilde{\gamma}_1$. Note that

$$\text{supp } \tilde{\psi} \cap \tilde{\tilde{A}} \times \mathbb{R}^d \subset S = \{\tilde{x} \in \mathbb{R}^d : |\tilde{x}_1 - 1| < 9/10, \quad |\tilde{x}'|_{\ell^\infty} < 9/10\} \times \mathbb{R}^d.$$

Every point $(\tilde{x}, \tilde{\xi})$ of S satisfies $\tilde{p}_\varepsilon(\tilde{x}, \tilde{\xi}) \neq 0$ or Sogge curvature conditions (Assumption 3). Indeed, if $(\tilde{x}, \tilde{\xi})$ satisfies $\tilde{p}_\varepsilon(\tilde{x}, \tilde{\xi}) = 0$, then uniformly in ε , by (VI.11)

$$\left| \nabla_{\tilde{\xi}} \tilde{p}_\varepsilon(\tilde{x}, \tilde{\xi}) \right| = 2 \left| B_\varepsilon(\tilde{x}) \tilde{\xi} \right| = 2\sqrt{c} \sqrt{|V_\varepsilon(\tilde{x})|} \geq 2c.$$

Furthermore, for all ε and \tilde{x}

$$\{\tilde{\xi} \in \mathbb{R}^d : \tilde{p}_\varepsilon(\tilde{x}, \tilde{\xi}) = 0\} = \{\tilde{\xi} \in \mathbb{R}^d : \langle \tilde{\xi}, B_\varepsilon(\tilde{x})\tilde{\xi} \rangle = |V_\varepsilon(\tilde{x})|\}$$

has a positive curvature which is bounded and bounded away from 0 uniformly in ε . Hence, by Theorem III.1 and Theorem V.2, Assumption 1 holds for $q, s = s_{\text{Sogge}}(q, d), t = 0$ and $\alpha = \alpha_{\text{Sogge}}(q, d)$ on the set S . By Remark 8 applied to S , to $\Omega = \tilde{A}$, to $\chi = \tilde{\psi}$, to $(q, s_{\text{Sogge}}(q, d), 0, \alpha_{\text{Sogge}}(q, d))$ and to the operator $\gamma = \chi_{\tilde{A}} \tilde{\gamma} \chi_{\tilde{A}}$

$$\begin{aligned} \|\rho_{\tilde{\gamma}_1}\|_{L^{q/2}(\mathbb{R}^d)} &= \|\rho_{\tilde{\psi}^w \chi_{\tilde{A}} \tilde{\gamma} \chi_{\tilde{A}} \tilde{\psi}^w}\|_{L^{q/2}(\mathbb{R}^d)} = \|\rho_{\tilde{\psi}^w \chi_{\tilde{A}} \chi_{\tilde{A}} \tilde{\gamma} \chi_{\tilde{A}} \chi_{\tilde{A}} \tilde{\psi}^w}\|_{L^{q/2}(\mathbb{R}^d)} \\ &\lesssim \tilde{h}^{-2s_{\text{Sogge}}(q,d)} \left\| (1 + \tilde{P}^* \tilde{P} / \tilde{h}^2)^{1/2} \chi_{\tilde{A}} \tilde{\gamma} \chi_{\tilde{A}} (1 + \tilde{P}^* \tilde{P} / \tilde{h}^2)^{1/2} \right\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}}. \end{aligned}$$

Estimate of the term $\tilde{\gamma}_2$. Recall that

$$\|\rho_{\tilde{\gamma}_2}\|_{L^{q/2}(\mathbb{R}^d)} = \sup_{W \in L^{2(q/2)' }(\mathbb{R}^d)} \frac{\|W(1 - \tilde{\psi}^w)\chi_A\sqrt{\tilde{\gamma}}\|_{\mathfrak{S}^2}^2}{\|W\|_{L^{2(q/2)' }(\mathbb{R}^d)}^2}.$$

By the Hölder and Kato-Seiler-Simon inequalities (Lemma II.21) then applied successively, we have for any $2 \leq q \leq \frac{2d}{d-2}$ (since $\frac{2d}{d-2} < \frac{2d}{(d-4)_+}$)

$$\begin{aligned} \|W(1 - \tilde{\psi}^w)\chi_A\sqrt{\tilde{\gamma}}\|_{\mathfrak{S}^2} &\leq \|W(1 - \tilde{h}^2\Delta)^{-1}\|_{\mathfrak{S}^{2(q/2)' }} \| (1 - \tilde{h}^2\Delta)(1 - \tilde{\psi}^w)\chi_A\sqrt{\tilde{\gamma}} \|_{\mathfrak{S}^{q/2}}^{1/2} \\ &\lesssim h^{-d(\frac{1}{2}-\frac{1}{q})} \|W\|_{L^{2(q/2)' }(\mathbb{R}^d)} \| (1 - \tilde{h}^2\Delta)(1 - \tilde{\psi}^w)\chi_A\sqrt{\tilde{\gamma}} \|_{\mathfrak{S}^{q/2}}^{1/2}. \end{aligned}$$

Now let us give a estimate of the right side of the previous bound.

Fait VI.10. *There exist $C > 0$ and $\tilde{h}_0 > 0$ such that for any $0 < \tilde{h} \leq \tilde{h}_0$ and any $0 \leq \varepsilon \leq \varepsilon_0$, one has for all $\alpha \geq 1$*

$$\| (1 - \tilde{h}^2\Delta)(1 - \tilde{\psi}^w)\chi_A\sqrt{\tilde{\gamma}} \|_{\mathfrak{S}^\alpha} \leq C \left(\| \tilde{P}\chi_A\sqrt{\tilde{\gamma}} \|_{\mathfrak{S}^\alpha} + \tilde{h} \| \chi_A\sqrt{\tilde{\gamma}} \|_{\mathfrak{S}^\alpha} \right).$$

Proof of Fact VI.10. Let $\alpha \geq 1$.

1) Let us first show that it is enough to do everything with right quantization by replacing $(1 - \tilde{\psi}^w)$ by $(1 - \tilde{\psi}^R)$ into Fact VI.10. By Proposition II.8 applied to the symbol $\tilde{\psi}$, there exists $\tilde{r} \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$ such that

$$(1 - \tilde{\psi}^w) - (1 - \tilde{\psi}^R) = \tilde{\psi}^R - \tilde{\psi}^w = \tilde{h}\tilde{r}^w.$$

We can now write

$$\begin{aligned} (1 - \tilde{h}^2\Delta)(1 - \tilde{\psi}^w)\chi_A\sqrt{\tilde{\gamma}} &= (1 - \tilde{h}^2\Delta) \left((1 - \tilde{\psi}^R)\chi_A\sqrt{\tilde{\gamma}} + \text{Op}_h^{1/2}(\mathcal{O}_{\mathcal{S}}(\tilde{h}))\chi_A\sqrt{\tilde{\gamma}} \right) \\ &= (1 - \tilde{h}^2\Delta)(1 - \tilde{\psi}^R)\chi_A\sqrt{\tilde{\gamma}} + \mathcal{O}_{L^2 \rightarrow L^2}(\tilde{h})\chi_A\sqrt{\tilde{\gamma}}. \end{aligned}$$

2) It remains to show fact VI.10 by replacing $\tilde{\psi}^w$ by $\tilde{\psi}^R$.

Let $\tilde{m}_0(\tilde{x}, \tilde{\xi}) = \langle \tilde{\xi} \rangle^2$. Let us first notice that the operator \tilde{p}_ε is elliptic on the support of $(1 - \tilde{\psi})\chi_{\tilde{A}}$. Indeed, the function $(1 - \tilde{\psi})\chi_{\tilde{A}}$ is supported into $\tilde{K}^c \cap (\tilde{A} \times \mathbb{R}^d)$ and by definition of \tilde{K} , for all $\varepsilon \in [0, \varepsilon_0]$ and for all $(\tilde{x}, \tilde{\xi}) \in \tilde{K}^c \cap (\tilde{A} \times \mathbb{R}^d)$ we have

$$\tilde{p}_\varepsilon(\tilde{x}, \tilde{\xi}) > \frac{\min(1, c)}{2} \tilde{m}_0(\tilde{x}, \tilde{\xi}).$$

Thus, we get the ellipticity (uniform in ε) of \tilde{p}_ε on $\tilde{K}^c \cap (\tilde{A} \times \mathbb{R}^d)$ and thus on $\text{supp}((1 - \tilde{\psi})\chi_{\tilde{A}})$. By Lemma II.10 applied to $(1 - \tilde{\psi})\chi_{\tilde{A}} \in S(1)$ and to $p \in S(\tilde{m}_0)$, there exist $\tilde{b} \in S(\tilde{m}_0^{-1})$ and $\tilde{r} = \mathcal{O}_{S(1)}(\tilde{h}^\infty)$ such that

$$(1 - \tilde{\psi})^R\chi_{\tilde{A}} = \tilde{b}^R\tilde{P}(1 - \tilde{\psi}^R)\chi_{\tilde{A}} + \tilde{r}^R.$$

Note that $\chi_A = \chi_{\tilde{A}}\chi_A$. We compose by $(1 - \tilde{h}^2\Delta)$ on the left and $\chi_A\sqrt{\tilde{\gamma}}$ on the right to infer

$$\begin{aligned} (1 - \tilde{h}^2\Delta)(1 - \tilde{\psi})^R\chi_A\sqrt{\tilde{\gamma}} &= \underbrace{(1 - \tilde{h}^2\Delta)\tilde{b}^R\tilde{P}(1 - \tilde{\psi}^R)\chi_A\sqrt{\tilde{\gamma}}}_{=\mathcal{O}_{L^2 \rightarrow L^2}(1)} + \underbrace{(1 - \tilde{h}^2\Delta)\tilde{r}^R(1 - \tilde{h}^2\Delta)^{-1}(1 - \tilde{h}^2\Delta)\chi_A\sqrt{\tilde{\gamma}}}_{=\mathcal{O}_{L^2 \rightarrow L^2}(\tilde{h}^\infty)}. \end{aligned}$$

Let us write $\tilde{P}(1 - \tilde{\psi}^R)\chi_A\sqrt{\tilde{\gamma}}$ in two parts

$$\tilde{P}(1 - \tilde{\psi}^R)\chi_A\sqrt{\tilde{\gamma}} = \underbrace{(1 - \tilde{\psi}^R)}_{=\mathcal{O}_{L^2 \rightarrow L^2}(1)} \tilde{P}\chi_A\sqrt{\tilde{\gamma}} - \underbrace{[\tilde{P}, \tilde{\psi}^R]}_{=\mathcal{O}_{L^2 \rightarrow L^2}(\tilde{h})} \chi_A\sqrt{\tilde{\gamma}}.$$

In addition, the term $(1 - \tilde{h}^2\Delta)\chi_A\sqrt{\tilde{\gamma}}$ is also divided into two parts

$$(1 - \tilde{h}^2\Delta)\chi_A\sqrt{\tilde{\gamma}} = \underbrace{(1 - \tilde{h}^2\Delta)\tilde{\psi}^R}_{=\mathcal{O}_{L^2 \rightarrow L^2}(1)} \chi_A\sqrt{\tilde{\gamma}} + (1 - \tilde{h}^2\Delta)(1 - \tilde{\psi}^R)\chi_A\sqrt{\tilde{\gamma}}.$$

Putting everything together and moving to the Schatten norm

$$\begin{aligned} \left\| (1 - \tilde{h}^2\Delta)(1 - \tilde{\psi}^R)\chi_A\sqrt{\tilde{\gamma}} \right\|_{\mathfrak{S}^\alpha} &\lesssim \left\| \tilde{P}\chi_A\sqrt{\tilde{\gamma}} \right\|_{\mathfrak{S}^\alpha} + \tilde{h} \left\| \chi_A\sqrt{\tilde{\gamma}} \right\|_{\mathfrak{S}^\alpha} \\ &\quad + \mathcal{O}(\tilde{h}^\infty) \left\| (1 - \tilde{h}^2\Delta)(1 - \tilde{\psi}^R)\chi_A\sqrt{\tilde{\gamma}} \right\|_{\mathfrak{S}^\alpha}. \end{aligned}$$

Then, we conclude by taking \tilde{h} small enough

$$\left\| (1 - \tilde{h}^2\Delta)(1 - \tilde{\psi}^R)\chi_A\sqrt{\tilde{\gamma}} \right\|_{\mathfrak{S}^\alpha} \lesssim \left\| \tilde{P}\chi_A\sqrt{\tilde{\gamma}} \right\|_{\mathfrak{S}^\alpha} + \tilde{h} \left\| \chi_A\sqrt{\tilde{\gamma}} \right\|_{\mathfrak{S}^\alpha}.$$

That ends the proof of Fact VI.10. \square

We apply it to $\alpha = q/2$ and we apply Lemma VI.11

Lemma VI.11. *Let m be an order function. Let $p \in S(m)$ and $P := p^w(x, hD)$. For any $\alpha \geq 1$ and non-negative density matrix γ on $L^2(\mathbb{R}^d)$*

$$\begin{aligned} \left\| (1 + P^*P/h^2)^{1/2}\gamma(1 + P^*P/h^2)^{1/2} \right\|_{\mathfrak{S}^\alpha} &\leq \|\gamma\|_{\mathfrak{S}^\alpha} + \frac{1}{h^2} \|P^*\gamma P\|_{\mathfrak{S}^\alpha} \\ &\leq 2 \left\| (1 + P^*P/h^2)^{1/2}\gamma(1 + P^*P/h^2)^{1/2} \right\|_{\mathfrak{S}^\alpha}. \end{aligned}$$

Hence, we get for any $2 \leq q \leq \frac{2d}{d-2}$

$$\begin{aligned} \|\rho_{\tilde{\gamma}_2}\|_{L^{q/2}(\mathbb{R}^d)} &\lesssim \tilde{h}^{2-2d(\frac{1}{2}-\frac{1}{q})} \left(\|\chi_A\tilde{\gamma}\chi_A\|_{\mathfrak{S}^{q/2}} + \frac{1}{h^2} \left\| \tilde{P}^*\chi_A\tilde{\gamma}\chi_A\tilde{P} \right\|_{\mathfrak{S}^{q/2}} \right) \\ &\lesssim \tilde{h}^{2-2d(\frac{1}{2}-\frac{1}{q})} \left\| (1 + \tilde{P}^*\tilde{P}/\tilde{h}^2)^{1/2}\chi_A\tilde{\gamma}\chi_A(1 + \tilde{P}^*\tilde{P}/\tilde{h}^2)^{1/2} \right\|_{\mathfrak{S}^{q/2}}. \end{aligned}$$

Estimate of the crossed terms $\tilde{\gamma}_{3,1}$ and $\tilde{\gamma}_{3,2}$. We deduce the estimates on the crossed terms $\tilde{\gamma}_{3,1}$ and $\tilde{\gamma}_{3,2}$ from those of $\tilde{\gamma}_1$ and $\tilde{\gamma}_2$. For example for $\tilde{\gamma}_{3,1}$, noting $C := \sqrt{\tilde{\gamma}}\chi_A(1 - \tilde{\psi}^w)$ and $B := \sqrt{\tilde{\gamma}}\chi_A\tilde{\psi}^w$

$$\begin{aligned} &|\mathrm{Tr}_{L^2}(W\tilde{\gamma}_{3,1}W)| \\ &= \left| \mathrm{Tr}_{L^2} \left(W(1 - \tilde{\psi}^w)\chi_A\tilde{\gamma}\chi_A\tilde{\psi}^wW \right) \right| = |\mathrm{Tr}_{L^2}(WC^*BW)| \\ &\leq |\mathrm{Tr}_{L^2}(WC^*CW)|^{1/2} |\mathrm{Tr}_{L^2}(WB^*BW)|^{1/2} \\ &\leq \left(\|W\|_{L^{2(q/2)'(\mathbb{R}^d)}}^2 \|\rho_{C^*C}\|_{L^{q/2}(\mathbb{R}^d)} \right)^{1/2} \left(\|W\|_{L^{2(q/2)'(\mathbb{R}^d)}}^2 \|\rho_{B^*B}\|_{L^{q/2}(\mathbb{R}^d)} \right)^{1/2} \\ &\leq \|W\|_{L^{2(q/2)'(\mathbb{R}^d)}}^2 \|\rho_{(1-\tilde{\psi}^w)\chi_A\tilde{\gamma}\chi_A(1-\tilde{\psi}^w)}\|_{L^{q/2}(\mathbb{R}^d)}^{1/2} \|\rho_{\tilde{\psi}^w\chi_A\tilde{\gamma}\chi_A\tilde{\psi}^w}\|_{L^{q/2}(\mathbb{R}^d)}^{1/2} \\ &\lesssim \tilde{h}^{1-d(\frac{1}{2}-\frac{1}{q})-s_{\mathrm{Sogge}}(q,d)} \|W\|_{L^{2(q/2)'(\mathbb{R}^d)}}^2 \left\| (1 + \tilde{P}^*\tilde{P}/\tilde{h}^2)^{1/2}\chi_A\tilde{\gamma}\chi_A(1 + \tilde{P}^*\tilde{P}/\tilde{h}^2)^{1/2} \right\|_{\mathfrak{S}^{\alpha_{\mathrm{Sogge}}(q,d)}}. \end{aligned}$$

For any $2 \leq q \leq \frac{2d}{d-2}$

$$\|\rho_{\tilde{\gamma}_3}\|_{L^{q/2}(\mathbb{R}^d)} \lesssim \tilde{h}^{1-d\left(\frac{1}{2}-\frac{1}{q}\right)-s_{\text{Sogge}}(q,d)} \left\| (1 + \tilde{P}^* \tilde{P} / \tilde{h}^2)^{1/2} \chi_A \tilde{\gamma} \chi_A (1 + \tilde{P}^* \tilde{P} / \tilde{h}^2)^{1/2} \right\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}}.$$

□

Step 1. The scaling. Let us deduce from Lemma VI.9 the same kind of result but on the boxes A_ε^k by a scaling argument. The following lemma controls the $L^{q/2}$ norm of the density on the boxes A_ε^k .

Lemma VI.12. *Let $d \geq 2$ and $2 \leq q \leq \frac{2d}{d-2}$. Then, there exists $C > 0$ such that for any $0 < h \leq h_0$, for any $\varepsilon \in [Mh^{2/3}, \delta/2]$ and for any $k \in \mathbb{Z}^{d-1}$ such that $|k|_{\ell^\infty} < \delta/\varepsilon - 1$, there exists $\chi_{\tilde{A}_\varepsilon^k} \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d, [0, 1])$ supported into \tilde{A}_ε^k , such that any bounded self-adjoint non-negative operator γ on $L^2(\mathbb{R}^d)$*

$$\|\rho_\gamma\|_{L^{q/2}(A_\varepsilon^k)} \leq Ch^{-2s_{\text{Sogge}}(q,d)} \varepsilon^{-2\mu(q,d)} \left(\left\| \chi_{\tilde{A}_\varepsilon^k} \gamma \chi_{\tilde{A}_\varepsilon^k} \right\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}} + \frac{\varepsilon}{h^2} \left\| \chi_{\tilde{A}_\varepsilon^k} P \gamma P^* \chi_{\tilde{A}_\varepsilon^k} \right\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}} \right),$$

where $\mu(q, d)$ is given by the formula

$$\mu(q, d) := d \left(\frac{1}{2} - \frac{1}{q} \right) - \frac{3s_{\text{Sogge}}(q, d)}{2}. \quad (\text{VI.12})$$

Proof of Lemma VI.12. Recall that h_0 and M were already fixed above. We will make additional constraints on them along this proof. Let $h \in (0, h_0]$, $\varepsilon \in [Mh^{2/3}, \delta/2]$ and $k \in \mathbb{Z}^{d-1}$ such that $|k|_{\ell^\infty} < \delta/\varepsilon - 1$. Let $\chi_{\tilde{A}} \in C_c^\infty(\mathbb{R}^d, [0, 1])$ be a cut-off function equal to 1 on \tilde{A} and supported into \tilde{A} . Let $\chi_{\tilde{A}} \in C_c^\infty(\mathbb{R}^d, [0, 1])$ be a cut-off function equal to 1 on $\text{supp } \chi_{\tilde{A}}$ and supported into \tilde{A} . Define for any $\tilde{x} \in \mathbb{R}^d$

$$B_\varepsilon(\tilde{x}) := \left(\begin{array}{c|c} 1 & 0 \cdots 0 \\ \hline 0 & \\ \vdots & (a_{ij}(\varepsilon \tilde{x}_1, \varepsilon \tilde{x}' + \varepsilon k))_{2 \leq i, j \leq d} \\ 0 & \end{array} \right), \quad V_\varepsilon(\tilde{x}) := -\tilde{x}_1 c(\varepsilon \tilde{x}_1, \varepsilon \tilde{x}' + \varepsilon k) \chi_{\tilde{A}}(\tilde{x}).$$

By our assumptions on $(a_{ij})_{2 \leq i, j \leq d}$ and c , $\{(B_\varepsilon, V_\varepsilon)\}_\varepsilon$ satisfies the assumptions of Lemma VI.9 with $\varepsilon_0 = \delta/2$ (notice that for our choice of ε and k , $|(\varepsilon \tilde{x}_1, \varepsilon \tilde{x}' + \varepsilon k)| < \delta$ for all $\tilde{x} \in \tilde{A}$). Hence, let $C > 0$ and $\tilde{h}_0 > 0$ such that for all $0 < \tilde{h} \leq \tilde{h}_0$ and all bounded self-adjoint non-negative operator $\tilde{\gamma}$ on $L^2(\mathbb{R}^d)$

$$\|\rho_{\tilde{\gamma}}(\tilde{x})\|_{L^{q/2}(A)} \leq C \tilde{h}^{-2s_{\text{Sogge}}(q,d)} \left\| (1 + \tilde{P}^* \tilde{P} / \tilde{h}^2)^{1/2} \chi_A \tilde{\gamma} \chi_A (1 + \tilde{P}^* \tilde{P} / \tilde{h}^2)^{1/2} \right\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}},$$

where $\tilde{P} = p_\varepsilon^R(\tilde{x}, \tilde{h} D_{\tilde{x}})$ and $p_\varepsilon(\tilde{x}, \tilde{\xi}) = \langle \tilde{\xi}, B_\varepsilon(\tilde{x}) \tilde{\xi} \rangle + V_\varepsilon(\tilde{x})$. Moreover, we have the following fact (which proof is given below).

Fait VI.13. *Let $\alpha \geq 1$. Then, there exists $C > 0$ such for all $\tilde{h} \in (0, \tilde{h}_0]$, for all $\varepsilon \in [0, \varepsilon_0]$ and for all bounded self-adjoint non-negative operator $\tilde{\gamma}$*

$$\left\| (1 + \tilde{P}^* \tilde{P} / \tilde{h}^2)^{1/2} \chi_A \tilde{\gamma} \chi_A (1 + \tilde{P}^* \tilde{P} / \tilde{h}^2)^{1/2} \right\|_{\mathfrak{S}^\alpha} \leq C \left(\left\| \chi_{\tilde{A}} \tilde{\gamma} \chi_{\tilde{A}} \right\|_{\mathfrak{S}^\alpha} + \frac{1}{\tilde{h}^2} \left\| \chi_{\tilde{A}} \tilde{P} \tilde{\gamma} \tilde{P}^* \chi_{\tilde{A}} \right\|_{\mathfrak{S}^\alpha} \right).$$

We deduce that for all bounded self-adjoint non-negative operator $\tilde{\gamma}$ on $L^2(\mathbb{R}^d)$, we have

$$\|\rho_{\tilde{\gamma}}(\tilde{x})\|_{L^{q/2}(A)} \leq C\tilde{h}^{-2s_{\text{Sogge}}(q,d)} \left(\|\chi_{\tilde{A}}\tilde{\gamma}\chi_{\tilde{A}}\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}} + \frac{1}{\tilde{h}^2} \|\chi_{\tilde{A}}\tilde{P}\tilde{\gamma}\tilde{P}^*\chi_{\tilde{A}}\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}} \right).$$

Since $\chi_{\tilde{A}}\chi_{\tilde{A}} = \chi_{\tilde{A}}$, the same bound holds when there is no factor $\chi_{\tilde{A}}$ in V_ε . We still denote by \tilde{P} the resulting operator. Now, let γ be a bounded self-adjoint non-negative operator on $L^2(\mathbb{R}^d)$. We apply the above bound to $\tilde{\gamma} = (U_\varepsilon^k)^* \gamma U_\varepsilon^k$, where U_ε^k is the unitary transformation defined by

$$\begin{aligned} U_\varepsilon^k : L^2(\mathbb{R}^d) &\rightarrow L^2(\mathbb{R}^d) \\ f &\mapsto \left(x \mapsto \varepsilon^{-d/2} f\left(\frac{x_1}{\varepsilon}, \frac{x' - \varepsilon k}{\varepsilon}\right) \right). \end{aligned}$$

Since we have

$$\|\rho_{\tilde{\gamma}}\|_{L^{q/2}(A)} = \varepsilon^{2d(1/2-1/q)} \|\rho_\gamma\|_{L^{q/2}(A_\varepsilon^k)},$$

and $U_\varepsilon^k \tilde{P} (U_\varepsilon^k)^* = P/\varepsilon$, we deduce that

$$\begin{aligned} &\|\rho_\gamma\|_{L^{q/2}(A_\varepsilon^k)} \\ &\leq C\tilde{h}^{-2s_{\text{Sogge}}(q,d)} \varepsilon^{-2d(1/2-1/q)} \left(\|\chi_{\tilde{A}_\varepsilon^k} \gamma \chi_{\tilde{A}_\varepsilon^k}\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}} + \frac{1}{(\varepsilon\tilde{h})^2} \|\chi_{\tilde{A}_\varepsilon^k} P \gamma P^* \chi_{\tilde{A}_\varepsilon^k}\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}} \right), \end{aligned}$$

with $\chi_{\tilde{A}_\varepsilon^k} = U_\varepsilon^k \chi_{\tilde{A}} (U_\varepsilon^k)^*$, i.e. $\chi_{\tilde{A}_\varepsilon^k}(x) = \chi_{\tilde{A}}\left(\frac{x_1}{\varepsilon}, \frac{x' - \varepsilon k}{\varepsilon}\right)$. Now assume that $M \geq \tilde{h}_0^{-2/3}$ and let $h \in (0, h_0]$ (where we recall that $h_0 > 0$ was chosen such that $Mh_0^{2/3} < \delta/2$). We apply the above bound to $\tilde{h} = h/\varepsilon^{3/2}$, which indeed satisfies $\tilde{h} \leq \tilde{h}_0$ since $\varepsilon \geq Mh^{2/3}$ implies $\tilde{h} \leq M^{-3/2} \leq \tilde{h}_0$. Finally, we obtain

$$\begin{aligned} &\|\rho_\gamma\|_{L^{q/2}(A_\varepsilon^k)} \\ &\leq C(h/\varepsilon^{3/2})^{-2s_{\text{Sogge}}(q,d)} \varepsilon^{-2d(1/2-1/q)} \left(\|\chi_{\tilde{A}_\varepsilon^k} \gamma \chi_{\tilde{A}_\varepsilon^k}\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}} + \frac{\varepsilon}{h^2} \|\chi_{\tilde{A}_\varepsilon^k} P \gamma P^* \chi_{\tilde{A}_\varepsilon^k}\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}} \right) \\ &= Ch^{-2s_{\text{Sogge}}(q,d)} \varepsilon^{-2\mu(q,d)} \left(\|\chi_{\tilde{A}_\varepsilon^k} \gamma \chi_{\tilde{A}_\varepsilon^k}\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}} + \frac{\varepsilon}{h^2} \|\chi_{\tilde{A}_\varepsilon^k} P \gamma P^* \chi_{\tilde{A}_\varepsilon^k}\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}} \right). \end{aligned}$$

□

We now give the missing proof of Fact VI.13.

Proof of Fact VI.13.

• It is essentially enough to understand why this inequality is true for the one-body case. The bound to prove is

$$\|\tilde{P}\chi_A \tilde{u}\|_{L^2(\mathbb{R}^d)} \lesssim \|\chi_{\tilde{A}} \tilde{P}\tilde{u}\|_{L^2(\mathbb{R}^d)} + \tilde{h} \|\chi_{\tilde{A}} \tilde{u}\|_{L^2(\mathbb{R}^d)}.$$

We already notice that

$$\begin{aligned} \tilde{P}\chi_A &= \chi_A \tilde{P} - \tilde{h}^2 (\partial_{\tilde{x}_1}^2 \chi_A) - 2\tilde{h} (\partial_{\tilde{x}_1} \chi_A) (\tilde{h} \partial_{\tilde{x}_1}) \\ &\quad - \tilde{h}^2 \sum_{2 \leq i, j \leq d} (\partial_{\tilde{x}_i} \partial_{\tilde{x}_j} \chi_A) a_{ij}(\varepsilon \tilde{x}_1, \varepsilon x' + \varepsilon k) - \tilde{h} \left\langle \nabla \chi_A, (a_{ij}(\varepsilon \tilde{x}_1, \varepsilon x' + \varepsilon k))_{i,j} \tilde{h} \nabla \right\rangle. \end{aligned}$$

On the one hand, since $a_{ij} \in L^\infty(\mathbb{R}^d)$

$$\begin{aligned} &\|\tilde{h}^2 (\partial_{\tilde{x}_1}^2 \chi_A) \tilde{u}\|_{L^2(\mathbb{R}^d)} + \|\tilde{h}^2 \sum_{2 \leq i, j \leq d} (\partial_{\tilde{x}_i} \partial_{\tilde{x}_j} \chi_A) a_{ij}(\varepsilon \tilde{x}_1, \varepsilon x' + \varepsilon k) \tilde{u}\|_{L^2(\mathbb{R}^d)} \\ &\lesssim \tilde{h}^2 \|\chi_{\tilde{A}} \tilde{u}\|_{L^2(\mathbb{R}^d)}. \end{aligned}$$

On the other hand, since \tilde{P} is elliptic in the sense of [KTZ07, Lem. 2.6], we have

$$\sum_{|\alpha|=1} \|(\tilde{h}D)^\alpha \tilde{u}\|_{L^2(A)} \lesssim \|\tilde{u}\|_{L^2(\tilde{A})} + \|\tilde{P}\tilde{u}\|_{L^2(\tilde{A})},$$

(by using again that $a_{ij} \in L^\infty(\mathbb{R}^d)$) so that

$$\begin{aligned} & \|\tilde{h}(\partial_{\tilde{x}_1} \chi_A)(\tilde{h}\partial_{\tilde{x}_1})\|_{L^2(\mathbb{R}^d)}^2 + \|\tilde{h} \left\langle \nabla \chi_A, (a_{ij}(\varepsilon \tilde{x}_1, \varepsilon \tilde{x}' + \varepsilon k))_{i,j}(\tilde{h}\nabla \tilde{u}) \right\rangle\|_{L^2(\mathbb{R}^d)}^2 \\ & \lesssim \tilde{h}^2 \|\tilde{h}D_{\tilde{x}_1} \tilde{u}\|_{L^2(A)}^2 + \tilde{h}^2 \|(a_{ij}(\varepsilon \tilde{x}_1, \varepsilon \tilde{x}' + \varepsilon k))_{i,j}(\tilde{h}\nabla \tilde{u})\|_{L^2(\tilde{A})} \\ & \lesssim \tilde{h}^2 \left(\|\tilde{u}\|_{L^2(\tilde{A})}^2 + \|\tilde{P}\tilde{u}\|_{L^2(\tilde{A})}^2 \right) \\ & \lesssim \tilde{h}^2 \left(\|\chi_{\tilde{A}} \tilde{u}\|_{L^2(\mathbb{R}^d)}^2 + \|\chi_{\tilde{A}} \tilde{P}\tilde{u}\|_{L^2(\mathbb{R}^d)}^2 \right). \end{aligned}$$

Hence,

$$\begin{aligned} \|\tilde{P}\chi_A \tilde{u}\|_{L^2(\mathbb{R}^d)} & \lesssim \|\chi_{\tilde{A}} \tilde{P}\tilde{u}\|_{L^2(\mathbb{R}^d)} + \tilde{h} \left(\|\chi_{\tilde{A}} \tilde{P}\tilde{u}\|_{L^2(\mathbb{R}^d)} + \|\chi_{\tilde{A}} \tilde{u}\|_{L^2(\mathbb{R}^d)} \right) \\ & \lesssim \|\chi_{\tilde{A}} \tilde{P}\tilde{u}\|_{L^2(\mathbb{R}^d)} + \tilde{h} \|\chi_{\tilde{A}} \tilde{u}\|_{L^2(\mathbb{R}^d)}. \end{aligned}$$

- Let us now extend the result to density matrices. We have shown the inequality of operators

$$\left(\tilde{P}\chi_A \right)^* \left(\tilde{P}\chi_A \right) \lesssim \tilde{h}^2 \chi_{\tilde{A}}^2 + \left(\chi_{\tilde{A}} \tilde{P} \right)^* \chi_{\tilde{A}} \tilde{P}.$$

In other words

$$\chi_A \tilde{P}^* \tilde{P} \chi_A \lesssim \tilde{h}^2 \chi_{\tilde{A}}^2 + \tilde{P}^* \chi_{\tilde{A}}^2 \tilde{P}.$$

Then for all $\alpha \geq 1$ and all bounded self-adjoint non-negative operator $\tilde{\gamma}$ on $L^2(\mathbb{R}^d)$

$$\left\| \sqrt{\tilde{\gamma}} \chi_A (1 + \tilde{P}^* \tilde{P} / \tilde{h}^2) \chi_A \sqrt{\tilde{\gamma}} \right\|_{\mathfrak{S}^\alpha} \lesssim \left\| \sqrt{\tilde{\gamma}} \chi_{\tilde{A}}^2 \sqrt{\tilde{\gamma}} \right\|_{\mathfrak{S}^\alpha} + \frac{1}{\tilde{h}^2} \left\| \sqrt{\tilde{\gamma}} \tilde{P}^* \chi_{\tilde{A}}^2 \tilde{P} \sqrt{\tilde{\gamma}} \right\|_{\mathfrak{S}^\alpha}.$$

This concludes the proof of Fact VI.13. \square

Step 2. The summation of the boxes. With the results on boxes of size ε , we will now have the following result.

Lemma VI.14. *Let $d \geq 2$ and $2 \leq q \leq \frac{2d}{d-2}$. Then, there exists $C > 0$ such that for any $\varepsilon \in [Mh^{2/3}, \delta/2]$, for any $h \in (0, h_0]$, and for any bounded self-adjoint non-negative operator γ on $L^2(\mathbb{R}^d)$ we have*

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(A_\varepsilon)} \leq Ch^{-2s_{\text{Sogge}}(q,d)} \varepsilon^{1/2-2\mu(q,d)} \left\| \left(1 + \frac{1}{h^2} P^* P \right)^{1/2} \gamma \left(1 + \frac{1}{h^2} P^* P \right)^{1/2} \right\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}},$$

where $\mu(q, d)$ is given by (VI.12).

Proof of Lemma VI.14. Since $\pi_x \text{supp } \chi \subset B_{\delta/2}$, we have for all $2 \leq q \leq \infty$

$$\|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(B_\varepsilon)} = \mathcal{O}(h^\infty) \|\gamma\|_{\mathfrak{S}^{q/2}}.$$

By Lemma VI.12, we have for non-negative operators γ

$$\begin{aligned} \|\rho\chi^w\gamma\chi^w\|_{L^{q/2}(A_\varepsilon\cap B_\delta)} &= \left(\sum_{|k|_{\ell^\infty} \leq \delta/\varepsilon-1} \|\rho\chi^w\gamma\chi^w\|_{L^{q/2}(A_\varepsilon^k)}^{q/2} \right)^{2/q} \\ &\lesssim h^{-2s_{\text{Sogge}}(q,d)} \varepsilon^{-2\mu(q,d)} \times \\ &\quad \times \underbrace{\left(\sum_{k \in \mathbb{Z}^{d-1}} \left\| \chi_{\tilde{A}_\varepsilon^k} \chi^w \gamma \chi^w \chi_{\tilde{A}_\varepsilon^k} \right\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}}^{q/2} \right)^{2/q}}_{= \left\| \chi_{\tilde{A}_\varepsilon^k} \chi^w \gamma \chi^w \chi_{\tilde{A}_\varepsilon^k} \right\|_{\ell_k^{q/2} \mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}}} + \frac{\varepsilon}{h^2} \underbrace{\left(\sum_{k \in \mathbb{Z}^{d-1}} \left\| \chi_{\tilde{A}_\varepsilon^k} P \chi^w \gamma \chi^w P^* \chi_{\tilde{A}_\varepsilon^k} \right\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}}^{q/2} \right)^{2/q}}_{= \left\| \chi_{\tilde{A}_\varepsilon^k} P \chi^w \gamma \chi^w P^* \chi_{\tilde{A}_\varepsilon^k} \right\|_{\ell_k^{q/2} \mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}}}. \end{aligned}$$

▷ The first step consists on showing that for $q \geq 2$, for any bounded self-adjoint operator γ

$$\begin{aligned} &\left\| \chi_{\tilde{A}_\varepsilon^k} \chi^w \gamma \chi^w \chi_{\tilde{A}_\varepsilon^k} \right\|_{\ell_k^{q/2} \mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}} + \frac{\varepsilon}{h^2} \left\| \chi_{\tilde{A}_\varepsilon^k} P \chi^w \gamma \chi^w P^* \chi_{\tilde{A}_\varepsilon^k} \right\|_{\ell_k^{q/2} \mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}} \\ &\lesssim \|\chi_{2\varepsilon} \chi^w \gamma \chi^w \chi_{2\varepsilon}\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}} + \frac{\varepsilon}{h^2} \|\chi_{2\varepsilon} P \chi^w \gamma \chi^w P^* \chi_{2\varepsilon}\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}}. \end{aligned}$$

In fact, we prove more precisely that for all non-negative Γ

$$\sum_{k \in \mathbb{Z}^{d-1}} \left\| \chi_{\tilde{A}_\varepsilon^k} \Gamma \chi_{\tilde{A}_\varepsilon^k} \right\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}}^{q/2} \leq C \|\chi_{2\varepsilon} \Gamma \chi_{2\varepsilon}\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}}^{q/2}.$$

Recall that $\text{supp } \chi_{\tilde{A}_\varepsilon^k} \subset \tilde{A}_\varepsilon^k \times \mathbb{R}^d$, $\chi_{2\varepsilon}(x_1) = 1$ when $x_1 \leq 2\varepsilon$. Hence, we have

$$\chi_{\tilde{A}_\varepsilon^k} = \chi_{\tilde{A}_\varepsilon^k} \chi_{2\varepsilon}$$

and thus we only have to show that

$$\sum_{k \in \mathbb{Z}^{d-1}} \left\| \chi_{\tilde{A}_\varepsilon^k} \Gamma \chi_{\tilde{A}_\varepsilon^k} \right\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}}^{q/2} \leq C \|\Gamma\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}}^{q/2}.$$

1) Let us check first that

$$\left\| \chi_{\tilde{A}_\varepsilon^k} \Gamma \chi_{\tilde{A}_\varepsilon^k} \right\|_{\ell_k^1 \mathfrak{S}^1} \lesssim \|\Gamma\|_{\mathfrak{S}^1}.$$

Since $\chi_{\tilde{A}_\varepsilon^k} \in \mathcal{C}^\infty(\mathbb{R}^d, [0, 1])$ and $\text{supp } \chi_{\tilde{A}_\varepsilon^k} \subset \tilde{A}_\varepsilon^k$, there exists $C > 0$ such that for all $\varepsilon > 0$,

$$\sum_{k \in \mathbb{Z}^{d-1}} \chi_{\tilde{A}_\varepsilon^k}^2 \leq C.$$

We recall that:

- if we have two non-negative operators A and B such that $A \leq B$ then $\sqrt{A} \leq \sqrt{B}$,
- for all trace-class operators A and B , $A \leq B \implies \text{Tr}(A) \leq \text{Tr}(B)$.

So if Γ is a non-negative operator

$$\begin{aligned} \left\| \chi_{A_\varepsilon^k} \Gamma \chi_{A_\varepsilon^k} \right\|_{\ell_k^1 \mathfrak{S}^1} &= \sum_{k \in \mathbb{Z}^{d-1}} \text{Tr}_{L^2} \left(\chi_{A_\varepsilon^k} \Gamma \chi_{A_\varepsilon^k} \right) \\ &= \sum_{k \in \mathbb{Z}^{d-1}} \text{Tr}_{L^2} \left(\sqrt{\Gamma} \chi_{\tilde{A}_\varepsilon^k}^2 \sqrt{\Gamma} \right) \\ &\leq \text{Tr}_{L^2} \left(\sqrt{\Gamma} \sum_{k \in \mathbb{Z}^{d-1}} \chi_{\tilde{A}_\varepsilon^k}^2 \sqrt{\Gamma} \right) \\ &\leq C \text{Tr}_{L^2} \Gamma = C \|\Gamma\|_{\mathfrak{S}^1}. \end{aligned}$$

We can pass to a general trace-class Γ by decomposing $\Gamma = \Gamma_+ - \Gamma_-$ with $\Gamma_+, \Gamma_- \geq 0$ and we obtain

$$\begin{aligned} \left\| \chi_{A_\varepsilon^k} \Gamma \chi_{A_\varepsilon^k} \right\|_{\ell_k^1 \mathfrak{S}^1} &\leq \left\| \chi_{A_\varepsilon^k} \Gamma_+ \chi_{A_\varepsilon^k} \right\|_{\ell_k^1 \mathfrak{S}^1} + \left\| \chi_{A_\varepsilon^k} \Gamma_- \chi_{A_\varepsilon^k} \right\|_{\ell_k^1 \mathfrak{S}^1} \\ &\lesssim \|\Gamma_+\|_{\mathfrak{S}^1} + \|\Gamma_-\|_{\mathfrak{S}^1} \\ &\lesssim \|\Gamma\|_{\mathfrak{S}^1}. \end{aligned}$$

2) Notice that we always have

$$\left\| \chi_{\tilde{A}_\varepsilon^k} \Gamma \chi_{\tilde{A}_\varepsilon^k} \right\|_{\ell_k^\infty \mathfrak{S}^\infty} \lesssim \|\Gamma\|_{\mathfrak{S}^\infty}.$$

3) The interpolation of

$$\begin{cases} \left\| \chi_{\tilde{A}_\varepsilon^k} \Gamma \chi_{\tilde{A}_\varepsilon^k} \right\|_{\ell_k^1 \mathfrak{S}^1} &\lesssim \|\Gamma\|_{\mathfrak{S}^1} \\ \left\| \chi_{\tilde{A}_\varepsilon^k} \Gamma \chi_{\tilde{A}_\varepsilon^k} \right\|_{\ell_k^\infty \mathfrak{S}^\infty} &\lesssim \|\Gamma\|_{\mathfrak{S}^\infty} \end{cases}$$

gives

$$\forall 1 \leq \alpha \leq \infty \quad \left\| \chi_{\tilde{A}_\varepsilon^k} \Gamma \chi_{\tilde{A}_\varepsilon^k} \right\|_{\ell_k^\alpha \mathfrak{S}^\alpha} \lesssim \|\Gamma\|_{\mathfrak{S}^\alpha}.$$

Hence, for any $2 \leq q \leq \infty$ and any $1 \leq \alpha \leq q/2$

$$\begin{aligned} \left\| \chi_{\tilde{A}_\varepsilon^k} \Gamma \chi_{\tilde{A}_\varepsilon^k} \right\|_{\ell_k^{q/2} \mathfrak{S}^\alpha} &\leq \left\| \chi_{\tilde{A}_\varepsilon^k} \Gamma \chi_{\tilde{A}_\varepsilon^k} \right\|_{\ell_k^\alpha \mathfrak{S}^\alpha} \\ &\lesssim \|\Gamma\|_{\mathfrak{S}^\alpha}. \end{aligned}$$

Now for any $2 \leq q \leq \infty$, we have $1 \leq \alpha_{\text{Sogge}}(q, d) \leq q/2$, hence for any $2 \leq q \leq \frac{2d}{d-2}$ we have

$$\begin{aligned} &\left\| \rho_{\chi^w \gamma \chi^w} \right\|_{L^{q/2}(A_\varepsilon \cap B_\delta)} \\ &\lesssim h^{-2s_{\text{Sogge}}(q, d)} \varepsilon^{-2\mu(q, d)} \left(\|\chi_{2\varepsilon} \chi^w \gamma \chi^w \chi_{2\varepsilon}\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q, d)}} + \frac{\varepsilon}{h^2} \|\chi_{2\varepsilon} P \chi^w \gamma \chi^w P^* \chi_{2\varepsilon}\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q, d)}} \right). \end{aligned}$$

▷ By the Hölder inequality and Corollary VI.6, we have for any $\alpha \geq 1$,

$$\|\chi_{2\varepsilon} \chi^w \gamma \chi^w \chi_{2\varepsilon}\|_{\mathfrak{S}^\alpha} \lesssim \varepsilon^{1/2} \left\| (1 + P^* P/h^2)^{1/2} \gamma (1 + P^* P/h^2)^{1/2} \right\|_{\mathfrak{S}^\alpha}.$$

Besides for any $\alpha \geq 1$,

$$\begin{aligned} \|\chi_{2\varepsilon} P \chi^w \gamma \chi^w P^* \chi_{2\varepsilon}\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q, d)}} &\lesssim \|P \gamma P^*\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q, d)}} \\ &\lesssim \left\| (1 + P^* P/h^2)^{1/2} \gamma (1 + P^* P/h^2)^{1/2} \right\|_{\mathfrak{S}^\alpha}. \end{aligned}$$

Thus, with the triangle inequality for any $2 \leq q \leq \frac{2d}{d-2}$

$$\begin{aligned} &\left\| \rho_{\chi^w \gamma \chi^w} \right\|_{L^{q/2}(A_\varepsilon \cap B_\delta)} \\ &\lesssim h^{-2s_{\text{Sogge}}(q, d)} \varepsilon^{-2\mu(q, d)} \left(\|\chi_{2\varepsilon} \chi^w \gamma \chi^w \chi_{2\varepsilon}\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q, d)}} + \frac{\varepsilon}{h^2} \|\chi_{2\varepsilon} P \chi^w \gamma \chi^w P^* \chi_{2\varepsilon}\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q, d)}} \right) \\ &\lesssim h^{-2s_{\text{Sogge}}(q, d)} \varepsilon^{1/2-2\mu(q, d)} \left\| (1 + P^* P/h^2)^{1/2} \gamma (1 + P^* P/h^2)^{1/2} \right\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q, d)}}. \end{aligned}$$

That finishes the proof of Lemma VI.14. \square

Step 3. The final summation. Finally, by Lemma VI.14 we are in position to obtain the estimates

$$\begin{aligned} \|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\Omega_{\delta/2} \setminus \Omega_{Mh^{2/3}})} &\leq \|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(\cup_k A_{2^k h^{2/3}})} \\ &\leq \left(\sum_{k=\lfloor \log_2(M) \rfloor}^{K(h)} \|\rho_{\chi^w \gamma \chi^w}\|_{L^{q/2}(A_{2^k h^{2/3}})}^{q/2} \right)^{2/q} \\ &\lesssim \left(\sum_{k=\lfloor \log_2(M) \rfloor}^{K(h)} C_{h, 2^k h^{2/3}}^q \right)^{2/q} \left\| (1 + P^* P/h^2)^{1/2} \gamma (1 + P^* P/h^2)^{1/2} \right\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}}, \end{aligned}$$

where $C_{h,\varepsilon} = h^{-s_{\text{Sogge}}(q,d)} \varepsilon^{1/4 - \mu(q,d)}$. Hence

$$\|\rho_\gamma\|_{L^{q/2}(\Omega_{\delta/2} \setminus \Omega_{Mh^{2/3}})} \lesssim C_h^2 \left\| (1 + P^* P/h^2)^{1/2} \gamma (1 + P^* P/h^2)^{1/2} \right\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}}$$

where

$$\begin{aligned} C_h &= \left(\sum_{k=\lfloor \log_2(M) \rfloor}^{K(h)} C_{h, 2^k h^{2/3}}^q \right)^{1/q} \\ &= \left(\sum_{k=\lfloor \log_2(M) \rfloor}^{K(h)} h^{-q(s_{\text{Sogge}}(q,d) + 2/3(\mu(q,d) - 1/4))} 2^{qk(1/4 - \mu(q,d))} \right)^{1/q} \\ &\lesssim \begin{cases} h^{-\frac{(d-1)}{2}(\frac{1}{2} - \frac{1}{q})} & \text{if } 2 \leq q < \frac{2(d+3)}{d+1}, \\ \log^{\frac{d+1}{2(d+3)}}(1/h) h^{-\frac{d-1}{2(d+3)}} & \text{if } q = \frac{2(d+3)}{d+1}, \\ h^{\frac{1}{6} - \frac{2d}{3}(\frac{1}{2} - \frac{1}{q})} & \text{if } \frac{2(d+3)}{d+1} < q \leq \frac{2d}{d-2}. \end{cases} \end{aligned}$$

That ends the proof of Lemma VI.8.

VII APPLICATIONS TO SPECTRAL CLUSTERS

In this section, we apply the results of the preceding sections on microlocalized quasimodes to spectral clusters. As we will see, this allows to get rid the microlocalization and leads to global estimates.

VII.1 Notation

- Let $\varepsilon \in (0, 1)$ and $h_0 \in (0, \varepsilon/2)$.
- Let $E \in \mathbb{R}$ and $h \in (0, h_0]$.
- Let $I_{h,E} := [E - h, E + h]$.
- Let $t_{\text{gene}}, s_{\text{gene}} \geq 0$ and $\alpha_{\text{gene}} \geq 1$ be given by the formulas in the statement of Theorem IV.2.
- Let $s_{\text{Sogge}} \geq 0$ and $\alpha_{\text{Sogge}} \geq 1$ be given by the formulas in the statement of Theorem V.2.
- Let $t_{\text{TP}}, s_{\text{TP}} \geq 0$ and $\alpha_{\text{TP}} \geq 1$ be given by the formulas in the statement of Theorem VI.2.

VII.2 Statement of the results

Let us add an additional assumption on the potential V , that will imply that the operator $-h^2\Delta + V$ has a compact resolvent.

Definition VII.1 (Polynomial growth). A potential $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$ has a *polynomial growth* if it satisfies Definition (II.3) and if there exist $k \in \mathbb{N}^*$ and $R > 0$ such that

$$\forall x \in \mathbb{R}^d, \forall |x| \geq R, \quad V(x) \geq c \langle x \rangle^k \quad (\text{VII.1})$$

Theorem VII.2. (i) Let $d \geq 1$. Let $p(x, \xi) = |\xi|^2 + V(x)$ with $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$ with a polynomial growth (Definition VII.1). For $h > 0$ and $E \in \mathbb{R}$, let us define $P := p^w(x, hD)$ and the spectral projector Π_h by

$$\Pi_h := \mathbb{1}(P \in I_{h,E}).$$

Let $E \in \mathbb{R}$. Then, there exist $C > 0$ and $h_0 > 0$ such that, for any $0 < h \leq h_0$, any $2 \leq q \leq \infty$ and any bounded self-adjoint non-negative operator γ on $L^2(\mathbb{R}^d)$

$$\|\rho_{\Pi_h \gamma \Pi_h}\|_{L^{q/2}(\mathbb{R}^d)} \leq C \log(1/h)^{2t_{\text{gene}}(q,d)} h^{-2s_{\text{gene}}(q,d)} \|\gamma\|_{\mathfrak{S}^{\alpha_{\text{gene}}(q,d)}(L^2(\mathbb{R}^d))}, \quad (\text{VII.2})$$

(ii) Let $d \geq 2$. There exist $C > 0$ and $h_0 > 0$ such that, for any $0 < h \leq h_0$, any $2 \leq q \leq \infty$ and any bounded self-adjoint non-negative operator γ on $L^2(\mathbb{R}^d)$

$$\|\rho_{\Pi_h \gamma \Pi_h}\|_{L^{q/2}(\{x \in \mathbb{R}^d : |V(x) - E| > \varepsilon\})} \leq Ch^{-2s_{\text{Sogge}}(q,d)} \|\gamma\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}}, \quad (\text{VII.3})$$

(iii) Let $d \geq 2$. Under the additional assumption that

$$\forall x \in \mathbb{R}^d, \quad V(x) = E \quad \implies \quad \nabla_x V(x) \neq 0, \quad (\text{VII.4})$$

there exist $C > 0$ and $h_0 > 0$ such that, for any $0 < h \leq h_0$, any $2 \leq q \leq \infty$ and any bounded self-adjoint non-negative operator γ on $L^2(\mathbb{R}^d)$

$$\|\rho_{\Pi_h \gamma \Pi_h}\|_{L^{q/2}(\{x \in \mathbb{R}^d : |V(x) - E| \leq \varepsilon\})} \leq C \log(1/h)^{2t_{TP}(q,d)} h^{-2s_{TP}(q,d)} \|\gamma\|_{\mathfrak{S}^{\alpha_{TP}(q,d)}}. \quad (\text{VII.5})$$

Remark 28. The constant C appearing in the above theorem can be chosen to be uniform in the energy level E when it varies in a compact set.

Remark 29. One can split the $L^{q/2}$ -norm of $\rho_{\Pi_h \gamma \Pi_h}$ on $\{x \in \mathbb{R}^d : |V(x) - E| > \varepsilon\}$ into two parts: on the classically allowed region $\{x \in \mathbb{R}^d : V(x) < E - \varepsilon\}$ and on the classically forbidden region $\{x \in \mathbb{R}^d : V(x) > E + \varepsilon\}$. When $d \geq 2$, there exist $C > 0$ and $h_0 > 0$ such that for any $0 < h \leq h_0$, any $2 \leq q \leq \infty$ and bounded self-adjoint non-negative operator γ on $L^2(\mathbb{R}^d)$,

$$\|\rho_{\Pi_h \gamma \Pi_h}\|_{L^{q/2}(\{x \in \mathbb{R}^d : V(x) - E < -\varepsilon\})} \leq Ch^{-2s_{\text{Sogge}}(q,d)} \|\gamma\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q,d)}(L^2(\mathbb{R}^d))}. \quad (\text{VII.6})$$

We will see below that, as one can expect, we have (for any $d \geq 1$)

$$\|\rho_{\Pi_h \gamma \Pi_h}\|_{L^{q/2}(\{x \in \mathbb{R}^d : V(x) - E > \varepsilon\})} = \mathcal{O}(h^\infty) \|\gamma\|_{\mathfrak{S}^\infty}. \quad (\text{VII.7})$$

We do not know if one can improve the $\mathcal{O}(h^\infty)$ to $\mathcal{O}(e^{-c/h})$ for some $c > 0$ in the spirit of Agmon estimates (c.f. for instance [DS99, Chap. 6]), since we are dealing with quasimodes and not exact eigenfunctions.

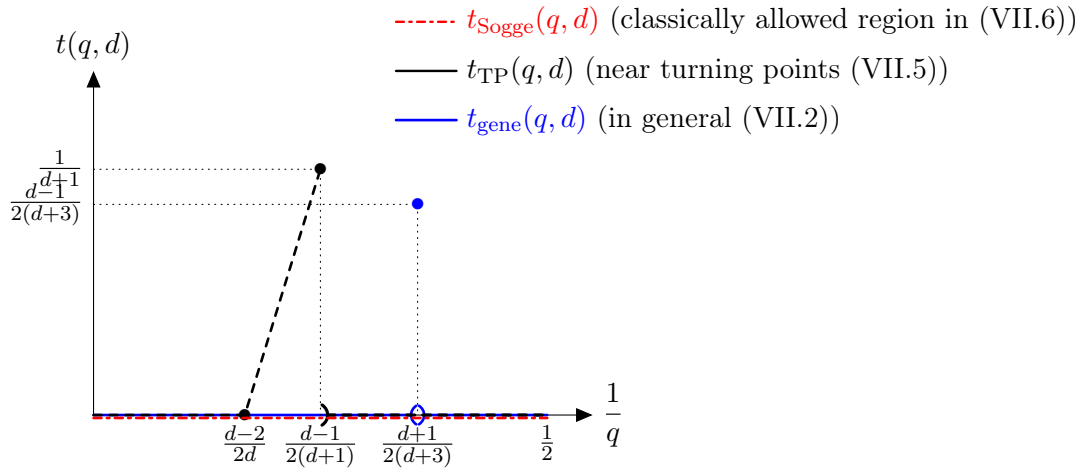


Figure 1.10 – Concentration logarithm exponent $t(q, d)$ when $d \geq 3$

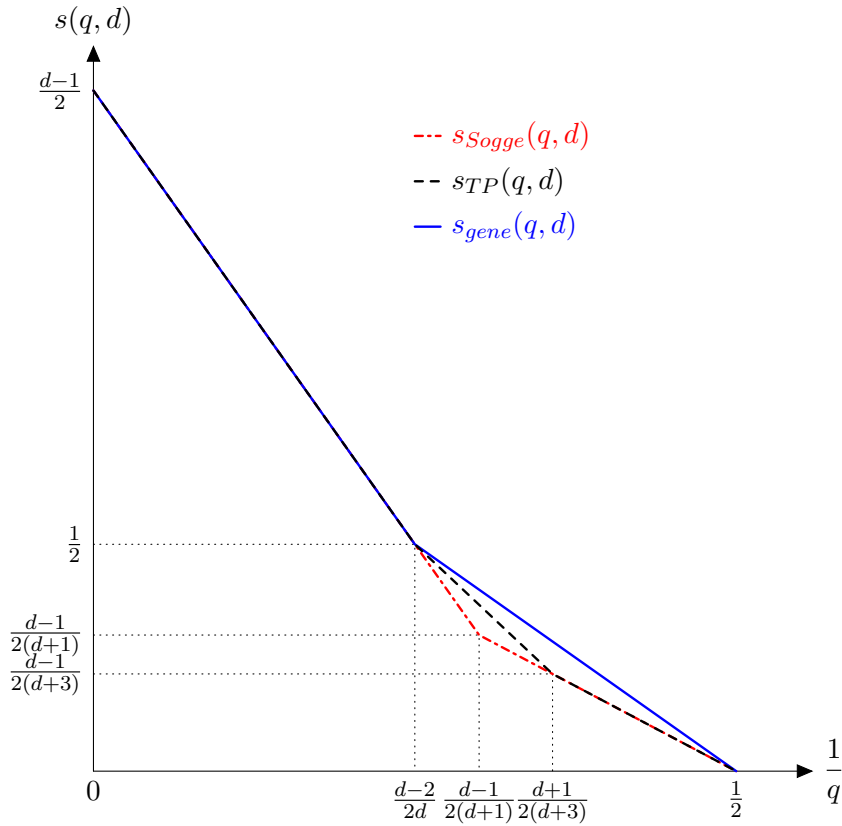
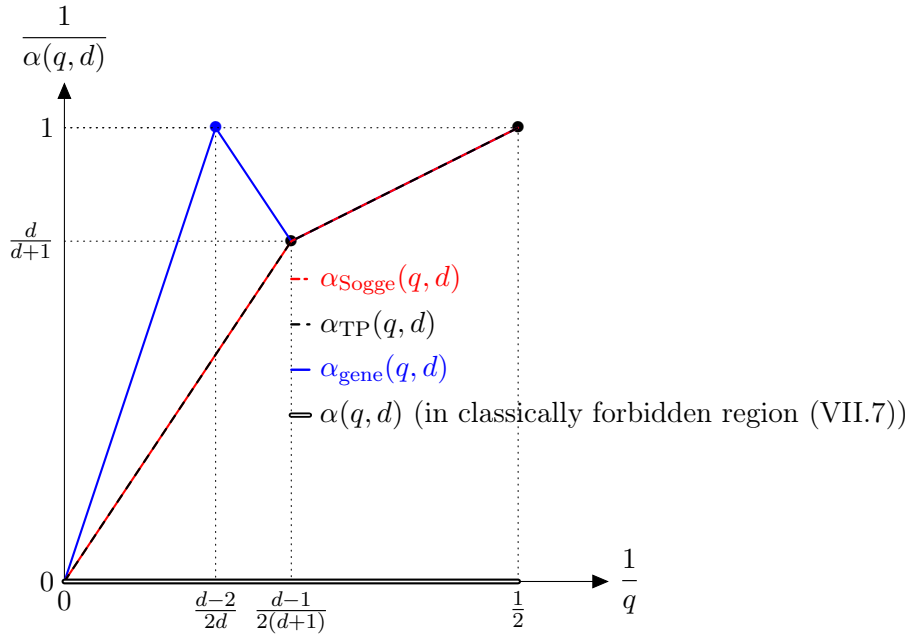


Figure 1.11 – Concentration exponent $s(q, d)$ when $d \geq 3$

VII.3 Proof of Theorem VII.2

Microlocalization of γ . We first explain why we only need to consider the microlocalized density matrix $\chi^w \Pi_h \gamma \Pi_h \chi^w$ for some $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ instead of the full one $\Pi_h \gamma \Pi_h$.

Let $f \in \mathcal{C}_c^\infty(\mathbb{R}, [0, 1])$ such that $f = 1$ on $I_{h_0, E}$ and $\text{supp } f \subset I_{\varepsilon/2, E}$. If we assume that

Figure 1.12 – Schatten exponent $\alpha(q, d)$ when $d \geq 3$

$h \in (0, h_0]$, we thus have

$$\Pi_h = f(P)\Pi_h.$$

By functional calculus Theorem II.11, $f(P)$ can be written as the Weyl quantization of a symbol $\tilde{\chi} \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$. Furthermore, for all $N \in \mathbb{N}$, there exists $\tilde{\chi}_N \in \mathcal{C}_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ and $r_N \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$, such that $\text{supp } \tilde{\chi}_N \subset \text{supp } f \circ p$ (note that $\text{supp } f \circ p$ is compact since $p(x, \xi) \rightarrow \infty$ when $|(x, \xi)| \rightarrow \infty$) and

$$\tilde{\chi}(x, \xi) = \tilde{\chi}_N(x, \xi) + h^N r_N(x, \xi).$$

Let us write the decomposition

$$\Pi_h = \tilde{\chi}_N^w \Pi_h + h^N r_N^w \Pi_h. \quad (\text{VII.8})$$

On the one hand, by the fact that $r_N^w = \mathcal{O}_{\mathcal{S}' \rightarrow \mathcal{S}}(1)$ and Kato-Seiler-Simon Lemma II.21 applied to $k \in \mathbb{N}$ such that $k(q/2)' > d$, for any $W \in L^{2(q/2)'(\mathbb{R}^d)}$

$$\begin{aligned} & \left\| h^N W r_N^w \Pi_h \sqrt{\gamma} \right\|_{\mathfrak{S}^2(L^2(\mathbb{R}^d))} \\ & \leq h^N \left\| W (1 - h^2 \Delta)^{-k/2} \right\|_{\mathfrak{S}^{2(q/2)'(L^2(\mathbb{R}^d))}} \left\| (1 - h^2 \Delta)^{k/2} r_N^w \Pi_h \right\|_{\mathfrak{S}^\infty(L^2(\mathbb{R}^d))} \left\| \sqrt{\gamma} \right\|_{\mathfrak{S}^q(L^2(\mathbb{R}^d))} \\ & \lesssim h^{N-d/2} \|W\|_{L^{2(q/2)'(\mathbb{R}^d)}} \|\gamma\|_{\mathfrak{S}^{q/2}(L^2(\mathbb{R}^d))}^{1/2}. \end{aligned}$$

By duality, we deduce that for all $N \in \mathbb{N}$

$$\left\| \rho_{(1-\tilde{\chi}_N^w)\Pi_h \gamma \Pi_h (1-\tilde{\chi}_N^w)} \right\|_{L^{q/2}(\mathbb{R}^d)} \leq C h^{2N-d} \|\gamma\|_{\mathfrak{S}^{q/2}(L^2(\mathbb{R}^d))},$$

hence, it remains to estimate $\rho_{\tilde{\chi}_N^w \Pi_h \gamma \Pi_h \tilde{\chi}_N^w}$ on various regions with perhaps additional assumptions on V .

(o) **Microlocalized estimates in the classically forbidden region.** Notice that since

$$\text{supp}(f \circ p) \cap (\{x \in \mathbb{R}^d : V(x) - E > \varepsilon\} \times \mathbb{R}^d) = \emptyset,$$

we have

$$\|\rho_{\tilde{\chi}_N^w} \Pi_h \gamma \Pi_h \tilde{\chi}_N^w\|_{L^{q/2}(\{x \in \mathbb{R}^d : V(x) - E > \varepsilon\})} = \mathcal{O}(h^\infty) \|\gamma\|_{\mathfrak{S}^{q/2}}.$$

By Weyl's law (Proposition II.16), we have

$$\|\Pi_h \gamma \Pi_h\|_{\mathfrak{S}^{q/2}} \leq \|\gamma\|_{\mathfrak{S}^\infty} \|\Pi_h\|_{\mathfrak{S}^{q/2}} \leq Ch^{-2d/q} \|\gamma\|_{\mathfrak{S}^\infty},$$

and thus, we deduce (VII.7).

(i) **General microlocalized estimates.** Note that all $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$ satisfy the non-degeneracy Assumption 2 for the symbol $p_E := p - E$. By Theorem IV.2, Assumption 1 is thus satisfied for $S = \mathbb{R}^d \times \mathbb{R}^d$, $q \in [2, \infty]$, $s = s_{\text{gene}}(q, d)$, $t = 0$ and $\alpha = \alpha_{\text{gene}}(q, d)$. We apply Theorem II.24 to these parameters $(q, s_{\text{gene}}(q, d), 0, \alpha_{\text{gene}}(q, d))$ and to $\chi = \tilde{\chi}_N$, that gives us

$$\begin{aligned} \|\rho_{\tilde{\chi}_N^w} \Pi_h \gamma \Pi_h \tilde{\chi}_N^w\|_{L^{q/2}(\mathbb{R}^d)} &\leq C \log(1/h)^{2t_{\text{gene}}(q, d)} h^{-2s_{\text{gene}}(q, d)} \times \\ &\quad \times \left(\|\Pi_h \gamma \Pi_h\|_{\mathfrak{S}^{\alpha_{\text{gene}}(q, d)}} + \frac{1}{h^2} \|(P - E) \Pi_h \gamma \Pi_h (P - E)\|_{\mathfrak{S}^{\alpha_{\text{gene}}(q, d)}} \right) \\ &\leq C' \log(1/h)^{2t_{\text{gene}}(q, d)} h^{-2s_{\text{gene}}(q, d)} \|\gamma\|_{\mathfrak{S}^{\alpha_{\text{gene}}(q, d)}}, \end{aligned}$$

which is exactly (VII.2).

(ii) **Microlocalized estimates in the classically allowed region.** Let $d \geq 2$. Let $S = \{(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d : |V(x) - E| > \varepsilon\}$. Any $(x_0, \xi_0) \in S$ satisfies either the ellipticity condition $p_E(x_0, \xi_0) \neq 0$ or Assumption 3 for the symbol p_E . By Theorem III.1 and Theorem V.2, the set S thus satisfies Assumption 1 for all $q \in [2, \infty]$, $s = s_{\text{Sogge}}(q, d)$, $t = 0$ and $\alpha = \alpha_{\text{Sogge}}(q, d)$. We apply Theorem II.25 to these parameters, $\Omega = \{x \in \mathbb{R}^d : |V(x) - E| > \varepsilon\}$ and $\chi = \tilde{\chi}_N$. Then, there exist $C > 0$ and $h_0 > 0$ such that for any $0 < h \leq h_0$ and $2 \leq q \leq \infty$

$$\|\rho_{\tilde{\chi}_N^w} \Pi_h \gamma \Pi_h \tilde{\chi}_N^w\|_{L^{q/2}(\{|V-E|>\varepsilon\})} \leq Ch^{-2s_{\text{Sogge}}(q, d)} \|\gamma\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q, d)}},$$

where we got rid of the operator $P - E$ in the Schatten norm by the same method as in the previous step. We thus get (VII.3).

(iii) **Microlocalized estimates near the turning points.** Let $d \geq 2$. Let $S = \{(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d : |V(x) - E| \leq \varepsilon\}$. Any $(x_0, \xi_0) \in S$ satisfies either the ellipticity condition $p_E(x_0, \xi_0) \neq 0$, Assumption 3, or Assumption 19 for the symbol p_E . By Theorem III.1, Theorem V.2, and Theorem VI.2, the set S thus satisfies Assumption 1 for all $q \in [2, \infty]$, $s = s_{\text{TP}}(q, d)$, $t = t_{\text{TP}}(q, d)$ and $\alpha = \alpha_{\text{TP}}(q, d)$. We apply Theorem II.25 to these parameters, $\Omega = \{x \in \mathbb{R}^d : |V(x) - E| \leq \varepsilon\}$ and $\chi = \tilde{\chi}_N$. As above, there exist $C > 0$ and $h_0 > 0$ such that for any $0 < h \leq h_0$ and $2 \leq q \leq \infty$

$$\|\rho_{\tilde{\chi}_N^w} \Pi_h \gamma \Pi_h \tilde{\chi}_N^w\|_{L^{q/2}(\{|V-E|\leq\varepsilon\})} \leq C \log(1/h)^{2t_{\text{TP}}(q, d)} h^{-2s_{\text{TP}}(q, d)} \|\gamma\|_{\mathfrak{S}^{\alpha_{\text{TP}}(q, d)}},$$

showing (VII.3).

VIII OPTIMALITY

In this section, we discuss the optimality of the concentration exponents $s(q, d)$ and $\alpha(q, d)$, appearing in the estimates of Theorem VII.2. We first explain why the exponents $s(q, d)$ are sharp for all values of q and d . To do so, we will see that it is enough to consider the one-body case $\text{rank } \gamma = 1$ for which only the exponent $s(q, d)$ appears. In many cases, this optimality was known in the literature, but we provide some details here. On the contrary, the optimality of the exponent $\alpha(q, d)$ is only proved in a restricted range of cases.

VIII.1 One-body optimality

Let V satisfying Definition VII.1, $h > 0$, $P = -h^2\Delta + V$ and $E \in \mathbb{R}$. In this section, we explain several concentration scenarii of functions u_h , which saturate the various one-body L^q bounds. All the saturating scenarii happen in the bulk $\{V - E < -\varepsilon\}$, meaning that they satisfy lower bounds of the type

$$\|u_h\|_{L^q(\{V-E < -\varepsilon\})} \geq Ch^{-s(q,d)} \left(\|u_h\|_{L^2(\mathbb{R}^d)} + \frac{1}{h} \|(P-E)u_h\|_{L^2(\mathbb{R}^d)} \right). \quad (\text{VIII.1})$$

The different saturation scenarii according to the values of $s(q, d)$ are summarized in Figure 1.16 and Figures 1.13, 1.14 and 1.15. The optimality of the estimates in the turning point region $\{|V - E| \leq \varepsilon\}$ is much more delicate. In [KT05], the optimality in the case $V(x) = |x|^2$ is proved for the estimates in the dyadic regions of size $2^j h^{2/3}$ (see the proof of Theorem VI.2) for fixed j . The optimality in the full region $\{|V - E| \leq \varepsilon\}$ (that is, when we sum over j), as well as the optimality in the small neighborhood $\Omega_{Mh^{2/3}}$ of a turning point seem open to us.

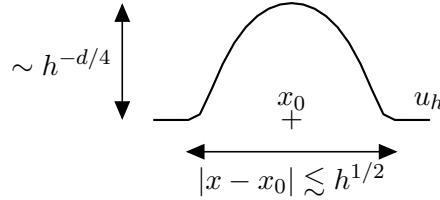


Figure 1.13 – Concentration of a gaussian ground state

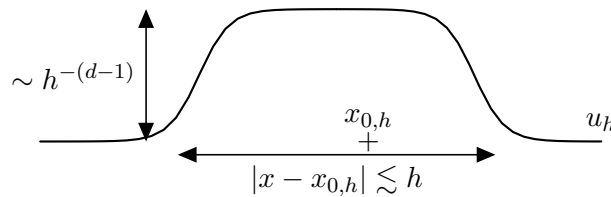


Figure 1.14 – Concentration of a zonal-type quasimode

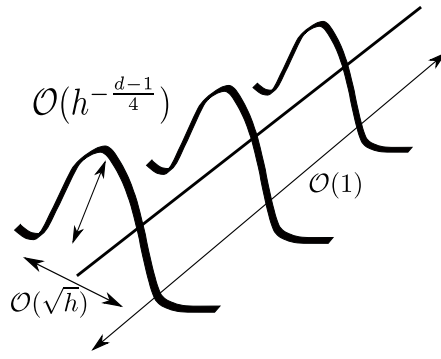


Figure 1.15 – Gaussian beams: concentration around a curve

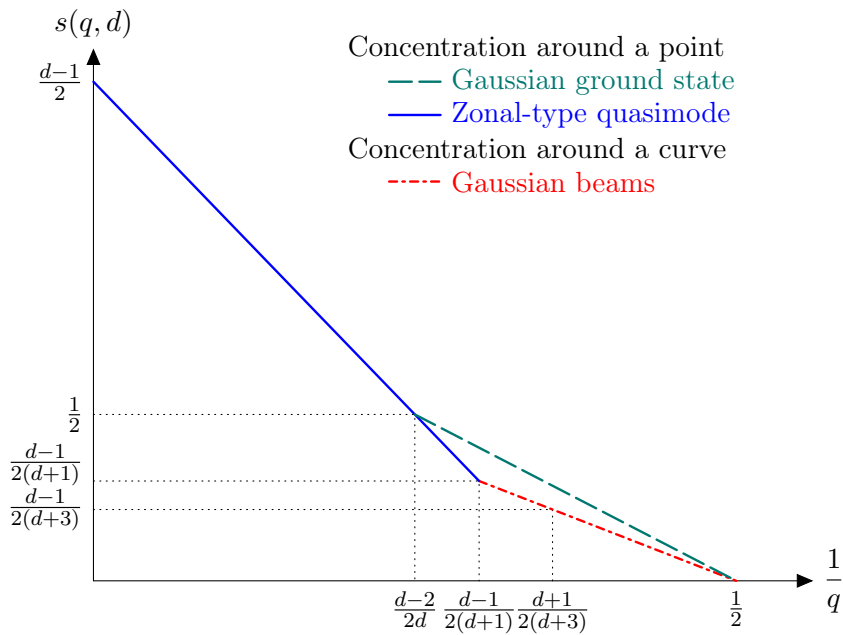


Figure 1.16 – Saturation of $s(q, d)$ for $d \geq 3$

Gaussian ground state

We begin with explaining why the exponent $s_{\text{gene}}(q, d)$ is sharp (that is, it cannot be lowered). We do so, by exhibiting a family of functions that saturates the inequalities in which $s_{\text{gene}}(q, d)$ appears. We will see that in this case, the saturation scenario happens for functions concentrating around a non-degenerate local minimum of the potential, exactly like the ground state of a harmonic oscillator. Such a construction is well-known (see for instance [Hel06, Chap. 2], [DS99, Thm 4.23] and [KTZ07, Exemple 2]), but we recall here for completeness.

Proposition VIII.1. *Let $d \geq 1$ and $2 \leq q \leq \infty$. Let $p(x, \xi) := |\xi|^2 + V(x)$ where $V \in \mathcal{C}^\infty(\mathbb{R}^d, \mathbb{R})$ is as in Definition VII.1. For any $h > 0$, define $P = p^w(x, hD)$. Let $E \in \mathbb{R}$ such that there exists $x_0 \in \mathbb{R}^d$ such that*

$$V(x_0) = E, \quad \nabla_x V(x_0) = 0, \quad \partial_x^2 V(x_0) \text{ definite positive} .$$

Then, there exist $C > 0$ and $h_0 > 0$, such that the normalized ground state of the operator $-h^2\Delta + \langle x - x_0, \sqrt{\partial_x^2 V(x_0)}(x - x_0) \rangle$

$$u_h(x) := (2\pi\sqrt{h})^{-d/2} \det(\partial_x^2 V(x_0))^{-1/4} e^{-\frac{\langle x - x_0, \sqrt{\partial_x^2 V(x_0)}(x - x_0) \rangle}{2h}}$$

associated to the eigenfunction $\lambda_h := h \operatorname{Tr}_{\mathbb{R}^d} \sqrt{\partial_x^2 V(x_0)}$ satisfies the bound for any $h \in (0, h_0]$

$$\|u_h\|_{L^2(\mathbb{R}^d)} = 1, \quad \|(P - E)u_h\|_{L^2(\mathbb{R}^d)} \leq Ch, \quad \|u_h\|_{L^q(\mathbb{R}^d)} \geq (1/C)h^{-\frac{d}{2}\left(\frac{1}{2} - \frac{1}{q}\right)}. \quad (\text{VIII.2})$$

The function u_h concentrates around x_0 at a scale \sqrt{h} with a height $\sim h^{-d/4}$ (c.f. Figure 1.13).

Remark 30. The previous proposition gives the optimality of the exponent $s_{\text{gene}}(q, d)$

- when $d = 1$: for $2 \leq q \leq \infty$,
- when $d = 2$: for $2 \leq q < \infty$,
- when $d \geq 3$: for $2 \leq q \leq 2d/(d - 2)$.

Indeed, recall that in these cases we have $s_{\text{gene}}(q, d) = \frac{d}{2} \left(\frac{1}{2} - \frac{1}{q} \right)$, which is the exponent appearing in (VIII.2). More precisely, this proves that one cannot take a smaller $s(q, d)$ in Theorem IV.1. Notice that this theorem applies to microlocalized functions, which is not the case for our quasimode u_h above. However, since u_h is an eigenfunction of a Schrödinger operator with a quadratic potential, there exists $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ such that $u_h = \chi^w u_h + \mathcal{O}(h^\infty)$ as in the proof of Theorem VII.2. Any point (x_0, ξ_0) in the support of χ satisfies either $p(x_0, \xi_0) \neq 0$ or Assumption 2. Hence, it shows that $\{u_h\}_{h \in (0, h_0]}$ actually saturates the bound of Theorem IV.1 but in its version of Theorem II.24.

Remark 31. In the special case where V is quadratic (meaning that $\partial_x^2 V$ is constant), u_h (more precisely $\gamma_h = |u_h\rangle \langle u_h|$) saturates also the bound (VII.2) in Theorem VII.2 because in this case it satisfies $\Pi_h u_h = u_h$. Notice that in this one-body setting, no logarithm appears in this estimate as we recall in Section IV.

Proof of Proposition VIII.1. Let $2 \leq q \leq \infty$ and $h > 0$. Let φ_1 the normalized gaussian on $L^2(\mathbb{R}^d)$

$$\varphi_1(x) := (2\pi)^{-d/2} e^{-|x|^2/2}.$$

When we replace the potential $|x|^2$ by $V_{x_0}(x) := \frac{1}{2} \langle x - x_0, \partial_x^2 V(x_0)(x - x_0) \rangle$ in the harmonic oscillator, the normalized ground state associated to the eigenvalue $\lambda_h = h \operatorname{Tr}_{\mathbb{R}^d} \sqrt{\partial_x^2 V(x_0)}$ of $P_0 := -h^2\Delta + V_{x_0}(x)$ is given by the formula

$$u_h(x) = h^{-d/4} (\det(\partial_x^2 V(x_0)))^{-1/4} \varphi_1(h^{-1/2}(\partial_x^2 V(x_0))^{1/4}(x - x_0)).$$

Moreover, for any compact K neighborhood of x_0 , there exists $C(d, K, h_0) > 0$ such that for $0 < h \leq h_0$ and any $2 \leq q \leq \infty$

$$\begin{aligned} \|u_h\|_{L^q(K)} &= (\det(\partial_x^2 V(x_0)))^{-1/4} h^{-d/4} \|\varphi_1(h^{-1/2}(\partial_x^2 V(x_0))^{1/4}(x - x_0))\|_{L^q(K)} \\ &\geq C(d, K) h^{-\frac{d}{2}\left(\frac{1}{2} - \frac{1}{q}\right)} \underbrace{\|\varphi_1\|_{L^q(h_0^{-1/2}(\partial_x^2 V(x_0))^{-1/4}(K+x_0))}}_{>0} \\ &\geq C(d, K, h_0) h^{-\frac{d}{2}\left(\frac{1}{2} - \frac{1}{q}\right)}. \end{aligned}$$

We have for any $h_0 > 0$, $C > 0$ such that for any $h \in (0, h_0]$ and any $2 \leq q \leq \infty$

$$\|u_h\|_{L^q(\mathbb{R}^d)} \geq Ch^{-\frac{d}{2}\left(\frac{1}{2}-\frac{1}{q}\right)} \left(\|u_h\|_{L^2(\mathbb{R}^d)} + \frac{1}{h} \|(P_0 - \lambda_h)u_h\|_{L^2(\mathbb{R}^d)} \right).$$

It remains to show that u_h is a quasimode of the operator $P - E$

$$(P - E)u_h = \mathcal{O}_{L^2}(h).$$

By Taylor formula of V at $x = x_0$, we have for any $x \in \mathbb{R}^d$

$$V(x) = E + V_{x_0}(x) + \mathcal{O}(|x - x_0|^3).$$

Thus, one can estimate $(V - E - V_{x_0})u_h$

$$\begin{aligned} \|(V - E - V_{x_0})u_h\|_{L^2(\mathbb{R}^d)}^2 &= \int_{\mathbb{R}^d} |(V - E - V_{x_0})(x)u_h(x)|^2 dx \\ &= \int_{\mathbb{R}^d} \left| (V - E - V_{x_0})(x_0 + \sqrt{h}x)u_1(x_0 + \sqrt{h}x) \right|^2 dx. \end{aligned}$$

On the one hand, since $\{y \in \mathbb{R}^d : y = x_0 + \sqrt{h}x \text{ and } x \in \mathbb{R}^d, |x| \leq 1/\sqrt{h}\} \subset \{y \in \mathbb{R}^d : |y| \leq |x_0| + 2\}$ is a compact set of \mathbb{R}^d , we have by Taylor formula and by $\varphi_1 \in \mathcal{S}(\mathbb{R}^d)$

$$\begin{aligned} &\int_{|x| \leq \frac{1}{\sqrt{h}}} \left| (V - E - V_{x_0})(x_0 + \sqrt{h}x)u_1(x_0 + \sqrt{h}x) \right|^2 dx \\ &\leq Ch^3 \int_{|x| \leq \frac{1}{\sqrt{h}}} |x|^6 \left| u_1(x_0 + \sqrt{h}x) \right|^2 dx \\ &\leq Ch^3 \int_{\mathbb{R}^d} |x|^6 \left| \varphi_1((\partial_x^2 V(x_0))^{1/4}x) \right|^2 (\det((\partial_x^2 V(x_0))))^{-1/2} dx \\ &\leq C'h^3 \underbrace{\int_{\mathbb{R}^d} |x|^6 |\varphi_1(x)|^2 dx}_{< \infty}. \end{aligned}$$

On the other hand, by the growth assumption (II.1) on the potential V

$$\begin{aligned} &\int_{|x| > \frac{1}{\sqrt{h}}} \left| (V - E - V_{x_0})(x_0 + \sqrt{h}x)u_1(x_0 + \sqrt{h}x) \right|^2 dx \\ &= \int_{|x| > \frac{1}{\sqrt{h}}} \left| V(x_0 + \sqrt{h}x) - E + h \langle x, \partial_x^2 V(x_0)x \rangle \right|^2 \left| u_1(x_0 + \sqrt{h}x) \right|^2 dx \\ &\leq C \int_{|x| > \frac{1}{\sqrt{h}}} (1 + |x_0 + \sqrt{h}x|^k + h \langle x, \partial_x^2 V(x_0)x \rangle)^2 \left| u_1(x_0 + \sqrt{h}x) \right|^2 dx \\ &\leq C' \int_{|x| > \frac{1}{\sqrt{h}}} \left| \varphi_1((\partial_x^2 V(x_0))^{1/4}x) \right|^2 (\det((\partial_x^2 V(x_0))))^{-1/2} dx \\ &\leq C'' \int_{|x| > \frac{c'}{\sqrt{h}}} |\varphi_1(x)|^2 dx = \mathcal{O}(e^{-c/h}) = \mathcal{O}(h^\infty). \end{aligned}$$

Thus,

$$\|(V - E - V_{x_0})u_h\|_{L^2(\mathbb{R}^d)} = \mathcal{O}(h^{3/2}).$$

We finally get

$$\begin{aligned} (P - E)u_h &= (P_0 - \lambda_h)u_h + \lambda_h u_h + (V - E - V_{x_0})u_h \\ &= \mathcal{O}_{L^2}(h). \end{aligned}$$

This concludes the proof. \square

Zonal-type quasimode

We now prove the sharpness of the exponent $s_{\text{Sogge}}(q, d)$ for large values of q . We will see that the saturation phenomenon is obtained for a sequence of functions concentrating around a point (with a rate different from the one of the gaussian ground state of the preceding section). For the harmonic potential $V(x) = |x|^2$, such functions have already been constructed in [KT05, Sec. 5.2]. Our example which relies on the Weyl law is valid for a more general class of potentials. It is inspired by the construction in [Sog17a, Eq. (5.1.12)].

Proposition VIII.2. *Let $d \geq 2$. Let $E_0 > 0$ such that $E_0 > \min V$. Let $\varepsilon_0 := E_0 - \min V$. Assume that*

$$\lim_{\varepsilon \rightarrow 0} \left| \{x \in \mathbb{R}^d : |V(x) - \lambda| \leq \varepsilon\} \right| = 0 \quad (\text{VIII.3})$$

uniformly for λ in a neighborhood of E_0 . Then, there exist $h_0 > 0$, energies $\{E_h\}_{h \in (0, h_0]} \subset [E_0 - \varepsilon_0/2, E_0 + \varepsilon_0/2]$, $\varepsilon \in (0, \varepsilon_0/4)$ and points $\{x_{0,h}\}_{h \in (0, h_0]} \subset \{V \leq E_h - \varepsilon\}$ such that the family of functions defined by

$$u_h := \Pi_h(x_{0,h}, \cdot)$$

where Π_h denotes the spectral projector

$$\Pi_h := \mathbf{1}(P \in I_{h, E_h}) = \mathbf{1}(P \in [E_h - h, E_h + h]),$$

satisfies along a sequence $h_n \rightarrow 0$ that for any $2 \leq q \leq \infty$

$$\|u_h\|_{L^2(\mathbb{R}^d)} \leq Ch^{-\frac{(d-1)}{2}}, \quad \|u_h\|_{L^q(\{x \in \mathbb{R}^d : V(x) - E_h \leq \varepsilon\})} \geq (1/C)h^{-(d-1) + \frac{d}{q}}.$$

Remark 32. As a consequence, we get that

$$\limsup_{h \rightarrow 0} h^{d(1/2 - 1/q) - 1/2} \frac{\|u_h\|_{L^q(\{x \in \mathbb{R}^d : V(x) - E_h \leq \varepsilon\})}}{\|u_h\|_{L^2(\mathbb{R}^d)}} > 0,$$

which proves the optimality of the exponent $s_{\text{Sogge}}(q, d)$ (which is equal to $d(1/2 - 1/q) - 1/2$ when $2(d+1)/(d-1) \leq q \leq \infty$) in the estimate (VII.3).

Remark 33. Assumption (VIII.3) is satisfied for instance when:

- $\nabla_x V(x_0)$ does not vanish for the points $x_0 \in \{V = \lambda\}$,
- or when the Hessian $\partial_x^2 V(x_0)$ is non-degenerate for the points $x_0 \in \{V = \lambda\}$,

for λ in a neighborhood of E_0 . In the first case, we have $|\{|V - \lambda| \leq \varepsilon\}| = \mathcal{O}(\varepsilon)$. We even expect that the condition holds if for any x_0 such that $V(x_0)$ belongs to a neighborhood of E_0 , the Taylor expansion of V at x_0 is not identically zero. On the contrary, if V is constant in a neighborhood of x_0 , then Assumption (VIII.3) is not satisfied.

Remark 34. The lower bound on the L^q norm of u_h comes the pointwise estimate

$$\forall x \in \mathbb{R}^d, |x - x_{0,h}| \leq ch \implies |u_h(x)| \geq Ch^{1-d}. \quad (\text{VIII.4})$$

In other words, the function u_h concentrates around $x_{0,h}$ at a scale h with a height $\sim h^{-(d-1)}$ (such that in Figure 1.14). This motivates the name *zonal-type quasimode* because they concentrate similarly to the zonal harmonics, which are known to saturate the Sogge L^q estimates in the same regime of q . This originally appeared in [Sog85].

Before proving Proposition VIII.2, we first provide a lemma which is an easy consequence of the integrated Weyl law, which is well known in the high energy regime and that we state here in the semiclassical setting. This result gives an interval of size h with the maximal number of eigenvalues inside. It will also be useful for the many-body optimality.

For any $I \subset \mathbb{R}$, recall that $N_h(I)$ denotes the number of eigenvalues of P in I .

Lemma VIII.3. *Let $a < b$ such that $|p^{-1}([a, b])| > 0$. Then*

$$\limsup_{h \rightarrow 0} \sup_{J_h \subset [a, b], |J_h| = 2h} h^{d-1} N_h(J_h) > 0.$$

Proof of Lemma VIII.3. Assume by contradiction that

$$\limsup_{h \rightarrow 0} \sup_{J_h \subset [a, b], |J_h| = 2h} h^{d-1} N_h(J_h) = 0$$

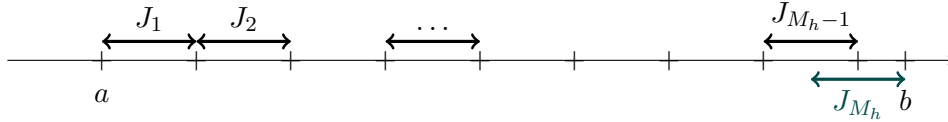
i.e. for all $\varepsilon > 0$, there exists $\tilde{h} > 0$ such that for all $h \in (0, \tilde{h})$ and for all interval $J_h \subset [a, b]$ such that $|J_h| = 2h$

$$h^{d-1} N_h(J_h) \leq \varepsilon.$$

One can cover $[a, b]$ by a finite set of intervals of length $2h$:

$$\{J_j\}_{j=1}^{M_h} \subset [a, b], \quad [a, b] \subset \bigcup_{j=1}^{M_h} J_j.$$

For example, for $2h < |b - a|$, one can take $M_h = \left\lfloor \frac{|b-a|}{2h} \right\rfloor - 1$, define the $M_h - 1$ first intervals by $J_j := [a + 2(j-1)h, a + 2jh]$ and define the M_h -th one $J_{M_h} := [b - 2h, b]$.



Finally,

$$N_h([a, b]) \leq \sum_{j=1}^{M_h} N_h(J_j) \lesssim M_h \varepsilon h^{-(d-1)} \sim \varepsilon |b - a| h^{-d}.$$

When ε goes to 0, we get

$$\lim_{h \rightarrow 0} h^d N_h([a, b]) = 0.$$

However, by the Weyl law (Proposition II.16) $h^d N_h([a, b])$ is equivalent to $(2\pi)^{-d} |p^{-1}([a, b])|$, which is positive. That is in contradiction with the original assumption. \square

Remark 35 (Broken dream). One can hope to find a fixed energy set $E \in [a, b]$ such that

$$\limsup_{h \rightarrow 0} h^{d-1} N_h([E - 2h, E + 2h]) > 0.$$

Actually, it is not clear that this is possible. Let us try a reasoning (which will not succeed). By Lemma VIII.3, we can find $\alpha > 0$ and a sequence $\{h_n\}_{n \in \mathbb{N}^*}$ that tends to 0 such that

$$\sup_{n \rightarrow \infty} \sup_{I_n \subset [a, b], |I_n| = 2h_n} h_n^{d-1} N_{h_n}(I_n) = \alpha.$$

Thus, there exists $N \in \mathbb{N}$ such that for any $n \geq N$ and any interval I_n of length $2h_n$

$$h_n^{d-1} N_{h_n}(I_n) \geq \frac{\alpha}{2}.$$

Denote by c_n the center of the interval $J_n := [c_n - h_n, c_n + h_n]$. The sequence $\{c_n\}_{n \in \mathbb{N}}$ is contained into the compact $[a, b]$. Up to an extraction of subsequence, $\{c_n\}_{n \in \mathbb{N}}$ admits a limit $E \in [a, b]$. Let us then define $\tilde{h}_n > h_n$ that tends also to 0

$$\forall n \geq N, \quad \tilde{h}_n := h_n + |c_n - E|.$$

Therefore,

$$\begin{aligned} \forall n \geq N, \quad \tilde{h}_n^{d-1} N_{\tilde{h}_n}([E - \tilde{h}_n, E + \tilde{h}_n]) &\geq h_n^{d-1} N_{h_n}([E - \tilde{h}_n, E + \tilde{h}_n]) \\ &\geq \frac{\alpha}{2}. \end{aligned}$$

Our dream would become true if $N_{\tilde{h}_n}(J) \geq N_{h_n}(J)$ for any interval $J \subset \mathbb{R}$, and more generally

$$N_{\tilde{h}}(J) \geq N_h(J) \quad \forall \tilde{h} > h.$$

However, it is not the case at all (indeed $h \mapsto N_h(J)$ is even decreasing). Consequently, the center c_h of the intervals J_h can move at the semiclassical limit.

Proof of Proposition VIII.2. Let $R > 0$ such that for any $\lambda \in [E_0 - R, E_0 + R]$, we have (VIII.3). Let $c_0 := \min\left(\frac{1}{4}, \frac{R}{2\varepsilon_0}\right)$. Define the intervals $I_0 := [E_0 - c_0\varepsilon_0, E_0 + c_0\varepsilon_0]$. Given the definition of ε_0 and c_0 , we have $I_0 \subset (\min V, \infty)$. Thus, $|p^{-1}(I_0)| > 0$. We begin to take $h_0 \in (0, c_0\varepsilon_0/2)$ (of course, we will lower it afterwards). By Lemma VIII.3 (up to a sequence $\{h_n\}_{n \in \mathbb{N}} \subset \mathbb{R}_+^*$ with $h_n \rightarrow 0$ when $n \rightarrow \infty$) there exists $h_0 > 0$, $\{E_h\}_{h \in (0, h_0]} \subset I_0$ and $C' > 0$ such that for any $h \in (0, h_0]$

$$\|\rho_{\Pi_h}\|_{L^1(\mathbb{R}^d)} \geq C' h^{-(d-1)}.$$

Let $\varepsilon > 0$ such that $\varepsilon < \text{dist}(E_0 - c_0\varepsilon_0, \min V)/2 = (1 - c_0)\varepsilon_0/2$. By the L^∞ estimates (see for instance Theorem VII.2), there exists $C > 0$ such that for any $h \in (0, h_0]$

$$\begin{aligned} \|\rho_{\Pi_h}\|_{L^1(\{|V - E_h| \leq \varepsilon\})} &\leq |\{|V - E_h| \leq \varepsilon\}| \|\rho_{\Pi_h}\|_{L^\infty(\mathbb{R}^d)} \\ &\leq C h^{-(d-1)} |\{|V - E_h| \leq \varepsilon\}|. \end{aligned}$$

By (VIII.3), let us fix $\varepsilon \in (0, (1 - c_0)\varepsilon_0/2)$ such that $C |\{|V - E_h| \leq \varepsilon\}| \leq C'/2$. Besides, by (VII.7), there exists $C_\varepsilon > 0$ such that for any $h \in (0, h_0]$

$$\|\rho_{\Pi_h}\|_{L^1(\{V \geq E_h + \varepsilon\})} \leq C_\varepsilon h^{-(d-2)}.$$

Finally, by the triangle inequality and the previous estimates there exists $h_0 > 0$ such that for any $h \in (0, h_0]$

$$\begin{aligned} \|\rho_{\Pi_h}\|_{L^1(\{V \leq E_h - \varepsilon\})} &= \|\rho_{\Pi_h}\|_{L^1(\mathbb{R}^d)} - \|\rho_{\Pi_h}\|_{L^1(\{|V - E_h| < \varepsilon\})} - \|\rho_{\Pi_h}\|_{L^1(\{V \geq E_h + \varepsilon\})} \\ &\geq \frac{1}{4} C' h^{-(d-1)}. \end{aligned} \tag{VIII.5}$$

For any $h \in (0, h_0]$, let us define $x_{0,h}$ as a maximizer of the function ρ_{Π_h} on the compact set $\{V \leq E_h - \varepsilon\}$. We thus have for any $h \in (0, h_0]$

$$\begin{aligned} \Pi_h(x_{0,h}, x_{0,h}) &= \rho_{\Pi_h}(x_{0,h}) \geq \frac{1}{|\{V \leq E_h - \varepsilon\}|} \|\rho_{\Pi_h}\|_{L^1(\{V \leq E_h - \varepsilon\})} \\ &\geq \frac{C'/4}{|\{V \leq E_0 + c_0\varepsilon_0\}|} h^{-(d-1)} = C'' h^{-(d-1)}. \end{aligned}$$

By the definition of u_h and the L^∞ estimate (see for instance Theorem IV.2) there exists $C > 0$ such that for any $h \in (0, h_0]$

$$\|u_h\|_{L^2(\mathbb{R}^d)} = \rho_{\Pi_h}(x_{0,h}) \leq \|\rho_{\Pi_h}\|_{L^\infty(\mathbb{R}^d)}^{1/2} \leq Ch^{-(d-1)/2}.$$

Let us now prove that there exists $C_1 > 0$ and $h_0 > 0$ such that for any $h \in (0, h_0]$

$$\sup_{x,y \in B(x_{0,h},h)} |\nabla_y \Pi_h(x,y)| \leq C_1 h^{-d}. \quad (\text{VIII.6})$$

This implies that for any $h \in (0, h_0]$ and for any $x \in B(x_{0,h}, \min(1, \frac{C''}{2C_1})h)$

$$\begin{aligned} |u_h(x)| &= |\Pi_h(x_{0,h}, x)| \\ &\geq \Pi_h(x_{0,h}, x_{0,h}) - |\Pi_h(x_{0,h}, x) - \Pi_h(x_{0,h}, x_{0,h})| \\ &\geq \Pi_h(x_{0,h}, x_{0,h}) - \|\nabla_y \Pi_h(x_{0,h}, \cdot)\|_{L^\infty(B(x_{0,h},h))} |x - x_{0,h}| \\ &\geq \frac{C''}{2} h^{-(d-1)}. \end{aligned}$$

That gives us (VIII.4). Let us prove now the estimate (VIII.6). Denote

$$\Pi_h^{(0)} := \mathbb{1}(-h^2 \Delta + V(x_{0,h}) \in I_{h,E_h}).$$

For all $x, y \in \mathbb{R}^d$, we have

$$\Pi_h^{(0)}(x,y) = \frac{1}{(2\pi h)^d} \int_{E_h - V(x_{0,h}) - h \leq |\xi|^2 \leq E_h - V(x_{0,h}) + h} e^{\frac{i}{h} \langle \xi, x-y \rangle} d\xi.$$

Hence,

$$\begin{aligned} \left| \nabla_y \Pi_h^{(0)}(x,y) \right| &\leq |y| Ch^{-d-1} \left((E_h - V(x_{0,h}) + h)^{d/2} - (E_h - V(x_{0,h}) - h)_+^{d/2} \right) \\ &\leq |y| C_\varepsilon h^{-d}. \end{aligned}$$

We next prove that

$$\sup_{x,y \in B(x_{0,h},h)} \left| \nabla_y \Pi_h(x,y) - \nabla_y \Pi_h^{(0)}(x,y) \right| \leq Ch^{-d}$$

by showing that

$$\sup_{x,y \in B(x_{0,h},h)} \left| \nabla_y \Pi_{h, \leq E_h \pm h}(x,y) - \nabla_y \Pi_{h, \leq E_h \pm h}^{(0)}(x,y) \right| \leq Ch^{-d},$$

where for any $E \in \mathbb{R}$, $\Pi_{h, \leq E} := \mathbb{1}(P \leq E)$ and $\Pi_{h, \leq E}^{(0)} := \mathbb{1}(-h^2 \Delta + V(x_{0,h}) \leq E)$. Introducing

$$K_{h, \leq E}(x,y) := \Pi_{h, \leq E}(x_{0,h} + hx, x_{0,h} + hy), \quad K_{h, \leq E}^{(0)}(x,y) := \Pi_{h, \leq E}^{(0)}(x_{0,h} + hx, x_{0,h} + hy),$$

it is enough to show that

$$\sup_{x,y \in B(0,1)} \left| \nabla_y K_{h, \leq E_h \pm h}(x,y) - \nabla_y K_{h, \leq E_h \pm h}^{(0)}(x,y) \right| \leq Ch^{-(d-1)}.$$

This is given by [DL21, Rem. 1.2]. Notice that in this work, the parameter $x_{0,h}$ and E_h are independent of h . However, the result still holds when $x_{0,h}$ and E_h depend on h in such a way that they belong to a h -independent compact set and are such that $V(x_{0,h}) \leq E_h - \delta$ for some h -independent $\delta > 0$. \square

Gaussian beams

We now explain the optimality of the exponent $s_{\text{Sogge}}(q, d)$ for low values of q , in the case $V(x) = |x|^2$. The saturating functions already appeared in [KT05, Sec. 5.1], and we just provide the computational details here. This example only works for the harmonic oscillator since the argument relies on separation of variables. However, we expect that this exponent is also sharp for more general V , using for instance the argument of [Sog89]. Here, the saturation phenomenon happens for a family of functions concentrating around a curve, similarly to gaussian beams on spheres [Sog85].

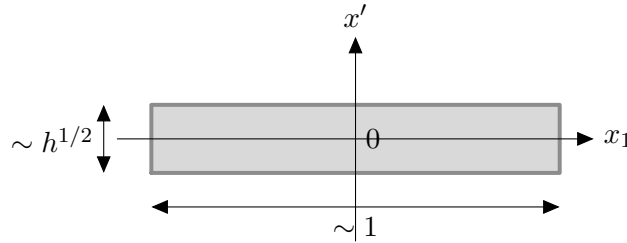
Proposition VIII.4. *Let $d \geq 2$ and $2 \leq q \leq \infty$. Let $p(x, \xi) = |\xi|^2 + |x|^2$. Let $E_{\text{exc}} > 0$. For any $h > 0$, define $P := p^w(x, hD)$ and $E_h := E_{\text{exc}} + (d-1)h$. For any $n \in \mathbb{N}$, let us denote $h_n := E_{\text{exc}}/(2n+1)$ and φ_n the normalized eigenfunction associated to the eigenvalue E_{exc} of the scalar harmonic oscillator $-h_n^2 \frac{d^2}{dy^2} + y^2$ on $L^2(\mathbb{R})$. For any $n \in \mathbb{N}$, define*

$$u_n(x) := (2\pi)^{-(d-1)/2} h_n^{-(d-1)/4} e^{-\frac{|x'|^2}{2h_n}} \varphi_n(x_1), \quad x = (x_1, x') \in \mathbb{R} \times \mathbb{R}^{d-1}.$$

Then, for all $n \in \mathbb{N}$, we have $\|u_n\|_{L^2(\mathbb{R}^d)} = 1$, $Pu_n = E_{h_n}u_n$, and there exists $\varepsilon > 0$ and $C > 0$ such that for n large enough

$$\|u_n\|_{L^q(\{x \in \mathbb{R}^d : |x|^2 - E_{h_n} < \varepsilon\})} \geq Ch_n^{-\frac{d-1}{2}(\frac{1}{2} - \frac{1}{q})}.$$

Remark 36. These eigenfunctions concentrate along the curve $\{x' = 0\}$ at scale \sqrt{h} in the orthogonal direction (c.f. Figure 1.15). Indeed, due to the well-known asymptotics of the Hermite functions, $\varphi_n(x_1)$ is essentially constant (up to oscillations which average out when taking the L^q norm) for x_1 in a neighborhood of 0.



Remark 37. This proves the optimality of the exponent $s_{\text{Sogge}}(q, d)$ for low regime $2 \leq q \leq 2(d+1)/(d-1)$ in the classically allowed region and also the optimality of the exponent $s_{\text{TP}}(q, d) = s_{\text{Sogge}}(q, d)$ for lower regime $2 \leq q \leq 2(d+3)/(d+1)$ around the turning points $\{V = E_{h_n}\}$ on Theorem VII.2 when $V(x) = |x|^2$, by taking $\gamma_{h_n} = |u_n\rangle \langle u_n|$.

Proof of Proposition VIII.4. Let $\varepsilon = E_{\text{exc}}/2$. First, defining for any $h > 0$

$$\varphi_{h,\text{ground}}(x') := (2\pi)^{-(d-1)/2} h^{-(d-1)/4} e^{-\frac{|x'|^2}{2h}},$$

there exists $C_d > 0$ such that for any $h > 0$

$$\|\varphi_{h,\text{ground}}\|_{L^q(\{x' \in \mathbb{R}^{d-1} : |x'| \leq h^{1/2}\})} = C_d h^{-\frac{d-1}{4} + \frac{d-1}{2q}}.$$

On the other hand, by Liouville-Green asymptotics (see for instance Chapter 6 in [Olv97]), we have for any $x_1 \in [-\sqrt{E_{\text{exc}}}/2, \sqrt{E_{\text{exc}}}/2]$

$$\varphi_n(x_1) = \frac{C_{h_n}}{(E_{\text{exc}} - x_1^2)^{1/4}} \begin{cases} \cos(h_n^{-1} \int_0^{x_1} \sqrt{E_{\text{exc}} - t^2} dt) (1 + e_{h_n}(x_1)) & \text{if } n \text{ is even,} \\ \sin(h_n^{-1} \int_0^{x_1} \sqrt{E_{\text{exc}} - t^2} dt) (1 + e_{h_n}(x_1)) & \text{if } n \text{ is odd,} \end{cases}$$

where $C_{h_n} \in \mathbb{R}$ be a normalization constant such that $\lim_{n \rightarrow \infty} C_{h_n} > 0$ and

$$\|e_{h_n}\|_{L^\infty([- \sqrt{E_{\text{exc}}}/2, \sqrt{E_{\text{exc}}}/2])} = \mathcal{O}(h_n).$$

Let us now show that $\liminf_{n \rightarrow \infty} \|\varphi_n\|_{L^q([0, \delta])} > 0$ for $\delta = \sqrt{E_{\text{exc}}}/2$, which then proves the result since for n large enough

$$\begin{aligned} \|u_n\|_{L^q(x \in \mathbb{R}^d : V(x) - E_{h_n} \leq \varepsilon)} &\geq \|u_n\|_{L^q([0, \delta] \times B_{\mathbb{R}^{d-1}}(0, \sqrt{h_n}))} \\ &\geq \|\varphi_n\|_{L^q([0, \delta])} \|\varphi_{h_n, \text{ground}}\|_{L^q(B_{\mathbb{R}^{d-1}}(0, \sqrt{h_n}))} \\ &\gtrsim h_n^{-\frac{d-1}{4} + \frac{d-1}{2q}}. \end{aligned}$$

Suppose for instance that n is even (the cas n odd is similar). For any $n \in \mathbb{N}$ and any $x_1 \in [0, \delta]$, define

$$f_{h_n}(x_1) := (E_{\text{exc}} - x_1^2)^{-1/4} \cos\left(h_n^{-1} \int_0^{x_1} \sqrt{E_{\text{exc}} - t^2} dt\right).$$

Given the estimate on the error term e_{h_n} , we have

$$\|\varphi_n - f_{h_n}\|_{L^q([0, \delta])} = \mathcal{O}(h_n).$$

Let us denote

$$S(x_1) := \int_0^{x_1} \sqrt{E_{\text{exc}} - t^2} dt.$$

Since its derivative S' is positive on $[0, \delta]$, we have

$$\begin{aligned} \|f_{h_n}\|_{L^q([0, \delta])}^q &= \int_0^\delta S'(x_1)^{-q/2} |\cos(h_n^{-1} S(x_1))|^q dx_1 \\ &\gtrsim \int_0^\delta |\cos(h_n^{-1} S(x_1))|^q S'(x_1) dx_1 \\ &= \int_0^{S(\delta)} |\cos(h_n^{-1} y)|^q dy = \int_0^{S(\delta)} (1 + \cos(2h_n^{-1} y))^{q/2} dy. \end{aligned}$$

Since $q/2 \geq 1$, the function $g = (1 + \cos(2\cdot))^{q/2}$ is π -periodic and \mathcal{C}^1 . Hence, its Fourier coefficients

$$c_k(g) := \frac{1}{\pi} \int_0^{h_n \pi} e^{-2ikt} g(t) dt$$

are summable over $k \in \mathbb{Z}$. As a consequence,

$$\int_0^{S(\delta)} g(h_n^{-1} y) dy = \sum_{k \in \mathbb{Z}} c_k(g) \int_0^{S(\delta)} e^{2iky/h_n} dy = S(\delta) c_0(g) + \mathcal{O}(h_n),$$

which finishes the proof. \square

VIII.2 Many-body optimality

We now turn to the optimality of the Schatten exponent α . We show that the exponent $\alpha = \alpha_{\text{Sogge}}$ is sharp in the estimates where it appears together with the exponent $s = s_{\text{Sogge}}$. The saturation scenario here is a family of operators γ such that ρ_γ is delocalized in the bulk region of the potential. We will see that it happens for the maximal family $\gamma = \Pi_h$, in the same spirit as in [FS17b, Rem. 11]. The optimality of the other Schatten exponents α_{gene} or α_{TP} (when they are not equal to α_{Sogge}) is a very challenging problem since $\gamma = \Pi_h$ does not saturate the inequalities where they appear.

Proposition VIII.5 (Many-body optimality of the Sogge exponent). *Let $d \geq 2$. Let $p(x, \xi) = |\xi|^2 + V(x)$ with $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$ satisfying Definition VII.1. Let $E_0 > \min V$ such that we have (VIII.3). Then, there exist $h_0 > 0$, $\{E_h\}_{h \in (0, h_0]}$ in a compact neighborhood of E_0 on $(\inf V, \infty)$, $\varepsilon > 0$ and $C > 0$ such that for any $h \in (0, h_0]$ and any $2 \leq q \leq \infty$ (along a sequence $h_n \rightarrow 0$ when $n \rightarrow \infty$)*

$$\|\rho_{\Pi_h}\|_{L^{q/2}(\{x \in \mathbb{R}^d : V(x) \leq E_h - \varepsilon\})} \geq Ch^{-(d-1)}, \quad (\text{VIII.7})$$

where Π_h denotes the spectral projector $\Pi_h := \mathbf{1}(P \in I_{h, E_h})$.

Remark 38. Due to the L^∞ estimates (VII.2) in the case $q = \infty$, we always have $\|\rho_h\|_{L^\infty(\mathbb{R}^d)} \leq Ch^{-(d-1)}$. Together with (VIII.7), this shows that all the $L^{q/2}$ norms of ρ_{Π_h} are of the order $h^{-(d-1)}$ in the bulk region $\{V < E_h - \varepsilon\}$, indicating that ρ_{Π_h} behaves like a (large) constant in this region.

Remark 39. This result also proves that the Schatten exponent $\alpha_{\text{Sogge}}(q, d)$ is optimal for instance in the estimate (VII.3). Indeed, for $\gamma = \Pi_h$, (VIII.7) shows that the left side of (VII.3) is of order $h^{-(d-1)}$, while the right side is order

$$h^{-2s_{\text{Sogge}}(q, d)} \|\Pi_h\|_{\mathfrak{S}^{\alpha_{\text{Sogge}}(q, d)}} \lesssim h^{-2s_{\text{Sogge}}(q, d)} h^{-(d-1)/\alpha_{\text{Sogge}}(q, d)} = h^{-(d-1)}.$$

Here, we used that $\text{rank}(\Pi_h) \leq Ch^{-(d-1)}$ which follows from the fact that

$$\text{rank}(\Pi_h) = \|\rho_{\Pi_h}\|_{L^1(\mathbb{R}^d)} = \|\rho_{\Pi_h}\|_{L^1(\{V \leq E_h + \varepsilon\})} + \|\rho_{\Pi_h}\|_{L^1(\{V > E_h + \varepsilon\})}$$

and the estimates (VII.2) in the case $q = \infty$ and (VII.7).

Proof of Proposition (VIII.5). Let $\varepsilon_0 := E_0 - \min V$. Here, we take $\{E_h\}_{h \in (0, h_0]} \subset [E_0 - \varepsilon_0/2, E_0 + \varepsilon_0/2]$ and $\varepsilon \in (0, \varepsilon_0/4)$ as in Proposition VIII.2. They are chosen to satisfy the lower bound (VIII.5). Thus, there exists $C' > 0$ such that for any $h \in (0, h_0]$ and any $2 \leq q \leq \infty$

$$\begin{aligned} \|\rho_{\Pi_h}\|_{L^{q/2}(\{V \leq E_h - \varepsilon\})} &\geq |\{V \leq E_h - \varepsilon\}|^{-1/(q/2)'} \|\rho_{\Pi_h}\|_{L^1(\{V \leq E_h - \varepsilon\})} \\ &\geq |\{V \leq E_0 + 3\varepsilon_0/4\}|^{-1/(q/2)'} \|\rho_{\Pi_h}\|_{L^1(\{V \leq E_h - \varepsilon\})} \\ &\geq C'h^{-(d-1)}. \end{aligned}$$

□

Chapter 2

Interacting particles : Weyl law

Abstract

In this chapter, we consider grand-canonical fermionic systems in a mean-field regime. We provide the grand-canonical version of Fournais-Lewin-Solovej's results [FLS18] for trapping potentials. In particular, we prove the convergence of the densities of the grand-canonical Hartree-Fock ground state to the Thomas-Fermi ground state at the semiclassical limit $\hbar \rightarrow 0$. As an application, it gives the first order term of the Weyl law in the case with interaction.

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I INTRODUCTION

We consider grand-canonical systems of fermionic particles. They are confined in an external trapping potential $V : \mathbb{R}^d \rightarrow \mathbb{R}$, i.e. $V(x) \rightarrow \infty$ as $|x| \rightarrow \infty$ and they are subject to a two body interaction $w : \mathbb{R}^d \rightarrow \mathbb{R}$. We look at the particles at a given energy $E \in \mathbb{R}$ and at the mean-field regime, which is a regime where a particle of the system sees the interaction with the others as an averaging of the interactions of all. We are particularly interested in the leading order term of

the ground state of the system. That is what did Fournais, Lewin, Solovej [FLS18] in a canonical setting with the constraints of the number of particles. In our case, we focus on the Hartree-Fock ground state, which is simpler.

Objects at play Let us start giving all the definitions of the objects at play in order to provide a more precise formulation of our problem.

	V	confining exterior potential on \mathbb{R}^d	Assumption 5
	$E \in \mathbb{R}$	chemical potential on \mathbb{R}^d	
	w	potential of interaction	
	$h > 0$	semiclassical parameter, reduced Plank constant	
	$\mathcal{E}_h^{\text{HF}}$	h -Hartree-Fock energy functional	see (I.1)
	$\mathcal{E}_h^{\text{rHF}}$	h -reduced Hartree-Fock energy functional	
	\mathcal{E}^{TF}	Thomas-Fermi energy functional	see (I.6)
	$\mathcal{E}^{\text{Vlas}}$	Vlasov energy functional	see (I.9)
Notation	e_h^{HF}	h -Hartree-Fock ground state energy	see (I.4)
	e_h^{rHF}	h -reduced Hartree-Fock ground state energy	
	e^{TF}	Thomas-Fermi ground state energy	see (I.8)
	e^{Vlas}	Vlasov ground state energy	see (I.11)
	\mathcal{X}	energy space of Hartree-Fock functional	see (I.2)
	\mathcal{K}	admissible states of Hartree-Fock energy	see (I.3)
	$\mathcal{K}^{\text{Vlas}}$	admissible states of Vlasov energy	see (I.10)
	\mathcal{X}^{TF}	energy space of Thomas-Fermi functional	see (I.7)
	$H_{\gamma,h}, H_\gamma$	h -semiclassical mean-field operator	see (I.5)

Associated definitions We focus essentially on the semiclassical limit $h \rightarrow 0$ of the h -Hartree-Fock energy functional denoted by

$$\mathcal{E}_{h,V-E,w}^{\text{HF}}(\gamma) := \text{Tr}((-h^2\Delta + V - E)\gamma) + \frac{h^d}{2} (D_w(\rho_\gamma, \rho_\gamma) - \text{Ex}_w(\gamma)), \quad (\text{I.1})$$

where D_w and Ex_w respectively denote the *direct term* and *exchange term* defined by

$$D_w(\rho_\gamma, \rho_{\tilde{\gamma}}) := \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \rho_\gamma(x) \rho_{\tilde{\gamma}}(y) w(x-y) dx dy, \quad \text{Ex}_w(\gamma) := \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} |\gamma(x,y)|^2 w(x-y) dx dy.$$

Here, $\text{Tr}((-h^2\Delta + V - E)\gamma)$ means for $V \geq 0$

$$\text{Tr}((-h^2\Delta + V - E)\gamma) := \text{Tr}(\sqrt{-h^2\Delta + V + 1}\gamma\sqrt{-h^2\Delta + V + 1}) - (1 + E) \text{Tr}(\gamma).$$

Notice that the mean-field regime appears in the coupling term h^d before the interaction part $\gamma \mapsto \frac{1}{2}D_w(\rho_\gamma, \rho_\gamma) - \text{Ex}_w(\gamma)$ of the Hartree-Fock energy. By abuse of notation, without any possible conflict, we sometimes denote $\mathcal{E}_h^{\text{HF}}$ instead of $\mathcal{E}_{h,V-E,w}^{\text{HF}}$. We show (in Section III.1) that $\mathcal{E}_h^{\text{HF}}$ is defined on the set

$$\mathcal{X} := \{\gamma \in \mathfrak{S}^1 : \left\| (-\Delta + V + 1)^{1/2} \gamma (-\Delta + V + 1)^{1/2} \right\|_{\mathfrak{S}^1} < +\infty\}, \quad (\text{I.2})$$

endowed with the norm

$$\|\gamma\|_{\mathcal{X}} := \left\| (-\Delta + V + 1)^{1/2} \gamma (-\Delta + V + 1)^{1/2} \right\|_{\mathfrak{S}^1}.$$

It turns out that we study the generalized Hartree-Fock problem, but to lighten the notations, we will just call and note it Hartree-Fock. Let us define its fermionic subset

$$\mathcal{K} := \{\gamma \in \mathcal{X} : 0 \leq \gamma \leq 1\}, \quad (\text{I.3})$$

where we look at the minimization problem for a fixed $h > 0$

$$\inf_{\gamma \in \mathcal{K}} \mathcal{E}_h^{\text{HF}}(\gamma) =: e_h^{\text{HF}}. \quad (\text{I.4})$$

We denote by e_h^{HF} this ground state energy (we explain in Sections III.2 and III.3 why it is well-posed for the considered potentials V, w). When they exist, minimizers of Hartree-Fock are strongly related to the *mean-field operator* (see Section III.4)

$$H_\gamma := (-h^2 \Delta + V - E) + h^d [(\rho_\gamma * w)(x) - X_w(\gamma)], \quad (\text{I.5})$$

defined on \mathcal{X} , with X_w which is the integral operator on $L^2(\mathbb{R}^d)$ defined by the kernel $X_w(\gamma)(x, y) := w(x - y)\gamma(x, y)$.

In the semiclassical limit $h \rightarrow 0$, the exchange term of $\mathcal{E}_h^{\text{HF}}$ becomes negligible (see for instance [Bac92] who proved in a grand-canonical setting. It is what we prove in Lemma IV.2). Therefore, it will therefore be easier to work with the *reduced Hartree-Fock* functional $\mathcal{E}_h^{\text{rHF}}$ which is the Hartree-Fock functional without its exchange term. We denote by e_h^{rHF} its associated ground state energy.

As in [FLS18], we will prove that the h -Hartree-Fock model is very connected to the Thomas-Fermi approximation when $h \rightarrow 0$. For any $d \geq 1$, defining

$$c_{\text{TF}} := 4\pi^2 \left(\frac{d}{|\mathbb{S}^{d-1}|} \right)^{2/d},$$

we set the *Thomas-Fermi energy functional* to be for any $\rho \in L^1(\mathbb{R}^d, \mathbb{R}_+)$

$$\begin{aligned} \mathcal{E}_{V-E,w}^{\text{TF}}(\rho) &= \frac{d}{d+2} c_{\text{TF}} \int_{\mathbb{R}^d} \rho(x)^{1+2/d} dx + \int_{\mathbb{R}^d} (V(x) - E)\rho(x) dx \\ &\quad + \frac{1}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} w(x-y)\rho(x)\rho(y) dx dy. \end{aligned} \quad (\text{I.6})$$

This energy is defined for good enough w on the set

$$\mathcal{X}_V^{\text{TF}} := \inf \left\{ \rho \in L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d), \rho \geq 0 : \int_{\mathbb{R}^d} V(x)\rho(x) dx < \infty \right\}. \quad (\text{I.7})$$

We denote by e^{TF} its ground state energy

$$e_{V-E,w}^{\text{TF}} := \inf_{\rho \in \mathcal{X}_V^{\text{TF}}} \mathcal{E}_{V-E,w}^{\text{TF}}(\rho). \quad (\text{I.8})$$

Let us introduce now the *Vlasov energy* functional

$$\begin{aligned} \mathcal{E}_{V-E,w}^{\text{Vlas}}(m) &:= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} |\xi|^2 m(x, \xi) dx d\xi + \int_{\mathbb{R}^d} (V(x) - E)\rho_m(x) dx \\ &\quad + \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \rho_m(x) w(x-y)\rho_m(y) dx dy, \end{aligned} \quad (\text{I.9})$$

defined on the phase-space densities set

$$\mathcal{K}_V^{\text{Vlas}} := \inf \left\{ m \in L^1(\mathbb{R}^d \times \mathbb{R}^d), 0 \leq m \leq 1, \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + V(x))m(x)d\xi dx < \infty \right\}, \quad (\text{I.10})$$

for

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

We define its ground state energy

$$e_{V-E, m}^{\text{Vlas}} := \inf_{m \in \mathcal{K}_V^{\text{Vlas}}} \mathcal{E}_{V-E, w}^{\text{Vlas}}(m). \quad (\text{I.11})$$

As we can see in Section II.2, Vlasov and Thomas-Fermi functionals are closely related. In particular, the Vlasov energy is used to study the Hartree-Fock ground state and thus relate it to the Thomas-Fermi model.

Assumptions on the potentials Without loss of generality, let us assume that V is non-negative and that satisfies a polynomial growth (in order to be in the setting of the Weyl's law).

Assumption 5 (Polynomial growth). Let $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$ such that there exists $k > 1$ and $R > 0$ such that

$$\forall \alpha \in \mathbb{N}^d, \exists C_\alpha > 0, \forall x \in \mathbb{R}^d \quad |\partial^\alpha V(x)| \leq C_\alpha \langle x \rangle^k$$

and such that there exists and $c > 0$

$$\forall x \in \mathbb{R}^d, |x| \geq R \quad V(x) \geq c|x|^k. \quad (\text{I.12})$$

We detail below definitions of repulsivity on the interaction potential.

Assumption 6 (Repulsive potential). Let w an even real-valued function on \mathbb{R}^d such that

$$\forall \rho \geq 0 \quad D_w(\rho, \rho) \geq 0.$$

Note that when w does not satisfy Assumption 6, the associated Thomas-Fermi ground state energy is not bounded by below for dimensions $d \geq 3$ where the contribution of the direct term is more important than the one of the kinetic one

$$e_{V-E, w}^{\text{TF}} = -\infty.$$

In this case, if we prove that the ground state behaves as the Thomas-Fermi model at the first order term, then the ground state of the system diverges. Therefore, Assumption 6 ensures that the Thomas-Fermi ground state energy is finite.

Assumption 7 (Alternative of repulsive potential for dimensions $d = 1, 2$). Let $p \in (\max(1, d/2), \infty)$. Let $w \in L^1 \cap L^p(\mathbb{R}^d)$ an even real-valued function such that

$$\|(\hat{w})_-\|_{L^\infty(\mathbb{R}^d)} < \frac{1}{2} \begin{cases} (2\sqrt{\pi})^{-1} & \text{if } d = 1, \\ (2\pi)^{-1} C_{\text{LT}}^{-2} & \text{if } d = 2. \end{cases} \quad (\text{I.13})$$

Remark 40. When the potential w is non-negative, the direct term $D_w(\rho_\gamma, \rho_\gamma)$ is always non-negative (c.f. Lemma III.5). Moreover, $D_w(\rho_\gamma, \rho_\gamma) \geq \text{Ex}_w(\gamma)$. Moreover V is trapping, then there exists $C > 0$ such that for any $\gamma \in \mathcal{K}$

$$\mathcal{E}_{h,V-E,w}^{\text{HF}}(\gamma) \geq \text{Tr}((-h^2\Delta + V - E)\gamma) \geq \text{Tr}((-h^2\Delta + V - E)_-) \geq -C.$$

Therefore, the energy $\inf_{\gamma \in \mathcal{K}} \mathcal{E}_{h,V-E,w}^{\text{HF}}(\gamma)$ is always bounded by below for any $h > 0$. We will show that it remains true under more general assumptions. It is that we prove in Lemma III.4 of Section III.

In the statement of our results, there appears also the following assumption¹.

Definition I.1. Let $p \in [1, \infty]$. A function $w \in L^p(\mathbb{R}^d) + L_\varepsilon^\infty(\mathbb{R}^d)$ if for any $\varepsilon > 0$, there exist $w_1 \in L^p(\mathbb{R}^d)$ and $w_2 \in L^\infty(\mathbb{R}^d)$ such that $\|w_2\|_{L^\infty(\mathbb{R}^d)} \leq \varepsilon$ and $w = w_1 + w_2$.

We will state in Section III, conditions on p that guarantee the well-definition of the Hartree-Fock energy functional and the well-posedness of the related minimization problem.

Motivation and the non-interacting case Provided that the energy functional $\mathcal{E}_{h,V,w}^{\text{HF}}$ is well-posed and that it is possible to minimize it, we would like to have information of the ground state $e_{h,V-E,w}^{\text{HF}}$ at the semiclassical limit $h \rightarrow 0$. Let us comment the non-interacting case $w = 0$ when V the external potential is confining, i.e. which satisfies Assumption 5. In this case, for any $h > 0$

$$\begin{aligned} e_{h,V-E,w=0}^{\text{HF}} &= \inf_{\gamma_h \in \mathcal{K}} \text{Tr}((-h^2\Delta + V - E)\gamma_h) = -\text{Tr}((-h^2\Delta + V - E)_-) \\ &\underset{h \rightarrow 0}{\sim} \frac{1}{(2\pi h)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + V(x) - E)_- dx d\xi \\ &= \frac{2|\mathbb{S}^{d-1}|}{d(d+2)(2\pi h)^d} \int_{\mathbb{R}^d} [(E - V(x))_-]^{1+2/d} dx \\ &= \frac{|B_{\mathbb{R}^d}(0,1)|}{(2\pi \hbar)^d} \int_{\mathbb{R}^d} [(E - V(x))_-]^{1+2/d} dx d\xi. \end{aligned}$$

Furthermore, $\mathcal{E}_{h,V,w=0}^{\text{HF}}$ is minimized by the spectral projector $\gamma_h = \mathbb{1}(-h^2\Delta + V \leq E)$. By the Weyl law (see for instance [Zwo12, Chap.6]), one has the leading order term convergence

$$\text{Tr}(\gamma_h) = \#\{\text{eigenvalues of } h^2\Delta + V \leq E\} \underset{h \rightarrow 0}{\sim} \frac{|B_{\mathbb{R}^d}(0,1)|}{(2\pi \hbar)^d} \int_{\mathbb{R}^d} [(E - V(x))_-]^{2/d} dx. \quad (\text{I.14})$$

Note that this asymptotic remains true if we consider even density matrices $\gamma_h \in \mathcal{K}$ that approaches minimizers of the Hartree-Fock functional, that we call its *almost minimizers*. That means that there exists $\varepsilon_h = o(h^{-d})$ such that

$$\mathcal{E}_{h,V-E,w}^{\text{HF}}(\gamma_h) = e_{h,V-E,w}^{\text{HF}} + \varepsilon_h. \quad (\text{I.15})$$

We are interested when $w \neq 0$ in the asymptotics as $h \rightarrow 0$ of the ground state energy $h^d e_{h,V-E,w}^{\text{HF}}$ and of a version of the Weyl law with interaction.

¹We will see that it is needed for the lower bound on the limit of the ground state energy in Theorem 1.

Main results on Hartree-Fock

In the first section, we state useful tools, with which we can carry out the proof of our results. Then, in Section III, we explain why the Hartree-Fock energy is well-defined, admit minimizers, and we discuss their form (Theorem III.10). Then in Section IV, we prove some asymptotics on the Hartree-Fock energy functional. Notably, the first order term of the h -Hartree-Fock ground state energy e_h^{HF} is the ground state energy of the Thomas-Fermi functional.

Theorem 1. *Let $d \geq 1$ and $p \in (\max(d/2), \infty)$. For any $E \in \mathbb{R}$, any $V : \mathbb{R}^d \rightarrow \mathbb{R}$ which satisfy respectively Assumptions 5 and $w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ which satisfy respectively Assumptions 5 and 6 (or $w \in L^1(\mathbb{R}^d) \cap L^p(\mathbb{R}^d)$ with Assumption 7 for $d = 1, 2$)*

$$\lim_{h \rightarrow 0} h^d e_{h,V-E,w}^{\text{HF}} = \lim_{h \rightarrow 0} h^d e_{h,V-E,w}^{\text{rHF}} = e_{V-E,w}^{\text{TF}}.$$

The result is the same as in [FLS18] in a simpler case where the magnetic field $A = 0$ and that consider the Hartree-Fock energy instead of the one of the many-body system. Moreover, they consider an interaction potential $w \in L^{1+d/2}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$, whereas in our case, the result can be extended to more general exponent p (the same as in Facts III.1 and III.2).

Note that the repulsivity conditions 6 and 7 just ensure that the fundamental Thomas-Fermi energy is well-defined and thus that the semiclassical finite is fine. However, if they are not verified, we have $e_{V-E,w}^{\text{TF}} = -\infty$, the limit is still true if we replace the conclusion by

$$\limsup_{h \rightarrow 0} h^d e_{h,V-E,w}^{\text{HF}} = \limsup_{h \rightarrow 0} h^d e_{h,V-E,w}^{\text{rHF}} = -\infty.$$

Furthermore, the proof of the convergence of the energies involves trial states and the so-called almost minimizers.

Theorem 2 (Weak semiclassical limit of the density). *Let $E \in \mathbb{R}$, $V : \mathbb{R}^d \rightarrow \mathbb{R}$ satisfying Assumption 5 and $w \in L^{1+d/2}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ satisfying Assumption 6 (or in dimensions $d = 1, 2$, $w \in L^1(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ with Assumption 7). Let $\{\gamma_h\}_h \subset \mathcal{K}$ be a sequence such that for any $h > 0$, γ_h is an approximate minimizer of the h -Hartree-Fock energy $\mathcal{E}_{h,V-E,w}^{\text{HF}}$, defined in (I.15). Then, there exist ρ_{TF} a minimizer of the Thomas-Fermi energy $\mathcal{E}_{V-E,w}^{\text{TF}}$ and a decreasing subsequence $\{h_n\}_n \subset \mathbb{R}_+^*$ such that $h_n \rightarrow 0$ as $n \rightarrow \infty$ and such that $h_n^d \rho_{\gamma_{h_n}} \rightharpoonup \rho_{\text{TF}}$ weakly in $L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d)$ as $n \rightarrow \infty$.*

Remark 41 (Assumptions on w). We restrict the exponent p that appears in Theorem 1

$$w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d) \quad (\text{or } w \in L^1(\mathbb{R}^d) \cap L^p(\mathbb{R}^d))$$

to $p = 1 + d/2$ so that the sequence of almost Hartree-Fock minimizers' densities $\rho_{\gamma_h} \in L^{1+2/d}(\mathbb{R}^d)$. Therefore, that ensures them to be trial states of the Thomas-Fermi functional and that the limit is well defined.

Remark 42 (About the convergence in Theorem 2). One could dream of the strong convergence $h^d \rho_{\gamma_h} \rightarrow \rho_{\text{TF}}$ in $L^q(\mathbb{R}^d)$ for any $1 \leq q < d/(d-2)_+$. Unfortunately, unlike for the minimizers of $\mathcal{E}_h^{\text{HF}}$ for any fixed $h > 0$, it is not trivial that the sequence $\{h^d \rho_{\gamma_h}\}_h$ is bounded on $H^1(\mathbb{R}^d)$ (indeed the Hoffmann-Ostenhof inequality is not semiclassical). Thus, it is not clear that $\{h^d \rho_{\gamma_h}\}_h$ is bounded into $L^q(\mathbb{R}^d)$.

From this weak convergence, we deduce an equivalent of the Weyl law (I.14) for the Hartree-Fock approximation.

Theorem 3 (Integrated Weyl law). *Let $E \in \mathbb{R}$, $V : \mathbb{R}^d \rightarrow \mathbb{R}$ which satisfies Assumption 5 and $w \in L^{1+d/2}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ satisfying Assumption 6 (or in dimensions $d = 1, 2$, $w \in L^1(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ satisfies Assumption 7). Let $\{\gamma_h\}_{h>0} \subset \mathcal{K}$ be a sequence of almost minimizers of the h -Hartree-Fock energy $\mathcal{E}_{h,V-E,w}^{\text{HF}}$. Then, we have the semiclassical asymptotic (up to a decreasing subsequence $\{h_n\}_n \subset \mathbb{R}_+^*$, $h_n \rightarrow 0$)*

$$h^d \text{Tr}(\gamma_h) \underset{h \rightarrow 0}{\sim} \int_{\mathbb{R}^d} \rho_{\text{TF}}(x) dx,$$

for ρ_{TF} be a minimizer of the Thomas-Fermi energy $\mathcal{E}_{V-E,w}^{\text{TF}}$ (the one in Theorem 2).

Remark 43 (Heuristic interpretation of Theorem 3). One could naively say that the $\text{Tr}(\gamma_h)$ is the eigenvalue counting function $N_{h,V-E,w}((-\infty, 0])$ of the h -mean-field operator H_{γ_h} associated to the minimizer γ_h . This would mean that γ_h satisfies the Euler-Lagrange equation. Actually, we do not know whether E is an eigenvalue of the operator H_{γ_h} or not, and by Theorem III.10 this equation is satisfied by the projectors $\mathbb{1}(\gamma_h \leq E)$ or $\mathbb{1}(\gamma_h < E)$. That is why the value $N_{h,V-E,w}((-\infty, 0])$ could be equal to $\text{Tr}(\gamma_h)$ minus the multiplicity of the eigenvalue E for H_{γ_h} and just not $\text{Tr}(\gamma_h)$.

II REVIEW OF KNOWN RESULTS

II.1 Useful estimates

Before stating functional bounds, let us state Peter-Paul inequalities, which are basic but useful for some error calculus.

Fact II.1 (Peter-Paul). *For $x, y \geq 0$ and $a, b \in [1, \infty]$ such that $\frac{1}{a} + \frac{1}{b} = 1$*

$$xy \leq \varepsilon \frac{x^a}{a} + \varepsilon^{-b/a} \frac{y^b}{b}.$$

In particular, for any $0 \leq \theta \leq 1$, any $\varepsilon > 0$ and any $x, y \geq 0$

$$x^\theta y^{1-\theta} \leq \theta \varepsilon x + \varepsilon^{-\theta/(1-\theta)} (1-\theta) y.$$

We recall also the relative compactness of $\mathcal{B}(L^2(\mathbb{R}^d))$.

Fact II.2. *Let a sequence of operators $\{\gamma_n\}_n$ on $L^2(\mathbb{R}^d)$ such that $0 \leq \gamma_n \leq 1$ for any $n \in \mathbb{N}$. Then, there exists $0 \leq \gamma \leq 1$ such that and $\gamma_n \rightarrow \gamma$ weakly in $\mathfrak{S}^\infty(L^2(\mathbb{R}^d)) = \mathcal{B}(L^2(\mathbb{R}^d))$, i.e. for any $A \in \mathfrak{S}^1(L^2(\mathbb{R}^d))$, $\text{Tr}(A\gamma_n) \rightarrow \text{Tr}(A\gamma)$.*

We recall now functional inequalities.

Proposition II.3 (Gagliardo-Nirenberg-Sobolev inequality). *When $d > 2$, there exists $C_{\text{GNS}} > 0$ such that for any $2 \leq q \leq 2d/(d-2)$ and any $u \in H^1(\mathbb{R}^d)$*

$$\|u\|_{L^q(\mathbb{R}^d)} \leq C_{\text{GNS}} \|\nabla u\|_{L^2(\mathbb{R}^d)}^{d(1/2-1/q)} \|u\|_{L^2(\mathbb{R}^d)}^{1-d(1/2-1/q)}.$$

We recall also the Lieb-Thirring kinetic energy inequality, which is an alternative to the Gagliardo-Nirenberg-Sobolev inequality.

Proposition II.4 (Lieb-Thirring inequality). *There exists $C_{\text{LT}} > 0$ such that for any $\gamma \geq 0$ on $L^2(\mathbb{R}^d)$*

$$\|\rho_\gamma\|_{L^{1+2/d}(\mathbb{R}^d)} \leq C_{\text{LT}} \text{Tr}((-\Delta)\gamma)^{\frac{d}{d+2}} \|\gamma\|_{\mathfrak{S}^\infty}^{\frac{2}{d+2}}.$$

The following lemma gives a Sobolev estimate on the square root of the density matrices $\sqrt{\rho_\gamma}$ of the elements of \mathcal{X} , $\sqrt{\rho_\gamma} \in H^1(\mathbb{R}^d)$. It is usually called the Hoffmann-Ostenhof inequality [HOHO77].

Lemma II.5 (Hoffmann-Ostenhof inequality). *For any $\gamma \in \mathcal{X}$, we have the bound*

$$\langle \sqrt{\rho_\gamma}, (-\Delta)\sqrt{\rho_\gamma} \rangle_{L^2} \leq \text{Tr}((-\Delta)\gamma).$$

Proof of Lemma II.5. From [LL01, Thm. 7.8],

$$\forall f, g \in H^1(\mathbb{R}^d) \quad \int_{\mathbb{R}^d} \left| \nabla \sqrt{|f(x)|^2 + |g(x)|^2} \right|^2 dx \leq \int_{\mathbb{R}^d} (|\nabla f(x)|^2 + |\nabla g(x)|^2) dx.$$

Writing $\gamma = \sum_j \lambda_j |\varphi_j\rangle \langle \varphi_j|$, we apply the inequality to the functions $\sqrt{\lambda_j} \varphi_j$ (by induction):

$$\begin{aligned} \langle \sqrt{\rho_\gamma}, (-\Delta)\sqrt{\rho_\gamma} \rangle_{L^2} &= \int_{\mathbb{R}^d} \left| \nabla \sqrt{\rho_\gamma(x)} \right|^2 dx = \int_{\mathbb{R}^d} \left| \nabla \sqrt{\sum_{j \in \mathbb{N}} \lambda_j |\varphi_j(x)|^2} \right|^2 dx \\ &\leq \int_{\mathbb{R}^d} \sum_{j \in \mathbb{N}} \lambda_j |\nabla \varphi_j(x)|^2 dx = \sum_{j \in \mathbb{N}} \lambda_j \|\varphi_j\|_{L^2(\mathbb{R}^d)}^2 = \sum_{j \in \mathbb{N}} \lambda_j \langle \varphi_j, (-\Delta)\varphi_j \rangle_{L^2} \\ &= \text{Tr}((-\Delta)\gamma). \end{aligned}$$

□

A L^p -bound of the density can be deduced from the Hoffmann-Ostenhof inequality.

Proposition II.6. *Let $\gamma \in \mathcal{K}$ and let $q \geq 1$ such that*

- $1 \leq q \leq d/(d-2)_+$ for $d = 1$ and $d \geq 3$,
- $1 \leq q < \infty$ for $d = 2$,

and such that $\rho_\gamma \in L^q(\mathbb{R}^d)$. Then, there exists $C > 0$ such that for any $\gamma \geq 0$

$$\|\rho_\gamma\|_{L^q(\mathbb{R}^d)} \leq C [\text{Tr}((-\Delta)\gamma) + \text{Tr}(\gamma)].$$

Proof of Proposition (II.6). Let $\gamma \in \mathcal{X}$. By the Hoffmann-Ostenhof (Lemma II.5), $\sqrt{\rho_\gamma} \in H^1(\mathbb{R}^d)$. By Sobolev's embedding, $\sqrt{\rho_\gamma} \in L^{2q}(\mathbb{R}^d)$ for any $1 \leq q \leq d/(d-2)_+$ for $d = 1$ and $d \geq 3$, and $1 \leq q < \infty$ for $d = 2$:

$$\begin{aligned} \|\rho_\gamma\|_{L^q(\mathbb{R}^d)} &= \|\sqrt{\rho_\gamma}\|_{L^{2q}(\mathbb{R}^d)}^2 \leq C \|\sqrt{\rho_\gamma}\|_{H^1(\mathbb{R}^d)}^2 = C \left(\|\nabla \sqrt{\rho_\gamma}\|_{L^2(\mathbb{R}^d)}^2 + \|\sqrt{\rho_\gamma}\|_{L^2(\mathbb{R}^d)}^2 \right) \\ &\leq C' [\text{Tr}((-\Delta)\gamma) + \text{Tr}(\gamma)]. \end{aligned}$$

□

Lemma II.7 (Kato-Seiler-Simon, [Sim05, Thm. 4.1]). *Let $\alpha \geq 2$. Then, for all functions $f, g \in L^\alpha(\mathbb{R}^d)$, the operator $f(x)g(-i\nabla)$ is in $\mathfrak{S}^\alpha(L^2(\mathbb{R}^d))$ and*

$$\|f(x)g(-i\nabla)\|_{\mathfrak{S}^\alpha(L^2(\mathbb{R}^d))} \leq (2\pi)^{-d/\alpha} \|f\|_{L^\alpha(\mathbb{R}^d)} \|g\|_{L^\alpha(\mathbb{R}^d)}.$$

Lemma II.8 (Araki-Lieb-Thirring, [Ara90, Thm. 1], [LT76, Thm. 9]). *For any operators $A, B \geq 0$ and scalars $q \geq 0$, $r \in [0, 1]$*

$$\text{Tr}((A^r B^r A^r)^q) \leq \text{Tr}((ABA)^{rq}).$$

We now state L^q -estimates of density in the scalar case. The proof is the same as for [LS15, Lem. 9] and relies on the Kato-Seiler-Simon and the Araki-Lieb-Thirring inequalities.

Lemma II.9. *For any self-adjoint operator γ on $L^2(\mathbb{R})$ such that $0 \leq \gamma \leq 1$ and any $1 \leq q \leq \infty$*

$$\|\rho_\gamma\|_{L^q(\mathbb{R})} \leq 2^{-1/q'} \left[\text{Tr} \left(\left(\sqrt{1-\Delta} \gamma \sqrt{1-\Delta} \right)^{q/q'} \right) \right]^{1/q}.$$

Proof of Lemma II.9. By duality, we have to prove the bound for any real-valued $W \in L^{q'}(\mathbb{R})$

$$\text{Tr}(W\gamma) \leq (2\pi^2)^{-1} \|W\|_{L^{q'}(\mathbb{R})} \left\| \sqrt{1-\Delta} \gamma \sqrt{1-\Delta} \right\|_{\mathfrak{S}^{q/q'}(L^2(\mathbb{R}))}^{1/q'}. \quad (\text{II.1})$$

Let $W \in L^{q'}(\mathbb{R})$. By the Hölder inequality on Schatten spaces and using that $\gamma \leq 1$

$$\begin{aligned} \text{Tr}(W\gamma) &\leq \text{Tr}(|W|\gamma) \\ &\leq \text{Tr}(|W|\gamma^{1/q'}) = \text{Tr} \left((1-\Delta)^{-\frac{1}{2q'}} |W| (1-\Delta)^{-\frac{1}{2q'}} (1-\Delta)^{\frac{1}{2q'}} \gamma^{\frac{1}{q'}} (1-\Delta)^{\frac{1}{2q'}} \right) \\ &\leq \left\| (1-\Delta)^{-\frac{1}{2q'}} |W| (1-\Delta)^{-\frac{1}{2q'}} \right\|_{\mathfrak{S}^{q'}(L^2(\mathbb{R}))} \left\| (1-\Delta)^{\frac{1}{2q'}} \gamma^{\frac{1}{q'}} (1-\Delta)^{\frac{1}{2q'}} \right\|_{\mathfrak{S}^q(L^2(\mathbb{R}))} \end{aligned}$$

On the one hand, by the Hölder inequality and the Kato-Seiler-Simon inequality (Lemma II.7) with the exponent $\alpha = 2q'$

$$\begin{aligned} \left\| (1-\Delta)^{-\frac{1}{2q'}} |W| (1-\Delta)^{-\frac{1}{2q'}} \right\|_{\mathfrak{S}^{q'}(L^2(\mathbb{R}))} &= \left\| (1-\Delta)^{-\frac{1}{2q'}} \sqrt{|W|} \right\|_{\mathfrak{S}^{2q'}(L^2(\mathbb{R}))}^2 \\ &\leq (2\pi)^{-1/q'} \|(1+x^2)^{-1}\|_{L^1(\mathbb{R})}^{1/q'} \|W\|_{L^{q'}(\mathbb{R})} \\ &= 2^{-1/q'} \|W\|_{L^{q'}(\mathbb{R})}. \end{aligned}$$

On the other hand, we apply the Araki-Lieb-Thirring (Lemma II.8) to $A = \sqrt{1-\Delta}$, $B = \gamma$, $r = 1/q'$

$$\begin{aligned} \left\| (1-\Delta)^{\frac{1}{2q'}} \gamma^{\frac{1}{q'}} (1-\Delta)^{\frac{1}{2q'}} \right\|_{\mathfrak{S}^q(L^2(\mathbb{R}))} &= \text{Tr} \left[\left((1-\Delta)^{\frac{1}{2q'}} \gamma^{\frac{1}{q'}} (1-\Delta)^{\frac{1}{2q'}} \right)^q \right]^{1/q} \\ &\leq \text{Tr} \left[\left(\sqrt{1-\Delta} \gamma \sqrt{1-\Delta} \right)^{q/q'} \right]^{1/q}. \end{aligned}$$

Finally, we obtain (II.1) by recovering all the elements together, that concludes the proof of Lemma II.9. \square

II.2 Links between the Vlasov and the Thomas-Fermi energy functionals

We give in this section some relations between Vlasov and Thomas-Fermi energy functionals. We will detail their proof for more completeness.

Claim II.10. *Let ρ be a trial function for the Thomas-Fermi energy $\mathcal{E}_{V,w}^{\text{TF}}$. Then, $m(x, \xi) := \mathbb{1}(|\xi|^2 \leq c_{\text{TF}} \rho(x)^{2/d})$ is a trial function for the Vlasov energy $\mathcal{E}_{V,w}^{\text{Vlas}}$ and we have the following equalities*

$$\rho = \rho_m$$

and

$$\frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |\xi|^2 m(x, \xi) dx d\xi = \frac{d}{d+2} c_{\text{TF}} \int_{\mathbb{R}^d} \rho(x)^{1+2/d} dx.$$

As a consequence,

$$\mathcal{E}_{V,w}^{\text{TF}}(\rho) = \mathcal{E}_{V,w}^{\text{Vlas}}(\mathbb{1}(|\xi|^2 \leq c_{\text{TF}}\rho(x)^{2/d})),$$

and we have the lower bound of the Thomas-Fermi energy

$$e_{V,w}^{\text{TF}} \geq e_{V,w}^{\text{Vlas}}.$$

Proof of Claim II.10. Recall that $c_{\text{TF}} := 4\pi^2 \left(\frac{d}{|\mathbb{S}^{d-1}|} \right)^{2/d}$. Let $\rho \geq 0$ a trial function for the Thomas-Fermi energy $\mathcal{E}_{V,w}^{\text{TF}}$. Let $m(x, \xi) := \mathbb{1}(|\xi|^2 \leq c_{\text{TF}}\rho(x)^{2/d})$. Let us show that

$$\frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} |\xi|^2 m(x, \xi) dx d\xi = \frac{d}{d+2} c_{\text{TF}} \int_{\mathbb{R}^d} \rho(x)^{1+2/d} dx.$$

We have

$$\begin{aligned} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |\xi|^2 m(x, \xi) dx d\xi &= \int_{\mathbb{R}^d} dx \int_{\mathbb{R}^d} |\xi|^2 \mathbb{1}(|\xi|^2 \leq c_{\text{TF}}\rho(x)^{2/d}) d\xi \\ &= \int_{\mathbb{R}^d} dx \int_0^{\sqrt{c_{\text{TF}}\rho(x)^{1/d}}} r^{d-1} dr \int_{\mathbb{S}^{d-1}} |r\omega|^2 d\omega \\ &= \int_{\mathbb{R}^d} dx \int_0^{\sqrt{c_{\text{TF}}\rho(x)^{1/d}}} r^{d+1} dr \int_{\mathbb{S}^{d-1}} |\omega|^2 d\omega \\ &= \int_{\mathbb{R}^d} \frac{(\sqrt{c_{\text{TF}}\rho(x)^{1/d}})^{d+2}}{d+2} |\mathbb{S}^{d-1}| dx \\ &= |\mathbb{S}^{d-1}| c_{\text{TF}}^{d/2} \frac{c_{\text{TF}}}{d+2} \int_{\mathbb{R}^d} \rho(x)^{1+2/d} dx \\ &= (2\pi)^d \frac{d}{d+2} c_{\text{TF}} \int_{\mathbb{R}^d} \rho(x)^{1+2/d} dx. \end{aligned}$$

As well, by an equivalent calculation

$$\rho_m(x) = \rho(x).$$

Indeed

$$\begin{aligned} \int_{\mathbb{R}^d} m(x, \xi) d\xi &= \int_{\mathbb{R}^d} \mathbb{1}(|\xi|^2 \leq c_{\text{TF}}\rho(x)^{2/d}) d\xi \\ &= \int_0^{\sqrt{c_{\text{TF}}\rho(x)^{1/d}}} r^{d-1} dr \int_{\mathbb{S}^{d-1}} d\omega = |\mathbb{S}^{d-1}| \int_0^{\sqrt{c_{\text{TF}}\rho(x)^{1/d}}} r^{d-1} dr \\ &= |\mathbb{S}^{d-1}| \frac{(\sqrt{c_{\text{TF}}\rho(x)^{1/d}})^d}{d} = \frac{|\mathbb{S}^{d-1}| c_{\text{TF}}^{d/2}}{d} \rho(x) \\ &= (2\pi)^d \rho(x). \end{aligned}$$

We deduce that

$$\int_{\mathbb{R}^d} V(x)\rho(x) dx = \int_{\mathbb{R}^d} V(x)\rho_m(x) dx, \quad D_w(\rho, \rho) = D_w(\rho_m, \rho_m).$$

Therefore, $\mathcal{E}_{V,w}^{\text{Vlas}}(m) = \mathcal{E}_{V,w}^{\text{TF}}(\rho)$. □

The following lemma shows that the Vlasov and Thomas-Fermi ground state energies are actually equal.

Lemma II.11. *Let m an admissible state for the Vlasov energy functional $\mathcal{E}_{V,w}^{\text{Vlas}}$. Then $\rho := \rho_m$ is an admissible state for the Thomas-Fermi energy functional $\mathcal{E}_{V,w}^{\text{TF}}$. Moreover, setting*

$$\tilde{m}(x, \xi) := \mathbf{1} \left((x, \xi) : |\xi|^2 \leq c_{\text{TF}} \rho(x)^{2/d} \right),$$

we have

$$\mathcal{E}_{V,w}^{\text{Vlas}}(m) \geq \mathcal{E}_{V,w}^{\text{Vlas}}(\tilde{m}) = \mathcal{E}_{V,w}^{\text{TF}}(\rho),$$

and the equality holds if and only if $m = \tilde{m}$. In particular, the ground state energies

$$e_{V,w}^{\text{Vlas}} = e_{V,w}^{\text{TF}},$$

and if m is a minimizer of $\mathcal{E}_{V,w}^{\text{Vlas}}$, then $m = \tilde{m}$ and ρ_m is a minimizer of $\mathcal{E}_{V,w}^{\text{TF}}$.

Proof of Lemma II.11. First, notice that $\rho_m = \rho_{\tilde{m}} = \rho$. We deduce that ρ is a trial function of $\mathcal{E}_{V,w}^{\text{TF}}$. Let us write

$$\mathcal{E}_{V,w}^{\text{Vlas}}(m) = \mathcal{E}_{V,w}^{\text{Vlas}}(\tilde{m}) + r(m, \rho),$$

with

$$r(m, \rho) = \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |\xi|^2 (m(x, \xi) - \tilde{m}(x, \xi)) dx d\xi.$$

Let us prove that $r(m, \rho) \geq 0$. To do it, we write

$$\begin{aligned} \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 - c_{\text{TF}} \rho(x)^{2/d}) m(x, \xi) dx d\xi &= \iint_{\{|\xi|^2 \leq c_{\text{TF}} \rho(x)^{2/d}\}} (|\xi|^2 - c_{\text{TF}} \rho(x)^{2/d}) dx d\xi \\ &+ \iint_{\{|\xi|^2 \leq c_{\text{TF}} \rho(x)^{2/d}\}} (|\xi|^2 - c_{\text{TF}} \rho(x)^{2/d}) (m(x, \xi) - 1) dx d\xi \\ &+ \iint_{\{|\xi|^2 \geq c_{\text{TF}} \rho(x)^{2/d}\}} (|\xi|^2 - c_{\text{TF}} \rho(x)^{2/d}) m(x, \xi) dx d\xi, \end{aligned}$$

and the definition of \tilde{m}

$$\iint_{\{|\xi|^2 \leq c_{\text{TF}} \rho(x)^{2/d}\}} (|\xi|^2 - c_{\text{TF}} \rho(x)^{2/d}) dx d\xi = \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 - c_{\text{TF}} \rho(x)^{2/d}) \tilde{m}(x, \xi) dx d\xi.$$

We deduce that the error can be decomposed into

$$\begin{aligned} (2\pi)^d r(m, \rho) &= \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 - c_{\text{TF}} \rho(x)^{2/d}) m(x, \xi) dx d\xi \\ &- \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 - c_{\text{TF}} \rho(x)^{2/d}) \tilde{m}(x, \xi) dx d\xi \\ &+ \iint_{\mathbb{R}^d \times \mathbb{R}^d} c_{\text{TF}} \rho(x)^{2/d} (m(x, \xi) - \tilde{m}(x, \xi)) dx d\xi \\ &= \iint_{|\xi|^2 \leq c_{\text{TF}} \rho(x)^{2/d}} (|\xi|^2 - c_{\text{TF}} \rho(x)^{2/d}) (m(x, \xi) - 1) dx d\xi \\ &+ \iint_{|\xi|^2 \geq c_{\text{TF}} \rho(x)^{2/d}} (|\xi|^2 - c_{\text{TF}} \rho(x)^{2/d}) m(x, \xi) dx d\xi. \end{aligned}$$

We have used the fact that m and \tilde{m} satisfy the relation $\rho_m = \rho_{\tilde{m}}$, which ensures that the last term in the first equality

$$\iint_{\mathbb{R}^d \times \mathbb{R}^d} c_{\text{TF}} \rho(x)^{2/d} (m(x, \xi) - \tilde{m}(x, \xi)) dx d\xi = (2\pi)^d \int_{\mathbb{R}^d} c_{\text{TF}} \rho(x)^{2/d} (\rho_m(x) - \rho_{\tilde{m}}(x)) dx = 0.$$

Hence, $r(m, \rho)$ non-negative because it is a sum of two non-negative integrals. As a consequence,

$$\mathcal{E}_{V,w}^{\text{Vlas}}(m) \geq \mathcal{E}_{V,w}^{\text{Vlas}}(\tilde{m}).$$

Assume now that $m \in \mathcal{K}_V^{\text{Vlas}}$ be a minimizer of $\mathcal{E}_{V,w}^{\text{Vlas}}$. Then, by the previous inequality $m = \tilde{m}$. Let us prove that ρ is a minimizer of the Thomas-Fermi energy. Since m is a minimizer of $\mathcal{E}_{V,w}^{\text{Vlas}}$, then $r(m, \rho) \leq 0$. Thus, this quantity must be equal to 0. In particular $m = \tilde{m} = 1$ in $\{(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d : |\xi|^2 \leq c_{\text{TF}} \rho(x)^{2/d}\} = \text{supp}(\tilde{m})$ and $m = 0$ in $\{(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d : |\xi|^2 \geq c_{\text{TF}} \rho(x)^{2/d}\}$. Besides, the set $\{(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d : |\xi|^2 - c_{\text{TF}} \rho(x)^{2/d} = 0\}$ is negligible with respect to the Lebesgue measure of $\mathbb{R}^d \times \mathbb{R}^d$.² Therefore, we obtain the desired equality $m = \tilde{m}$. By Claim II.10

$$\mathcal{E}_{V,w}^{\text{TF}}(\rho) = \mathcal{E}_{V,w}^{\text{Vlas}}(\tilde{m}) = \mathcal{E}_{V,w}^{\text{Vlas}}(m) = e_{V,w}^{\text{Vlas}} \leq e_{V,w}^{\text{TF}},$$

we deduce that ρ is a minimizer of the Thomas-Fermi functional $\mathcal{E}_{V,w}^{\text{TF}}$. That proves Lemma II.11. \square

As a consequence of Claim II.10 and Lemma II.11, the Thomas-Fermi and Vlasov functional minimization problems are equivalent.

Corollary II.12. *The Thomas-Fermi and Vlasov ground state energies coincide*

$$e_{V,w}^{\text{TF}} = e_{V,w}^{\text{Vlas}}.$$

II.3 Semiclassical tools

Let us introduce in this section definitions of coherent states, Husimi measures and some properties which will be useful for proving the wanted asymptotics on ground state energies and densities. Indeed, the main idea is to look instead at the limit of the sequences of Husimi measures associated with the sequences of minimizers or approximate minimizers of the h -Hartree-Fock functional. We will see later that they are even minimizing sequences for the Vlasov energy.

Definition II.13. Let $f \in H^1(\mathbb{R}^d)$ be a real-valued even function such that $\|f\|_{L^2(\mathbb{R}^d)} = 1$. Denote by f^h , the normalized function

$$f^h(y) := h^{-d/4} f\left(\frac{y}{\sqrt{h}}\right).$$

For any $x, \xi \in \mathbb{R}^d$, denote by $f_{x,\xi}^h$ the *coherent state*

$$f_{x,\xi}^h(y) := h^{-d/4} f\left(\frac{x-y}{\sqrt{h}}\right) e^{-i\frac{\xi \cdot y}{h}}.$$

²For any fixed $x \in \mathbb{R}^d$, the quantity $\int_{\mathbb{R}^d} \mathbb{1}\left(\{(x, \xi) : |\xi|^2 - c_{\text{TF}} \rho(x)^{2/d} = 0\}\right) d\xi = \left|\{\xi \in \mathbb{R}^d : |\xi|^2 - c_{\text{TF}} \rho(x)^{2/d} = 0\}\right|$ corresponds to the \mathbb{R}^d -Lebesgue measure of the $d-1$ -sphere of radius $c_{\text{TF}} \rho(x)^{2/d}$, which is equal to 0. Thus,

$$\left|\{(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d : |\xi|^2 - c_{\text{TF}} \rho(x)^{2/d} = 0\}\right| = \int_{\mathbb{R}^d} \underbrace{\left(\int_{\mathbb{R}^d} \mathbb{1}\left(\{(x, \xi) : |\xi|^2 - c_{\text{TF}} \rho(x)^{2/d} = 0\}\right) d\xi\right)}_{=0} dx = 0.$$

Let us introduce the *Husimi transform* defined for any operator $0 \leq \gamma \leq 1$ on $L^2(\mathbb{R}^d)$

$$m_{h,\gamma,f}(x, \xi) := \left\langle f_{x,\xi}^h, \gamma f_{x,\xi}^h \right\rangle.$$

For any $m : \mathbb{R}^d \times \mathbb{R}^d \rightarrow [0, 1]$, let us denote by ρ_m the density

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

Before stating properties of the Husimi measure, let us start by providing facts of weak continuity of the application $m \mapsto \rho_m$ and a consequence.

Claim II.14. *Let $m_h : \mathbb{R}^d \times \mathbb{R}^d \rightarrow [0, 1]$ such that $\iint |\xi|^2 m_h(x, \xi) dx d\xi$ is uniformly bounded as $h \rightarrow 0$. Let us assume that there exists $m : \mathbb{R}^d \times \mathbb{R}^d \rightarrow [0, 1]$ such that $m_h \rightharpoonup m$ weakly-* in $L^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ as $h \rightarrow 0$. Then, the density $\rho_{m_h} \rightarrow \rho_m$ in $\mathcal{D}'(\mathbb{R}^d)$.*

Proof of Claim II.14. Let $\varphi \in \mathcal{C}_c^\infty(\mathbb{R}^d, \mathbb{R}_+)$. First, note that for any $r > 0$

$$\begin{aligned} \left| \int_{\mathbb{R}^d \times \mathbb{R}^d \setminus B_r} \varphi(x) m_h(x, \xi) dx d\xi \right| &= \left| \int_{\mathbb{R}^d \times \mathbb{R}^d \setminus B_r} |\xi|^{-2} \varphi(x) |\xi|^2 m_h(x, \xi) dx d\xi \right| \\ &\leq r^{-2} \|\varphi\|_{L^\infty(\mathbb{R}^d)} \| |\xi|^2 m_h \|_{L^1(\mathbb{R}^d \times \mathbb{R}^d)}. \end{aligned}$$

Let us fix now $\varepsilon > 0$. We set $r > 0$ independent of h , large enough to have for all $h > 0$ (that is possible since $\| |\xi|^2 m_h \|_{L^1(\mathbb{R}^d \times \mathbb{R}^d)} \lesssim 1$)

$$\left| \int_{\mathbb{R}^d \times \mathbb{R}^d \setminus B_r} \varphi(x) m_h(x, \xi) dx d\xi \right| \leq \varepsilon.$$

Since φ is compactly supported and since $m_h \rightharpoonup m$ weakly-* on $L^\infty(\mathbb{R}^d \times \mathbb{R}^d)$, there exists $h_0 > 0$ such that for any $h \in (0, h_0]$

$$\left| \int_{\mathbb{R}^d \times B_r} \varphi(x) (m_h(x, \xi) - m(x, \xi)) dx d\xi \right| \leq \varepsilon.$$

Then, the triangle inequality provides the desired limit

$$\begin{aligned} \lim_{h \rightarrow 0} \int_{\mathbb{R}^d} \rho_{m_h}(x) \varphi(x) dx &= \lim_{h \rightarrow 0} \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} m_h(x, \xi) \varphi(x) dx d\xi \\ &= \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} m(x, \xi) \varphi(x) dx d\xi = \int_{\mathbb{R}^d} \rho_m(x) \varphi(x) dx. \end{aligned}$$

□

Remark 44. Claim II.14 can be applied to any bounded sequence $\{m_h\}_{h>0}$ (up to a subsequence $\{h_n\}_n \subset \mathbb{R}_+^*$ that $h_n \rightarrow 0$ as $n \rightarrow \infty$) of $\mathcal{K}_V^{\text{Vlas}}$ such that $m_h \rightharpoonup m$ weakly-* on $L^\infty(\mathbb{R}^d \times \mathbb{R}^d)$.

We now state useful formulas between operators and their associated Husimi measure.

Claim II.15. *For any $u \in L^2(\mathbb{R}^d)$*

$$\left\langle f_{x,\xi}^h, u \right\rangle = (2\pi h)^{d/2} \mathcal{F}_h[f^h(\cdot - x)u](\xi). \tag{II.2}$$

Furthermore, for any $0 \leq \gamma_h \leq 1$ and $m_h := m_{\gamma_h, h, f}$

$$\rho_{m_h} = h^d \rho_{\gamma_h} * (|f^h|^2). \tag{II.3}$$

Details of (II.3). Indeed, writing $\gamma_h = \sum_{j \in \mathbb{N}} \lambda_j \left| \varphi_j^h \right\rangle \left\langle \varphi_j^h \right|$ where $\{\varphi_j^h\}_{j \in \mathbb{N}}$ is an orthonormal basis of $L^2(\mathbb{R}^d)$ and using (II.2), we have

$$\begin{aligned} m_h(x, \xi) &= \left\langle f_{x, \xi}^h, \gamma_h f_{x, \xi}^h \right\rangle = \left\langle f_{x, \xi}^h, \sum_{j \in \mathbb{N}} \lambda_j \left\langle \varphi_j^h, f_{x, \xi}^h \right\rangle \varphi_j^h \right\rangle \\ &= \sum_{j \in \mathbb{N}} \lambda_j \left\langle \varphi_j^h, f_{x, \xi}^h \right\rangle \left\langle f_{x, \xi}^h, \varphi_j^h \right\rangle = \sum_{j \in \mathbb{N}} \lambda_j \left\langle f_{x, \xi}^h, \varphi_j^h \right\rangle \overline{\left\langle f_{x, \xi}^h, \varphi_j^h \right\rangle} \\ &= \sum_{j \in \mathbb{N}} \lambda_j \left| \left\langle f_{x, \xi}^h, \varphi_j^h \right\rangle \right|^2 = (2\pi h)^d \sum_{j \in \mathbb{N}} \lambda_j \left| \mathcal{F}_h[f^h(\cdot - x)\varphi_j^h](\xi) \right|^2. \end{aligned}$$

Thus, by the Plancherel equality

$$\begin{aligned} \rho_{m_h}(x) &= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} m_h(x, \xi) d\xi = h^d \int_{\mathbb{R}^d} \sum_{j \in \mathbb{N}} \lambda_j \left| \mathcal{F}_h[f^h(\cdot - x)\varphi_j^h](\xi) \right|^2 d\xi \\ &= h^d \int_{\mathbb{R}^d} \sum_{j \in \mathbb{N}} \lambda_j \left| f^h(y - x)\varphi_j^h(y) \right|^2 dy = h^d \int_{\mathbb{R}^d} \left| f^h(y - x) \right|^2 \left(\sum_{j \in \mathbb{N}} \lambda_j \left| \varphi_j^h(y) \right|^2 \right) dy \\ &= h^d \int_{\mathbb{R}^d} \left| f^h(y - x) \right|^2 \rho_\gamma(y) dy = h^d \rho_{\gamma_h} * (|f^h|^2)(x). \end{aligned}$$

That gives us the desired equality. \square

The following claim gives some implication on the weak convergence of $\{\rho_{m_h}\}_h$ in the case where $\{h^d \rho_{\gamma_h}\}_h$ has a weak limit.

Claim II.16. *Let $1 < q \leq \infty$, a sequence $\{\gamma_h\}_h \subset \mathfrak{S}^1(L^2(\mathbb{R}^d))$ such that $0 \leq \gamma_h \leq 1$ for all $h > 0$ and a density $\rho : \mathbb{R}^d \rightarrow \mathbb{R}_+$ be such that $h^d \rho_{\gamma_h} \rightharpoonup \rho$*

- *weakly on $L^q(\mathbb{R}^d)$ if $q \in [1, \infty)$*
- *or weakly- $*$ on $L^\infty(\mathbb{R}^d)$ if $q = \infty$.*

Then,

- *if $q \in (1, \infty)$, the sequence $\rho_{m_h} \rightharpoonup \rho$ weakly on $L^q(\mathbb{R}^d)$,*
- *if $q = \infty$, the sequence $\rho_{m_h} \rightharpoonup \rho$ weakly- $*$ on $L^\infty(\mathbb{R}^d)$.*

Proof of Claim II.16. For any $\varphi \in L^{q'}(\mathbb{R}^d)$, since $\{|f^h|^2\}_h$ is an approximation of the identity, we have $\varphi * |f^h|^2 \rightarrow \varphi$ strongly in $L^{q'}(\mathbb{R}^d)$. Thus,

$$\begin{aligned} \int_{\mathbb{R}^d} (\rho_{m_h} - \rho)\varphi dx &= \int_{\mathbb{R}^d} (h^d \rho_{\gamma_h} * |f^h|^2 - \rho)\varphi dx \\ &= \int_{\mathbb{R}^d} h^d \rho_{\gamma_h} (\varphi * |f^h|^2 - \varphi) dx + \int_{\mathbb{R}^d} (h^d \rho_{\gamma_h} - \rho)\varphi dx \\ &\xrightarrow{h \rightarrow 0} 0. \end{aligned}$$

\square

Now let us give some assumptions of the sequence on the operator γ_h so that the associated Husimi transform m_h is an integrable measure on the phase-space $\mathbb{R}^d \times \mathbb{R}^d$ with the Pauli exclusion constraint $0 \leq m_h \leq 1$.

Claim II.17. Assume that $0 \leq \gamma_h \leq 1$ and $h^d \text{Tr}(\gamma_h) \lesssim 1$. Then, the associated sequence of Husimi transforms $\{m_h\}_h$ is bounded on $L^1(\mathbb{R}^d \times \mathbb{R}^d)$ and $0 \leq m_h \leq 1$ for all $h > 0$.

Proof of Claim II.17. The boundedness in $L^1(\mathbb{R}^d)$ comes from (II.3). Moreover, by the assumption $h^d \text{Tr}(\gamma_h) \lesssim 1$ and $\| |f^h|^2 \|_{L^1(\mathbb{R}^d)} = 1$,

$$\begin{aligned} \forall h > 0 \quad \|m_h\|_{L^1(\mathbb{R}^d \times \mathbb{R}^d)} &= (2\pi)^d \int_{\mathbb{R}^d} \rho_{m_h}(x) dx = (2\pi)^d \int_{\mathbb{R}^d} h^d \rho_{\gamma_h} * (|f^h|^2)(x) dx \\ &\leq (2\pi)^d h^d \text{Tr}(\gamma_h) \| |f^h|^2 \|_{L^1(\mathbb{R}^d)} \leq C. \end{aligned}$$

Moreover, m_h is non-negative and for almost every $(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d$

$$m_h(x, \xi) = \left\langle f_{x,\xi}^h, \gamma_h f_{x,\xi}^h \right\rangle \leq \|f_{x,\xi}^h\|_{L^2}^2 \|\gamma_h\|_{\mathfrak{S}^\infty} \leq 1.$$

□

Let us state and prove a crucial relation, which links the kinetic part of the h -Hartree-Fock energy $\mathcal{E}_{h,\tilde{V},w}^{\text{HF}}$ of γ_h to the kinetic part of the Vlasov energy $\mathcal{E}_{\tilde{V},w}^{\text{Vlas}}$ of the associated Husimi transform m_h .

Lemma II.18. For any $h > 0$, any $0 \leq \gamma_h \leq 1$, $m_h := m_{\gamma_h, h, f}$ and any $\tilde{V} \in \mathcal{C}_c^\infty(\mathbb{R}^d)$

$$\frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} \tilde{V}(x) m_h(x, \xi) dx d\xi = h^d \int_{\mathbb{R}^d} \rho_{\gamma_h}(x) (\tilde{V} * (|f^h|^2))(x) dx.$$

and

$$\frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |\xi|^2 m_h(x, \xi) dx d\xi = h^d \text{Tr}(-h^2 \Delta \gamma_h) + h^{d+1} \text{Tr}(\gamma_h) \|\nabla f\|_{L^2(\mathbb{R}^d)}^2. \quad (\text{II.4})$$

Proof of Lemma II.18.

- On the one hand, by (II.3),

$$\begin{aligned} \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} \tilde{V}(x) m_h(x, \xi) dx d\xi &= \int_{\mathbb{R}^d} \tilde{V}(x) \rho_{m_h}(x) dx \\ &= \int_{\mathbb{R}^d} \tilde{V}(x) (h^d \rho_{\gamma_h} * (|f^h|^2))(x) dx \\ &= h^d \int_{\mathbb{R}^d} \rho_{\gamma_h}(x) (\tilde{V} * (|f^h|^2))(x) dx. \end{aligned}$$

- On the other hand, let us show that (II.4). Writing $\gamma_h = \sum_{j \in \mathbb{N}} \lambda_j \left| \varphi_j^h \right\rangle \left\langle \varphi_j^h \right|$, using the Plancherel formula, integration by part, that $\{f^h\}_h$ is a normalized family on $L^2(\mathbb{R}^d)$ and the invariance of

the Lebesgue measure through translations

$$\begin{aligned}
& \frac{1}{(2\pi h)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |\xi|^2 m_h(x, \xi) dx d\xi \\
&= dx \sum_{j \in \mathbb{N}} \int_{\mathbb{R}^d} |\xi|^2 \left| \mathcal{F}_h[f^h(\cdot - x)\varphi_j^h](\xi) \right|^2 d\xi \\
&= \int_{\mathbb{R}^d} dx \sum_{j \in \mathbb{N}} \int_{\mathbb{R}^d} \left| \frac{h}{i} \nabla_y [f^h(\cdot - x)\varphi_j^h](y) \right|^2 dy \\
&= \int_{\mathbb{R}^d} dx \sum_{j \in \mathbb{N}} \int_{\mathbb{R}^d} \left| h f^h(\cdot - x) \nabla_y \varphi_j^h(y) + \varphi_j^h(y) \nabla_y f^h(y - x) \right|^2 dy \\
&= \int_{\mathbb{R}^d} dx \left(\int_{\mathbb{R}^d} \sum_{j \in \mathbb{N}} \left| h \nabla_y \varphi_j^h(y) \right|^2 \left| f^h(x - y) \right|^2 dy + \int_{\mathbb{R}^d} h \sum_{j \in \mathbb{N}} \left| \varphi_j^h(y) \right|^2 \left| \nabla f^h(x - y) \right|^2 dy \right. \\
&\quad \left. + 2h \int_{\mathbb{R}^d} (\varphi_j^h(y) \nabla_y \varphi_j^h(y)) \cdot (f^h(y - x) \nabla_y f^h(y - x)) dy \right) \\
&= \int_{\mathbb{R}^d} dy \left(\sum_{n \in \mathbb{N}} \left| h \nabla_y \varphi_j^h(y) \right|^2 \right) \underbrace{\int_{\mathbb{R}^d} \left| f^h(x - y) \right|^2 dx}_{=1} \\
&\quad + h \int_{\mathbb{R}^d} dy \left(\sum_{n \in \mathbb{N}} \left| \varphi_j^h(y) \right|^2 \right) \underbrace{\int_{\mathbb{R}^d} h \left| \nabla_y f^h(x - y) \right|^2 dx}_{= \int_{\mathbb{R}^d} |\nabla_y f(x - y)|^2 dx} \\
&\quad - \int_{\mathbb{R}^d} dy \sum_{n \in \mathbb{N}} \left(\left| \nabla_y \varphi_j^h(y) \right|^2 + h^2 \varphi_j^h(y) \Delta_y \varphi_j^h(y) \right) \underbrace{\int_{\mathbb{R}^d} \left| f^h(x - y) \right|^2 dx}_{=1} \\
&= h \int_{\mathbb{R}^d} dy \rho_{\gamma_h}(y) \|\nabla f(\cdot - y)\|_{L^2(\mathbb{R}^d)}^2 + \text{Tr}(-h^2 \Delta \gamma_h) \\
&= h \text{Tr}(\gamma_h) + \text{Tr}(-h^2 \Delta \gamma_h).
\end{aligned}$$

□

Furthermore, we have the relation on the direct term that links the densities $h^d \rho_{\gamma_h}$ and ρ_{m_h} .

Lemma II.19. *For any $h > 0$, $w \in L^\infty(\mathbb{R}^d)$, $\gamma_h \in \mathfrak{S}^1(L^2(\mathbb{R}^d))$ such that $0 \leq \gamma_h \leq 1$ and $m_h := m_{\gamma_h, h, f}$*

$$D_w(\rho_{\gamma_h}, \rho_{\gamma_h}) = h^{-2d} D_w(\rho_{m_h}, \rho_{m_h}) + D_{w - w * |f^h|^2 * |f^h|^2}(\rho_{\gamma_h}, \rho_{\gamma_h}).$$

Proof of Lemma II.19. Using (II.3) and Fubini's formula

$$\begin{aligned}
h^{-2d} D_w(\rho_{m_h}, \rho_{m_h}) &= h^{-2d} D_w(h^d \rho_{\gamma_h} * (|f^h|^2), h^d \rho_{\gamma_h} * (|f^h|^2)) \\
&= \iint_{\mathbb{R}^d \times \mathbb{R}^d} w(x - y) (\rho_{\gamma_h} * (|f^h|^2))(x) (\rho_{\gamma_h} * (|f^h|^2))(y) dx dy \\
&= \iint_{\mathbb{R}^d \times \mathbb{R}^d} (w * |f^h|^2 * |f^h|^2)(x - y) \rho_{\gamma_h}(x) \rho_{\gamma_h}(y) dx dy \\
&= D_{w * |f^h|^2 * |f^h|^2}(\rho_{\gamma_h}, \rho_{\gamma_h}).
\end{aligned}$$

We conclude by the linearity of $w \mapsto D_w(\rho_{\gamma_h}, \rho_{\gamma_h})$.

□

We state here a special case of the semiclassical Weyl law for compactly supported potentials (see for instance the proof of [Lew22, Thm. 5.51]).

Proposition II.20 (Semiclassical Weyl lay for negative eigenvalues in a bounded domain). *Let $d \geq 1$. Let $\Omega \subset \mathbb{R}^d$ be an open cube. Let V be a smooth real-valued function compactly supported on Ω and let $-\Delta_\Omega$ be the Dirichlet Laplace operator on Ω . Then,*

$$\mathrm{Tr}((-h^2\Delta_\Omega + V)_-) \underset{h \rightarrow 0}{\sim} \frac{1}{(2\pi h)^d} \iint_{\Omega \times \mathbb{R}^d} (|\xi|^2 + V(x))_- dx d\xi.$$

III BASIC PROPERTIES THE HARTREE-FOCK FUNCTIONAL

We state and prove in this section some basic properties on the Hartree-Fock functional: that it is well-defined in the good space, the existence of minimizers and the structure of the minimizers.

We study for a fixed h , the variational problem

$$\inf_{\gamma \in \mathcal{K}} \mathcal{E}_{h,V,w}^{\mathrm{HF}}(\gamma)$$

on the convex closed set \mathcal{K} .

To do so, we will follow the same ideas as in [LL10].

First, we prove that for any fixed $h > 0$, this energy $\mathcal{E}_h^{\mathrm{HF}}$ admits a minimizer on the variational set

$$\mathcal{K} := \{0 \leq \gamma \leq 1 : \mathrm{Tr}((-\Delta + V + 1)\gamma) < \infty\}.$$

We ask notably w to satisfy the condition below.

Assumption 8 (Hypothesis on the interaction potential). Let $p \in [1, \infty]$ such that

$$p \in \begin{cases} (1, \infty) & \text{if } d = 1, 2, \\ [\frac{d}{2}, \infty] & \text{if } d \geq 3. \end{cases}$$

w is an even real-valued function on \mathbb{R}^d such that $w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$.

III.1 Setting and well-posedness of the Hartree-Fock energy

First, let us verify that $\mathcal{E}_h^{\mathrm{HF}}$ is well-defined on the space \mathcal{X} . It is the case for the linear term $\gamma \mapsto \mathrm{Tr}((-h^2\Delta + V - E)\gamma)$. Now, let us show that the direct term $D_w(\rho_\gamma, \rho_\gamma)$ and the exchange term $\mathrm{Ex}_w(\gamma)$ are controlled by the \mathcal{X} -norm.

Fact III.1 (Bound on the direct term). *Let $d \geq 1$ and*

$$p \in \begin{cases} [1, \infty] & \text{for } d = 1, 3, 4, \\ \{1\} & \text{for } d = 2, \\ [\frac{d}{4}, \infty] & \text{for } d \geq 5. \end{cases} \quad (\text{III.1})$$

(i) *Let $w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$. Then, there exists $C > 0$ such that for any $0 \leq \gamma \leq 1$*

$$|D_w(\rho_\gamma, \rho_\gamma)| \leq C [\mathrm{Tr}((-\Delta)\gamma)^2 + \mathrm{Tr}(\gamma)^2]. \quad (\text{III.2})$$

(ii) Assume that $d \in \{1, 2\}$ and let $w \in L^p(\mathbb{R}^d)$. Then, for any $h > 0$ and any $\gamma \in \mathfrak{S}^1(L^1(\mathbb{R}^d))$ such that $0 \leq \gamma \leq 1$

$$-C_{\gamma,h}(d)\|(\hat{w})_-\|_{L^\infty(\mathbb{R}^d)} \leq h^d D_w(\rho_\gamma, \rho_\gamma) \leq C_{\gamma,h}(d)\|(\hat{w})_+\|_{L^\infty(\mathbb{R}^d)}, \quad (\text{III.3})$$

with

$$C_{\gamma,h}(d) = (2\pi)^{d/2} \begin{cases} 2 \operatorname{Tr}((1 - h^2 \Delta)\gamma) & \text{if } d = 1, \\ C_{\text{LT}}^2 \operatorname{Tr}((-h^2 \Delta)\gamma) & \text{if } d = 2. \end{cases}$$

Remark 45. We make the constants explicit for the bounds for dimensions $d = 1, 2$, since one can deduce from them conditions such that the Hartree-Fock energy is bounded by below in \mathcal{K} (see later Lemma III.4).

Remark 46. Notice that when $d = 1, 2$, one can also have a bound for any $p \in [1, \infty]$ (by interpolation of the L^1 -norm of ρ_γ and the Lieb-Thirring inequality). But we lose on the exponent of $\operatorname{Tr}(\gamma)$

$$\forall w \in L^p(\mathbb{R}^d) \quad |D_w(\rho_\gamma, \rho_\gamma)| \leq \|w\|_{L^p(\mathbb{R}^d)} C_{\text{LT}}^2 \left[\frac{d+2}{4p} \operatorname{Tr}((-\Delta)\gamma)^{2/3} + \left(1 - \frac{d+2}{4p}\right) \operatorname{Tr}(\gamma)^2 \right].$$

More roughly, one has (III.2) for any $p \leq \max(1, d/4)$.

Proof of Fact III.1. The idea is to combine the Young inequality and estimates on the L^q -norms of ρ_γ for $q \geq 1$ such that $1/p + 2/q = 2$

$$\forall w \in L^p(\mathbb{R}^d), \quad |D_w(\rho_\gamma, \rho_\gamma)| \leq \|w\|_{L^p(\mathbb{R}^d)} \|\rho_\gamma\|_{L^q(\mathbb{R}^d)}^2.$$

Notice that taking $p \in [1, \infty]$ forces $q \in [1, 2]$.

1) Let us write $w = w_1 + w_\infty$ with $w_1 \in L^p(\mathbb{R}^d)$ and $w_\infty \in L^\infty(\mathbb{R}^d)$. On the one hand,

$$|D_{w_\infty}(\rho_\gamma, \rho_\gamma)| \leq \|w_\infty\|_{L^\infty(\mathbb{R}^d)} \|\rho_\gamma\|_{L^1(\mathbb{R}^d)}^2 = \|w_\infty\|_{L^\infty(\mathbb{R}^d)} \operatorname{Tr}(\gamma)^2.$$

In the other hand, notice that $1 + 2/(d-2) \geq 2$ if and only if $d \leq 4$. Thus, for

$$\begin{cases} p \geq 1 & \text{if } d = 1, 3, 4, \\ p = 1 & \text{if } d = 2, \\ p \geq d/4 & \text{if } d \geq 5, \end{cases}$$

the consequence of the Hoffmann-Ostenhof inequality (Proposition II.6) implies

$$|D_{w_1}(\rho_\gamma, \rho_\gamma)| \leq 2C_{\text{HO}}^2 \|w_1\|_{L^p(\mathbb{R}^d)} [\operatorname{Tr}((-\Delta)\gamma)^2 + \operatorname{Tr}(\gamma)^2].$$

2) Assume that $d \in \{1, 2\}$ and $w \in L^p(\mathbb{R}^d)$. we write

$$\begin{aligned} D_w(\rho_\gamma, \rho_\gamma) &= (2\pi)^{d/2} \int_{\mathbb{R}^d} \hat{w}(k) |\hat{\rho}_\gamma(k)|^2 dk \\ &= (2\pi)^{d/2} \int_{\mathbb{R}^d} (\hat{w}(k))_+ |\hat{\rho}_\gamma(k)|^2 dk - (2\pi)^{d/2} \int_{\mathbb{R}^d} (\hat{w}(k))_- |\hat{\rho}_\gamma(k)|^2 dk. \end{aligned}$$

By the Hölder inequality and the Plancherel formula

$$\begin{aligned} \int_{\mathbb{R}^d} (\hat{w}(k))_\pm |\hat{\rho}_\gamma(k)|^2 &\leq (2\pi)^{d/2} \|(\hat{w})_\pm\|_{L^\infty(\mathbb{R}^2)} \|\hat{\rho}_\gamma\|_{L^2(\mathbb{R}^2)}^2 \\ &= (2\pi)^{d/2} \|(\hat{w})_\pm\|_{L^\infty(\mathbb{R}^2)} \|\rho_\gamma\|_{L^2(\mathbb{R}^2)}^2. \end{aligned}$$

We use Lemma II.9 for $q = 2^3$ and the Lieb-Thirring inequality (Proposition II.4) for $d = 2$

$$\|\rho_\gamma\|_{L^2(\mathbb{R}^d)} \leq \begin{cases} \sqrt{2} \operatorname{Tr}((1 - \Delta)\gamma)^{1/2} & \text{if } d = 1, \\ C_{\text{LT}} \operatorname{Tr}((-\Delta)\gamma)^{1/2} & \text{if } d = 2. \end{cases}$$

Now, let us make appear in the L^2 -bound of ρ_γ the semiclassical parameter h . For instance for any $0 \leq \gamma \leq 1$, let us denote

$$\gamma_h := U_h \gamma U_h^*,$$

where U_h is the unitary transformation on $L^2(\mathbb{R}^d)$ defined by $U_h f := h^{d/2} f(h \cdot)$. The integral kernel of γ_h is

$$\gamma_h(x, y) = h^d \gamma(hx, hy) \quad \text{a.e.}$$

and

$$\begin{aligned} \|\rho_{\gamma_h}\|_{L^2(\mathbb{R}^d)} &= h^{d/2} \|\rho_\gamma\|_{L^2(\mathbb{R}^d)}, & \operatorname{Tr}(\gamma_h) &= \operatorname{Tr}(\gamma), \\ \operatorname{Tr}((-\Delta)\gamma_h) &= \operatorname{Tr}(\sqrt{-\Delta}\gamma_h\sqrt{-\Delta}) = \operatorname{Tr}(h^2\sqrt{-\Delta}\gamma\sqrt{-\Delta}) = \operatorname{Tr}((-h^2\Delta)\gamma). \end{aligned}$$

Then, by writing the L^2 -bound of γ_h in function of γ

$$\|\rho_\gamma\|_{L^2(\mathbb{R}^d)} \leq h^{-d/2} \begin{cases} \sqrt{2} \operatorname{Tr}((1 - h^2\Delta)\gamma)^{1/2} & \text{if } d = 1, \\ C_{\text{LT}} \operatorname{Tr}((-h^2\Delta)\gamma)^{1/2} & \text{if } d = 2. \end{cases}$$

Therefore, we deduce the bound (III.3). \square

Fact III.2 (Bound on the exchange term). *Let $d \geq 1$ and*

$$p \in \begin{cases} [1, +\infty] & \text{if } d = 1, \\ (1, +\infty] & \text{if } d = 2, \\ [\frac{d}{2}, +\infty] & \text{if } d \geq 3. \end{cases} \quad (\text{III.4})$$

For any $w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$, there exists $C > 0$ such that for any $0 \leq \gamma \leq 1$ and any $\varepsilon > 0$

$$|\operatorname{Ex}_w(\gamma)| \leq C \left[\varepsilon \operatorname{Tr}((-\Delta)\gamma) + (1 + \varepsilon^{-\frac{d}{2p-d}}) \operatorname{Tr}(\gamma) \right]. \quad (\text{III.5})$$

As a consequence, assuming $p > 1$ when $d = 1$, there exists $\varepsilon_h, \tilde{\varepsilon}_h > 0$ such that $\varepsilon_h, \tilde{\varepsilon}_h = o_h(1)$, such that for any $\gamma \in \mathcal{X}$

$$h^d |\operatorname{Ex}_w(\gamma)| \leq C \left[\varepsilon_h \operatorname{Tr}((-h^2\Delta)\gamma) + \tilde{\varepsilon}_h \operatorname{Tr}(\gamma) \right]. \quad (\text{III.6})$$

The second bound states that the kinetic term of the Hartree-Fock energy can absorb the exchange term.

Remark 47. The assumption on p here imply that

$$2 \leq 2p' \begin{cases} \leq \infty & \text{if } d = 1, \\ < \infty & \text{if } d = 2, \\ \leq \frac{2d}{d-2} & \text{if } d \geq 3, \end{cases}$$

this is very useful to use the Sobolev embedding $H^1(\mathbb{R}^d) \hookrightarrow L^{2p'}(\mathbb{R}^d)$. One can also prove that

$$|\operatorname{Ex}_w(\gamma)| \leq C \left[\operatorname{Tr}((-\Delta)\gamma)^{\frac{d}{p}} + \operatorname{Tr}(\gamma)^{2-\frac{d}{p}} + \operatorname{Tr}(\gamma) \right].$$

³The only way to control $\|\sqrt{1 - \Delta}\gamma\sqrt{1 - \Delta}\|_{\mathfrak{S}^{q/q'}}^{1/q'}$ by $\operatorname{Tr}((1 - \Delta)\gamma) = \operatorname{Tr}(\sqrt{1 - \Delta}\gamma\sqrt{1 - \Delta})^{1/2}$ is to choose q such that $q/q' \geq 1$ i.e. $q \geq 2$. Moreover, we have a second constraint that $q \in [1, 2]$. Therefore, we must take $q = 2$.

Before doing the proof, let us recall two useful bounds.

For any trace-class γ operator on $L^2(\mathbb{R}^d)$ such that $0 \leq \gamma \leq 1$ with an integral kernel $H^1(\mathbb{R}^d \times \mathbb{R}^d)$, we have

$$\|\nabla_x \gamma(x, y)\|_{L^2_{x,y}(\mathbb{R}^d \times \mathbb{R}^d)}, \|\nabla_y \gamma(x, y)\|_{L^2_{x,y}(\mathbb{R}^d \times \mathbb{R}^d)} \leq \text{Tr}((-\Delta)\gamma)^{1/2}. \quad (\text{III.7})$$

Details why (III.7) holds. Denote $\gamma = \sum_{j \in \mathbb{N}} \lambda_j |\varphi_j\rangle \langle \varphi_j|$. Note that $\lambda_j \subset [0, 1]$. Since $\{\varphi_j\}_j$ is an orthonormal family of $L^2(\mathbb{R}^d)$ and $0 \leq \lambda_j \leq \sqrt{\lambda_j}$

$$\begin{aligned} \|\nabla_x \gamma(x, y)\|_{L^2_{x,y}(\mathbb{R}^d \times \mathbb{R}^d)}^2 &= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \left| \sum_{j \in \mathbb{N}} \lambda_j \nabla_x \varphi_j(x) \overline{\varphi_j(y)} \right|^2 dx dy \\ &= \sum_{j \in \mathbb{N}} \int_{\mathbb{R}^d} \lambda_j^2 |\nabla_x \varphi_j(x)|^2 dx \\ &\leq \sum_{j \in \mathbb{N}} \int_{\mathbb{R}^d} \lambda_j |\nabla_x \varphi_j(x)|^2 dx = \sum_{j \in \mathbb{N}} \lambda_j \|\nabla_x \varphi_j\|_{L^2(\mathbb{R}^d)}^2 = \text{Tr}((-\Delta)\gamma). \end{aligned}$$

We obtain the bound on $\nabla_y \gamma$ similarly by symmetry. \square

Lemma III.3. *Let $q \in [2, \infty]$ such that*

$$2 \leq q \begin{cases} \leq \infty & \text{if } d = 1, \\ < \infty & \text{if } d = 2, \\ \leq \frac{2d}{d-2} & \text{if } d \geq 3, \end{cases} \quad (\text{III.8})$$

Then, there exists $C > 0$ such that for any $u \in H^1(\mathbb{R}^d)$

$$\|u\|_{L^q(\mathbb{R}^d)}^2 \leq C \left(\varepsilon \|\nabla u\|_{L^2(\mathbb{R}^d)}^2 + \varepsilon^{-\frac{d(q-2)}{2q-d(q-2)}} \|u\|_{L^2(\mathbb{R}^d)}^2 \right).$$

Notice that in Lemma III.3, the exponent $\frac{d(q-2)}{2q-d(q-2)} > 0$ for any q that satisfies (III.8) when $d = 1, 2$. For higher dimensions $d \geq 3$, it is positive if and only if $q < \frac{2d}{d-2}$.

Remark 48. In dimension $d > 2$, it is possible to prove this bound with Gagliardo-Nirenberg-Sobolev (Lemma II.3), which is true for any $2 \leq q \leq \frac{2d}{d-2}$

$$\begin{aligned} \|u\|_{L^q(\mathbb{R}^d)}^2 &\leq C_{\text{GNS}}^2 \|\nabla u\|_{L^2(\mathbb{R}^d)}^{2d\left(\frac{1}{2}-\frac{1}{q}\right)} \|u\|_{L^2(\mathbb{R}^d)}^{2-2d\left(\frac{1}{2}-\frac{1}{q}\right)} \\ &\leq C \left[\varepsilon \|\nabla u\|_{L^2(\mathbb{R}^d)}^2 + \varepsilon^{-\frac{d(q-2)}{2q-d(q-2)}} \|u\|_{L^2(\mathbb{R}^d)}^2 \right]. \end{aligned}$$

The last line is obtained with the Peter-Paul identity (Fact II.1)

$$\forall a, b \geq 0, \theta \in [0, 1], \varepsilon > 0 \quad a^\theta b^{1-\theta} \leq \varepsilon \theta a + \varepsilon^{-\frac{\theta}{1-\theta}} (1-\theta) b.$$

applied to $a = \|\nabla u\|_{L^2(\mathbb{R}^d)}^2$, $b = \|u\|_{L^2(\mathbb{R}^d)}^2$, $\theta = d(1/2 - 1/q)^4$.

⁴which is in $[0, 1]$ since $q \geq 2$ and $d \geq 2$

Proof of Lemma III.3. Let $2 \leq q \leq \infty$ that satisfies (III.8). By the Sobolev's embedding $H^1(\mathbb{R}^d) \hookrightarrow L^q(\mathbb{R}^d)$, there exists $C > 0$ such that for any $v \in H^1(\mathbb{R}^d)$

$$\|v\|_{L^q(\mathbb{R}^d)}^2 \leq C \left(\|\nabla v\|_{L^2(\mathbb{R}^d)}^2 + \|v\|_{L^2(\mathbb{R}^d)}^2 \right).$$

Then, for any $u \in H^1(\mathbb{R}^d)$ and any $\delta > 0$ (by taking for instance the scaling $v(x) := \delta^{d/q} u(\delta x)$)

$$\|u\|_{L^q(\mathbb{R}^d)}^2 \leq C \left(\delta^{\frac{2d}{q}-d+2} \|\nabla u\|_{L^2(\mathbb{R}^d)}^2 + \delta^{\frac{2d}{q}-d} \|u\|_{L^2(\mathbb{R}^d)}^2 \right).$$

Thus, we obtain the desired bound (by posing $\varepsilon = \delta^{\frac{2d}{q}-d+2}$)

$$\|u\|_{L^q(\mathbb{R}^d)}^2 \leq C \left(\varepsilon \|\nabla u\|_{L^2(\mathbb{R}^d)}^2 + \varepsilon^{-\frac{d(q-2)}{2q-d(q-2)}} \|u\|_{L^2(\mathbb{R}^d)}^2 \right).$$

□

Proof of Fact III.2.

1) Let us write $w = w_1 + w_\infty$ with $w_1 \in L^p(\mathbb{R}^d)$ and $w_\infty \in L^\infty(\mathbb{R}^d)$. We have to distinguish to cases:

- for $d = 1$, we prove the bound for $p \geq 1$,
- for $d = 2$, we prove the bound for $1 < p < \infty$,
- for $d > 2$, we chose $p \geq d/2$ so that $2p' \leq 2d/(d-2)$.

On the one hand, by the Hölder inequality and the fact that $0 \leq \gamma \leq 1$

$$\begin{aligned} |\text{Ex}_{w_\infty}(\gamma)| &\leq \|w_\infty\|_{L^\infty} \left(\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} |\gamma(x, y)|^2 dx dy \right) = \|w_\infty\|_{L^\infty} \|\gamma\|_{\mathfrak{S}^2}^2 \\ &\leq \|w_\infty\|_{L^\infty} \text{Tr}(\gamma) \|\gamma\|_{\mathfrak{S}^\infty} \leq \|w_\infty\|_{L^\infty} \text{Tr}(\gamma). \end{aligned}$$

On another hand, by the Hölder inequality

$$\begin{aligned} |\text{Ex}_{w_1}(\gamma)| &= \left| \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w_1(x-y) |\gamma(x, y)|^2 dx dy \right| \\ &\leq \|w_1\|_{L^p(\mathbb{R}^d)} \int_{\mathbb{R}^d} \|\gamma(x, y)\|_{L_x^{2p'}(\mathbb{R}^d)}^2 dy. \end{aligned}$$

Finally, by the modified version of Sobolev embedding (Lemma III.3) with the function $u = \gamma(\cdot, y) \in H_x^1(\mathbb{R}^d)$ for almost fixed $y \in \mathbb{R}^d$ and $q = 2p'$, by (III.7) and the fact that $0 \leq \gamma \leq 1$

$$\begin{aligned} \int_{\mathbb{R}^d} \|\gamma(x, y)\|_{L_x^{2p'}(\mathbb{R}^d)}^2 dy &\leq C \left(\varepsilon \|\nabla_x \gamma\|_{L_{x,y}^2(\mathbb{R}^d \times \mathbb{R}^d)}^2 + \varepsilon^{-\frac{d}{2p-d}} \|\gamma\|_{L_{x,y}^2(\mathbb{R}^d \times \mathbb{R}^d)}^2 \right) \\ &\leq C \left(\varepsilon \text{Tr}(-\Delta \gamma) + \varepsilon^{-\frac{d}{2p-d}} \text{Tr}(\gamma) \right). \end{aligned}$$

Finally, there exists $C_w > 0$ such that for any $0 \leq \gamma \leq 1$

$$|\text{Ex}_w(\gamma)| \leq C_w \left[\varepsilon \text{Tr}((-\Delta)\gamma) + (1 + \varepsilon^{-\frac{d}{2p-d}}) \text{Tr}(\gamma) \right],$$

it is exactly (III.5).

2) Furthermore, assume that $p > 1$ when $d = 1$. We show now the bound (III.6). Let us denote $\varepsilon_h := C_w \varepsilon h^{d-2}$ and $\tilde{\varepsilon}_h := C_w (1 + \varepsilon^{-\frac{d}{2p-d}}) h^d$. Let $\alpha > 0$. We now explain why the following $\varepsilon > 0$ is well-chosen

$$\varepsilon := \begin{cases} \frac{h}{|\log h|^\alpha} & \text{if } d = 1, \\ \frac{1}{|\log h|} & \text{if } d = 2, \\ 1 & \text{if } d \geq 3. \end{cases}$$

One has

$$\varepsilon_h = C_w \begin{cases} \frac{1}{|\log h|^\alpha} & \text{if } d = 1, \\ \frac{1}{|\log h|} & \text{if } d = 2, \\ h^{d-2} & \text{if } d \geq 3, \end{cases} \quad \text{and} \quad \tilde{\varepsilon}_h = C_w \begin{cases} h + h^{1-\frac{1}{2p-1}} |\log h|^{\frac{\alpha}{2p-1}} & \text{if } d = 1, \\ h^2 + h^2 |\log h|^{\frac{1}{p-1}} & \text{if } d = 2, \\ 2h^d & \text{if } d \geq 3, \end{cases}$$

which tend to 0 when h goes to 0. □

III.2 Coercivity of the Hartree-Fock energy.

First, we prove that for any fixed $h > 0$, the energy $\mathcal{E}_h^{\text{HF}}$ is coercive on \mathcal{X} : that there exists $C_h, c_h > 0$ such that for any $0 \leq \gamma \leq 1$, we have $\mathcal{E}_h^{\text{HF}}(\gamma) \geq C_h \|\gamma\|_{\mathcal{X}} - c_h$. In particular, $\mathcal{E}_h^{\text{HF}}$ is bounded by below in \mathcal{X} , that implies that all minimizing sequences of $\mathcal{E}_h^{\text{HF}}$ are bounded with respect to the \mathcal{X} -norm.

Lemma III.4. *Let $p \in [1, \infty]$ such that*

$$p \in \begin{cases} (1, \infty] & \text{if } d = 1, 2, \\ [\frac{d}{2}, \infty] & \text{if } d \geq 3. \end{cases} \quad (\text{III.9})$$

Let $w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ satisfies Assumption 6. Otherwise, a second alternative for $d = 1, 2$ is to take $w \in L^1 \cap L^p(\mathbb{R}^d)$ satisfies Assumption 7. Then, there exists $C > 0$ and $h_0 > 0$ such that for any $h \in (0, h_0]$ and any $\gamma \in \mathcal{K}$

$$\mathcal{E}_h^{\text{HF}}(\gamma) \geq \frac{1}{4} \text{Tr}((-h^2 \Delta + V + 1)\gamma) - h^{-d} C.$$

Remark 49. The assumption (III.9) on p takes in account both (III.1) and (III.4) so that the direct and the exchange terms are well-defined in \mathcal{X} . It allows also (III.6) in order to control the exchange term by the direct term.

Remark 50. If w is nonnegative, we have the bound

$$\text{Ex}_w(\gamma) \leq D_w(\rho_\gamma, \rho_\gamma).$$

Otherwise, we can just have

$$\text{Ex}_w(\gamma) \leq D_{|w|}(\rho_\gamma, \rho_\gamma).$$

And that does not say anything.

Fact III.5. *For any $\gamma \geq 0$, we have almost everywhere $|\gamma(x, y)| \leq \rho_\gamma(x) \rho_\gamma(y)$.*

Proof. Indeed, if we write $\gamma = \sum_{j \in \mathbb{N}} \lambda_j |\varphi_j\rangle \langle \varphi_j|$ with $\{\lambda_j\}_j \subset \mathbb{R}_+$ and $\{\varphi_j\}_j$ an orthonormal basis of $L^2(\mathbb{R}^d)$, by the Cauchy-Schwarz inequality

$$\begin{aligned} |\gamma(x, y)|^2 &= \left| \sum_{j \in \mathbb{N}} \lambda_j \bar{\varphi}_j(y) \varphi_j(x) \right|^2 = \left| \sum_{j \in \mathbb{N}} \sqrt{\lambda_j} \bar{\varphi}_j(y) \sqrt{\lambda_j} \varphi_j(x) \right|^2 \\ &\leq \left(\sum_{j \in \mathbb{N}} \left| \sqrt{\lambda_j} \bar{\varphi}_j(y) \right|^2 \right) \left(\sum_{j \in \mathbb{N}} \left| \sqrt{\lambda_j} \varphi_j(x) \right|^2 \right) = \left(\sum_{j \in \mathbb{N}} \lambda_j |\bar{\varphi}_j(y)|^2 \right) \left(\sum_{j \in \mathbb{N}} \lambda_j |\varphi_j(x)|^2 \right) \\ &\leq \rho_\gamma(y) \rho_\gamma(x). \end{aligned}$$

□

Proof of Lemma III.4. Since we have Assumption 6, we only need to control the linear and the exchange term of the Hartree-Fock energy. As well, Assumption (I.13) for $d = 1, 2$ ensures that the direct term to be controlled by the linear term. Indeed,

$$\begin{aligned} \mathcal{E}_h^{\text{HF}}(\gamma) &\geq \text{Tr}((-h^2\Delta + V - E)\gamma) - \frac{h^d}{2} \|\hat{w}_-\|_{L^\infty(\mathbb{R}^d)} C_{\gamma, h}(d) - \frac{h^d}{2} \text{Ex}_w(\gamma) \\ &\geq \text{Tr}((-h^2\Delta + V - E)\gamma) - \frac{h^d}{2} \text{Ex}_w(\gamma) - \frac{1}{2} \begin{cases} \text{Tr}((1 - h^2\Delta)\gamma) & \text{if } d = 1, \\ \text{Tr}((-h^2\Delta)\gamma) & \text{if } d = 2, \end{cases} \\ &\geq -\frac{h^d}{2} \text{Ex}_w(\gamma) + \frac{1}{2} \begin{cases} \text{Tr}((-h^2\Delta + V - 2(E + 1))\gamma) & \text{if } d = 1, \\ \text{Tr}((-h^2\Delta + V - 2E)\gamma) & \text{if } d = 2. \end{cases} \end{aligned}$$

Let us bound by below the now the Hartree-Fock energy without its direct term. For convenience, let us treat only $\mathcal{E}_h^{\text{rHF}}$ (we recover the other cases by adding multiplicative constants and changing the value of E). For any $M > 0$, we denote the spectral projectors $\Pi_{M, h}^\pm$ by

$$\Pi_{M, h}^+ := \mathbf{1}(-h^2\Delta + V > M), \quad \Pi_{M, h}^- := \mathbf{1}(-h^2\Delta + V \leq M).$$

Notice that $\Pi_{M, h}^+ + \Pi_{M, h}^- = 1$. Furthermore, for any $\gamma \geq 0$ and $M \geq E$, there exists $C_M \geq 0$ such that

$$\text{Tr}((-h^2\Delta + V - E)\Pi_{M, h}^+\gamma) \geq (M - E) \text{Tr}(\gamma) - h^{-d} C_M. \quad (\text{III.10})$$

Proof of the formula (III.10). Indeed

$$\begin{aligned} \text{Tr}((-h^2\Delta + V - E)\Pi_{M, h}^+\gamma) &= \text{Tr}(((-h^2\Delta + V - M) + (M - E))\Pi_{M, h}^+\gamma) \\ &= \underbrace{\text{Tr}((-h^2\Delta + V - M)\Pi_{M, h}^+\gamma)}_{\geq 0} + (M - E) \text{Tr}((1 - \Pi_{M, h}^-)\gamma) \\ &\geq (M - E) \text{Tr}(\gamma) - (M - E) \text{Tr}(\Pi_{M, h}^-). \end{aligned}$$

By the Weyl's law, we have

$$\text{Tr}(\Pi_{M, h}^-) = (2\pi h)^{-d} \left| \{(x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d : |\xi|^2 + V(x) \leq M\} \right| + o_h(1).$$

□

On the one hand,

$$\text{Tr}((-h^2\Delta + V - E)\gamma) = \text{Tr}((-h^2\Delta + V + 1)\gamma) - (1 + E) \text{Tr}(\gamma).$$

On an other hand, by (III.10), the Hölder inequality and $0 \leq \gamma \leq 1$

$$\begin{aligned} \operatorname{Tr}((-h^2\Delta + V - E)\gamma) &= \operatorname{Tr}((-h^2\Delta + V - E)\Pi_{M,h}^+\gamma) + \operatorname{Tr}((-h^2\Delta + V - E)\Pi_{M,h}^-\gamma) \\ &\geq (M - E) \operatorname{Tr}(\gamma) - h^{-d}C_M + (\min V - E) \operatorname{Tr}(\Pi_{M,h}^-\gamma) \\ &\geq (M - 2E) \operatorname{Tr}(\gamma) - h^{-d}C_M. \end{aligned}$$

We obtain

$$\begin{aligned} \operatorname{Tr}((-h^2\Delta + V - E)\gamma) &= \left(\frac{1}{2} + \frac{1}{2}\right) \operatorname{Tr}((-h^2\Delta + V - E)\gamma) \\ &\geq \frac{1}{2} \operatorname{Tr}((-h^2\Delta + V + 1)\gamma) + \frac{1}{2}(M - 1 - 3E) \operatorname{Tr}(\gamma) - h^{-d}C_M. \end{aligned}$$

Furthermore, taking into account the bound on the exchange term (III.6) there exist $\varepsilon_h, \tilde{\varepsilon}_h = o_h(1)$ such that

$$\begin{aligned} \mathcal{E}_h^{\text{HF}}(\gamma) &\geq \frac{1}{2} \operatorname{Tr}((-h^2\Delta + V + 1)\gamma) - h^{-d}C_M \\ &\quad + \frac{1}{2}(M - 1 - 3E - 2\tilde{\varepsilon}_h) \operatorname{Tr}(\gamma) - \varepsilon_h \operatorname{Tr}((-h^2\Delta)\gamma). \end{aligned}$$

By taking $M = 1 + 3E$, there exists $C' > 0$ such that

$$\mathcal{E}_h^{\text{HF}}(\gamma) \geq \frac{1}{2} \operatorname{Tr}((-h^2\Delta + V + 1)\gamma) - h^{-d}C' - \varepsilon_h \operatorname{Tr}((-h^2\Delta)\gamma) - \tilde{\varepsilon}_h \operatorname{Tr}(\gamma).$$

We impose now that $h \in (0, h_0]$ for $h_0 > 0$ such that $1/2 - \max(\varepsilon_{h_0}, \tilde{\varepsilon}_{h_0}) > 1/4$. That ends the proof of Lemma III.4. \square

III.3 Convergence of minimizing sequences

Let a fixed $h > 0$. Notice that all the arguments of this section will be the same as for $h = 1$. Let $e_h^{\text{HF}} := \inf_{\gamma \in \mathcal{K}} \mathcal{E}_h^{\text{HF}}$. We have shown that the functional $\mathcal{E}_h^{\text{HF}}$ is coercive in \mathcal{K} , that then implies that the ground state energy e_h^{HF} is finite. The idea now is to consider a minimizing sequence $\{\gamma_{n,h}\}_n$ of $\mathcal{E}_h^{\text{HF}}$ on \mathcal{K} .

$$\lim_{n \rightarrow \infty} \mathcal{E}_h^{\text{HF}}(\gamma_{n,h}) = e_h^{\text{HF}}.$$

The coercivity of $\mathcal{E}_h^{\text{HF}}$ (Lemma III.4) implies the boundedness of the sequence with respect to the \mathcal{X} -norm. Recall that \mathcal{K} is a convex and closed subspace of \mathcal{X} , there exists $\gamma_h \in \mathcal{K}$ such that $\gamma_{n,h} \rightharpoonup \gamma_h$ weakly-* and weakly in \mathcal{X} : that means that for any $A \in \mathfrak{S}^\infty(L^2(\mathbb{R}^d))$

$$\begin{aligned} \lim_{n \rightarrow \infty} \operatorname{Tr}((-\Delta + V + 1)^{1/2} \gamma_{n,h} (-\Delta + V + 1)^{1/2} A) \\ = \operatorname{Tr}((-\Delta + V + 1)^{1/2} \gamma_h (-\Delta + V + 1)^{1/2} A). \end{aligned}$$

We will prove that $\mathcal{E}_h^{\text{HF}}$ is weakly lower semi-continuous in \mathcal{X} . We will deduce

$$e_h^{\text{HF}} = \liminf_{n \rightarrow \infty} \mathcal{E}_h^{\text{HF}}(\gamma_{n,h}) \geq \mathcal{E}_h^{\text{HF}}(\gamma_h) \geq e_h^{\text{HF}},$$

that gives us $\mathcal{E}_h^{\text{HF}}(\gamma_h) = e_h^{\text{HF}}$, i.e. that γ_h is a minimizer of the Hartree-Fock functional in \mathcal{K} . We will see that that quadratic term is strongly-* continuous (Facts III.8 and III.9)

$$\lim_{n \rightarrow \infty} \frac{h^d}{2} (D_w(\rho_{\gamma_{n,h}}, \rho_{\gamma_{n,h}}) - \operatorname{Ex}_w(\gamma_{n,h})) = \frac{h^d}{2} (D_w(\rho_{\gamma_h}, \rho_{\gamma_h}) - \operatorname{Ex}_w(\gamma_h)).$$

Basic properties on the minimizing sequences of $\mathcal{E}_h^{\text{HF}}$.

Remark 51. Note that every $\gamma \in \mathcal{X}$ satisfies $\rho_\gamma \in L^1(\mathbb{R}^d)$ and $V\rho_\gamma \in L^1(\mathbb{R}^d)$. Furthermore, by the Lieb-Thirring inequality $\rho_\gamma \in L^{1+2/d}(\mathbb{R}^d)$. More generally, we will see that $\rho_\gamma \in L^q(\mathbb{R}^d)$ for any $1 \leq q \leq d/(d-2)$.

We deduce from the Hoffmann-Ostenhof inequality (Lemma II.5) that (up to a subsequence) $\sqrt{\rho_{\gamma_{n,h}}} \xrightarrow{n \rightarrow \infty} \sqrt{\rho_{\gamma_h}}$ weakly in $H^1(\mathbb{R}^d)$.

Details. Since the sequence $\{\sqrt{\rho_{\gamma_{n,h}}}\}_n$ is bounded on $H^1(\mathbb{R}^d)$, there exists $f \in H^1(\mathbb{R}^d)$ such that up to a subsequence, $\sqrt{\rho_{\gamma_{n,h}}} \xrightarrow{n \rightarrow \infty} f$ in $H^1(\mathbb{R}^d)$. Let us prove that this limit is actually $\sqrt{\rho_{\gamma_h}}$. In particular, $\sqrt{\rho_{\gamma_{n,h}}} \xrightarrow{n \rightarrow \infty} f$ strongly in $L^2_{\text{loc}}(\mathbb{R}^d)$, so $\rho_{\gamma_{n,h}} \xrightarrow{n \rightarrow \infty} f^2$ strongly in $L^1_{\text{loc}}(\mathbb{R}^d)$. Then, for any test function $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^d)$

$$\text{Tr}(\gamma_{n,h}\chi) = \int_{\mathbb{R}^d} \rho_{\gamma_{n,h}}(x)\chi(x)dx \xrightarrow{n \rightarrow \infty} \int_{\mathbb{R}^d} f(x)^2\chi(x)dx$$

Moreover, since $\{\rho_{\gamma_{n,h}}\}_n$ is bounded on \mathcal{X} and that V is confining, the operator $\sqrt{-\Delta + V + 1}^{-1}\chi\sqrt{-\Delta + V + 1}^{-1}$ is compact, that gives the limit

$$\begin{aligned} \text{Tr}(\gamma_{n,h}\chi) &= \text{Tr} \left(\sqrt{-\Delta + V + 1}\gamma_{n,h}\sqrt{-\Delta + V + 1} \frac{1}{\sqrt{-\Delta + V + 1}}\chi\frac{1}{\sqrt{-\Delta + V + 1}} \right) \\ &\xrightarrow{n \rightarrow \infty} \text{Tr} \left(\sqrt{-\Delta + V + 1}\gamma_h\sqrt{-\Delta + V + 1} \frac{1}{\sqrt{-\Delta + V + 1}}\chi\frac{1}{\sqrt{-\Delta + V + 1}} \right) \\ &= \text{Tr}(\gamma_h\chi) = \int_{\mathbb{R}^d} \rho_{\gamma_h}(x)\chi(x)dx. \end{aligned}$$

Finally, $f^2 = \rho_{\gamma_h}$ almost everywhere. □

Furthermore, by the Rellich-Kondrachov theorem $\rho_{\gamma_{n,h}} \xrightarrow{n \rightarrow \infty} \rho_{\gamma_h}$ strongly in $L^p_{\text{loc}}(\mathbb{R}^d)$ for any $1 \leq p < d/(d-2)$. That implies the pointwise convergence $\rho_{\gamma_{n,h}}(x) \xrightarrow{n \rightarrow \infty} \rho_{\gamma_h}(x)$ almost everywhere.

The trapping condition on V actually gives a stronger convergence of the sequence $\{\rho_{\gamma_{n,h}}\}_n$.

Lemma III.6. *Let $d \geq 2$. Let $V : \mathbb{R}^d \rightarrow \mathbb{R}$ that satisfies Assumption 5. Then, for any $1 \leq q < d/(d-2)$, $\rho_{\gamma_{n,h}} \xrightarrow{n \rightarrow \infty} \rho_{\gamma_h}$ strongly in $L^q(\mathbb{R}^d)$.*

Proof of Lemma III.6. Fix $R > 0$ as in (I.12). By the triangle inequality,

$$\|\rho_{\gamma_{n,h}} - \rho_{\gamma_h}\|_{L^q(\mathbb{R}^d)} \leq \|\rho_{\gamma_{n,h}} - \rho_{\gamma_h}\|_{L^q(\{|x| \leq R\})} + \|\rho_{\gamma_{n,h}} - \rho_{\gamma_h}\|_{L^q(\{|x| > R\})}.$$

On the one hand, by the Rellich-Kondrachov theorem $\|\rho_{\gamma_{n,h}} - \rho_{\gamma_h}\|_{L^q(\{|x| \leq R\})} \xrightarrow{n \rightarrow \infty} 0$ for any $1 \leq q < d/(d-2)$. On the other hand, using that $\{V(\rho_{\gamma_{n,h}} - \rho_{\gamma_h})\}_n$ is bounded on $L^1(\mathbb{R}^d)$ and the bound (I.12), there exists $k \in \mathbb{N}^*$ and $C > 0$ such that

$$\|\rho_{\gamma_{n,h}} - \rho_{\gamma_h}\|_{L^1(\{|x| > R\})} \leq \|V^{-1}\|_{L^\infty(\{|x| > R\})}\|V(\rho_{\gamma_{n,h}} - \rho_{\gamma_h})\|_{L^1(\mathbb{R}^d)} \leq CR^{-k}.$$

Finally, we make $R \rightarrow \infty$, and the L^1 -norm of $\rho_{\gamma_{n,h}} - \rho_{\gamma_h}$ tends to 0. Then, we deduce by interpolation⁵ that $\rho_{\gamma_{n,h}} \xrightarrow{n \rightarrow \infty} \rho_{\gamma_h}$ strongly in L^q for all $1 \leq q < d/(d-2)$. That concludes the proof of the lemma. □

⁵For any $1 \leq q < d/(d-2)$, there exists $\tilde{q} \in (q, d/(d-2))$. Let $\theta \in (0, 1)$ such that $\frac{1}{q} = \theta + \frac{1-\theta}{\tilde{q}}$. Since

Weak-* lower continuity of each term.

Fact III.7. *The linear term $\gamma \mapsto \text{Tr}((-h^2\Delta + V - E)\gamma)$ is weakly-* lower semi-continuous in \mathcal{X} .*

$$\forall \gamma_n \rightharpoonup \gamma \text{ weakly-* in } \mathcal{X}, \quad \liminf_{n \rightarrow \infty} \text{Tr}(P_{h,E}\gamma_n) \geq \text{Tr}(P_{h,E}\gamma).$$

Proof. Let us write $-h^2\Delta + V - E = (-h^2\Delta + V - E)_+ - (-h^2\Delta + V - E)_-$. On the one hand,

$$\liminf_{n \rightarrow \infty} \text{Tr}((-h^2\Delta + V - E)_+\gamma_n) \geq \text{Tr}((-h^2\Delta + V - E)_+\gamma).$$

Indeed, there exists $\{\lambda_j\}_j \subset \mathbb{R}_+$ and $\{\varphi_j\}_j$ a L^2 -orthonormal basis of eigenfunctions of $-h^2\Delta + V$, so that $(-h^2\Delta + V - E)_+ = \sum_{j \in \mathbb{N}} \lambda_j |\varphi_j\rangle\langle\varphi_j|$. Then, by Fatou's lemma

$$\begin{aligned} \liminf_{n \rightarrow \infty} \text{Tr}((-h^2\Delta + V - E)_+\gamma_n) &= \liminf_{n \rightarrow \infty} \text{Tr}(\sqrt{\gamma_n}(-h^2\Delta + V - E)_+\sqrt{\gamma_n}) \\ &= \liminf_{n \rightarrow \infty} \sum_{j \in \mathbb{N}} \lambda_j \langle \sqrt{\gamma_n}\varphi_j, \sqrt{\gamma_n}\varphi_j \rangle_{L^2} \\ &= \liminf_{n \rightarrow \infty} \sum_{j \in \mathbb{N}} \lambda_j \langle \varphi_j, \gamma_n\varphi_j \rangle_{L^2} \\ &\geq \sum_{j \in \mathbb{N}} \lambda_j \liminf_{n \rightarrow \infty} \langle \varphi_j, \gamma_n\varphi_j \rangle_{L^2} = \sum_{j \in \mathbb{N}} \lambda_j \langle \varphi_j, \gamma\varphi_j \rangle_{L^2} \\ &= \text{Tr}((-h^2\Delta + V - E)_+\gamma). \end{aligned}$$

Moreover, since the operator $(-h^2\Delta + V - E)_-$ has a finite rank (in particular, it is trace-class) and that $\gamma_n \rightharpoonup \gamma$ weakly-* in $\mathcal{B}(L^2(\mathbb{R}^d))$, we have the strong convergence

$$\lim_{n \rightarrow \infty} \text{Tr}((-h^2\Delta + V - E)_-\gamma_n) = \text{Tr}((-h^2\Delta + V - E)_-\gamma).$$

□

Fact III.8. *Let $\max(1, \frac{d}{4}) < p \leq \infty$. In particular, $1 \leq p \leq \infty$ for $d \in \{1, 2, 3\}$ and $p > d/4$ when $d \geq 4$. For any $w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$, the direct term $\gamma \mapsto D_w(\rho_\gamma, \rho_\gamma)$ is strongly continuous on \mathcal{K} .*

Remark 52. The assumption on the exponent $p \in [1, \infty]$ are more restrictive than the one of Fact III.1, since the key compactness ingredient for the limit here is Rellich-Kondrachov theorem.

Proof of Fact III.8. Let a sequence $\gamma_n \rightharpoonup \gamma$ in \mathcal{X} . By the triangle inequality,

$$\begin{aligned} &|D_w(\rho_{\gamma_n}, \rho_{\gamma_n}) - D_w(\rho_\gamma, \rho_\gamma)| \\ &= \left| \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} (\rho_{\gamma_n}(x)\rho_{\gamma_n}(y) - \rho_\gamma(x)\rho_\gamma(y))w(x-y)dx dy \right| \\ &\leq \left| \int_{\mathbb{R}^d} (\rho_{\gamma_n}(x) - \rho_\gamma(x))\rho_\gamma(y)w(x-y)dx dy \right| + \left| \int_{\mathbb{R}^d} \rho_{\gamma_n}(x)(\rho_\gamma(y) - \rho_{\gamma_n}(y))w(x-y)dy \right|. \end{aligned}$$

$\{\rho_{\gamma_n, h} - \rho_{\gamma_h}\}_{n \in \mathbb{N}}$ is uniformly bounded on $L^{\tilde{q}}(\mathbb{R}^d)$,

$$\begin{aligned} \|\rho_{\gamma_n, h} - \rho_{\gamma_h}\|_{L_y^2 L_x^{\tilde{q}}(\mathbb{R}^d \times \mathbb{R}^d)} &\leq \|\rho_{\gamma_n, h} - \rho_{\gamma_h}\|_{L_y^2 L_x^1(\mathbb{R}^d \times \mathbb{R}^d)}^\theta \|\rho_{\gamma_n, h} - \rho_{\gamma_h}\|_{L_y^2 L_x^{\tilde{q}}(\mathbb{R}^d \times \mathbb{R}^d)}^{1-\theta} \\ &\xrightarrow{n \rightarrow \infty} 0. \end{aligned}$$

We write $w = w_1 + w_\infty$ with $w_1 \in L^p(\mathbb{R}^d)$ and $w_\infty \in L^\infty(\mathbb{R}^d)$. Let $q \geq 1$ which satisfies the relation $1/p + 2/q = 2$. By definition of p , q satisfies $1 \leq q < d/(d-2)$, then $\{\rho_{\gamma_n}\}_n$ is bounded on $L^q(\mathbb{R}^d)$. Moreover, by Lemma III.6, $\rho_{\gamma_n} \rightarrow \rho_\gamma$ strongly in $L^q(\mathbb{R}^d)$. Hence, by the Young inequality

$$\begin{aligned} & |D_w(\rho_{\gamma_n}, \rho_{\gamma_n}) - D_w(\rho_\gamma, \rho_\gamma)| \\ & \leq 2\|w_\infty\|_{L^\infty(\mathbb{R}^d)}\|\rho_\gamma\|_{L^1(\mathbb{R}^d)}\underbrace{\|\rho_{\gamma_n} - \rho_\gamma\|_{L^1(\mathbb{R}^d)}}_{\rightarrow 0} \\ & \quad + \|w_1\|_{L^p(\mathbb{R}^d)}\left(\|\rho_\gamma\|_{L^q(\mathbb{R}^d)} + \|\rho_{\gamma_n}\|_{L^q(\mathbb{R}^d)}\right)\underbrace{\|\rho_{\gamma_n} - \rho_\gamma\|_{L^q(\mathbb{R}^d)}}_{\rightarrow 0}. \end{aligned}$$

Finally, we get $D_w(\rho_{\gamma_n}, \rho_{\gamma_n}) \xrightarrow{n \rightarrow \infty} D_w(\rho_\gamma, \rho_\gamma)$. \square

Fact III.9. *Let $w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ with $\max(1, d/2) \leq p \leq \infty$ such that $1 \leq p \leq \infty$ when $d = 1$ and $d/2 < p \leq \infty$ when $d \geq 2$. Then, the exchange term Ex_w is strongly continuous on \mathcal{K} .*

Remark 53. As for Fact III.1, the assumption on the exponent $p \in [1, \infty]$ are more restrictive than the one of Fact III.2, since we must fit the assumption Rellich-Kondrachov theorem.

Proof of Fact III.9. By non-negativity of V , the operator $\frac{\sqrt{1-\Delta}}{\sqrt{-\Delta+V+1}} \in \mathfrak{S}^\infty(L^2(\mathbb{R}^d))$.⁶ For any $\gamma \in \mathcal{K}$, $\sqrt{-\Delta+V+1}\gamma \in \mathfrak{S}^2(L^2(\mathbb{R}^d))$. Thus, by the Hölder inequality, $\sqrt{1-\Delta}\gamma \in \mathfrak{S}^2(L^2(\mathbb{R}^d))$. Using now the property $0 \leq \gamma \leq 1$

$$\sqrt{1-\Delta}\gamma^2\sqrt{1-\Delta} \leq \sqrt{1-\Delta}\gamma\sqrt{1-\Delta} \in \mathfrak{S}^1(L^2(\mathbb{R}^d)),$$

in other words, $\sqrt{1-\Delta}\gamma$ is Hilbert-Schmidt. Hence,

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \left| \sqrt{1-\Delta_x}\gamma(x, y) \right|^2 dx dy < \infty,$$

i.e.

$$(\sqrt{1-\Delta_x} + \sqrt{1-\Delta_y})\gamma \in L^2_{x,y}(\mathbb{R}^d \times \mathbb{R}^d). \quad (\text{III.11})$$

We deduce that $\gamma \in H^1_{x,y}(\mathbb{R}^d \times \mathbb{R}^d)$. As well, $\sqrt{V}\gamma^2\sqrt{V} \leq \sqrt{V}\gamma\sqrt{V} \in \mathfrak{S}^1(L^2(\mathbb{R}^d))$. Thus, $\sqrt{V}\gamma \in \mathfrak{S}^2(L^2(\mathbb{R}^d))$

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} (1 + V(x) + V(y)) |\gamma(x, y)|^2 dx dy < \infty. \quad (\text{III.12})$$

Let $\{\gamma_n\}_n \subset \mathcal{K}$ and $\gamma \in \mathcal{K}$ a sequence such that $\gamma_n \rightharpoonup \gamma$ weakly-* in \mathcal{X} . By the Hölder inequality

$$\begin{aligned} |\text{Ex}_w(\gamma_n) - \text{Ex}_w(\gamma)| &= \left| \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} (|\gamma_n(x, y)|^2 - |\gamma(x, y)|^2) w(x-y) dx dy \right| \\ &\leq \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \left| |\gamma_n(x, y)|^2 - |\gamma(x, y)|^2 \right| |w(x-y)| dx dy \\ &\leq \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} |\gamma_n(x, y) - \gamma(x, y)| (|\gamma_n(x, y)| + |\gamma(x, y)|) |w(x-y)| dx dy \\ &\leq \text{Ex}_{|w|}(\gamma_n - \gamma) \text{Ex}_{|w|}(|\gamma_n| + |\gamma|) \\ &\leq 2\text{Ex}_{|w|}(\gamma_n - \gamma) (\text{Ex}_{|w|}(\gamma_n) + \text{Ex}_{|w|}(\gamma)). \end{aligned}$$

⁶It follows from the bound

$$\forall u \in L^2(\mathbb{R}^d), \quad \|\sqrt{1-\Delta}u\|_{L^2(\mathbb{R}^d)} \leq \|\sqrt{-\Delta+V+1}u\|_{L^2(\mathbb{R}^d)},$$

which is true since

$$\|\sqrt{1-\Delta}u\|_{L^2(\mathbb{R}^d)}^2 = \langle u, (1-\Delta)u \rangle_{L^2(\mathbb{R}^d)} \leq \langle u, (-\Delta+V+1)u \rangle_{L^2(\mathbb{R}^d)} = \|\sqrt{-\Delta+V+1}u\|_{L^2(\mathbb{R}^d)}^2.$$

Writing $w = w_1 + w_\infty$ with $w_1 \in L^p(\mathbb{R}^d)$ and $w_\infty \in L^\infty(\mathbb{R}^d)$, we get

$$\begin{aligned} & |\text{Ex}_w(\gamma_n) - \text{Ex}_w(\gamma)| \\ & \leq 2\|w_\infty\|_{L^\infty(\mathbb{R}^d)}^2 \|\gamma_n - \gamma\|_{L_y^2 L_x^2(\mathbb{R}^d \times \mathbb{R}^d)} \left(\|\gamma_n\|_{L_y^2 L_x^2(\mathbb{R}^d \times \mathbb{R}^d)} + \|\gamma\|_{L_y^2 L_x^2(\mathbb{R}^d \times \mathbb{R}^d)} \right) \\ & \quad + 2\|w_1\|_{L^p(\mathbb{R}^d)}^2 \|\gamma_n - \gamma\|_{L_y^2 L_x^{2p'}(\mathbb{R}^d \times \mathbb{R}^d)} \left(\|\gamma_n\|_{L_y^2 L_x^{2p'}(\mathbb{R}^d \times \mathbb{R}^d)} + \|\gamma\|_{L_y^2 L_x^{2p'}(\mathbb{R}^d \times \mathbb{R}^d)} \right). \end{aligned}$$

Recall that we consider the following values of p

- $p = 1$ when $d = 1^7$,
- $p > d/2$ when $d \geq 2$.

This implies

$$\begin{cases} 2p' = \infty & \text{when } d = 1, \\ 2 \leq 2p' < \frac{2d}{d-2} & \text{when } d \geq 2. \end{cases}$$

By (III.11) the sequence of integral kernels $\{\gamma_n\}_n$ and γ are bounded on $H_{x,y}^1(\mathbb{R}^d \times \mathbb{R}^d)$. Furthermore, since we are under the assumptions of the Sobolev embedding $H_x^1(\mathbb{R}^d) \hookrightarrow L_x^{2p'}(\mathbb{R}^d)$ ⁸

$$\begin{aligned} & |\text{Ex}_w(\gamma_n) - \text{Ex}_w(\gamma)| \\ & \lesssim \|\gamma_n - \gamma\|_{L_y^2 L_x^2(\mathbb{R}^d \times \mathbb{R}^d)} \left(\|\gamma_n\|_{L_y^2 L_x^2(\mathbb{R}^d \times \mathbb{R}^d)} + \|\gamma\|_{L_y^2 L_x^2(\mathbb{R}^d \times \mathbb{R}^d)} \right) \\ & \quad + \|\gamma_n - \gamma\|_{L_y^2 H_x^1(\mathbb{R}^d \times \mathbb{R}^d)} \left(\|\gamma_n\|_{L_y^2 H_x^1(\mathbb{R}^d \times \mathbb{R}^d)} + \|\gamma\|_{L_y^2 H_x^1(\mathbb{R}^d \times \mathbb{R}^d)} \right) \\ & \lesssim \|\gamma_n - \gamma\|_{L_y^2 L_x^2(\mathbb{R}^d \times \mathbb{R}^d)} + \|\gamma_n - \gamma\|_{L_y^2 L_x^{2p'}(\mathbb{R}^d \times \mathbb{R}^d)}. \end{aligned}$$

▷ By the Rellich-Kondrachov compact injection, $\gamma_n \rightarrow \gamma$ strongly in $L_{\text{loc}}^2(\mathbb{R}^d \times \mathbb{R}^d)$. In particular, for any $R > 0$

$$\lim_{n \rightarrow \infty} \|\gamma_n - \gamma\|_{L_{x,y}^2(|x| \leq R, |y| \leq R)} = 0.$$

Take now $R > 0$ and $k \in \mathbb{N}^*$ which satisfy (I.12). By (III.12), the sequence $\{(x, y) \mapsto \sqrt{1 + V(x) + V(y)} \gamma_n(x, y)\}_n$ and $(x, y) \mapsto \sqrt{1 + V(x) + V(y)} \gamma(x, y)$ are bounded on $L_{x,y}^2(\mathbb{R}^d \times \mathbb{R}^d)$. Hence applying the Hölder inequality and the previous remarks, we have for any $n \in \mathbb{N}$

$$\begin{aligned} & \|\gamma_n - \gamma\|_{L_{x,y}^2(|x| \leq R, |y| \geq R)} + \|\gamma_n - \gamma\|_{L_{x,y}^2(|x| \geq R, |y| \leq R)} + \|\gamma_n - \gamma\|_{L_{x,y}^2(|x| \geq R, |y| \geq R)} \\ & \leq 3 \left\| (1 + V(x) + V(y))^{-1/2} \right\|_{L_{x,y}^\infty(\mathbb{R}^d \times \{|y| \geq R\})} \left\| (\gamma_n - \gamma)(1 + V(x) + V(y))^{1/2} \right\|_{L_{x,y}^2(\mathbb{R}^d \times \mathbb{R}^d)} \\ & \leq CR^{-k/2}. \end{aligned}$$

Finally with the limit $R \rightarrow \infty$, we obtain $\gamma_n \rightarrow \gamma$ strongly in $L^2(\mathbb{R}^d \times \mathbb{R}^d)$.

⁷We obtain the continuity for $1 < p \leq \infty$ by interpolation.

⁸We used also the continuous injection $L_y^2 H_x^1(\mathbb{R}^d \times \mathbb{R}^d) \hookrightarrow H_{x,y}^1(\mathbb{R}^d \times \mathbb{R}^d)$. Indeed, for any $f \in H_{c,r}^1(\mathbb{R}^d \times \mathbb{R}^d)$

$$\begin{aligned} \|f\|_{L_y^2 H_x^1}^2 &= \|f\|_{L_{y,x}^2}^2 + \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} |\nabla_x f(x, y)|^2 dx dy \\ &\leq \|f\|_{L_{y,x}^2}^2 + \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} (|\nabla_x f(x, y)|^2 + |\nabla_y f(x, y)|^2) dx dy \\ &= \|f\|_{L_{x,y}^2}^2 + \|\nabla_{x,y} f\|_{L_{x,y}^2}^2 = \|f\|_{H_{x,y}^1}^2. \end{aligned}$$

▷ Let us explain the term $\|\gamma_n - \gamma\|_{L_y^2 L_x^{2p'}(\mathbb{R}^d \times \mathbb{R}^d)}$ tends to 0 also. Let us explain how it follows from the strong limit $\gamma_n \rightarrow \gamma$ in $L^2(\mathbb{R}^d \times \mathbb{R}^d)$.

- When $d = 1$, $2p' = 2$ and we have already proved that $\gamma_n \rightarrow \gamma$ strongly in $L^2(\mathbb{R}^d \times \mathbb{R}^d)$.
- When $d = 2$, for any $p > 1$, there exists $\tilde{p} \in (1, p)$ so that $2 \leq 2p' < 2\tilde{p}' < \infty$ and $\theta \in (0, 1)$ ⁹ such that

$$\|\gamma_n - \gamma\|_{L_y^2 L_x^{2p'}(\mathbb{R}^d \times \mathbb{R}^d)} \leq C \|\gamma_n - \gamma\|_{L_y^2 L_x^2(\mathbb{R}^d \times \mathbb{R}^d)}^\theta \|\gamma_n - \gamma\|_{L_y^2 L_x^{2\tilde{p}'}(\mathbb{R}^d \times \mathbb{R}^d)}^{1-\theta}$$

which tends to 0 since $\{\gamma_n - \gamma\}_n$ is bounded in $L_y^2 L_x^{2\tilde{p}'}(\mathbb{R}^d \times \mathbb{R}^d)$.

- When¹⁰ $d > 2$, by the Gagliardo-Nirenberg-Sobolev inequality (Proposition II.3) and the strong L^2 -convergence

$$\begin{aligned} \|\gamma_n - \gamma\|_{L_y^2 L_x^{2p'}(\mathbb{R}^d \times \mathbb{R}^d)} &\leq C \|\gamma_n - \gamma\|_{L_y^2 L_x^2(\mathbb{R}^d \times \mathbb{R}^d)}^{1-\frac{d}{2p}} \|\nabla_x(\gamma_n - \gamma)\|_{L_y^2 L_x^2(\mathbb{R}^d \times \mathbb{R}^d)}^{\frac{d}{2p}} \\ &\leq C \|\gamma_n - \gamma\|_{L_y^2 L_x^2(\mathbb{R}^d \times \mathbb{R}^d)}^{1-\frac{d}{2p}} \|\gamma_n - \gamma\|_{H_{x,y}^1(\mathbb{R}^d \times \mathbb{R}^d)}^{\frac{d}{2p}}, \end{aligned}$$

which tends to 0 since $\{\gamma_n - \gamma\}_n$ is bounded in $H_{x,y}^1(\mathbb{R}^d \times \mathbb{R}^d)$.

That concludes the proof of Fact III.9. □

III.4 Nonlinear equation of the minimizers

In this section, we discuss the form of the minimizers of the h -Hartree-Fock functional. Recall that $H_\gamma = H_{\gamma,h,V-E,w}$ refers to the semiclassical mean-field operator (see (I.5)). We state in the result that any minimizer of the Hartree-Fock energy must ‘almost’ satisfy a non-linear equation

$$\gamma_h = \mathbb{1}(H_{\gamma_h} \leq 0) \text{ or } \gamma_h = \mathbb{1}(H_{\gamma_h} < 0).$$

Such an equation may be seen as an *Euler-Lagrange* equations for the Hartree-Fock minimizers. This means that γ_h is a projector on the eigenspaces associated to all negative eigenvalues of its associated mean-field operator H_{γ_h} or all the negative eigenvalues without the bigger one. However, we will see that there exists projector P_h which minimizes the h -Hartree-Fock energy. In this case, it is true that it satisfies exactly the Euler-Lagrange equation.

Theorem III.10. *Let $p > \max(1, d/2)$. Assume that $w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ is even and positive. Then, for any minimizer γ_h of $\mathcal{E}_h^{\text{HF}}$ in \mathcal{K} , there exists a self-adjoint operator $0 \leq Q_h \leq 1$ on $L^2(\mathbb{R}^d)$ such that*

$$\gamma_h = \mathbb{1}(H_{\gamma_h} < 0) + Q_h,$$

with $\text{range}(Q_h) \subset \ker(H_{\gamma_h})$. Furthermore, there exists a projector P_h that minimizes $\mathcal{E}_h^{\text{HF}}$ and that satisfies

$$P_h = \mathbb{1}(H_{P_h} \leq 0) \text{ or } \mathbb{1}(H_{P_h} < 0).$$

This kind of results is for instance done by Lenzmann and Lewin [LL10, Thm.2] for minimizers for Hartree-Fock-Bogoliubov functionals.

Remark 54. Here, we take $p \in [1, \infty]$ such that we have not only assumptions of both Facts III.7, III.8 and III.9, that ensure the existence of the minimizers. Secondly, the repulsive condition $w > 0$ is sufficient to have the rank of the projector of the error Q_h on $(0, 1)$ be at most equal to 1. However, it is not clear that we can weaken it.

Let us now prove Theorem III.10.

⁹ $2p' = \frac{\theta}{2} + \frac{1-\theta}{2\tilde{p}'}$

¹⁰Notice that one can also use the same kind of interpolation as in dimension 2 but with $2\tilde{p}' \in (p, 2d/(d-2))$.

Step 1. We first prove that any minimizer γ_h of $\mathcal{E}_h^{\text{HF}}$ minimizes the energy $\text{Tr}(H_{\gamma_h} \cdot)$ on the set of self-adjoint operators of \mathcal{K} .

Lemma III.11. *For any self-adjoint operators $\gamma, \tilde{\gamma} \in \mathcal{X}$*

$$\mathcal{E}_h^{\text{HF}}(\gamma + \tilde{\gamma}) - \mathcal{E}_h^{\text{HF}}(\gamma) = \text{Tr}(H_{\gamma} \tilde{\gamma}) + \frac{h^d}{2} [D_w(\rho_{\tilde{\gamma}}, \rho_{\tilde{\gamma}}) - \text{Ex}_w(\tilde{\gamma})].$$

Proof of Lemma III.11. Let $\gamma, \tilde{\gamma} \in \mathcal{X}$. Let us write each term of $\mathcal{E}_h^{\text{HF}}(\gamma + \tilde{\gamma})$. For the linear term, we have

$$\text{Tr}((-h^2\Delta + V - E)(\gamma + \tilde{\gamma})) = \text{Tr}((-h^2\Delta + V - E)\gamma) + \text{Tr}((-h^2\Delta + V - E)\tilde{\gamma}).$$

Moreover, since the interaction potential w is even, the direct term is expressed by

$$\begin{aligned} D_w(\rho_{\gamma+\tilde{\gamma}}, \rho_{\gamma+\tilde{\gamma}}) &= D_w(\rho_{\gamma}, \rho_{\gamma}) + D_w(\rho_{\gamma}, \rho_{\tilde{\gamma}}) + D_w(\rho_{\tilde{\gamma}}, \rho_{\gamma}) + D_w(\rho_{\tilde{\gamma}}, \rho_{\tilde{\gamma}}) \\ &= D_w(\rho_{\gamma}, \rho_{\gamma}) + 2D_w(\rho_{\gamma}, \rho_{\tilde{\gamma}}) + D_w(\rho_{\tilde{\gamma}}, \rho_{\tilde{\gamma}}). \end{aligned}$$

Besides, we compute the exchange term

$$\text{Ex}_w(\gamma + \tilde{\gamma}, \gamma + \tilde{\gamma}) = \text{Ex}_w(\gamma) + 2 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y) \text{Re} \left(\gamma(x, y) \overline{\tilde{\gamma}(x, y)} \right) dx dy + \text{Ex}_w(\tilde{\gamma}).$$

Thus, we obtain

$$\begin{aligned} \mathcal{E}_h^{\text{HF}}(\gamma + \tilde{\gamma}) - \mathcal{E}_h^{\text{HF}}(\gamma) &= \left[\text{Tr}((-h^2\Delta + V - E)\tilde{\gamma}) + h^d (D_w(\rho_{\gamma}, \rho_{\tilde{\gamma}}) - \text{Ex}_w(\text{Re}(\gamma\tilde{\gamma}))) \right] \\ &\quad + \frac{h^d}{2} [D_w(\rho_{\tilde{\gamma}}, \rho_{\tilde{\gamma}}) - \text{Ex}_w(\tilde{\gamma})]. \end{aligned}$$

Since w is even

$$\begin{aligned} D_w(\rho_{\gamma}, \rho_{\tilde{\gamma}}) &= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} w(x-y) \rho_{\gamma}(x) \rho_{\tilde{\gamma}}(y) dx dy = \int_{\mathbb{R}^d} \left(\int_{\mathbb{R}^d} w(-z) \rho_{\gamma}(y-z) dz \right) \rho_{\tilde{\gamma}}(y) dy \\ &= \int_{\mathbb{R}^d} \left(\int_{\mathbb{R}^d} w(z) \rho_{\gamma}(y-z) dz \right) \rho_{\tilde{\gamma}}(y) dy \\ &= \int_{\mathbb{R}^d} (w * \rho_{\gamma})(y) \rho_{\tilde{\gamma}}(y) dx = \text{Tr}((w * \rho_{\gamma})\tilde{\gamma}). \end{aligned}$$

Furthermore, note that

$$\begin{aligned} \text{Ex}_w(\gamma\tilde{\gamma}) &= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} X_w(\gamma)(x, y) \overline{\tilde{\gamma}(x, y)} dx dy = \int_{\mathbb{R}^d} \left(\int_{\mathbb{R}^d} X_w(\gamma)(x, y) (\tilde{\gamma})^*(y, x) dy \right) dx \\ &= \int_{\mathbb{R}^d} (X_w(\gamma)\tilde{\gamma}^*)(x) dx = \text{Tr}(X_w(\gamma)\tilde{\gamma}^*). \end{aligned}$$

Then, we get

$$2\text{Ex}_w(\gamma\tilde{\gamma}) = \text{Tr}(X_w(\gamma)\tilde{\gamma}^* + X_w(\gamma)^*\tilde{\gamma}).$$

If γ and $\tilde{\gamma}$ are self-adjoint, their kernel is real, and we have

$$2\text{Ex}_w(\gamma\tilde{\gamma}) = 2 \text{Tr}(X_w(\gamma)\tilde{\gamma}).$$

Finally, we have

$$\text{Tr}((-h^2\Delta + V - E)\tilde{\gamma}) + h^d (D_w(\rho_{\gamma}, \rho_{\tilde{\gamma}}) - \text{Ex}_w(\text{Re}(\gamma\tilde{\gamma}))) = H_{\gamma}(\tilde{\gamma}).$$

□

Then, we deduce the following corollary.

Corollary III.12. *For any self-adjoint $\gamma_h, \tilde{\gamma} \in \mathcal{X}$*

$$\lim_{t \rightarrow 0, t \in (0,1]} \frac{\mathcal{E}_h^{\text{HF}}(\gamma_h + t(\tilde{\gamma} - \gamma_h)) - \mathcal{E}_h^{\text{HF}}(\gamma_h)}{t} = \text{Tr}(H_{\gamma_h}(\tilde{\gamma} - \gamma_h)).$$

Proof. We apply Lemma III.11 to $\gamma = \gamma_h$ and $\tilde{\gamma} = t(\tilde{\gamma} - \gamma_h)$, and we conclude by dividing the equality by t and taking the limit $t \rightarrow 0$.

$$\begin{aligned} & \lim_{t \rightarrow 0, t \in (0,1]} \frac{\mathcal{E}_h^{\text{HF}}(\gamma_h + t(\tilde{\gamma} - \gamma_h)) - \mathcal{E}_h^{\text{HF}}(\gamma_h)}{t} \\ &= \text{Tr}(H_{\gamma_h}(\tilde{\gamma} - \gamma_h)) + \lim_{t \rightarrow 0, t \in (0,1]} t \frac{h^d}{2} [D_w(\rho_{\tilde{\gamma} - \gamma_h}, \rho_{\tilde{\gamma} - \gamma_h}) - \text{Ex}_w(\tilde{\gamma} - \gamma_h)]. \end{aligned}$$

□

Since γ_h is minimizer of $\mathcal{E}_h^{\text{HF}}$ on \mathcal{K} , for any $\tilde{\gamma} \in \mathcal{K}$ and $t \in [0, 1]$, we have $\mathcal{E}_h^{\text{HF}}(\gamma_h + t(\tilde{\gamma} - \gamma_h)) \geq \mathcal{E}_h^{\text{HF}}(\gamma_h)$. By Corollary III.12 and the linearity of the trace, for any self-adjoint $\tilde{\gamma} \in \mathcal{K}$

$$\text{Tr}(H_{\gamma_h} \tilde{\gamma}) \geq \text{Tr}(H_{\gamma_h} \gamma_h).$$

Step 2. Let us prove that $P_-^{\gamma_h} := \mathbb{1}(H_{\gamma_h} < 0)$ ¹¹ is a minimizer of $\text{Tr}(H_{\gamma_h} \cdot)$.

Let us define also $P_+^{\gamma_h} := 1 - P_-^{\gamma_h}$. For any operator γ on $L^2(\mathbb{R}^d)$, let us denote $\gamma_{\pm\pm} := P_{\pm}^{\gamma_h} \gamma P_{\pm}^{\gamma_h}$ and $\gamma_{\pm\mp} := P_{\pm}^{\gamma_h} \gamma P_{\mp}^{\gamma_h}$.

Let $\tilde{\gamma} \in \mathcal{K}$. Using the relation

$$P_{\pm}^{\gamma_h} H_{\gamma_h} P_{\pm}^{\gamma_h} = \pm P_{\pm}^{\gamma_h} |H_{\gamma_h}| P_{\pm}^{\gamma_h}$$

the trace's cyclicity, the non-negativity of $|H_{\gamma_h}| \tilde{\gamma}_{++}$ and $\tilde{\gamma}_{--} \leq P_-^{\gamma_h}$ (since $0 \leq \tilde{\gamma} \leq 1$)

$$\begin{aligned} \text{Tr}(H_{\gamma_h} \tilde{\gamma}) &= \text{Tr}(H_{\gamma_h} \tilde{\gamma}_{++}) + \text{Tr}(H_{\gamma_h} \tilde{\gamma}_{--}) = \text{Tr}(|H_{\gamma_h}| \tilde{\gamma}_{++}) - \text{Tr}(|H_{\gamma_h}| \tilde{\gamma}_{--}) \\ &\geq -\text{Tr}(|H_{\gamma_h}| \tilde{\gamma}_{--}) \\ &\geq -\text{Tr}(|H_{\gamma_h}| P_-^{\gamma_h}) = -\text{Tr}(|H_{\gamma_h}| (P_-^{\gamma_h})^2) = -\text{Tr}(P_-^{\gamma_h} |H_{\gamma_h}| P_-^{\gamma_h}) = \text{Tr}(H_{\gamma_h} P_-^{\gamma_h}). \end{aligned}$$

This bound is true for any $\tilde{\gamma}$, that proves that the projector $P_-^{\gamma_h}$ is a minimizer of $\text{Tr}(H_{\gamma_h} \cdot)$ on \mathcal{K} .

Step 3. Properties of $Q_h := \gamma_h - P_-^{\gamma_h}$. Let us now explain why the range of $Q_h := \gamma_h - P_-^{\gamma_h}$ is included in the kernel of H_{γ_h} . For this, it remains to prove the inclusion $\text{Im } H_{\gamma_h} \subset \ker Q_h$. The wanted inclusion follows by orthogonality.

Since γ_h and $P_-^{\gamma_h}$ are minimizers of $\text{Tr}(H_{\gamma_h} \cdot)$ on \mathcal{K} , we have $\text{Tr}(H_{\gamma_h} Q_h) = 0$. Now, let us bound by below $\text{Tr}(H_{\gamma_h} Q_h)$.

$$\text{Tr}(H_{\gamma_h} Q_h) = \text{Tr}(|H_{\gamma_h}| (Q_{h,++} - Q_{h,--})) \geq \text{Tr}(|H_{\gamma_h}| Q_h^2).$$

The last inequality came from the non-negativity of $|H_{\gamma_h}|$ and the following lemma.

Lemma III.13. *The operator Q_h satisfies the inequality*

$$Q_{h,++} - Q_{h,--} \geq Q_h^2.$$

¹¹One can show with the same argument, that it is also true for $\mathbb{1}(H_{\gamma_h} \leq 0)$.

Proof of Lemma III.13. Recall that $Q_h + P_-^{\gamma_h} = \gamma_h$ and $0 \leq \gamma_h \leq 1$. Then,

$$0 \leq (Q_h + P_-^{\gamma_h})^2 \leq Q_h + P_-^{\gamma_h}.$$

Moreover,

$$(Q_h + P_-^{\gamma_h})^2 = Q_h^2 + P_-^{\gamma_h} + Q_h P_-^{\gamma_h} + P_-^{\gamma_h} Q_h.$$

We recall that $P_-^{\gamma_h^-} + P_+^{\gamma_h^-} = 1$, and we deduce

$$\begin{aligned} Q_h^2 &\leq Q_h^2 + P_-^{\gamma_h} \\ &\leq Q_h - P_-^{\gamma_h} - Q_h P_-^{\gamma_h} - P_-^{\gamma_h} Q_h \\ &= Q_{h,++} + Q_{h,--} + Q_{h,+} + Q_{h,+} - Q_{h,--} - Q_{h,+} - Q_{h,--} - Q_{h,+} \\ &= Q_{h,++} - Q_{h,--}. \end{aligned}$$

□

Since the operator H_{γ_h} is self-adjoint and has a compact resolvent on $L^2(\mathbb{R}^d)$, there exists a L^2 -orthonormal basis of $|H_{\gamma_h}|$'s eigenfunctions $\{\varphi_j^h\}_{j \in \mathbb{N}}$. Let $\{\lambda_j^h\}_{j \in \mathbb{N}}$ the sequence of the associated eigenvalues. Furthermore, since γ_h and $P_-^{\gamma_h}$ are self-adjoint, Q_h is self-adjoint too. We have $|H_{\gamma_h}|, Q_h^2 \geq 0$. Then, $|H_{\gamma_h}| Q_h^2$ is also a non-negative operator. Hence, for any $j \in \mathbb{N}$

$$\begin{aligned} 0 = \text{Tr}(|H_{\gamma_h}| Q_h^2) &\geq \left\langle \varphi_j^h, |H_{\gamma_h}| Q_h^2 \varphi_j^h \right\rangle_{L^2} = \left\langle |H_{\gamma_h}| \varphi_j^h, Q_h^2 \varphi_j^h \right\rangle_{L^2} \\ &= \lambda_j^h \left\langle \varphi_j^h, Q_h^2 \varphi_j^h \right\rangle_{L^2} = \lambda_j^h \|Q_h \varphi_j^h\|_{L^2(\mathbb{R}^d)}^2. \end{aligned}$$

From the eigenvalues λ_j^h such that $\lambda_j > 0$, we obtain $Q_h \varphi_j^h = 0$. That implies that $\text{range}(H_{\gamma_h}) \subset \ker(Q_h)$. Hence, $\text{range}(Q_h) \subset \ker(H_{\gamma_h})$.

Step 4. Assume that w is positive almost everywhere in \mathbb{R}^d . Let us show that the number of eigenvalues of Q_h in $(0, 1)$ is at most 1. We will follow the same argument as [Bac92, Cor. 1].

Let $u_h, v_h \in L^2(\mathbb{R}^d)$ an orthonormal pair in $L^2(\mathbb{R}^d)$ and $\lambda_h, \mu_h \in (0, 1)$ such that $Q_h u_h = \mu_h u_h$ and $Q_h v_h = \lambda_h v_h$. Assume that u_h and v_h are linearly independent. Defining A_h to be the operator $|u_h\rangle \langle u_h| - |v_h\rangle \langle v_h|$, we have $A_h(x, y) = u_h(x) \overline{u_h(y)} - v_h(x) \overline{v_h(y)}$ for almost all $x, y \in \mathbb{R}^d$. We deduce

$$\begin{aligned} \rho_{A_h}(x) \rho_{A_h}(y) &= (|u_h(x)|^2 - |v_h(x)|^2)(|u_h(y)|^2 - |v_h(y)|^2) \\ &= |u_h(x)|^2 |u_h(y)|^2 + |v_h(x)|^2 |v_h(y)|^2 - |u_h(x)|^2 |v_h(y)|^2 - |v_h(x)|^2 |u_h(y)|^2, \end{aligned}$$

and

$$\begin{aligned} |A_h(x, y)|^2 &= |u_h(x)|^2 |u_h(y)|^2 + |v_h(x)|^2 |v_h(y)|^2 - u_h(x) \overline{u_h(y)} \overline{v_h(x)} v_h(y) - v(x) \overline{v_h(y)} \overline{u_h(x)} u_h(y) \\ &= |u_h(x)|^2 |u_h(y)|^2 + |v_h(x)|^2 |v_h(y)|^2 - u_h(x) v_h(y) \overline{u_h(y)} \overline{v_h(x)} - \overline{u_h(x)} v_h(y) \overline{u_h(y)} v_h(x) \\ &= |u_h(x)|^2 |u_h(y)|^2 + |v_h(x)|^2 |v_h(y)|^2 - 2 \text{Re} \left(u_h(x) v_h(y) \overline{u_h(y)} \overline{v_h(x)} \right). \end{aligned}$$

From their definition and the previous step, we have $u_h, v_h \in \ker(H_{\gamma_h})$. Thus, $\text{Tr}(H_{\gamma_h} A_h) = 0$.

By Lemma III.11

$$\begin{aligned}
 & \mathcal{E}_h^{\text{HF}}(\gamma_h + \delta |u_h\rangle \langle u_h| - \delta |v_h\rangle \langle v_h|) - \mathcal{E}_h^{\text{HF}}(\gamma_h) \\
 &= \delta \text{Tr}(H_{\gamma_h} A_h) + \frac{\delta^2 h^2}{2} [D_w(\rho_{A_h}, \rho_{A_h}) - \text{Ex}_w(A_h)] \\
 &= -\frac{\delta^2 h^2}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} w(x-y) \times \\
 & \quad \times \left(|u_h(x)|^2 |v_h(y)|^2 + |v_h(x)|^2 |u_h(y)|^2 - 2 \text{Re}(u_h(x)v_h(y)\overline{u_h(y)v_h(x)}) \right) dx dy \\
 &= -\frac{\delta^2 h^2}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} w(x-y) |u_h(x)v_h(y) - u_h(y)v_h(x)|^2 dx dy.
 \end{aligned}$$

Since w is positive and u_h and v_h are not proportional, the Lebesgue measure of the set $\{(x, y) \in \mathbb{R}^d \times \mathbb{R}^d \mid w(x-y) |u_h(x)v_h(y) - u_h(y)v_h(x)|^2 \neq 0\}$ is not equal to 0. Thus, we have for any $\delta > 0$,

$$\mathcal{E}_h^{\text{HF}}(\gamma_h + \delta |u_h\rangle \langle u_h| - \delta |v_h\rangle \langle v_h|) - \mathcal{E}_h^{\text{HF}}(\gamma_h) < 0.$$

Let $\{\nu_j^h\}_j \subset [0, 1]$ and $\{\varphi_j^h\}_j$ an orthonormal basis such that $\gamma_h = \sum_j \nu_j^h |\varphi_j^h\rangle \langle \varphi_j^h|$. Thus, for any $\delta = \min(\mu, 1 - \lambda)$

$$\begin{aligned}
 & \gamma_h + \delta |u_h\rangle \langle u_h| - \delta |v_h\rangle \langle v_h| \\
 &= \sum_{j: \varphi_j^h \neq u_h, \varphi_j^h \neq v_h} \nu_j^h |\varphi_j^h\rangle \langle \varphi_j^h| + \underbrace{(\lambda_h + \delta)}_{\in [0,1]} |u_h\rangle \langle u_h| + \underbrace{(\mu_h - \delta)}_{\in [0,1]} |v_h\rangle \langle v_h| \in \mathcal{K}.
 \end{aligned}$$

That leads to a contradiction since γ_h is a minimizer of the Hartree-Fock energy on \mathcal{K} . Hence, the operator Q_h admits at most one eigenfunction in the interval $(0, 1)$.

Step 5. Let us now explain why for any minimizer γ_h of $\mathcal{E}_h^{\text{HF}}$ on \mathcal{K} , one can build a projector P_h that minimizes also $\mathcal{E}_h^{\text{HF}}$. Let P_1^h be the projector on the eigenspace $\ker(Q_h - \text{Id})$. By the previous step, there exists $\theta \in \{0, 1\}$, $\lambda_h \in (0, 1)$ and u_h a L^2 -normalized eigenfunction of Q_h such that $Q_h = P_1^h + \theta \lambda_h |u_h\rangle \langle u_h|$. The operator $P_h = \gamma_h - \theta \lambda_h |u_h\rangle \langle u_h| = \mathbf{1}(H_{\gamma_h} < 0) + P_1^h$ is a projector since $\text{range}(P_1^h) \subset \ker(H_{\gamma_h})$. Let us explain why P_h is a minimizer of $\mathcal{E}_h^{\text{HF}}$.

- If $\theta = 0$, $\gamma_h = \mathbf{1}(H_{\gamma_h} < 0) + P_1^h$ and this is over.
- Assume that $\theta = 1$. Using the inclusion $u_h \in \text{range}(Q_h) \subset \ker(H_{\gamma_h})$, P_h satisfies the relation $\mathcal{E}_h^{\text{HF}}(\gamma_h - \lambda_h |u_h\rangle \langle u_h|) = \mathcal{E}_h^{\text{HF}}(\gamma_h)$, and then is a minimizer of $\mathcal{E}_h^{\text{HF}}$.

Step 6. Finally, there remains to prove why P_h satisfies the Euler-Lagrange equation. Since $w > 0$, one can write $P_h = \mathbf{1}(H_{P_h} < 0) + \tilde{Q}_h$ with $0 \leq \tilde{Q}_h \leq 1$, which is also a projector, and $\text{range}(\tilde{Q}_h) \subset \ker(P_h)$. Let us prove that $\tilde{Q}_h = 0$ or \tilde{Q}_h is the projector on $\ker(H_{P_h})$. Assume that there exists an orthonormal family functions $\{u_h, v_h\}$ on $L^2(\mathbb{R}^d)$ such that $\tilde{Q}_h u_h = 0$ and $\tilde{Q}_h v_h = v_h$. Recall that $u_h, v_h \in \ker(P_h)$ since there are in the image of \tilde{Q}_h . Notice that $0 \leq P_h + |u_h\rangle \langle u_h| - |v_h\rangle \langle v_h| \leq 1$. Similarly as in Step 4, $P_h + |u_h\rangle \langle u_h| - |v_h\rangle \langle v_h| \in \mathcal{K}$ ¹² and

$$\mathcal{E}_h^{\text{HF}}(P_h + |u_h\rangle \langle u_h| - |v_h\rangle \langle v_h|) < \mathcal{E}_h^{\text{HF}}(P_h),$$

¹²By definition $P_h + |u_h\rangle \langle u_h| - |v_h\rangle \langle v_h| \in \mathcal{X}$. Again, we write the projector $P_h = \sum_{j \geq 2} |\varphi_j^h\rangle \langle \varphi_j^h|$ with $\{\varphi_j^h\}_{j \in \mathbb{N}}$ an orthonormal basis of $L^2(\mathbb{R}^d)$ that includes u_h and v_h (for convenience $\varphi_0^h = v_h$ and $\varphi_1^h = u_h$). We can now write

$$P_h + |u_h\rangle \langle u_h| - |v_h\rangle \langle v_h| = \sum_{j \geq 1} |\varphi_j^h\rangle \langle \varphi_j^h|,$$

which remains a projector, hence $0 \leq P_h + |u_h\rangle \langle u_h| - |v_h\rangle \langle v_h| \leq 1$.

this is a contradiction with the fact that P_h minimizes $\mathcal{E}_h^{\text{HF}}$ on \mathcal{K} . Therefore, we have either $\tilde{Q}_h = 0$ or \tilde{Q}_h must be the spectral projector on the kernel of P_h .

That concludes the proof of Theorem III.10.

IV PROOF OF THE SEMICLASSICAL LIMIT OF THE HARTREE-FOCK GROUND STATE ENERGY

We prove in this section the convergence to the Hartree-Fock ground state energy to the Thomas-Fermi ground state energy.

IV.1 To the reduced Hartree-Fock energy

The main idea of the proof of Theorem 1 consists on getting back to the reduced Hartree-Fock ground state. Indeed, we can deal the asymptotics at the semiclassical limit. In [FLS18], Fournais, Lewin and Solovej proved bounds on densities matrices γ with a fixed trace $\text{Tr} \gamma = N$ (with the relation $N = h^{-d}$) and then take the limit (or limsup, or liminf) $N \rightarrow \infty$. Here, we do not fix the trace, but it is relevant to consider

Assumption 9. $\gamma \in \mathcal{K}$ such that there exists $C > 0$ so that $\text{Tr}(-h^2 \Delta \gamma), \text{Tr}(\gamma) < Ch^{-d}$.

Example IV.1. The previous assumption is valid for example for $0 \leq \gamma \leq 1$ such that $\mathcal{E}_h^{\text{HF}}(\gamma_h) \leq Ch^{-d}$. This condition is actually satisfies for almost-optimizers of the Hartree-Fock energy. (For minimizers, we would have more specifically $\mathcal{E}_h^{\text{HF}}(\gamma_h) \leq 0$.) In this case, there exists $C' > 0$ such that

$$\text{Tr}((-h^2 \Delta + V + 1)\gamma_h) \leq C'h^{-d}.$$

The Assumption 9 is necessary to have the next lemma, that states that at the limits of $h^d \mathcal{E}_h^{\text{HF}}(\gamma)$ and $h^d \mathcal{E}_h^{\text{rHF}}(\gamma)$ are the same when $h \rightarrow 0$.

Lemma IV.2. *There exists $\{r_h\}_h \subset \mathbb{R}_+^*$ such that $r_h \rightarrow 0$ as $h \rightarrow 0$ and such that for any $\gamma \in \mathcal{K}$ satisfying Assumption 9*

$$|\mathcal{E}_h^{\text{HF}}(\gamma) - \mathcal{E}_h^{\text{rHF}}(\gamma)| \leq h^{-d} r_h.$$

Proof of Lemma IV.2. The bound is a direct consequence of Assumption 9 and the bound (III.6): there exists $\varepsilon_h = o_h(1)$ and $\tilde{\varepsilon}_h = o_h(1)$

$$|\mathcal{E}_h^{\text{HF}}(\gamma) - \mathcal{E}_h^{\text{rHF}}(\gamma)| \leq \frac{h^d}{2} |\text{Ex}_w(\gamma)| \leq \underbrace{\varepsilon_h \text{Tr}(-h^2 \Delta \gamma)}_{=o_h(h^{-d})} + \underbrace{\tilde{\varepsilon}_h \text{Tr}(\gamma)}_{=o_h(h^{-d})}.$$

□

IV.2 The upper bound

The idea for the upper bound consists in bounding by above the h -Hartree-Fock functional by the h -reduced Hartree-Fock functional up to an error depending on h , and taking a suitable element $\tilde{\gamma}_h \in \mathcal{K}$ that satisfies the desired limit for the reduced Hartree-Fock functional $\lim_{h \rightarrow 0} h^d \mathcal{E}_{h,V-E,w}^{\text{rHF}}(\tilde{\gamma}_h) = e_{V-E,w}^{\text{TF}}$. Hence,

$$\limsup_{h \rightarrow 0} h^d e_{h,V-E,w}^{\text{HF}} \leq \limsup_{h \rightarrow 0} h^d \mathcal{E}_{h,V-E,w}^{\text{HF}}(\tilde{\gamma}_h) \leq \limsup_{h \rightarrow 0} h^d \mathcal{E}_{h,V-E,w}^{\text{rHF}}(\tilde{\gamma}_h) = e_{V-E,w}^{\text{TF}}.$$

This is essentially the same proof as in Fournais-Lewin-Solovej [FLS18, Sec. 3.1].

Step 1. To the reduced Hartree-Fock energy. For any $h > 0$ and γ satisfying Assumption 9, by Lemma IV.2, there exist $r_h > 0$ such that $r_h = o_h(1)$ such that we have for any $\gamma \in \mathcal{K}$

$$e_{h,V-E,w}^{\text{HF}} \leq \mathcal{E}_{h,V-E,w}^{\text{HF}}(\gamma) \leq \mathcal{E}_{h,V-E,w}^{\text{rHF}}(\gamma) + h^{-d}r_h. \quad (\text{IV.1})$$

Step 2. Semiclassical limit with the trial state. Let $\rho \in C_c^\infty(\mathbb{R}^d, \mathbb{R}_+)$ trial state of the Thomas-Fermi energy functional. Actually, we will construct $\tilde{\gamma}_h$ that satisfies Assumption 9 and such that $h^d \mathcal{E}_h^{\text{rHF}}(\tilde{\gamma}_h) \rightarrow \mathcal{E}^{\text{TF}}(\rho)$. We introduce also the density

$$m(x, \xi) := \mathbb{1} \left(|\xi|^2 \leq c_{\text{TF}} \rho(x)^{2/d} \right).$$

Note that $\rho_m(x) := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} m(x, \xi) d\xi$ is equal to ρ . Moreover, by definition, m is a trial state the Vlasov energy functional $\mathcal{E}^{\text{Vlas}}$ associated to given ρ . We have

$$\mathcal{E}_{V-E,w}^{\text{Vlas}}(m) = \mathcal{E}_{V-E,w}^{\text{TF}}(\rho) = e_{V-E,w}^{\text{TF}}.$$

Notation. Let $R > 0$ such that $\text{supp } \rho$ is contained on the cube $C_R = (-R/2, R/2)^d$. Denote by Δ_{C_R} the Dirichlet Laplace operator on C_R . Let $\tilde{\gamma}_h$ be the operator which extends by zero outside C_R the operator

$$\gamma_h = \mathbb{1} \left(-h^2 \Delta_{C_R} - c_{\text{TF}} \rho(x)^{2/d} \leq 0 \right).$$

Let us detail what it means and the expression of $\tilde{\gamma}_h$ with orthonormal functions. Recall that the semiclassical Schrödinger operator $P_{C_R} = -h^2 \Delta_{C_R} - c_{\text{TF}} \rho(x)^{2/d}$ on $L^2(C_R)$ admits a discrete spectrum and that we can take an orthonormal family of eigenfunctions $\{u_j^h\}_{1 \leq j \leq N_h} \subset H^2(C_R) \cap H_0^1(C_R)$ of P_{C_R} (associated to negative eigenvalues of P_{C_R}) so that

$$\gamma_h = \sum_{j=1}^{N_h} |u_j^h\rangle \langle u_j^h|.$$

Let us define, for each $1 \leq j \leq N_h$

$$\tilde{u}_j^h(x) := \begin{cases} u_j(x) & \text{in } C_R, \\ 0 & \text{in } (C_R)^c, \end{cases}$$

which is also $L^2(\mathbb{R}^d)$ -normalized and in $H^1(\mathbb{R}^d)$. Furthermore, the family $\{u_j^h\}_{1 \leq j \leq N_h}$ is orthonormalized in $L^2(\mathbb{R}^d)$. At last, we set the spectral projector of rank N_h

$$\tilde{\gamma}_h := \sum_{j=1}^{N_h} |\tilde{u}_j^h\rangle \langle \tilde{u}_j^h|.$$

Proposition IV.3 ([FLS18, Lem. 3.2]). *Under the assumptions and notation above, we have Assumption 9,*

$$\lim_{h \rightarrow 0} h^d \text{Tr}(-h^2 \Delta \tilde{\gamma}_h) = \frac{d}{d+2} c_{\text{TF}} \int_{\mathbb{R}^d} \rho(x)^{1+2/d} dx \quad (\text{IV.2})$$

and

$$\lim_{h \rightarrow 0} h^d \text{Tr} \tilde{\gamma}_h = \int_{\mathbb{R}^d} \rho(x) dx. \quad (\text{IV.3})$$

Furthermore, up to a subsequence $h^d \rho_{\tilde{\gamma}_h} \rightharpoonup \rho$ weakly-* in $L^\infty(\mathbb{R}^d)$.

Before detailing the proof of Proposition IV.3, we explain why the upper bound (IV.1) and the analysis on the cube C_R implies the semiclassical limit $\limsup_{h \rightarrow 0} h^d \mathcal{E}_{h, V-E, w}^{\text{HF}}(\tilde{\gamma}_h) = \mathcal{E}_{V-E, w}^{\text{TF}}(\rho)$. First, by the previous proposition $\tilde{\gamma}_h$ satisfies Assumption 9. Thus, the limit of $h^d \mathcal{E}_h^{\text{HF}}$ is the same that $h^d \mathcal{E}_h^{\text{HF}}$. Moreover, by (IV.2)

$$\lim_{h \rightarrow 0} h^d \text{Tr}((-h^2 \Delta) \tilde{\gamma}_h) = \frac{d}{d+2} c_{\text{TF}} \int_{\mathbb{R}^d} \rho(x)^{1+2/d} dx.$$

We also recall that $\rho_{\tilde{\gamma}_h}$ and ρ are supported on the cube C_R , which is bounded. Thus, using that $h^d \rho_{\tilde{\gamma}_h} \rightharpoonup \rho$ weakly-* in $L^\infty(\mathbb{R}^d)$ and that $V - E \in L^1_{\text{loc}}(\mathbb{R}^d)$

$$\begin{aligned} h^d \int_{\mathbb{R}^d} (V(x) - E) \rho_{\tilde{\gamma}_h}(x) dx &= \int_{C_R} (V(x) - E) h^d \rho_{\tilde{\gamma}_h}(x) dx \\ &\xrightarrow{h \rightarrow 0} \int_{C_R} (V(x) - E) \rho(x) dx = \int_{\mathbb{R}^d} (V(x) - E) \rho(x) dx. \end{aligned}$$

Let us focus on the limit of the direct term. As w is even, $\rho * w \in L^\infty(\mathbb{R}^d)$ (since w is in $L^1_{\text{loc}}(\mathbb{R}^d)$ and $\text{supp } \rho$ is compact) and $h^d \rho_{\tilde{\gamma}_h} \rightharpoonup \rho$ weakly in $L^1(\mathbb{R}^d)$

$$\int_{C_R} h^d \rho_{\tilde{\gamma}_h}(x) (\rho * w)(x) dx \xrightarrow{h \rightarrow 0} \int_{C_R} \rho(x) (\rho * w)(x) dx.$$

Furthermore, we use again that $w \in L^1_{\text{loc}}(\mathbb{R})$, $(h^d \rho_{\tilde{\gamma}_h} - \rho)$ is bounded in $L^\infty(C_R)$ and $(h^d \rho_{\tilde{\gamma}_h} - \rho) * w \rightarrow 0$ strongly in $L^1(C_R)$ by dominated convergence ¹³

$$\begin{aligned} &\left| \int_{C_R} (h^d \rho_{\tilde{\gamma}_h}(x) - \rho(x)) ((h^d \rho_{\tilde{\gamma}_h} - \rho) * w)(x) dx \right| \\ &\leq \left(\int_{C_R} \left| \int_{C_R} w(x-y) (h^d \rho_{\tilde{\gamma}_h}(y) - \rho(y)) dy \right| dx \right) \|h^d \rho_{\tilde{\gamma}_h} - \rho\|_{L^\infty(C_R)} \\ &= \|(h^d \rho_{\tilde{\gamma}_h} - \rho) * w\|_{L^1(C_r)} \|h^d \rho_{\tilde{\gamma}_h} - \rho\|_{L^\infty(C_R)} \\ &\xrightarrow{h \rightarrow 0} 0. \end{aligned}$$

Hence,

$$\begin{aligned} h^{2d} D_w(\rho_{\tilde{\gamma}_h}, \rho_{\tilde{\gamma}_h}) &= \iint_{C_R \times C_R} w(x-y) (h^d \rho_{\tilde{\gamma}_h}(x)) (h^d \rho_{\tilde{\gamma}_h}(y)) dx dy \\ &= \int_{C_R} h^d \rho_{\tilde{\gamma}_h}(x) (\rho * w)(x) dx + \int_{C_R} h^d \rho_{\tilde{\gamma}_h}(x) ((h^d \rho_{\tilde{\gamma}_h} - \rho) * w)(x) dx \\ &= \int_{C_R} h^d \rho_{\tilde{\gamma}_h}(x) (\rho * w)(x) dx + \int_{C_R} \rho(x) ((h^d \rho_{\tilde{\gamma}_h} - \rho) * w)(x) dx \\ &\quad + \int_{C_R} (h^d \rho_{\tilde{\gamma}_h}(x) - \rho(x)) ((h^d \rho_{\tilde{\gamma}_h} - \rho) * w)(x) dx \\ &= \int_{C_R} h^d \rho_{\tilde{\gamma}_h}(x) (\rho * w)(x) dx + \int_{C_R} (h^d \rho_{\tilde{\gamma}_h}(x) - \rho(x)) (\rho * w)(x) dx \\ &\quad + \int_{C_R} (h^d \rho_{\tilde{\gamma}_h}(x) - \rho(x)) ((h^d \rho_{\tilde{\gamma}_h} - \rho) * w)(x) dx \\ &\xrightarrow{h \rightarrow 0} \int_{C_R} \rho(x) (\rho * w)(x) dx = D_w(\rho, \rho). \end{aligned}$$

¹³Indeed $(h^d \rho_{\tilde{\gamma}_h} - \rho) * w \rightarrow 0$ a.e. and $\{(h^d \rho_{\tilde{\gamma}_h} - \rho) * w\}_h$ bounded in C_R .

Finally, by (IV.1)

$$\begin{aligned}
 & \limsup_{h \rightarrow 0} h^d \mathcal{E}_{h, V-E, w}^{\text{HF}}(\tilde{\gamma}_h) \\
 & \leq \limsup_{h \rightarrow 0} \left(h^d \text{Tr}((-h^2 \Delta) \tilde{\gamma}_h) + h^d \int_{\mathbb{R}^d} (V(x) - E) \rho_{\tilde{\gamma}_h}(x) dx + \frac{h^{2d}}{2} D_w(\rho_{\tilde{\gamma}_h}, \rho_{\tilde{\gamma}_h}) \right) \\
 & = \frac{d}{d+2} c_{\text{TF}} \int_{\mathbb{R}^d} \rho(x)^{1+2/d} dx + \int_{\mathbb{R}^d} (V(x) - E) \rho(x) dx + \frac{1}{2} D_w(\rho, \rho) \\
 & = \mathcal{E}_{V-E, w}^{\text{TF}}(\rho).
 \end{aligned}$$

This bound is hold for any trial state $\rho \in C_c^\infty(\mathbb{R}^d, \mathbb{R}_+)$ of the Thomas-Fermi energy functional. Thus, by minimizing on all these trial states, we obtain the desired upper bound proof.

Proof of Proposition IV.3. We present now a proof of Proposition IV.3.

1) First, we verify that the operator $\tilde{\gamma}_h$ is in the set \mathcal{K} . Since $\tilde{\gamma}_h$ is a spectral projector, the condition $0 \leq \tilde{\gamma}_h \leq 1$ is immediately satisfied.

Claim IV.4 (First properties on $\tilde{\gamma}_h$). *For almost all $x \in \mathbb{R}^d$,*

$$\rho_{\tilde{\gamma}_h}(x) = \begin{cases} \rho_{\gamma_h}(x) & \text{if } x \in C_R, \\ 0 & \text{if } x \notin C_R. \end{cases}$$

Furthermore, we have

$$\text{Tr}_{L^2(\mathbb{R}^d)}((-\Delta) \tilde{\gamma}_h) = \text{Tr}_{L^2(C_R)}((-\Delta_{C_R}) \gamma_h).$$

Proof of Claim IV.4. The first inequality comes from the definition of γ_h and $\tilde{\gamma}_h$. Furthermore, recall that $\tilde{u}_j^h \in H^1(\mathbb{R}^d)$ and

$$\nabla \tilde{u}_j^h(x) = \begin{cases} \nabla u_j^h(x) & \text{if } x \in C_R, \\ 0 & \text{if } x \notin C_R. \end{cases}$$

Let us prove the second equality. Looking in the way of quadratic forms and using the equality on the gradients

$$\begin{aligned}
 \text{Tr}_{L^2(\mathbb{R}^d)}((-\Delta) \tilde{\gamma}_h) &= \text{Tr}_{L^2(\mathbb{R}^d)}(\sqrt{-\Delta} \tilde{\gamma}_h \sqrt{-\Delta}) = \int_{\mathbb{R}^d} \sum_{j=1}^{N_h} |\nabla \tilde{u}_j^h(x)|^2 dx = \int_{C_R} \sum_{j=1}^{N_h} |\nabla u_j^h(x)|^2 dx \\
 &= \text{Tr}_{L^2(C_R)}(\sqrt{-\Delta_{C_R}} \gamma_h \sqrt{-\Delta_{C_R}}) = \text{Tr}_{L^2(C_R)}((-\Delta) \gamma_h).
 \end{aligned}$$

□

This remains to prove that $\tilde{\gamma}_h$ is in the domain \mathcal{X} of $\mathcal{E}_h^{\text{HF}}$. We will treat the estimate on $\text{Tr}(\tilde{\gamma}_h)$, $\text{Tr}(V \tilde{\gamma}_h)$ and $\text{Tr}(-\Delta \tilde{\gamma}_h)$ in the second point.

2) To do so, we show that the sequence $\{h^d \rho_{\tilde{\gamma}_h}\}_h$ is bounded on $L^\infty(C_R)$ (and that it implies also Assumption 9). The idea is to use Feynman-Kac formula and the spectral properties of the Dirichlet Laplacian Δ_{C_R} on C_R . For any $\beta > 0$,

$$\gamma_h = \mathbf{1} \left(-h^2 \Delta_{C_R} - c_{\text{TF}} \rho^{2/d} \leq 0 \right) \leq e^{-\beta(-h^2 \Delta_{C_R} - c_{\text{TF}} \rho^{2/d})},$$

it is true also for the densities

$$\forall x \in \mathbb{R}^d, \quad \rho_{\tilde{\gamma}_h}(x) \leq \left| e^{-\beta(-h^2\Delta_{C_R} - c_{\text{TF}}\rho^{2/d})(x, x)} \right|.$$

Let us explain how we get by hand

$$\left| e^{-\beta(-h^2\Delta_{C_R} - c_{\text{TF}}\rho^{2/d})(x, y)} \right| \leq e^{c_{\text{TF}}\beta\|\rho\|_{L^\infty}^{2/d}} e^{h^2\Delta_{C_R}(x, y)}. \quad (\text{IV.4})$$

Details. For any $n \in \mathbb{N}^*$, we write the kernel of the non-negative operator $(e^{\beta h^2\Delta_{C_R}/n} e^{\beta c_{\text{TF}}\rho^{2/d}(x)/n})^n$

$$\begin{aligned} & \left| (e^{\beta h^2\Delta_{C_R}/n} e^{\beta c_{\text{TF}}\rho^{2/d}(x)/n})^n(x, y) \right| \\ &= \left| \int_{(C_R)^{n-1}} e^{\beta h^2/n\Delta_{C_R}(x, x_1)} e^{\beta/n c_{\text{TF}}\rho(x_1)^{2/d}} \dots e^{\beta h^2/n\Delta_{C_R}(x_{n-1}, y)} e^{\beta/n c_{\text{TF}}\rho(y)^{2/d}} dx_1 \dots dx_{n-1} \right| \\ &\leq \|e^{\beta/n c_{\text{TF}}\rho^{2/d}}\|_{L^\infty}^n \int_{(C_R)^{n-1}} \left| e^{\beta h^2/n\Delta_{C_R}(x, x_1)} \right| \dots \left| e^{\beta h^2/n\Delta_{C_R}(x_{n-1}, y)} \right| dx_1 \dots dx_{n-1} \\ &= e^{\beta c_{\text{TF}}\|\rho\|_{L^\infty}^{2/d}} \int_{(C_R)^{n-1}} e^{\beta h^2/n\Delta_{C_R}(x, x_1)} \dots e^{\beta h^2/n\Delta_{C_R}(x_{n-1}, y)} dx_1 \dots dx_{n-1} \\ &= e^{\beta c_{\text{TF}}\|\rho\|_{L^\infty}^{2/d}} (e^{\beta h^2\Delta_{C_R}/n})^n(x, y) = e^{\beta c_{\text{TF}}\|\rho\|_{L^\infty}^{2/d}} e^{\beta h^2\Delta_{C_R}(x, y)}. \end{aligned}$$

Here, we used that the explicit expression of the operator $e^{\beta h^2\Delta_{C_R}/n} e^{\beta c_{\text{TF}}\rho^{2/d}(x)/n}$'s integral kernel and that the kernel $e^{\beta c_{\text{TF}}\rho^{2/d}(x)/n}$ is non-negative. Furthermore, the last equality follows from the properties of the semigroup $\{e^{t\Delta_{C_R}}\}_{t \geq 0}$ on $L^2(C_R)$. We apply now the Trotter-Kato formula

$$e^{A+B} = \lim_{n \rightarrow \infty} \left(e^{A/n} e^{B/n} \right)^n \quad \text{in } \mathfrak{S}^\infty(L^2(C_R)),$$

to the non-negative operators $A = \beta h^2\Delta_{C_R}$ and the multiplication operator $B = \beta c_{\text{TF}}\rho^{2/d}(x)$. Hence, given the previous estimate, we obtain the bound (IV.4). \square

Let $\{(\frac{2}{R})^{d/2} \prod_{j=1}^d \sin(n_j \frac{2\pi}{R}(x_j - \frac{2}{R}))\}_{n \in (\mathbb{N} \setminus \{0\})^d}$ a family of normalized eigenfunctions of Δ_{C_R} , they are associated to the eigenvalues $\frac{\pi^2}{(R/2)} \sum_{j=1}^d n_j^2$. Thus, we get by the functional calculus

$$\begin{aligned} e^{h^2\beta\Delta_{C_R}(x, x)} &\leq \left(\frac{2}{R}\right)^d \sum_{n_1, \dots, n_d \in \mathbb{N} \setminus \{0\}} e^{-h^2\beta \frac{\pi^2}{(R/2)^2} \sum_{j=1}^d n_j^2} \underbrace{\prod_{j=1}^d \sin\left(n_j \frac{2\pi}{R}\left(x_j - \frac{2}{R}\right)\right)}_{\leq 1} \\ &\leq \left(\frac{2}{R}\right)^d \left(\sum_{n \in \mathbb{N}} e^{-h^2\beta \frac{\pi^2}{(R/2)^2} |n|^2} \right)^d \\ &\leq \left(\frac{2}{R}\right)^d \left(\int_{\mathbb{R}} e^{-h^2\beta \frac{\pi^2}{(R/2)^2} |t|^2} dt \right)^d = \left(\frac{2}{R}\right)^d h^{-d} (\beta\pi^2)^{-d/2} \left(\frac{R}{2}\right)^d \pi^{d/2} \\ &= h^{-d} \beta^{-d/2} \pi^{-d/2}. \end{aligned}$$

By (IV.4), for any $\beta > 0$ and any $x \in \mathbb{R}^d$

$$\rho_{\tilde{\gamma}_h}(x) \leq h^{-d} \pi^{-d/2} e^{\beta c_{\text{TF}}\|\rho\|_{L^\infty}^{2/d}} \beta^{-d/2}.$$

Now, after optimizing on β . For instance with $\beta = c_{\text{TF}}^{-1} \|\rho\|_{L^\infty}^{-2/d}$, we have for any $h > 0$ and any $x \in \mathbb{R}^{d14}$

$$\rho_{\tilde{\gamma}_h}(x) \leq h^{-d} e^{(\pi c_{\text{TF}})^{-d/2}} \|\rho\|_{L^\infty}. \quad (\text{IV.5})$$

Let us now estimate $\text{Tr}(\gamma_h)$, $\text{Tr}(V\gamma_h)$ and $\text{Tr}(-h^2\Delta_{C_R}\gamma_h)$. Since $\rho_{\tilde{\gamma}_h}$ is compactly supported in C_R ,

$$\text{Tr}_{L^2(\mathbb{R}^d)}(\tilde{\gamma}_h) = \int_{\mathbb{R}^d} \rho_{\tilde{\gamma}_h}(x) dx = \int_{C_R} \rho_{\tilde{\gamma}_h}(x) dx = \int_{C_R} \rho_{\gamma_h}(x) dx \leq |C_R| \|\rho_{\gamma_h}\|_{L^\infty(\mathbb{R}^d)} \leq Ch^{-d}.$$

As well,

$$\int_{\mathbb{R}^d} V(x) \rho_{\tilde{\gamma}_h}(x) dx \leq \|V\|_{L^\infty(C_R)} \text{Tr}(\tilde{\gamma}_h) \leq Ch^{-d}.$$

As a consequence of the boundedness of $\{h^d \rho_{\tilde{\gamma}_h}\}_h$ in $L^\infty(\mathbb{R}^d)$ uniformly in h , there exists $\tilde{\rho}$ such that up to a subsequence, $h^d \rho_{\tilde{\gamma}_h} \rightharpoonup \tilde{\rho}$ weakly-* in $L^\infty(\mathbb{R}^d)$. We got almost (IV.3) but with $\tilde{\rho}$ instead of ρ

$$h^d \text{Tr}(\tilde{\gamma}_h) = h^d \int_{\mathbb{R}^d} \rho_{\tilde{\gamma}_h}(x) dx = h^d \int_{C_R} \rho_{\tilde{\gamma}_h}(x) dx \xrightarrow{h \rightarrow 0} \int_{C_R} \tilde{\rho}(x) dx = \int_{\mathbb{R}^d} \tilde{\rho}(x) dx.$$

Furthermore, notice that

$$\begin{aligned} & h^d \text{Tr}_{L^2(C_R)}(-h^2\Delta_{C_R}\gamma_h) - c_{\text{TF}} h^d \int_{C_R} \rho(x) \rho_{\gamma_h}(x) dx \\ &= h^d \text{Tr}_{L^2(C_R)}((-h^2\Delta_{C_R} - c_{\text{TF}}\rho^{2/d})\gamma_h) \\ &= -h^d \text{Tr}_{L^2(C_R)}((-h^2\Delta_{C_R} - c_{\text{TF}}\rho^{2/d})_-) \\ &\leq 0. \end{aligned} \quad (\text{IV.6})$$

Combining the previous inequality with by (IV.5), we deduce the uniform bound

$$\begin{aligned} h^d \text{Tr}_{L^2(\mathbb{R}^d)}(-h^2\Delta\tilde{\gamma}_h) &= h^d \text{Tr}_{L^2(C_R)}(-h^2\Delta_{C_R}\gamma_h) \\ &\leq c_{\text{TF}} h^d \int_{C_R} \rho(x) \rho_{\gamma_h}(x) dx \leq c_{\text{TF}} \|\rho\|_{L^1} \|h^d \rho_{\gamma_h}\|_{L^\infty} \\ &\leq e\pi^{-d/2} c_{\text{TF}}^{1-d/2} \|\rho\|_{L^1} \|\rho\|_{L^\infty}. \end{aligned}$$

Thus, we get Assumption 9.

3) It is now time to show that $\tilde{\rho} = \rho$. This equality will imply the asymptotics (IV.3). It is here where appear Husimi transform and coherent states.

Let $f \in H^1(\mathbb{R}^d)$ be an even real-valued function such that $\|f\|_{L^2(\mathbb{R}^d)} = 1$. Let us set the semiclassical measure $m_h := m_{\gamma_h, h, f}$. From the relation (II.3) and Claim II.16, we deduce the weak-* limit $\rho_{\tilde{m}_h} \rightharpoonup \tilde{\rho}$ on $L^\infty(\mathbb{R}^d)$.

By Claim II.17, we have that $\{m_h\}_h \subset L^1(\mathbb{R}^d \times \mathbb{R}^d)$ is bounded and $0 \leq m_h \leq 1$. Thus, up to extraction of a subsequence, $\{m_h\}_h$ admits a weak-* limit \tilde{m} on $L^\infty(\mathbb{R}^d)$. Then, to prove that $\tilde{\rho} = \rho_m$, it remains to show that $\tilde{m} = m$ and that $\rho_{m_h} \rightharpoonup \rho_{\tilde{m}}$. To do so, we use Lemma II.18 applied to $\tilde{\gamma}_h$, which links the kinetic part of the Vlasov energy $\mathcal{E}_{V,w}^{\text{Vlas}}$ of m_h to the kinetic part of the h -Hartree-Fock energy $\mathcal{E}_{h, \tilde{V}, w}^{\text{HF}}$ of $\tilde{\gamma}_h$ and Claim II.14. The last result relies on the weak

¹⁴This bound is also held by ρ_{γ_h} on C_R .

convergence of m_h to \tilde{m} and the fact that $\iint |\xi|^2 m_h(x, \xi) dx d\xi$ is uniformly bounded. Indeed, by Assumption 9 and the equality (II.4)

$$\forall h > 0 \quad \iint_{\mathbb{R}^d \times \mathbb{R}^d} |\xi|^2 m_h(x, \xi) dx d\xi = (2\pi h)^d \left[\text{Tr}(-h^2 \Delta \tilde{\gamma}_h) + h \text{Tr}(\tilde{\gamma}_h) \|\nabla f\|_{L^2(\mathbb{R}^d)}^2 \right] \lesssim 1.$$

By Assumption 9, we have $h^{d+1} \text{Tr}(\tilde{\gamma}_h) = \mathcal{O}(h)$. Furthermore, using that $\{|f_h|^2\}_h$ is an approximation of the identity, for any $\tilde{V} \in C_c^\infty(\mathbb{R}^d)$

$$\begin{aligned} h^d \left| \int_{\mathbb{R}^d} (\tilde{V}(x) - (\tilde{V} * |f_h|^2)(x)) \rho_{\tilde{\gamma}_h}(x) dx \right| &= h^d \left| \int_{C_R} (\tilde{V}(x) - (\tilde{V} * |f_h|^2)(x)) \rho_{\tilde{\gamma}_h}(x) dx \right| \\ &\leq \|\tilde{V} - \tilde{V} * |f_h|^2\|_{L^\infty(\mathbb{R}^d)} h^d \text{Tr}(\tilde{\gamma}_h) \\ &\leq C \|\tilde{V} - \tilde{V} * |f_h|^2\|_{L^\infty(\mathbb{R}^d)} \\ &\xrightarrow{h \rightarrow 0} 0. \end{aligned}$$

From Lemma II.18, Fatou's lemma and Claim II.14 with the test function $-c_{\text{TF}} \rho^{2/d}$

$$\begin{aligned} &\lim_{h \rightarrow 0} h^d \text{Tr}_{L^2(\mathbb{R}^d)}((-h^2 \Delta - c_{\text{TF}} \rho(x)^{2/d}) \tilde{\gamma}_h) \\ &= \lim_{h \rightarrow 0} \left[\frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 - c_{\text{TF}} \rho(x)^{2/d}) m_h(x, \xi) dx d\xi \right. \\ &\quad \left. - h^{d+1} \text{Tr}(\gamma_h) \|\nabla f\|_{L^2(\mathbb{R}^d)}^2 + h^d \int_{\mathbb{R}^d} (c_{\text{TF}} \rho(x)^{2/d} * |f_h|^2)(x) - c_{\text{TF}} \rho(x)^{2/d} \rho_{\gamma_h}(x) dx \right] \\ &= \lim_{h \rightarrow 0} \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 - c_{\text{TF}} \rho(x)^{2/d}) m_h(x, \xi) dx d\xi \\ &\geq \liminf_{h \rightarrow 0} \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |\xi|^2 m_h(x, \xi) dx d\xi - \lim_{h \rightarrow 0} \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} c_{\text{TF}} \rho(x)^{2/d} m_h(x, \xi) dx d\xi \\ &\geq \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 - c_{\text{TF}} \rho(x)^{2/d}) \tilde{m}(x, \xi) dx d\xi. \end{aligned}$$

Besides, by (IV.6), the integrated Weyl law (Proposition II.20 applied to $\Omega = C_R$) and Claim IV.4

$$\begin{aligned} &\lim_{h \rightarrow 0} h^d \text{Tr}_{L^2(\mathbb{R}^d)}((-h^2 \Delta - c_{\text{TF}} \rho(x)^{2/d}) \gamma_h) = \lim_{h \rightarrow 0} h^d \text{Tr}_{L^2(C_R)}((-h^2 \Delta_{C_R} - c_{\text{TF}} \rho(x)^{2/d}) \tilde{\gamma}_h) \\ &= \lim_{h \rightarrow 0} -h^d \text{Tr}_{L^2(C_R)}((-h^2 \Delta_{C_R} - c_{\text{TF}} \rho(x)^{2/d})_-) \\ &= -\frac{1}{(2\pi)^d} \iint_{C_R \times \mathbb{R}^d} (|\xi|^2 - c_{\text{TF}} \rho(x)^{2/d})_- dx d\xi = -\frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 - c_{\text{TF}} \rho(x)^{2/d})_- dx d\xi \\ &= \inf_{0 \leq m' \leq 1} \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 - c_{\text{TF}} \rho(x)^{2/d}) m'(x, \xi) dx d\xi \\ &= \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 - c_{\text{TF}} \rho(x)^{2/d}) m(x, \xi) dx d\xi. \end{aligned}$$

Thus, we deduce that \tilde{m} must be equal to the unique minimum $m(x, \xi) = \mathbf{1}(|\xi|^2 \leq c_{\text{TF}} \rho(x)^{2/d})$ of the Vlasov energy $\mathcal{E}_{-c_{\text{TF}} \rho^{2/d}, 0}^{\text{Vlas}}$. This implies with Claim II.14 the equality $\tilde{\rho} = \rho_{\tilde{m}} = \rho_m = \rho$.

Hence, with the previous equality

$$\begin{aligned} & \lim_{h \rightarrow 0} h^d \operatorname{Tr}(-h^2 \Delta_{C_R} \tilde{\gamma}_h) \\ &= \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |\xi|^2 m(x, \xi) dx d\xi + c_{\text{TF}} \underbrace{\lim_{h \rightarrow 0} \int_{\mathbb{R}^d} \rho(x)^{2/d} (h^d \rho_{\tilde{\gamma}_h}(x) - \rho_m(x)) dx}_{=0} \\ &= \frac{d}{d+2} c_{\text{TF}} \int_{\mathbb{R}^d} \rho(x)^{1+2/d} dx. \end{aligned}$$

That ends the proof of Proposition IV.3.

IV.3 The lower bound

As in the proof above of the upper bound, we get back to the limit of the reduced Hartree-Fock ground state energy (IV.7) and then

$$\liminf_{h \rightarrow 0} h^d e_{h,V-E,w}^{\text{HF}} \geq \liminf_{h \rightarrow 0} h^d e_{h,V-E,w}^{\text{rHF}} = e_{V-E,w}^{\text{TF}}.$$

Step 1. To the reduced Hartree-Fock energy. We have shown with the upper bound that

$$\limsup_{h \rightarrow 0} \inf_{\tilde{\gamma}_h \in \mathcal{K}} h^d \mathcal{E}_{h,V-E,w}^{\text{HF}}(\tilde{\gamma}_h) = e_{V-E,w}^{\text{TF}}.$$

In particular, there exists $h_0 > 0$ such that for all $h \in (0, h_0]$, the minimizers $\{\tilde{\gamma}_h\}_h$ of $\mathcal{E}_h^{\text{HF}}$ satisfy Assumption 9 (c.f. Example IV.1). Then, by Lemma IV.2, there exists $r_h \in \mathbb{R}$ such that $r_h \rightarrow 0$ as $h \rightarrow 0$

$$h^d e_{h,V-E,w}^{\text{HF}} = h^d \mathcal{E}_{h,V-E,w}^{\text{HF}}(\tilde{\gamma}_h) \geq h^d \mathcal{E}_{h,V-E,w}^{\text{rHF}}(\tilde{\gamma}_h) - r_h \geq h^d e_{h,V-E,w}^{\text{rHF}} - r_h.$$

Since $\{\tilde{\gamma}_h\}_h$ is bounded on \mathcal{K} . Hence,

$$\liminf_{h \rightarrow 0} h^d e_{h,V-E,w}^{\text{HF}} \geq \liminf_{h \rightarrow 0} h^d e_{h,V-E,w}^{\text{rHF}}.$$

Step 2. The asymptotics of the reduced Hartree-Fock ground state. It remains to prove now the semiclassical limit to the Thomas-Fermi ground state

$$\lim_{h \rightarrow 0} h^d e_{h,V-E,w}^{\text{rHF}} = e_{V-E,w}^{\text{TF}}. \quad (\text{IV.7})$$

For any $h > 0$, let $\gamma_h \in \mathcal{K}$ be an almost minimizer of the h -Hartree-Fock energy:

$$\mathcal{E}_{h,V-E,w}^{\text{HF}}(\gamma_h) = e_{h,V-E,w}^{\text{HF}} + o(h^{-d}).$$

In particular, we get $\mathcal{E}_h^{\text{HF}}(\gamma_h) \leq Ch^{-d}$, so that γ_h satisfies Assumption 9 (c.f. Example IV.1). Furthermore,

$$\lim_{h \rightarrow 0} h^d \mathcal{E}_{h,V-E,w}^{\text{HF}}(\gamma_h) = \lim_{h \rightarrow 0} h^d e_{h,V-E,w}^{\text{HF}} = \lim_{h \rightarrow 0} h^d e_{h,V-E,w}^{\text{rHF}}.$$

That limit coincides with the limit of the first order term of the h -reduced Hartree-Fock functional $h^d e_h^{\text{rHF}}$. We have shown in the upper bound proof that there exists a sequence $\{\tilde{\gamma}_h\}_h \subset \mathcal{K}$ (c.f. the consequence of Proposition IV.3) such that

$$\lim_{h \rightarrow 0} h^d \mathcal{E}_{h,V-E,w}^{\text{HF}}(\tilde{\gamma}_h) = e_{V-E,w}^{\text{TF}},$$

Thus,

$$\lim_{h \rightarrow 0} h^d e_{h,V-E,w}^{\text{HF}} = \lim_{h \rightarrow 0} h^d e_{h,V-E,w}^{\text{rHF}} \leq \lim_{h \rightarrow 0} h^d \mathcal{E}_{h,V-E,w}^{\text{rHF}}(\tilde{\gamma}_h) = e_{V-E,w}^{\text{TF}}.$$

Let $f_{x,\xi}^h$ be a coherent state defined above with the additional assumption $f \in \mathcal{S}(\mathbb{R}^d)$ and even. Define the Husimi measure m_h associated to γ_h and f .

Claim IV.5. *The sequence $\{m_h\}_h$ is a bounded sequence of trial functions for the Vlasov energy $\mathcal{E}_{V-E,w}^{\text{Vlas}}$. There exists $C > 0$ such that for any $h > 0$*

$$0 \leq m_h \leq 1, \quad \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + V(x) + 1)m_h(x, \xi) dx d\xi \leq C.$$

Proof of Claim IV.5. First, note that

$$\int_{\mathbb{R}^d} \langle x \rangle^k \rho_{\gamma_h}(x) dx \lesssim h^{-d}. \quad (\text{IV.8})$$

Details of (IV.8). Indeed, we have that $\text{Tr}(\gamma) \lesssim h^{-d}$ and $\text{Tr}(V\gamma) \lesssim h^{-d}$. Furthermore, since V has a polynomial growth (Assumption 5) and $f \in \mathcal{S}(\mathbb{R}^d)$ $|x|^k \lesssim V(x)$ for any $|x| \geq R$. Thus,

$$\begin{aligned} \int_{\mathbb{R}^d} \langle x \rangle^k \rho_{\gamma_h}(x) dx &\leq \|\langle x \rangle^k\|_{L^\infty(B_R)} \text{Tr}(\gamma_h) + C \int_{B_R} V(x) \rho_{\gamma_h}(x) dx \\ &\leq C' [\text{Tr}(\gamma_h) + \text{Tr}(V\gamma_h)] \\ &\leq C'' h^{-d}. \end{aligned}$$

□

Since V has a polynomial growth (Assumption 5)

$$\forall x \in \mathbb{R}^d, \quad |V(x)| \leq C \langle x \rangle^k,$$

and $|f^h|^2$ is L^1 -normalized, then $V * |f^h|^2$ has at most the same growth

$$\forall h > 0, \forall x \in \mathbb{R}^d, \quad |V * |f^h|^2(x)| \leq C \langle x \rangle^k.$$

Thus, by the same computations as in Lemma II.18, by (IV.8) and by Assumption 9

$$\begin{aligned} &\frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + V(x) + 1)m_h(x, \xi) dx d\xi \\ &= h^d \text{Tr}(-h^2 \Delta \gamma_h) + h^d \int_{\mathbb{R}^d} (1 + V(x) + (V * |f^h|^2)(x)) \rho_{\gamma_h}(x) dx \\ &\quad + h^{d+1} \text{Tr}(\gamma_h) \|\nabla f\|_{L^2(\mathbb{R}^d)}^2 \lesssim 1. \end{aligned}$$

□

To have the limit (IV.7), there remains to get the lower bound ¹⁵. To do so, we have to prove that

$$h^d \mathcal{E}_{h,V-E,w}^{\text{rHF}}(\gamma_h) = \mathcal{E}_{V-E,w}^{\text{Vlas}}(m_h) + \varepsilon_h, \quad (\text{IV.9})$$

Let us express the linear term and the direct term of $\mathcal{E}_h^{\text{rHF}}$ with respect to m_h and ρ_{γ_h} . By Lemma II.18,

$$\begin{aligned} h^d \text{Tr}((-h^2 \Delta + V - E)\gamma_h) &= \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + V(x) - E)m_h(x, \xi) dx d\xi \\ &\quad - h^{d+1} \text{Tr}(\gamma_h) \|\nabla f\|_{L^2(\mathbb{R}^d)}^2 + h^d \int_{\mathbb{R}^d} (V - V * (|f^h|^2))(x) \rho_{\gamma_h}(x) dx. \end{aligned}$$

¹⁵One can prove

$$h^d \mathcal{E}_{h,V-E,w}^{\text{rHF}}(\gamma_h) \geq \mathcal{E}_{V-E,w}^{\text{Vlas}}(m_h) + \varepsilon_h,$$

on a truncated function $V_M \in L^\infty(\mathbb{R}^d)$ as in [FLS18], however it is more convenient here to use the polynomial growth of V .

Thus, with Lemma II.19 for any $h \in (0, h_0]$

$$\begin{aligned} h^d \mathcal{E}_{h,V-E,w}^{\text{rHF}}(\gamma_h) &= h^d \text{Tr}((-h^2 \Delta + V - E)\gamma_h) + \frac{h^{2d}}{2} D_w(\rho_{\gamma_h}, \rho_{\gamma_h}) \\ &= \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + V - E) m_h(x, \xi) dx d\xi + \frac{1}{2} D_w(\rho_{m_h}, \rho_{m_h}) + \varepsilon_h \\ &= \mathcal{E}_{V-E,w}^{\text{Vlas}}(m_h) + \varepsilon_h, \end{aligned}$$

where

$$\begin{aligned} \varepsilon_h &= -h^{d+1} \text{Tr}(\gamma_h) \|\nabla f\|_{L^2(\mathbb{R}^d)}^2 \\ &\quad + h^d \int_{\mathbb{R}^d} (V - V * (|f^h|^2))(x) \rho_{\gamma_h}(x) dx + \frac{h^{2d}}{2} D_{w * |f^h|^2 * |f^h|^2 - w}(\rho_{\gamma_h}, \rho_{\gamma_h}). \end{aligned}$$

This remains to explain why $\varepsilon_h = o_h(1)$. It does follow from Assumption 9 and $f \in H^1(\mathbb{R}^d)$ that

$$\lim_{h \rightarrow 0} h^{d+1} \text{Tr}(\gamma_h) \|\nabla f\|_{L^2(\mathbb{R}^d)}^2 = 0.$$

Since $w \in L^p(\mathbb{R}^d) + L^\infty_\varepsilon(\mathbb{R}^d)$, for a fixed $\varepsilon > 0$, there exist $w_1 \in L^p(\mathbb{R}^d)$ and $w_\infty \in L^\infty(\mathbb{R}^d)$ such that $w = w_1 + w_\infty$ and $\|w_\infty\|_{L^\infty(\mathbb{R}^d)} \leq \varepsilon$. Since $\{|f^h|^2\}_{h>0}$ is an approximation of the unity, $w_1 - w_1 * |f^h|^2 * |f^h|^2 \rightarrow 0$ strongly in $L^p(\mathbb{R}^d)$. Furthermore, one has $\|w_\infty - w_\infty * |f^h|^2 * |f^h|^2\|_{L^\infty(\mathbb{R}^d)} \leq 2\varepsilon$. By Fact III.1

$$\begin{aligned} &\left| D_{w - w * |f^h|^2 * |f^h|^2}(\rho_{\gamma_h}, \rho_{\gamma_h}) \right| \\ &\leq C \left(\left\| w_1 - w_1 * |f^h|^2 * |f^h|^2 \right\|_{L^p(\mathbb{R}^d)} + 2\varepsilon \right) (\text{Tr}(-h^2 \Delta \gamma_h)^2 + \text{Tr}(\gamma_h)^2) \\ &\leq C'' h^{-2d} (o_h(1) + \varepsilon). \end{aligned}$$

Thus, by making $\varepsilon \rightarrow 0$

$$\lim_{h \rightarrow 0} h^{2d} D_{w - w * |f^h|^2 * |f^h|^2}(\rho_{\gamma_h}, \rho_{\gamma_h}) = 0.$$

Furthermore, using the definition of f^h and that f is normalized in $L^2(\mathbb{R}^d)$

$$\begin{aligned} V(x) - (V * |f^h|^2)(x) &= \int_{\mathbb{R}^d} (V(x) - V(x - \sqrt{h}y)) |f(y)|^2 dy \\ &= \sqrt{h} \int_{\mathbb{R}^d} \left(\int_0^1 y \cdot \nabla V(x - \sqrt{h}(1-\theta)y) d\theta \right) |f(y)|^2 dy. \end{aligned}$$

By Assumption 5, there exists $C > 0$ such that for any $x, y \in \mathbb{R}^d$, for any $\theta \in [0, 1]$

$$\left| \nabla V(x - \sqrt{h}(1-\theta)y) \right| \leq C \left(\langle x \rangle^k + \langle y \rangle^k \right).$$

Finally, using again that $f \in \mathcal{S}(\mathbb{R}^d)$, (IV.8) and Assumption 9

$$\begin{aligned} &\int_{\mathbb{R}^d} (V(x) - (V * |f^h|^2)(x)) \rho_{\gamma_h}(x) dx \\ &\leq C \sqrt{h} \left[\left(\int_{\mathbb{R}^d} \langle x \rangle^k \rho_{\gamma_h}(x) dx \right) \left(\int_{\mathbb{R}^d} |y| |f(y)|^2 dy \right) + \text{Tr}(\gamma_h) \left(\int_{\mathbb{R}^d} \langle y \rangle^{k+1} |f(y)|^2 dy \right) \right] \\ &= \mathcal{O}(h^{1/2-d}). \end{aligned}$$

That ends the proof of (IV.7).

V PROOF OF THE WEYL LAW FOR THE HARTREE-FOCK FUNCTIONAL

V.1 Weak semiclassical limit of the density: proof of Theorem 2

Before proving Theorem 2, let us state and prove a crucial ingredient: the weak lower semi-continuity of the Vlasov functional.

Lemma V.1. *Let $E \in \mathbb{R}$, $V : \mathbb{R}^d \rightarrow \mathbb{R}$ which satisfying Assumption 5 and $w \in L^{1+d/2}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ satisfying Assumption 6 (or in dimensions $d = 1, 2$, $w \in L^1(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ that satisfies Assumption 7). For any $E \in \mathbb{R}$ and any bounded sequence $\{m_h\}_h \subset \mathcal{K}_V^{\text{Vlas}}$ such that $m_h \rightharpoonup m$ weakly-* on $L^\infty(\mathbb{R}^d \times \mathbb{R}^d)$,*

$$\liminf_{h \rightarrow 0} \mathcal{E}_{V-E,w}^{\text{Vlas}}(m_h) \geq \mathcal{E}_{V-E,w}^{\text{Vlas}}(m).$$

Proof of Lemma V.1.

1) We first show that the kinetic energy $m \mapsto \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + V(x) - E)m(x, \xi) dx d\xi$ is weakly-* lower semi-continuous in $L^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ ¹⁶. Let us treat the two terms of the functional

$$\begin{aligned} & \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + V(x) - E)m_h(x, \xi) dx d\xi \\ &= \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + V(x) - E)_+ m_h(x, \xi) dx d\xi - \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + V(x) - E)_- m_h(x, \xi) dx d\xi. \end{aligned}$$

Let us introduce a radial decreasing function $\chi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d, [0, 1])$, which is equal to 1 in the ball $B_{\mathbb{R}^d \times \mathbb{R}^d}(0, 1)$ and for any $R > 0$ the cut-off function $\chi_R(x) := \chi(x/R)$. On the one hand,

$$\iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + V(x) - E)_+ m_h(x, \xi) dx d\xi \geq \iint_{\mathbb{R}^d \times \mathbb{R}^d} \chi_R(x, \xi) (|\xi|^2 + V(x) - E)_+ m_h(x, \xi) dx d\xi.$$

By taking first the limit $h \rightarrow 0$ of the left-hand side term and then $R \rightarrow \infty$ by the monotone convergence theorem

$$\liminf_{h \rightarrow 0} \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + V(x) - E)_+ m_h(x, \xi) dx d\xi \geq \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + V(x) - E)_+ m(x, \xi) dx d\xi.$$

On the other hand, since V is a confining potential, the function $(x, \xi) \mapsto (|\xi|^2 + V(x) - E)_-$ has a compact support and then is in $L^1(\mathbb{R}^d \times \mathbb{R}^d)$. Thus, using that $m_h \rightharpoonup m$ weakly-* in $L^\infty(\mathbb{R}^d \times \mathbb{R}^d)$

$$\begin{aligned} & \lim_{h \rightarrow 0} \left(- \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + V(x) - E)_- m_h(x, \xi) dx d\xi \right) \\ &= - \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + V(x) - E)_- m(x, \xi) dx d\xi. \end{aligned}$$

Finally, we recover the lower semi-continuity by adding the two limits

$$\liminf_{h \rightarrow 0} \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + V(x) - E)m_h(x, \xi) dx d\xi \geq \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + V(x) - E)m(x, \xi) dx d\xi.$$

¹⁶It is actually also true in L^q .

2) We prove now that the direct term $m \mapsto D_w(\rho_m, \rho_m)$ is strongly continuous. By Claim II.14, $\rho_{m_h} \rightharpoonup \rho_m$ weakly in $L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d)$. The choice of w makes the sequence $\{w * \rho_{m_h}\}_h$ be bounded in $L^\infty(\mathbb{R}^d)$, $w * \rho_{m_h} \rightarrow w * \rho_m$ a.e. and the weak convergence $w * \rho_{m_h} \rightharpoonup w * \rho$ in $L^1_{\text{loc}}(\mathbb{R}^d) \cap L^{1+2/d}_{\text{loc}}(\mathbb{R}^d)$. Besides, we write

$$D_w(\rho_{m_h}, \rho_{m_h}) = \int_{\mathbb{R}^d} (w * \rho_{m_h})(x) \rho_{m_h}(x) dx,$$

which can be split into two parts $\int_{B_R} (w * \rho_{m_h})(x) \rho_{m_h}(x) dx$ and $\int_{\mathbb{R}^d \setminus B_R} (w * \rho_{m_h})(x) \rho_{m_h}(x) dx$. For any fixed $R > 0$, the first part tends to $\int_{B_R} (w * \rho_m)(x) \rho_m(x) dx$ as $h \rightarrow 0$. Besides, since the sequences $\{w * \rho_{m_h}\}_h \subset L^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ and $\{V \rho_{m_h}\}_h \subset L^1(\mathbb{R}^d)$ are bounded as $h \rightarrow 0$ and V satisfies Assumption 5, there exists $C' > 0$ such that for any $R > 0$ as in Assumption 5 and any $h > 0$

$$\begin{aligned} \left| \int_{\mathbb{R}^d \setminus B_R} (w * \rho_{m_h})(x) \rho_{m_h}(x) dx \right| &\leq \left| \int_{\mathbb{R}^d} (w * \rho_{m_h})(x) \mathbb{1}(|x| \geq R) V(x)^{-1} V(x) \rho_{m_h}(x) dx \right| \\ &\leq C \langle R \rangle^{-k} \|w * \rho_{m_h}\|_{L^\infty(\mathbb{R}^d)} \int_{\mathbb{R}^d} V(x) \rho_{m_h}(x) dx \\ &< C' \langle R \rangle^{-k}. \end{aligned}$$

Therefore, as $R \rightarrow \infty$, we obtain the limit $D_w(\rho_{m_h}, \rho_{m_h}) \rightarrow D_w(\rho_m, \rho_m)$. That ends the proof of Lemma V.1. \square

Proof of Theorem 2. Let $\{\gamma_h\}_h \subset \mathcal{K}$ be an approximate minimizing sequence of the h -Hartree-Fock energies associated to the potentials $V - E$ and w . Then, there exists $\rho \geq 0$ such that $V\rho \in L^1(\mathbb{R}^d)$ and $h^d \rho_{\gamma_h} \rightharpoonup \rho$ weakly in $L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d)$ ¹⁷. In particular, ρ is a trial function of the Thomas-Fermi energy $\mathcal{E}_{V-E,w}^{\text{TF}}$. Let us explain now why ρ is a minimizer of the Thomas-Fermi energy. To do so, we link it again to the associated Vlasov energy $\mathcal{E}_{V-E,w}^{\text{Vlas}}$. Let m_h be the Husimi transform associated to γ_h and the L^2 -normalized function $f \in \mathcal{S}(\mathbb{R}^d)$. The equality (II.3) yields that $\{\rho_{m_h}\}_h \subset L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d)$ is bounded. Furthermore, by Claim II.16, we have that $\rho_{m_h} \rightharpoonup \rho$ weakly in $L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d)$. We have seen in the proof of the lower bound in Theorem 1 (see Claim IV.5 and (IV.9)) that $\{m_h\}_h$ is a minimizing sequence of the Vlasov energy:

$$\lim_{h \rightarrow 0} \mathcal{E}_{V-E,w}^{\text{Vlas}}(m_h) = \lim_{h \rightarrow 0} h^d \mathcal{E}_{h,V-E,w}^{\text{HF}}(\gamma_h) = e_{V-E,w}^{\text{TF}} = e_{V-E,w}^{\text{Vlas}}.$$

In addition since $\{m_h\}_h$ is bounded, there exists $0 \leq m \leq 1$ such that $m_h \rightharpoonup m$ weakly-* in $L^\infty(\mathbb{R}^d \times \mathbb{R}^d)$. By Lemma V.1, we deduce that the limit m is a minimizer of the Vlasov energy. Then, by Lemma II.11 there exists a minimizer ρ_{TF} of the Thomas-Fermi energy such that

$$m(x, \xi) = \mathbb{1} \left((x, \xi) : |\xi|^2 \leq c_{\text{TF}} \rho_{\text{TF}}(x)^{2/d} \right).$$

Notice, that this minimizer is nothing but ρ_m . Eventually, since the limit of $\{h^d \rho_{\gamma_h}\}_h$ and $\{\rho_{m_h}\}_h$ have the same weak limit on $L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d)$ (and that the limits are respectively ρ and ρ_m), one has $\rho = \rho_m$. Thus, the weak limit of $\{h^d \rho_{\gamma_h}\}_h$ is $\rho = \rho_{\text{TF}}$. That ends the proof of Theorem 2.

¹⁷By Example IV.1 $h^d \text{Tr}((-h^2 \Delta + V + 1)\gamma_h)$ is uniformly bounded in h . This inequality combined with the Lieb-Thirring inequality (Proposition II.4) implies that the associated sequence of densities $\{h^d \rho_{\gamma_h}\}_h$ is bounded in $L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d)$ and in $L^1(\mathbb{R}^d, V(x)dx)$.

V.2 Proof of the semiclassical integrated Weyl law (Theorem 3)

Let $\{\gamma_h\}_h$ be a sequence of almost minimizers of $\mathcal{E}_{V-E,w}^{\text{HF}}$. Let us write once again

$$\begin{aligned} & h^d \text{Tr}(\gamma_h) - \int_{\mathbb{R}^d} \rho_{\text{TF}}(x) dx \\ &= \int_{\mathbb{R}^d} (h^d \rho_{\gamma_h}(x) - \rho_{\text{TF}}(x)) dx \\ &= \int_{B_R} (h^d \rho_{\gamma_h}(x) - \rho_{\text{TF}}(x)) dx + \int_{\mathbb{R}^d \setminus B_R} (h^d \rho_{\gamma_h}(x) - \rho_{\text{TF}}(x)) dx. \end{aligned}$$

Let us explain why we can restrict ourselves to the limit of the integral on a ball. For any $R > 0$ greater than the one in Assumption 5, for any $h > 0$

$$\begin{aligned} & \left| \int_{\mathbb{R}^d \setminus B_R} (h^d \rho_{\gamma_h}(x) - \rho_{\text{TF}}(x)) dx \right| \\ &= \left| \int_{\mathbb{R}^d} \mathbf{1}(|x| \geq R) V(x)^{-1} V(x) (h^d \rho_{\gamma_h}(x) - \rho_{\text{TF}}(x)) dx \right| \\ &\leq C \langle R \rangle^{-k} \|V(h^d \rho_{\gamma_h} - \rho_{\text{TF}})\|_{L^1(\mathbb{R}^d)} \leq C' \langle R \rangle^{-k}. \end{aligned}$$

Here, we used that $\{V \rho_{\gamma_h}\}_h$ is bounded in $L^1(\mathbb{R}^d)$ and $V \rho_{\text{TF}} \in L^1(\mathbb{R}^d)$. Let $\varepsilon > 0$, we fix now $R > 0$ large enough so that

$$\left| \int_{\mathbb{R}^d \setminus B_R} (h^d \rho_{\gamma_h}(x) - \rho_{\text{TF}}(x)) dx \right| \leq \varepsilon.$$

Moreover, Theorem 2 yields that $h^d \rho_{\gamma_h} \rightharpoonup \rho_{\text{TF}}$ in $L^1(\mathbb{R}^d)$ that implies that

$$\lim_{h \rightarrow 0} \int_{B_R} (h^d \rho_{\gamma_h}(x) - \rho_{\text{TF}}(x)) dx = 0.$$

Thus,

$$\lim_{h \rightarrow 0} h^d \text{Tr}(\gamma_h) = \int_{\mathbb{R}^d} \rho_{\text{TF}}(x) dx.$$

That proves Theorem 3.

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