Semi-classical limits of large fermionic systems

A modern approach based on de Finetti theorems

Peter Skovlund Madsen

PhD dissertation
July 2019

Supervised by Søren Fournais

Department of mathematics
Aarhus University

Resumé

I denne afhandling undersøges to forskellige modeller beslægtet med mange-legeme kvantemekanik. Vi betragter store systemer af fermioniske partikler i en middelfelt-skalering og med meget generelle potentialer. Ved brug af de Finetti-teknikker introduceret for nylig i en artikel af Fournais, Lewin og Solovej, udledes effektive tæthedsfunktionaler i grænsen hvor antallet af partikler vokser mod uendelig, imens systemet er koblet til en semiklassisk grænse.

Den ene model, som betragtes, omhandler systemer af spin-$\frac{1}{2}$ fermioner i stærke, homogene magnetfelter, og med generelle betingelser på både det eksterne potential og interaktionspotentialet. For enkelthedens skyld betragtes dog kun eksterne potentialer, som vokser mod uendelig i uendelig (på engelsk "confining potentials"). I den semiklassiske grænse bevises konvergens af grundtilstandsenergien for store systemer i forskellige parameter-regimer mod grundtilstandsenergien for både et Thomas-Fermi-funktional og et Vlasov-funktional på faserummet, til ledende orden. Derudover opnår vi konvergensresultater for positionstæthederne for approksimative grundtilstande mod konvekse kombinationer af produkter af minimerende funktioner for det tilsvarende Thomas-Fermi-funktional.

Den anden model, som betragtes i denne afhandling, beskriver store systemer af spinløse fermioner ved positiv temperatur. Vi introducerer og analyserer et Vlasov-funktional på faserummet ved positiv temperatur, og vi beviser eksistensen af minimerende funktioner. Med generelle betingelser på det eksterne potential (som dog skal vokse i uendelig), og under antagelse af, at Fouriertransformationen af interaktionspotentialet er ikke-negativ, beviser vi konvergens til ledende orden af den minimale frie energi for kvantesystemet mod den minimale energi af Vlasov-funktionalet in den semiklassiske grænse. Vi opnår ydermere konvergensresultater af positionstætheder for følger af approksimative Gibbs-tilstande mod produkter af den (entydige) minimerende funktion for et Thomas-Fermi-funktional ved positiv temperatur.

Afslutningsvis indeholder afhandlingen også et kort kapitel om termodynamiske grænser for systemer af ikke-interagerende fermioner ved positiv temperatur.

Abstract

In this thesis, two different types of operators related to many-body quantum mechanics are investigated. We consider large systems of fermionic particles in a mean-field scaling and with very general potentials. Coupled to a semi-classical limit, effective density functional theories are derived in the limit as the number of particles tends to infinity, using de Finetti techniques introduced in a recent paper by Fournais, Lewin, and Solovej.

The first model considered concerns confined systems of spin-$\frac{1}{2}$ fermions in strong homogeneous magnetic fields, and with general assumptions on both the confining external potential and the inter-particle interaction potential. In the semi-classical limit, in different scaling regimes, we prove convergence of the ground state energy of large systems to that of both a Thomas-Fermi type functional and a Vlasov type functional on phase space, to leading order. We also obtain convergence results for the position densities of approximate ground states to convex combinations of products of minimizers of the corresponding Thomas-Fermi functional.

The other model considered describes large systems of spinless fermions at positive temperature. We introduce and analyse a positive temperature Vlasov type functional on phase space, and we prove the existence of minimizers. With general conditions on the (confining) external potential, and under the assumption that the interaction potential has non-negative Fourier transform, we prove convergence of minimum free energy of the quantum system to the minimum energy of the Vlasov functional in the semi-classical limit, to leading order. Furthermore, we obtain results on the convergence of states for sequences of approximate Gibbs states towards products of the (unique) minimizer of a positive temperature Thomas-Fermi functional.

Finally, the thesis contains a short chapter on thermodynamic limits of systems on non-interacting fermions at positive temperature.

Contents

Preface

I present in this thesis the results that I have obtained during my time as a graduate student at the Department of Mathematics at Aarhus University. The project was supervised by Søren Fournais.

The thesis contains a short introduction to de Finetti theorems and their applications, a presentation and discussion of the results obtained during my studies, and two papers which are to be considered the main contribution of the dissertation. The papers are

- **Paper A: Semi-classical limit of confined fermionic systems in homogeneous magnetic fields.** Submitted to Annales Henri Poincaré. Available at arXiv:1907.00629.
- **Paper B: Semi-classical limit of large fermionic systems at positive temperature.** Submitted to the Journal of Mathematical Physics. Available at arXiv:1902.00310.

Paper A is co-authored with my supervisor, Søren Fournais. While we had many fruitful discussions and did many of calculations in cooperation, I was the one to actually write the paper (except maybe for a few paraghraphs). Parts of the contents of Paper A were contained in the progress report for my qualifying exam, but the results have since been considerably generalized. The version included here is the same as the version on arXiv (which is the same as the version submitted to AHP), *except for the appendix*, which is only included in this thesis. Apart from adding the appendix, only cosmetic changes have been made to the paper, such as formatting and numbering of equations, and a few typos have been corrected as well.

Paper B is the outcome of a longer reseach stay at the University of Paris-Dauphine where I visited Mathieu Lewin to work with him and his graduate student, Arnaud Triay. Mathieu and Arnaud are both co-authors on the paper, and we all took equal part in the research, as well as the writing. The version of the paper included here is, modulo cosmetic changes and correction of a few typos, the same as the version submitted to JMP.

Finally, I have also for completeness included a supplement to the second paper where I recall and prove a few results that we use in the paper without proof. The contents of the supplement are to be considered well-known, and they do not represent new research. I have included it here because I do not know any good references that contain the exact results that we need in Paper B.

Aknowlegdements

My studies were mostly funded by the Independent Reseach Fund Denmark, but I also received financial support from the Department of Mathematics at Aarhus University while travelling, for which I am grateful.

I would like to first and foremost thank my supervisor, Søren Fournais, for his expert guidance and for the untold amount of hours spent discussing with me both technical details as well as the bigger scheme of things. Your insight has been invaluable.

I am grateful to the University of Paris-Dauphine, Mathieu Lewin, and Arnaud Triay for their hospitality during my three month stay in Paris in 2017, and also during my subsequent shorter stays in October 2018 and July 2019. I have learned a lot from both Mathieu and Arnaud during our many long discussions.

I wish to thank the Mittag-Leffler Institute, Stockholm, for hosting me during the programme "Spectral Methods in Mathematical Physics" in spring 2019. The programme was filled to the brim with exciting seminars, and it was an honor to be able to work in such inspiring surroundings.

A special thanks goes to the people who have shared office space with me the last couple of years, especially Helene and Søren (not to forget all the other beautiful nerds who have crossed my path during my time in Aarhus). You have made my time in Aarhus both exciting and enjoyable.

I also want to give thanks to Lars "daleif" Madsen for helping me set up the thesis. You truly are a LaTeX-nical sorcerer, and your help is much appreciated.

Last, but not least, I wish to thank my family and friends who have supported me unconditionally during my studies, even when they claim to not understand anything that I do.

Peter Skovlund Madsen
July 2019, Aarhus.

Chapter 1

A short introduction to de Finetti theorems

In this first chapter, I briefly introduce the theory of de Finetti theorems, mostly without proof. I will mainly follow [38] which contains a thorough introduction to the subject, and I refer the reader to this set of notes for additional details and references.

Classical de Finetti theorems

Denote by Ω a locally compact and separable metric space (one may think of Ω as being a locally compact subset of $\mathbb{R}^d$). For any topological space X, we let $\mathcal{P}(X)$ denote the space of Borel probability measures endowed with the weak-$*$ topology. Finally, for $N \in \mathbb{N}$ we let $\mathcal{P}_s(\Omega^N)$ denote the space of symmetric Borel probability measures on Ω^N, i.e. the set of measures $\mu \in \mathcal{P}(\Omega^N)$ satisfying

$$\mu(A_1, \ldots, A_N) = \mu(A_{\sigma(1)}, \ldots, A_{\sigma(N)})$$

for any permutation σ in the symmetric group $\mathcal{S}_N$, and for all Borel sets $A_i \subseteq \Omega$. This definition extends in an obvious way to measures on $\Omega^{\mathbb{N}}$.

Classically, de Finetti theorems (in the context of this thesis) describe the structure of sequences of symmetric probability measures. Loosely, one might say that a symmetric measure $\mu \in \mathcal{P}_s(\Omega^N)$ is close to a convex combination of product measures when N is large. The following theorem, due to Hewitt and Savage [14], is a generalization of de Finettis original theorem [7, 8].

Theorem 1.1 (Hewitt-Savage). *Suppose that Ω is a locally compact, separable metric space, and that $\mu \in \mathcal{P}_s(\Omega^{\mathbb{N}})$. Let $\mu^{(n)}$ be its n-th marginal,*

$$\mu^{(n)}(A_1 \times \cdots \times A_n) = \mu(A_1 \times \cdots \times A_n \times \Omega \times \cdots).$$

Then there exists a unique Borel probability measure P_μ *on* $\mathcal{P}(\Omega)$ *such that for all* $n \in \mathbb{N}$,

$$\mu^{(n)} = \int_{\mathcal{P}(\Omega)} \rho^{\otimes n} \,\mathrm{dP}_\mu(\rho),$$

where $\rho^{\otimes n}$ *is the* n*-fold product measure of* ρ.

The Hewitt-Savage theorem may be proven in several different ways. One approach is to use a quantitative approximation result at finite N, due to Diaconis and Freedman [9]. The approximation is given in terms of the total variation norm, which for non-negative measures μ on Ω is given by

$$\|\mu\|_{\mathrm{TV}} = \sup_{\substack{\phi \in C(\Omega) \\ \|\phi\|_\infty \leq 1}} \left| \int_\Omega \phi \,\mathrm{d}\mu \right| = \sup_{A \subseteq \Omega} |\mu(A)|,$$

where the last supremum is taken over all Borel subsets $A \subseteq \Omega$.

Theorem 1.2 (Diaconis-Freedman). *Let* $\mu_N \in \mathcal{P}_s(\Omega^N)$ *be a symmetric probability measure. There exists a measure* $\mathrm{P}_{\mu_N} \in \mathcal{P}(\mathcal{P}(\Omega))$ *such that, denoting*

$$\widetilde{\mu}_N := \int_{\mathcal{P}(\Omega)} \rho^{\otimes N} \,\mathrm{dP}_{\mu_N}(\rho),$$

we have

$$\left\| \mu_N^{(n)} - \widetilde{\mu}_N^{(n)} \right\|_{\mathrm{TV}} \leq 2\frac{n(n-1)}{N} \tag{1.1}$$

for $1 \leq n \leq N$.

The measure P_{μ_N} can be constructed explicitly using empirical measures (convex conbinations of Dirac delta measures). For compact Ω, one can easily prove existence in Theorem 1.1 by applying Theorem 1.2 to the marginals of μ. Because $\mathcal{P}(\mathcal{P}(\Omega))$ is also compact in this case, the de Finetti measure P_μ arises as a weak limit of the measures from Theorem 1.2. When Ω is only a locally compact, separable metric space, one can still conlude through a compactification argument.

The usefulness of de Finetti theorems has long been known in classical statistical mechanics [5, 42, 36, 6, 17]. Sometimes, the qualitative bound (1.1) can be useful for more than just proving the Hewitt-Savage theorem. Classical log-gases in a mean-field limit coupled to low temperature is an example of this [38].

The following version of the theorem, which is the one applied in the papers included in the thesis, is essentially [10, Theorem 2.6]. Because I will need a slightly more general formulation, I also include the proof, which is still essentially the proof in [10], only with a few more details.

Theorem 1.3. *Let* Ω *be a locally compact, separable metric space, and* ω *any non-zero, outer regular, and* σ*-finite Borel measure on* Ω. *Furthermore, let* $m^{(k)} \in L^1(\Omega^k)$

be a family of symmetric positive densities (with respect to ω) satisfying for some $c > 0$ and all $k \geq 1$ that $0 \leq m^{(k)} \leq 1$, and

$$c \int_\Omega m^{(k)}(\xi_1, \ldots, \xi_k)\,\mathrm{d}\omega(\xi_k) = m^{(k-1)}(\xi_1, \ldots, \xi_{k-1}) \tag{1.2}$$

with $m^{(0)} = 1$. Then there exists a unique Borel probability measure P *on the set*

$$\mathcal{S} = \left\{\mu \in L^1(\Omega) \,\middle|\, 0 \leq \mu \leq 1,\ c \int_\Omega \mu(\xi)\,\mathrm{d}\omega(\xi) = 1\right\}$$

such that for all $k \geq 1$, in the sense of measures,

$$m^{(k)} = \int_{\mathcal{S}} \mu^{\otimes k}\,\mathrm{dP}(\mu). \tag{1.3}$$

Proof. Denote by $\mathscr{B}(\Omega)$ the Borel σ-algebra on Ω. By the Kolmogorov extension theorem (see e.g. [44, Theorem 2.4.3]), there is a unique Borel probability measure m on $\Omega^{\mathbb{N}}$ such that

$$c^k m^{(k)}(A_1, \ldots, A_k) = m(A_1, \ldots, A_k, \Omega, \ldots)$$

for all $k \geq 1$ and Borel sets $A_i \in \mathscr{B}(\Omega)$. Note that the measure m is symmetric since all the $m^{(k)}$ are. Because Ω is a locally compact separable metric space, Theorem 1.1 now yields a unique Borel probability measure P on $\mathcal{P}(\Omega)$, satisfying

$$c^k m^{(k)} = \int_{\mathcal{P}(\Omega)} \rho^{\otimes k}\,\mathrm{dP}(\rho). \tag{1.4}$$

Hence we just have to show that P is supported on $\mathcal{S}$. To this end, we will show that the set $\{\rho \in \mathcal{P}(\Omega) \mid \exists A \in \mathscr{B}(\Omega)$ such that $\rho(A) > c\,\omega(A)\}$ is a null set with respect to the measure P.

Since the bound $m^{(k)} \leq 1$ implies for all $A \in \mathscr{B}(\Omega)$ that

$$m^{(k)}(A^k) \leq \omega^{\otimes k}(A^k),$$

we get for fixed A with $0 < \omega(A) < \infty$, and all $k \geq 1$ that

$$\int_{\mathcal{P}(\Omega)} \Big(\frac{\rho(A)}{c\,\omega(A)}\Big)^k \mathrm{dP}(\rho) = \frac{1}{(c\,\omega(A))^k} \int_{\mathcal{P}(\Omega)} \rho(A)^k\,\mathrm{dP}(\rho) = \frac{m^{(k)}(A^k)}{\omega^{\otimes k}(A^k)} \leq 1.$$

Consider for $n \in \mathbb{N}$ the sets

$$B_n := \{\rho \in \mathcal{P}(\Omega) \mid \rho(A) \geq c\,\omega(A)(1 + 1/n)\}.$$

Then, since P is a probability measure,

$$\begin{aligned} 1 \geq \int_{\mathcal{P}(\Omega)} \Big(\frac{\rho(A)}{c\,\omega(A)}\Big)^k \mathrm{dP}(\rho) &\geq \int_{B_n} \Big(\frac{\rho(A)}{c\,\omega(A)}\Big)^k \mathrm{dP}(\rho) \\ &\geq (1 + 1/n)^k \mathrm{P}(B_n). \end{aligned}$$

Since k is arbitrary, this forces B_n to be a P-null set for each $n \in \mathbb{N}$, implying that

$$\{\rho \in \mathcal{P}(\Omega) \mid \rho(A) > c\,\omega(A)\} = \bigcup_{n\in\mathbb{N}} B_n$$

is also a null set with respect to P.

Since Ω is a separable metric space, there exists a countable base $\mathscr{V}$ for the topology of Ω (one can e.g. choose $\mathscr{V}$ to be a collection of open balls). Let $\mathscr{A} \subseteq \mathscr{B}(\Omega)$ be the collection of finite unions of sets from $\mathscr{V}$. Then we have:

Claim. If $\rho \in \mathcal{P}(\Omega)$ satisfies $\rho(A) > c\,\omega(A)$ for some $A \in \mathscr{B}(\Omega)$, then there is a set $\widetilde{A} \in \mathscr{A}$ such that $\rho(\widetilde{A}) > c\,\omega(\widetilde{A})$.

The validity of this claim is easily checked using the outer regularity of the measure ω, along with the fact that $\mathscr{V}$ generates the topology on Ω. Indeed, suppose that $\rho(A) > c\,\omega(A)$, and assume for simplicity that $\rho(A)$ is finite. Then by the outer regularity of ω we may choose an open set B satisfying $A \subseteq B$ and $c\,\omega(B) \leq c\,\omega(A) + \varepsilon < \rho(B) + \varepsilon$. Writing $B = \bigcup_{i\geq 1} B_i$ with $B_i \in \mathscr{V}$, we may choose n such that $c\,\omega\big(\bigcup_{i=1}^n B_i\big) < \rho\big(\bigcup_{i=1}^n B_i\big) + 2\varepsilon$. Now, simply choosing $\varepsilon < \frac{1}{2}(\rho(A) - c\,\omega(A))$ proves the claim.

The claim implies that

$$\begin{aligned}&\{\rho \in \mathcal{P}(\Omega) \mid \exists A \in \mathscr{B}(\Omega) \text{ such that } \rho(A) > c\,\omega(A)\} \\ &\quad \subseteq \bigcup_{\widetilde{A}\in\mathscr{A}} \{\rho \in \mathcal{P}(\Omega) \mid \rho(\widetilde{A}) > c\,\omega(\widetilde{A})\}.\end{aligned}$$

Note that $\mathscr{A}$ is the union of countably many countable sets, so it is itself countable. Hence the right hand side above is a countable union of P-null sets, so P is supported on

$$\{\rho \in \mathcal{P}(\Omega) \mid \rho(A) \leq c\,\omega(A) \text{ for all } A \in \mathscr{B}(\Omega)\}.$$

Each measure ρ in this set is absolutely continuous with respect to ω, so since ω is σ-finite, ρ is given by a density function $\mu \in L^1(\Omega)$. Now, $\rho(A) \leq c\,\omega(A)$ for all $A \in \mathscr{B}(\Omega)$ implies that the density μ satisfies $0 \leq \mu \leq c$, and thus (up to scaling by c^{-1}) lies in $\mathcal{S}$. Finally, combining this with (1.4), we obtain (1.3). $\square$

In Paper A we will take $\Omega = \mathbb{R}^3 \times \mathbb{R} \times \mathbb{N}_0 \times \{\pm 1\}$ with ω being the product of the Lebesgue measure in the continuous variables with the counting measure in the discrete variables. In Paper B, Ω is the usual phase space $\Omega = \mathbb{R}^d \times \mathbb{R}^d$ equipped with the Lebesgue measure.

If the measures $m^{(k)}$ do not satisfy the compatibility relation (1.2), or are not probability measures, then we still have a weak version of the theorem. This is useful for handling non-confined systems where mass can be lost at infinity. The theorem below is taken verbatim from [10, Theorem 2.7].

Theorem 1.4 (weak de Finetti). *Let $m_N^{(N)}$ be a sequence of symmetric positive densities in $L^1(M^N)$, with $M \subseteq \mathbb{R}^d$, and let $m_N^{(k)}$ be its marginals defined recursively by (1.2). We assume that $m^{(0)} = 1$, that $0 \leq m_N^{(k)} \leq 1$ for every $1 \leq k \leq N$, and that $m_N^{(k)} \rightharpoonup m^{(k)}$ weakly for every fixed $k \geq 1$, as $N \to \infty$. Then there exists a Borel probability measure* P *on the set $\mathcal{B} := \{\mu \in L^1(M) \mid 0 \leq \mu \leq 1,\ c\int_M \mu \leq 1\}$ such that*

$$m^{(k)} = \int_{\mathcal{B}} \mu^{\otimes k} \, \mathrm{dP}(\mu),$$

for all $k \geq 1$.

Quantum de Finetti theorems

There are also quantum versions of the de Finetti theorem, applicable to symmetric quantum states instead of measures. However, since quantum de Finetti theorems are mostly useful for dealing with bosons, and this thesis is concerned exclusively with fermions, I will only briefly mention them in passing.

The first versions of the quantum de Finetti theorem were proven by Størmer [43] and Hudson-Moody [15]. The theorems formulated below, however, are taken from [38]. The second theorem (weak quantum de Finetti) was proven in [18] (see also [1, 2, 3] for more general results implying Theorem 1.6 below).

Let $\mathcal{H}$ be a complex, separable Hilbert space and for $n \in \mathbb{N}_0$, denote by $\mathcal{H}_s^n := \bigotimes_s^n \mathcal{H}$ the corresponding bosonic (symmetric) n-particle space (with the convention $\mathcal{H}_s^0 = \mathbb{C}$). A *bosonic state* with infinitely many particles is a sequence $(\gamma^{(n)})_{n\in\mathbb{N}_0}$ of bosonic n-particle states, that is, satisfying that $\gamma^{(n)} \in \mathfrak{S}_1(\mathcal{H}_s^n)$ is self-adjoint, positive, and $\operatorname{Tr}_{\mathcal{H}_s^n} \gamma^{(n)} = 1$, and furthermore satisfying the consistency relation

$$\operatorname{Tr}_{n+1} \gamma^{(n+1)} = \gamma^{(n)},$$

where Tr_{n+1} denotes the partial trace with respect to the last variable in $\mathcal{H}^{n+1}$.

Theorem 1.5 (Strong quantum de Finetti). *Let $\mathcal{H}$ be a separable Hilbert space and $(\gamma^{(n)})_{n\in\mathbb{N}_0}$ a bosonic state with infinitely many particles on $\mathcal{H}$. There exists a unique Borel probability measure $\mu \in \mathcal{P}(S\mathcal{H})$ on the sphere $S\mathcal{H} = \{u \in \mathcal{H} \mid \|u\| = 1\}$ of $\mathcal{H}$, invariant under the action of S^1, such that*

$$\gamma^{(n)} = \int_{S\mathcal{H}} |u^{\otimes n}\rangle\langle u^{\otimes n}| \, \mathrm{d}\mu(u)$$

for all $n \geq 0$.

Theorem 1.6 (Weak quantum de Finetti). *Let $\mathcal{H}$ be a separable Hilbert space and $(\Gamma_N)_{N\in\mathbb{N}_0}$ a sequence of bosonic states with $\Gamma_N \in \mathfrak{S}_1(\mathcal{H}_s^N)$. We assume that for all $n \in \mathbb{N}$*

$$\Gamma_N^{(n)} \rightharpoonup_* \gamma^{(n)}$$

in $\mathfrak{S}_1(\mathcal{H}_s^N)$*. Then there exists a unique probability measure* $\mu \in \mathcal{P}(B\mathcal{H})$ *on the unit ball* $B\mathcal{H} = \{u \in \mathcal{H} \mid \|u\| \leq 1\}$ *of* $\mathcal{H}$*, invariant under the action of* S^1*, such that*

$$\gamma^{(n)} = \int_{B\mathcal{H}} |u^{\otimes n}\rangle\langle u^{\otimes n}| \, \mathrm{d}\mu(u)$$

for all $n \geq 0$*.*

When dealing with bosonic systems, one has the advantage that the quantum de Finetti theorems are applicable directly to the quantum states of the system. However, in the case of fermionic systems, one usually has to reduce the problem to a case where a classical de Finetti theorem is applicable, since the quantum theorems do not work on anti-symmetric states. Hence, in the fermionic case, one tends to only obtain information on position (or momentum) density functions, instead of the true quantum states.

The parts of the de Finetti theorems concerning uniqueness will not be important in the context of this thesis, since we will be considering only stationary problems. In time-dependent cases, however, uniquess can be very useful [1, 2, 3].

Chapter 2

The papers

In this chapter, I summarize the results obtained in the papers included in the thesis. Even though one paper concerns systems in strong magnetic fields while the other deals with systems at positive temperature, the models considered and the methods used in the papers feature many similarities. Both papers concern the semi-classical limits of large fermionic systems in mean-field scaling in a canonical setting. The operators considered are of the form

$$H_N = \sum_{j=1}^{N} T_j + V_j + \frac{1}{N} \sum_{1 \le j < k \le N} w_{jk}, \tag{2.1}$$

where T is a kinetic energy operator acting on a one-particle Hilbert space $\mathcal{H}$ (in both papers some appropriate L^2 space), V is an external potential, and w models a pairwise particle interaction. The operator acts a priori on the N-fold tensor product $\mathcal{H}^{\otimes N} = \bigotimes^N \mathcal{H}$, but since the papers deal exclusively with fermions, we restrict H_N to the subspace of anti-symmetric tensors $\bigwedge^N \mathcal{H}$. In the notation above, T_j denotes the operator

$$T_j = \mathbb{1}^{\otimes(j-1)} \otimes T \otimes \mathbb{1}^{\otimes(N-j)}$$

acting on the jth component of $\mathcal{H}^{\otimes N}$, with $\mathbb{1}$ being the identity on $\mathcal{H}$. The kinetic energy T is coupled to a semi-classical parameter (omitted from the notation here) that we let tend to zero in the large N limit.

In both papers the aim is to evaluate the ground state energy to leading order in N, as well as to obtain convergence results for sequences of approximate minimizers in the large N limit. We ignore all questions concerning dynamics, and deal exclusively with the stationary case. Many-body operators like (2.1) quickly become difficult to handle explicitly when N is large, so it is natural to derive effective theories exhibiting properties similar to the true quantum mechanical model. In the context of fermions, these are usually density functional theories like Thomas-Fermi or Vlasov type theories [26, 37, 13, 10]. For bosons, the mean-field limit can usually be described using Hartree or Gross-Pitaevski theory [18, 40, 4, 31, 32].

A crucial tool in both Papers A and B is the application of a de Finetti theorem to achieve good lower bounds on the energy, and to obtain information on the structure of approximate ground states in the $N \to \infty$ limit. The idea of using de Finetti theorems in the context of many-body quantum mechanics was recently developed in a series of papers by Lewin, Nam, and Rougerie for bosons [18, 19, 20], and by Fournais, Lewin, and Solovej for fermions [10]. However, applications in classical statistical mechanics have been known for a longer time [5, 42, 36, 6, 17], as previously mentioned in Chapter 1.

De Finetti techniques are particularly useful for controlling the contribution of general interactions to the ground state energy. In the case of Coulomb systems, one would typically resort to the Lieb-Oxford inequality [23], or something similar, to achieve a good lower bound on the interaction energy using a one-body potential. However, the application of de Finetti techniques opens up the possibility of handling much more general interactions that cannot easily be approximated using one-body potentials.

Various versions of the Lieb-Thirring inequality [29, 30, 28, 24] constitute another important, though well-known, tool. Being able to control the kinetic energy in terms of one-body position densities is extremely useful, and forms the backbone of many approximation arguments.

2.1 Paper A: Semi-classical limit of confined fermionic systems in homogeneous magnetic fields

In this paper, we consider three-dimensional systems in the presence of a strong homogeneous magnetic field, at zero temperature. For simplicity, we deal only with confined systems, but our results should be easily generalizable to also include non-confining external potentials. Because we want to allow for strong magnetic fields, it is important to account for the spin of the particles. Therefore, the kinetic energy of a particle is described by the Pauli operator

$$H(\hbar, b) = (\boldsymbol{\sigma} \cdot (-i\hbar\nabla + bA(x)))^2$$

acting on spinor-valued functions $L^2(\mathbb{R}^3; \mathbb{C}^2)$, where $\hbar > 0$ is a semi-classical parameter, $b \geq 0$ the magnetic field strength, and $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ denotes the vector of Pauli spin matrices

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

The magnetic potential is denoted by A, and since the magnetic field is homogeneous, we settle on the canonical choice $A(x) = \frac{1}{2}(-x_2, x_1, 0)$ giving rise to the constant field $\boldsymbol{B} = \operatorname{curl} bA = (0, 0, b)$. Because of the well-known decomposition of the spectrum of

$H(\hbar, b)$ into Landau bands

$$p^2 + 2\hbar b j, \qquad p \in \mathbb{R},\, j \in \mathbb{N}_0,$$

the phase space naturally becomes

$$\Omega = \mathbb{R}^3 \times \mathbb{R} \times \mathbb{N}_0 \times \{\pm 1\}.$$

Here, $\mathbb{R}^3$ is interpreted as position variables, $\mathbb{R} \times \mathbb{N}_0$ as momentum variables, and $\{\pm 1\}$ as a spin variable.

The Hamiltonian for the N-body system is

$$H_{N,\hbar,b} := \sum_{j=1}^{N} (\boldsymbol{\sigma} \cdot (-i\hbar\nabla_j + bA(x_j)))^2 + V(x_j) + \frac{1}{N}\sum_{j<k}^{N} w(x_j - x_k),$$

acting on the Hilbert space $\bigwedge^N L^2(\mathbb{R}^3; \mathbb{C}^2) \simeq \bigwedge^N L^2(\mathbb{R}^3 \times \{\pm 1\}; \mathbb{C})$, where V and w are functions on $\mathbb{R}^3$. This operator has been considered in [46, 27, 28] in the case where w is a Coulomb interaction, $w(x) = |x|^{-1}$. In [27] the magnetic field strength grows so quickly that semi-classical analysis breaks down, and this regime is not considered in our paper. The main motivation for this work is partly to generalize the results obtained in [28], and partly to generalize de Finetti techniques [10] to magnetic semi-classics.

In the regime we consider, the parameters $\hbar$ and b can be parametrized by

$$\hbar = N^{-\frac{1}{3}}(1 + \beta_N)^{\frac{1}{5}}, \qquad b = N^{\frac{1}{3}}\beta_N(1 + \beta_N)^{-\frac{3}{5}}, \tag{2.2}$$

where $(\beta_N)_N$ is a sequence of positive numbers with $\beta := \lim_{N\to\infty} \beta_N \in (0, \infty)$, and we denote $H_{N,\beta_N} = H_{N,\hbar,b}$ when $\hbar$ and b satisfy (2.2). This choice of scaling may seem strange at first glance, but it ensures that the terms of H_{N,β_N} are of the same order in N, and furthermore, it coincides with the notation in [28]. I refer the reader to Section A.1 for some heuristic arguments explaining why this scaling is reasonable. We also deal with the extreme cases $\beta = 0$ and $\beta = \infty$, but for simplicity I will omit the finer details of these cases from this summary and refer the reader to the paper.

The ground state energy of H_{N,β_N} is denoted by

$$E(N, \beta_N) := \inf \sigma_{\bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)}(H_{N,\beta_N}).$$

In the $N \to \infty$ limit, we find that $E(N, \beta_N)$ to is described leading order by a magnetic Thomas-Fermi type functional. It is given by

$$\begin{aligned} \widetilde{\mathcal{E}}_\beta^{\mathrm{MTF}}(\rho) = {} & \sum_{s=\pm 1} \int_{\mathbb{R}^3} \widetilde{\tau}_\beta(\rho(x,s), s)\,\mathrm{d}x + \sum_{s=\pm 1} \int_{\mathbb{R}^3} V(x)\rho(x,s)\,\mathrm{d}x \\ & + \frac{1}{2} \sum_{s_1,s_2=\pm 1} \iint_{\mathbb{R}^6} w(x-y)\rho(x,s_1)\rho(y,s_2)\,\mathrm{d}x\,\mathrm{d}y, \end{aligned}$$

defined on an appropriate set of densities $\rho \in L^1(\mathbb{R}^3 \times \{\pm 1\})$. The kinetic energy density $\widetilde{\tau}_\beta$ is given by the Legendre transform of a scaled pressure function,

$$\widetilde{\tau}_\beta(t, s) = \sup_{\nu \geq 0}(t\nu - (1+\beta)^{-\frac{3}{5}} \widetilde{P}_{k_\beta}(\nu, s)),$$

where $k_\beta := \beta(1+\beta)^{-2/5} = \lim_{N\to\infty} \hbar b$ is half the distance between the Landau bands in the limit, and for $B, \nu \geq 0$, and $s = \pm 1$, the pressure is given by

$$\widetilde{P}_B(\nu, s) = \frac{B}{3\pi^2} \sum_{j=0}^{\infty} [B(2j+1+s) - \nu]_-^{\frac{3}{2}}.$$

The corresponding Thomas-Fermi ground state energy is

$$\widetilde{E}^{\mathrm{MTF}}(\beta) = \inf\big\{\widetilde{\mathcal{E}}_\beta^{\mathrm{MTF}}(\rho) \,\big|\, 0 \leq \rho \in L^1(\mathbb{R}^3 \times \{\pm 1\}), \int \rho = 1\big\}.$$

This magnetic Thomas-Fermi functional is very similar to the one in [28], the only difference being that we keep account of the spin variable. The functional in [28] is recovered by instead using the spin-summed pressure $P_B(\nu) = \widetilde{P}_B(\nu, -1) + \widetilde{P}_B(\nu, 1)$ in the definition of the kinetic energy density above.

The main results of the paper are the following (in the case $\beta \neq 0, \infty$):

Theorem 2.1 (Convergence of energy). *Let $w \in L^{5/2}(\mathbb{R}^3) + L^\infty_\varepsilon(\mathbb{R}^3)$ be an even function, and $V \in L^{5/2}_{\mathrm{loc}}(\mathbb{R}^3)$ with $V(x) \to \infty$ as $|x| \to \infty$. Let (β_N) be a sequence of positive real numbers satisfying $\beta_N \to \beta \in (0, \infty)$. Then we have convergence of the ground state energy per particle*

$$\lim_{N\to\infty} \frac{E(N, \beta_N)}{N} = \widetilde{E}^{\mathrm{MTF}}(\beta).$$

Recall that $L^{5/2}(\mathbb{R}^3) + L^\infty_\varepsilon(\mathbb{R}^3)$ is the space of functions f satisfying that for each $\varepsilon > 0$ there exist $f_1 \in L^{5/2}(\mathbb{R}^3)$ and $f_2 \in L^\infty(\mathbb{R}^3)$ such that $\|f_2\|_\infty \leq \varepsilon$ and $f = f_1 + f_2$. I also recall the k-particle reduced position density of a wave function $\Psi \in \bigwedge^N L^2(\mathbb{R}^3; \mathbb{C}^2)$,

$$\widetilde{\rho}_\Psi^{(k)}(z_1, \ldots, z_k) = \binom{N}{k} \int_{(\mathbb{R}^3 \times \{\pm 1\})^{(N-k)}} |\Psi(z_1, \ldots, z_N)|^2 \,\mathrm{d}z_{k+1} \cdots \mathrm{d}z_N.$$

Theorem 2.2 (Convergence of states). *Suppose that the assumptions of Theorem 2.1 are satisfied. Let $\Psi_N \in \bigwedge^N L^2(\mathbb{R}^3; \mathbb{C}^2)$ be a sequence of normalized approximate ground states, i.e. satisfying $\langle \Psi_N, H_{N,\beta_N} \Psi_N \rangle = E(N, \beta_N) + o(N)$. Denote by $\mathcal{M}_\beta$ the set of minimizers of the magnetic Thomas-Fermi functional,*

$$\mathcal{M}_\beta = \big\{0 \leq \rho \in L^1(\mathbb{R}^3 \times \{\pm 1\}) \,\big|\, \widetilde{\mathcal{E}}_\beta^{\mathrm{MTF}}(\rho) = \widetilde{E}^{\mathrm{MTF}}(\beta), \int \rho = 1\big\},$$

Then there exist a subsequence $(N_\ell) \subseteq \mathbb{N}$ and a Borel probability measure $\mathscr{P}$ on $\mathcal{M}_\beta$ such that for $\varphi \in L^{5/2}(\mathbb{R}^3 \times \{\pm 1\}) + L^\infty(\mathbb{R}^3 \times \{\pm 1\})$ if $k = 1$, and for any bounded and uniformly continuous function φ on $(\mathbb{R}^3 \times \{\pm 1\})^k$ if $k \geq 2$, we have

$$\frac{k!}{N_\ell^k} \sum_{s \in \{\pm 1\}^k} \int_{\mathbb{R}^{3k}} \widetilde{\rho}^{(k)}_{\Psi_{N_\ell}}(x,s)\varphi(x,s)\,\mathrm{d}x \longrightarrow \int_{\mathcal{M}_\beta} \left(\sum_{s \in \{\pm 1\}^k} \int_{\mathbb{R}^{3k}} \rho^{\otimes k}(x,s)\varphi(x,s)\,\mathrm{d}x \right) \mathrm{d}\mathscr{P}(\rho),$$

as ℓ tends to infinity.

We also obtain analogous results if the parameter β_N tends to either zero or infinity, where, in the latter case, we also impose the additional condition $N^{-1/3}\beta_N^{1/5} \to 0$, in order to stay in the semi-classical regime, $\hbar \to 0$. In the $\beta = 0$ case, we derive the usual non-magnetic Thomas-Fermi functional in the limit, and for $\beta = \infty$, the limit is described using a strong-field Thomas-Fermi functional where only the lowest Landau band contributes to the kinetic energy.

If the interaction potential w is of positive type (i.e. has non-negative Fourier transform), then the limiting Thomas-Fermi functional is convex, so any minimizer is in this case unique. Hence the de Finetti measure $\mathscr{P}$ above is forced to be a Dirac delta $\mathscr{P} = \delta_\rho$, where ρ minimizes $\widetilde{\mathcal{E}}^{\mathrm{MTF}}_\beta$. In other words, the integral over $\mathcal{M}_\beta$ above disappears, and the k-particle position densities $\widetilde{\rho}^{(k)}_{\Psi_{N_\ell}}$ factorize completely in the limit. This is the case e.g. for Coulomb interactions, which corresponds nicely to the convergence of states result in [28] for $k = 1$. Our results for the convergence of states for $k \geq 2$ seem to be new. To the best of my knowledge, the convergence of energy was until now only proven for Coulomb interactions in the case where the external potential vanishes at infinity [28], and the same goes for the convergence of states for $k = 1$.

The upper bound on $E(N, \beta_N)$ is shown by constructing a sequence of trial states, utilizing the Weyl asymptotics for the Pauli operator obtained in [28]. The trial states can all be taken to be Slater determinants, also known as Hartree-Fock states [25, 33, 41], which are the simplest form of trial states for fermionic systems.

To prove the corresponding lower bound on the energy, a crucial step is the construction of a coherent state map $(u, p, j, s) \mapsto P^{\hbar,b}_{u,p,j,s}$ from the phase space $\Omega = \mathbb{R}^3 \times \mathbb{R} \times \mathbb{N}_0 \times \{\pm 1\}$ to the bounded operators on $L^2(\mathbb{R}^3; \mathbb{C}^2)$, satisfying

$$\frac{b}{(2\pi\hbar)^2} \sum_{s=\pm 1} \sum_{j=0}^{\infty} \iint_{\mathbb{R}^3 \times \mathbb{R}} P^{\hbar,b}_{u,p,j,s}\,\mathrm{d}u\,\mathrm{d}p = \mathbb{1}_{L^2(\mathbb{R}^3;\mathbb{C}^2)},$$

and allowing us to calculate the kinetic energy of a state (wave function) in terms of semi-classical measures on phase space.

Our coherent state operators are very similar to the ones used in [28], but there is one key difference. While the coherent states in [28] are constructed directly using

Landau band projections for the Pauli operator, our construction is instead based on Landau band projections for the magnetic Laplacian $(-i\hbar\nabla + bA)^2$ acting on $L^2(\mathbb{R}^3;\mathbb{C})$, in order to separately keep track of contributions from spin.

Using the coherent states, we define k-particle semi-classical (Husimi) measures corresponding to a state $\Psi \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ on phase space Ω^k as in [10] by

$$m^{(k)}_{f,\Psi}(\xi_1,\ldots,\xi_k) = \frac{N!}{(N-k)!}\big\langle \Psi, P^{\hbar,b}_{\xi_1}\otimes\cdots\otimes P^{\hbar,b}_{\xi_k}\otimes \mathbb{1}_{N-k}\Psi\big\rangle_{L^2(\mathbb{R}^{3N};\mathbb{C}^{2^N})},$$

where $\xi_\ell = (u_\ell, p_\ell, j_\ell, s_\ell) \in \Omega$. The presence of f on the left hand side is explained by the fact that we use some auxiliary function $f \in L^2(\mathbb{R}^3)$ in the construction of the coherent state operators, for localization purposes. The measures have the following useful properties:

Lemma 2.3 (Position densities and kinetic energy). *Let $\Psi \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ be normalized, and suppose that $f \in C^\infty_c(\mathbb{R}^3)$ is real-valued, L^2-normalized and even. Then we can recover the k-particle reduced position density of Ψ,*

$$\frac{b^k}{(2\pi\hbar)^{2k}}\sum_{j\in(\mathbb{N}_0)^k}\int_{\mathbb{R}^k} m^{(k)}_{f,\Psi}(u,p,j,s)\,\mathrm{d}p = k!\big(\widetilde{\rho}^{(k)}_\Psi * (|f^\hbar|^2)^{\otimes k}\big)(u,s),$$

where the convolution on the right hand side is the ordinary position space convolution in each spin component of $\widetilde{\rho}^{(k)}_\Psi$. Furthermore, the kinetic energy in the state Ψ can be calculated by

$$\begin{aligned}\Big\langle \Psi, \sum_{j=1}^N (\boldsymbol{\sigma}\cdot(-i\hbar\nabla_j + bA(x_j)))^2\Psi\Big\rangle &= -\hbar N\int_{\mathbb{R}^3}(\nabla f(u))^2\,\mathrm{d}u \\ &+ \frac{b}{(2\pi\hbar)^2}\sum_{s=\pm1}\sum_{j=0}^\infty\int_{\mathbb{R}}\int_{\mathbb{R}^3}(p^2 + \hbar b(2j+1+s))m^{(1)}_{f,\Psi}(u,p,j,s)\,\mathrm{d}u\,\mathrm{d}p.\end{aligned}$$

Then, after analysing sequences of such semi-classical measures, we apply a classical de Finetti theorem (Theorem 1.3) to a hierarchy of limiting measures, obtaining a de Finetti measure supported on the set of minimizers of a Vlasov type functional on phase space.

Having the external potential V to be confining simplifies the last part of the argument significantly, since the sequences of semi-classical measures in this case are tight at infinity, meaning that no mass can be lost in the limit. If V is not confining, but instead just satisfies $V \in L^{1+d/2}(\mathbb{R}^d) + L^\infty_\varepsilon(\mathbb{R}^d)$, then Theorem 2.1 should still hold exactly as stated, and Theorem 2.2 should still hold with minor modifications. In this case, a weak version of the de Finetti theorem (Theorem 1.4) is still applicable, but the convergence of the interaction energy term is more subtle. Convergence of states for non-confining V is dealt with in [10] in the case of weak magnetic fields, and the methods applied there (which are based on localization methods in Fock space) should also work for homogeneous magnetic fields.

2.2 Paper B: Semi-classical limit of large fermionic systems at positive temperature

In this paper, we consider large systems of spinless fermions in $\mathbb{R}^d$, at positive temperature. As in Paper A, we work in a mean-field scaling. The system (at zero temperature) is described by a Hamiltonian of the form

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

acting on the anti-symmetric space $\bigwedge^N L^2(\mathbb{R}^d)$. We allow for a magnetic potential in the kinetic energy, but like in [10], the assumptions on A will be weak enough such that its presence has no effect on the ground state energy to leading order. We call A a magnetic potential, even though it can also have a different physical origin (which is the case e.g. when describing the Coriolis effect for gases in a rotating frame). At inverse temperature $\beta > 0$, the free energy functional is given by

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

defined on the set of fermionic quantum states $\Gamma \in \mathfrak{S}_1(\bigwedge^N L^2(\mathbb{R}^d))$ satisfying $0 \leq \Gamma$ and $\mathrm{Tr}\,\Gamma = 1$. Because of the presence of the entropy term, we have to assume that the external potential V is confining, in order for the free energy to be bounded from below. More precisely, we work under assumptions ensuring that $\mathrm{Tr}\, e^{-\beta H_{N,\hbar}} < \infty$. If this is satisfied, the infimum of $\mathcal{E}^{N,\hbar}_{\mathrm{Can}}$ over all fermionic states is attained uniquely at the Gibbs state

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

where $Z := \mathrm{Tr}\, e^{-\beta H_{N,\hbar}}$ is the partition function, and the minimum energy is

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

The main purpose of the paper is to investigate $e^{\beta}_{\mathrm{Can}}(\hbar, N)$ to leading order in the coupled limit where $N \to \infty$ and $\hbar^d N \to \rho$ for some $\rho > 0$. The mean-field limit for fermions at positive temperature is different from the similar mean-field limit for bosons, where the free energy is known to not be affected to leading order by the temperature, but that an effect can be observed to next to leading order [18, 22].

In the coupled limit where $N \to \infty$ and $\hbar \to 0$, we derive a Vlasov type density functional on phase space $\mathbb{R}^3 \times \mathbb{R}^3$. For $\beta, \rho > 0$, the Vlasov functional is defined on measures m on phase space by

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

where $s(t)=t\log t+(1-t)\log(1-t)$ is the fermionic (Fermi-Dirac) entropy, and

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

is the position density of m. The functional is defined on measures satisfying

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

along with the Pauli principle $0\le m\le 1$. The minimal free energy is denoted by

$$e^{\beta}_{\text{Vla}}(\rho):=\inf_{\substack{0\le m\le 1\\(2\pi)^{-d}\iint_{\mathbb{R}^{2d}}m=\rho}}\mathcal{E}^{\beta,\rho}_{\text{Vla}}(m). \tag{2.3}$$

To aid us in the analysis of the mean-field problem, we do a thorough analysis of the Vlasov functional under very general assumptions on the potentials. In particular, we want to be able to include a delta distribution in the interaction w. This is useful when dealing with *dilute* limits of the quantum system, where the range of the interaction becomes small as $N\to\infty$. The main result for the Vlasov functional is the following.

Theorem 2.4 (Minimizers of the Vlasov functional). *Fix $\rho,\beta_0>0$. Suppose that $V_-\in L^{d/2}(\mathbb{R}^d)\cap L^{1+d/2}(\mathbb{R}^d)$, $A\in L^1_{\text{loc}}(\mathbb{R}^d)$ and that $V_+\in L^1_{\text{loc}}(\mathbb{R}^d)$ satisfies $\int_{\mathbb{R}^d}e^{-\beta_0V_+(x)}\,\mathrm{d}x<\infty$. Let*

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

Then, for all $\beta>\beta_0$, there are minimizers for the Vlasov problem (2.3). Any minimizer m_0 solves the nonlinear equation

$$m_0(x,p)=\frac{1}{1+\exp\big(\beta(|p+A(x)|^2+V(x)+\rho^{-1}w*\rho_{m_0}(x)-\mu)\big)}, \tag{2.4}$$

for some Lagrange multiplier μ. The minimum can be expressed in terms of m_0 and μ as

$$\begin{aligned}e^{\beta}_{\text{Vla}}(\rho)=&-\frac{1}{(2\pi)^d\beta}\iint_{\mathbb{R}^{2d}}\log\big(1+e^{-\beta(|p|^2+V(x)+\rho^{-1}w*\rho_{m_0}(x)-\mu)}\big)\,\mathrm{d}x\,\mathrm{d}p\\&+\mu\rho-\frac{1}{2\rho}\iint_{\mathbb{R}^{2d}}w(x-y)\rho_{m_0}(x)\rho_{m_0}(y)\,\mathrm{d}x\,\mathrm{d}y.\end{aligned}$$

Furthermore, if $\widehat{w} \geq 0$, then $\mathcal{E}_{\mathrm{Vla}}^{\beta,\rho}$ is strictly convex and therefore has a unique minimizer. In this case, for $\rho' > 0$ define

$$F_{\mathrm{Vla}}^{\beta}(\rho, \rho') := \inf_{\substack{0 \leq m \leq 1 \\ (2\pi)^{-d} \iint_{\mathbb{R}^{2d}} m = \rho}} \mathcal{E}_{\mathrm{Vla}}^{\beta,\rho'}(m).$$

Then, for any $\rho' > 0$, $F_{\mathrm{Vla}}^{\beta}(\,\cdot\,, \rho')$ is C^1 on $\mathbb{R}_+$ and the multiplier appearing in (2.4) is given by

$$\mu = \frac{\partial F_{\mathrm{Vla}}^{\beta}}{\partial \rho}(\rho, \rho')\Big|_{\rho'=\rho}$$

The conditions on the external potential in the theorem are chosen exactly such that the minimizer m_0 has both finite mass and finite free energy. In the case where there is no interaction, the assertions of Theorem 2.4 follow easily from simple convexity arguments. The case $w \neq 0$ is more cumbersome, but can still be dealt with using standard functional analysis techniques.

Of course, the minimization problem (2.3) can also be stated in terms of a positive temperature Thomas-Fermi model by first minimizing over measures with a fixed position density, and afterwards minimizing over a set of appropriate position densities. See Subsection B.2.1 for details.

In the canonical setting (as in the present paper) there is not much to be found in the mathematical literature concerning the mean-field limit for fermions at positive temperature. However, there are multiple rigorous works at zero temperature for atoms [25, 26] and for pseudo-relativistic stars [31, 32], along with the very general recent paper [10]. Positive temperature Thomas-Fermi theory has been treated before [37, 35, 45], and it has been derived rigorously from quantum mechanics in the case atoms in a grand canonical setting in [37], and also in the presence of a constant magnetic field [13].

The main result of the paper is the convergence of energy and of approximate minimizers in the mean-field limit. In the statement of Theorem 2.5 below, two different types of semi-classical measures appear. One of them is the Husimi measure [16, 10] defined using the usual coherent states

$$f_{x,p}^{\hbar}(y) = \hbar^{-\frac{d}{4}} f(\hbar^{-\frac{1}{2}}(x-y)) e^{i\frac{p \cdot y}{\hbar}},$$

where $f \in L^2(\mathbb{R}^d)$ is normalized and real-valued, and $(x,p) \in \mathbb{R}^d \times \mathbb{R}^d$. Denoting $P_{x,p}^{\hbar} = |f_{x,p}^{\hbar}\rangle\langle f_{x,p}^{\hbar}|$ the projection onto $f_{x,p}^{\hbar}$, the k-particle Husimi measure of a state Γ is given by

$$m_{f,\Gamma}^{(k)}(x_1, p_1, \ldots, x_k, p_k) = \frac{N!}{(N-k)!} \operatorname{Tr}(P_{x_1,p_1}^{\hbar} \otimes \cdots \otimes P_{x_k,p_k}^{\hbar} \otimes \mathbb{1}_{N-k} \Gamma),$$

for $x_1, p_1, \dots, x_k, p_k \in \mathbb{R}^d$. The other measure is the k-particle Wigner measure [34, 11, 10] of Γ defined by

$$\begin{aligned}\mathcal{W}_\Gamma^{(k)}&(x_1, p_1, \dots, x_k, p_k)\\ &= \int_{\mathbb{R}^{dk}} \int_{\mathbb{R}^{d(N-k)}} \Gamma\big((x + \frac{\hbar}{2}y, z); (x - \frac{\hbar}{2}y, z)\big) e^{-ip\cdot y}\, \mathrm{d}z\, \mathrm{d}y,\end{aligned}$$

where $x = (x_1, \dots x_k), p = (p_1, \dots, p_k) \in \mathbb{R}^{dk}$, and $\Gamma(\cdot;\cdot)$ is the kernel of the operator Γ. Both types of measures were studied at length in [10].

Theorem 2.5 (Mean-field limit). *Let $\beta_0, \rho > 0$. Assume that $V \in L^{1+d/2}_{\mathrm{loc}}(\mathbb{R}^d)$ is such that $V(x) \to \infty$ at infinity and that $\int e^{-\beta_0 V_+(x)}\, \mathrm{d}x < \infty$. Furthermore, assume $|A|^2, w \in L^{1+d/2}(\mathbb{R}^d) + L^\infty_\varepsilon(\mathbb{R}^d)$ with w even and satisfying $\widehat{w} \geq 0$. Then, for all $\beta > \beta_0$ we have the convergence*

$$\boxed{\lim_{\substack{N\to\infty \\ \hbar^d N \to \rho}} \hbar^d e^\beta_{\mathrm{Can}}(\hbar, N) = e^\beta_{\mathrm{Vla}}(\rho).}$$

Moreover, if (Γ_N) is a sequence of approximate Gibbs states, that is, satisfying

$$\mathcal{E}^{N,\hbar}_{\mathrm{Can}}(\Gamma_N) = e^\beta_{\mathrm{Can}}(\hbar, N) + o(1),$$

then the one-particle density of Γ_N satisfies the following convergence

$$\hbar^d \rho^{(1)}_{\Gamma_N} \rightharpoonup \rho_{m_0} \qquad \text{weakly in } L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d),$$

and

$$\begin{aligned} m^{(1)}_{f,\Gamma_N} &\longrightarrow m_0 && \text{strongly in } L^1(\mathbb{R}^{2d}),\\ \rho_{m^{(1)}_{f,\Gamma_N}} &\longrightarrow \rho_{m_0} && \text{strongly in } L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d),\end{aligned}$$

where $m^{(k)}_{f,\Gamma_N}$ is the k-particle Husimi function of Γ_N and m_0 is the unique minimizer of the Vlasov functional in (2.4). The k-particle Husimi functions converge weakly in the sense that

$$\int_{\mathbb{R}^{2dk}} m^{(k)}_{f,\Gamma_N} \varphi \to \int_{\mathbb{R}^{2dk}} m_0^{\otimes k} \varphi$$

for all $\varphi \in L^1(\mathbb{R}^{2dk}) + L^\infty(\mathbb{R}^{2dk})$. Similarly, if we denote by $\mathcal{W}^{(k)}_{\Gamma_N}$ the k-particle Wigner measure of Γ_N, we also have,

$$\int_{\mathbb{R}^{2dk}} \mathcal{W}^{(k)}_{\Gamma_N} \varphi \to \int_{\mathbb{R}^{2dk}} m_0^{\otimes k} \varphi,$$

for all φ satisfying $\partial^{\alpha_1}_{x_1} \cdots \partial^{\alpha_k}_{x_k} \partial^{\beta_1}_{p_1} \cdots \partial^{\beta_k}_{p_k} \varphi \in L^\infty(\mathbb{R}^{2dk})$, where $\alpha_j, \beta_j \leq 1$ for all $1 \leq j \leq k$.

We prove the upper bound on the free energy by constructing a sequence of trial states for the variational problem, following ideas of [39]. The strategy is to divide $\mathbb{R}^d$ into cubes and use the minimizer of the free energy in each cube with periodic boundary conditions. This choice allows us to control the one-body density, which will be almost constant in each cube. We then add correlations by hand (which are only needed to handle the dilute limit, see Theorem 2.6 below), and anti-symmetrize to obtain a trial state on the whole space.

Our proof of the lower bound on the free energy relies on the strong assumption that the interaction potential is of positive type ($\widehat{w} \geq 0$), but the proof of the upper bound works for general w. Without the assumption $\widehat{w} \geq 0$, we still have weak convergence of the semi-classical measures to an average of measures with respect to a de Finetti measure. That is, there exists a measure $\mathcal{P}$ on the set of densities $\mathcal{S} = \{m \in L^1(\mathbb{R}^{2d}) \,|\, 0 \leq m \leq 1,\ (2\pi)^{-d} \iint m = \rho\}$, such that, along a (not displayed) subsequence,

$$m^{(k)}_{f,\Gamma_N} \rightharpoonup \int_{\mathcal{S}} m^{\otimes k} \, \mathrm{d}\mathcal{P}(m),$$

in the same sense as in Theorem 2.5. If the entropy satisfies the following Fatou-type inequality

$$\liminf_{\substack{N\to\infty \\ \hbar^d N \to \rho}} \hbar^d \operatorname{Tr} \Gamma_N \log \Gamma_N \geq \frac{1}{(2\pi)^d} \int_{\mathcal{S}} \Big(\int_{\mathbb{R}^{2d}} s(m) \Big) \, \mathrm{d}\mathcal{P}(m),$$

then we can remove the assumption $\widehat{w} \geq 0$ from the theorem. In our proof we only obtain the weaker bound

$$\liminf_{\substack{N\to\infty \\ \hbar^d N \to \rho}} \hbar^d \operatorname{Tr} \Gamma_N \log \Gamma_N \geq \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} s\Big(\int_{\mathcal{S}} m \, \mathrm{d}\mathcal{P}(m) \Big).$$

However, when $\widehat{w} \geq 0$, it is possible to show that $\mathcal{P}$ is a point measure supported on the unique minimizer of the Vlasov functional, in which case the right hand sides of the two inequalities coincide. We do this by first proving the strong convergence of the one-particle Husimi measures towards the Vlasov minimizer, using coercive properties of the entropy. Afterwards, we use a perturbation argument inspired by a new technique recently introduced in [21] to conclude that $\mathcal{P}$ is a point measure.

Finally, we also obtain results for dilute systems where the range of the interaction depends on N. Usually, this is modelled by choosing an interaction of the form

$$w_N(x) := N^{d\eta} w(N^\eta x)$$

for some fixed parameter $\eta > 0$. In the dilute regime, the interaction often has a trivial effect in the limit, due to the Pauli principle, except in the presence of spin, or if the system contains multiple species of particles [12]. Our result in this case is as follows:

Theorem 2.6 (Dilute limit). *Let $\beta_0, \rho > 0$. We assume that $V \in L^{1+d/2}_{\mathrm{loc}}(\mathbb{R}^d)$ is such that $V(x) \to \infty$ at infinity and that $\int e^{-\beta_0 V_+(x)}\,\mathrm{d}x < \infty$. Furthermore, assume that $|A|^2 \in L^{1+d/2}(\mathbb{R}^d) + L^\infty_\varepsilon(\mathbb{R}^d)$ and $w \in L^1(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ is even.*

- *If $0 < \eta < 1/d$ and $\widehat{w} \geq 0$ then, for all $\beta > \beta_0$ we have*

$$\lim_{\substack{N\to\infty \\ \hbar^d N \to \rho}} \hbar^d e^\beta_{\mathrm{Can}}(\hbar, N) = e^{\beta, (\int_{\mathbb{R}^d} w)\delta_0}_{\mathrm{Vla}}(\rho)$$

  where $e^{\beta, (\int_{\mathbb{R}^d} w)\delta_0}_{\mathrm{Vla}}(\rho)$ is the minimum of the Vlasov energy with interaction potential $(\int_{\mathbb{R}^d} w)\delta_0$.

- *If $\eta > 1/d$, $d \geq 3$ and $w \geq 0$ is compactly supported, then for all $\beta > \beta_0$ we have*

$$\lim_{\substack{N\to\infty \\ \hbar^d N \to \rho}} \hbar^d e^\beta_{\mathrm{Can}}(\hbar, N) = e^{\beta, 0}_{\mathrm{Vla}}(\rho)$$

  where $e^{\beta,0}_{\mathrm{Vla}}(\rho)$ is the minimum of the Vlasov energy without interaction potential.

In both cases, we have the same convergence of approximate Gibbs states as in Theorem 2.5.

Compared to Theorem 2.5, the proof of Theorem 2.6 does not rely on any additional techniques, the only exception being the construction of trial states, where we take correlations into account.

Bibliography

[1] Z. Ammari and F. Nier. *Mean Field Limit for Bosons and Infinite Dimensional Phase-Space Analysis. Ann. Henri Poincaré*, **9**:1503–1574, 2008. ISSN 1424-0637. doi:10.1007/s00023-008-0393-5.

[2] Z. Ammari and F. Nier. *Mean field limit for bosons and propagation of Wigner measures. J. Math. Phys.*, **50**(4):042107, 2009.

[3] Z. Ammari and F. Nier. *Mean field propagation of Wigner measures and BBGKY hierarchies for general bosonic states. J. Math. Pures Appl.*, **95**(6):585–626, 2011.

[4] R. Benguria and E. H. Lieb. *Proof of the Stability of Highly Negative Ions in the Absence of the Pauli Principle. Phys. Rev. Lett.*, **50**:1771–1774, 1983. doi:10.1103/PhysRevLett.50.1771.

[5] W. Braun and K. Hepp. *The Vlasov dynamics and its fluctuations in the* $1/N$ *limit of interacting classical particles. Comm. Math. Phys.*, **56**(2):101–113, 1977. ISSN 0010-3616.

[6] E. Caglioti, P.-L. Lions, C. Marchioro, and M. Pulvirenti. *A special class of stationary flows for two-dimensional Euler equations: a statistical mechanics description. Comm. Math. Phys.*, **143**(3):501–525, 1992. ISSN 0010-3616.

[7] B. de Finetti. *Funzione caratteristica di un fenomeno aleatorio.* Atti della R. Accademia Nazionale dei Lincei, 1931. Ser. 6, Memorie, Classe di Scienze Fisiche, Matematiche e Naturali.

[8] B. de Finetti. *La prévision : ses lois logiques, ses sources subjectives. Ann. Inst. H. Poincaré*, **7**(1):1–68, 1937. ISSN 0365-320X.

[9] P. Diaconis and D. Freedman. *Finite exchangeable sequences. Ann. Probab.*, **8**(4):745–764, 1980. ISSN 0091-1798.

[10] S. Fournais, M. Lewin, and J. P. Solovej. *The semi-classical limit of large fermionic systems. Calc. Var. Partial Differ. Equ.*, pages 57–105, 2018. doi:10.1007/s00526-018-1374-2.

[11] J. Fröhlich, S. Graffi, and S. Schwarz. *Mean-Field and Classical Limit of Many-Body Schrödinger Dynamics for Bosons. Comm. Math. Phys.*, **271**(3):681–697, 2007. ISSN 0010-3616. doi:10.1007/s00220-007-0207-5.

[12] S. Giorgini, L. P. Pitaevskii, and S. Stringari. *Theory of ultracold atomic Fermi gases. Rev. Mod. Phys.*, **80**:1215–1274, 2008. doi:10.1103/RevModPhys.80.1215.

[13] B. Hauksson and J. Yngvason. *Asymptotic Exactness of Magnetic Thomas–Fermi Theory at Nonzero Temperature. Journal of Statistical Physics*, **116**(1):523–546, 2004. ISSN

1572-9613. doi:10.1023/B:JOSS.0000037223.74597.4e.

[14] E. Hewitt and L. J. Savage. *Symmetric measures on Cartesian products. Trans. Amer. Math. Soc.*, **80**:470–501, 1955. ISSN 0002-9947.

[15] R. L. Hudson and G. R. Moody. *Locally normal symmetric states and an analogue of de Finetti's theorem. Z. Wahrscheinlichkeitstheor. und Verw. Gebiete*, **33**(4):343–351, 1975/76.

[16] K. Husimi. *Some Formal Properties of the Density Matrix. Proc. Phys. Math. Soc. Japan*, **22**:264, 1940.

[17] M. K.-H. Kiessling. *Statistical mechanics of classical particles with logarithmic interactions. Comm. Pure. Appl. Math.*, **46**:27–56, 1993.

[18] M. Lewin, P. T. Nam, and N. Rougerie. *Derivation of Hartree's theory for generic mean-field Bose systems. Adv. Math.*, **254**:570–621, 2014. doi:10.1016/j.aim.2013.12.010.

[19] M. Lewin, P. T. Nam, and N. Rougerie. *Remarks on the quantum de Finetti theorem for bosonic systems. Appl. Math. Res. Express (AMRX)*, **2015**(1):48–63, 2015. doi:10.1093/amrx/abu006.

[20] M. Lewin, P. T. Nam, and N. Rougerie. *The mean-field approximation and the non-linear Schrödinger functional for trapped Bose gases. Trans. Amer. Math. Soc*, **368**(9):6131–6157, 2016. doi:10.1090/tran/6537.

[21] M. Lewin, P. T. Nam, and N. Rougerie. *Classical field theory limit of 2D many-body quantum Gibbs states. ArXiv e-prints*, 2018.

[22] M. Lewin, P. T. Nam, S. Serfaty, and J. P. Solovej. *Bogoliubov spectrum of interacting Bose gases. Comm. Pure Appl. Math.*, **68**(3):413–471, 2015. doi:10.1002/cpa.21519.

[23] E. H. Lieb and S. Oxford. *Improved lower bound on the indirect Coulomb energy. Int. J. Quantum Chem.*, **19**(3):427–439, 1981. doi:10.1002/qua.560190306.

[24] E. H. Lieb and R. Seiringer. *The Stability of Matter in Quantum Mechanics.* Cambridge Univ. Press, 2010.

[25] E. H. Lieb and B. Simon. *The Hartree-Fock theory for Coulomb systems. Commun. Math. Phys.*, **53**(3):185–194, 1977. ISSN 0010-3616.

[26] E. H. Lieb and B. Simon. *The Thomas-Fermi theory of atoms, molecules and solids. Adv. Math.*, **23**(1):22–116, 1977. ISSN 0001-8708.

[27] E. H. Lieb, J. P. Solovej, and J. Yngvason. *Asymptotics of heavy atoms in high magnetic fields: I. Lowest Landau band regions. Comm. Pure Appl. Math.*, **47**(4):513–591, 1994.

[28] E. H. Lieb, J. P. Solovej, and J. Yngvason. *Asymptotics of heavy atoms in high magnetic fields: II. Semiclassical regions. Comm. Math. Phys.*, **161**(1):77–124, 1994.

[29] E. H. Lieb and W. E. Thirring. *Bound on kinetic energy of fermions which proves stability of matter. Phys. Rev. Lett.*, **35**:687–689, 1975.

[30] E. H. Lieb and W. E. Thirring. *Inequalities for the moments of the eigenvalues of the Schrödinger hamiltonian and their relation to Sobolev inequalities*, pages 269–303. Studies in Mathematical Physics. Princeton University Press, 1976.

[31] E. H. Lieb and W. E. Thirring. *Gravitational collapse in quantum mechanics with relativistic kinetic energy. Ann. Physics*, **155**(2):494–512, 1984. ISSN 0003-4916.

[32] E. H. Lieb and H.-T. Yau. *The Chandrasekhar theory of stellar collapse as the limit of*

quantum mechanics. Commun. Math. Phys., **112**(1):147–174, 1987. ISSN 0010-3616.

[33] P.-L. Lions. *Solutions of Hartree-Fock equations for Coulomb systems. Commun. Math. Phys.*, **109**(1):33–97, 1987. ISSN 0010-3616.

[34] P.-L. Lions and T. Paul. *Sur les mesures de Wigner. Rev. Mat. Iberoamericana*, **9**(3):553–618, 1993. ISSN 0213-2230. doi:10.4171/RMI/143.

[35] J. Messer. *Temperature Dependent Thomas-Fermi Theory*, volume 147 of *Lecture Notes in Physics*. Springer-Verlag, 1981. ISBN 9783540108757.

[36] J. Messer and H. Spohn. *Statistical mechanics of the isothermal Lane-Emden equation. J. Statist. Phys.*, **29**(3):561–578, 1982. ISSN 0022-4715. doi:10.1007/BF01342187.

[37] H. Narnhofer and W. Thirring. *Asymptotic exactness of finite temperature Thomas-Fermi theory. Ann. Phys.*, **134**(1):128 – 140, 1981. ISSN 0003-4916. doi:10.1016/0003-4916(81)90008-7.

[38] N. Rougerie. *De Finetti theorems, mean-field limits and Bose-Einstein condensation. ArXiv e-prints*, 2015.

[39] R. Seiringer. *A correlation estimate for quantum many-body systems at positive temperature. Rev. Math. Phys.*, **18**(3):233–253, 2006. ISSN 0129-055X. doi:10.1142/S0129055X06002632.

[40] J. P. Solovej. *Asymptotics for bosonic atoms. Lett. Math. Phys.*, **20**(2):165–172, 1990. ISSN 0377-9017. doi:10.1007/BF00398282.

[41] J. P. Solovej. *The ionization conjecture in Hartree-Fock theory. Ann. of Math. (2)*, **158**(2):509–576, 2003. ISSN 0003-486X.

[42] H. Spohn. *On the Vlasov hierarchy. Math. Methods Appl. Sci.*, **3**(4):445–455, 1981. ISSN 0170-4214. doi:10.1002/mma.1670030131.

[43] E. Størmer. *Symmetric states of infinite tensor products of C^*-algebras. J. Functional Analysis*, **3**:48–68, 1969.

[44] T. Tao. *An Introduction to Measure Theory.* Graduate studies in Mathematics. American Mathematical Soc., 2013. ISBN 9780821884287.

[45] W. Thirring. *A Course in Mathematical Physics: Quantum mechanics of large systems.* A Course in Mathematical Physics. Springer-Verlag, 1983. ISBN 9780387817019.

[46] J. Yngvason. *Thomas-Fermi theory for matter in a magnetic field as a limit of quantum mechanics. Lett. Math. Phys.*, **22**(2):107–117, 1991.

Paper A

Semi-classical limit of confined fermionic systems in homogeneous magnetic fields

By S. Fournais and P. S. Madsen

Available at arXiv:1907.00629.

Abstract

We consider a system of N interacting fermions in $\mathbb{R}^3$ confined by an external potential and in the presence of a homogeneous magnetic field. The intensity of the interaction has the mean-field scaling $1/N$. With a semi-classical parameter $\hbar \sim N^{-1/3}$, we prove convergence in the large N limit to the appropriate Magnetic Thomas-Fermi type model with various strength scalings of the magnetic field.

A.1 Introduction and main results

We consider a system of N fermionic particles in $\mathbb{R}^3$ with an exterior potential V, and with the particles interacting pairwise through a potential w. The system is in the presence of a homogeneous magnetic field pointing along the z-direction, i.e. of the form $\boldsymbol{B} = (0, 0, b)$ for some $b > 0$. That is, we can take the magnetic vector potential to be $bA(x) = \frac{b}{2}(-x_2, x_1, 0)$.

A.1.1 The quantum mechanical model

Given parameters $\hbar, b > 0$, we consider the mean-field Hamiltonian operator

$$H_{N,\hbar,b} := \sum_{j=1}^{N} \big((\boldsymbol{\sigma} \cdot (-i\hbar\nabla_j + bA(x_j)))^2 + V(x_j) \big) + \frac{1}{N} \sum_{j<k}^{N} w(x_j - x_k), \tag{A.1}$$

where $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the vector of Pauli spin matrices

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

Since we are dealing with fermions, the operator $H_{N,\hbar,b}$ must be restricted to the subspace $\bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2) \subseteq L^2\big(\mathbb{R}^{3N};\mathbb{C}^{2^N}\big)$ of anti-symmetric wave functions. The anti-symmetry is due to the Pauli exclusion principle, stating that two identical fermionic particles cannot occupy the same quantum state. The fact that the system is in a mean-field scaling is expressed by the prefactor $1/N$ in front of the interaction. In mathematics, many-body fermionic systems in strong homogeneous magnetic fields have been considered before [19, 20, 21, 27, 7, 6] with Coulomb interactions, and also at positive temperature [8] in the context of pressure functionals. For references to the physics literature, see e.g. [19, 20].

Remark A.1 (Relation between parameters). *If the magnetic field strength is small or vanishing (more precisely, if $\hbar b \to 0$), and the system is confined to a bounded domain, then the kinetic energy satisfies the usual Lieb-Thirring inequality*

$$\begin{aligned}\Big\langle \Psi, \sum_{j=1}^N (\boldsymbol{\sigma}\cdot(-i\hbar\nabla_j + bA(x_j)))^2\Psi\Big\rangle \\ \geq c\hbar^2 \int_{\mathbb{R}^3} \big(\rho_\Psi^{(1)}(x)\big)^{\frac{5}{3}}\,\mathrm{d}x - \hbar b N \geq \tilde{c}\hbar^2 N^{\frac{5}{3}} - \hbar b N,\end{aligned}$$

(here the boundedness of the domain is used to get the second inequality) where $\rho_\Psi^{(1)}$ is the one-particle reduced position density of the normalized wave function $\Psi \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$, defined in (A.22) below. This means, in order for the terms in (A.1) to be of the same order in N, that we need to take $\hbar$ of order

$$\hbar \sim N^{-\frac{1}{3}}. \tag{A.2}$$

In the opposite case with a strong magnetic field (that is, $\hbar b \gg 1$), one expects, by the magnetic Lieb-Thirring inequality ((A.24) below),

$$\Big\langle \Psi, \sum_{j=1}^N (\boldsymbol{\sigma}\cdot(-i\hbar\nabla_j + bA(x_j)))^2\Psi\Big\rangle \gtrsim c\hbar^2 \frac{1}{(b/\hbar)^2} \int \big(\rho_\Psi^{(1)}(x)\big)^3\,\mathrm{d}x.$$

This inequality is not rigorous, but it is reasonable in a strong magnetic field where all particles are confined to the lowest Landau level. Assuming the inequality to hold, we get

$$\Big\langle \Psi, \sum_{j=1}^N (\boldsymbol{\sigma}\cdot(-i\hbar\nabla_j + bA(x_j)))^2\Psi\Big\rangle \geq \tilde{c}\frac{\hbar^4}{b^2}N^3 = \tilde{c}\frac{(\hbar^3 N)^2}{(\hbar b)^2}N,$$

so in order to have energy balance we take in this case

$$\hbar^3 N \sim \hbar b. \tag{A.3}$$

Based on the observations of Remark A.1, we introduce a new parameter $\beta \geq 0$ and define $\hbar$ and b by

$$\hbar := N^{-\frac{1}{3}}(1+\beta)^{\frac{1}{5}}, \qquad b := N^{\frac{1}{3}}\beta(1+\beta)^{-\frac{3}{5}}, \tag{A.4}$$

or, equivalently, by the relations

$$\hbar b = \beta(1+\beta)^{-\frac{2}{5}}, \qquad \hbar^3 N = (1+\beta)^{\frac{3}{5}}, \qquad \frac{b}{\hbar^2 N} = \frac{\beta}{1+\beta}. \tag{A.5}$$

This scaling convention interpolates between the two extreme cases (A.2) ($\beta = 0$) and (A.3) ($\beta \gg 1$). The notation is chosen to fit the notation in [20], see also Remark A.2 below.

In this paper we analyze the semi-classical limit of (A.1) as the number of particles tends to infinity and $\hbar$ tends to zero. In light of (A.4) we must thus require that

$$\lim_{N\to\infty} N^{-\frac{1}{3}}\beta^{\frac{1}{5}} = 0, \tag{A.6}$$

in order to stay in the semi-classical regime, $\hbar \to 0$.

When $\hbar$ and b satisfy the scaling convention (A.4), we will instead denote the Hamiltonian (A.1) by $H_{N,\beta}$, and the ground state energy of $H_{N,\beta}$ restricted to $\bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ will be denoted by

$$E(N,\beta) := \inf \sigma_{\bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)}(H_{N,\beta}). \tag{A.7}$$

Remark A.2. *Physical systems do not usually come with a mean-field scaling, but the Hamiltonian in question can sometimes be put in the form (A.1) by rescaling appropriately. This is true e.g. for atoms [17, 18, 20] and non-relativistic white dwarfs [22, 23], with or without magnetic fields. In the case of an atom in a homogeneous magnetic field of strength B, the Hamiltonian is*

$$H_{N,B,Z} = \sum_{j=1}^{N}\Big((\boldsymbol{\sigma}\cdot(-i\nabla_j + BA(x_j)))^2 - \frac{Z}{|x_j|}\Big) + \sum_{1\leq j<k\leq N}\frac{1}{|x_j - x_k|}.$$

Choosing parameters $\beta := BZ^{-4/3}$ and $\ell := Z^{-1/3}(1+\beta)^{-2/5}$, then $H_{N,B,Z}$ is for $Z = N$ unitarily equivalent to $Z\ell^{-1}H_{N,\beta}$, where $H_{N,\beta}$ is given by (A.1) with $V(x) = w(x) = |x|^{-1}$, and $\hbar$ and b defined by (A.4).

The analysis naturally splits into three cases, depending on the asymptotics of the parameter β. In the first case, when $\beta \to 0$, the presence of the magnetic field has no effect on the ground state energy of $H_{N,\beta}$ to leading order, and the energy in the limit is described by the usual non-magnetic Thomas-Fermi theory. In the second case, when $\beta \to \beta_0$ for some $\beta_0 \in (0,\infty)$, the energy in the semi-classical limit is described by a magnetic Thomas-Fermi theory, as already seen in [20] in the case of Coulomb interactions. In the third case, when β goes to infinity, corresponding to a strong magnetic field, all particles are forced to stay in the lowest Landau band of the magnetic Laplacian, and the limit is described by a strong-field Thomas-Fermi theory.

Suitable upper bounds on the energy $E(N,\beta)$ will be provided by constructing appropriate trial states. Corresponding lower bounds are obtained using coherent states along with a fermionic (classical) de Finetti-Hewitt-Savage theorem. The usefulness of classical de Finetti theorems [3, 9, 4] has been known for a long time in the context of classical mechanics (e.g. [1, 28, 25, 2, 11]). Recently, quantum de Finetti type theorems [29, 10] have also been used to study mean-field problems in quantum mechanics in works by Lewin, Nam and Rougerie [13, 14, 15], where the ground state energy of a mean-field *Bose* system under rather general assumptions is shown to converge to the Hartree energy of the system. The idea is further developed by Fournais, Lewin and Solovej in [5], where it is used to treat the case of spinless fermions in weak magnetic fields, and by Lewin, Triay, and the second author of the present article to treat the case of Fermi systems at positive temperature, also in weak magnetic fields [12]. See also [26] for a thorough discussion of de Finetti theorems. One of the main motivations for the present work is to extend the de Finetti technique to magnetic semiclassics.

We briefly remind the reader of the well-known fact that the spectrum of the Pauli operator $(\boldsymbol{\sigma}\cdot(-i\hbar\nabla_j+bA(x_j)))^2$ is parametrized by the Landau bands

$$p^2+2\hbar bj, \qquad p\in\mathbb{R},\ j\in\mathbb{N}_0.$$

Therefore, the phase space naturally becomes

$$\Omega=\mathbb{R}^3\times\mathbb{R}\times\mathbb{N}_0\times\{\pm1\}, \tag{A.8}$$

where $\mathbb{R}^3$ is interpreted as position variables, $\mathbb{R}\times\mathbb{N}_0$ as momentum variables, and $\{\pm1\}$ as a spin variable. We will denote components of vectors $\xi\in\Omega^k$ by $\xi_\ell=(u_\ell,p_\ell,j_\ell,s_\ell)\in\Omega$. For notational convenience, we will sometimes rearrange the variables by separating them into position and momentum components, i.e.

$$\xi=(u,p,j,s), \tag{A.9}$$

with $u\in\mathbb{R}^{3k}$, $p\in\mathbb{R}^k$, $j\in\mathbb{N}_0^k$, and $s\in\{\pm1\}^k$. Integration over Ω^k will be done with respect to its natural measure, using the Lebesgue measure in the continuous variables and the counting measure in the discrete variables.

A.1.2 Magnetic Thomas-Fermi theories

We recall that the pressure of the free Landau gas [20, equation (4.47)], i.e. a gas of non-interacting fermions in a homogeneous magnetic field, at chemical potential $\nu\geq0$ is given by

$$P_B(\nu)=\frac{B}{3\pi^2}\Big(\nu^{\frac32}+2\sum_{j=1}^{\infty}[2jB-\nu]_-^{\frac32}\Big), \tag{A.10}$$

where $B > 0$ is the magnetic field strength, and $\gamma_- := \max(-\gamma, 0)$ denotes the negative part of a number $\gamma \in \mathbb{R}$. Clearly, P_B is a convex and continuously differentiable function with derivative

$$P_B'(\nu) = \frac{B}{2\pi^2}\Big(\nu^{\frac{1}{2}} + 2\sum_{j=1}^{\infty}[2jB - \nu]_-^{\frac{1}{2}}\Big). \tag{A.11}$$

In the mean-field scaling we will take $B = \beta(1+\beta)^{-2/5}$, and the pressure will come with an additional prefactor $(1+\beta)^{-3/5}$.

Definition A.3 (Magnetic Thomas-Fermi energy). Let $V \in L^{5/2}_{\mathrm{loc}}(\mathbb{R}^3)$ satisfy $V(x) \to \infty$ as $|x| \to \infty$, and let $w \in L^{5/2}(\mathbb{R}^3) + L^\infty_\varepsilon(\mathbb{R}^3)$ be even. We define the magnetic Thomas-Fermi energy functional with parameter $\beta > 0$ by

$$\begin{aligned}\mathcal{E}_\beta^{\mathrm{MTF}}(\rho) = &\int_{\mathbb{R}^3} \tau_\beta(\rho(x))\,\mathrm{d}x + \int_{\mathbb{R}^3} V(x)\rho(x)\,\mathrm{d}x \\ &+ \frac{1}{2}\iint_{\mathbb{R}^6} w(x-y)\rho(x)\rho(y)\,\mathrm{d}x\,\mathrm{d}y\end{aligned} \tag{A.12}$$

on the set

$$\mathcal{D}^{\mathrm{MTF}} = \big\{\rho \in L^1(\mathbb{R}^3) \cap L^{\frac{5}{3}}(\mathbb{R}^3) \,\big|\, 0 \le \rho,\ V\rho \in L^1(\mathbb{R}^3)\big\},$$

where the energy density τ_β is given by the Legendre transform of the scaled pressure

$$\tau_\beta(t) = \sup_{\nu \ge 0}\big(t\nu - (1+\beta)^{-\frac{3}{5}} P_{k_\beta}(\nu)\big), \tag{A.13}$$

with $k_\beta = \beta(1+\beta)^{-2/5}$. Furthermore, the magnetic Thomas-Fermi ground state energy is defined as the infimum

$$E^{\mathrm{MTF}}(\beta) = \inf\big\{\mathcal{E}_\beta^{\mathrm{MTF}}(\rho) \,\big|\, \rho \in \mathcal{D}^{\mathrm{MTF}},\ \int_{\mathbb{R}^3} \rho(x)\,\mathrm{d}x = 1\big\}. \tag{A.14}$$

Recall that the space $L^{5/2}(\mathbb{R}^3) + L^\infty_\varepsilon(\mathbb{R}^3)$ consists of functions f satisfying that for each $\varepsilon > 0$ there exist $f_1 \in L^{5/2}(\mathbb{R}^3)$ and $f_2 \in L^\infty(\mathbb{R}^3)$ with $\|f_2\|_\infty \le \varepsilon$ and $f = f_1 + f_2$.

Remark A.4. *For any $0 \le \rho \in L^1(\mathbb{R}^3)$ and $\beta > 0$ it is well known [20, Proposition 4.2] that $\rho \in L^{5/3}(\mathbb{R}^3)$ if and only if $\int \tau_\beta(\rho(x))\,\mathrm{d}x$ is finite. In particular, we have the bound*

$$\begin{aligned}\int_{\mathbb{R}^3} \rho(x)^{\frac{5}{3}}\,\mathrm{d}x \le \kappa_1(1+\beta)^{\frac{2}{5}} &\int_{\mathbb{R}^3} \tau_\beta(\rho(x))\,\mathrm{d}x \\ &+ \kappa_2\Big(\frac{\beta}{1+\beta}\Big)^{\frac{2}{5}} \|\rho\|_1^{\frac{2}{3}} \Big(\int_{\mathbb{R}^3} \tau_\beta(\rho(x))\,\mathrm{d}x\Big)^{\frac{1}{3}}\end{aligned} \tag{A.15}$$

for some constants $\kappa_1, \kappa_2 > 0$. It follows that the domain of $\mathcal{E}_\beta^{\mathrm{MTF}}$ indeed is as stated above. Furthermore, it is not difficult to show that the functional is bounded from below on $\mathcal{D}^{\mathrm{MTF}} \cap \{\rho | \int \rho \le M\}$ for each $M > 0$, when V and w satisfy the assumptions stated above.

Similarly, we also define the *strong Thomas-Fermi functional*

$$\begin{aligned}\mathcal{E}^{\mathrm{STF}}(\rho) = \frac{4\pi^4}{3}\int_{\mathbb{R}^3}\rho(x)^3\,\mathrm{d}x + \int_{\mathbb{R}^3} V(x)\rho(x)\,\mathrm{d}x \\ + \frac{1}{2}\iint_{\mathbb{R}^6} w(x-y)\rho(x)\rho(y)\,\mathrm{d}x\,\mathrm{d}y,\end{aligned}$$

along with the ordinary non-magnetic *Thomas-Fermi functional*

$$\begin{aligned}\mathcal{E}^{\mathrm{TF}}(\rho) = \frac{3}{5}c_{\mathrm{TF}}\int_{\mathbb{R}^3}\rho(x)^{\frac{5}{3}}\,\mathrm{d}x + \int_{\mathbb{R}^3} V(x)\rho(x)\,\mathrm{d}x \\ + \frac{1}{2}\iint_{\mathbb{R}^6} w(x-y)\rho(x)\rho(y)\,\mathrm{d}x\,\mathrm{d}y,\end{aligned}$$

where $c_{\mathrm{TF}} = (3\pi^2)^{2/3}$, and with corresponding ground state energies E^{STF} and E^{TF}, both defined in complete analogy to (A.14).

MTF theory with spin

We also introduce a version of the magnetic Thomas-Fermi functional that keeps better track of the spin dependence. We will mostly need this for the formulation of our main result, and most of the proofs in the paper will be done using the spin-summed version defined above. We use a tilde ($\sim$) to distinguish the relevant spin-dependent quantities from the corresponding spin-independent (or spin-summed) ones. The pressure of the free Laundau gas with complete spin polarization is

$$\widetilde{P}_B(\nu, s) = \frac{B}{3\pi^2}\sum_{j=0}^{\infty}[B(2j+1+s)-\nu]_-^{\frac{3}{2}}, \tag{A.16}$$

where $B > 0$ is the magnetic field strength and $s \in \{\pm 1\}$ denotes the spin variable. As in the spin-summed case, $\widetilde{P}_B$ is convex and continuously differentiable with derivative

$$\widetilde{P}'_B(\nu, s) := \frac{\partial \widetilde{P}_B}{\partial \nu}(\nu, s) = \frac{B}{2\pi^2}\sum_{j=0}^{\infty}[B(2j+1+s)-\nu]_-^{\frac{1}{2}}. \tag{A.17}$$

Again, the kinetic energy density is the Legendre transform of the scaled pressure

$$\widetilde{\tau}_\beta(t, s) = \sup_{\nu\geq 0}\big(t\nu - (1+\beta)^{-\frac{3}{5}}\widetilde{P}_{k_\beta}(\nu, s)\big), \tag{A.18}$$

and the corresponding energy functional

$$\begin{aligned}\widetilde{\mathcal{E}}_\beta^{\mathrm{MTF}}(\rho) = \sum_{s=\pm 1}\int_{\mathbb{R}^3}\widetilde{\tau}_\beta(\rho(x,s), s)\,\mathrm{d}x + \sum_{s=\pm 1}\int_{\mathbb{R}^3} V(x)\rho(x,s)\,\mathrm{d}x \\ + \frac{1}{2}\sum_{s_1,s_2=\pm 1}\iint_{\mathbb{R}^6} w(x-y)\rho(x,s_1)\rho(y,s_2)\,\mathrm{d}x\,\mathrm{d}y\end{aligned} \tag{A.19}$$

is defined on the set of densities

$$\widetilde{\mathcal{D}}^{\mathrm{MTF}} = \big\{\rho \in L^1(\mathbb{R}^3 \times \{\pm 1\}) \cap L^{\frac{5}{3}}(\mathbb{R}^3 \times \{\pm 1\}) \,\big|\, 0 \le \rho,\ V\rho \in L^1(\mathbb{R}^3 \times \{\pm 1\})\big\}.$$

The fact that $\widetilde{\mathcal{E}}_\beta^{\mathrm{MTF}}$ is well defined on $\widetilde{\mathcal{D}}^{\mathrm{MTF}}$ is easily seen by showing the elementary bounds

$$2\widetilde{\tau}_\beta(t,-1) \le \tau_\beta(2t) \le \widetilde{\tau}_\beta(t,-1) + \widetilde{\tau}_\beta(t,1) \le 2\widetilde{\tau}_\beta(t,-1) + 4k_\beta t$$

for each $t \ge 0$, and combining with the description of the domain of the spin-summed magnetic Thomas-Fermi functional in Remark A.4. In Section A.2 we will argue that the spin-dependent functional has the same ground state energy as the spin-independent functional,

$$\widetilde{E}^{\mathrm{MTF}}(\beta) = E^{\mathrm{MTF}}(\beta),$$

and that they both also coincide with the ground state energy of a Vlasov type functional on the phase space $\Omega = \mathbb{R}^3 \times \mathbb{R} \times \mathbb{N}_0 \times \{\pm 1\}$, which will be introduced in (A.39).

A.1.3 Main results

The main results of this paper are the asymptotics of the ground state energy of the N-body Hamiltonian (A.1) to leading order in N, along with weak convergence of approximate ground states to convex combinations of factorized states.

Theorem A.5 (Convergence of energy). *Let $w \in L^{5/2}(\mathbb{R}^3) + L^\infty_\varepsilon(\mathbb{R}^3)$ be an even function, and $V \in L^{5/2}_{\mathrm{loc}}(\mathbb{R}^3)$ with $V(x) \to \infty$ as $|x| \to \infty$. Let (β_N) be a sequence of positive real numbers satisfying $\beta_N \to \beta \in [0,\infty]$ and (A.6). Then we have convergence of the ground state energy per particle*

$$\lim_{N\to\infty} \frac{E(N,\beta_N)}{N} = \begin{cases} E^{\mathrm{TF}}, & \text{if } \beta = 0, \\ E^{\mathrm{MTF}}(\beta), & \text{if } 0 < \beta < \infty, \\ E^{\mathrm{STF}}, & \text{if } \beta = \infty. \end{cases} \tag{A.20}$$

For the next theorem we recall that the k-particle position density of a function $\Psi \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2) \simeq \bigwedge^N L^2(\mathbb{R}^3 \times \{\pm 1\};\mathbb{C})$ is given by

$$\widetilde{\rho}_\Psi^{(k)}(z_1,\ldots,z_k) = \binom{N}{k} \int_{(\mathbb{R}^3\times\{\pm 1\})^{(N-k)}} |\Psi(z_1,\ldots,z_N)|^2 \,\mathrm{d}z_{k+1}\cdots \mathrm{d}z_N. \tag{A.21}$$

We will also need the spin-summed densities

$$\rho_\Psi^{(k)}(x_1,\ldots,x_k) = \binom{N}{k} \sum_{s\in\{\pm 1\}^N} \int_{\mathbb{R}^{3(N-k)}} |\Psi(x_1,\ldots,x_N;s)|^2 \,\mathrm{d}x_{k+1}\cdots \mathrm{d}x_N. \tag{A.22}$$

For the result on convergence of states below, we would like to call attention to the fact that the phase space changes in the extreme cases $\beta = 0$ and $\beta = \infty$. When $\beta_N \to 0$, the distance between the Landau bands (which is $2\hbar b = 2\beta_N(1+\beta_N)^{-2/5}$) also tends to zero, in which case we recover the usual phase space $\mathbb{R}^3 \times \mathbb{R}^3$. In the other extreme case, where $\beta_N \to \infty$, the magnetic field is so strong that all particles are confined to the lowest Landau band with spin pointing downwards, so the phase space here becomes $\mathbb{R}^3 \times \mathbb{R}$.

Theorem A.6 (Convergence of states). *Suppose that the assumptions of Theorem A.5 are satisfied. Let $\Psi_N \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ be a sequence of normalized approximate ground states, i.e. satisfying $\langle \Psi_N, H_{N,\beta_N}\Psi_N\rangle = E(N,\beta_N) + o(N)$. Denote by $\mathcal{M}_\beta$ the set of minimizers of the corresponding classical functional describing the ground state energy in the limit, that is,*

$$\mathcal{M}_\beta = \begin{cases} \{0 \le \rho \in L^1 \mid \int \rho = 1,\ \mathcal{E}^{\mathrm{TF}}(\rho) = E^{\mathrm{TF}}\}, & \text{if } \beta = 0,\\ \{0 \le \rho \in L^1 \mid \int \rho = 1,\ \widetilde{\mathcal{E}}^{\mathrm{MTF}}_\beta(\rho) = \widetilde{E}^{\mathrm{MTF}}(\beta)\}, & \text{if } 0 < \beta < \infty,\\ \{0 \le \rho \in L^1 \mid \int \rho = 1,\ \mathcal{E}^{\mathrm{STF}}(\rho) = E^{\mathrm{STF}}\}, & \text{if } \beta = \infty, \end{cases}$$

where $\rho \in L^1$ means $\rho \in L^1(\mathbb{R}^3)$ if $\beta = 0$ or $\beta = \infty$, and $\rho \in L^1(\mathbb{R}^3 \times \{\pm 1\})$ if $0 < \beta < \infty$.

Then there exist a subsequence $(N_\ell) \subseteq \mathbb{N}$ and a Borel probability measure $\mathscr{P}$ on $\mathcal{M}_\beta$ such that for $\varphi \in L^{5/2}(\mathbb{R}^3 \times \{\pm1\}) + L^\infty(\mathbb{R}^3 \times \{\pm1\})$ if $k = 1$, and for any bounded and uniformly continuous function φ on $(\mathbb{R}^3 \times \{\pm1\})^k$ if $k \ge 2$, we have as ℓ tends to infinity,

$$\frac{k!}{N_\ell^k} \sum_{s \in \{\pm1\}^k} \int_{\mathbb{R}^{3k}} \widetilde{\rho}^{(k)}_{\Psi_{N_\ell}}(x,s)\varphi(x,s)\,\mathrm{d}x \longrightarrow \int_{\mathcal{M}_\beta} \Big(\int_{\mathbb{R}^{3k}} G^{\beta,k}_{\rho,\varphi}(x)\,\mathrm{d}x \Big)\,\mathrm{d}\mathscr{P}(\rho). \tag{A.23}$$

The function $G^{\beta,k}_{\rho,\varphi}$ is given by

$$G^{\beta,k}_{\rho,\varphi}(x) = \begin{cases} \sum\limits_{s \in \{\pm1\}^k} 2^{-k}\rho^{\otimes k}(x)\varphi(x,s), & \text{if } \beta = 0,\\ \sum\limits_{s \in \{\pm1\}^k} \rho^{\otimes k}(x,s)\varphi(x,s), & \text{if } 0 < \beta < \infty,\\ \rho^{\otimes k}(x)\varphi(x,(-1)^{\times k}), & \text{if } \beta = \infty, \end{cases}$$

where $(-1)^{\times k}$ denotes the k-dimensional vector whose entries are all equal to -1. Its presence is an expression of the fact that all the particles in this regime are confined to the lowest Landau band, with all spins pointing downwards.

The convergence of energy and the convergence of states for $k = 1$ were both previously known in the case where the interaction w is Coulomb, and $V \in L^{5/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ with V tending to zero at infinity [20, Theorems 5.1–5.3]. The convergence of states result for $k > 1$ and the generality of the interaction w seem to be new.

Remark A.7. *If the interaction w is of positive type, that is, if it has non-negative Fourier transform (which is the case e.g. for Coulomb interactions), then the limiting Thomas-Fermi functional is (strictly) convex in all three cases. This implies that any minimizer must be unique, so the de Finetti measures in Theorem A.6 are forced to be supported on a single point. In other words, the outer integral in* (A.23) *disappears, and thus in this case the k-particle densities converge weakly to pure tensor products of the unique Thomas-Fermi minimizers.*

Remark A.8. *Analogues of Theorems A.5 and A.6 also hold if the external potential V is not confining, but for brevity we will omit this generalization. In this case, the convergence of energy is the same as in Theorem A.5, but the statement for convergence of states is slightly different. Instead of being supported on the set of minimizers of the classical functional, the de Finetti measure in Theorem A.6 will be supported on the set of weak limits of minimizing sequences for the functional. In this case, the lack of compactness at infinity forces one to use a weak version of the de Finetti theorem. See [5] for details in the case where there is no strong magnetic field.*

Organization of the paper

In Section A.2 we will recall a few results and preliminary observations that will be important for the later analysis. Section A.3 is devoted to proving the upper energy bounds of Theorem A.5 through construction of appropriate trial states. In Section A.4 we will construct semi-classical measures which in Section A.5 will allow us to prove the lower energy bounds of Theorem A.5 along with Theorem A.6 in the case of strong magnetic fields, i.e. when $\beta_N \to \beta \in (0, \infty]$. Finally, in Section A.6 we will treat the case $\beta_N \to 0$ where the spin is negligible, so we can in this case use the semi-classical measures constructed in [5] on the usual phase space $\mathbb{R}^3 \times \mathbb{R}^3$.

Acknowledgement

The authors were partially supported by the Sapere Aude grant DFF–4181-00221 from the Independent Research Fund Denmark. Part of this work was carried out while both authors visited the Mittag-Leffler Institute in Stockholm, Sweden.

A.2 Preliminary observations

We start out by recalling a few results on Pauli operators and the magnetic Thomas-Fermi functional that will be important for our analysis.

A.2.1 The semi-classical approximation and Lieb-Thirring bounds

Here we briefly recall a few useful tools obtained in [20]. We denote by $V_-(x) = \max(-V(x), 0)$ the negative part of the potential V. Supposing that $V_- \in L^{3/2}(\mathbb{R}^3) \cap L^{5/2}(\mathbb{R}^3)$ and denoting by $e_j(\hbar, b, V)$, $j \geq 1$, the negative eigenvalues for the operator

$$H(\hbar, b) = (\boldsymbol{\sigma} \cdot (-i\hbar\nabla + bA(x)))^2 + V(x), \tag{A.24}$$

then we have the magnetic Lieb-Thirring inequality [20, Theorem 2.1]

$$\sum_{j=1}^{\infty} |e_j(\hbar, b, V)| \leq L_1 \frac{b}{\hbar^2} \int_{\mathbb{R}^3} V_-(x)^{\frac{3}{2}} \, \mathrm{d}x + L_2 \frac{1}{\hbar^3} \int_{\mathbb{R}^3} V_-(x)^{\frac{5}{2}} \, \mathrm{d}x, \tag{A.25}$$

where for each $0 < \delta < 1$ one can choose $L_1 = \frac{4}{3}(\pi(1-\delta))^{-1}$ and $L_2 = 8\sqrt{6}(5\pi\delta^2)^{-1}$. The inequality can also be stated in terms of the 1-particle position density $\rho_\Psi^{(1)}$ of a many-body state $\Psi \in \bigwedge^N L^2(\mathbb{R}^3; \mathbb{C}^2)$. Namely, letting F_B denote the Legendre transform of the function $v \mapsto L_1 B v^{3/2} + L_2 v^{5/2}$, that is,

$$F_B(t) = \sup_{v \geq 0} (tv - L_1 B v^{\frac{3}{2}} - L_2 v^{\frac{5}{2}}), \tag{A.26}$$

then we have the lower bound [20, Corollary 2.2]

$$\Big\langle \Psi, \sum_{j=1}^{N} (\boldsymbol{\sigma} \cdot (-i\hbar\nabla_j + bA(x_j)))^2 \Psi \Big\rangle \geq \hbar^2 \int_{\mathbb{R}^3} F_{\frac{b}{\hbar}}(\rho_\Psi^{(1)}(x)) \, \mathrm{d}x \tag{A.27}$$

on the kinetic energy of the state Ψ. We also have Weyl asymptotics for the Pauli operator [20, Theorem 3.1]

$$\lim_{\hbar \to 0} \frac{\sum_j e_j(\hbar, b, V)}{E_{\mathrm{scl}}(\hbar, b, V)} = 1, \tag{A.28}$$

uniformly in the magnetic field strength b, where $E_{\mathrm{scl}}(\hbar, b, V)$ is the semi-classical expression for the sum of negative eigenvalues

$$E_{\mathrm{scl}}(\hbar, b, V) = -\frac{1}{\hbar^3} \int_{\mathbb{R}^3} P_{\hbar b}(V_-(x)) \, \mathrm{d}x, \tag{A.29}$$

with $P_{\hbar b}$ given in (A.10). In our case, with the scaling relations (A.5), the Weyl asymptotics take the following form:

Corollary A.9. *Suppose $V_- \in L^{3/2}(\mathbb{R}^3) \cap L^{5/2}(\mathbb{R}^3)$, let (β_N) be a sequence of positive real numbers satisfying $\beta_N \to \beta \in [0, \infty]$ and (A.6), and define $\hbar$ and b by (A.4). Then the Weyl asymptotics (A.28) take the form*

$$\lim_{N \to \infty} \frac{1}{N} \sum_j e_j(\hbar, b, V) = \begin{cases} -\frac{2}{15\pi^2} \int V_-(x)^{\frac{5}{2}} \, \mathrm{d}x, & \text{if } \beta = 0, \\ -(1+\beta)^{-\frac{3}{5}} \int P_{k_\beta}(V_-(x)) \, \mathrm{d}x, & \text{if } 0 < \beta < \infty, \\ -\frac{1}{3\pi^2} \int V_-(x)^{\frac{3}{2}} \, \mathrm{d}x, & \text{if } \beta = \infty. \end{cases} \tag{A.30}$$

The details of the proof, which mainly consists of applying the dominated convergence theorem to (A.28), will be omitted.

Remark A.10. *The Weyl asymptotics in* (A.28) *and Corollary A.9 also hold true if the Pauli operator* $(\boldsymbol{\sigma}\cdot(-i\hbar\nabla+bA(x)))^2$ *is replaced by the Pauli operator in a cube* $C_R=\left(-\frac{R}{2},\frac{R}{2}\right)^3$ *with Dirichlet boundary conditions, denoted by* $(\boldsymbol{\sigma}\cdot(-i\hbar\nabla+bA(x)))^2_{C_R}$*, (and* V *is replaced by a potential defined on* C_R*). For further details on this, see e.g. [24].*

Applying the generalized Lieb-Thirring inequality Eqs. (A.24) and (A.27) yields the following important estimates. The proof is a step-by-step imitation of the proof of [5, Lemma 3.4].

Lemma A.11. *If* $V_-,w_-\in L^{5/2}(\mathbb{R}^3)+L^\infty(\mathbb{R}^3)$ *and* $\beta_N>0$*, then*

$$H_{N,\beta_N}\geq\sum_{j=1}^N\Big(\frac{1}{2}(\boldsymbol{\sigma}\cdot(-i\hbar\nabla_j+bA(x_j)))^2+V_+(x_j)\Big)-CN\Big(\frac{b+1}{\hbar^2N}+1\Big)\tag{A.31}$$

and for any normalized fermionic wave function $\Psi\in\bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$*,*

$$\begin{aligned}\Big\langle\Psi,\sum_{j=1}^N\big((\boldsymbol{\sigma}\cdot(-i\hbar\nabla_j+bA(x_j)))^2+V_+(x_j)\big)\Psi\Big\rangle+\hbar^2\int F_{\frac{b}{\hbar}}(\rho_\Psi^{(1)}(x))\,\mathrm{d}x\\ \leq 2\langle\Psi,H_{N,\beta_N}\Psi\rangle+CN\Big(\frac{b+1}{\hbar^2N}+1\Big),\end{aligned}\tag{A.32}$$

with $F_{b/\hbar}$ *given by* (A.26)*. Furthermore, if* $\Psi_N\in\bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ *is a sequence satisfying* $\langle\Psi_N,H_{N,\beta_N}\Psi_N\rangle\leq CN$*, then for any* $f=f_1+f_2\in L^{3/2}(\mathbb{R}^3)\cap L^{5/2}(\mathbb{R}^3)+L^\infty(\mathbb{R}^3)$*, we have that*

$$\begin{aligned}\frac{1}{N}\int_{\mathbb{R}^3}f(x)\rho_{\Psi_N}^{(1)}(x)\,\mathrm{d}x+\frac{1}{N^2}\iint_{\mathbb{R}^6}f(x-y)\rho_{\Psi_N}^{(2)}(x,y)\,\mathrm{d}x\,\mathrm{d}y\\ \leq\tilde{C}\Big(\frac{b+1}{\hbar^2N}+\frac{1}{\hbar^3N}+1\Big)(\|f_1\|_{\frac{3}{2}}+\|f_1\|_{\frac{5}{2}}+\|f_2\|_\infty).\end{aligned}\tag{A.33}$$

Proof. The argument goes along the same lines as the proof of [5, Lemma 3.4]. We write $V_-=V_1+V_2$ and $w_-=w_1+w_2$ with $V_1,w_1\in L^{5/2}(\mathbb{R}^3)\cap L^{3/2}(\mathbb{R}^3)$ and $V_2,w_2\in L^\infty(\mathbb{R}^3)$. We clearly have that

$$\Big\langle\Psi,\sum_{j=1}^N-V_2(x_j)\Psi\Big\rangle\geq-\|V_2\|_\infty N\tag{A.34}$$

for any normalized wave function Ψ. Briefly denoting by H_{V_1} the operator $H_{V_1}:=\frac{1}{4}(\boldsymbol{\sigma}\cdot(-i\hbar\nabla+bA))^2-V_1$ and applying the magnetic Lieb-Thirring inequality (A.24), we obtain

$$\Big\langle \Psi, \sum_{j=1}^{N} H_{V_1} \Psi \Big\rangle \geq \operatorname{Tr}(H_{V_1})_- \\ \geq -2L_1 \frac{b}{\hbar^2} \int_{\mathbb{R}^3} V_1(x)^{\frac{3}{2}} \,\mathrm{d}x - 8L_2 \frac{1}{\hbar^3} \int_{\mathbb{R}^3} V_1(x)^{\frac{5}{2}} \,\mathrm{d}x. \tag{A.35}$$

Note that by symmetry we have

$$\Big\langle \Psi, \frac{1}{N} \sum_{1 \leq k < \ell \leq N} w_-(x_k - x_\ell)\Psi \Big\rangle = \frac{N-1}{2} \Big\langle \Psi, w_-(x_1 - x_2)\Psi \Big\rangle \\ = \frac{1}{2} \Big\langle \Psi, \sum_{j=2}^{N} w_-(x_1 - x_j)\Psi \Big\rangle,$$

so applying what we have just shown to the last $N-1$ variables, we get

$$\Big\langle \Psi, \Big(\sum_{j=1}^{N} \frac{1}{4} (\boldsymbol{\sigma} \cdot (-i\hbar\nabla_j + bA(x_j)))^2 - \frac{1}{2} \sum_{j=2}^{N} w_1(x_1 - x_j) \Big) \Psi \Big\rangle \\ \geq \Big\langle \Psi, \Big(\sum_{j=2}^{N} \frac{1}{4} (\boldsymbol{\sigma} \cdot (-i\hbar\nabla_j + bA(x_j)))^2 - \frac{1}{2} w_1(x_1 - x_j) \Big) \Psi \Big\rangle \\ \geq -C_1 \frac{b}{\hbar^2} \int_{\mathbb{R}^3} w_1(x)^{\frac{3}{2}} \,\mathrm{d}x - C_2 \frac{1}{\hbar^3} \int_{\mathbb{R}^3} w_1(x)^{\frac{5}{2}} \,\mathrm{d}x.$$

Hence we see that

$$\sum_{j=1}^{N} \frac{1}{4} (\boldsymbol{\sigma} \cdot (-i\hbar\nabla_j + bA(x_j)))^2 + \frac{1}{N} \sum_{1 \leq k < \ell \leq N} w(x_k - x_\ell) \\ \geq -C_1 \frac{b}{\hbar^2} \int_{\mathbb{R}^3} w_1(x)^{\frac{3}{2}} \,\mathrm{d}x - C_2 \frac{1}{\hbar^3} \int_{\mathbb{R}^3} w_1(x)^{\frac{5}{2}} \,\mathrm{d}x - \frac{N-1}{2} \|w_2\|_\infty. \tag{A.36}$$

Combining (A.34)-(A.36) yields (A.31). We obtain (A.32) directly from (A.31) by applying the Lieb-Thirring inequality (A.27).

Let us turn our attention towards the proof of (A.33). Note that it suffices to prove the estimate for non-negative functions f. We will prove the one-body part of the estimate first. Clearly, since Ψ_N is normalized,

$$\frac{1}{N} \int_{\mathbb{R}^3} f_2(x) \rho^{(1)}_{\Psi_N}(x) \,\mathrm{d}x \leq \|f_2\|_\infty, \tag{A.37}$$

so we may consider only $f_1 \in L^{3/2}(\mathbb{R}^3) \cap L^{5/2}(\mathbb{R}^3)$. For any $v \geq 0$ we have by definition,

$$\rho^{(1)}_{\Psi_N}(x) v - L_1 \frac{b}{\hbar} v^{\frac{3}{2}} - L_2 v^{\frac{5}{2}} \leq F_{\frac{b}{\hbar}}(\rho^{(1)}_{\Psi_N}(x)),$$

so we replace v by $\frac{1}{\varepsilon}f_1(x)$, integrate and apply (A.32) to obtain

$$\begin{aligned}\int_{\mathbb{R}^3} f_1(x)\rho^{(1)}_{\Psi_N}(x) - \frac{L_1}{\varepsilon^{\frac{1}{2}}}\frac{b}{\hbar}f_1(x)^{\frac{3}{2}} - \frac{L_2}{\varepsilon^{\frac{3}{2}}}f_1(x)^{\frac{5}{2}}\,\mathrm{d}x \\ \le \varepsilon\int_{\mathbb{R}^3} F_{\frac{b}{\hbar}}(\rho^{(1)}_{\Psi_N}(x))\,\mathrm{d}x \le \frac{CN}{\hbar^2}\Big(\frac{b+1}{\hbar^2 N}+3\Big)\varepsilon,\end{aligned}$$

implying the bound

$$\int_{\mathbb{R}^3} f_1(x)\rho^{(1)}_{\Psi_N}(x)\,\mathrm{d}x \le \frac{CN}{\hbar^2}\Big(\frac{b+1}{\hbar^2 N}+3\Big)\varepsilon + L_1\frac{b}{\hbar\varepsilon^{\frac{1}{2}}}\|f_1\|^{\frac{3}{2}}_{\frac{3}{2}} + L_2\frac{1}{\varepsilon^{\frac{3}{2}}}\|f_1\|^{\frac{5}{2}}_{\frac{5}{2}}.$$

With the choice $\varepsilon = (\|f_1\|_{\frac{3}{2}} + \|f_1\|_{\frac{5}{2}})\hbar^2$, we get

$$\frac{1}{N}\int_{\mathbb{R}^3} f_1(x)\rho^{(1)}_{\Psi_N}(x)\,\mathrm{d}x \le \tilde{C}\Big(\frac{b+1}{\hbar^2 N}+\frac{1}{\hbar^3 N}+1\Big)\big(\|f_1\|_{\frac{3}{2}}+\|f_1\|_{\frac{5}{2}}\big) \tag{A.38}$$

for some constant $\tilde{C} > 0$, showing the one-body part of (A.33). To obtain the two-body estimate, we apply (A.36) with w replaced by $\frac{1}{\varepsilon}f_1$ and use the anti-symmetry of Ψ_N to get

$$\begin{aligned}&-C_1\frac{b}{\hbar^2\varepsilon^{\frac{3}{2}}}\int_{\mathbb{R}^3} f_1(x)^{\frac{3}{2}}\,\mathrm{d}x - C_2\frac{1}{\hbar^3\varepsilon^{\frac{5}{2}}}\int_{\mathbb{R}^3} f_1(x)^{\frac{5}{2}}\,\mathrm{d}x \\ &\quad\le \Big\langle \Psi_N, \Big(\sum_{j=1}^N \frac{1}{4}(\boldsymbol{\sigma}\cdot(-i\hbar\nabla_j + bA(x_j)))^2 - \frac{1}{2}\sum_{j=2}^N \frac{1}{\varepsilon}f_1(x_1-x_j)\Big)\Psi_N\Big\rangle \\ &\quad\le CN\Big(\frac{b+1}{\hbar^2 N}+3\Big) - \frac{1}{\varepsilon N}\iint_{\mathbb{R}^6} f_1(x-y)\rho^{(2)}_{\Psi_N}(x,y)\,\mathrm{d}x\,\mathrm{d}y,\end{aligned}$$

where the second inequality holds by (A.32). Now we simply take $\varepsilon = \|f_1\|_{\frac{3}{2}} + \|f_1\|_{\frac{5}{2}}$ and rearrange to obtain

$$\frac{1}{N^2}\iint_{\mathbb{R}^6} f_1(x-y)\rho^{(2)}_{\Psi_N}(x,y)\,\mathrm{d}x\,\mathrm{d}y \le \widetilde{C}\Big(\frac{b+1}{\hbar^2 N}+\frac{1}{\hbar^3 N}+1\Big)\big(\|f_1\|_{\frac{3}{2}}+\|f_1\|_{\frac{5}{2}}\big).$$

Combining this with the fact that

$$\frac{1}{N^2}\iint_{\mathbb{R}^6} f_2(x-y)\rho^{(2)}_{\Psi_N}(x,y)\,\mathrm{d}x\,\mathrm{d}y \le \|f_2\|_\infty\frac{1}{N^2}\binom{N}{2}\|\Psi_N\|_2^2 \le \frac{1}{2}\|f_2\|_\infty,$$

we get the two-body estimate in (A.33), finishing the proof. □

Corollary A.12 (to LT inequality). *If $\Psi \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ is an N-particle state with finite kinetic energy, then $\rho^{(1)}_\Psi \in L^{5/3}(\mathbb{R}^3)$.*

Proof. Note first that for any $M > 0$, we have by Markov's inequality,

$$\begin{aligned}\int (\rho^{(1)}_\Psi(x)\mathbb{1}_{\{\rho^{(1)}_\Psi \le M\}}(x))^{\frac{5}{3}}\,\mathrm{d}x &\le \int_{\{\rho^{(1)}_\Psi \le 1\}} (\rho^{(1)}_\Psi(x))^{\frac{5}{3}}\,\mathrm{d}x + M^{\frac{5}{3}}|\{\rho^{(1)}_\Psi \ge 1\}| \\ &\le \big(1+M^{\frac{5}{3}}\big)\int_{\mathbb{R}^3}\rho^{(1)}_\Psi(x)\,\mathrm{d}x,\end{aligned}$$

so $\rho_\Psi^{(1)}\mathbb{1}_{\{\rho_\Psi^{(1)}\le M\}} \in L^{5/3}(\mathbb{R}^3)$. Since Ψ has finite kinetic energy, it follows from (A.27) that

$$\int_{\mathbb{R}^3} \rho_\Psi^{(1)}(x)f(x) - L_1\frac{b}{\hbar}f(x)^{\frac{3}{2}} - L_2 f(x)^{\frac{5}{2}}\,\mathrm{d}x \le C$$

for any $0 \le f \in L^{3/2}(\mathbb{R}^3)\cap L^{5/2}(\mathbb{R}^3)$, where C is independent of f, and L_2 can be chosen such that $0 < L_2 < 1$ by the Lieb-Thirring inequality (A.24). Choosing $f = (\rho_\Psi^{(1)}\mathbb{1}_{\{\rho_\Psi^{(1)}\le M\}})^{2/3}$, we get

$$(1-L_2)\int_{\{\rho_\Psi^{(1)}\le M\}} \rho_\Psi^{(1)}(x)^{\frac{5}{3}}\,\mathrm{d}x \le C + L_1\frac{b}{\hbar}\int_{\{\rho_\Psi^{(1)}\le M\}} \rho_\Psi^{(1)}(x)\,\mathrm{d}x.$$

Taking M to infinity finishes the proof. $\square$

Lemma A.13. *Suppose that $\Psi_N \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ is a sequence satisfying the kinetic energy bound*

$$\Big\langle \Psi_N, \Big(\sum_{j=1}^N (\boldsymbol{\sigma}\cdot(-i\hbar\nabla_j + bA(x_j)))^2\Big)\Psi_N\Big\rangle \le \widetilde{C}N,$$

where $\hbar$ and b satisfy the scaling relations (A.4). Then there exists a $C > 0$ such that $\|\rho_{\Psi_N}^{(1)}\|_{\frac{5}{3}} \le CN$ for all N. In particular, if $\frac{1}{N}\rho_{\Psi_N}^{(1)} \rightharpoonup \rho$ weakly as functionals on $C_c(\mathbb{R}^3)$, then $\rho \in L^1(\mathbb{R}^3)\cap L^{5/3}(\mathbb{R}^3)$ and for any test function $\varphi \in L^{5/2}(\mathbb{R}^3)+L^\infty_\varepsilon(\mathbb{R}^3)$ we have $\int \frac{1}{N}\rho_{\Psi_N}^{(1)}\varphi \to \int \rho\varphi$.

Proof. For the duration of the proof we will denote $\rho_N = \rho_{\Psi_N}^{(1)}$. For any $0 \le f \in L^{3/2}(\mathbb{R}^3)\cap L^{5/2}(\mathbb{R}^3)$ we have by (A.27) that

$$\hbar^2\int_{\mathbb{R}^3} \rho_N(x)f(x) - L_1\frac{b}{\hbar}f(x)^{\frac{3}{2}} - L_2 f(x)^{\frac{5}{2}}\,\mathrm{d}x \le \widetilde{C}N.$$

Hence, noting by (A.24) that we can take $L_2 < 1$, and choosing $f = \varepsilon^2\rho_N^{2/3}$ with $0 < \varepsilon < 1$, we obtain

$$\varepsilon^2(1-L_2\varepsilon^3)\int_{\mathbb{R}^3}\rho_N(x)^{\frac{5}{3}}\,\mathrm{d}x \le \widetilde{C}\frac{N}{\hbar^2} + \varepsilon^3 L_1\frac{b}{\hbar}\int_{\mathbb{R}^3}\rho_N(x)\,\mathrm{d}x.$$

Inserting the definitions of $\hbar$ and b (A.4) yields

$$\|\rho_N\|_{\frac{5}{3}}^{\frac{5}{3}} \le \frac{\widetilde{C}N}{\varepsilon^2(1-L_2)}\Big(\frac{1}{\hbar^2} + \varepsilon^3\frac{b}{\hbar}\Big) = C'N^{\frac{5}{3}}\Big(\frac{1}{\varepsilon^2(1+\beta_N)^{\frac{2}{5}}} + \frac{\varepsilon\beta_N}{(1+\beta_N)^{\frac{4}{5}}}\Big),$$

so simply choosing $\varepsilon = (1+\beta_N)^{-1/5}$ gives the desired bound.

The last part of the lemma follows easily from standard methods in functional analysis, and the details will be omitted. $\square$

A.2.2 Energy functionals on phase space

Instead of working with a functional on position densities, it will in some situations be much more convenient to use a functional defined on densities on phase space. Hence we introduce the Vlasov energy functional, and note its connection to the magnetic Thomas-Fermi functionals.

Definition A.14 (Magnetic Vlasov functional). We put $\Omega = \mathbb{R}^3 \times \mathbb{R} \times \mathbb{N}_0 \times \{\pm 1\}$, and for $\beta > 0$,

$$\mathcal{D}^{\mathrm{Vla}} = \{m \in L^1(\Omega) \mid 0 \le m \le 1,\ V\rho_m, (w * \rho_m)\rho_m \in L^1(\mathbb{R}^3)\},$$

where

$$\rho_m(x) = \frac{1}{(2\pi)^2}\frac{\beta}{1+\beta}\sum_{s=\pm 1}\sum_{j=0}^{\infty}\int_{\mathbb{R}} m(x,p,j,s)\,\mathrm{d}p.$$

Putting $k_\beta = \beta(1+\beta)^{-2/5}$, we define a functional

$$\begin{aligned}\mathcal{E}_\beta^{\mathrm{Vla}}(m) = &\frac{1}{(2\pi)^2}\frac{\beta}{1+\beta}\sum_{\substack{j\ge 0\\ s=\pm 1}}\int_{\mathbb{R}}\int_{\mathbb{R}^3}(p^2 + k_\beta(2j+1+s))m(x,p,j,s)\,\mathrm{d}x\,\mathrm{d}p\\ &+\int_{\mathbb{R}^3} V(x)\rho_m(x)\,\mathrm{d}x + \frac{1}{2}\iint_{\mathbb{R}^6} w(x-y)\rho_m(x)\rho_m(y)\,\mathrm{d}x\,\mathrm{d}y. \end{aligned}\tag{A.39}$$

Furthermore, we define the Vlasov ground state energy

$$E^{\mathrm{Vla}}(\beta) = \inf\big\{\mathcal{E}_\beta^{\mathrm{Vla}}(m)\ \big|\ m \in \mathcal{D}^{\mathrm{Vla}}, \frac{1}{(2\pi)^2}\frac{\beta}{1+\beta}\int_\Omega m(\xi)\,\mathrm{d}\xi = 1\big\}.$$

Lemma A.15. *Suppose that $\rho \in \mathcal{D}^{\mathrm{MTF}}$ and define a measure on $\Omega = \mathbb{R}^3 \times \mathbb{R} \times \mathbb{N}_0 \times \{\pm 1\}$ with density*

$$m_\rho(x,p,j,s) = \mathbb{1}_{\{p^2 + k_\beta(2j+1+s) \le r(x)\}},\tag{A.40}$$

where for (almost) each $x \in \mathbb{R}^3$, $r(x)$ is the unique solution to the equation

$$\rho(x) = \frac{1}{2\pi^2}\frac{\beta}{1+\beta}\Big(r(x)^{\frac{1}{2}} + 2\sum_{j=1}^{\infty}[2k_\beta j - r(x)]_-^{\frac{1}{2}}\Big) = (1+\beta)^{-\frac{3}{5}}P'_{k_\beta}(r(x)).\tag{A.41}$$

Then $m_\rho \in \mathcal{D}^{\mathrm{Vla}}$ and satisfies for almost all $x \in \mathbb{R}^3$

$$\rho_{m_\rho}(x) := \frac{1}{(2\pi)^2}\frac{\beta}{1+\beta}\sum_{s=\pm 1}\sum_{j=0}^{\infty}\int_{\mathbb{R}} m_\rho(x,p,j,s)\,\mathrm{d}p = \rho(x),$$

$$\frac{1}{(2\pi)^2}\frac{\beta}{1+\beta}\sum_{s=\pm 1}\sum_{j=0}^{\infty}\int_{\mathbb{R}}(p^2 + k_\beta(2j+1+s))m_\rho(x,p,j,s)\,\mathrm{d}p = \tau_\beta(\rho(x)),\tag{A.42}$$

and $\mathcal{E}_\beta^{\mathrm{MTF}}(\rho) = \mathcal{E}_\beta^{\mathrm{Vla}}(m_\rho)$.

On the other hand, if $m \in \mathcal{D}^{\mathrm{Vla}}$, then $\rho_m \in \mathcal{D}^{\mathrm{MTF}}$ and $\mathcal{E}_\beta^{\mathrm{MTF}}(\rho_m) \le \mathcal{E}_\beta^{\mathrm{Vla}}(m)$. In particular,

$$E^{\mathrm{MTF}}(\beta) = E^{\mathrm{Vla}}(\beta).$$

Remark A.16. *The assertions of the lemma also hold true when the magnetic Thomas-Fermi functional is replaced by the spin dependent functional $\widetilde{\mathcal{E}}_\beta^{\mathrm{MTF}}$. In particular,*

$$\widetilde{E}^{\mathrm{MTF}}(\beta) = E^{\mathrm{Vla}}(\beta) = E^{\mathrm{MTF}}(\beta).$$

The proof is exactly the same is in the spin-summed case, except that in this case, the equation

$$\widetilde{\rho}(x,s) = (1+\beta)^{-\frac{3}{5}} \widetilde{P}'_{k_\beta}(\widetilde{r}(x,s),s)$$

does not uniquely define $\widetilde{r}$ everywhere, because $\widetilde{P}'_{k_\beta}(\nu,1) = 0$ for $0 \le \nu \le 2k_\beta$. However, this can easily be remedied by instead defining

$$\widetilde{r}(x,s) = \max\left\{r \ge 0 \mid \widetilde{\tau}_\beta(\rho(x,s),s) = \rho(x,s)r - (1+\beta)^{-\frac{3}{5}} \widetilde{P}_{k_\beta}(r,s)\right\},$$

but we omit the details.

Proof. The idea is to fix a position density and minimize the Vlasov problem for each fixed position $x \in \mathbb{R}^3$. For any $\nu \ge 0$, we calculate the measure of the set

$$\begin{aligned} &|\{(p,j,s) \in \mathbb{R} \times \mathbb{N}_0 \times \{\pm 1\} \mid p^2 + k_\beta(2j+1+s) \le \nu\}| \\ &\qquad = \sum_{j=0}^{\infty} |\{p^2 \le \nu - 2k_\beta(j+1)\}| + \sum_{j=0}^{\infty} |\{p^2 \le \nu - 2k_\beta j\}| \\ &\qquad = 2t^{\frac{1}{2}} + 4\sum_{j=1}^{\infty} [2k_\beta j - \nu]_-^{\frac{1}{2}} = \frac{(2\pi)^2}{k_\beta} P'_{k_\beta}(\nu). \end{aligned} \tag{A.43}$$

Supposing that $\rho \in \mathcal{D}^{\mathrm{MTF}}$, then for each $x \in \mathbb{R}^3$ we may choose $r(x) \ge 0$ to be the unique solution of (A.41) and define m_ρ as in (A.40). The calculation above then clearly shows

$$\begin{aligned} &\frac{1}{(2\pi)^2} \frac{\beta}{1+\beta} \sum_{s=\pm 1} \sum_{j=0}^{\infty} \int_{\mathbb{R}} m_\rho(x,p,j,s)\,\mathrm{d}p \\ &\qquad = \frac{1}{(2\pi)^2} \frac{\beta}{1+\beta} \sum_{s=\pm 1} \sum_{j=0}^{\infty} \int_{\mathbb{R}} \mathbb{1}_{\{p^2 + k_\beta(2j+1+s) \le r(x)\}}\,\mathrm{d}p = \rho(x). \end{aligned}$$

To see that (A.42) holds, note that the supremum in (A.13) is attained exactly at the point $r(x) \ge 0$, that is,

$$\tau_\beta(\rho(x)) = \rho(x)r(x) - (1+\beta)^{-\frac{3}{5}} P_{k_\beta}(r(x)). \tag{A.44}$$

Furthermore, using $[2k_\beta j - r(x)]_-^{3/2} = (r(x) - 2k_\beta j)[2k_\beta j - r(x)]_-^{1/2}$ along with the definition of the pressure P_{k_β}, we also have

$$2\sum_{j=1}^{\infty} 2k_\beta j [2k_\beta j - r(x)]_-^{\frac{1}{2}} = \frac{2\pi^2}{k_\beta} P'_{k_\beta}(r(x)) r(x) - \frac{3\pi^2}{k_\beta} P_{k_\beta}(r(x)).$$

With this in mind, we calculate, using the definition of m_ρ,

$$
\begin{aligned}
\sum_{s=\pm1}\sum_{j=0}^{\infty}\int_{\mathbb{R}}&(p^2+k_\beta(2j+1+s))m_\rho(x,p,j,s)\,\mathrm{d}p \\
&= \int_{\mathbb{R}} p^2\mathbb{1}_{\{p^2\le r(x)\}}\,\mathrm{d}p + 2\sum_{j=1}^{\infty}\int_{\mathbb{R}}(p^2+2k_\beta j)\mathbb{1}_{\{p^2+2k_\beta j\le r(x)\}}\,\mathrm{d}p \\
&= \frac{2\pi^2}{k_\beta}P_{k_\beta}(r(x)) + 4\sum_{j=1}^{\infty}2k_\beta j[2k_\beta j - r(x)]_-^{\frac{1}{2}} \\
&= \frac{(2\pi)^2}{k_\beta}(P'_{k_\beta}(r(x))r(x) - P_{k_\beta}(r(x))) \qquad\qquad (A.45) \\
&= (2\pi)^2\frac{1+\beta}{\beta}\tau_\beta(\rho(x)),
\end{aligned}
$$

showing (A.42). This implies that $m_\rho \in \mathcal{D}^{\mathrm{Vla}}$ and $\mathcal{E}_\beta^{\mathrm{MTF}}(\rho) = \mathcal{E}_\beta^{\mathrm{Vla}}(m_\rho)$, and hence $E^{\mathrm{MTF}}(\beta) \ge E^{\mathrm{Vla}}(\beta)$.

On the other hand, for any $m \in \mathcal{D}^{\mathrm{Vla}}$ we may consider $\rho_m \in \mathcal{D}^{\mathrm{MTF}}$ and construct as above the measure $m_{\rho_m} \in \mathcal{D}^{\mathrm{Vla}}$. Then for each $x \in \mathbb{R}^3$, $m_{\rho_m}(x,\cdot)$ is by construction a minimizer of the functional

$$\mathcal{E}(\widetilde{m}) := \frac{1}{(2\pi)^2}\frac{\beta}{1+\beta}\sum_{s=\pm1}\sum_{j=0}^{\infty}\int_{\mathbb{R}}(p^2+k_\beta(2j+1+s))\widetilde{m}(p,j,s)\,\mathrm{d}p$$

defined on the set of densities $\widetilde{m} \in L^1(\mathbb{R}\times\mathbb{N}_0\times\{\pm1\})$ satisfying $0 \le \widetilde{m} \le 1$ and

$$\frac{1}{(2\pi)^2}\frac{\beta}{1+\beta}\sum_{s=\pm1}\sum_{j=0}^{\infty}\int_{\mathbb{R}}\widetilde{m}(p,j,s)\,\mathrm{d}p = \rho_m(x).$$

(This is the bathtub principle [16, Theorem 1.14]). Hence for almost every $x \in \mathbb{R}^3$,

$$
\begin{aligned}
\sum_{s=\pm1}\sum_{j=0}^{\infty}\int_{\mathbb{R}}&(p^2+k_\beta(2j+1+s))m_{\rho_m}(x,p,j,s)\,\mathrm{d}p \\
&\le \sum_{s=\pm1}\sum_{j=0}^{\infty}\int_{\mathbb{R}}(p^2+k_\beta(2j+1+s))m(x,p,j,s)\,\mathrm{d}p,
\end{aligned}
$$

implying that $\mathcal{E}_\beta^{\mathrm{MTF}}(\rho_m) = \mathcal{E}_\beta^{\mathrm{Vla}}(m_{\rho_m}) \le \mathcal{E}_\beta^{\mathrm{Vla}}(m)$. We conclude that $E^{\mathrm{MTF}}(\beta) \le E^{\mathrm{Vla}}(\beta)$, so we have the desired result. □

To handle the extreme cases where $\beta_N \to \infty$ or $\beta_N \to 0$, we need to introduce a couple of extra Vlasov type functionals.

Definition A.17 (Strong field Vlasov energy). Define a functional by

$$\begin{aligned}\mathcal{E}^{\mathrm{Vla}}_{\infty}(m) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}}\int_{\mathbb{R}^3} p^2 m(x,p)\,\mathrm{d}x\,\mathrm{d}p + \int_{\mathbb{R}^3} V(x)\rho_m(x)\,\mathrm{d}x \\ + \frac{1}{2}\iint_{\mathbb{R}^6} w(x-y)\rho_m(x)\rho_m(y)\,\mathrm{d}x\,\mathrm{d}y\end{aligned}$$

on the set

$$\mathcal{D}^{\mathrm{Vla}}_{\infty} = \{m \in L^1(\mathbb{R}^3\times\mathbb{R}) \mid 0 \le m \le 1,\ V\rho_m, (w*\rho_m)\rho_m \in L^1(\mathbb{R}^3)\},$$

where

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

The functional has ground state energy

$$E^{\mathrm{Vla}}(\infty) = \inf\big\{\mathcal{E}^{\mathrm{Vla}}_{\infty}(m) \bigm| m \in \mathcal{D}^{\mathrm{Vla}}_{\infty}, \frac{1}{(2\pi)^2}\iint_{\mathbb{R}^3\times\mathbb{R}} m(x,p)\,\mathrm{d}x\,\mathrm{d}p = 1\big\}.$$

Lemma A.18. *Suppose that ρ is in the domain of the strong Thomas-Fermi functional $\mathcal{E}^{\mathrm{STF}}$ and define a measure on $\mathbb{R}^3\times\mathbb{R}$ with density $m_\rho(x,p) = \mathbb{1}_{\{p^2\le 4\pi^4\rho(x)^2\}}$. Then $m_\rho \in \mathcal{D}^{\mathrm{Vla}}_{\infty}$ and satisfies*

$$\rho_{m_\rho}(x) := \frac{1}{(2\pi)^2}\int_{\mathbb{R}} m_\rho(x,p)\,\mathrm{d}p = \rho(x),$$

$$\frac{1}{(2\pi)^2}\int_{\mathbb{R}} p^2 m_\rho(x,p)\,\mathrm{d}p = \frac{4\pi^4}{3}\rho(x)^3, \tag{A.46}$$

and $\mathcal{E}^{\mathrm{STF}}(\rho) = \mathcal{E}^{\mathrm{Vla}}_{\infty}(m_\rho)$. On the other hand, if $m \in \mathcal{D}^{\mathrm{Vla}}_{\infty}$, then $\mathcal{E}^{\mathrm{STF}}(\rho_m) \le \mathcal{E}^{\mathrm{Vla}}_{\infty}(m)$. In particular, $E^{\mathrm{STF}} = E^{\mathrm{Vla}}(\infty)$.

This result is proved in exactly the way as Lemma A.15, using the bathtub principle.

Definition A.19 (Weak field Vlasov energy). Let $b \ge 0$ and define a functional by

$$\begin{aligned}\mathcal{E}^{\mathrm{Vla}}_{0}(m) = \frac{1}{(2\pi)^3}\sum_{s=\pm1}\iint_{\mathbb{R}^6}(p+bA(x))^2 m(x,p,s)\,\mathrm{d}x\,\mathrm{d}p \\ + \int_{\mathbb{R}^3} V(x)\rho_m(x)\,\mathrm{d}x + \frac{1}{2}\iint_{\mathbb{R}^6} w(x-y)\rho_m(x)\rho_m(y)\,\mathrm{d}x\,\mathrm{d}y\end{aligned}$$

on the set

$$\mathcal{D}^{\mathrm{Vla}}_{0} = \{m \in L^1(\mathbb{R}^6\times\{\pm1\}) \mid 0 \le m \le 1,\ V\rho_m, (w*\rho_m)\rho_m \in L^1(\mathbb{R}^3)\},$$

where

$$\rho_m(x) := \frac{1}{(2\pi)^3} \sum_{s=\pm 1} \int_{\mathbb{R}^3} m(x,p,s)\,\mathrm{d}p.$$

The functional has ground state energy

$$E_0^{\mathrm{Vla}} = \inf\Big\{\mathcal{E}_0^{\mathrm{Vla}}(m) \,\Big|\, m \in \mathcal{D}_0^{\mathrm{Vla}}, \frac{1}{(2\pi)^3} \sum_{s=\pm 1} \iint_{\mathbb{R}^6} m(x,p,s)\,\mathrm{d}x\,\mathrm{d}p = 1\Big\}.$$

Lemma A.20. *Suppose that ρ is in the domain of the usual Thomas-Fermi functional $\mathcal{E}^{\mathrm{TF}}$ and define a measure m_ρ on $\mathbb{R}^3 \times \mathbb{R}^3 \times \{\pm 1\}$ with density $m_\rho(x,p,s) = \mathbb{1}_{\{(p+bA(x))^2 \leq c_{\mathrm{TF}}\rho(x)^{2/3}\}}$, where $c_{\mathrm{TF}} = (3\pi^2)^{2/3}$. Then $m_\rho \in \mathcal{D}_0^{\mathrm{Vla}}$ and satisfies*

$$\rho_{m_\rho}(x) := \frac{1}{(2\pi)^3} \sum_{s=\pm 1} \int_{\mathbb{R}^3} m_\rho(x,p,s)\,\mathrm{d}p = \rho(x),$$

$$\frac{1}{(2\pi)^3} \sum_{s=\pm 1} \int_{\mathbb{R}^3} (p+bA(x))^2 m_\rho(x,p,s)\,\mathrm{d}p = \frac{3}{5} c_{\mathrm{TF}} \rho(x)^{\frac{5}{3}}, \tag{A.47}$$

and $\mathcal{E}^{\mathrm{TF}}(\rho) = \mathcal{E}_0^{\mathrm{Vla}}(m_\rho)$. On the other hand, if $m \in \mathcal{D}_0^{\mathrm{Vla}}$, then $\mathcal{E}^{\mathrm{TF}}(\rho_m) \leq \mathcal{E}_0^{\mathrm{Vla}}(m)$. In particular, $E^{\mathrm{TF}} = E_0^{\mathrm{Vla}}$.

Remark A.21. *For any fixed density $0 \leq \rho \in L^1(\mathbb{R}^3)$, it follows from the uniqueness statement in [16, Theorem 1.14] that for each fixed $x \in \mathbb{R}^3$, the measure $m_\rho(x,\,\cdot\,)$ on $\mathbb{R}^3 \times \{\pm 1\}$ constructed above is the* unique *minimizer of the functional*

$$m \mapsto \frac{1}{(2\pi)^3} \sum_{s=\pm 1} \int_{\mathbb{R}^3} (p+bA(x))^2 m(p,s)\,\mathrm{d}p$$

under the constraints $0 \leq m \leq 1$ and $\sum_{s=\pm 1} \int_{\mathbb{R}^3} m(p,s)\,\mathrm{d}p = (2\pi)^3 \rho(x)$. In particular, if m_0 is a minimizer of the Vlasov functional $\mathcal{E}_0^{\mathrm{Vla}}$, then the uniquess statement implies that

$$m_0(x,p,s) = \mathbb{1}_{\{(p+bA(x))^2 \leq c_{\mathrm{TF}}\rho_{m_0}(x)^{2/3}\}},$$

so the minimizers of $\mathcal{E}_0^{\mathrm{Vla}}$ are independent of the spin variable.

A.3 Upper energy bounds

This section is devoted to proving the upper bounds in Theorem A.5, i.e.

Proposition A.22. *With the assumptions in Theorem A.5, we have*

$$\limsup_{N\to\infty} \frac{E(N,\beta_N)}{N} \leq \begin{cases} E^{\mathrm{TF}}, & \text{if } \beta_N \to 0, \\ E^{\mathrm{MTF}}(\beta), & \text{if } \beta_N \to \beta \in (0,\infty), \\ E^{\mathrm{STF}}, & \text{if } \beta_N \to \infty. \end{cases} \tag{A.48}$$

We will prove Proposition A.22 by constructing an appropriate trial state for the variational problem. Let $(f_j)_{j=1}^N$ be functions in the magnetic Sobolev space $H^1_{\hbar^{-1}bA}(\mathbb{R}^3;\mathbb{C}^2)$, orthonormal in $L^2(\mathbb{R}^3;\mathbb{C}^2)$. Consider the corresponding Hartree-Fock state (abbrv. HF state) $\Psi \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ defined by

$$\Psi(x,s) = \frac{1}{\sqrt{N!}}\det[f_i(x_j,s_j)] = \frac{1}{\sqrt{N!}}\sum_{\sigma\in S_N}\operatorname{sgn}(\sigma)\prod_{j=1}^N f_{\sigma(j)}(x_j,s_j),$$

where S_N is the symmetric group of N elements. The function Ψ is normalized in $L^2\big(\mathbb{R}^{3N};\mathbb{C}^{2^N}\big)$ and its one-particle density matrix is $\gamma_\Psi = \sum_{j=1}^N |f_j\rangle\langle f_j|$, so $\operatorname{Tr}[\gamma_\Psi] = N$ and γ_Ψ is the orthogonal projection onto the subspace in $L^2(\mathbb{R}^3;\mathbb{C}^2)$ spanned by the f_j's. Furthermore, γ_Ψ has integral kernel

$$\gamma_\Psi(x_1,s_1;x_2,s_2) = \sum_{j=1}^N f_j(x_1,s_1)\overline{f_j(x_2,s_2)},$$

and the one-particle position density is $\rho_\Psi^{(1)}(x) = \sum_{s=\pm1}\sum_{j=1}^N |f_j(x,s)|^2$. Note that $\|\gamma_\Psi\|_2^2 = \operatorname{Tr}[\gamma_\Psi] = N$ since the f_j's are orthonormal. One easily calculates the expectation of the energy in the state Ψ to be

$$\begin{aligned}\langle\Psi, H_{N,\beta_N}\Psi\rangle = {}& \operatorname{Tr}[(\boldsymbol{\sigma}\cdot(-i\hbar\nabla + bA))^2\gamma_\Psi] + \int_{\mathbb{R}^3} V(x)\rho_\Psi^{(1)}(x)\,\mathrm{d}x \\ & + \frac{1}{2N}\iint_{\mathbb{R}^6} w(x-y)\rho_\Psi^{(1)}(x)\rho_\Psi^{(1)}(y)\,\mathrm{d}x\,\mathrm{d}y \\ & - \frac{1}{2N}\sum_{s_1,s_2=\pm1}\iint_{\mathbb{R}^6} w(x-y)|\gamma_\Psi(x,s_1;y,s_2)|^2\,\mathrm{d}x\,\mathrm{d}y \end{aligned} \tag{A.49}$$

We proceed to derive a bound on the exchange term involving $|\gamma_\Psi|^2$.

Lemma A.23 (Bound on the exchange term). *Let $w \in L^{5/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. There is a constant $C > 0$ such that for each $N \geq 1$,*

$$\begin{aligned}&\frac{1}{2N}\sum_{s_1,s_2=\pm1}\iint_{\mathbb{R}^6} |w(x-y)||\gamma_\Psi(x,s_1;y,s_2)|^2\,\mathrm{d}x\,\mathrm{d}y \\ &\qquad \leq CN^{\frac{2}{3}}\Big(\frac{1}{N}\operatorname{Tr}[(\boldsymbol{\sigma}\cdot(-i\hbar\nabla + bA))^2\gamma_\Psi] + \beta_N(1+\beta_N)^{-\frac{4}{5}} + 1\Big).\end{aligned} \tag{A.50}$$

Proof. We mimic the proof of the analogous bound in [5, Proposition 3.1]. Writing $w = w_1 + w_2$ with $w_1 \in L^{3/2}(\mathbb{R}^3)\cap L^{5/2}(\mathbb{R}^3)$ and $w_2 \in L^\infty(\mathbb{R}^3)$. Note that the contribution from w_2 is bounded by

$$\frac{1}{2N}\sum_{s_1,s_2=\pm1}\iint_{\mathbb{R}^6} |w_2(x-y)||\gamma_\Psi(x,s_1;y,s_2)|^2\,\mathrm{d}x\,\mathrm{d}y \leq \frac{\|w_2\|_\infty}{2}, \tag{A.51}$$

so we concentrate on controlling the contribution from w_1.

Now, for any function f in the magnetic Sobolev space $H^1_{\hbar^{-1}bA}(\mathbb{R}^3)$, the diamagnetic inequality implies that $|f| \in H^1(\mathbb{R}^3)$. Defining $f_\varepsilon(x) := \varepsilon^{1/2} f(\varepsilon x)$ for $\varepsilon > 0$, we have $\|f_\varepsilon\|_6 = \|f\|_6$, $\|f_\varepsilon\|_2^2 = \varepsilon^{-2}\|f\|_2^2$, and $\|\nabla|f_\varepsilon|\|_2^2 = \|\nabla|f|\|_2^2$, so by the diamagnetic and Gagliardo-Nirenberg-Sobolev inequalities,

$$\begin{aligned}\|f\|_6^2 = \|f_\varepsilon\|_6^2 &\le C(\|\nabla|f_\varepsilon|\|_2^2 + \|f_\varepsilon\|_2^2) = C(\|\nabla|f|\|_2^2 + \varepsilon^{-2}\|f\|_2^2)\\ &\le C(\hbar^{-2}\|(-i\hbar\nabla + bA)f\|_2^2 + \varepsilon^{-2}\|f\|_2^2).\end{aligned}$$

Combining this with the Hölder inequality, we obtain

$$\int_{\mathbb{R}^3} |w_1(x)||f(x)|^2 \,\mathrm{d}x \le C\|w_1\|_{\frac{3}{2}} (\hbar^{-2}\|(-i\hbar\nabla + bA)f\|_2^2 + \varepsilon^{-2}\|f\|_2^2).$$

We will apply this to the function $\gamma_\Psi(\,\cdot\,, s_1; y, s_2)$ for fixed y, so we calculate

$$\sum_{s_1,s_2=\pm1} \int_{\mathbb{R}^3} \|(-i\hbar\nabla_x + bA(x))\gamma_\Psi(\,\cdot\,, s_1; y, s_2)\|_2^2 \,\mathrm{d}y = \mathrm{Tr}[(-i\hbar\nabla + bA)^2\gamma_\Psi].$$

Briefly noting that $(\boldsymbol{\sigma}\cdot(-i\hbar\nabla+bA))^2 = (-i\hbar\nabla+bA)^2\mathbb{1}_{\mathbb{C}^2} + \hbar b\sigma_3$ and $\mathrm{Tr}[\sigma_3\gamma_\Psi] \ge -N$, we combine the bounds above to obtain

$$\begin{aligned}&\sum_{s_1,s_2=\pm1} \iint_{\mathbb{R}^6} |w_1(x-y)||\gamma_\Psi(x,s_1;y,s_2)|^2 \,\mathrm{d}x\,\mathrm{d}y\\ &\qquad\le C\|w_1\|_{\frac{3}{2}}\Big(\frac{1}{\hbar^2}\mathrm{Tr}[(\boldsymbol{\sigma}\cdot(-i\hbar\nabla + bA))^2\gamma_\Psi] - \frac{1}{\hbar^2}\mathrm{Tr}[\hbar b\sigma_3\gamma_\Psi] + \varepsilon^{-2}N\Big)\\ &\qquad\le C\|w_1\|_{\frac{3}{2}}\Big(\frac{1}{\hbar^2}\mathrm{Tr}[(\boldsymbol{\sigma}\cdot(-i\hbar\nabla + bA))^2\gamma_\Psi] + \frac{b}{\hbar}N + \varepsilon^{-2}N\Big).\end{aligned}$$

Now, choosing $\varepsilon^2 = \hbar/b$ and recalling the definitions of $\hbar$ and b (A.4), we get

$$\begin{aligned}&\frac{1}{2N}\sum_{s_1,s_2=\pm1} \iint_{\mathbb{R}^6} |w_1(x-y)||\gamma_\Psi(x,s_1;y,s_2)|^2 \,\mathrm{d}x\,\mathrm{d}y\\ &\qquad\le C\|w_1\|_{\frac{3}{2}} N^{\frac{2}{3}}\Big(\frac{1}{N}\mathrm{Tr}[(\boldsymbol{\sigma}\cdot(-i\hbar\nabla + bA))^2\gamma_\Psi] + \beta_N(1+\beta_N)^{-\frac{4}{5}}\Big),\end{aligned}$$

so combining with (A.51), we obtain (A.50). □

Continuing (A.49), recalling (A.6) (the assumption $N^{-1/3}\beta_N^{1/5} \to 0$), and applying the min-max principle, we get the bound

$$\begin{aligned}&\limsup_{N\to\infty} \frac{E(N,\beta_N)}{N}\\ &\quad\le \limsup_{N\to\infty} \inf_{\substack{\Psi\ \text{HF-}\\ \text{state}}} \Big\{\frac{1+CN^{-\frac{1}{3}}}{N}\mathrm{Tr}[(\boldsymbol{\sigma}\cdot(-i\hbar\nabla + bA))^2\gamma_\Psi]\\ &\qquad + \frac{1}{N}\int_{\mathbb{R}^3} V(x)\rho_\Psi^{(1)}(x)\,\mathrm{d}x + \frac{1}{2N^2}\iint_{\mathbb{R}^6} w(x-y)\rho_\Psi^{(1)}(x)\rho_\Psi^{(1)}(y)\,\mathrm{d}x\,\mathrm{d}y\Big\}. \quad (A.52)\end{aligned}$$

We proceed to construct an appropriate trial state for this variational problem. For $R > 0$ we denote by $(\boldsymbol{\sigma} \cdot (-i\hbar\nabla + bA))^2_{C_R}$ the Pauli operator in the cube $C_R = (-R/2, R/2)^3$ with Dirichlet boundary conditions.

Lemma A.24. *Suppose that $\beta_N \to \beta \in (0, \infty)$ and let $0 \le \rho \in C_c(C_R)$ be any function with $\int_{\mathbb{R}^3} \rho(x)\,\mathrm{d}x = 1$. Define $r(x)$ to be the solution to the equation*

$$\rho(x) = (1+\beta)^{-\frac{3}{5}} P'_{k_\beta}(r(x)),$$

where P_{k_β} is the pressure of the free Landau gas (A.10) and $k_\beta = \beta(1+\beta)^{-2/5}$, cf. Lemma A.15. Then the sequence of density matrices γ_N given by the spectral projections

$$\gamma_N := \mathbb{1}_{(-\infty,0]}((\boldsymbol{\sigma} \cdot (-i\hbar\nabla + bA))^2_{C_R} - r(x)), \tag{A.53}$$

satisfies

$$\lim_{N\to\infty} \frac{1}{N} \operatorname{Tr}[(\boldsymbol{\sigma} \cdot (-i\hbar\nabla + bA))^2 \gamma_N] = \int_{\mathbb{R}^3} \tau_\beta(\rho(x))\,\mathrm{d}x \tag{A.54}$$

and

$$\lim_{N\to\infty} \frac{1}{N} \operatorname{Tr}[\gamma_N] = \int_{\mathbb{R}^3} \rho(x)\,\mathrm{d}x = 1. \tag{A.55}$$

Moreover, the densities $\frac{1}{N}\rho_{\gamma_N}$ converge to ρ weakly in $L^1(\mathbb{R}^3)$ and $L^{5/3}(\mathbb{R}^3)$, and the same conclusions also hold if γ_N is replaced by the projection $\tilde{\gamma}_N$ onto the N lowest eigenvectors of the operator $(\boldsymbol{\sigma} \cdot (-i\hbar\nabla + bA))^2_{C_R} - r(x)$.

Proof. For the duration of the proof, we will employ the notation $T^{\beta_N}_{C_R} = (\boldsymbol{\sigma} \cdot (-i\hbar\nabla + bA))^2_{C_R}$. By domain inclusions it is not difficult to see that in the sense of quadratic forms $\operatorname{Tr}[T^{\beta_N}_{C_R}\gamma_N] = \operatorname{Tr}[(\boldsymbol{\sigma} \cdot (-i\hbar\nabla + bA))^2\gamma_N]$, and that the same equality holds when γ_N is replaced by $\tilde{\gamma}_N$. Thus, it is sufficient to show (A.54) using $T^{\beta_N}_{C_R}$ instead of the Pauli operator on the whole space.

Note also that the quadratic form domain of $T^{\beta_N}_{C_R} - r(x)$, $H^1_0(C_R; \mathbb{C}^2)$, is compactly embedded in $L^2(C_R; \mathbb{C}^2)$, so that $T^{\beta_N}_{C_R} - r(x)$ has compact resolvent, and hence it has purely discrete spectrum. This implies that γ_N is a projection onto a finite-dimensional subspace of $L^2(C_R)$, and hence ρ_{γ_N} is an L^1-function.

Using the Weyl asymptotics from Corollary A.9 and Remark A.10 and recalling (A.44), we obtain in the semi-classical limit

$$\begin{aligned} \lim_{N\to\infty} \frac{1}{N} \operatorname{Tr}[(T^{\beta_N}_{C_R} - r(x))\gamma_N] &= -(1+\beta)^{-\frac{3}{5}} \int_{C_R} P_{k_\beta}(r(x))\,\mathrm{d}x \\ &= \int_{C_R} \tau_\beta(\rho(x))\,\mathrm{d}x - \int_{C_R} \rho(x) r(x)\,\mathrm{d}x. \end{aligned} \tag{A.56}$$

Let now $g \in L^\infty(C_R)$ be real and non-negative. We shall see that

$$\lim_{N\to\infty} \frac{1}{N} \operatorname{Tr}[g(x)\gamma_N] = \int_{C_R} g(x)\rho(x)\,\mathrm{d}x. \tag{A.57}$$

To see this, note first for any real δ that any function in the range of γ_N is also in the domain of $T_{C_R}^{\beta_N} - r(x) + \delta g(x)$. Hence we have by the variational principle

$$\operatorname{Tr}[(T_{C_R}^{\beta_N} - r(x) + \delta g(x))\gamma_N] \geq \operatorname{Tr}(T_{C_R}^{\beta_N} - r(x) + \delta g(x))_-,$$

so that

$$\delta \operatorname{Tr}[g(x)\gamma_N] \geq \operatorname{Tr}(T_{C_R}^{\beta_N} - r(x) + \delta g(x))_- - \operatorname{Tr}(T_{C_R}^{\beta_N} - r(x))_-. \tag{A.58}$$

Hence for $\delta < 0$, we get by Corollary A.9,

$$\begin{aligned}
&\limsup_{N\to\infty} \frac{1}{N} \operatorname{Tr}[g(x)\gamma_N] \\
&\qquad \leq \frac{1}{\delta} \lim_{N\to\infty} \frac{1}{N}\big(\operatorname{Tr}(T_{C_R}^{\beta_N} - r(x) + \delta g(x))_- - \operatorname{Tr}(T_{C_R}^{\beta_N} - r(x))_-\big) \\
&\qquad = (1+\beta)^{-\frac{3}{5}} \int_{C_R} \frac{P_{k_\beta}(r(x) - \delta g(x)) - P_{k_\beta}(r(x))}{-\delta g(x)} g(x)\,\mathrm{d}x.
\end{aligned}$$

Since g is non-negative and P_{k_β} is convex and increasing, the integrand above decreases pointwise to $P_{k_\beta}'(r(x))$ as $\delta \to 0_-$, on the set where $g(x) \neq 0$. This implies by the monotone convergence theorem and definition of r that

$$\begin{aligned}
\limsup_{N\to\infty} \frac{1}{N} \operatorname{Tr}[g(x)\gamma_N] &\leq (1+\beta)^{-\frac{3}{5}} \int_{C_R} P_{k_\beta}'(r(x))g(x)\,\mathrm{d}x \\
&= \int_{C_R} \rho(x)g(x)\,\mathrm{d}x.
\end{aligned}$$

In the same way we get from (A.58) for positive δ, that

$$\begin{aligned}
&\liminf_{N\to\infty} \frac{1}{N} \operatorname{Tr}[g(x)\gamma_N] \\
&\qquad \geq (1+\beta)^{-\frac{3}{5}} \int_{C_R} \frac{P_{k_\beta}([r(x) - \delta g(x)]_+) - P_{k_\beta}(r(x))}{-\delta g(x)} g(x)\,\mathrm{d}x \\
&\qquad \xrightarrow{\delta\to 0_+} (1+\beta)^{-\frac{3}{5}} \int_{C_R} P_{k_\beta}'(r(x))g(x)\,\mathrm{d}x = \int_{C_R} \rho(x)g(x)\,\mathrm{d}x,
\end{aligned}$$

since the fraction in the integral this time increases to $P_{k_\beta}'(r(x))$ on the set where $g(x) \neq 0$. It follows that (A.57) holds, and by extension that for arbitrary $g \in L^\infty(\mathbb{R}^3)$, we have

$$\int_{\mathbb{R}^3} g(x)\frac{\rho_{\gamma_N}(x)}{N}\,\mathrm{d}x = \frac{1}{N}\operatorname{Tr}[(g\mathbb{1}_{C_R})(x)\gamma_N] \to \int_{\mathbb{R}^3} g(x)\rho(x)\,\mathrm{d}x,$$

as N tends to infinity, so $\frac{1}{N}\rho_{\gamma_N} \rightharpoonup \rho$ weakly in $L^1(\mathbb{R}^3)$, as advertised. Taking $g = \mathbb{1}_{C_R}$ in (A.57) yields (A.55), implying that $T_{C_R}^{\beta_N} - r(x)$ has $N + o(N)$ negative eigenvalues.

Noting that r is bounded by construction, we can take $g = r$ in (A.57) and combine with (A.56) to obtain

$$\lim_{N\to\infty} \frac{1}{N} \operatorname{Tr}[T_{C_R}^{\beta_N} \gamma_N] = \int_{C_R} \tau_\beta(\rho(x))\,\mathrm{d}x. \tag{A.59}$$

Finally, applying Lemma A.13 to get weak convergence in $L^{5/3}(\mathbb{R}^3)$, we have proven the lemma for γ_N.

We want to see that the assertions of the lemma also hold for $\tilde{\gamma}_N$. The fact that the dimension of the range of γ_N is $N+o(N)$ immediately implies that $\|\rho_{\gamma_N} - \rho_{\tilde{\gamma}_N}\|_1 = \operatorname{Tr}[|\gamma_N - \tilde{\gamma}_N|] = o(N)$. Hence for any $g \in L^\infty(\mathbb{R}^3)$ we have

$$\operatorname{Tr}[g(x)(\gamma_N - \tilde{\gamma}_N)] = o(N). \tag{A.60}$$

In other words, $\frac{1}{N}\rho_{\tilde{\gamma}_N}$ has the same weak limit in $L^1(\mathbb{R}^3)$ as $\frac{1}{N}\rho_{\gamma_N}$. Note by (A.11) that P'_{k_β} is continuous and increasing, which along with continuity of ρ implies that r is continuous. Also, it is clear that $\operatorname{supp} r = \operatorname{supp} \rho \subseteq C_R$, so we get by uniform continuity that for each $\delta > 0$ there is some $\varepsilon \in (0, \delta]$ such that for all $x \in C_R$, we have

$$(1+\beta)^{-\frac{3}{5}} |P'_{k_\beta}([r(x) \pm \varepsilon]_+) - P'_{k_\beta}(r(x))| \le \delta. \tag{A.61}$$

Use this ε to define

$$\gamma_{N,\pm\varepsilon} := \mathbb{1}_{(-\infty,\pm\varepsilon]}(T_{C_R}^{\beta_N} - r(x)) = \mathbb{1}_{(-\infty,0]}(T_{C_R}^{\beta_N} - (r(x) \pm \varepsilon)).$$

Redoing the argument used to prove (A.57), we obtain

$$\lim_{N\to\infty} \frac{1}{N} \operatorname{Tr}[\gamma_{N,\pm\varepsilon}] = (1+\beta)^{-\frac{3}{5}} \int_{C_R} P'_{k_\beta}([r(x) \pm \varepsilon]_+)\,\mathrm{d}x,$$

and since P'_{k_β} strictly increasing on $[0, \infty)$, we have

$$\eta_\pm := \pm(1+\beta)^{-\frac{3}{5}} \int_{C_R} P'_{k_\beta}([r(x) \pm \varepsilon]_+) - P'_{k_\beta}(r(x))\,\mathrm{d}x > 0$$

as long as ε is small enough, implying

$$\lim_{N\to\infty} \frac{1}{N} \operatorname{Tr}[\gamma_{N,-\varepsilon}] \le 1 - \eta_- \le 1 + \eta_+ \le \lim_{N\to\infty} \frac{1}{N} \operatorname{Tr}[\gamma_{N,\varepsilon}].$$

These bounds yield for N large enough that $\operatorname{Tr}[\gamma_{N,-\varepsilon}] \le N \le \operatorname{Tr}[\gamma_{N,\varepsilon}]$, so

$$\gamma_{N,-\varepsilon} \le \tilde{\gamma}_N \le \gamma_{N,\varepsilon}. \tag{A.62}$$

Similarly, using (A.61) along with the fact that P'_{k_β} is increasing, we have

$$1 - \delta R^3 \le \lim_{N\to\infty} \frac{1}{N} \operatorname{Tr}[\gamma_{N,-\varepsilon}] \le \lim_{N\to\infty} \frac{1}{N} \operatorname{Tr}[\gamma_{N,\varepsilon}] \le 1 + \delta R^3.$$

Now, for each $N \geq 1$, there are two cases; either $\tilde{\gamma}_N$ is a subprojection of γ_N, or the converse is true. In case $\tilde{\gamma}_N \leq \gamma_N$, we have $\gamma_N - \tilde{\gamma}_N \geq \gamma_N - \gamma_{N,-\varepsilon}$, where the latter is the spectral projection of $T^{\beta_N}_{C_R} - r(x)$ corresponding to the interval $(-\varepsilon, 0]$. Hence we have

$$\begin{aligned} 0 &\geq \operatorname{Tr}[(T^{\beta_N}_{C_R} - r(x))(\gamma_N - \tilde{\gamma}_N)] \geq \operatorname{Tr}[(T^{\beta_N}_{C_R} - r(x))(\gamma_N - \gamma_{N,-\varepsilon})] \\ &\geq -\varepsilon \operatorname{Tr}[\gamma_N - \gamma_{N,-\varepsilon}] \geq -\varepsilon(\delta R^3 N + o(N)). \end{aligned}$$

The other case, where $\gamma_N \leq \tilde{\gamma}_N$, is handled similarly. Here we get the bound

$$\begin{aligned} 0 &\leq -\operatorname{Tr}[(T^{\beta_N}_{C_R} - r(x))(\gamma_N - \tilde{\gamma}_N)] \leq \operatorname{Tr}[[T^{\beta_N}_{C_R} - r(x)](\gamma_{N,\varepsilon} - \gamma_N)] \\ &\leq \varepsilon \operatorname{Tr}[\gamma_{N,\varepsilon} - \gamma_N] \leq \varepsilon(\delta R^3 N + o(N)). \end{aligned}$$

In either case,

$$\operatorname{Tr}[(T^{\beta_N}_{C_R} - r(x))(\gamma_N - \tilde{\gamma}_N)] = o(N),$$

so combining with (A.60), we obtain $\operatorname{Tr}[T^{\beta_N}_{C_R}(\gamma_N - \tilde{\gamma}_N)] = o(N)$, meaning that (A.59) also holds for $\tilde{\gamma}_N$, finishing the proof. □

In the regimes where either $\beta_N \to 0$ or $\beta_N \to \infty$, we modify the proof above to obtain similar results:

Lemma A.25. *Let $0 \leq \rho \in C_c(C_R)$ be any function with $\int_{\mathbb{R}^3} \rho(x)\,\mathrm{d}x = 1$.*

(1) If $\beta_N \to 0$, then the sequence of density matrices γ_N given by the spectral projections

$$\gamma_N := \mathbb{1}_{(-\infty,0]}\big((\boldsymbol{\sigma} \cdot (-i\hbar\nabla + bA))^2_{C_R} - c_{\mathrm{TF}}\rho(x)^{\frac{2}{3}}\big)$$

satisfies

$$\lim_{N\to\infty} \frac{1}{N} \operatorname{Tr}[(\boldsymbol{\sigma} \cdot (-i\hbar\nabla + bA))^2 \gamma_N] = \frac{3}{5} c_{\mathrm{TF}} \int_{\mathbb{R}^3} \rho(x)^{\frac{5}{3}}\,\mathrm{d}x.$$

(2) If $\beta_N \to \infty$ and (A.6) holds, then the sequence of density matrices γ_N given by the spectral projections

$$\gamma_N := \mathbb{1}_{(-\infty,0]}((\boldsymbol{\sigma} \cdot (-i\hbar\nabla + bA))^2_{C_R} - 4\pi^4\rho(x)^2)$$

satisfies

$$\lim_{N\to\infty} \frac{1}{N} \operatorname{Tr}[(\boldsymbol{\sigma} \cdot (-i\hbar\nabla + bA))^2 \gamma_N] = \frac{4\pi^4}{3} \int_{\mathbb{R}^3} \rho(x)^3\,\mathrm{d}x.$$

Moreover, in both cases we have

$$\lim_{N\to\infty} \frac{1}{N} \operatorname{Tr}[\gamma_N] = \int_{\mathbb{R}^3} \rho(x)\,\mathrm{d}x = 1,$$

and the densities $\frac{1}{N}\rho_{\gamma_N}$ *converge to* ρ *weakly in* $L^1(\mathbb{R}^3)$ *and in* $L^{5/3}(\mathbb{R}^3)$*. The same conclusions also hold if* γ_N *is replaced by the projection* $\tilde{\gamma}_N$ *onto the* N *lowest eigenvectors of the operator used to define* γ_N*.*

Proof. The proof of Lemma A.24 also holds mutatis mutandis for this lemma, and we omit the details. □

Using the trial states constructed above we can now show the upper bound on the energy.

Proof of Proposition A.22.. Let $0 \le \rho \in C_c(\mathbb{R}^3)$ with $\int \rho(x)\,\mathrm{d}x = 1$, and take $\tilde{\gamma}_N$ as in either Lemma A.24 or Lemma A.25, depending on the sequence (β_N). Since $V \in L^{5/2}_{\mathrm{loc}}(\mathbb{R}^3)$ and $\rho_{\tilde{\gamma}_N}$ is supported inside the box C_R, we get by weak convergence of $\frac{1}{N}\rho_{\tilde{\gamma}_N}$ that

$$\frac{1}{N}\int_{\mathbb{R}^3} V(x)\rho_{\tilde{\gamma}_N}(x)\,\mathrm{d}x \longrightarrow \int_{C_R} V(x)\rho(x)\,\mathrm{d}x$$

as N tends to infinity. By the Stone-Weierstrass theorem, we may approximate $w(x-y)$ in $L^{\frac{5}{2}}(C_R^2)$ by a function of the form $w_0 = \sum_{j=1}^k g_j \otimes h_j$ with $g_j, h_j \in C(C_R)$. By a standard approximation argument we conclude that

$$\frac{1}{N^2}\iint_{\mathbb{R}^6} w(x-y)\rho_{\tilde{\gamma}_N}(x)\rho_{\tilde{\gamma}_N}(y)\,\mathrm{d}x\,\mathrm{d}y \longrightarrow \iint_{C_R^2} w(x-y)\rho(x)\rho(y)\,\mathrm{d}x\,\mathrm{d}y.$$

Hence, continuing from (A.52) with $\gamma_\Psi = \tilde{\gamma}_N$, we find (for instance in the case where $\beta_N \to \beta \in (0,\infty)$)

$$\limsup_{N\to\infty} \frac{E(N,\beta_N)}{N} \le \mathcal{E}^{\mathrm{MTF}}_\beta(\rho).$$

If $\beta_N \to 0$, or $\beta_N \to \infty$, we obtain analogous bounds by appealing to Lemma A.25. This concludes the proof since the Thomas-Fermi ground state energy can be obtained by minimizing over compactly supported, continuous functions, and $\rho \in C_c(\mathbb{R}^3)$ is arbitrary. □

A.4 Semi-classical measures

Having established the upper bound on the energy, we turn our attention towards proving the lower bound. In order to do this, we will construct semi-classical measures using coherent states, and see that these measures have some very nice properties in the limit as the number of particles tends to infinity. Afterwards, a de Finetti theorem may be applied to yield general information about the structure in the limit. The constructions in this section are only useful for dealing with the case where $\beta_N \to \beta > 0$. In the case where $\beta_N \to 0$, it is more convenient to use the same semi-classical measures as in [5]. This case is treated in Section A.6.

The first step is to diagonalize the three-dimensional magnetic Laplacian, i.e., we consider

$$H_A = (-i\nabla + A)^2 = H_{A^\perp} - \partial_{x_3}^2, \tag{A.63}$$

where $A^\perp(x_1, x_2) = \frac{1}{2}(-x_2, x_1)$, and $H_{A^\perp} := (-i\nabla + A^\perp)^2$ acts on $L^2(\mathbb{R}^2)$. Letting $\mathcal{F}_2$ denote the partial Fourier transform in the second variable on $L^2(\mathbb{R}^2)$, and T the unitary operator on $L^2(\mathbb{R}^2)$ defined by $(T\varphi)(x_1, \xi) = \varphi(x_1 + \xi, \xi)$, an elementary calculation shows that

$$H_{A^\perp} e^{i\frac{1}{2}x_1x_2}\mathcal{F}_2^{-1}T = e^{i\frac{1}{2}x_1x_2}\mathcal{F}_2^{-1}T\Big(\Big(-\frac{\mathrm{d}^2}{\mathrm{d}x_1^2} + x_1^2\Big) \otimes \mathbb{1}_{L^2(\mathbb{R})}\Big). \tag{A.64}$$

It is very well known that the harmonic oscillator admits an orthonormal basis of eigenfunctions $(f_j)_{j\geq 0}$ for $L^2(\mathbb{R})$, with $(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2)f_j = (2j+1)f_j$ and $f_0(x) = \pi^{-\frac{1}{4}}e^{-\frac{1}{2}x^2}$. In particular, equation (A.64) means for any $j \geq 0$ and any normalized Schwartz function v on $\mathbb{R}$, that $e^{i\frac{1}{2}x_1x_2}\mathcal{F}_2^{-1}T(f_j \otimes v)$ is a normalized eigenfunction for $H_{A^\perp}$ with corresponding eigenvalue $2j+1$.

Suppose that φ is an eigenfunction for $H_{A^\perp}$ corresponding to $2j+1$. If we scale the magnetic field and instead consider $H_{BA^\perp} = (-i\nabla + BA^\perp)^2$, and denote $x \times y = x_1y_2 - x_2y_1$ for $x, y \in \mathbb{R}^2$, we see for any fixed $y \in \mathbb{R}^2$ that $\widetilde{\varphi}_{y,B}(x) := \sqrt{B}e^{-i\frac{B}{2}y\times x}u_j(\sqrt{B}(x-y))$ is an eigenfunction for $H_{BA^\perp}$ corresponding to the eigenvalue $B(2j+1)$.

A.4.1 Coherent states

Throughout this subsection, $\hbar$ and b will denote arbitrary positive numbers, that is, the scaling relations (A.5) will not be needed. For $f \in L^2(\mathbb{R}^3)$ we denote by $f^\hbar$ the function

$$f^\hbar(y) = \hbar^{-\frac{3}{4}}f(\hbar^{-\frac{1}{2}}y).$$

Definition A.26. We fix a normalized $f \in L^2(\mathbb{R}^3)$, and for each $j \in \mathbb{N}_0$ we choose any normalized eigenfunction φ_j in the j'th Landau level of $H_{A^\perp}$. For fixed $x \in \mathbb{R}^2$, $u \in \mathbb{R}^3$, $p \in \mathbb{R}$, and $\hbar, b > 0$, we define functions $\varphi_{x,j}^{\hbar,b}$ on $\mathbb{R}^2$ and $f_{x,u,p,j}^{\hbar,b}$ on $\mathbb{R}^3$ by

$$\varphi_{x,j}^{\hbar,b}(y_\perp) = \hbar^{-\frac{1}{2}}b^{\frac{1}{2}}e^{-i\frac{b}{2\hbar}x\times y_\perp}\varphi_j(\hbar^{-\frac{1}{2}}b^{\frac{1}{2}}(y_\perp - x)), \tag{A.65}$$

and

$$f_{x,u,p,j}^{\hbar,b}(y) = \varphi_{x,j}^{\hbar,b}(y_\perp)f^\hbar(y-u)e^{i\frac{py_3}{\hbar}}, \tag{A.66}$$

where $y_\perp = (y_1, y_2)$ denotes the part of y orthogonal to the magnetic field.

Note that $\varphi^{\hbar,b}_{x,j}$ is an eigenfunction for the operator $H_{\hbar^{-1}bA^\perp}$ corresponding to the eigenvalue $\hbar^{-1}b(2j+1)$. Later we will put further assumptions on the function f, but for now it can be any normalized L^2-function.

We will use (A.65) and (A.66) to build Landau level projections and some resolutions of the identity. Recall that for any normalized function $v \in L^2(\mathbb{R})$ we have a resolution of the identity

$$\frac{1}{2\pi}\int_{\mathbb{R}^2} |v_{x,p}\rangle\langle v_{x,p}|\,\mathrm{d}x\,\mathrm{d}p = \mathbb{1}_{L^2(\mathbb{R})}, \tag{A.67}$$

where $v_{x,p}(y) = v(y-x)e^{ipy}$, $x, p \in \mathbb{R}$. We will use shortly that if $u \in L^2(\mathbb{R})$ is any other function, then

$$\begin{aligned}\frac{1}{2\pi}&\int_{\mathbb{R}^2} \langle \psi, v_{x,p}\rangle\langle u_{x,p}, \psi\rangle\,\mathrm{d}x\,\mathrm{d}p \\ &= \frac{1}{2\pi}\int_{\mathbb{R}^2} \langle u, \psi_{-x,-p}\rangle\langle \psi_{-x,-p}, v\rangle\,\mathrm{d}x\,\mathrm{d}p = \langle u, v\rangle\|\psi\|^2.\end{aligned} \tag{A.68}$$

Lemma A.27. *Let $\Pi^{(2)}_j$ denote the projection onto the j'th Landau level of the operator $H_{\hbar^{-1}bA^\perp}$. We have that*

$$\frac{b}{2\pi\hbar}\sum_{j=0}^{\infty}\int_{\mathbb{R}^2} |\varphi^{\hbar,b}_{x,j}\rangle\langle \varphi^{\hbar,b}_{x,j}|\,\mathrm{d}x = \mathbb{1}_{L^2(\mathbb{R}^2)}, \tag{A.69}$$

and

$$\frac{b}{2\pi\hbar}\int_{\mathbb{R}^2} |\varphi^{\hbar,b}_{x,j}\rangle\langle \varphi^{\hbar,b}_{x,j}|\,\mathrm{d}x = \Pi^{(2)}_j. \tag{A.70}$$

Proof. For $\varphi \in L^2(\mathbb{R}^2)$ we denote $\widetilde{\varphi}_x(y) = e^{-\frac{i}{2}x\times y}\varphi(y-x)$, and recalling the isomorphism (A.64), we furthermore define a unitary operator $U := T^*\mathcal{F}_2 e^{-i\frac{1}{2}(\cdot)_1(\cdot)_2}$. Utilizing the usual properties of the Fourier transform, we have for any function φ that

$$\begin{aligned}&\mathcal{F}_2\big[e^{-\frac{i}{2}(\cdot)_1(\cdot)_2}\widetilde{\varphi}_x\big](y_1,\xi)\\ &\quad= e^{-\frac{i}{2}x_1x_2}\mathcal{F}_2\big[e^{-\frac{i}{2}((\cdot)_1+x_1)((\cdot)_2-x_2)}\varphi(\,\cdot\,-x)\big](y_1,\xi)\\ &\quad= e^{-\frac{i}{2}x_1x_2}e^{-ix_2\xi}\mathcal{F}_2\big[e^{-\frac{i}{2}((\cdot)_1+x_1)(\cdot)_2}\varphi((\,\cdot\,)_1-x_1,(\,\cdot\,)_2)\big](y_1,\xi)\\ &\quad= e^{-\frac{i}{2}x_1x_2}e^{-ix_2\xi}\mathcal{F}_2\big[e^{-\frac{i}{2}(\cdot)_1(\cdot)_2}\varphi\big](y_1-x_1,\xi+x_1),\end{aligned}$$

and so

$$(U\widetilde{\varphi}_x)(y_1,\xi) = e^{-\frac{i}{2}x_1x_2}e^{-ix_2\xi}(U\varphi)(y_1,\xi+x_1). \tag{A.71}$$

Introducing the parameter $\alpha := b/\hbar$ and denoting by V_α the unitary operator given by $(V_\alpha\psi)(y) := \sqrt{\alpha}\psi(\sqrt{\alpha}y)$, then $\varphi^{\hbar,b}_{x,j}(y) = (V_\alpha\varphi^{1,1}_{\sqrt{\alpha}x,j})(y)$. Since $U\varphi_j$ is an eigenvector corresponding to the j'th eigenvalue of $(-\frac{\mathrm{d}^2}{\mathrm{d}x_1^2} + x_1^2) \otimes \mathbb{1}_{L^2(\mathbb{R})}$, we can write

$$U\varphi_j = \sum_{k=1}^{\infty} c_k f_j \otimes v_k,$$

where (v_k) is any orthonormal basis of $L^2(\mathbb{R})$, and $\sum_k |c_k|^2 = 1$. Combining this with (A.71) and using (A.68), we obtain

$$\begin{aligned}
&\frac{b}{2\pi\hbar}\int_{\mathbb{R}^2} \left|\langle \varphi^{\hbar,b}_{-x,j}, \psi\rangle\right|^2 \mathrm{d}x \\
&\quad = \frac{\alpha}{2\pi}\int_{\mathbb{R}^2} \left|\langle U\varphi_j((\,\cdot\,)_1, (\,\cdot\,)_2 - \sqrt{\alpha}x_1)e^{i\sqrt{\alpha}x_2(\cdot)_2}, UV_\alpha^*\psi\rangle\right|^2 \mathrm{d}x \\
&\quad = \frac{1}{2\pi}\int_{\mathbb{R}^2} \sum_{\ell,k} \overline{c_\ell} c_k \langle f_j \otimes (v_\ell)_{x_1,x_2}, UV_\alpha^*\psi\rangle \langle UV_\alpha^*\psi, f_j \otimes (v_k)_{x_1,x_2}\rangle \,\mathrm{d}x \\
&\quad = \sum_{\ell,k} \overline{c_\ell} c_k \langle UV_\alpha^*\psi, (|f_j\rangle\langle f_j| \otimes \langle v_\ell, v_k\rangle \mathbb{1}_{L^2(\mathbb{R})})UV_\alpha^*\psi\rangle \\
&\quad = \langle UV_\alpha^*\psi, (|f_j\rangle\langle f_j| \otimes \mathbb{1}_{L^2(\mathbb{R})})UV_\alpha^*\psi\rangle.
\end{aligned}$$

This actually shows (A.70), since $\Pi_j^{(2)} = V_\alpha U^*(|f_j\rangle\langle f_j| \otimes \mathbb{1}_{L^2(\mathbb{R})})UV_\alpha^*$ by the unitary equivalence (A.64). Summing over all j, we also get

$$\frac{b}{2\pi\hbar}\sum_{j=0}^{\infty}\int_{\mathbb{R}^2} \left|\langle \varphi^{\hbar,b}_{x,j}, \psi\rangle\right|^2 \mathrm{d}x = \|UV_\alpha^*\psi\|^2 = \|\psi\|^2,$$

concluding the proof. □

Definition A.28. Using the functions from (A.66), we define operators on $L^2(\mathbb{R}^3)$ by

$$P^{\hbar,b}_{u,p,j} := \int_{\mathbb{R}^2} |f^{\hbar,b}_{x,u,p,j}\rangle\langle f^{\hbar,b}_{x,u,p,j}| \,\mathrm{d}x. \tag{A.72}$$

Applying the lemma above and using (A.67), it is easy to show the following

Lemma A.29. *The $P^{\hbar,b}_{u,p,j}$ yield a resolution of the identity on $L^2(\mathbb{R}^3)$, i.e.,*

$$\frac{b}{(2\pi\hbar)^2}\sum_{j=0}^{\infty}\int_{\mathbb{R}}\int_{\mathbb{R}^3} P^{\hbar,b}_{u,p,j}\,\mathrm{d}u\,\mathrm{d}p = \mathbb{1}_{L^2(\mathbb{R}^3)}.$$

Furthermore, $P^{\hbar,b}_{u,p,j}$ is a trace class operator with $\mathrm{Tr}(P^{\hbar,b}_{u,p,j}) = 1$.

Proof. Recall that for $y \in \mathbb{R}^3$ we denote by $y_\perp = (y_1, y_2) \in \mathbb{R}^2$ the coordinates of y orthogonal to the magnetic field. Let $\psi \in L^2(\mathbb{R}^3)$ and define an auxiliary function

$$\begin{aligned}
g^{\hbar}_{u,p}(y_\perp) :=& \langle f^{\hbar}(y_\perp - u_\perp, \,\cdot\, - u_3)e^{i\frac{p}{\hbar}(\cdot)}, \psi(y_\perp, \,\cdot\,)\rangle_{L^2(\mathbb{R})} \\
=& \sqrt{2\pi}\mathcal{F}_3\left[\overline{f^{\hbar}(\,\cdot\, - u)}\psi\right](y_\perp, \frac{p}{\hbar}),
\end{aligned} \tag{A.73}$$

with $\mathcal{F}_3$ being the partial Fourier transform in the third variable. Using Lemma A.27, we calculate

$$\begin{aligned}\langle\psi, P^{\hbar,b}_{u,p,j}\psi\rangle &= \int_{\mathbb{R}^2}\big|\langle f^{\hbar,b}_{x,u,p,j},\psi\rangle\big|^2\,\mathrm{d}x\\ &= \int_{\mathbb{R}^2}\big|\langle\varphi^{\hbar,b}_{x,j}, g^{\hbar}_{u,p}\rangle\big|^2\,\mathrm{d}x = \frac{2\pi\hbar}{b}\langle g^{\hbar}_{u,p},\Pi^{(2)}_j g^{\hbar}_{u,p}\rangle,\end{aligned}\tag{A.74}$$

implying that

$$\begin{aligned}&\frac{b}{(2\pi\hbar)^2}\sum_{j=0}^{\infty}\int_{\mathbb{R}}\int_{\mathbb{R}^3}\langle\psi, P^{\hbar,b}_{u,p,j}\psi\rangle\,\mathrm{d}u\,\mathrm{d}p\\ &\quad= \frac{1}{2\pi\hbar}\sum_{j=0}^{\infty}\int_{\mathbb{R}}\int_{\mathbb{R}^3}\langle g^{\hbar}_{u,p},\Pi^{(2)}_j g^{\hbar}_{u,p}\rangle\,\mathrm{d}u\,\mathrm{d}p\\ &\quad= \frac{1}{\hbar}\int_{\mathbb{R}}\int_{\mathbb{R}^3}\int_{\mathbb{R}^2}\big|\mathcal{F}_3\big[\overline{f^{\hbar}(\,\cdot\,-u)}\psi\big]\big(y_\perp,\frac{p}{\hbar}\big)\big|^2\,\mathrm{d}y_\perp\,\mathrm{d}u\,\mathrm{d}p\\ &\quad= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}|f^{\hbar}(y-u)\psi(y)|^2\,\mathrm{d}y\,\mathrm{d}u = \langle\psi,\psi\rangle.\end{aligned}$$

To calculate the trace of $P^{\hbar,b}_{u,p,j}$, we take an arbitrary orthonormal basis (ψ_ℓ) of $L^2(\mathbb{R}^3)$ and use the definition of the coherent states (A.65) and (A.66)

$$\begin{aligned}\mathrm{Tr}(P^{\hbar,b}_{u,p,j}) &= \sum_{\ell=1}^{\infty}\langle\psi_\ell, P^{\hbar,b}_{u,p,j}\psi_\ell\rangle = \int_{\mathbb{R}^2}\big\|f^{\hbar,b}_{x,u,p,j}\big\|_2^2\,\mathrm{d}x\\ &= \int_{\mathbb{R}^2}\int_{\mathbb{R}^3}\frac{b}{\hbar}|\varphi_j(\hbar^{-\frac12}b^{\frac12}(y_\perp-x))|^2|f^{\hbar}(y-u)|^2\,\mathrm{d}y\,\mathrm{d}x = 1.\end{aligned}$$

□

A.4.2 Semi-classical measures on phase space

Let $\mathcal{P}_{\pm1}$ denote the projections onto the spin-up and spin-down components in $\mathbb{C}^2$, that is,

$$\mathcal{P}_1 = \begin{pmatrix}1&0\\0&0\end{pmatrix},\qquad \mathcal{P}_{-1} = \begin{pmatrix}0&0\\0&1\end{pmatrix}.$$

We recall that the phase space is $\Omega = \mathbb{R}^3\times\mathbb{R}\times\mathbb{N}_0\times\{\pm1\}$, and that we use the notational convention (A.9). We define k-particle semi-classical measures as follows.

Definition A.30. For $\Psi_N\in\bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ normalized and $1\le k\le N$, the k-particle semi-classical measure on Ω^k is the measure with density

$$m^{(k)}_{f,\Psi_N}(\xi) = \frac{N!}{(N-k)!}\Big\langle\Psi_N,\Big(\bigotimes_{\ell=1}^{k}P^{\hbar,b}_{u_\ell,p_\ell,j_\ell}\mathcal{P}_{s_\ell}\Big)\otimes\mathbb{1}_{N-k}\Psi_N\Big\rangle_{L^2(\mathbb{R}^{3N};\mathbb{C}^{2^N})},$$

where $\mathbb{1}_{N-k}$ is the identity acting on the last $N-k$ components of Ψ_N.

The semi-classical measures have the following basic properties. The upper bound in (A.75) below is a manifestation of the Pauli exclusion principle.

Lemma A.31. *The function $m^{(k)}_{f,\Psi_N}$ is symmetric on Ω^k and satisfies*

$$0 \le m^{(k)}_{f,\Psi_N} \le 1, \tag{A.75}$$

$$\frac{b^k}{(2\pi\hbar)^{2k}} \int_{\Omega^k} m^{(k)}_{f,\Psi_N}(\xi)\,\mathrm{d}\xi = \frac{N!}{(N-k)!}, \tag{A.76}$$

and for $k \ge 2$,

$$\frac{b}{(2\pi\hbar)^2} \int_{\Omega} m^{(k)}_{f,\Psi_N}(\xi_1,\dots,\xi_k)\,\mathrm{d}\xi_k = (N-k+1)m^{(k-1)}_{f,\Psi_N}(\xi_1,\dots,\xi_{k-1}). \tag{A.77}$$

Proof. We will start out by proving (A.75), and we will concentrate on the case $k=1$, since the proof easily generalizes to $k \ge 2$. Note that $0 \le m^{(k)}_{f,\Psi_N}$ obviously holds, as the $P^{\hbar,b}_{u,p,j}$'s are positive operators. Since $P^{\hbar,b}_{u,p,j}$ is trace class, we may write $P^{\hbar,b}_{u,p,j} = \sum_k \lambda_k |\psi_k\rangle\langle\psi_k|$, where the ψ_k constitute an orthonormal basis of $L^2(\mathbb{R}^3)$, and $\sum_k \lambda_k = \mathrm{Tr}(P^{\hbar,b}_{u,p,j}) = 1$. Note that for any $\psi \in L^2(\mathbb{R}^3)$ we can rewrite, as operators acting on $\bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$,

$$N(|\psi\rangle\langle\psi|\mathcal{P}_s \otimes \mathbb{1}_{N-1}) = \sum_{k=1}^N \mathbb{1}_{k-1} \otimes |\psi\rangle\langle\psi|\mathcal{P}_s \otimes \mathbb{1}_{N-k},$$

where

$$\begin{aligned}\Big(\sum_{k=1}^N \mathbb{1}_{k-1} \otimes |\psi\rangle\langle\psi|\mathcal{P}_s \otimes \mathbb{1}_{N-k}\Big)^2 &= \sum_{k=1}^N \mathbb{1}_{k-1} \otimes |\psi\rangle\langle\psi|\mathcal{P}_s \otimes \mathbb{1}_{N-k} \\ &\quad + 2\sum_{1\le k<\ell\le N} \mathbb{1}_{k-1} \otimes |\psi\rangle\langle\psi|\mathcal{P}_s \otimes \mathbb{1}_{\ell-k-1} \otimes |\psi\rangle\langle\psi|\mathcal{P}_s \otimes \mathbb{1}_{N-\ell}.\end{aligned}$$

Each term in the last sum acts as zero on anti-symmetric functions, implying for any $\psi \in L^2(\mathbb{R}^3)$ that $N|\psi\rangle\langle\psi|\mathcal{P}_s \otimes \mathbb{1}_{N-1}$ is an orthogonal projection on $\bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$. We arrive at the conclusion that

$$m^{(1)}_{f,\Psi_N}(u,p,j,s) = \sum_{k=0}^\infty \lambda_k N\big\langle \Psi_N, (|\psi_k\rangle\langle\psi_k|\mathcal{P}_s \otimes \mathbb{1}_{N-1})\Psi_N\big\rangle \le 1.$$

The result for general k follows by applying what we have just shown k times, so (A.75) holds.

The compatibility relation (A.77) follows by applying Lemma A.29:

$$\begin{aligned}&\frac{b}{(2\pi\hbar)^2}\int_\Omega m^{(k)}_{f,\Psi_N}(\xi_1,\dots,\xi_k)\,\mathrm{d}\xi_k \\ &\quad= \frac{N!}{(N-k)!}\sum_{s_k=\pm1}\Big\langle \Psi_N, \Big(\bigotimes_{\ell=1}^{k-1} P^{\hbar,b}_{u_\ell,p_\ell,j_\ell}\mathcal{P}_{s_\ell}\Big) \otimes \mathcal{P}_{s_k} \otimes \mathbb{1}_{N-k}\Psi_N\Big\rangle \\ &\quad= (N-k+1)m^{(k-1)}_{f,\Psi_N}(\xi_1,\dots,\xi_{k-1}).\end{aligned}$$

Finally, (A.76) is obtained by repeating this $k-1$ more times. $\square$

The next two lemmas assert some particularly nice properties of the semi-classical measures, which will prove to be of great importance later. The first one states that the position densities of the measures are like the position densities (A.21) of the wave function Ψ_N.

Lemma A.32 (Position densities). *Let $\Psi \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ be any normalized wave function, and suppose that that f is a real, L^2-normalized and even function, we have for $1 \le k \le N$ that*

$$\frac{b^k}{(2\pi\hbar)^{2k}} \sum_{j\in(\mathbb{N}_0)^k} \int_{\mathbb{R}^k} m^{(k)}_{f,\Psi}(u,p,j,s)\,\mathrm{d}p = k!\big(\widetilde{\rho}^{(k)}_{\Psi} * (|f^\hbar|^2)^{\otimes k}\big)(u,s), \tag{A.78}$$

where the convolution in the right hand side is the ordinary position space convolution in each spin component of $\widetilde{\rho}^{(k)}_{\Psi}$.

Proof. For notational convenience we introduce an arbitrary $\Phi \in L^2(\mathbb{R}^{3N})$. Think of Φ as being one of the spin components of Ψ. Note first that

$$P^{\hbar,b}_{u_1,p_1,j_1} \otimes \cdots \otimes P^{\hbar,b}_{u_k,p_k,j_k} = \int_{\mathbb{R}^{2k}} |\otimes_{\ell=1}^k f^{\hbar,b}_{x_\ell,u_\ell,p_\ell,j_\ell}\rangle\langle \otimes_{\ell=1}^k f^{\hbar,b}_{x_\ell,u_\ell,p_\ell,j_\ell}|\,\mathrm{d}x,$$

and that for each fixed $y \in \mathbb{R}^{3(N-k)}$ we have as in (A.73) that

$$\begin{aligned}
&\big\langle \otimes_{\ell=1}^k f^{\hbar,b}_{x_\ell,u_\ell,p_\ell,j_\ell}, \Phi(\,\cdot\,,y)\big\rangle_{L^2(\mathbb{R}^{3k})} \\
&\qquad = (2\pi)^{\frac{k}{2}} \big\langle \otimes_{\ell=1}^k \varphi^{\hbar,b}_{x_\ell,j_\ell}, \mathcal{F}_3^{\otimes k}\big[(f^\hbar)^{\otimes k}(\,\cdot\, - u)\Phi(\,\cdot\,,y)\big](\,\cdot\,,\hbar^{-\frac{1}{2}}p)\big\rangle_{L^2(\mathbb{R}^{2k})}.
\end{aligned}$$

Combining these observations and using Lemma A.27, we get

$$\begin{aligned}
&\frac{1}{(2\pi)^k} \sum_{j\in(\mathbb{N}_0)^k} \int_{\mathbb{R}^k} \big\langle \Phi, (P^{\hbar,b}_{u_1,p_1,j_1} \otimes \cdots \otimes P^{\hbar,b}_{u_k,p_k,j_k}) \otimes \mathbb{1}_{N-k}\Phi\big\rangle\,\mathrm{d}p \\
&\quad = \frac{1}{(2\pi)^k} \sum_{j\in(\mathbb{N}_0)^k} \int_{\mathbb{R}^k}\int_{\mathbb{R}^{3(N-k)}}\int_{\mathbb{R}^{2k}} \big|\big\langle \otimes_{\ell=1}^k f^{\hbar,b}_{x_\ell,u_\ell,p_\ell,j_\ell}, \Phi(\cdot,y)\big\rangle\big|^2\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}p \\
&\quad = \frac{(2\pi\hbar)^k}{b^k} \int_{\mathbb{R}^k}\int_{\mathbb{R}^{3(N-k)}} \big\|\mathcal{F}_3^{\otimes k}\big[(f^\hbar)^{\otimes k}(\,\cdot\, - u)\Phi(\,\cdot\,,y)\big](\,\cdot\,,\hbar^{-\frac{1}{2}}p)\big\|^2_{L^2(\mathbb{R}^{2k})}\,\mathrm{d}y\,\mathrm{d}p \\
&\quad = \frac{(2\pi)^k\hbar^{2k}}{b^k} \int_{\mathbb{R}^{3(N-k)}} \big\|(f^\hbar)^{\otimes k}(\,\cdot\, - u)\Phi(\,\cdot\,,y)\big\|^2_{L^2(\mathbb{R}^{3k})}\,\mathrm{d}y.
\end{aligned}$$

Applying this to Ψ and using that f is even, we obtain

$$\begin{aligned}
&\sum_{j\in(\mathbb{N}_0)^k}\int_{\mathbb{R}^k} m^{(k)}_{f,\Psi}(u,p,j,s)\,\mathrm{d}p \\
&\quad= \sum_{r\in\{\pm1\}^N}\sum_{j\in(\mathbb{N}_0)^k}\int_{\mathbb{R}^k}\frac{N!}{(N-k)!}\Big\langle \Psi(\,\cdot\,;r),\Big(\bigotimes_{\ell=1}^{k-1}P^{\hbar,b}_{u_\ell,p_\ell,j_\ell}\mathcal{P}_{s_\ell}\Big)\Psi(\,\cdot\,;r)\Big\rangle\,\mathrm{d}p \\
&\quad= \frac{(2\pi\hbar)^{2k}N!}{b^k(N-k)!}\sum_{r\in\{\pm1\}^{N-k}}\int_{\mathbb{R}^{3(N-k)}}\big\|(f^\hbar)^{\otimes k}(\,\cdot\,-u)\Psi(\,\cdot\,,y;s,r)\big\|^2_{L^2(\mathbb{R}^{3k})}\,\mathrm{d}y \\
&\quad= \frac{(2\pi\hbar)^{2k}}{b^k}k!\big(\widetilde{\rho}^{(k)}_\Psi * (|f^\hbar|^2)^{\otimes k}\big)(u,s),
\end{aligned}$$

concluding the proof. □

Lemma A.33 (Kinetic energy). *Let $\Psi\in\bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ be normalized, and suppose that $f\in C_c^\infty(\mathbb{R}^3)$ is real-valued, L^2-normalized and even. Then we have*

$$\begin{aligned}
\Big\langle \Psi,\sum_{j=1}^N(\boldsymbol{\sigma}\cdot(-i\hbar\nabla_j+bA(x_j)))^2\Psi\Big\rangle &= -\hbar N\int_{\mathbb{R}^3}(\nabla f(u))^2\,\mathrm{d}u \\
&\quad+\frac{b}{(2\pi\hbar)^2}\sum_{s=\pm1}\sum_{j=0}^\infty\int_{\mathbb{R}}\int_{\mathbb{R}^3}(p^2+\hbar b(2j+1+s))m^{(1)}_{f,\Psi}(u,p,j,s)\,\mathrm{d}u\,\mathrm{d}p. \qquad (A.79)
\end{aligned}$$

Proof. The assumption that f is both smooth and compactly supported is far from optimal, but it will be sufficient for our purposes. The assertion of the lemma will hold as long as $f^\hbar$ satisfies the following version of the IMS localization formula [20, equation (3.18)]

$$\big\langle\psi,f^\hbar(-i\hbar\nabla+bA)^2f^\hbar\psi\big\rangle = \big\langle\psi,(f^\hbar)^2(-i\hbar\nabla+bA)^2\psi\big\rangle+\hbar^2\big\langle\psi,(\nabla f^\hbar)^2\psi\big\rangle \qquad (A.80)$$

for any ψ in the domain of $(-i\hbar\nabla+bA)^2$. Since f is normalized, the IMS formula yields

$$\begin{aligned}
\big\langle\psi,(-i\hbar\nabla+bA)^2\psi\big\rangle &= \int_{\mathbb{R}^3}\big\langle\psi,f^\hbar(\,\cdot\,-u)^2(-i\hbar\nabla+bA)^2\psi\big\rangle\,\mathrm{d}u \\
&= \int_{\mathbb{R}^3}\big\langle\psi,f^\hbar(\,\cdot\,-u)(-i\hbar\nabla+bA)^2f^\hbar(\cdot-u)\psi\big\rangle\,\mathrm{d}u \\
&\quad-\hbar\|\psi\|_2^2\int_{\mathbb{R}^3}(\nabla f(u))^2\,\mathrm{d}u. \qquad (A.81)
\end{aligned}$$

Returning to the semi-classical measures, note by (A.73) and (A.74) that

$$\begin{aligned}\frac{b}{(2\pi\hbar)^2}\sum_{j=0}^{\infty}\int_{\mathbb{R}}\int_{\mathbb{R}^3} p^2\langle\psi, P_{u,p,j}^{\hbar,b}\psi\rangle\,\mathrm{d}u\,\mathrm{d}p &= \frac{1}{2\pi\hbar}\int_{\mathbb{R}}\int_{\mathbb{R}^3} p^2\langle g_{u,p}^{\hbar}, g_{u,p}^{\hbar}\rangle\,\mathrm{d}u\,\mathrm{d}p \\ &= \frac{1}{\hbar}\int_{\mathbb{R}}\int_{\mathbb{R}^3}\int_{\mathbb{R}^2} p^2\big|\mathcal{F}_3\big[f^{\hbar}(\,\cdot\,-u)\psi\big](y,\hbar^{-1}p)\big|^2\,\mathrm{d}y\,\mathrm{d}u\,\mathrm{d}p \\ &= \hbar^2\int_{\mathbb{R}}\int_{\mathbb{R}^3}\int_{\mathbb{R}^2}\big|\mathcal{F}_3\big[\partial_3^2(f^{\hbar}(\,\cdot\,-u)\psi)\big](y,p)\big|^2\,\mathrm{d}y\,\mathrm{d}u\,\mathrm{d}p \\ &= \int_{\mathbb{R}^3}\big\langle f^{\hbar}(\,\cdot\,-u)\psi, -\hbar^2\partial_3^2(f^{\hbar}(\,\cdot\,-u)\psi)\big\rangle\,\mathrm{d}u.\end{aligned}$$

Similarly, also using (A.73) and (A.74), and recalling (A.63), we get

$$\begin{aligned}&\frac{b}{(2\pi\hbar)^2}\sum_{j=0}^{\infty}\int_{\mathbb{R}}\int_{\mathbb{R}^3}\hbar b(2j+1)\langle\psi, P_{u,p,j}^{\hbar,b}\psi\rangle\,\mathrm{d}u\,\mathrm{d}p \\ &\quad= \frac{\hbar}{2\pi}\sum_{j=0}^{\infty}\int_{\mathbb{R}}\int_{\mathbb{R}^3}\langle g_{u,p}^{\hbar}, H_{\hbar^{-1}bA^{\perp}}\Pi_j^{(2)} g_{u,p}^{\hbar}\rangle\,\mathrm{d}u\,\mathrm{d}p \\ &\quad= \frac{\hbar}{2\pi}\int_{\mathbb{R}}\int_{\mathbb{R}^3}\langle g_{u,p}^{\hbar}, H_{\hbar^{-1}bA^{\perp}} g_{u,p}^{\hbar}\rangle\,\mathrm{d}u\,\mathrm{d}p \\ &\quad= \int_{\mathbb{R}^3}\big\langle f^{\hbar}(\,\cdot\,-u)\psi, \hbar^2(H_{\hbar^{-1}bA^{\perp}}\otimes\mathbb{1}_{L^2(\mathbb{R})})(f^{\hbar}(\,\cdot\,-u)\psi)\big\rangle\,\mathrm{d}u.\end{aligned}$$

Since $(-i\hbar\nabla+bA)^2 = \hbar^2(H_{\hbar^{-1}bA^{\perp}}-\partial_3^2)$, combining these with (A.81) yields

$$\begin{aligned}\big\langle\psi,(-i\hbar\nabla+bA)^2\psi\big\rangle &= -\hbar\|\psi\|_2^2\int_{\mathbb{R}^3}(\nabla f(u))^2\,\mathrm{d}u \\ &\quad+\frac{b}{(2\pi\hbar)^2}\sum_{j=0}^{\infty}\int_{\mathbb{R}}\int_{\mathbb{R}^3}(p^2+\hbar b(2j+1))\langle\psi, P_{u,p,j}^{\hbar,b}\psi\rangle\,\mathrm{d}u\,\mathrm{d}p.\end{aligned}$$

Now, since $(\boldsymbol{\sigma}\cdot(-i\hbar\nabla+bA))^2 = (-i\hbar\nabla+bA)^2\mathbb{1}_{\mathbb{C}^2}+\hbar b\sigma_3$, we get for $\Phi\in L^2(\mathbb{R}^3;\mathbb{C}^2)$,

$$\begin{aligned}&\big\langle\Phi,(\boldsymbol{\sigma}\cdot(-i\hbar\nabla+bA))^2\Phi\big\rangle \\ &\quad= \frac{b}{(2\pi\hbar)^2}\sum_{j=0}^{\infty}\int_{\mathbb{R}}\int_{\mathbb{R}^3}(p^2+\hbar b(2j+1))\langle\Phi, P_{u,p,j}^{\hbar,b}\mathbb{1}_{\mathbb{C}^2}\Phi\rangle+\hbar b\langle\Phi, P_{u,p,j}^{\hbar,b}\sigma_3\Phi\rangle\,\mathrm{d}u\,\mathrm{d}p \\ &\qquad-\hbar\|\Phi\|_{L^2(\mathbb{R}^3;\mathbb{C}^2)}^2\int_{\mathbb{R}^3}(\nabla f(u))^2\,\mathrm{d}u \\ &\quad= \frac{b}{(2\pi\hbar)^2}\sum_{s=\pm1}\sum_{j=0}^{\infty}\int_{\mathbb{R}}\int_{\mathbb{R}^3}(p^2+\hbar b(2j+1+s))\langle\Phi, P_{u,p,j}^{\hbar,b}\mathcal{P}_s\Phi\rangle\,\mathrm{d}u\,\mathrm{d}p \\ &\qquad-\hbar\|\Phi\|_{L^2(\mathbb{R}^3;\mathbb{C}^2)}^2\int_{\mathbb{R}^3}(\nabla f(u))^2\,\mathrm{d}u.\end{aligned}$$

Applying this to the first component of the wave function Ψ while keeping all other variables fixed, we finally obtain

$$\begin{aligned}
&\Big\langle \Psi, \sum_{j=1}^{N} (\boldsymbol{\sigma}\cdot(-i\hbar\nabla_j + bA(x_j)))^2\Psi\Big\rangle \\
&\quad = N\int_{(\mathbb{R}^3\times\{\pm1\})^{N-1}} \big\langle \Psi(\,\cdot\,,z), (\boldsymbol{\sigma}\cdot(-i\hbar\nabla + bA))^2\Psi(\,\cdot\,,z)\big\rangle_{L^2(\mathbb{R}^3;\mathbb{C}^2)}\,\mathrm{d}z \\
&\quad = \frac{b}{(2\pi\hbar)^2}\sum_{s=\pm1}\sum_{j=0}^{\infty}\int_{\mathbb{R}}\int_{\mathbb{R}^3}(p^2+\hbar b(2j+1+s))N\big\langle \Psi, P^{\hbar,b}_{u,p,j}\mathcal{P}_s\Psi\big\rangle\,\mathrm{d}u\,\mathrm{d}p \\
&\qquad - \hbar N\int_{\mathbb{R}^3}(\nabla f(u))^2\,\mathrm{d}u,
\end{aligned}$$

finishing the proof. □

A.4.3 Limiting measures, strong magnetic fields

We now fix a real-valued, even and normalized function $f\in L^2(\mathbb{R}^3)$, along with a sequence $(\Psi_N)_{N\geq 1}$ of normalized functions with $\Psi_N\in\bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ for each N. We investigate the measures $m^{(k)}_{f,\Psi_N}$ in the limit as N tends to infinity, when β_N is a sequence with $\beta_N\to\beta$, $0<\beta\leq\infty$. This corresponds to the regime where the distance between the Landau bands of the Pauli operator remains bounded from below.

Lemma A.34. *For each $k\geq 1$ there is a symmetric function $m^{(k)}_f\in L^1(\Omega^k)\cap L^\infty(\Omega^k)$ with $0\leq m^{(k)}_f\leq 1$ such that, along a common (not displayed) subsequence in N,*

$$\int_{\Omega^k} m^{(k)}_{f,\Psi_N}(\xi)\varphi(\xi)\,\mathrm{d}\xi \longrightarrow \int_{\Omega^k} m^{(k)}_f(\xi)\varphi(\xi)\,\mathrm{d}\xi \tag{A.82}$$

for all $\varphi\in L^1(\Omega^k)+L^\infty_\varepsilon(\Omega^k)$, as N tends to infinity.

The proof of this lemma is a standard exercise in functional analysis, using the boundedness of the sequence $(m^{(k)}_{f,\Psi_N})_{N\geq k}$ both in $L^1(\Omega^k)$ and in $L^\infty(\Omega^k)$, and we leave the details to the reader.

If the sequence of measures $(m^{(k)}_{f,\Psi_N})_{N\geq k}$ is *tight*, that is, if

$$\lim_{R\to\infty}\limsup_{N\to\infty}\int_{|\xi_1|+\cdots+|\xi_k|\geq R} m^{(k)}_{f,\Psi_N}(\xi)\,\mathrm{d}\xi = 0.$$

then all the properties of the measures in Lemma A.31 carry over to the limit, and the weak convergence in Lemma A.34 is strengthened. We collect these observations in the lemma below, but the proof (which is elementary) will be omitted. The key ingredient for the proof is the fact that

$$\int_{|\xi|\leq R} m^{(k)}_{f,\Psi_N}(\xi)\,\mathrm{d}\xi \xrightarrow{R\to\infty} \int_{\Omega^k} m^{(k)}_{f,\Psi_N}(\xi)\,\mathrm{d}\xi = \frac{(2\pi\hbar)^{2k}}{b^k}\frac{N!}{(N-k)!}$$

uniformly in N as R tends to infinity, whenever $(m^{(k)}_{f,\Psi_N})_{N\geq k}$ is tight.

Lemma A.35. *Suppose that $(m^{(1)}_{f,\Psi_N})_{N\in\mathbb{N}}$ is a tight sequence. Then we have*

(1) $(m^{(k)}_{f,\Psi_N})_{N\geq k}$ is also tight for each $k \geq 1$.

(2) The limit measures $m^{(k)}_f$ are probability measures. More precisely,

$$\frac{1}{(2\pi)^{2k}} \frac{\beta^k}{(1+\beta)^k} \int_{\Omega^k} m^{(k)}_f(\xi)\,\mathrm{d}\xi = 1. \tag{A.83}$$

(3) The compatibility relation (A.77) is preserved in the limit, that is, for $k \geq 2$ and almost every $\xi \in \Omega^{k-1}$,

$$\frac{1}{(2\pi)^2} \frac{\beta}{1+\beta} \int_{\Omega} m^{(k)}_f(\xi, \xi_k)\,\mathrm{d}\xi_k = m^{(k-1)}_f(\xi). \tag{A.84}$$

(4) The convergence in (A.82) holds on all of $L^1(\Omega^k) + L^\infty(\Omega^k)$.

We now formulate the de Finetti theorem which serves as the main abstract tool in our proof of the lower bound of the energy in Theorem A.5. The version of the theorem below is essentially [5, Theorem 2.6] For some additional details, see e.g. [24].

Theorem A.36 (de Finetti). *Let $M \subseteq \Omega$ be a locally compact subset, and $m^{(k)} \in L^1(M^k)$ a family of symmetric positive densities satisfying for some $c > 0$ and all $k \geq 1$ that $0 \leq m^{(k)} \leq 1$, and*

$$c \int_M m^{(k)}(\xi_1, \ldots, \xi_k)\,\mathrm{d}\xi_k = m^{(k-1)}(\xi_1, \ldots, \xi_{k-1})$$

with $m^{(0)} = 1$. Then there exists a unique Borel probability measure P on the set

$$\mathcal{S} = \left\{\mu \in L^1(M) \,\middle|\, 0 \leq \mu \leq 1, \quad c\int_M \mu(\xi)\,\mathrm{d}\xi = 1\right\}$$

such that for all $k \geq 1$, in the sense of measures,

$$m^{(k)} = \int_{\mathcal{S}} \mu^{\otimes k}\,\mathrm{dP}(\mu). \tag{A.85}$$

A.5 Lower energy bounds, strong fields

Throughout this section we suppose that the potentials V and w satisfy the assumptions of Theorem A.5, and that (β_N) is a sequence satisfying $\beta_N \to \beta$ with $0 < \beta \leq \infty$ and (A.6). We further assume that the auxiliary function f is smooth and compactly supported.

Lemma A.37. *Suppose that $\Psi_N \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ is a sequence satisfying the energy bound $\langle \Psi_N, H_{N,\beta_N}\Psi_N\rangle \le CN$. Then the corresponding semi-classical measures $(m^{(k)}_{f,\Psi_N})_{N\ge k}$ are tight.*

Proof. The proof is straightforward, and we only outline it. One first uses the energy bound combined with (A.6) and the Lieb-Thirring bound (A.32) to conclude that $\frac{1}{N}\widetilde{\rho}^{(1)}_{\Psi_N}$ is a tight sequence. It is essential at this point that V is a confining potential. Then, applying Lemma A.32 and the fact that f is well localized, it follows that $(m^{(1)}_{f,\Psi_N})_{N\ge 1}$ is tight in the position variable.

On the other hand, using (A.32) to bound the kinetic energy and then combining with the expression for the kinetic energy from Lemma A.33, it follows that $(m^{(1)}_{f,\Psi_N})_{N\ge 1}$ is also tight in the momentum variables $(p,j)\in\mathbb{R}\times\mathbb{N}_0$. Now by Lemma A.35, the sequences $(m^{(k)}_{f,\Psi_N})_{N\ge k}$ are all tight for $k\ge 1$. □

We once again remind the reader of the notational convention (A.9).

Proposition A.38 (Convergence of states). *Let $\Psi_N \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ be a sequence satisfying the energy bound $\langle \Psi_N, H_{N,\beta_N}\Psi_N\rangle \le CN$. Then there exist a subsequence $(N_\ell)\subseteq\mathbb{N}$ and a unique Borel probability measure P on the set*

$$\mathcal{S}=\Big\{\mu\in L^1(\Omega)\;\Big|\;0\le\mu\le 1,\ \frac{1}{(2\pi)^2}\frac{\beta}{1+\beta}\int_\Omega \mu(\xi)\,\mathrm{d}\xi=1\Big\},$$

such that for each $k\ge 1$ the following holds:

(1) For all $\varphi\in L^1(\Omega^k)+L^\infty(\Omega^k)$,

$$\int_{\Omega^k} m^{(k)}_{f,\Psi_{N_\ell}}(\xi)\varphi(\xi)\,\mathrm{d}\xi \longrightarrow \int_{\mathcal{S}}\Big(\int_{\Omega^k}\mu^{\otimes k}(\xi)\varphi(\xi)\,\mathrm{d}\xi\Big)\,\mathrm{dP}(\mu). \tag{A.86}$$

as ℓ tends to infinity.

(2) For $U\in L^{5/2}(\mathbb{R}^3\times\{\pm1\})+L^\infty(\mathbb{R}^3\times\{\pm1\})$ if $k=1$, and for any bounded and uniformly continuous function U on $(\mathbb{R}^3\times\{\pm1\})^k$ if $k\ge 2$, as ℓ tends to infinity,

$$\begin{aligned}\frac{k!}{N_\ell^k}&\sum_{s\in\{\pm1\}^k}\int_{\mathbb{R}^{3k}}\widetilde{\rho}^{(k)}_{\Psi_{N_\ell}}(x,s)U(x,s)\,\mathrm{d}x\\ &\longrightarrow \int_{\mathcal{S}}\Big(\sum_{s\in\{\pm1\}^k}\int_{\mathbb{R}^{3k}}\rho_\mu^{\otimes k}(x,s)U(x,s)\,\mathrm{d}x\Big)\,\mathrm{dP}(\mu),\end{aligned} \tag{A.87}$$

where ρ_μ is the position density

$$\rho_\mu(x,s)=\frac{1}{(2\pi)^2}\frac{\beta}{1+\beta}\sum_{j=0}^{\infty}\int_{\mathbb{R}}\mu(x,p,j,s)\,\mathrm{d}p.$$

Proof. Consider the subsequence (N_ℓ) along with the limit measures $(m_f^{(k)})$ from Lemma A.34. Throughout the proof, we will suppress the subsequence from the notation. By Lemma A.37, the measures $(m_{f,\Psi_N}^{(k)})_{N\geq k}$ are tight, the limit measures are ensured by Lemma A.35 to satisfy the compatibility relation

$$c\int_\Omega m_f^{(k)}(\xi_1,\ldots,\xi_k)\,\mathrm{d}\xi_k = m_f^{(k-1)}(\xi_1,\ldots,\xi_{k-1}),$$

with $c = \frac{1}{(2\pi)^2}\frac{\beta}{1+\beta}$. Hence by the de Finetti Theorem A.36 we have a unique Borel probability measure P on $\mathcal{S}$ such that

$$m_f^{(k)} = \int_{\mathcal{S}} \mu^{\otimes k}\,\mathrm{dP}(\mu).$$

It follows that (A.86) holds, since

$$\int_{\Omega^k} m_f^{(k)}(\xi)\varphi(\xi)\,\mathrm{d}\xi = \int_{\mathcal{S}}\Big(\int_{\Omega^k}\mu^{\otimes k}(\xi)\varphi(\xi)\,\mathrm{d}\xi\Big)\,\mathrm{dP}(\mu)$$

for each $\varphi\in L^1(\Omega^k)+L^\infty(\Omega^k)$, by definition of the measure $\int_{\mathcal{S}}\mu^{\otimes k}\,\mathrm{dP}(\mu)$.

Now, if U is a bounded function on $(\mathbb{R}^3\times\{\pm1\})^k$, we define $\varphi\in L^\infty(\Omega^k)$ by $\varphi(x,p,j,s) := U(x,s)$. Then by (A.86) we have as N tends to infinity,

$$\begin{aligned}
&\sum_{s\in\{\pm1\}^k}\int_{\mathbb{R}^{3k}}\rho_{m_{f,\Psi_N}^{(k)}}(x,s)U(x,s)\,\mathrm{d}x\\
&\qquad\longrightarrow \frac{1}{(2\pi)^{2k}}\frac{\beta^k}{(1+\beta)^k}\int_{\mathcal{S}}\Big(\int_{\Omega^k}\mu^{\otimes k}(\xi)\varphi(\xi)\,\mathrm{d}\xi\Big)\,\mathrm{dP}(\mu)\\
&\qquad= \int_{\mathcal{S}}\Big(\sum_{s\in\{\pm1\}^k}\int_{\mathbb{R}^{3k}}\rho_\mu^{\otimes k}(x,s)U(x,s)\,\mathrm{d}x\Big)\,\mathrm{dP}(\mu),
\end{aligned}\tag{A.88}$$

so in order to show (A.87) it suffices to see that $\frac{k!}{N^k}\widetilde{\rho}_{\Psi_N}^{(k)}$ has the same weak limit as $\rho_{m_{f,\Psi_N}^{(k)}}$ on the set of bounded, uniformly continuous functions on $(\mathbb{R}^3\times\{\pm1\})^k$. However, by Lemma A.32,

$$\rho_{m_{f,\Psi_N}^{(k)}}(x,s) = \frac{\beta^k}{(1+\beta)^k}\frac{\hbar^{2k}N^k}{b^k}\frac{k!}{N^k}\big(\widetilde{\rho}_{\Psi_N}^{(k)} * (|f^\hbar|^2)^{\otimes k}\big)(x,s),$$

where $\frac{\beta^k}{(1+\beta)^k}\frac{\hbar^{2k}N^k}{b^k}\to 1$ when $N\to\infty$, so it suffices to show that $\frac{k!}{N^k}\widetilde{\rho}_{\Psi_N}^{(k)}$ and $\frac{k!}{N^k}\widetilde{\rho}_{\Psi_N}^{(k)} * (|f^\hbar|^2)^{\otimes k}$ have the same weak limit. However, this follows easily from the boundedness of $\frac{k!}{N^k}\widetilde{\rho}_{\Psi_N}^{(k)}$ in $L^1((\mathbb{R}^3\times\{\pm1\})^k)$, and from the fact that $\lim_{\hbar\to0}\|U - U*(|f^\hbar|^2)^{\otimes k}\|_\infty = 0$ whenever U is a uniformly continuous and bounded function on $(\mathbb{R}^3\times\{\pm1\})^k$.

For $k=1$ we appeal to Lemma A.13 and the tightness of $\frac{1}{N}\widetilde{\rho}_{\Psi_N}^{(1)}$ to obtain convergence for test functions $U\in L^{5/2}(\mathbb{R}^3\times\{\pm1\})+L^\infty(\mathbb{R}^3\times\{\pm1\})$. □

In the case where $\beta_N \to \infty$ we can further refine the assertions of Proposition A.38 above.

Corollary A.39 (Convergence of states, strong field regime). *Suppose that (β_N) satisfies $\beta_N \to \infty$ and (A.6), and that $\Psi_N \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ is a sequence satisfying the energy bound $\langle \Psi_N, H_{N,\beta_N}\Psi_N\rangle \le CN$. Then the measure P from Proposition A.38 is supported on the set*

$$\widetilde{\mathcal{S}} = \big\{\mu \in L^1(\mathbb{R}^3\times\mathbb{R}) \,\big|\, 0 \le \mu \le 1,\ \frac{1}{(2\pi)^2}\iint_{\mathbb{R}^3\times\mathbb{R}} \mu(x,p)\,\mathrm{d}x\,\mathrm{d}p = 1\big\},$$

where each $\widetilde{\mu} \in \widetilde{\mathcal{S}}$ is identified with a density $\mu \in \mathcal{S}$ by

$$\mu(x,p,j,s) = \begin{cases} \widetilde{\mu}(x,p), & \text{if } j = 0 \text{ and } s = -1,\\ 0, & \text{otherwise,}\end{cases}$$

and for each $k \ge 1$ the following holds:

(1) For all $\varphi \in L^1(\Omega^k) + L^\infty(\Omega^k)$, as ℓ tends to infinity,

$$\int_{\Omega^k} m^{(k)}_{f,\Psi_{N_\ell}}(\xi)\varphi(\xi)\,\mathrm{d}\xi \longrightarrow \int_{\widetilde{\mathcal{S}}}\Big(\int_{\mathbb{R}^{4k}} \mu^{\otimes k}(x,p)\varphi(x,p,0^{\times k},(-1)^{\times k})\,\mathrm{d}x\,\mathrm{d}p\Big)\,\mathrm{d}\mathrm{P}(\mu), \tag{A.89}$$

where $0^{\times k}$ and $(-1)^{\times k}$ are the k-dimensional vectors whose entries are all equal to 0 and -1, respectively.

(2) For $U \in L^{5/2}(\mathbb{R}^3\times\{\pm1\}) + L^\infty(\mathbb{R}^3\times\{\pm1\})$ if $k=1$, and for any bounded and uniformly continuous function U on $(\mathbb{R}^3\times\{\pm1\})^k$ if $k\ge 2$, as ℓ tends to infinity,

$$\frac{k!}{N_\ell^k}\sum_{s\in\{\pm1\}^k}\int_{\mathbb{R}^{3k}} \widetilde{\rho}^{(k)}_{\Psi_{N_\ell}}(x,s)U(x,s)\,\mathrm{d}x \longrightarrow \int_{\widetilde{\mathcal{S}}}\Big(\int_{\mathbb{R}^{3k}} \rho_\mu^{\otimes k}(x)U(x,(-1)^{\times k})\,\mathrm{d}x\Big)\,\mathrm{d}\mathrm{P}(\mu), \tag{A.90}$$

where

$$\rho_\mu(x) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}} \mu(x,p)\,\mathrm{d}p.$$

Proof. Using that $\hbar b \to \infty$ since $\beta_N \to \infty$, along with the expression for the kinetic energy in Lemma A.33, the Lieb-Thirring bound (A.32), and the energy bound from the assumptions, we obtain in particular for any $n \in \mathbb{N}$ that

$$\sum_{s=\pm1}\sum_{j=0}^{n}\int_{\mathbb{R}^3}\int_{\mathbb{R}}(j+1+s)m^{(1)}_f(x,p,j,s)\,\mathrm{d}p\,\mathrm{d}x = \lim_{N\to\infty}\sum_{s=\pm1}\sum_{j=0}^{n}\int_{\mathbb{R}^3}\int_{\mathbb{R}}(j+1+s)m^{(1)}_{f,\Psi_N}(x,p,j,s)\,\mathrm{d}p\,\mathrm{d}x = 0$$

implying that $m_f^{(1)}(x,p,j,s) = 0$ unless $j = 0$ and $s = -1$. It follows that

$$\int_{\mathcal{S}} \Big(\int_{\mathbb{R}^3\times\mathbb{R}\times\{0\}\times\{-1\}} \mu(\xi)\,\mathrm{d}\xi \Big)\,\mathrm{dP}(\mu) \\ = \int_\Omega m_f^{(1)}(\xi)\,\mathrm{d}\xi = \int_{\mathcal{S}} \Big(\int_\Omega \mu(\xi)\,\mathrm{d}\xi \Big)\,\mathrm{dP}(\mu),$$

so for P-almost every $\mu \in \mathcal{S}$, we have

$$\int_{\mathbb{R}^3\times\mathbb{R}\times\{0\}\times\{-1\}} \mu(\xi)\,\mathrm{d}\xi = \int_\Omega \mu(\xi)\,\mathrm{d}\xi,$$

and hence P is supported on $\widetilde{\mathcal{S}}$. The rest of the corollary follows directly from Lemma A.38. □

We now finally have the tools to give a proof of the lower bounds in Theorem A.5 in the case when $\beta_N \to \beta \in (0,\infty]$. The proof will be split into a few lemmas, each giving a lower bound on part of the energy. Note that if $\Psi_N \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ is a sequence of fermionic wave functions satisfying $\langle \Psi_N, H_{N,\beta_N}\Psi_N\rangle = E(N,\beta_N) + o(N)$, then by the upper energy bound of Proposition A.22 we have $\langle \Psi_N, H_{N,\beta_N}\Psi_N\rangle \le CN$, so that Proposition A.38 and Corollary A.39 are applicable.

Lemma A.40. *Suppose that the assumptions in Theorem A.5 are satisfied, and that we have a sequence $\Psi_N \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ with $\langle \Psi_N, H_{N,\beta_N}\Psi_N\rangle = E(N,\beta_N) + o(N)$.*

(1) If $\beta_N \to \beta \in (0,\infty)$, then, with $\mathcal{S}$ as in Proposition A.38,

$$\begin{aligned} C &\ge \liminf_{N\to\infty} \Big\langle \Psi_N, \frac{1}{N}\sum_{j=1}^N (\boldsymbol{\sigma}\cdot(-i\hbar\nabla + bA(x_j)))^2 \Psi_N \Big\rangle \\ &\ge \frac{1}{(2\pi)^2}\frac{\beta}{1+\beta} \int_{\mathcal{S}} \Big(\int_\Omega (p^2 + k_\beta(2j+1+s))\mu(\xi)\,\mathrm{d}\xi \Big)\,\mathrm{dP}(\mu). \end{aligned} \tag{A.91}$$

(2) If $\beta_N \to \infty$, then, with $\widetilde{\mathcal{S}}$ as in Corollary A.39,

$$\begin{aligned} C &\ge \liminf_{N\to\infty} \Big\langle \Psi_N, \frac{1}{N}\sum_{j=1}^N (\boldsymbol{\sigma}\cdot(-i\hbar\nabla + bA(x_j)))^2 \Psi_N \Big\rangle \\ &\ge \frac{1}{(2\pi)^2} \int_{\widetilde{\mathcal{S}}} \Big(\int_{\mathbb{R}^3\times\mathbb{R}} p^2 \mu(x,p)\,\mathrm{d}p\,\mathrm{d}x \Big)\,\mathrm{dP}(\mu). \end{aligned} \tag{A.92}$$

Proof. Suppose first that $\beta_N \to \beta < \infty$. By Lemma A.11 the kinetic energy per particle is bounded, so applying Lemma A.33 and Proposition A.38 we obtain for any positive R,

$$
\begin{aligned}
C &\geq \liminf_{N\to\infty} \Big\langle \Psi_N, \frac{1}{N}\sum_{j=1}^{N} (\boldsymbol{\sigma}\cdot(-i\hbar\nabla + bA(x_j)))^2 \Psi_N \Big\rangle \\
&\geq \liminf_{N\to\infty} \frac{1}{(2\pi)^2}\frac{b}{\hbar^2 N}\int_{|u|+|p|+j\leq R} (p^2 + \hbar b(2j+1+s)) m^{(1)}_{f,\Psi_N}(\xi)\,\mathrm{d}\xi \\
&= \frac{1}{(2\pi)^2}\frac{\beta}{1+\beta}\int_{\mathcal{S}} \Big(\int_{|u|+|p|+j\leq R} (p^2 + k_\beta(2j+1+s))\mu(\xi)\,\mathrm{d}\xi \Big)\,\mathrm{dP}(\mu).
\end{aligned}
$$

Taking $R\to\infty$, monotone convergence implies (A.91).

The bound (A.92) follows in exactly the same way by simply discarding the term $\hbar b(2j+1+s)$ in the integrand above, and applying Corollary A.39. $\square$

Lemma A.41. *Suppose that* (β_N) *satisfies* (A.6) *and* $\beta_N \to \beta \in (0,\infty]$. *With the assumptions in Theorem A.5 and a sequence* $\Psi_N \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ *satisfying* $\langle \Psi_N, H_{N,\beta_N}\Psi_N\rangle = E(N,\beta_N) + o(N)$, *we have*

$$
\liminf_{N\to\infty} \Big\langle \Psi_N, \frac{1}{N}\sum_{j=1}^{N} V(x_j)\Psi_N \Big\rangle \geq \int_{\mathcal{S}} \Big(\int_{\mathbb{R}^3} V(x)\rho_\mu(x)\,\mathrm{d}x \Big)\,\mathrm{dP}(\mu), \tag{A.93}
$$

and

$$
\begin{aligned}
\lim_{N\to\infty} &\Big\langle \Psi_N, \frac{1}{N^2}\sum_{1\leq j<k\leq N} w(x_j - x_k)\Psi_N \Big\rangle \\
&= \frac{1}{2}\int_{\mathcal{S}} \Big(\int_{\mathbb{R}^6} w(x-y)\rho_\mu(x)\rho_\mu(y)\,\mathrm{d}x\,\mathrm{d}y \Big)\,\mathrm{dP}(\mu).
\end{aligned} \tag{A.94}
$$

Proof. By Lemma A.11 the potential energy per particle is bounded, so for $R>0$ large enough we have by the weak convergence of $\frac{1}{N}\rho^{(1)}_{\Psi_N}$ in $L^{5/2}(\mathbb{R}^3)$ that

$$
\begin{aligned}
C &\geq \liminf_{N\to\infty} \Big\langle \Psi_N, \frac{1}{N}\sum_{j=1}^{N} V(x_j)\Psi_N \Big\rangle \\
&\geq \liminf_{N\to\infty} \frac{1}{N}\int_{|x|\leq R} V(x)\rho^{(1)}_{\Psi_N}(x)\,\mathrm{d}x = \int_{\mathcal{S}} \Big(\int_{|x|\leq R} V(x)\rho_\mu(x)\,\mathrm{d}x \Big)\,\mathrm{dP}(\mu).
\end{aligned}
$$

Taking $R\to\infty$ yields (A.93) by the monotone convergence theorem.

For the interaction part, write $w = w_1 + w_2 \in L^{3/2}(\mathbb{R}^3)\cap L^{5/2}(\mathbb{R}^3) + L^\infty_\varepsilon(\mathbb{R}^3)$ and approximate w_1 in $L^{3/2}(\mathbb{R}^3)$ and $L^{5/2}(\mathbb{R}^3)$ by some $w_0 \in C_c(\mathbb{R}^3)$. By the Lieb-Thirring estimate (A.33), we have

$$
\begin{aligned}
\Big| \Big\langle \Psi_N, &\frac{1}{N^2}\sum_{j<k}^{N} \big(w - w_0\big)(x_j - x_k)\Psi_N \Big\rangle \Big| \\
&= \frac{1}{N^2}\Big| \iint_{\mathbb{R}^6} \big(w - w_0\big)(x-y)\rho^{(2)}_{\Psi_N}(x,y)\,\mathrm{d}x\,\mathrm{d}y \Big| \\
&\leq C(\|w_1 - w_0\|_{\frac{3}{2}} + \|w_1 - w_0\|_{\frac{5}{2}} + \|w_2\|_\infty).
\end{aligned} \tag{A.95}
$$

Note that by the bathtub principle (Lemmas A.15 and A.18) and the upper bound on kinetic energy Lemma A.40 it follows that either

$$\int_{\mathcal{S}}\Big(\int_{\mathbb{R}^3}\tau_\beta(\rho_\mu(x))\,\mathrm{d}x\Big)\,\mathrm{dP}(\mu) \\ \leq \frac{1}{(2\pi)^2}\frac{\beta}{1+\beta}\int_{\mathcal{S}}\Big(\int_\Omega(p^2+k_\beta(2j+1+s))\mu(\xi)\,\mathrm{d}\xi\Big)\,\mathrm{dP}(\mu)<\infty,$$

or

$$\frac{4\pi^4}{3}\int_{\widetilde{\mathcal{S}}}\Big(\int_{\mathbb{R}^3}\rho_\mu(x)^3\,\mathrm{d}x\Big)\,\mathrm{dP}(\mu) \leq \frac{1}{(2\pi)^2}\int_{\widetilde{\mathcal{S}}}\Big(\iint_{\mathbb{R}^3\times\mathbb{R}}p^2\mu(x,p)\,\mathrm{d}p\,\mathrm{d}x\Big)\,\mathrm{dP}(\mu)<\infty,$$

depending on the sequence (β_N). Applying either the bound (A.15) or Markov's inequality leads to the conclusion that

$$\int_{\mathcal{S}}\|\rho_\mu\|_{\frac{5}{3}}\,\mathrm{dP}(\mu)<\infty.$$

Hence we can use Young's inequality to obtain

$$\Big|\int_{\mathcal{S}}\Big(\int_{\mathbb{R}^6}(w-w_0)(x-y)\rho_\mu(x)\rho_\mu(y)\,\mathrm{d}x\,\mathrm{d}y\Big)\,\mathrm{dP}(\mu)\Big| \\ \leq \int_{\mathcal{S}}\|w_1-w_0\|_{\frac{5}{2}}\|\rho_\mu\|_{\frac{5}{3}}+\|w_2\|_\infty\,\mathrm{dP}(\mu)<\infty.$$

This bound together with (A.95) implies that it suffices to show (A.94) for $w\in C_c(\mathbb{R}^3)$. However, the convergence holds in this case by Proposition A.38 and Corollary A.39, since the function $(x,y)\mapsto w(x-y)$ is bounded and uniformly continuous on $\mathbb{R}^3\times\mathbb{R}^3$. $\square$

Proof of Theorem A.5 (and Theorem A.6) for strong fields. Assume first that $\beta_N\to\beta\in(0,\infty)$. It follows from Lemmas A.40 and A.41 that for any sequence $\Psi_N\in\bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ satisfying $\langle\Psi_N,H_{N,\beta_N}\Psi_N\rangle=E(N,\beta_N)+o(N)$, then along the subsequence N_ℓ from Proposition A.38,

$$\liminf_{\ell\to\infty}\frac{\langle\Psi_{N_\ell},H_{N_\ell,\beta_{N_\ell}}\Psi_{N_\ell}\rangle}{N_\ell}\geq\int_{\mathcal{S}}\mathcal{E}_\beta^{\mathrm{Vla}}(\mu)\,\mathrm{dP}(\mu)\geq E^{\mathrm{MTF}}(\beta),$$

where the last inequality follows from Lemma A.15 and the fact that P is a probability measure. Assume for the sake of contradiction that $E^{\mathrm{MTF}}(\beta)>\liminf_N\frac{E(N,\beta_N)}{N}$, and take a sequence $M_k\in\mathbb{N}$ satisfying

$$\lim_{k\to\infty}\frac{E(M_k,\beta_{M_k})}{M_k}=\liminf_N\frac{E(N,\beta_N)}{N}.$$

Since we might as well have proven Lemma A.34 and Proposition A.38 starting from this sequence, we may assume that N_ℓ is a subsequence of M_k. Hence

$$E^{\mathrm{MTF}}(\beta)>\liminf_{N\to\infty}\frac{E(N,\beta_N)}{N}=\liminf_{\ell\to\infty}\frac{\langle\Psi_{N_\ell},H_{N_\ell,\beta_{N_\ell}}\Psi_{N_\ell}\rangle}{N_\ell}\geq E^{\mathrm{MTF}}(\beta),$$

which is absurd, so we must have equality everywhere (using the already proven upper energy bound in Proposition A.22), concluding the proof of Theorem A.5 for $0 < \beta < \infty$. In particular, we also have

$$\int_{\mathcal{S}} \mathcal{E}_{\beta}^{\mathrm{Vla}}(\mu) - E^{\mathrm{MTF}}(\beta)\,\mathrm{dP}(\mu) = 0,$$

so P is supported on the set of minimizers of the Vlasov energy functional. Hence P induces a probability measure on the set of minimizers of the magnetic Thomas-Fermi functional, completing the proof of the first part of Theorem A.6.

In the case where (β_N) satisfies $\beta_N \to \infty$ and (A.6), we apply the same argument, obtaining

$$E^{\mathrm{STF}} \geq \liminf_{N\to\infty} \frac{\langle \Psi_N, H_{N,\beta_N}\Psi_N\rangle}{N} \geq \int_{\widetilde{\mathcal{S}}} \mathcal{E}_{\infty}^{\mathrm{Vla}}(\mu)\,\mathrm{dP}(\mu) \geq E^{\mathrm{STF}}.$$

In this case P induces a measure on the set of minimizers of the strong Thomas-Fermi functional, completing the proof of Theorem A.6, except for the case when $\beta_N \to 0$. □

A.6 Lower energy bounds, weak fields

Here we consider the case where $\beta_N \to 0$ as $N \to \infty$. Again, suppose that V and w satisfy the assumptions of Theorem A.5, and let $f \in C_c^{\infty}(\mathbb{R}^3)$ be a real-valued, even and L^2-normalized function. Since the distance between the Landau bands of $(\boldsymbol{\sigma}\cdot(-i\hbar\nabla + bA(x)))^2$ is $2\hbar b$, and $\beta_N \to 0$ is equivalent to $\hbar b = \beta_N(1+\beta_N)^{-2/5} \to 0$, we can argue without diagonalising the magnetic Laplacian as in the beginning of Section A.4. In other words, we get the usual phase space $\mathbb{R}^3 \times \mathbb{R}^3 \times \{\pm 1\}$.

This means that we can follow [5] in our construction of the semi-classical measures, but we do, however, need a slight rescaling. In addition to $\hbar > 0$, we also introduce an auxiliary parameter $\alpha > 0$ and put

$$f_{x,p}^{\hbar,\alpha}(y) = (\hbar\alpha)^{-\frac{3}{4}} f\Big(\frac{y-x}{\sqrt{\hbar\alpha}}\Big) e^{i\frac{p\cdot y}{\hbar}},$$

and we further define $f^{\hbar\alpha} = f_{0,0}^{\hbar,\alpha}$ and $g^{\hbar,\alpha} = \mathcal{F}_{\hbar}[f^{\hbar\alpha}]$. Then we have a resolution of the identity

$$\frac{1}{(2\pi\hbar)^3}\iint_{\mathbb{R}^3\times\mathbb{R}^3} |f_{x,p}^{\hbar,\alpha}\rangle\langle f_{x,p}^{\hbar,\alpha}|\,\mathrm{d}x\,\mathrm{d}p = \mathbb{1}_{L^2(\mathbb{R}^3)}.$$

Now, denoting $P_{x,p}^{\hbar,\alpha} = |f_{x,p}^{\hbar,\alpha}\rangle\langle f_{x,p}^{\hbar,\alpha}|\mathbb{1}_{\mathbb{C}^2}$, we define the k-particle semi-classical measures

$$m_{f,\Psi_N}^{(k)}(x,p,s) = \frac{N!}{(N-k)!}\Big\langle \Psi_N, \Big(\bigotimes_{\ell=1}^{k} P_{x_\ell,p_\ell}^{\hbar,\alpha}\mathcal{P}_{s_\ell}\Big)\otimes \mathbb{1}_{N-k}\Psi_N\Big\rangle_{L^2(\mathbb{R}^{3N};\mathbb{C}^{2^N})},$$

where $\Psi_N \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ is any wave function. The parameter α is arbitrary for now, but later we will settle on a specific choice, see (A.101) below. Going through the proofs of Lemmas 2.2, 2.4 and 2.5 in [5] we get the same properties of the semi-classical measures as before:

Lemma A.42. *The function $m^{(k)}_{f,\Psi_N}$ is symmetric on $(\mathbb{R}^3\times\mathbb{R}^3\times\{\pm1\})^k$ and satisfies*

$$0 \le m^{(k)}_{f,\Psi_N} \le 1, \tag{A.96}$$

$$\frac{1}{(2\pi\hbar)^{3k}} \sum_{s\in\{\pm1\}^k} \iint_{\mathbb{R}^{3k}\times\mathbb{R}^{3k}} m^{(k)}_{f,\Psi_N}(x,p,s)\,\mathrm{d}x\,\mathrm{d}p = \frac{N!}{(N-k)!}, \tag{A.97}$$

and for $k\ge 2$,

$$\begin{aligned}\frac{1}{(2\pi\hbar)^3}\sum_{s_k=\pm1}\iint_{\mathbb{R}^3\times\mathbb{R}^3} & m^{(k)}_{f,\Psi_N}(x_1,p_1,s_1,\dots,x_k,p_k,s_k)\,\mathrm{d}x_k\,\mathrm{d}p_k \\ &= (N-k+1)m^{(k-1)}_{f,\Psi_N}(x_1,p_1,s_1,\dots,x_{k-1},p_{k-1},s_{k-1}).\end{aligned} \tag{A.98}$$

Lemma A.43 (Position densities). *Supposing that f is real, L^2-normalized and even, we have for $1\le k\le N$ and any normalized Ψ_N that*

$$\frac{1}{(2\pi\hbar)^{3k}}\int_{\mathbb{R}^{3k}} m^{(k)}_{f,\Psi_N}(x,p,s)\,\mathrm{d}p = k!(\widetilde{\rho}^{(k)}_{\Psi_N} * (|f^{\hbar\alpha}|^2)^{\otimes k})(x,s). \tag{A.99}$$

Lemma A.44 (Kinetic energy). *Suppose that $\Psi_N \in \bigwedge^N H^1_{\hbar b^{-1}A}(\mathbb{R}^3)$ is normalized in L^2 and satisfies $A\Psi_N \in L^2(\mathbb{R}^3;\mathbb{R}^3)$, and that $f\in C^\infty_c(\mathbb{R}^3)$ is real-valued, L^2-normalised and even. Then we have*

$$\begin{aligned}\Big\langle \Psi_N, \sum_{j=1}^N (\boldsymbol{\sigma}\cdot(-i\hbar\nabla_j + bA(x_j)))^2\Psi_N\Big\rangle \\ = \frac{1}{(2\pi\hbar)^3}\sum_{s=\pm1}\iint_{\mathbb{R}^6} |p+bA(x)|^2 m^{(1)}_{f,\Psi_N}(x,p,s)\,\mathrm{d}x\,\mathrm{d}p \\ + \hbar b N\big\langle\Psi_N,\sigma_3\Psi_N\big\rangle - \frac{\hbar}{\alpha}N\int|\nabla f|^2 \\ + 2b\mathrm{Re}\Big\langle\Psi_N,\sum_{j=1}^N\big(A - A*|f^{\hbar\alpha}|^2\big)(x_j)\cdot(-i\hbar\nabla_j)\Psi_N\Big\rangle \\ + b^2\Big\langle\Psi_N,\sum_{j=1}^N\big(|A|^2 - |A|^2 * |f^{\hbar\alpha}|^2\big)(x_j)\Psi_N\Big\rangle.\end{aligned} \tag{A.100}$$

Lemma A.45 (Estimation of error terms). *With our specific choice of magnetic potential, $A(x) = \frac{1}{2}(-x_2,x_1,0)$, we have*

$$\Big\langle\Psi_N,\sum_{j=1}^N\big(A - A*|f^{\hbar\alpha}|^2\big)(x_j)\cdot(-i\hbar\nabla_j)\Psi_N\Big\rangle = 0,$$

and

$$\Big|\Big\langle \Psi_N, \sum_{j=1}^{N} \big(|A|^2 - |A|^2 * |f^{\hbar\alpha}|^2\big)(x_j)\Psi_N \Big\rangle\Big| \le CN\hbar\alpha.$$

Proof. By direct computation,

$$|A|^2(x) - |A|^2(y) - \nabla |A|^2(x)\cdot(x-y) = -\frac{1}{4}(x_\perp - y_\perp)^2,$$

implying for any $x \in \mathbb{R}^3$, since f is even, that

$$\begin{aligned}
&\big||A|^2(x) - |A|^2 * |f^{\hbar\alpha}|^2(x)\big| \\
&\quad = \Big|\int (|A|^2(x) - |A|^2(y))|f^{\hbar\alpha}(x-y)|^2\,\mathrm{d}y\Big| \\
&\quad = \Big|\int (\nabla|A|^2(x)\cdot(x-y) - \frac{1}{4}(x_\perp - y_\perp)^2)|f^{\hbar\alpha}(x-y)|^2\,\mathrm{d}y\Big| \\
&\quad = \frac{1}{4}\int y_\perp^2 |f^{\hbar\alpha}(y)|^2\,\mathrm{d}y = C\hbar\alpha.
\end{aligned}$$

On the other hand, since A is linear and f is even,

$$\begin{aligned}
A(x) - A * |f^{\hbar\alpha}|^2(x) &= \int (A(x) - A(y))|f^{\hbar\alpha}(x-y)|^2\,\mathrm{d}y \\
&= \int A(y)|f^{\hbar\alpha}(y)|^2\,\mathrm{d}y = 0,
\end{aligned}$$

so the error term in (A.100) involving $A - A * |f^{\hbar\alpha}|^2$ is simply not present in our case. $\square$

At this point, we need to distinguish two cases, depending on how fast the parameter β_N tends to zero. If $b = N^{1/3}\beta_N(1+\beta_N)^{-3/5}$ is bounded from above, we can take $\alpha = 1$. If, on the other hand, β_N goes to zero slowly enough such that $b \to \infty$, we instead take $\alpha = b^{-1}$. Then all the error terms in (A.100) will be of order at most $\hbar b$, and furthermore $\hbar\alpha \to 0$, so $|f^{\hbar\alpha}|^2$ is still an approximate identity. For the sake of brevity we will treat both cases simultaneously by choosing

$$\alpha = (1+b)^{-1}. \tag{A.101}$$

By combining Lemmas A.44 and A.45 we have, since also $\hbar\alpha^{-1} \to 0$,

$$\begin{aligned}
&\Big\langle \Psi_N, \sum_{j=1}^{N} (\boldsymbol{\sigma}\cdot(-i\hbar\nabla_j + bA(x_j)))^2 \Psi_N \Big\rangle \\
&\qquad = \frac{1}{(2\pi\hbar)^3}\sum_{s=\pm 1}\iint_{\mathbb{R}^6} |p + bA(x)|^2 m^{(1)}_{f,\Psi_N}(x,p,s)\,\mathrm{d}x\,\mathrm{d}p + o(N).
\end{aligned} \tag{A.102}$$

When b is unbounded, a slight complication arises from the fact that we cannot obtain tightness in the momentum variables of the semi-classical measures, due to the presence of $bA(x)$ in the above approximation. We can, however, circumvent this by doing a simple translation in the momentum variables. Note that doing this will not change the position densities of the measures.

For $x \in \mathbb{R}^{3k}$ we denote $\widetilde{A}(x) = (A(x_1), \ldots, A(x_k))$ and define

$$\widetilde{m}_N^{(k)}(x,p,s) = m_{f,\Psi_N}^{(k)}(x, p - b\widetilde{A}(x), s).$$

Then the family of sequences $(\widetilde{m}_N^{(k)})_{N\geq k}$ still satisfies Lemmas A.42 and A.43, and in exactly the same way as in Lemma A.34, we obtain (symmetric) weak limits $\widetilde{m}^{(k)} \in L^1((\mathbb{R}^6 \times \{\pm1\})^k) \cap L^\infty((\mathbb{R}^6 \times \{\pm1\})^k)$ with $0 \leq \widetilde{m}^{(k)} \leq 1$ such that

$$\sum_{s\in\{\pm1\}^k} \int_{\mathbb{R}^{6k}} \widetilde{m}_N^{(k)}(x,p,s)\varphi(x,p,s)\,\mathrm{d}x\,\mathrm{d}p \longrightarrow \sum_{s\in\{\pm1\}^k} \int_{\mathbb{R}^{6k}} \widetilde{m}^{(k)}(x,p,s)\varphi(x,p,s)\,\mathrm{d}x\,\mathrm{d}p \tag{A.103}$$

for all $\varphi \in L^1((\mathbb{R}^6 \times \{\pm1\})^k) + L^\infty_\varepsilon((\mathbb{R}^6 \times \{\pm1\})^k)$, as N tends to infinity.

Lemma A.46. *Suppose that $\Psi_N \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ is a sequence satisfying the energy bound $\langle \Psi_N, H_{N,\beta_N}\Psi_N\rangle \leq CN$. Then we have*

(1) The sequence $(\widetilde{m}_N^{(k)})_{N\geq k}$ is tight for each $k \geq 1$.

(2) The limit measures $\widetilde{m}^{(k)}$ are probability measures, i.e.,

$$\frac{1}{(2\pi)^{3k}} \sum_{s\in\{\pm1\}^k} \iint_{\mathbb{R}^{3k}\times\mathbb{R}^{3k}} \widetilde{m}^{(k)}(x,p,s)\,\mathrm{d}x\,\mathrm{d}p = 1. \tag{A.104}$$

(3) The compatibility relation (A.98) is preserved in the limit, that is, for $k \geq 2$ and almost every $(x,p,s) \in (\mathbb{R}^3 \times \mathbb{R}^3 \times \{\pm1\})^{k-1}$,

$$\frac{1}{(2\pi)^3} \sum_{s_k=\pm1} \iint_{\mathbb{R}^6} \widetilde{m}^{(k)}(x,x_k;p,p_k;s,s_k)\,\mathrm{d}x_k\,\mathrm{d}p_k = \widetilde{m}^{(k-1)}(x,p,s). \tag{A.105}$$

(4) The convergence in (A.103) holds for any φ in $L^1((\mathbb{R}^6 \times \{\pm1\})^k) + L^\infty((\mathbb{R}^6 \times \{\pm1\})^k)$.

Proof. We will only prove that $(\widetilde{m}_N^{(1)})$ is a tight sequence. The rest follows in exactly the same way as in Lemma A.35. Supposing that f is supported on a ball with radius

K centred at the origin, we have by Lemma A.43 for $\hbar\alpha$ small that

$$\begin{aligned}\int_{|x|\geq R}\int_{\mathbb{R}^3} &\widetilde{m}_N^{(1)}(x,p,s)\,\mathrm{d}p\,\mathrm{d}x \\ &= (2\pi\hbar)^3\int_{|x|\geq R}\int_{\operatorname{supp} f^{\hbar\alpha}} \widetilde{\rho}_{\Psi_N}^{(1)}(x-y,s)|f^{\hbar\alpha}(y)|^2\,\mathrm{d}y\,\mathrm{d}x \\ &\leq C\int_{|x|\geq R-K}\frac{1}{N}\widetilde{\rho}_{\Psi_N}^{(1)}(x,s)\,\mathrm{d}x.\end{aligned}$$

Now, combining Lemma A.11 with the fact that V is a confining potential, it follows that the right hand side above tends to zero uniformly in N as R tends to infinity, implying that $(\widetilde{m}_N^{(1)})$ is tight in the position variable. Using the kinetic energy bound (A.32) combined with (A.102) we also obtain

$$\begin{aligned}\int_{|p|\geq R}\int_{\mathbb{R}^3}\widetilde{m}_N^{(1)}(x,p,s)\,\mathrm{d}x\,\mathrm{d}p &= \int_{\mathbb{R}^3}\int_{|p+bA(x)|\geq R} m_{f,\Psi_N}^{(1)}(x,p,s)\,\mathrm{d}p\,\mathrm{d}x \\ &\leq \frac{1}{R^2}\iint_{\mathbb{R}^6}|p+bA(x)|^2 m_{f,\Psi_N}^{(1)}(x,p,s)\,\mathrm{d}x\,\mathrm{d}p \leq \frac{C}{R^2},\end{aligned}$$

showing that $(\widetilde{m}_N^{(1)})$ is also tight in the momentum variable. □

Proposition A.47 (Convergence of states). *Suppose that $\beta_N \to 0$, and that $\Psi_N \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ is a sequence of normalized wave functions satisfying the energy bound $\langle \Psi_N, H_{N,\beta_N}\Psi_N\rangle \leq CN$. Then there exist a subsequence $(N_\ell)\subseteq\mathbb{N}$ and a unique Borel probability measure* P *on the set*

$$\mathcal{S} = \big\{\mu\in L^1(\mathbb{R}^6\times\{\pm1\}) \,\big|\, 0\leq\mu\leq 1,\ \frac{1}{(2\pi)^3}\|\mu\|_1 = 1\big\},$$

such that for each $k\geq 1$ the following holds:

(1) For all $\varphi\in L^1((\mathbb{R}^6\times\{\pm1\})^k)+L^\infty((\mathbb{R}^6\times\{\pm1\})^k)$, as ℓ tends to infinity,

$$\begin{aligned}\sum_{s\in\{\pm1\}^k}&\iint_{\mathbb{R}^{6k}}\widetilde{m}_{N_\ell}^{(k)}(x,p,s)\varphi(x,p,s)\,\mathrm{d}x\,\mathrm{d}p \\ &\longrightarrow \int_{\mathcal{S}}\Big(\sum_{s\in\{\pm1\}^k}\iint_{\mathbb{R}^{6k}}\mu^{\otimes k}(x,p,s)\varphi(x,p,s)\,\mathrm{d}x\,\mathrm{d}p\Big)\,\mathrm{dP}(\mu).\end{aligned}$$

(2) For $U\in L^{5/2}(\mathbb{R}^3\times\{\pm1\})+L^\infty(\mathbb{R}^3\times\{\pm1\})$ if $k=1$, and for any bounded and uniformly continuous function U on $(\mathbb{R}^3\times\{\pm1\})^k$ if $k\geq 2$, as ℓ tends to infinity,

$$\begin{aligned}\frac{k!}{N_\ell^k}\sum_{s\in\{\pm1\}^k}&\int_{\mathbb{R}^{3k}}\widetilde{\rho}_{\Psi_{N_\ell}}^{(k)}(x,s)U(x,s)\,\mathrm{d}x \\ &\longrightarrow \int_{\mathcal{S}}\Big(\sum_{s\in\{\pm1\}^k}\int_{\mathbb{R}^{3k}}\widetilde{\rho}_\mu^{\otimes k}(x,s)U(x,s)\,\mathrm{d}x\Big)\,\mathrm{dP}(\mu), \qquad \text{(A.106)}\end{aligned}$$

where

$$\widetilde{\rho}_\mu(x,s) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\mu(x,p,s)\,\mathrm{d}p.$$

Lemma A.48. *Suppose that we have a sequence $\Psi_N \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ satisfying $\langle \Psi_N, H_{N,\beta_N}\Psi_N\rangle = E(N,\beta_N)+o(N)$. Then, denoting by ρ_μ the spin-summed position density of μ, we have*

$$\liminf_{N\to\infty}\Big\langle \Psi_N, \frac{1}{N}\sum_{j=1}^N(\boldsymbol{\sigma}\cdot(-i\hbar\nabla + bA(x_j)))^2\Psi_N\Big\rangle \geq \frac{1}{(2\pi)^3}\int_{\mathcal{S}}\Big(\sum_{s=\pm1}\iint_{\mathbb{R}^6}p^2\mu(x,p,s)\,\mathrm{d}p\,\mathrm{d}x\Big)\,\mathrm{dP}(\mu),$$

$$\liminf_{N\to\infty}\Big\langle \Psi_N, \frac{1}{N}\sum_{j=1}^N V(x_j)\Psi_N\Big\rangle \geq \int_{\mathcal{S}}\Big(\int_{\mathbb{R}^3}V(x)\rho_\mu(x)\,\mathrm{d}x\Big)\,\mathrm{dP}(\mu),$$

and

$$\lim_{N\to\infty}\Big\langle \Psi_N, \frac{1}{N^2}\sum_{1\leq j<k\leq N}w(x_j-x_k)\Psi_N\Big\rangle = \frac{1}{2}\int_{\mathcal{S}}\Big(\int_{\mathbb{R}^6}w(x-y)\rho_\mu(x)\rho_\mu(y)\,\mathrm{d}x\,\mathrm{d}y\Big)\,\mathrm{dP}(\mu).$$

Proof. For the kinetic energy term, simply use that

$$\Big\langle \Psi_N, \sum_{j=1}^N(\boldsymbol{\sigma}\cdot(-i\hbar\nabla_j + bA(x_j)))^2\Psi_N\Big\rangle = \frac{1}{(2\pi\hbar)^3}\sum_{s=\pm1}\iint_{\mathbb{R}^6}p^2\widetilde{m}_N^{(1)}(x,p,s)\,\mathrm{d}x\,\mathrm{d}p + o(N),$$

and proceed as in the proof of Lemma A.40. The convergence of the potential energy terms follows exactly as in Lemma A.41. ☐

Proof of Theorem A.5 and Theorem A.6, weak fields. We find exactly as in the previous cases that

$$E_0^{\mathrm{Vla}} \geq \liminf_{N\to\infty}\frac{\langle \Psi_N, H_{N,\beta_N}\Psi_N\rangle}{N} \geq \int_{\mathcal{S}}\mathcal{E}_0^{\mathrm{Vla}}(\mu)\,\mathrm{dP}(\mu) \geq E_0^{\mathrm{Vla}},$$

finishing the proof of Theorem A.5, and implying that the de Finetti measure P is supported on the set of minimizers of $\mathcal{E}_0^{\mathrm{Vla}}$. Since these are independent of the spin variable by Remark A.21, the convergence of states (A.106) becomes

$$\frac{k!}{N_\ell^k}\sum_{s\in\{\pm1\}^k}\int_{\mathbb{R}^{3k}}\widetilde{\rho}^{(k)}_{\Psi_{N_\ell}}(x,s)U(x,s)\,\mathrm{d}x \longrightarrow \int_{\mathcal{S}}\Big(\frac{1}{2^k}\sum_{s\in\{\pm1\}^k}\int_{\mathbb{R}^{3k}}\rho_\mu^{\otimes k}(x)U(x,s)\,\mathrm{d}x\Big)\,\mathrm{dP}(\mu).$$

Using P to induce a measure on the set of minimizers of the Thomas-Fermi functional concludes the proof of Theorem A.6. □

A.7 Appendix: Weyl asymptotics for the Dirichlet Pauli operator

Here we give a proof of the generalization of Corollary A.9 advertised in Remark A.10. The idea of the proof is the same as in [20], but we spell out the details here for completeness. Assume that $\Lambda \subseteq \mathbb{R}^3$ is an open and connected set, and let V be any potential with $V_- \in L^{3/2}(\Lambda) \cap L^{5/2}(\Lambda)$. We denote by $(\boldsymbol{\sigma} \cdot (-i\hbar\nabla + bA))^2_\Lambda$ the Pauli operator acting on $L^2(\Lambda)$ with Dirichlet boundary conditions, and consider

$$H(\hbar, b, \Lambda) = (\boldsymbol{\sigma} \cdot (-i\hbar\nabla + bA))^2_\Lambda + V.$$

We denote by $e_j(\hbar, b, \Lambda)$, $j \geq 1$, the negative eigenvalues of $H(\hbar, b, \Lambda)$. Recall that the semi-classical expression for the sum of negative eigenvalues of $H(\hbar, b, \Lambda)$ is

$$E_{\mathrm{scl}}(\hbar, b, \Lambda) = -\frac{1}{\hbar^3} \int_\Lambda P_{\hbar b}(V_-(x))\, \mathrm{d}x, \tag{A.107}$$

with the pressure P_B given in (A.10).

Proposition A.49. *For any potential V on Λ with $V_- \in L^{3/2}(\Lambda) \cap L^{5/2}(\Lambda)$, we have*

$$\lim_{\hbar \to 0} \frac{\sum_j e_j(\hbar, b, \Lambda)}{E_{\mathrm{scl}}(\hbar, b, \Lambda)} = 1 \tag{A.108}$$

uniformly in the magnetic field strength b.

Remark A.50. *It actually follows from the proof that we have the error bound*

$$\sum_j e_j(\hbar, b, \Lambda) = E_{\mathrm{scl}}(\hbar, b, \Lambda) + o\Big(\frac{b}{\hbar^2} + \frac{1}{\hbar^3}\Big).$$

Proof. For the lower bound on the eigenvalues we will make use of the fact that the result is well-known for the Pauli operator

$$H(\hbar, b) = (\boldsymbol{\sigma} \cdot (-i\hbar\nabla + bA(x)))^2 + V(x)$$

on the full space [20, Theorem 3.1] (where we extend V to be zero outside of Λ). Denoting by $e_j(\hbar, b)$ the corresponding negative eigenvalues, we immediately get by the min-max principle and inclusion of quadratic form domains the inequalities

$$e_j(\hbar, b, \Omega) \geq e_j(\hbar, b), \quad j \geq 1,$$

and hence

$$\limsup_{\hbar\to 0} \frac{\sum_j e_j(\hbar, b, \Lambda)}{E_{\mathrm{scl}}(\hbar, b, \Lambda)} \le \limsup_{\hbar\to 0} \frac{\sum_j e_j(\hbar, b)}{E_{\mathrm{scl}}(\hbar, b)} = 1.$$

In fact, it is shown in the proof of [20, Theorem 3.1] that

$$\sum_j e_j(\hbar, b) \ge E_{\mathrm{scl}}(\hbar, b) + o\Big(\frac{b}{\hbar^2} + \frac{1}{\hbar^3}\Big),$$

implying one of the bounds in Remark A.50.

We will use the coherent states from Section A.4 to construct an appropriate trial state for the corresponding upper bound on the sum of eigenvalues, using the construction in [20] as a guide line. Let $f \in C_c^\infty(\mathbb{R}^3)$ with support contained in the unit ball $B(0,1)$, and denote by $\Lambda_\hbar = \{x \in \Lambda \mid d(x, \partial\Lambda) > 2\hbar^{1/2}\}$. We furthermore introduce

$$K_{\hbar,b} = \{(u,p,j,s) \in \mathbb{R}^3 \times \mathbb{R} \times \mathbb{N}_0 \times \{\pm 1\} \mid p^2 + \hbar b(2j+1+s) \le V_-(u)\},$$

and let $M_{\hbar,b}$ be the characteristic function of $K_{\hbar,b} \cap \{(u,p,j,s) \mid u \in \Lambda_\hbar\}$. We define the trial state $\gamma_\hbar$ by

$$\gamma_\hbar = \frac{b}{(2\pi\hbar)^2} \sum_{s=\pm 1} \sum_{j\ge 0} \int_{\mathbb{R}^3} \int_{\mathbb{R}} M_{\hbar,b}(u,p,j,s) P^{\hbar,b}_{u,p,j} \mathcal{P}_s \,\mathrm{d}p\,\mathrm{d}u. \tag{A.109}$$

Note by (A.74) for any $\psi \in L^2(\mathbb{R}^3; \mathbb{C}^2)$ that

$$\frac{b}{2\pi\hbar} \langle \psi, P^{\hbar,b}_{u,p,j} \mathcal{P}_s \psi\rangle = 2\pi \int_{\mathbb{R}^2} |\Pi^{(2)}_j \otimes \mathcal{F}_3\big[\overline{f^\hbar(\,\cdot\, - u)} \psi(\,\cdot\,, s)\big](y, \hbar^{-1}p)|^2 \,\mathrm{d}y,$$

where $\operatorname{supp} f^\hbar = \hbar^{1/2} \operatorname{supp} f \subseteq B(0, \hbar^{1/2})$. Hence, if $u \in \Lambda_\hbar$ and $d(\operatorname{supp}\psi(\cdot, s), \Lambda_\hbar) \ge \hbar^{1/2}$, then we have $\langle \psi, P^{\hbar,b}_{u,p,j} \mathcal{P}_s \psi\rangle = 0$, because in this case $f^\hbar(\,\cdot\, - u)\psi(\,\cdot\,, s) = 0$. It follows that $\gamma_\hbar$ indeed is a suitable trial state for the Dirichlet problem on Λ, so by the variational principle,

$$\begin{aligned}\sum_{j\ge 1} e_j(\hbar, b, \Lambda) &\le \operatorname{Tr}[H(\hbar, b, \Lambda)\gamma_\hbar] \\ &= \frac{b}{(2\pi\hbar)^2} \sum_{s=\pm 1} \sum_{j\ge 0} \int_{\mathbb{R}^3} \int_{\mathbb{R}} M_{\hbar,b}(u,p,j,s) \operatorname{Tr}[H(\hbar, b, \Lambda) P^{\hbar,b}_{u,p,j} \mathcal{P}_s] \,\mathrm{d}p\,\mathrm{d}u.\end{aligned}$$

We proceed to estimate the terms on the right hand side individually. For the potential energy term, note that by definition of the coherent states,

$$\begin{aligned}\operatorname{Tr}\big[V_+ P^{\hbar,b}_{u,p,j}\big] &= \operatorname{Tr}\big[V_+^{\frac12} P^{\hbar,b}_{u,p,j} V_+^{\frac12}\big] = \int_{\mathbb{R}^2} \big\|V_+^{\frac12} f^{\hbar,b}_{x,u,p,j}\big\|_2^2 \,\mathrm{d}x \\ &= \int_{\mathbb{R}^2} \int_{\mathbb{R}^3} V_+(y) |\varphi^{\hbar,b}_{x,j}(y_\perp)|^2 |f^\hbar(y-u)|^2 \,\mathrm{d}y\,\mathrm{d}x = V_+ * |f^\hbar|^2(u),\end{aligned}$$

with the same equality also holding for V_-. For the kinetic energy term we have, using the IMS localization formula (A.80),

$$
\begin{aligned}
\operatorname{Tr}[(-i\hbar\nabla + bA)^2 P^{\hbar,b}_{u,p,j}] &= \int_{\mathbb{R}^2} \big\|(-i\hbar\nabla + bA) f^{\hbar,b}_{x,u,p,j}\big\|_2^2 \,\mathrm{d}x \\
&= \int_{\mathbb{R}^2} \big\langle \varphi^{\hbar,b}_{x,j} \otimes e^{i\frac{p(\cdot)}{\hbar}}, f^{\hbar}(\,\cdot\, - u)(-i\hbar\nabla + bA)^2 f^{\hbar}(\,\cdot\, - u)\varphi^{\hbar,b}_{x,j} \otimes e^{i\frac{p(\cdot)}{\hbar}} \big\rangle \,\mathrm{d}x \\
&= \int_{\mathbb{R}^2} \big\langle \varphi^{\hbar,b}_{x,j} \otimes e^{i\frac{p(\cdot)}{\hbar}}, |f^{\hbar}(\,\cdot\, - u)|^2(-i\hbar\nabla + bA)^2 \varphi^{\hbar,b}_{x,j} \otimes e^{i\frac{p(\cdot)}{\hbar}} \big\rangle \\
&\quad + \hbar^2 \big\langle \varphi^{\hbar,b}_{x,j} \otimes e^{i\frac{p(\cdot)}{\hbar}}, |\nabla f^{\hbar}(\,\cdot\, - u)|^2 \varphi^{\hbar,b}_{x,j} \otimes e^{i\frac{p(\cdot)}{\hbar}} \big\rangle \,\mathrm{d}x \\
&= (p^2 + \hbar b(2j+1)) \int_{\mathbb{R}^2} \big\| f^{\hbar,b}_{x,u,p,j}\big\|_2^2 \,\mathrm{d}x + \hbar^2 \int_{\mathbb{R}^3} |\nabla f^{\hbar}|^2 \\
&= p^2 + \hbar b(2j+1) + \hbar \int_{\mathbb{R}^3} |\nabla f|^2,
\end{aligned}
$$

implying that

$$
\begin{aligned}
\operatorname{Tr}[(\boldsymbol{\sigma}\cdot(-i\hbar\nabla + bA))^2 P^{\hbar,b}_{u,p,j}\mathcal{P}_s] &= \operatorname{Tr}[((-i\hbar\nabla + bA)^2 \mathbb{1}_{\mathbb{C}^2} + \hbar b\sigma_3) P^{\hbar,b}_{u,p,j}\mathcal{P}_s] \\
&= p^2 + \hbar b(2j+1+s) + \hbar \int_{\mathbb{R}^3} |\nabla f|^2.
\end{aligned}
$$

Collecting the terms and using (A.43) and (A.45), we have shown

$$
\begin{aligned}
\sum_{j\geq 1} e_j(\hbar, b, \Lambda) \leq \frac{b}{(2\pi\hbar)^2} &\sum_{\substack{j\geq 0\\ s=\pm 1}} \int_{\Lambda_\hbar\times\mathbb{R}} (p^2 + \hbar b(2j+1+s)) \mathbb{1}_{K_{\hbar,b}} \,\mathrm{d}u\,\mathrm{d}p \\
&+ \frac{b}{(2\pi\hbar)^2} \sum_{\substack{j\geq 0\\ s=\pm 1}} \int_{\Lambda_\hbar\times\mathbb{R}} \Big(V * |f^{\hbar}|^2(u) + \hbar \int |\nabla f|^2\Big) \mathbb{1}_{K_{\hbar,b}} \,\mathrm{d}u\,\mathrm{d}p \\
&= \frac{1}{\hbar^3} \int_{\Lambda_\hbar} V_-(u) P'_{\hbar b}(V_-(u)) - P_{\hbar b}(V_-(u)) \,\mathrm{d}u \\
&\quad + \frac{1}{\hbar^3} \int_{\Lambda_\hbar} \Big(V * |f^{\hbar}|^2(u) + \hbar \int |\nabla f|^2\Big) P'_{\hbar b}(V_-(u)) \,\mathrm{d}u.
\end{aligned}
$$

To compare with the semi-classical expression for the sum of eigenvalues, we will need the bounds [20, Theorem 3.1]

$$
k_1 \frac{b}{\hbar^2} y^{\frac{1}{2}} + k_2 \frac{1}{\hbar^3} y^{\frac{3}{2}} \leq \frac{1}{\hbar^3} P'_{\hbar b}(y) \leq K_1 \frac{b}{\hbar^2} y^{\frac{1}{2}} + K_2 \frac{1}{\hbar^3} y^{\frac{3}{2}},
$$

valid for all $y \geq 0$, where k_1, k_2, K_1, K_2 are positive constants. These bounds also imply

$$
c_1 \frac{b}{\hbar^2} y^{\frac{3}{2}} + c_2 \frac{1}{\hbar^3} y^{\frac{5}{2}} \leq \frac{1}{\hbar^3} P_{\hbar b}(y) \leq C_1 \frac{b}{\hbar^2} y^{\frac{3}{2}} + C_2 \frac{1}{\hbar^3} y^{\frac{5}{2}},
$$

and

$$
\tilde{c}\Big(\frac{b}{\hbar^2} + \frac{1}{\hbar^3}\Big) \leq \int \frac{1}{\hbar^3} P_{\hbar b}(V_-(u)) \,\mathrm{d}u \leq \widetilde{C}\Big(\frac{b}{\hbar^2} + \frac{1}{\hbar^3}\Big). \tag{A.110}
$$

We obtain for the leading term

$$
\begin{aligned}
&-\frac{1}{\hbar^3}\int_{\Lambda_\hbar} P_{\hbar b}(V_-(u))\,\mathrm{d}u \\
&\qquad = -\frac{1}{\hbar^3}\int_{\Lambda} P_{\hbar b}(V_-(u))\,\mathrm{d}u + \int_{\Lambda\setminus\Lambda_\hbar} C_1\frac{b}{\hbar^2}V_-(u)^{\frac{3}{2}} + C_2\frac{1}{\hbar^3}V_-(u)^{\frac{5}{2}}\,\mathrm{d}u,
\end{aligned}
$$

and applying Hölder's inequality for the subleading terms,

$$
\begin{aligned}
\frac{1}{\hbar^3}\int_{\Lambda_\hbar} P_{\hbar b}'(V_-(u))\,\mathrm{d}u &\leq C\int_{\Lambda}\frac{b}{\hbar^2}V_-(u)^{\frac{3}{2}} + \frac{1}{\hbar^3}V_-(u)^{\frac{5}{2}}\,\mathrm{d}u \\
&\leq \frac{C}{\hbar^3}\big\|V_-\big\|_{\frac{3}{2}}^{\frac{3}{2}} + C\frac{b}{\hbar^2}|\Lambda|^{\frac{2}{3}}\Big(\int_\Omega V_-(u)^{\frac{3}{2}}\,\mathrm{d}u\Big)^{\frac{1}{3}},
\end{aligned}
$$

and

$$
\begin{aligned}
&\frac{1}{\hbar^3}\int_{\Lambda_\hbar}(V_-(u) + V*|f^\hbar|^2(u))P_{\hbar b}'(V_-(u))\,\mathrm{d}u \\
&\quad \leq C\int_{\operatorname{supp}V_-}(V_- + V*|f^\hbar|^2)\Big(\frac{b}{\hbar^2}V_-^{\frac{1}{2}} + \frac{1}{\hbar^3}V_-^{\frac{3}{2}}\Big)\,\mathrm{d}u \\
&\quad \leq C\frac{b}{\hbar^2}\Big(\int_\Lambda V_-^{\frac{3}{2}}\,\mathrm{d}u\Big)^{\frac{1}{3}}\Big(\int_{\operatorname{supp}V_-}\big|V*|f^\hbar|^2 - V\big|^{\frac{3}{2}}\,\mathrm{d}u\Big)^{\frac{2}{3}} \\
&\qquad + \frac{C}{\hbar^3}\Big(\int_\Lambda V_-^{\frac{5}{2}}\,\mathrm{d}u\Big)^{\frac{3}{5}}\Big(\int_{\operatorname{supp}V_-}\big|V*|f^\hbar|^2 - V\big|^{\frac{5}{2}}\,\mathrm{d}u\Big)^{\frac{2}{5}} \\
&\quad = C\frac{b}{\hbar^2}\big\|V_-\big\|_{\frac{3}{2}}^{\frac{1}{2}}\big\|V*|f^\hbar|^2 - V\big\|_{L^{\frac{3}{2}}(\operatorname{supp}V_-)} \\
&\qquad + \frac{C}{\hbar^3}\big\|V_-\big\|_{\frac{5}{2}}^{\frac{3}{2}}\big\|V*|f^\hbar|^2 - V\big\|_{L^{\frac{5}{2}}(\operatorname{supp}V_-)}.
\end{aligned}
$$

Collecting these bounds, we have

$$
\sum_{j\geq 1} e_j(\hbar, b, \Lambda) \leq -\frac{1}{\hbar^3}\int_\Lambda P_{\hbar b}(V_-(u))\,\mathrm{d}u + C\Big(\frac{b}{\hbar^2} + \frac{1}{\hbar^3}\Big)\varepsilon(\hbar), \tag{A.111}
$$

where $\varepsilon(\hbar)$ is independent of b, and $\lim_{\hbar\to 0}\varepsilon(\hbar) = 0$. Finally, by the upper bound in (A.110), we conclude

$$
\liminf_{\hbar\to 0}\frac{\sum_j e_j(\hbar, b, \Lambda)}{E_{\mathrm{scl}}(\hbar, b, \Lambda)} \geq 1
$$

uniformly in b. □

Lastly, we also include a proof of Corollary A.9, elaborating on the Weyl asymptotics when $\hbar$ and b satisfy the scaling relations (A.5). For this, it is very useful to know the error bound in Remark A.50.

Proof of Corollary A.9. We start out by considering the case $0 < \beta < \infty$. We wish to apply dominated convergence to the sequence $P_{\hbar b}(V_-(x))$. Note for each $j \geq 1$ that $\lim_{N\to\infty}[2\hbar b j - V_-(x)]_- = [2k_\beta j - V_-(x)]_-$ for almost every $x \in \mathbb{R}^3$. Note also for each x that the number of non-zero terms in the sum in the semi-classical expression (A.107) is bounded by $V_-(x)(2\hbar b)^{-1}$, and for each $j \geq 1$ we have $[2\hbar b j - V_-(x)]_- \leq [2\hbar b - V_-(x)]_-$. Hence we get the integrable pointwise bound

$$\sum_{j=1}^{\infty}[2\hbar bj - V_-(x)]_-^{\frac{3}{2}} \leq \frac{V_-(x)}{2\hbar b}[2\hbar b - V_-(x)]_-^{\frac{3}{2}} \leq \frac{V_-(x)^{\frac{5}{2}}}{2\hbar b},$$

so by dominated convergence,

$$\lim_{N\to\infty}\int_{\mathbb{R}^3}\hbar b\sum_{j=1}^{\infty}[2\hbar bj - V_-(x)]_-^{\frac{3}{2}}\,\mathrm{d}x = \int_{\mathbb{R}^3}k_\beta\sum_{j=1}^{\infty}[2k_\beta j - V_-(x)]_-^{\frac{3}{2}}\,\mathrm{d}x.$$

Combining this with the error bound in Remark A.50 and the definitions of $\hbar$ and b by (A.4), we obtain

$$\begin{aligned}
\lim_{N\to\infty}\frac{1}{N}\sum_j e_j(\hbar, b, V) &= \lim_{N\to\infty}\frac{1}{N}E_{\mathrm{scl}}(\hbar, b, V) \\
&= \lim_{N\to\infty} -\frac{1}{\hbar^3 N}\int_{\mathbb{R}^3}\frac{\hbar b}{3\pi^2}\Big(V_-(x)^{\frac{3}{2}} + 2\sum_{j=1}^{\infty}[2\hbar bj - V_-(x)]_-^{\frac{3}{2}}\Big)\,\mathrm{d}x \\
&= -(1+\beta)^{-\frac{3}{5}}\int_{\mathbb{R}^3}P_{k_\beta}(V_-(x))\,\mathrm{d}x.
\end{aligned}$$

For the case $\beta = 0$, note that the sum in the semi-classical expression becomes a Riemann sum, i.e.

$$\begin{aligned}
\lim_{N\to\infty}2\hbar b\sum_{j=1}^{\infty}[2\hbar bj - V_-(x)]_-^{\frac{3}{2}} &= \lim_{N\to\infty}2\hbar b\sum_{j=1}^{\lfloor V_-(x)(2\hbar b)^{-1}\rfloor}[2\hbar bj - V_-(x)]_-^{\frac{3}{2}} \\
&= \int_0^{V_-(x)}[y - V_-(x)]_-^{\frac{3}{2}}\,\mathrm{d}y = \frac{2}{5}V_-(x)^{\frac{5}{2}},
\end{aligned}$$

so we obtain the result in the same way by applying Remark A.50 as above.

In case $\beta_N \to \infty$, the contribution from all the higher Landau levels to the pressure $P_{\hbar b}$ goes to zero pointwise as N goes to infinity, so we conclude by monotone convergence and Remark A.50. □

References

[1] W. Braun and K. Hepp. *The Vlasov dynamics and its fluctuations in the* $1/N$ *limit of interacting classical particles.* *Comm. Math. Phys.*, **56**(2):101–113, 1977. ISSN 0010-3616.

[2] E. Caglioti, P.-L. Lions, C. Marchioro, and M. Pulvirenti. *A special class of stationary flows for two-dimensional Euler equations: a statistical mechanics description. Comm. Math. Phys.*, **143**(3):501–525, 1992. ISSN 0010-3616.

[3] B. de Finetti. *Funzione caratteristica di un fenomeno aleatorio.* Atti della R. Accademia Nazionale dei Lincei, 1931. Ser. 6, Memorie, Classe di Scienze Fisiche, Matematiche e Naturali.

[4] P. Diaconis and D. Freedman. *Finite exchangeable sequences. Ann. Probab.*, **8**(4):745–764, 1980. ISSN 0091-1798.

[5] S. Fournais, M. Lewin, and J. P. Solovej. *The semi-classical limit of large fermionic systems. Calc. Var. Partial Differ. Equ.*, pages 57–105, 2018. doi:10.1007/s00526-018-1374-2.

[6] C. Hainzl and R. Seiringer. *Bounds on One-Dimensional Exchange Energies with Application to Lowest Landau Band Quantum Mechanics. Letters in Mathematical Physics*, **55**(2):133–142, 2001. ISSN 1573-0530. doi:10.1023/A:1010951905548.

[7] C. Hainzl and R. Seiringer. *A Discrete Density Matrix Theory for Atoms in Strong Magnetic Fields. Communications in Mathematical Physics*, **217**(1):229–248, 2001. ISSN 1432-0916. doi:10.1007/s002200100373.

[8] B. Hauksson and J. Yngvason. *Asymptotic Exactness of Magnetic Thomas–Fermi Theory at Nonzero Temperature. Journal of Statistical Physics*, **116**(1):523–546, 2004. ISSN 1572-9613. doi:10.1023/B:JOSS.0000037223.74597.4e.

[9] E. Hewitt and L. J. Savage. *Symmetric measures on Cartesian products. Trans. Amer. Math. Soc.*, **80**:470–501, 1955. ISSN 0002-9947.

[10] R. L. Hudson and G. R. Moody. *Locally normal symmetric states and an analogue of de Finetti's theorem. Z. Wahrscheinlichkeitstheor. und Verw. Gebiete*, **33**(4):343–351, 1975/76.

[11] M. K.-H. Kiessling. *Statistical mechanics of classical particles with logarithmic interactions. Comm. Pure. Appl. Math.*, **46**:27–56, 1993.

[12] M. Lewin, P. S. Madsen, and A. Triay. *Semi-classical limit of large fermionic systems at positive temperature. ArXiv e-prints*, 2019.

[13] M. Lewin, P. T. Nam, and N. Rougerie. *Derivation of Hartree's theory for generic mean-field Bose systems. Adv. Math.*, **254**:570–621, 2014. doi:10.1016/j.aim.2013.12.010.

[14] M. Lewin, P. T. Nam, and N. Rougerie. *Remarks on the quantum de Finetti theorem for bosonic systems. Appl. Math. Res. Express (AMRX)*, **2015**(1):48–63, 2015. doi:10.1093/amrx/abu006.

[15] M. Lewin, P. T. Nam, and N. Rougerie. *The mean-field approximation and the non-linear Schrödinger functional for trapped Bose gases. Trans. Amer. Math. Soc*, **368**(9):6131–6157, 2016. doi:10.1090/tran/6537.

[16] E. H. Lieb and M. Loss. *Analysis*, volume 14 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI, 2nd edition, 2001. ISBN 0-8218-2783-9.

[17] E. H. Lieb and B. Simon. *The Hartree-Fock theory for Coulomb systems. Commun. Math. Phys.*, **53**(3):185–194, 1977. ISSN 0010-3616.

[18] E. H. Lieb and B. Simon. *The Thomas-Fermi theory of atoms, molecules and solids.*

Adv. Math., **23**(1):22–116, 1977. ISSN 0001-8708.

[19] E. H. Lieb, J. P. Solovej, and J. Yngvason. *Asymptotics of heavy atoms in high magnetic fields: I. Lowest Landau band regions. Comm. Pure Appl. Math.*, **47**(4):513–591, 1994.

[20] E. H. Lieb, J. P. Solovej, and J. Yngvason. *Asymptotics of heavy atoms in high magnetic fields: II. Semiclassical regions. Comm. Math. Phys.*, **161**(1):77–124, 1994.

[21] E. H. Lieb, J. P. Solovej, and J. Yngvason. *Ground states of large quantum dots in magnetic fields. Phys. Rev. B*, **51**:10646–10665, 1995. doi:10.1103/PhysRevB.51.10646.

[22] E. H. Lieb and W. E. Thirring. *Gravitational collapse in quantum mechanics with relativistic kinetic energy. Ann. Physics*, **155**(2):494–512, 1984. ISSN 0003-4916.

[23] E. H. Lieb and H.-T. Yau. *The Chandrasekhar theory of stellar collapse as the limit of quantum mechanics. Commun. Math. Phys.*, **112**(1):147–174, 1987. ISSN 0010-3616.

[24] P. Madsen. *In preparation.* Ph.D. thesis, Aarhus University, 2019.

[25] J. Messer and H. Spohn. *Statistical mechanics of the isothermal Lane-Emden equation. J. Statist. Phys.*, **29**(3):561–578, 1982. ISSN 0022-4715. doi:10.1007/BF01342187.

[26] N. Rougerie. *De Finetti theorems, mean-field limits and Bose-Einstein condensation. ArXiv e-prints*, 2015.

[27] R. Seiringer. *On the maximal ionization of atoms in strong magnetic fields. Journal of Physics A: Mathematical and General*, **34**(9):1943–1948, 2001. doi:10.1088/0305-4470/34/9/311.

[28] H. Spohn. *On the Vlasov hierarchy. Math. Methods Appl. Sci.*, **3**(4):445–455, 1981. ISSN 0170-4214. doi:10.1002/mma.1670030131.

[29] E. Størmer. *Symmetric states of infinite tensor products of C^*-algebras. J. Functional Analysis*, **3**:48–68, 1969.

Paper B

Semi-classical limit of large fermionic systems at positive temperature

By M. Lewin, P. S. Madsen, and A. Triay

Available at arXiv:1902.00310.

Abstract

We study a system of N interacting fermions at positive temperature in a confining potential. In the regime where the intensity of the interaction scales as $1/N$ and with an effective semi-classical parameter $\hbar = N^{-1/d}$ where d is the space dimension, we prove the convergence to the corresponding Thomas-Fermi model at positive temperature.

B.1 Introduction

In this article we study mean-field-type limits for a system of N fermions at temperature $T > 0$ in a fixed confining potential. We assume that the interaction has an intensity of the order $1/N$ and that there is an effective semi-classical parameter $\hbar = N^{-1/d}$ where d is the space dimension. In the limit $N \to \infty$ we obtain the nonlinear Thomas-Fermi problem at the same temperature $T > 0$. This paper is an extension of a recent work [18] by Fournais, Solovej and the first author where the case $T = 0$ was solved.

Physically, the Thomas-Fermi model is a rather crude approximation of quantum many-body systems in normal conditions, and it has to be refined in order to obtain a quantitative description of their equilibrium properties. However, certain physical systems in extreme conditions are rather well described by Thomas-Fermi theory.

It then becomes important to take into account the effect of the temperature. For instance, the positive-temperature Thomas-Fermi model has been thoroughly studied for very heavy atoms [17, 20, 30, 13, 53]. It has also played an important role in astrophysics, where the very high pressure encountered in the core of neutron stars and white dwarfs makes it valuable for all kinds of particles [48, 47, 12, 5]. Finally, the Thomas-Fermi model is also useful for ultracold dilute atomic Fermi gases, but the interaction often becomes negligible due to the Pauli principle, except in the presence of spin or of several interacting species [21].

In the regime considered in this paper, a mean-field scaling is coupled to a semi-classical limit. This creates some mathematical difficulties. Before [18], this limit has been rigorously considered at $T = 0$ for atoms by Lieb and Simon in [41, 40] and for pseudo-relativistic stars by Lieb, Thirring and Yau in [44, 45]. Upper and lower bounds on the next order correction have recently been derived in [26, 7], for particles evolving on the torus. The positive temperature Thomas-Fermi model was derived for confined gravitational systems in [29, 28, 50, 49, 51] and for atoms in [53]. There are several mathematical works on the time-dependent setting [52, 62, 4, 16, 1, 19, 10, 9, 6, 2, 54, 8, 22, 23, 15], in which the Schrödinger dynamics has been proved to converge to the time-dependent Vlasov equation in the limit $N \to \infty$. Finally, the first two terms in the expansion of the (free) energy of a Fermi gas with spin in the limit $\rho \to 0$ was provided in [39] at $T = 0$ and in [60] at $T > 0$.

The mean-field limit at positive temperature for fermions is completely different from the bosonic case. It was proved in [32] that in the similar mean-field regime for bosons, the leading order is the same at $T > 0$ as when $T = 0$. Only the next (Bogoliubov) correction depends on T [37]. In order to observe an effect of the temperature at the leading order of the bosonic free energy, one should take $T \sim N$, a completely different limit where nonlinear Gibbs measures arise [24, 33, 35, 36, 34, 57]. Without statistics (boltzons), the temperature does affect the leading order of the energy [31], and the same happens for fermions, as we will demonstrate.

Our method for studying the Fermi gas in the coupled mean-field/semi-classical limit relies on techniques previously introduced in [18]. Assuming that the interaction is positive-type ($\widehat{w} \geq 0$), the lower bound follows from using coherent states and inequalities on the entropy. We discuss later in Remark B.6 a conjectured inequality on the entropy of large fermionic systems which would imply the result for any interaction potential, not necessarily of positive-type. The upper bound is slightly more tedious. The idea is to construct a trial state with locally constant density in small boxes of side length much larger than $\hbar$, and to use the equivalence between the canonical and grand-canonical ensembles for the free Fermi gas. Finally, the convergence of states requires the tools recently introduced in [18] based on the classical de Finetti theorem for fermions.

The article is organized as follows. In the next section we introduce both the N-particle quantum Hamiltonian and the positive-temperature Thomas-Fermi theory which is obtained in the limit. We then state our main theorems, Theorem B.2 and

Theorem B.8. As an intermediate result for the upper bound, we show in Section B.3 how to approximate a classical density by an N body quantum state. In Section B.4, we use this trial state and some known results about the free Fermi gas at positive temperature to prove our main result in the non-interacting case. The interacting case is dealt with in Section B.5. Finally, in Section B.6 we study the Gibbs state and the minimizers of the Thomas-Fermi functional at positive temperature (Theorem B.1).

B.2 Models and main results

B.2.1 The Vlasov and Thomas-Fermi functionals at $T > 0$

For a given density $\rho > 0$ and an inverse temperature $\beta > 0$, the Vlasov functional at positive temperature is given by

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

where $s(t) = t \log t + (1-t) \log(1-t)$ is the fermionic entropy, and

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

is the spatial density of particles. Here m is a positive measure on the phase space $\mathbb{R}^d \times \mathbb{R}^d$, with the convention

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

and which is assumed to satisfy Pauli's principle $0 \leq m \leq 1$. For convenience we have added the factor $1/\rho$ in front of the interaction energy, because it will naturally arise in the mean-field limit. This dependence of the Vlasov functional is emphasized by adding the index ρ on $\mathcal{E}_{\text{Vla}}^{\beta,\rho}$, this density coincides with the mass constraint we impose on the semi-classical mesures even though it could be considered as independent. We denote the Vlasov minimum free energy by

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

Precise assumptions on A, V and w will be given later.

Similarly as in the case $T = 0$, we can rewrite the minimum as a two-step procedure where we first choose a density $\nu \in L^1(\mathbb{R}^d, \mathbb{R}_+)$ with $\int_{\mathbb{R}^d} \nu = \rho$ and minimize over all m such that $\rho_m = \nu$, before minimizing over ν. For any fixed constants $\nu \in \mathbb{R}_+$ and $A \in \mathbb{R}^d$ we can solve the problem at fixed x and obtain

$$\begin{aligned}\min_{\substack{0\le m(p)\le 1\\ (2\pi)^{-d}\int_{\mathbb{R}^d} m(p)\,\mathrm{d}p=\nu}} &\Big(\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}|p+A|^2 m(p)\,\mathrm{d}p + \frac{1}{(2\pi)^d\beta}\int_{\mathbb{R}^d} s(m(p))\,\mathrm{d}p\Big)\\ &= -\frac{1}{(2\pi)^d\beta}\int_{\mathbb{R}^d}\log\big(1+e^{-\beta(p^2-\mu_{\mathrm{FG}}(\beta,\nu))}\big)\,\mathrm{d}p + \mu_{\mathrm{FG}}(\beta,\nu)\nu\end{aligned}$$

where $\mu_{\mathrm{FG}}(\beta,\nu)$ is the unique solution to the implicit equation

$$\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\frac{1}{1+e^{\beta(p^2-\mu_{\mathrm{FG}}(\beta,\nu))}}\,\mathrm{d}p = \nu$$

and with the unique corresponding minimizer

$$m_{\nu,A}(p) = \frac{1}{1+e^{\beta(|p+A|^2-\mu_{\mathrm{FG}}(\beta,\nu))}}.$$

This is the uniform Fermi gas at density $\nu > 0$. For later purposes we introduce the free energy of the Fermi gas

$$F_\beta(\nu) := -\frac{1}{(2\pi)^d\beta}\int_{\mathbb{R}^d}\log\big(1+e^{-\beta(p^2-\mu_{\mathrm{FG}}(\beta,\nu))}\big)\,\mathrm{d}p + \mu_{\mathrm{FG}}(\beta,\nu)\nu. \tag{B.3}$$

Note that A only appears in the formula of the minimizer. It does not affect the value of the minimum $F_\beta(\nu)$.

All this allows us to reformulate the Vlasov minimization problem using only the density, leading to the Thomas-Fermi type minimization problem

$$\begin{aligned}e^\beta_{\mathrm{Vla}}(\rho) = \min_{\substack{\nu\in L^1(\mathbb{R}^d,\mathbb{R}_+)\\ \int_{\mathbb{R}^d}\nu(x)\,\mathrm{d}x=\rho}} \Big\{&\int_{\mathbb{R}^d} F_\beta(\nu(x))\,\mathrm{d}x + \int_{\mathbb{R}^d} V(x)\nu(x)\,\mathrm{d}x\\ &+\frac{1}{2\rho}\iint_{\mathbb{R}^{2d}} w(x-y)\nu(x)\nu(y)\,\mathrm{d}x\,\mathrm{d}y\Big\}.\end{aligned} \tag{B.4}$$

The Vlasov minimization (B.2) on phase space will be more tractable and we will almost never use the Thomas-Fermi formulation (B.4) of the problem.

Now we discuss the existence of a unique Vlasov minimizer for (B.2), under appropriate assumptions on V, A, w. We use everywhere the notation $V_\pm = \max(\pm V, 0)$ for the positive and negative parts of V, which are both positive functions by definition.

Theorem B.1 (Minimizers of the Vlasov functional). *Fix $\rho, \beta_0 > 0$. Suppose that $V_- \in L^{d/2}(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$, $A \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ and that $V_+ \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ satisfies $\int_{\mathbb{R}^d} e^{-\beta_0 V_+(x)}\,\mathrm{d}x < \infty$. Let*

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

Then, for all $\beta > \beta_0$, there are minimizers for the Vlasov problem (B.2)*. Any minimizer m_0 solves the nonlinear equation*

$$m_0(x,p) = \frac{1}{1+\exp\big(\beta(|p+A(x)|^2+V(x)+\rho^{-1}w*\rho_{m_0}(x)-\mu)\big)}, \tag{B.5}$$

for some Lagrange multiplier μ. The minimum can be expressed in terms of m_0 and μ as

$$\begin{aligned} e^{\beta}_{\rm Vla}(\rho) = &-\frac{1}{(2\pi)^d\beta}\iint_{\mathbb{R}^{2d}} \log\big(1+e^{-\beta(|p|^2+V(x)+\rho^{-1}w*\rho_{m_0}(x)-\mu)}\big)\,\mathrm{d}x\,\mathrm{d}p \\ &+\mu\rho-\frac{1}{2\rho}\iint_{\mathbb{R}^{2d}} w(x-y)\rho_{m_0}(x)\rho_{m_0}(y)\,\mathrm{d}x\,\mathrm{d}y. \end{aligned} \tag{B.6}$$

Furthermore, if $\widehat{w}\geq 0$, then $\mathcal{E}^{\beta,\rho}_{\rm Vla}$ is strictly convex and therefore has a unique minimizer. In this case, for $\rho'>0$ define

$$F^{\beta}_{\rm Vla}(\rho,\rho') := \inf_{\substack{0\leq m\leq 1\\ (2\pi)^{-d}\iint_{\mathbb{R}^{2d}} m=\rho}} \mathcal{E}^{\beta,\rho'}_{\rm Vla}(m). \tag{B.7}$$

Then, for any $\rho'>0$, $F^\beta_{\rm Vla}(\,\cdot\,,\rho')$ is C^1 on $\mathbb{R}_+$ and the multiplier appearing in (B.5) *is given by*

$$\mu = \frac{\partial F^\beta_{\rm Vla}}{\partial\rho}(\rho,\rho')\Big|_{\rho'=\rho} \tag{B.8}$$

We recall that, for $p\geq 1$, $f\in L^p(\mathbb{R}^3)+L^\infty_\varepsilon(\mathbb{R}^3)$ if and only if for all $\varepsilon>0$ we can write $f=f_1+f_2$ with $f_1\in L^p(\mathbb{R}^3)$ and $\|f_2\|_{L^\infty(\mathbb{R}^3)}\leq\varepsilon$. The proof of Theorem B.1 is classical and given for completeness in Section B.6. Note that the magnetic potential A has only a trivial effect on the minimization problem. The minimizers for a given A are exactly equal to the $m_0(x,p+A)$ with m_0 a minimizer for $A\equiv 0$. The value of the minimal energy, the density ρ_{m_0} and the Lagrange multiplier μ are unchanged under this transformation.

The two conditions $e^{-\beta V_+}\in L^1(\mathbb{R}^d)$ and $V_-\in L^{d/2}(\mathbb{R}^d)\cap L^{1+d/2}(\mathbb{R}^d)$ have been chosen to ensure that the minimizer has a finite total mass and a finite total energy. This is because

$$\begin{aligned} &\iint_{\mathbb{R}^{2d}} \frac{1}{1+e^{\beta(p^2+V_+(x)-V_-(x))}}\,\mathrm{d}x\,\mathrm{d}p \\ &\qquad\leq \iint_{\mathbb{R}^{2d}} \big(e^{-\beta(p^2/2+V_+(x))}+|\{p^2\leq 2V_-(x)\}|\big)\,\mathrm{d}x\,\mathrm{d}p \\ &\qquad\leq C\int_{\mathbb{R}^d}\big(\beta^{-\frac{d}{2}}e^{-\beta V_+(x)}+V_-(x)^{\frac{d}{2}}\big)\,\mathrm{d}x \end{aligned} \tag{B.9}$$

and, similarly,

$$\begin{aligned}
&\iint_{\mathbb{R}^{2d}} \log\big(1+e^{-\beta(p^2+V_+(x)-V_-(x))}\big)\,\mathrm{d}x\,\mathrm{d}p \\
&\qquad \le \iint_{\mathbb{R}^{2d}} e^{-\beta(p^2/2+V_+(x))}\,\mathrm{d}x\,\mathrm{d}p + C\iint_{\{p^2\le 2V_-(x)\}} (1+\beta V_-(x))\,\mathrm{d}x\,\mathrm{d}p \\
&\qquad \le C\int_{\mathbb{R}^d} \big(\beta^{-\frac{d}{2}}e^{-\beta V_+(x)} + V_-(x)^{\frac{d}{2}} + \beta V_-(x)^{1+\frac{d}{2}}\big)\,\mathrm{d}x.
\end{aligned}$$

B.2.2 The N-body Gibbs state and its limit

The aim of this paper is to understand the large–N limit of fermionic systems in a mean-field-type regime. We will end up with the Vlasov problem Eq. (B.1) introduced in the previous section.

The mean-field limit

Here we analyze the 'mean-field' limit where the interaction has a fixed range and a small intensity. We consider the following Hamiltonian

$$H_{N,\hbar} = \sum_{j=1}^{N} |i\hbar\nabla_{x_j} + A(x_j)|^2 + V(x_j) + \frac{1}{N}\sum_{1\le j<k\le N} w(x_j-x_k) \tag{B.10}$$

acting on the Hilbert space $\bigwedge_1^N L^2(\mathbb{R}^d)$ of anti-symmetric functions. For simplicity we neglect the spin variable. In the mean-field regime considered here, spin could be taken into account without changing the result (in the dilute limit considered later in section B.2.2 the presence of spin would affect the result). We suppose that

$$|A|^2, w \in L^{1+\frac{d}{2}}(\mathbb{R}^d) + L^\infty_\varepsilon(\mathbb{R}^d)$$

and that w is an even function. We also assume that the potential $V \in L^{1+d/2}_{\rm loc}(\mathbb{R}^d)$ is confining, that is, $V(x)\to\infty$ when $|x|\to\infty$, and that the divergence is so fast that $\int e^{-\beta_0 V_+(x)}\,\mathrm{d}x < \infty$ for some $\beta_0>0$. Note that this implies that V_- has a compact support, hence in particular $V_- \in L^{d/2}(\mathbb{R}^d)\cap L^{1+d/2}(\mathbb{R}^d)$. At inverse temperature $\beta>\beta_0$, the canonical free energy is given by the functional

$$\mathcal{E}^{N,\hbar}_{\rm Can}(\Gamma) = \mathrm{Tr}(H_{N,\hbar}\Gamma) + \frac{1}{\beta}\mathrm{Tr}(\Gamma\log\Gamma), \tag{B.11}$$

defined for all fermionic quantum states $\Gamma=\Gamma^*\ge 0$ with $\mathrm{Tr}(\Gamma)=1$. The minimum over all Γ is uniquely attained at the Gibbs state

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

where $Z = \operatorname{Tr} e^{-\beta H_{N,\hbar}}$, which leads to the minimum free energy

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

Our main result is the following.

Theorem B.2 (Mean-field limit). *Let $\beta_0, \rho > 0$. Assume that $V \in L^{1+d/2}_{\text{loc}}(\mathbb{R}^d)$ is such that $V(x) \to \infty$ at infinity and that $\int e^{-\beta_0 V_+(x)}\, \mathrm{d}x < \infty$. Furthermore, assume $|A|^2, w \in L^{1+d/2}(\mathbb{R}^d) + L^{\infty}_{\varepsilon}(\mathbb{R}^d)$ with w even and satisfying $\widehat{w} \geq 0$. Then, for all $\beta > \beta_0$ we have the convergence*

$$\lim_{\substack{N \to \infty \\ \hbar^d N \to \rho}} \hbar^d e^{\beta}_{\text{Can}}(\hbar, N) = e^{\beta}_{\text{Vla}}(\rho). \tag{B.12}$$

Moreover, if (Γ_N) is a sequence of approximate Gibbs states, that is, satisfying

$$\mathcal{E}^{N,\hbar}_{\text{Can}}(\Gamma_N) = e^{\beta}_{\text{Can}}(\hbar, N) + o(1), \tag{B.13}$$

then the one-particle density of Γ_N satisfies the following convergence

$$\hbar^d \rho^{(1)}_{\Gamma_N} \rightharpoonup \rho_{m_0} \qquad \textit{weakly in } L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d),$$

and

$$m^{(1)}_{f,\Gamma_N} \longrightarrow m_0 \qquad \textit{strongly in } L^1(\mathbb{R}^{2d}), \tag{B.14}$$

$$\rho_{m^{(1)}_{f,\Gamma_N}} \longrightarrow \rho_{m_0} \qquad \textit{strongly in } L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d), \tag{B.15}$$

where $m^{(k)}_{f,\Gamma_N}$ is the k-particle Husimi function of Γ_N and m_0 is the unique minimizer of the Vlasov functional in Eq. (B.5). The k-particle Husimi functions converge weakly in the sense that

$$\int_{\mathbb{R}^{2dk}} m^{(k)}_{f,\Gamma_N} \varphi \to \int_{\mathbb{R}^{2dk}} m_0^{\otimes k} \varphi \tag{B.16}$$

for all $\varphi \in L^1(\mathbb{R}^{2dk}) + L^{\infty}(\mathbb{R}^{2dk})$. Similarly, if we denote by $\mathcal{W}^{(k)}_{\Gamma_N}$ the k-particle Wigner measure of Γ_N, we also have,

$$\int_{\mathbb{R}^{2dk}} \mathcal{W}^{(k)}_{\Gamma_N} \varphi \to \int_{\mathbb{R}^{2dk}} m_0^{\otimes k} \varphi, \tag{B.17}$$

for all φ satisfying $\partial^{\alpha_1}_{x_1} \cdots \partial^{\alpha_k}_{x_k} \partial^{\beta_1}_{p_1} \cdots \partial^{\beta_k}_{p_k} \varphi \in L^{\infty}(\mathbb{R}^{2dk})$, where $\alpha_j, \beta_j \leq 1$ for all $1 \leq j \leq k$.

We have denoted by $\rho_\Gamma^{(1)}$ the one-particle density of the state Γ, which is the unique function such that

$$\mathrm{Tr}\Big(\sum_{j=1}^N F(x_j)\Big)\Gamma = \int_{\mathbb{R}^3} F(x)\rho_\Gamma^{(1)}(x)\,\mathrm{d}x.$$

for all bounded functions $F \in L^\infty(\mathbb{R}^3)$.

The Husimi function $m_{f,\Gamma_N}^{(k)}$ (based on a given shape function f) and the Wigner measure $\mathcal{W}_{\Gamma_N}^{(k)}$ are defined and studied at length in [18]. These are some natural semiclassical measures that can be associated with Γ_N in the k-particle phase space $\mathbb{R}^{2dk}$. We will recall their definition in the proof later in Section B.5.3.

Remark B.3. *For simplicity we work with a confining potential V but Theorems B.1 and B.2 hold the same when $\mathbb{R}^d$ is replaced by a bounded domain Ω with any boundary conditions.*

Remark B.4. *Our lower bound relies on the strong assumption that $\widehat{w} \geq 0$, but the upper bound does not. It is classical that a positive Fourier transform allows to easily bound the interaction from below by a one-body potential, see Eq.* (B.42) *below.*

Remark B.5. *As mentioned in* (B.13)*, we can handle approximate Gibbs states with a free energy close to the minimum with an error $o(1)$, although the energy is itself of order N. Our proof actually applies to the one-particle Husimi function under the weaker condition that $\mathcal{E}_{\rm Can}^{N,\hbar}(\Gamma_N) = e_{\rm Can}^{\beta}(\hbar, N) + o(N)$ but our argument does not easily generalize to higher order Husimi functions. Of course, for the exact quantum Gibbs state we have equality $\mathcal{E}_{\rm Can}^{N,\hbar}(\Gamma_{N,\hbar,\beta}) = e_{\rm Can}^{\beta}(\hbar, N)$.*

Remark B.6. *Without the assumption $\widehat{w} \geq 0$, the Vlasov functional $\mathcal{E}_{\rm Vla}^{\beta,\rho}$ can have several minimizers and the limit in Eq.* (B.16) *is believed to be an average over the set of minimizers of $\mathcal{E}_{\rm Vla}^{\beta,\rho}$. Namely there exists a so called de Finetti measure $\mathcal{P}$ [18], concentrated on the set $\mathcal{M}$ of minimizers for $e_{\rm Vla}^{\beta}$, such that*

$$m_{f,\Gamma_N}^{(k)} \rightharpoonup \int_{\mathcal{M}} m^{\otimes k}\,\mathrm{d}\mathcal{P}(m),$$

in the sense defined in Theorem B.2. We conjecture the following Fatou-type inequality on the entropy

$$\liminf_{\substack{N\to\infty \\ \hbar^d N \to \rho}} \hbar^d\,\mathrm{Tr}\,\Gamma_N \log \Gamma_N \geq \int_{\mathcal{M}} \Big(\int_{\mathbb{R}^{2d}} s(m)\Big)\,\mathrm{d}\mathcal{P}(m) \tag{B.18}$$

for general sequences (Γ_N) with de Finetti measure $\mathcal{P}$. Should this inequality be true, we could remove the assumption $\widehat{w} \geq 0$ in Theorem B.2. In fact, in our proof we show that the above inequality holds when the right-hand side is replaced by

$$\int_{\mathbb{R}^{2d}} s\Big(\int_{\mathcal{M}} m\,\mathrm{d}\mathcal{P}(m)\Big).$$

When there is a unique minimizer, the two coincide.

A completely different route for handling non positive-definite potentials would be to extend the method in [29, 28] where the (attractive) Newton potential was covered, using an approximation by a finite sum of rank-one interactions.

Example B.7 (Large atoms in a strong harmonic potential). The Hamiltonian in Eq. (B.10) can describe a large atom in a strong harmonic potential. Indeed, consider N electrons in a harmonic trap and interacting with a nucleus of charge Z. In the Born-Oppenheimer approximation, the N electrons are described by the Hamiltonian

$$\sum_{j=1}^{N} -\Delta_{x_j} + \omega^2|x_j|^2 - \frac{Z}{|x_j|} + \sum_{j<k} \frac{1}{|x_j - x_k|}.$$

Scaling length in the manner $x_j = N^{-1/3}x_j'$ we see that this Hamiltonian is unitarily equivalent to

$$N^{4/3}\left(\sum_{j=1}^{N} -N^{-\frac{2}{3}}\Delta_{x_j} + (\omega N^{-1})^2|x_j|^2 - \frac{ZN^{-1}}{|x_j|} + \frac{1}{N}\sum_{j<k} \frac{1}{|x_j - x_k|}\right).$$

Hence taking Z proportional to N and ω proportional to N, we obtain the Hamiltonian of Eq. (B.10) with $d = 3$, $A = 0$, $V(x) = |x|^2$ and $w(x) = |x|^{-1}$. In the limit we find the positive-temperature Thomas-Fermi model for an atom in a harmonic trap, which has stimulated many works in the Physics literature [17, 20, 30, 13]. This convergence has been proved for the first time by Narnhofer and Thirring in [53], but starting from the grand-canonical model instead of the canonical ensemble as we do here. This was generalized to strong magnetic fields in [27].

The dilute limit

In this section we deal with the case where the interaction potential has a range depending on N and tending to zero in our limit $N \to \infty$ with $\hbar^d N \to \rho$. This is classically taken into account by choosing the interaction in the form

$$w_N(x) := N^{d\eta}w(N^\eta x) \tag{B.19}$$

for a fixed w and a fixed parameter $\eta > 0$. In our confined system, the average distance between the particles is of order $N^{-1/d} \simeq \rho^{-1/d}\hbar$. The system is dilute when the particles interact rarely, that is, $\eta > 1/d$. For bosons in 3D, the limit involves the finite-range interaction $4\pi a\delta_0$ where $a = \int_{\mathbb{R}^d} w/(4\pi)$ for $\eta < 1$ and $a = a_s$, the s-wave scattering length a_s when $\eta = 1$. Due to the anti-symmetry the s-wave scattering length does not appear for fermions, except if there are several different species, e.g. with spin. This regime has been studied in [39] for the ground state and [60] at positive temperature, for the infinite translation-invariant gas. Here we extend these results to the confined case but do not consider any spin for shortness, hence we obtain a trivial limit. Our main result for dilute systems is the following.

Theorem B.8 (Dilute limit). *Let $\beta_0, \rho > 0$. We assume that $V \in L^{1+d/2}_{\mathrm{loc}}(\mathbb{R}^d)$ is such that $V(x) \to \infty$ at infinity and that $\int e^{-\beta_0 V_+(x)}\,\mathrm{d}x < \infty$. Furthermore, assume that $|A|^2 \in L^{1+d/2}(\mathbb{R}^d) + L^\infty_\varepsilon(\mathbb{R}^d)$ and $w \in L^1(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ is even.*

- *If $0 < \eta < 1/d$ and $\widehat{w} \geq 0$ then, for all $\beta > \beta_0$ we have*

$$\lim_{\substack{N\to\infty \\ \hbar^d N \to \rho}} \hbar^d e^{\beta}_{\mathrm{Can}}(\hbar, N) = e^{\beta, (\int_{\mathbb{R}^d} w)\delta_0}_{\mathrm{Vla}}(\rho)$$

  where $e^{\beta, (\int_{\mathbb{R}^d} w)\delta_0}_{\mathrm{Vla}}(\rho)$ is the minimum of the Vlasov energy with interaction potential $(\int_{\mathbb{R}^d} w)\delta_0$.

- *If $\eta > 1/d$, $d \geq 3$ and $w \geq 0$ is compactly supported, then for all $\beta > \beta_0$ we have*

$$\lim_{\substack{N\to\infty \\ \hbar^d N \to \rho}} \hbar^d e^{\beta}_{\mathrm{Can}}(\hbar, N) = e^{\beta, 0}_{\mathrm{Vla}}(\rho)$$

  where $e^{\beta, 0}_{\mathrm{Vla}}(\rho)$ is the minimum of the Vlasov energy without interaction potential.

In both cases, we have the same convergence of approximate Gibbs states as in Theorem B.2.

The proof of Theorem B.8 is given in Section B.5.

B.3 Construction of trial states

In this section we construct a trial state for the proof of the upper bound. In the dilute case this construction is similar to the one in [60] where the thermodynamic limit of non-zero spin interacting fermions were studied in the grand-canonical picture. This construction allows us to prove the following proposition.

Proposition B.9 (Trial states). *Let $\rho_0 \in C^\infty_c(\mathbb{R}^d)$ be such that $\int_{\mathbb{R}^d} \rho_0 = 1$. Assume $|A|^2 \in L^{1+d/2}(\mathbb{R}^d)$, $w \in L^1(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$. If $\eta d > 1$, we assume w to be compactly supported. Then, there is a sequence of states Γ_N on $\bigwedge_{i=1}^N L^2(\mathbb{R}^d)$ satisfying*

$$\hbar^d \Big(\mathrm{Tr} \sum_{i=1}^N (i\hbar\nabla + A)^2 \Gamma_N + \mathrm{Tr}\, \Gamma_N \log \Gamma_N \Big) \underset{\substack{N\to\infty \\ \hbar^d N \to 1}}{\longrightarrow} \int_{\mathbb{R}^d} F_\beta(\rho_0), \tag{B.20}$$

$$\Big\| \frac{1}{N} \rho^{(1)}_{\Gamma_N} - \rho_0 \Big\|_{L^1(\mathbb{R}^d)} \underset{\substack{N\to\infty \\ \hbar^d N \to 1}}{\longrightarrow} 0 \tag{B.21}$$

and

$$\frac{\hbar^d}{N}\int_{\mathbb{R}^{2d}} w_N(x-y)\rho^{(2)}_{\Gamma_N}(x,y)\,\mathrm{d}x\,\mathrm{d}y \underset{\substack{N\to\infty\\ \hbar^d N\to 1}}{\longrightarrow} \begin{cases} \int_{\mathbb{R}^d}(w*\rho_0)\rho_0 & \text{if } \eta=0\\ \left(\int_{\mathbb{R}^d} w\right)\int_{\mathbb{R}^d}\rho_0^2 & \text{if } 0<d\eta<1\\ 0 & \text{if } d\eta>1, d\geq 3.\end{cases} \tag{B.22}$$

Furthermore, we can take $\rho^{(1)}_{\Gamma_N}$ to be supported in a compact set which is independent of N and uniformly bounded in $L^\infty(\mathbb{R}^d)$ so that the convergence (B.21) holds in fact in all $L^p(\mathbb{R}^d)$ for $1\leq p<\infty$.

Proof. The proof consists in dividing the space into small cubes in which we take a correlated version of the minimizer for the free case (correlations are only needed for the case $d\eta>1$) and then do the thermodynamic limit in these cubes (or equivalently the limit where the effective Planck constant in front of the Laplacian tends to zero). This choice allows us to control the one-body density, which will be almost constant in these boxes. Without loss of generality, we will write the proof for $A=0$. The proof is the same for $A\neq 0$.

Step 1. Definition of the trial state

Let $\rho_0\in C^\infty_c(\mathbb{R}^d)$ and take $R>0$ such that $\operatorname{supp}\rho_0\subset[-R/2,R/2)^d=:C_R$. Divide C_R in small cubes of size $\ell>0$, $C_R\subset\bigcup_{z\in B(R\ell^{-1})\cap\mathbb{Z}^d}\Lambda_z$ with $\Lambda_z:=z\ell+[-\ell/2,\ell/2)^d$ and $B(R\ell^{-1})$ the ball centered at the origin with radius $R\ell^{-1}$. We will take later $1\gg\ell\gg\hbar$. For all z define $N_z:=\lfloor\hbar^d\ell^d\min_{x\in\Lambda_z}\rho_0(x)\rfloor$ so that $\sum_z N_z\leq N$. For $0<\varepsilon<\ell/4$ and for all z, define the box

$$\widetilde{\Lambda}_z:=z\ell+\Big[-\frac{\ell-\varepsilon}{2},\frac{\ell-\varepsilon}{2}\Big)^d\subset\Lambda_z$$

and denote by

$$\widetilde{\Gamma}_z=\frac{e^{-\beta(\sum_{i=1}^{N_z}-\hbar^2\Delta_i^{\rm per})}}{Z_z}=\sum_{k\in\mathcal{P}_{N_z}(\mathbb{Z}^d)}\lambda_k\,|e_{k_1}\wedge\cdots\wedge e_{k_{N_z}}\rangle\,\langle e_{k_1}\wedge\cdots\wedge e_{k_{N_z}}|$$

the canonical minimizer of the free energy at inverse temperature β of N_z free fermions in the box $\widetilde{\Lambda}_z$ with periodic boundary conditions, where $\mathcal{P}_n(E)$ denotes the set of all subsets of E with n elements. For $j\in\mathbb{Z}^d$,

$$e_j(x)=(\ell-\varepsilon)^{-d/2}e^{i\frac{2\pi}{\ell-\varepsilon}j\cdot x}$$

are the eigenfunctions of the periodic Laplacian in $\widetilde{\Lambda}_z$ and λ_k the eigenvalues of $\widetilde{\Gamma}_z$ associated with $e_k=e_{k_1}\wedge\cdots\wedge e_{k_{N_z}}$. Note that we omit the z dependence of λ_k and e_k. We now regularize these functions and construct a state in the slightly larger cube Λ_z with Dirichlet boundary condition. Let $\chi \in C^\infty(\mathbb{R}^d)$ such that $\chi \equiv 0$ in $\mathbb{R}^d \setminus B(0,1)$, $\chi \geq 0$ and $\int_{\mathbb{R}^d} \chi = 1$, denote $\chi_\varepsilon = \varepsilon^{-d}\chi(\varepsilon^{-1}\,\cdot\,)$ and define for $j \in \mathbb{Z}^d$

$$f_j := e_j \sqrt{\mathbb{1}_{\widetilde{\Lambda}_z} * \chi_\varepsilon}.$$

Note that

$$\begin{aligned}\int_{\Lambda_z} f_j \overline{f_k} &= \int e_j \overline{e_k}\,(\mathbb{1}_{\widetilde{\Lambda}_z} * \chi_\varepsilon) = \int \int_{\widetilde{\Lambda}_z} e_j(x)\overline{e_k}(x)\chi_\varepsilon(y-x)\,\mathrm{d}y\,\mathrm{d}x \\ &= \int_{\widetilde{\Lambda}_z} e_j \overline{e_k} \int_{\mathbb{R}^d} \chi = \delta_{j,k}.\end{aligned}$$

Hence the family $((_j)_j$ is still orthonormal and one can check that it satisfies $f_j \equiv e_j$ in $[-(\ell-2\varepsilon)/2, (\ell-2\varepsilon)/2)^d$ and as well as the Dirichlet boundary condition on Λ_z. Besides from having a state satisfying the Dirichlet boundary condition, we also want to add correlations in order to deal with the $d\eta > 1$ case. Let $\varphi \in C_c^\infty(\mathbb{R}^d)$ such that $\varphi \equiv 0$ in $B(0,1)$, $\varphi \equiv 1$ in $B(0,2)^c$ and $\varphi \leq 1$ almost everywhere and for $s > 0$ denote $\varphi_s = \varphi(s^{-1}\,\cdot\,)$. Following [60], we define the correlation function $F(x_1,\ldots,x_{N_z}) = \prod_{i<j}\varphi_s(x_i - x_j)$ and the state

$$\Gamma_z = \sum_{k \in \mathcal{P}_{N_z}(\mathbb{Z}^d)} \lambda_k Z_k^{-1} \left| F f_{k_1} \wedge \cdots \wedge f_{k_{N_z}} \right\rangle \left\langle F f_{k_1} \wedge \cdots \wedge f_{k_{N_z}} \right|,$$

where $Z_k = \|F f_{k_1} \wedge \cdots \wedge f_{k_{N_z}}\|^2_{L^2(\Lambda_z^{N_z})}$ are normalization factors. Now consider the state

$$\Gamma := \bigwedge_z \Gamma_z.$$

We will show that Γ satisfies the three limits Eq. (B.20), (B.21) and (B.22). This state does not have the exact number of particle N but satisfies $\sum_z N_z = N - \mathcal{O}(\ell N)$. Hence we will only have to correct the particle number by adding $\mathcal{O}(\ell N)$ uncorrelated particles of low energy, for instance outside the support of ρ_0. This will not modify the validity of the three limits. Now we focus on Γ and compute its free energy.

In the case $\eta d < 1$, we choose the following regime for the parameters introduced above.

$$s \ll \hbar \ll \varepsilon \ll \ell \ll N^{-\eta} \quad \text{and} \quad s\ell \ll \hbar^2.$$

One could in fact take $\Gamma_{F=1}$ (removing the factor F, see below) and remove the dependence in s. In the case $\eta d > 1$, the convergence holds in the regime

$$N^{-\eta} \ll s \ll \hbar \ll \varepsilon \ll \ell \quad \text{and} \quad s\ell \ll \hbar^2.$$

Step 2. Verification of (B.20)

We fix z and work in the cube Λ_z. Let us first compute the kinetic energy of the correlated Slater determinants appearing in the definition of Γ_z (note that this is not a eigenfunction decomposition due of the lack of orthogonality). Let us denote $X = (\sqrt{\mathbb{1}_{\widetilde{\Lambda}_z} * \chi_\varepsilon})^{\otimes N_z}$ so that $\Psi_k^z := f_{k_1} \wedge \cdots \wedge f_{k_{N_z}} = X e_{k_1} \wedge \cdots \wedge e_{k_{N_z}}$ (we will omit the superscript z when there is no ambiguity) and denote $\nabla, -\Delta$ the gradient and the Laplacian for all coordinates $x_1, \ldots, x_{N_z}$ in the box Λ_z with Dirichlet boundary condition, we can check that

$$\nabla(FXe_{k_1} \wedge \cdots \wedge e_{k_{N_z}}) = \Big(X\nabla F + F\nabla X + iFX\sum_{j=1}^{N_z}\frac{2\pi k_j}{\ell - \varepsilon}\Big)e_{k_1} \wedge \cdots \wedge e_{k_{N_z}}.$$

Hence,

$$\mathrm{Tr}(-\Delta)\Gamma_z = \sum_{k \in \mathcal{P}_{N_z}(\mathbb{Z}^d)} \frac{\lambda_k}{Z_k}\big(\epsilon_k + \|(X\nabla F + F\nabla X)e_{k_1} \wedge \cdots \wedge e_{k_{N_z}}\|^2_{L^2(\Lambda_z^{N_z})}\big)$$

where

$$\epsilon_k := \Big|2\pi(\ell-\varepsilon)^{-1}\sum_{j=1}^{N_z} k_j\Big|^2$$

is the eigenvalue of $-\Delta^{\mathrm{per}}$ associated with the eigenfunction e_k. Note that $\lambda_k \propto e^{-\beta\hbar^2\epsilon_k}$. We will show that $\sum_k \lambda_k Z_k^{-1}\epsilon_k \simeq \sum_k \lambda_k \epsilon_k = \mathrm{Tr}(-\Delta^{\mathrm{per}})\widetilde{\Gamma}$ and that the second summand above is an error term. For that we first need to estimate the normalization factors Z_k and then bound the factor with the ∇F and ∇X. We will use several times that for any sequence $0 < a_1, \ldots, a_p \leq 1$ we have

$$1 \geq \prod_{n=1}^{p}(1 - a_n) \geq 1 - \sum_{n=1}^{p} a_n. \tag{B.23}$$

Hence,

$$\begin{aligned}
Z_k &= \int_{\Lambda_z^{N_z}} \prod_{1 \leq n < m \leq N_z} \varphi_s(x_n - x_m)^2 |\Psi_k|^2 \,\mathrm{d}X \\
&\geq 1 - \int_{\Lambda_z^{N_z}} \sum_{1 \leq n < m \leq N_z} (1 - \varphi_s(x_n - x_m)^2)|\Psi_k|^2 \,\mathrm{d}X \\
&\geq 1 - \int_{\Lambda_z^2} (1 - \varphi_s(x_1 - x_2)^2)\rho^{(1)}_{\Psi_k}(x_1)\rho^{(1)}_{\Psi_k}(x_2)\,\mathrm{d}x_1\,\mathrm{d}x_2 \\
&\geq 1 - Cs^d\ell^d\hbar^{-2d},
\end{aligned} \tag{B.24}$$

where we used that $\rho^{(2)}_{\Psi_k}(x,y) \leq \rho^{(1)}_{\Psi_k}(x)\rho^{(1)}_{\Psi_k}(y)$ because Ψ_k is a Slater determinant, and that $\rho^{(1)}_{\Psi_k} = N_z\ell^{-d}\mathbb{1}_{\widetilde{\Lambda}_z} * \chi_\varepsilon \leq C\hbar^{-d}$.

Then we compute

$$|\nabla_{x_1}F|^2 = \sum_{\substack{m \neq n \\ m,n \geq 2}}^{N_z} \frac{\nabla\varphi_s(x_1 - x_m)\cdot\nabla\varphi_s(x_1 - x_n)}{\varphi_s(x_1 - x_m)\varphi_s(x_1 - x_m)}F^2 + \sum_{m \geq 2}^{N_z}\frac{|\nabla\varphi_s(x_1 - x_m)|^2}{\varphi_s(x_1 - x_m)^2}F^2$$

and obtain

$$
\begin{aligned}
&\|\nabla F\Psi_k\|^2_{L^2(\Lambda_z^{N_z})} \\
&\quad\leq C\int_{\Lambda_z^{3d}} |\nabla\varphi_s(x_1-x_2)||\nabla\varphi_s(x_1-x_3)|\rho^{(1)}_{\Psi_k}(x_1)\rho^{(1)}_{\Psi_k}(x_2)\rho^{(1)}_{\Psi_k}(x_3)\,\mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3 \\
&\qquad + C\int_{\Lambda_z^{2d}} |\nabla\varphi_s(x_1-x_2)|^2\rho^{(1)}_{\Psi_k}(x_1)\rho^{(1)}_{\Psi_k}(x_2)\,\mathrm{d}x_1\,\mathrm{d}x_2 \\
&\quad\leq Cs^{-2}(s^{2d}\ell^d\hbar^{-3d}+s^d\ell^d\hbar^{-2d}).
\end{aligned}
$$

Now we turn to the ∇X part. We have

$$
\nabla_{x_1}X(x_1,\ldots,x_{N_z}) = \frac{\nabla\sqrt{\mathbb{1}_{\widetilde{\Lambda}_z}*\chi_\varepsilon}(x_1)}{\sqrt{\mathbb{1}_{\widetilde{\Lambda}_z}*\chi_\varepsilon(x_1)}}X(x_1,\ldots,x_{N_z})
$$

and

$$
\begin{aligned}
\int_{\Lambda_z^{N_z}}|\nabla X|^2|e_{k_1}\wedge\cdots\wedge e_{k_{N_z}}|^2 &= \int_{\Lambda_z^{N_z}}\sum_{j=1}^{N_z}\left|\frac{\nabla\sqrt{\mathbb{1}_{\widetilde{\Lambda}_z}*\chi_\varepsilon}(x_1)}{\sqrt{\mathbb{1}_{\widetilde{\Lambda}_z}*\chi_\varepsilon(x_1)}}\right|^2|\Psi_k|^2 \\
&= \int_{\Lambda_z}\left|\frac{\nabla\sqrt{\mathbb{1}_{\widetilde{\Lambda}_z}*\chi_\varepsilon}(x_1)}{\sqrt{\mathbb{1}_{\widetilde{\Lambda}_z}*\chi_\varepsilon(x_1)}}\right|^2\rho^{(1)}_{\Psi_k} \\
&\leq C\int_{\Lambda_z}\left|\nabla\sqrt{\mathbb{1}_{\widetilde{\Lambda}_z}*\chi_\varepsilon}(x_1)\right|^2 N_z\ell^{-d} \\
&\leq CN_z\ell^{-d}\int_{\Lambda_z}\int|\nabla\sqrt{\chi_\varepsilon}|^2 \leq C\ell^d\hbar^{-d}\varepsilon^{-2},
\end{aligned}
$$

where we used the pointwise bound $|\nabla\sqrt{\mathbb{1}_{\widetilde{\Lambda}_z}*\chi_\varepsilon}(x_1)|^2\leq\int|\nabla\sqrt{\chi_\varepsilon}|^2$. Since X and F are both bounded by 1 we obtain

$$
\begin{aligned}
\operatorname{Tr}(-\Delta)\Gamma_z =\ & \operatorname{Tr}(-\Delta^{\mathrm{per}})\widetilde{\Gamma}_z \\
&+\mathcal{O}\Big(\frac{s^{2(d-1)}\ell^d\hbar^{-3d}+s^{d-2}\ell^d\hbar^{-2d}+\ell^d\hbar^{-d}\varepsilon^{-2}}{1-Cs^d\ell^d\hbar^{-2d}}+N_z^{1+2/d}s^d\ell^d\hbar^{-2d}\Big).
\end{aligned}
$$

We proceed with estimating the entropy of Γ_z. Thanks to [60, Lemma 2] we have

$$
\begin{aligned}
\operatorname{Tr}\Gamma_z\log\Gamma_z &\leq \operatorname{Tr}\widetilde{\Gamma}_z\log\widetilde{\Gamma}_z-\log\min_k Z_k \\
&= \operatorname{Tr}\widetilde{\Gamma}_z\log\widetilde{\Gamma}_z+\mathcal{O}(s^d\ell^d\hbar^{-2d}),
\end{aligned}
$$

where we used the estimate (B.24) on Z_k. Combining the last two estimates gives

$$\begin{aligned}
&\mathrm{Tr}(-\hbar^2\Delta)\Gamma + \mathrm{Tr}\,\Gamma\log\Gamma \\
&\quad = \sum_z \mathrm{Tr}(-\hbar^2\Delta)\Gamma_z + \mathrm{Tr}\,\Gamma\log\Gamma_z \\
&\quad \leq \sum_z e^{\beta,\mathrm{per}}_{\mathrm{Can}}(\widetilde{\Lambda}_z,\hbar,N_z) + \ell^{-d}\mathcal{O}(s^d\ell^d\hbar^{-2d}) + \mathcal{O}((\hbar^{-d}\ell^d)^{1+2/d}s^d\ell^d\hbar^{-2d}) \\
&\qquad + \hbar^2\ell^{-d}\mathcal{O}\Big(\frac{s^{2(d-1)}\ell^d\hbar^{-3d} + s^{d-2}\ell^d\hbar^{-2d} + \ell^d\hbar^{-d}\varepsilon^{-2}}{1 - Cs^d\ell^d\hbar^{-2d}}\Big),
\end{aligned}$$

where we used that $N_z \leq \|\rho_0\|_{L^\infty(\mathbb{R}^d)}\hbar^{-d}\ell^d$. It is a known fact [56, Proposition 2.1.3], [58, Part 3.4] (see also [46, 64] for more details) that

$$e^{\beta,\mathrm{per}}_{\mathrm{Can}}(\widetilde{\Lambda}_z,\hbar,N_z) = \hbar^{-d}\ell^d F_\beta(N_z/(\hbar^{-d}\ell^d)) + o(\hbar^{-d}\ell^d) \tag{B.25}$$

locally uniformly in $\rho_z := N_z\hbar^d\ell^{-d}$ as $\hbar \to 0$ under the condition $\hbar \ll \ell$. This is the thermodynamic limit of the free Fermi gas. By the continuity of F_β and the estimate $N_z/(\hbar^{-d}(\ell-\varepsilon)^d) = \rho(z) + \mathcal{O}(\varepsilon\ell^{-1})$ we obtain

$$\begin{aligned}
\hbar^d(\mathrm{Tr}(-\hbar^2\Delta)\Gamma + \mathrm{Tr}\,\Gamma\log\Gamma) &\leq \ell^d\sum_{z\in\mathbb{Z}^d} F_\beta(\rho(z)) + o(1) + \mathcal{O}(\varepsilon/\ell) \\
&\quad + \mathcal{O}((s\ell/\hbar^2)^d\ell^2) + \mathcal{O}(s/\hbar)^d + \mathcal{O}\Big(\frac{(s/\hbar)^{2(d-1)} + (s/\hbar)^{d-2} + (\hbar/\varepsilon)^2}{1 - C(s\ell/\hbar^2)^d}\Big).
\end{aligned}$$

If $s \ll \hbar \ll \varepsilon \ll \ell$ with the extra condition that $s\ell \ll \hbar^2$ we obtain the upper bound in (B.20) by passing to the limit and by identifying the first term above as a Riemann sum. The lower bound is obtained in the same fashion by seeing Γ_z as a trial state for the periodic case.

Step 3. Verification of (B.21)

Let us recall that $\Gamma_{F=1}$ is the uncorrelated version of the trial state (which corresponds to taking $\varphi \equiv 1$) and that we denote by $\rho^{(k)}_{F=1}$ its k-particle density, for $k \geq 1$. From (B.23) and using that $\Gamma_{F=1}$ is a sum of Slater determinants we have

$$\begin{aligned}
&N^{-1}\|\rho^{(1)}_\Gamma - \rho^{(1)}_{F=1}\|_{L^1(\mathbb{R}^d)} \\
&\quad \leq N^{-1}\sum_{z\in\mathbb{Z}^d}\sum_{k\in\mathcal{P}_{N_z}(\mathbb{Z}^d)} \lambda^z_k \iint_{\mathbb{R}^{2d}} (1-\varphi_s(x_1-x_2)^2)\rho^{(2)}_{\Psi^z_k}(x_1,x_2)\,\mathrm{d}x_1\,\mathrm{d}x_2 \\
&\quad \leq CN^{-1}\sum_{z\in\mathbb{Z}^d}\iint_{\Lambda_z^2}(1-\varphi_s(x_1-x_2)^2)N_z^2\ell^{-2d}\,\mathrm{d}x_1\,\mathrm{d}x_2 \\
&\quad \leq CN^{-1}\sum_{z\in\mathbb{Z}^d} s^d\ell^d N_z^2\ell^{-2d} \\
&\quad \leq C(s/\hbar)^d.
\end{aligned}$$

We also used that $\rho^{(2)}_{\Psi^z_k} \leq \rho^{(1)}_{\Psi^z_k} \otimes \rho^{(1)}_{\Psi^z_k} \leq \|\rho_0\|_{L^\infty(\mathbb{R}^d)} N_z^2 \ell^{-2d}$. Finally, denoting by $\Gamma_{z,F=1}$ the uncorrelated version of Γ_z and by $\rho^{(1)}_{z,F=1}$ its one-body density we have

$$\begin{aligned}\|N^{-1}\rho^{(1)}_{F=1} - \rho_0\|_{L^1(\mathbb{R}^d)} &\leq \sum_z \|N^{-1}\rho^{(1)}_{z,F=1} - \rho_0 \mathbb{1}_{\Lambda_z}\|_{L^1(\mathbb{R}^d)} \\ &\leq C\sum_z (\|\nabla\rho_0\|_{L^\infty(\mathbb{R}^d)} \ell^{d+1} + \|\rho_0\|_{L^\infty(\mathbb{R}^d)}\ell^{d-1}\varepsilon) \\ &\leq C(\ell + \varepsilon/\ell).\end{aligned}$$

We have used that in $z\ell + [-(\ell-2\varepsilon)/2, (\ell-2\varepsilon)/2)^d$,

$$N^{-1}\rho^{(1)}_{z,F=1} = N^{-1}\ell^{-d}\lfloor \hbar^{-d}\ell^d \min_{\Lambda_z}\rho_0 \rfloor = \rho_0 + \mathcal{O}(\hbar^d\ell^d) + \mathcal{O}(\|\nabla\rho_0\|_{L^\infty(\mathbb{R}^d)}\ell)$$

and that

$$\|N^{-1}\rho^{(1)}_{z,F=1} - \rho_0\mathbb{1}_{\Lambda_z}\|_{L^\infty(\Lambda_z)} \leq C\|\rho_0\|_{L^\infty(\mathbb{R}^d)}.$$

Under the stated conditions on $\hbar, \ell, s$ and ε we have $N^{-1}\rho^{(1)}_\Gamma \to \rho_0$ in $L^1(\mathbb{R}^d)$.

Step 4. Verification of (B.22)

Let us first turn to the case $0 \leq \eta d < 1$. Note that the two-particle density matrices satisfy

$$\begin{aligned}\Gamma^{(2)} &= \sum_{z\in\mathbb{Z}^d} \Gamma^{(2)}_z + \sum_{z\neq z'} \Gamma^{(1)}_z \otimes \Gamma^{(1)}_{z'} \\ &= \Gamma^{(1)} \otimes \Gamma^{(1)} + \sum_{z\in\mathbb{Z}^d} \Gamma^{(2)}_z - \Gamma^{(1)}_z \otimes \Gamma^{(1)}_z.\end{aligned} \tag{B.26}$$

In particular we obtain for the two-particle reduced density

$$\rho^{(2)}_\Gamma = \rho^{(1)}_\Gamma \otimes \rho^{(1)}_\Gamma + \sum_{z\in\mathbb{Z}^d} \rho^{(2)}_{\Gamma_z} - \rho^{(1)}_{\Gamma_z} \otimes \rho^{(1)}_{\Gamma_z}. \tag{B.27}$$

The second term above is negligible in our regime. Indeed, using the triangle inequality, the Lieb-Thirring inequality [42, 43] (the reader can refer to [18, Lem. 3.4] for the exact version of the LT inequality we use) and Young's inequality we obtain

$$\begin{aligned}&N^{-2}\Big|\sum_{z\in\mathbb{Z}^d}\int_{\mathbb{R}^d} w_N(x-y)\big(\rho^{(2)}_{\Gamma_z} - \rho^{(1)}_{\Gamma_z}\otimes\rho^{(1)}_{\Gamma_z}\big)\Big| \\ &\quad\leq CN^{-2}\|w_N\|_{L^{1+d/2}(\mathbb{R}^d)} \sum_{z\in\mathbb{Z}^d}\Bigg\{\|\rho^{(1)}_{\Gamma_z}\|_{L^{1+2/d}(\mathbb{R}^d)}\|\rho^{(1)}_{\Gamma_z}\|_{L^1(\mathbb{R}^d)} \\ &\qquad\qquad + N_z^2\left(\frac{\operatorname{Tr}\Gamma_z(\sum_{j=1}^{N_z} -\Delta_{z_j})}{N_z^{1+2/d}}\right)^{\frac{1}{1+2/d}}\Bigg\} \\ &\quad\leq CN^{-2}N^{d\eta\frac{d}{d+2}}\sum_{z\in\mathbb{Z}^d} N_z^2 \ell^{-\frac{2}{1+2/d}} \\ &\quad\leq C(N^\eta\ell)^d \ell^{d(1-\frac{1}{d+2})}\end{aligned}$$

where we used that $\rho^{(1)}_{\Gamma_z} \leq CN_z\ell^{-d} \leq C\|\rho_0\|_{L^\infty(\mathbb{R}^d)}\hbar^{-d}$ almost everywhere and the estimate on the kinetic energy of Γ_z computed before. Hence, if $N^{-1}\rho^{(1)}_\Gamma \to \rho_0$ in $L^1(\mathbb{R}^d)$ and if $\ell = o(N^{-\eta})$, since both $N^{-1}\rho^{(1)}_\Gamma$ and ρ_0 are bounded (uniformly in N) in $L^\infty(\mathbb{R}^d)$, by (B.27) and the use of Young's inequality we obtain (B.22) for $0 \leq \eta d < 1$.

The case $\eta d > 1$ is easier to handle since in this case $N^{-\eta} = o(s)$. Indeed, due to the correlation factor F and because w is compactly supported we will have $\operatorname{Tr} w_N(x-y)\Gamma = 0$ for N sufficiently large. □

B.4 Proof of Theorem B.2 in the non-interacting case $w \equiv 0$

In this section we prove the convergence (B.12) of the free energy in Theorem B.2 in the case where the interaction is dropped, that is $w \equiv 0$. We study the interacting case later in Section B.5. The convergence of states will be discussed in Section B.5.3.

The non-interacting case is well understood since the Hamiltonian is quadratic in creation and annihilation operators in the grand canonical picture. The minimizers are known to be the so-called quasi-free states [3]. For those we have an explicit formula and the argument of the proof is reduced to a usual semi-classical limit. The upper bound on the free energy is a consequence of Proposition B.9 from the previous section. The proof of the lower bound relies on localization and the use of coherent states.

We start with the following well-known lemma, the proof of which can for instance rely on Klein's inequality and the convexity of the fermionic entropy s [63].

Lemma B.10 (The minimal free energy of quasi-free states). *Let $\beta > 0$, and let H be a self-adjoint operator on a Hilbert space $\mathfrak{H}$ such that $\operatorname{Tr} e^{-\beta H} < \infty$. Then*

$$\min_{\substack{0\leq\gamma\leq 1\\ \gamma\in\mathfrak{S}_1(\mathfrak{H})}} \left(\operatorname{Tr} H\gamma + \frac{1}{\beta}\operatorname{Tr} s(\gamma)\right) = -\frac{1}{\beta}\operatorname{Tr}\log(1+e^{-\beta H}),$$

with the unique minimizer being $\gamma_0 = \frac{1}{1+e^{\beta H}}$.

With Lemma B.10 at hand we are able to provide the

Proof of Theorem B.2 in the non-interacting case.. Suppose that $w = 0$. We start out by proving the upper bound on the energy, using the trial states constructed in the previous section. Let $\rho > 0$ and $0 \leq \nu \in C^\infty_c(\mathbb{R}^d)$ with $\int_{\mathbb{R}^d}\nu(x)\,\mathrm{d}x = \rho$. By Proposition B.9 we then have a sequence (Γ_N) of canonical N-particle states satisfying

$$\hbar^d \operatorname{Tr}\Big(\sum_{j=1}^N |i\hbar\nabla_{x_j} + A(x_j)|^2\Gamma_N\Big) + \frac{\hbar^d}{\beta}\operatorname{Tr}\Gamma_N\log\Gamma_N \to \int_{\mathbb{R}^d} F_\beta(\nu(x))\,\mathrm{d}x.$$

The one-particle densities $\hbar^d \rho^{(1)}_{\Gamma_N}$ converge to ν strongly in $L^1(\mathbb{R}^d)$ and are uniformly bounded in $L^\infty(\mathbb{R}^d)$. Hence they converge strongly in all $L^p(\mathbb{R}^d)$ for $p \in [1,\infty)$. Since $V \in L^{1+d/2}_{\mathrm{loc}}(\mathbb{R}^d)$ and $\rho^{(1)}_{\Gamma_N}$ are, by construction, supported in a fixed compact set, we have

$$\hbar^d \operatorname{Tr} V(x)\Gamma_N^{(1)} = \hbar^d \int_{\mathbb{R}^d} V(x)\rho^{(1)}_{\Gamma_N}(x)\,\mathrm{d}x \to \int_{\mathbb{R}^d} V(x)\nu(x)\,\mathrm{d}x.$$

This means that

$$\hbar^d e^\beta_{\mathrm{Can}}(\hbar, N) \leq \hbar^d \mathcal{E}^{N,\hbar}_{\mathrm{Can}}(\Gamma_N) \to \int_{\mathbb{R}^d} F_\beta(\nu(x))\,\mathrm{d}x + \int_{\mathbb{R}^d} V(x)\nu(x)\,\mathrm{d}x,$$

and, since ν is arbitrary, we have shown that

$$\limsup_{\substack{N\to\infty \\ \hbar^d N \to \rho}} \hbar^d e^\beta_{\mathrm{Can}}(\hbar, N) \leq e^\beta_{\mathrm{Vla}}(\rho).$$

To prove the lower bound, we use the following bound [3, 63] on the entropy

$$\operatorname{Tr}\Gamma\log\Gamma \geq \operatorname{Tr}(\Gamma^{(1)}\log\Gamma^{(1)} + (1-\Gamma^{(1)})\log(1-\Gamma^{(1)})) = \operatorname{Tr} s(\Gamma^{(1)})$$

which follows from the fact that quasi-free states maximize the entropy at given one-particle density matrix $\Gamma^{(1)}$. The bound applies to any N-particle state Γ whose one-particle density is $\Gamma^{(1)}$. Applying Lemma B.10 above, we have for any $\mu \in \mathbb{R}$ and any N-body state Γ

$$\begin{aligned}\mathcal{E}^{N,\hbar}_{\mathrm{Can}}(\Gamma) &\geq \operatorname{Tr}(|i\hbar\nabla + A(x)|^2 + V(x) - \mu)\Gamma^{(1)} + \frac{1}{\beta}\operatorname{Tr} s(\Gamma^{(1)}) + \mu N \\ &\geq -\frac{1}{\beta}\operatorname{Tr}\log\big(1 + e^{-\beta(|i\hbar\nabla + A(x)|^2 + V(x) - \mu)}\big) + \mu N.\end{aligned}$$

Thus, we are left to using the known semi-classical convergence (whose proof is recalled below in Proposition B.11)

$$\begin{aligned}\liminf_{\hbar\to 0} -\frac{\hbar^d}{\beta}&\operatorname{Tr}\log\big(1 + e^{-\beta(|i\hbar\nabla + A(x)|^2 + V(x) - \mu)}\big) \\ &\geq -\frac{1}{(2\pi)^d\beta}\iint_{\mathbb{R}^{2d}} \log\big(1 + e^{-\beta(p^2 + V(x) - \mu)}\big)\,\mathrm{d}x\,\mathrm{d}p,\end{aligned} \tag{B.28}$$

and to take $\mu = \mu_{\mathrm{Vla}}(\rho)$. Recognizing the expression of the Vlasov free energy on the right-hand side we appeal to Theorem B.1 and immediately obtain

$$\liminf_{\substack{N\to\infty \\ \hbar^d N \to \rho}} \hbar^d e^\beta_{\mathrm{Can}}(\hbar, N) \geq e^\beta_{\mathrm{Vla}}(\rho),$$

concluding the proof of (B.12) in the non-interacting case. □

In (B.28) we have used the following well-known fact, which we prove for completeness.

Proposition B.11 (Semi-classical limit). *Let $\beta_0 > 0$, we assume that $|A|^2 \in L^{1+d/2}(\mathbb{R}^d) + L^\infty_\varepsilon(\mathbb{R}^d)$, $V \in L^{1+d/2}_{\rm loc}(\mathbb{R}^d)$ is such that $V(x) \to \infty$ at infinity and that $\int e^{-\beta_0 V_+(x)}\,\mathrm{d}x < \infty$. Then for any chemical potential $\mu \in \mathbb{R}$ and all $\beta > \beta_0$,*

$$\limsup_{\hbar\to 0} \frac{\hbar^d}{\beta} \operatorname{Tr}\log\big(1 + e^{-\beta((|i\hbar\nabla + A|^2 + V - \mu)}\big) \\ \leq \frac{1}{(2\pi)^d\beta} \iint_{\mathbb{R}^{2d}} \log\big(1 + e^{-\beta(p^2 + V(x) - \mu)}\big)\,\mathrm{d}x\,\mathrm{d}p. \tag{B.29}$$

This result is known [63] and the proof we provide here is essentially the one in [61], where however the von Neumann entropy $x\log(x)$ was used instead of the Fermi-Dirac entropy $x\log(x) + (1-x)\log(1-x)$. In fact, Theorem B.2 shows that the inequality (B.29) is indeed an equality.

Proof of Proposition B.11. Without loss of generality we may assume that $\mu = 0$. We also assume in a first step that $V_- \in L^\infty(\mathbb{R}^d)$ and then remove this assumption at the end of the proof. Due to technical issues involving the potential V, we need to localize the minimization problem on some bounded set. Let $\chi, \eta \in C^\infty(\mathbb{R}^d)$ satisfy $\chi^2 + \eta^2 = 1$, $\operatorname{supp}\chi \subseteq B(0,1)$ and $\operatorname{supp}\eta \subseteq B(0,\frac{1}{2})^c$. For $R > 0$, denote $\chi_R = \chi(\frac{\cdot}{R})$ and $\eta_R = \eta(\frac{\cdot}{R})$. Let $H_\hbar = |i\hbar\nabla + A|^2 + V$ and take $\gamma^\hbar = \frac{1}{1+e^{\beta H_\hbar}}$ as in Lemma B.10. By the IMS localization formula we have

$$\operatorname{Tr} H_\hbar\gamma^\hbar = \operatorname{Tr}(H_\hbar\chi_R\gamma^\hbar\chi_R) + \operatorname{Tr}(H_\hbar\eta_R\gamma^\hbar\eta_R) - \hbar^2\operatorname{Tr}(|\nabla\chi_R|^2 + |\nabla\eta_R|^2)\gamma^\hbar, \tag{B.30}$$

and using the convexity of s and [11, Theorem 14],

$$\operatorname{Tr} s(\gamma^\hbar) = \operatorname{Tr}\chi_R s(\gamma^\hbar)\chi_R + \operatorname{Tr}\eta_R s(\gamma^\hbar)\eta_R \\ \geq \operatorname{Tr} s(\chi_R\gamma^\hbar\chi_R) + \operatorname{Tr} s(\eta_R\gamma^\hbar\eta_R). \tag{B.31}$$

We first deal with the localization outside the ball. The operators we consider in $B(0,\frac{R}{2})^c$ are the ones with Dirichlet boundary condition. We obtain by Lemma B.10 that the remainder terms are bounded by

$$\begin{aligned}
&\operatorname{Tr}(H_\hbar\eta_R\gamma^\hbar\eta_R) + \frac{1}{\beta}\operatorname{Tr} s(\eta_R\gamma^\hbar\eta_R) \\
&\qquad \geq -\frac{1}{\beta}\operatorname{Tr}_{L^2(B(0,\frac{R}{2})^c)}\log\big(1 + e^{-\beta(|i\hbar\nabla + A|^2 + V - C)}\big) \\
&\qquad \geq -\frac{C}{\beta}\operatorname{Tr}_{L^2(B(0,\frac{R}{2})^c)} e^{-\beta((i\hbar\nabla + A)^2 + V)} \\
&\qquad \geq -\frac{C}{\beta}\operatorname{Tr}_{L^2(B(0,\frac{R}{2})^c)} e^{-\beta(-\hbar^2\Delta^D + V)} && \text{(B.32)} \\
&\qquad \geq -\frac{C}{\beta}\operatorname{Tr}_{L^2(\mathbb{R}^d)} e^{-\beta(-\hbar^2\Delta + (1-\alpha)V + \alpha\inf_{B(0,R)^c} V)} && \text{(B.33)} \\
&\qquad \geq -\frac{Ce^{-\beta\alpha\inf_{B(0,R)^c} V}}{(2\pi\hbar)^d}\iint_{\mathbb{R}^{2d}} e^{-\beta(p^2 + (1-\alpha)V(x))}\,\mathrm{d}x\,\mathrm{d}p, && \text{(B.34)}
\end{aligned}$$

where $\alpha > 0$ is such that $\beta(1-\alpha) > \beta_0$. The inequality (B.32) comes from the diamagnetic inequality [14] and (B.33) is obtained by the min-max characterization of the eigenvalues. The last inequality follows from Golden-Thompson's formula [55, Theorem VIII.30].

The error term in the IMS formula can be estimated by

$$\begin{aligned} -\operatorname{Tr}(|\nabla\chi_R|^2+|\nabla\eta_R|^2)\gamma^\hbar &\geq -\frac{C}{R}\operatorname{Tr}\gamma^\hbar \geq -\frac{C}{R}\operatorname{Tr}e^{-\beta H_\hbar} \\ &\geq -\frac{C}{R(2\pi\hbar)^d}\iint_{\mathbb{R}^{2d}} e^{-\beta(p^2+V(x))}\,\mathrm{d}x\,\mathrm{d}p, \end{aligned} \tag{B.35}$$

where we used again the diamagnetic and Golden-Thompson inequalities.

Next we derive a bound on the densities $\rho_{\gamma_R^\hbar}$, where $\gamma_R^\hbar = \chi_R\gamma^\hbar\chi_R$, using the Lieb-Thirring inequality [42, 43]. Combining (B.30), (B.31), (B.34) and (B.35) we have shown

$$\begin{aligned} \operatorname{Tr}H_\hbar\gamma_R^\hbar + \frac{1}{\beta}\operatorname{Tr}s(\gamma_R^\hbar) - \frac{\varepsilon(R)}{\hbar^d} &\leq \operatorname{Tr}H_\hbar\gamma^\hbar + \frac{1}{\beta}\operatorname{Tr}s(\gamma^\hbar) \\ &= -\frac{1}{\beta}\operatorname{Tr}\log(1+e^{-\beta H_\hbar}) \leq 0 \end{aligned} \tag{B.36}$$

where $\varepsilon(R)\to 0$ when $R\to\infty$. By Lemma B.10 we have

$$\begin{aligned} &\operatorname{Tr}H_\hbar\gamma_R^\hbar + \frac{1}{\beta}\operatorname{Tr}s(\gamma_R^\hbar) \\ &\qquad \geq \frac{1}{2}\operatorname{Tr}(-\hbar^2\Delta)\gamma_R^\hbar - \frac{1}{\beta}\operatorname{Tr}\log\big(1+e^{-\beta(|i\hbar\nabla+A|^2/2+V)}\big) - \frac{C}{\hbar^d} \end{aligned}$$

where, as in (B.34),

$$\operatorname{Tr}\log\big(1+e^{-\beta(|i\hbar\nabla+A|^2/2+V)}\big) \leq \frac{Ce^{-\alpha\beta\inf V}}{(2\pi\hbar)^d}\iint_{\mathbb{R}^{2d}} e^{-\beta(p^2/2+(1-\alpha)V(x))}\,\mathrm{d}x\,\mathrm{d}p.$$

This implies the following bound on the kinetic energy

$$\operatorname{Tr}(-\hbar^2\Delta)\gamma_R^\hbar \leq \frac{C}{\hbar^d}. \tag{B.37}$$

By the Lieb-Thirring inequality [18, Lem. 3.4], we obtain

$$\int_{\mathbb{R}^d}\rho_{\gamma_R^\hbar}(x)^{1+\frac{2}{d}}\,\mathrm{d}x \leq C\operatorname{Tr}(-\Delta\gamma_R^\hbar) \leq \frac{1}{\hbar^{d+2}}C. \tag{B.38}$$

We return to the estimate on the localized terms in (B.30) and (B.31), using coherent states. Let $f\in C_c^\infty(\mathbb{R}^d)$ be a real-valued and even function, and consider the coherent state $f_{x,p}^\hbar(y) = \hbar^{-d/4}f(\hbar^{-1/2}(y-x))e^{i\frac{p\cdot y}{\hbar}}$. The projections $|f_{x,p}^\hbar\rangle\langle f_{x,p}^\hbar|$ give rise to a resolution of the identity on $L^2(\mathbb{R}^d)$:

$$\frac{1}{(2\pi\hbar)^d}\int_{\mathbb{R}^{2d}}|f_{x,p}^\hbar\rangle\langle f_{x,p}^\hbar| = \mathrm{Id}_{L^2(\mathbb{R}^d)}. \tag{B.39}$$

Using this in combination with Jensen's inequality and the spectral theorem, we obtain

$$\begin{aligned} \operatorname{Tr} s(\chi_R \gamma^\hbar \chi_R) &= \frac{1}{(2\pi\hbar)^d} \iint_{\mathbb{R}^{2d}} \langle f^\hbar_{x,p}, s(\gamma^\hbar_R) f^\hbar_{x,p} \rangle \, \mathrm{d}x \, \mathrm{d}p \\ &\geq \frac{1}{(2\pi\hbar)^d} \iint_{\mathbb{R}^{2d}} s\big(\langle f^\hbar_{x,p}, \gamma^\hbar_R f^\hbar_{x,p} \rangle\big) \, \mathrm{d}x \, \mathrm{d}p. \end{aligned} \tag{B.40}$$

On the other hand, applying [18, Corollary 2.5] we have

$$\begin{aligned} \operatorname{Tr} H_\hbar \chi_R \gamma^\hbar \chi_R &= \frac{1}{(2\pi\hbar)^d} \iint_{\mathbb{R}^{2d}} \langle f^\hbar_{x,p}, H_\hbar \gamma^\hbar_R f^\hbar_{x,p} \rangle \, \mathrm{d}x \, \mathrm{d}p \\ &= \frac{1}{(2\pi\hbar)^d} \iint_{\mathbb{R}^{2d}} (|p + A|^2 + V(x)) \langle f^\hbar_{x,p}, \gamma^\hbar_R f^\hbar_{x,p} \rangle \, \mathrm{d}x \, \mathrm{d}p \\ &\quad + \int_{\mathbb{R}^d} \rho_{\gamma^\hbar_R} (A^2 - A^2 * |f^\hbar|^2) - 2\Re \operatorname{Tr}(A - A * |f^\hbar|^2) \cdot i\hbar\nabla\gamma^\hbar_R \\ &\quad - \hbar \int_{\mathbb{R}^d} |\nabla f|^2 + \int_{\mathbb{R}^d} \rho_{\gamma^\hbar_R} (V - V * |f^\hbar|^2) \end{aligned} \tag{B.41}$$

Since $\hbar^d \rho_{\gamma^\hbar_R}$ is supported in $B(0,R)$ and is uniformly bounded in $L^{1+2/d}(\mathbb{R}^d)$ by (B.38), and $V * |f^\hbar|^2$ converges to V locally in $L^{1+d/2}(\mathbb{R}^d)$. The same argument applied to A and $|A|^2$ combined with Hölder's inequality, the Lieb-Thirring inequality and (B.37) shows that the remainder terms above are $o(\hbar^{-d})$. At last, combining (B.36), (B.40) and (B.41) as well as a simple adaptation of Proposition B.16 to finite domains (Remark B.17) yields

$$\begin{aligned} &\limsup_{\hbar \to 0} \hbar^d \operatorname{Tr} \log\big(1 + e^{-\beta(|i\hbar\nabla + A|^2 + V)}\big) \\ &\qquad \leq \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} \log\big(1 + e^{-\beta(p^2 + V(x))}\big) \, \mathrm{d}x \, \mathrm{d}p + \varepsilon(R), \end{aligned}$$

where $\varepsilon(R) \to 0$ when $R \to \infty$. This concludes the proof in the case $V_- \in L^\infty(\mathbb{R}^d)$. We now remove this unnecessary assumption: let us consider a potential V satisfying the assumptions of Proposition B.11 (possibly unbounded below). For $K > 0$, we take the cut off potential $V_K = V \mathbb{1}_{\{V \geq -K\}}$ and for any $0 < \varepsilon < 1$ we obtain using Lemma B.10

$$\begin{aligned} &-\frac{1}{\beta} \operatorname{Tr} \log\big(1 + e^{-\beta(|i\hbar\nabla + A|^2 + V)}\big) \\ &\qquad \geq \min_{0 \leq \gamma \leq 1} \Big(\operatorname{Tr}((1-\varepsilon)|i\hbar\nabla + A|^2 + V_K)\gamma + \frac{1}{\beta} \operatorname{Tr} s(\gamma) \Big) \\ &\qquad\quad + \min_{0 \leq \gamma \leq 1} \operatorname{Tr}(\varepsilon |i\hbar\nabla + A|^2 + V - V_K)\gamma \\ &\qquad = -\frac{1}{\beta} \operatorname{Tr} \log\big(1 + e^{-\beta((1-\varepsilon)|i\hbar\nabla + A|^2 + V_K)}\big) \\ &\qquad\quad - \operatorname{Tr}(\varepsilon |i\hbar\nabla + A|^2 + V - V_K)_-. \end{aligned}$$

Applying the Lieb-Thirring inequality, we obtain

$$\operatorname{Tr}(\varepsilon|i\hbar\nabla + A|^2 + V - V_K)_- \leq C\hbar^{-d}\varepsilon^{-d/2}\int_{\mathbb{R}^d}(V - V_K)_-^{1+d/2}\,\mathrm{d}x.$$

This means that for any K and ε

$$\begin{aligned}\limsup_{\hbar\to 0}\hbar^d \operatorname{Tr}\log\big(1 + e^{-\beta(|i\hbar\nabla + A|^2 + V)}\big) \\ \leq \frac{1}{(2\pi)^d}\iint_{\mathbb{R}^{2d}}\log\big(1 + e^{-\beta((1-\varepsilon)p^2 + V_K(x))}\big)\,\mathrm{d}x\,\mathrm{d}p \\ + \varepsilon^{-d/2}C\int_{\mathbb{R}^d}(V - V_K)_-^{1+d/2}\,\mathrm{d}x.\end{aligned}$$

First taking $K \to \infty$ and afterwards $\varepsilon \to 0$, the result follows using the monotone convergence theorem. □

B.5 Proof of Theorem B.2 in the general case

In this section we deal with the interacting case $w \neq 0$. We first focus on the proof of Theorem B.2 (mean-field limit) before proving Theorem B.8 (dilute limit).

B.5.1 Convergence of the energy in the mean-field limit $\eta = 0$

Here we prove (B.12) in the case of general $w \in L^{1+d/2}(\mathbb{R}^d) + L^\infty_\varepsilon(\mathbb{R}^d)$. The upper bound on the canonical energy follows immediately from the trial states constructed in Proposition B.9, so we concentrate on proving the lower bound. This is the content of the following proposition.

Proposition B.12. *Let $\beta_0, \rho > 0$, $V \in L^{1+d/2}_{\mathrm{loc}}(\mathbb{R}^d)$ such that $V(x) \to \infty$ when $|x| \to \infty$ and $\int e^{-\beta_0 V_+(x)}\,\mathrm{d}x < \infty$. Furthermore, let $|A|^2, w \in L^{1+d/2}(\mathbb{R}^d) + L^\infty_\varepsilon(\mathbb{R}^d)$, w be even and satisfy $\widehat{w} \geq 0$. Then we have*

$$\liminf_{\substack{N\to\infty \\ \hbar^d N \to \rho}} \hbar^d e^\beta_{\mathrm{Can}}(\hbar, N) \geq e^\beta_{\mathrm{Vla}}(\rho).$$

Proof. The main idea of the proof is to replace w by an effective one-body potential, and then use the lower bound in the non-interacting case.

We begin by regularizing the interaction potential: let $\varphi \in C^\infty_c(\mathbb{R}^d)$ even and real-valued, define $\chi = \varphi * \varphi$ and $w_\varepsilon = w * \chi_\varepsilon$ with $\chi_\varepsilon = \varepsilon^{-d}\chi(\varepsilon^{-1}\,\cdot\,)$ for $\varepsilon > 0$. Note that $\widehat{w_\varepsilon} \geq 0$. Moreover, if $\alpha > 0$ and $w = w_1 + w_2$ with $w_1 \in L^{1+\frac{d}{2}}(\mathbb{R}^d)$ and $\|w_2\|_{L^\infty(\mathbb{R}^d)} \leq \alpha$ then $w_{1,\varepsilon} := w_1 * \chi_\varepsilon$ satisfies $\widehat{w_{1,\varepsilon}} \in L^1(\mathbb{R}^d)$ and $w_{2,\varepsilon} := w_2 * \chi_\varepsilon$ satisfies $\|w_{2,\varepsilon}\|_{L^\infty(\mathbb{R}^d)} \leq \alpha$. Then, using the Lieb-Thirring inequality, we can replace w by w_ε up to an error of order $\|w_1 - w_{1,\varepsilon}\|_{L^{1+d/2}(\mathbb{R}^d)} + C\alpha$, see for instance [18, Lem. 3.4]. It remains to let ε tend to zero and then let α tend to zero. We therefore assume for the rest of the proof that w satisfies $\widehat{w} \in L^1(\mathbb{R}^d)$.

Now, with $0 \leq \widehat{w} \in L^1(\mathbb{R}^d)$, it is classical that we can bound w from below by a one-body potential, see, e.g., [18, Lem. 3.6]. More precisely, we have for all $x_1, \dots, x_N \in \mathbb{R}^d$ and $\varphi \in C_c^\infty(\mathbb{R}^d)$

$$\int_{\mathbb{R}^d} \widehat{w} \Big| \mathcal{F}\Big[\sum_{i=1}^N \delta_{x_i} - \varphi \Big] \Big|^2 \geq 0,$$

with $\mathcal{F}[\,\cdot\,]$ also denoting the Fourier transform. After expanding, this is the same as

$$\sum_{1 \leq i < j \leq N} w(x_i - x_j) \geq \sum_{i=1}^N w * \varphi(x_i) - \frac{1}{2} \int_{\mathbb{R}^d} (\varphi * w)\varphi - \frac{N}{2} w(0). \tag{B.42}$$

Let m_0 be the minimizer of the semiclassical problem with density ρ, whose existence is guaranteed by Theorem B.1. For any N-body trial state Γ we obtain from (B.42)

$$\begin{aligned} \operatorname{Tr} H_{N,\hbar}\Gamma \geq\ & \operatorname{Tr}\big((i\hbar\nabla + A(x))^2 + V(x) + \rho^{-1} w * \rho_{m_0}(x) \big) \Gamma^{(1)} \\ & - \frac{N}{2\rho^2} \int_{\mathbb{R}^d} (\rho_{m_0} * w)\rho_{m_0} - \frac{1}{2} w(0), \end{aligned}$$

where $\Gamma^{(1)}$ is the 1-particle reduced density matrix of Γ. Let $\mu_{\mathrm{Vla}}(\rho)$ be the chemical potential corresponding to the minimizer m_0 and define $V^{\mathrm{eff}} = V + \rho^{-1} w * \rho_{m_0}(x) - \mu_{\mathrm{Vla}}(\rho)$. Denoting by $e_{\mathrm{Can}}^{\beta,\mathrm{eff}}(\hbar, N)$ the minimum of the canonical energy with potential V^{eff} and with no interaction, we obtain using the convergence shown for the non-interacting case in Section B.4,

$$\begin{aligned} \hbar^d e_{\mathrm{Can}}^{\beta}(\hbar, N) &\geq \hbar^d e_{\mathrm{Can}}^{\beta,\mathrm{eff}}(\hbar, N) - \frac{\hbar^d N}{2\rho^2} \int_{\mathbb{R}^d} (\rho_{m_0} * w)\rho_{m_0} + \mu_{\mathrm{Vla}}(\rho)\hbar^d N \\ & \xrightarrow[\substack{N\to\infty \\ \hbar^d N \to \rho}]{} -\frac{1}{\beta(2\pi)^d} \iint_{\mathbb{R}^{2d}} \log\big(1 + e^{-\beta(p^2 + V^{\mathrm{eff}}(x))}\big)\, \mathrm{d}x\, \mathrm{d}p \\ & \qquad - \frac{1}{2\rho} \int_{\mathbb{R}^d} (\rho_{m_0} * w)\rho_{m_0} + \mu_{\mathrm{Vla}}(\rho)\rho \\ & = e_{\mathrm{Vla}}^{\beta}(\rho), \end{aligned}$$

where the last equality is due to Theorem B.1. This concludes the proof of the convergence of energy in Theorem B.2. □

B.5.2 Convergence of the energy in the dilute limit $\eta > 0$

Here we prove the convergence of the energy in Theorem B.8 where $\eta > 0$. We first state a lemma about the regularity of the minimizers of (B.4) when the interaction has a Dirac component. It will be needed in the proof of the convergence of the energy in Theorem B.8 below.

Lemma B.13. *Let $\beta, a, \rho > 0$, let A, V satisfy the assumptions of Theorem B.1, let $w = a\delta_0$ for some $a > 0$. If $m \in L^1(\mathbb{R}^{2d})$ satisfies the non-linear equation (B.5), then $\rho_m \in L^{1+d/2}(\mathbb{R}^d)$.*

Proof. For simplicity and without loss of generality, we assume that $a = \rho = 1$, $\mu = 0$ and we take $w = \delta_0$ and $A = 0$. Since $\rho_m \in L^1(\mathbb{R}^d)$, it is sufficient to show that $\rho_m \mathbb{1}_{\{\rho_m(x) \geq 1\}}$ is in $L^{1+d/2}(\mathbb{R}^d)$. Recalling that m satisfies the equation

$$m(x,p) = \frac{1}{1 + e^{\beta(p^2 + V(x) + \rho_m(x))}}, \tag{B.43}$$

we immediately have

$$\rho_m(x) \leq \frac{e^{-\beta(V(x)+\rho_m(x))}}{(2\pi)^d} \int_{\mathbb{R}^d} e^{-\beta p^2}\, \mathrm{d}p = C_{d,\beta} e^{-\beta(V(x)+\rho_m(x))},$$

implying that

$$\rho_m(x) e^{\beta \rho_m(x)} \leq C_{d,\beta} e^{\beta V_-(x)}.$$

Hence

$$\rho_m \mathbb{1}_{\{\rho_m \geq 1\}} \leq (V_- + \log C_{d,\beta}) \mathbb{1}_{\{\rho_m \geq 1\}} \in L^{1+\frac{d}{2}}(\mathbb{R}^d),$$

since $V_- \in L^{1+\frac{d}{2}}(\mathbb{R}^d)$ and $\{\rho_m \geq 1\}$ has finite measure by Markov's inequality. □

Case $0 < \eta < 1/d$

In this case, we take $w \in L^1(\mathbb{R}^d)$ with $0 \leq \widehat{w} \in L^1(\mathbb{R}^d)$. Take $w_N = N^{d\eta} w(N^\eta \cdot)$ and consider the canonical model with this interaction. Denoting $a = \int_{\mathbb{R}^d} w(x)\, \mathrm{d}x$, Proposition B.9 implies that

$$\limsup_{\substack{N\to\infty \\ \hbar^d N \to \rho}} \hbar^d e^{\beta}_{\mathrm{Can}}(N, \hbar) \leq e^{\beta, a\delta_0}_{\mathrm{Vla}}(\rho).$$

To show the lower bound, we follow the argument of Proposition B.12. Denote by m_0 the minimizer of the Vlasov functional with the delta interaction $a\delta_0$, and let Γ_N be the Gibbs state minimizing the canonical free energy functional. Applying (B.42) with $\varphi = \frac{N}{\rho}\rho_{m_0}$, we obtain

$$\begin{aligned} \operatorname{Tr} H_{N,\hbar}\Gamma_N \geq\ & \operatorname{Tr}((i\hbar\nabla + A)^2 + V^{\mathrm{eff}})\Gamma_N^{(1)} + \frac{1}{\rho} \operatorname{Tr}(w_N * \rho_{m_0} - a\rho_{m_0})\Gamma_N^{(1)} \\ & - \frac{N}{2\rho^2} \int_{\mathbb{R}^d} (\rho_{m_0} * w_N)\rho_{m_0} + \mu^{a\delta_0}_{\mathrm{Vla}}(\rho) N + o(\hbar^{-d}), \end{aligned} \tag{B.44}$$

where $V^{\mathrm{eff}} = V + \frac{a}{\rho}\rho_{m_0} - \mu^{a\delta_0}_{\mathrm{Vla}}(\rho)$. Here, by Hölder's inequality, we have

$$\begin{aligned} & \hbar^d \operatorname{Tr}(w_N * \rho_{m_0} - a\rho_{m_0})\Gamma_N^{(1)} \\ & \quad = \hbar^d \int_{\mathbb{R}^d} (w_N * \rho_{m_0} - a\rho_{m_0}) \rho_{\Gamma_N^{(1)}} \\ & \quad \leq \|\hbar^d \rho_{\Gamma_N^{(1)}}\|_{L^{1+2/d}(\mathbb{R}^d)} \|w_N * \rho_{m_0} - a\rho_{m_0}\|_{L^{1+d/2}(\mathbb{R}^d)}, \end{aligned}$$

which tends to 0 since $\|\hbar^d \rho_{\Gamma_N^{(1)}}\|_{L^{1+2/d}(\mathbb{R}^d)}$ is bounded, by the Lieb-Thirring inequality, and since $\rho_{m_0} \in L^{1+\frac{d}{2}}(\mathbb{R}^d)$ by Lemma B.13. Finally we have,

$$\int_{\mathbb{R}^d} (\rho_{m_0} * w_N)\rho_{m_0} \longrightarrow a \int_{\mathbb{R}^d} \rho_{m_0}^2.$$

Hence, continuing from (B.44), we conclude that

$$\begin{aligned}\liminf_{\substack{N\to\infty \\ \hbar^d N \to \rho}} \hbar^d e^{\beta}_{\mathrm{Can}}(N,\hbar) \geq & -\frac{1}{(2\pi)^d \beta} \iint_{\mathbb{R}^{2d}} \log\left(1 + e^{-\beta(p^2 + V^{\mathrm{eff}}(x))}\right) \mathrm{d}x\, \mathrm{d}p \\ & + \mu^{a\delta_0}_{\mathrm{Vla}}(\rho)\rho - \frac{a}{2\rho}\int_{\mathbb{R}^d} \rho_{m_0}^2 \\ = & \, e^{\beta, a\delta_0}_{\mathrm{Vla}}(\rho).\end{aligned}$$

Case $\eta > 1/d$

Here we treat the dilute limit. Assume that $d \geq 3$, $0 \leq w \in L^1(\mathbb{R}^d)$, and that w is compactly supported. Then, since $w \geq 0$, we have the immediate lower bound

$$\liminf_{\substack{N\to\infty \\ \hbar^d N \to \rho}} \hbar^d e^{\beta}_{\mathrm{Can}}(N,\hbar) \geq \liminf_{\substack{N\to\infty \\ \hbar^d N \to \rho}} \hbar^d e^{\beta,0}_{\mathrm{Can}}(N,\hbar) = e^{\beta,0}_{\mathrm{Vla}}(\rho).$$

On the other hand, it follows from Proposition B.9 that we also have the corresponding upper bound, so

$$\lim_{\substack{N\to\infty \\ \hbar^d N \to \rho}} \hbar^d e^{\beta}_{\mathrm{Can}}(N,\hbar) = e^{\beta,0}_{\mathrm{Vla}}(\rho).$$

This finishes the proof of the convergence of the energy in the dilute limit.

B.5.3 Convergence of states

Strong convergence of the one-particle Husimi and Wigner measures

Here we concentrate on proving the limits (B.14) and (B.15) for the one-particle Husimi measure and the associated density. We start by briefly recalling the definitions.

For $f \in L^2(\mathbb{R}^d)$ a normalized, real-valued function and $(x,p) \in \mathbb{R}^{2d}$, $\hbar > 0$, we define $f^{\hbar}_{x,p}(y) = \hbar^{-d/4} f((x-y)/\hbar^{1/2}) e^{ip\cdot y/\hbar}$ and denote by $P^{\hbar}_{x,p} = |f^{\hbar}_{x,p}\rangle\langle f^{\hbar}_{x,p}|$ the orthogonal projection onto $f^{\hbar}_{x,p}$. For $k \geq 1$, we introduce the k-particle Husimi measure of a state Γ

$$m^{(k)}_{f,\Gamma}(x_1,p_1,\dots,x_k,p_k) = \frac{N!}{(N-k)!} \mathrm{Tr}(P^{\hbar}_{x_1,p_1} \otimes \cdots \otimes P^{\hbar}_{x_k,p_k} \otimes \mathbb{1}_{N-k}\Gamma),$$

for $x_1, p_1, \dots, x_k, p_k \in \mathbb{R}^{2dk}$. See [18] for alternative formulas of $m^{(k)}_{f,\Gamma}$. We also recall the definition of the Wigner measure,

$$\begin{aligned}\mathcal{W}^{(k)}_\Gamma&(x_1, p_1, \dots, x_k, p_k)\\ &= \int_{\mathbb{R}^{dk}} \int_{\mathbb{R}^{d(N-k)}} \Gamma\big((x + \frac{\hbar}{2}y, z); (x - \frac{\hbar}{2}y, z)\big) e^{-ip\cdot y} \,\mathrm{d}z \,\mathrm{d}y,\end{aligned}$$

where $x = (x_1, \dots x_k), p = (p_1, \dots, p_k) \in \mathbb{R}^{dk}$, and $\Gamma(\cdot, \cdot)$ is the kernel of the operator Γ.

Using [18, Theorem 2.7] and the fact that the Husimi measures are bounded both in the x and p variables, we obtain the existence of a Borel probability measure $\mathcal{P}$ on

$$\mathcal{S} = \left\{\mu \in L^1(\mathbb{R}^{2d}) \,\middle|\, 0 \le \mu \le 1, \int_{\mathbb{R}^{2d}} \mu = \rho\right\}$$

such that, up to a subsequence, we have

$$\int_{\mathbb{R}^{2dk}} m^{(k)}_{f,\Gamma_N} \varphi \to \int_{\mathcal{S}} \Big(\int_{\mathbb{R}^{2dk}} m^{\otimes k} \varphi\Big) \,\mathrm{d}\mathcal{P}(m),$$

for any $\varphi \in L^1(\mathbb{R}^{2dk}) + L^\infty(\mathbb{R}^{2dk})$ and similarly for the Wigner measures. There is no loss of mass in the limit due to the confining potential V. Our goal is to show that $\mathcal{P} = \delta_{m_0}$, where m_0 is the Vlasov minimizer from Theorem B.1.

We begin with the case $\eta = 0$. Using coherent states, the tightness of $(m^{(1)}_{f,\Gamma_N})_N$ and a finite volume approximation we obtain

$$\begin{aligned}\lim_{\substack{N_j \to \infty \\ \hbar^d N_j \to \rho}} \hbar^d e^\beta_{\mathrm{Can}}(\hbar, N_j) &\ge \frac{1}{(2\pi)^d} \int_{\mathcal{S}} \Big(\int_{\mathbb{R}^{2dk}} (p^2 + V(x)) m(x,p)\Big) \,\mathrm{d}\mathcal{P}(m)\\ &+ \frac{1}{2\rho} \int_{\mathcal{S}} \Big(\int_{\mathbb{R}^{2dk}} (w * \rho_m)\rho_m\Big) \,\mathrm{d}\mathcal{P}(m) + \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} s\Big(\int_{\mathcal{S}} m \,\mathrm{d}\mathcal{P}(m)\Big). \end{aligned} \tag{B.45}$$

The lower semi-continuity of the entropy term can be justified as in the proof of Lemma B.19. The case $0 < \eta < 1/d$ can be adapted using (B.42) with $\varphi = N\rho_{m_0}$ and the case $\eta > 1/d$ is even easier since the interaction is assumed non-negative and can therefore be dropped.

If we denote $\overline{m} = \int_{\mathcal{S}} m \,\mathrm{d}\mathcal{P}(m)$, the right side of (B.45) is not exactly $\mathcal{E}_{\mathrm{Can}}(\overline{m})$ because of the interaction term. In the case $0 \le \eta < 1/d$ we assumed $\widehat{w} \ge 0$, hence the following inequality follows from convexity:

$$\int_{\mathcal{S}} \Big(\int_{\mathbb{R}^{2dk}} w * \rho_m \rho_m\Big) \,\mathrm{d}\mathcal{P}(m) \ge \int_{\mathbb{R}^{2d}} w * \rho_{\overline{m}} \rho_{\overline{m}}. \tag{B.46}$$

The case $1/d < \eta$ is immediate since we assumed $w \ge 0$ and the limiting energy has no interaction term. Gathering the above inequalities we have

$$\lim_{\substack{N_j \to \infty \\ \hbar^d N_j \to \rho}} \hbar^d e^\beta_{\mathrm{Can}}(\hbar, N_j) \ge \mathcal{E}^{\beta,\rho,\bullet}_{\mathrm{Vla}}(\overline{m}) \ge e^{\beta,\bullet}_{\mathrm{Vla}}(\rho),$$

where $\mathcal{E}_{\rm Vla}^{\beta,\rho,\bullet}$ and $e_{\rm Vla}^{\beta,\bullet}(\rho)$ are the appropriate limiting functional and energy: i.e. $\bullet = w$ if $\eta = 0$, $\bullet = (\int_{\mathbb{R}^d} w)\delta_0$ if $0 < d\eta < 1$ and $\bullet = 0$ if $d\eta \geq 1$ and $d \geq 3$. Now, by Theorem B.2 and Theorem B.8 the above inequalities are in fact equalities and $\overline{m}$ is therefore the unique minimizer of $\mathcal{E}_{\rm Vla}^{\beta,\rho,\bullet}$ that is m_0. Since this limit does not depend on the subsequence we have taken, we conclude that the whole sequence $m^{(1)}_{f,\Gamma_N}$ converges weakly to m_0, and similarly for the Wigner measure.

Note that, when $\widehat{w} > 0$ and $0 < d\eta < 1$, the equality in (B.46) gives that $\mathcal{P}$ is concentrated on functions m which all share the same density ρ_{m_0}, by strict convexity. But this is the only information that we have obtained so far on $\mathcal{P}$. If the conjectured entropy inequality (B.18) was valid, then we would conclude immediately that $\mathcal{P} = \delta_{m_0}$. Since we do not have this inequality, we will have to go back later to the proof that $\mathcal{P} = \delta_{m_0}$.

So far the convergence of $m^{(1)}_{f,\Gamma_N}$ is only weak but it can be improved using the (one-particle) entropy. Going back to the previous estimates we now have

$$\hbar^d e^{\beta}_{\rm Can}(\hbar, N) = e_{\rm Vla}^{\beta,\bullet}(\rho) + \frac{1}{(2\pi)^d\beta}\iint_{\mathbb{R}^{2d}} (s(m^{(1)}_{f,\Gamma_N}) - s(m_0)) + o(1) \tag{B.47}$$

As before we denote by $e_{\rm Vla}^{\beta,\bullet}(\rho)$ the appropriate limiting energy, depending on the choice of η. Recall that in the case $\eta > 1/d$, the interaction potential is assumed to be non negative, so the interaction term is just dropped. We now focus on the second term in (B.47). Let us remark that

$$\begin{aligned}
&s(m^{(1)}_{f,\Gamma_N}) - s(m_0)\\
&\quad= m^{(1)}_{f,\Gamma_N}\log\left(\frac{m^{(1)}_{f,\Gamma_N}}{m_0}\right) + (1 - m^{(1)}_{f,\Gamma_N})\log\left(\frac{1 - m^{(1)}_{f,\Gamma_N}}{1-m_0}\right)\\
&\qquad + (m_0 - m^{(1)}_{f,\Gamma_N})\log\left(\frac{1-m_0}{m_0}\right)\\
&\quad\geq m_0\log\left(\frac{m^{(1)}_{f,\Gamma_N}}{m_0}\right) + \beta(m_0 - m^{(1)}_{f,\Gamma_N})(p^2 + V + \frac{1}{\rho}w_N * \rho_{m_0} - \mu + \beta^{-1}),
\end{aligned}$$

where we used the expression of m_0 (B.5) and the pointwise inequality $x\log(x/y) + (y-x) \geq 0$ for any $x, y > 0$. Integrating over x and p, we obtain on the right side the sum of the relative von Neumann entropy of $m^{(1)}_{f,\Gamma_N}$ and m_0, and a term which tends to zero, due to the weak convergence we have proven. By Pinsker's inequality and (B.47) we obtain

$$\hbar^d e^{\beta}_{\rm Can}(\hbar, N) - e_{\rm Vla}^{\beta,\bullet}(\rho) \geq \frac{1}{2(2\pi)^d\beta}\left(\int_{\mathbb{R}^{2d}} |m^{(1)}_{f,\Gamma_N} - m_0|\right)^2 + o(1).$$

The convergence of the energies gives the strong convergence in $L^1(\mathbb{R}^{2d})$ of $m^{(1)}_{f,\Gamma_N}$ towards the Vlasov minimizer m_0, hence in $L^p(\mathbb{R}^{2d})$ for all $1 \leq p < \infty$ since the

Husimi measures are bounded by 1. This automatically gives that $\rho_{m^{(1)}_{f,\Gamma_N}} \to \rho_{m_0}$ strongly in $L^1(\mathbb{R}^d)$. The weak convergence in $L^{1+2/d}(\mathbb{R}^d)$ follows from the (classical) Lieb-Thirring inequality

$$\|\rho_m\|_{L^{1+d/2}(\mathbb{R}^d)} \leq C\|m\|^{\frac{d}{d+2}}_{L^1(\mathbb{R}^{2d},p^2\,\mathrm{d}x\,\mathrm{d}p)}\|m\|^{\frac{2}{d+2}}_{L^\infty(\mathbb{R}^{2d})}$$

for any m in $L^1(\mathbb{R}^{2d})$.

Finally, by the Lieb-Thirring inequality $\hbar^d\rho^{(1)}_{\Gamma_N}$ is bounded in $L^1(\mathbb{R}^d)\cap L^{1+d/2}(\mathbb{R}^d)$, hence this sequence is weakly precompact in those spaces. On the other hand, for any $\varphi \in C^\infty_c(\mathbb{R}^d)$ we have by [18, Lemma 2.4]

$$\int_{\mathbb{R}^d}\rho_{m^{(1)}_{f,\Gamma_N}}\varphi = \int_{\mathbb{R}^d}\hbar^d\rho^{(1)}_{\Gamma_N}\varphi * |f^\hbar|^2.$$

Let $\widetilde{\rho}$ be an accumulation point for $\hbar^d\rho^{(1)}_{\Gamma_N}$. By passing to the limit in both sides we obtain

$$\int_{\mathbb{R}^d}\rho_{m_0}\varphi = \int_{\mathbb{R}^d}\widetilde{\rho}\varphi.$$

The test function φ being arbitrary, we conclude that $\hbar^d\rho^{(1)}_{\Gamma_N}$ has a single accumulation point and therefore converges weakly in $L^1(\mathbb{R}^d)\cap L^{1+d/2}(\mathbb{R}^d)$ towards ρ_{m_0}.

Weak convergence of the k-particle Husimi and Wigner measures

At this point we have proved the strong convergence of $m^{(1)}_{f,\Gamma_N}$ towards m_0 in $L^p(\mathbb{R}^{2d})$ for all $1 \leq p < \infty$. Our argument works for any sequence of approximate Gibbs states (Γ_N) in the sense that

$$\mathcal{E}^{N,\hbar}_{\mathrm{Can}}(\Gamma_N) = e^\beta_{\mathrm{Can}}(\hbar, N) + o(N).$$

Here we discuss the weak convergence of the higher order Husimi functions. This is not an easy fact in the canonical ensemble case. For instance, when $w \equiv 0$ one can use Wick's formula in the grand canonical case but there is no such formula in the canonical ensemble [59, 25]. Here we will use a Feynman-Hellmann-type argument, which forces us to consider the exact Gibbs state, and not only an approximate equilibrium state. We will come back to approximate Gibbs states at the end of the proof but our argument will require that they approach the right energy with an error of order $o(1)$ instead of $o(N)$.

In order to access the two-particle Husimi function, the usual Feynman-Hellmann argument is to perturb the N-body Hamiltonian by a positive two-body term of order N, multiplied by a small parameter ε. This modifies the effective Vlasov energy and, after taking the limit, one then look at the derivative at $\varepsilon = 0$. The problem here is to control negative values of ε. For atoms one can use the strong repulsion at the origin of the Coulomb interaction to control a negative two-body term, as was done in [53].[1] For a general interaction or even when $w \equiv 0$, such an argument fails. Another difficulty is the need to re-prove the existence of the limit with the perturbation, since in the canonical ensemble trial states are not so easy to construct.

We follow a different route and use instead an argument inspired of a new technique recently introduced in [34]. The idea is to perturb the energy by a one body term of order 1. This will not modify the leading order in the limit and will force us to look at the next order. Since we are only interested in deviations in ε, the existence of the limit for the one-particle Husimi measure will help us to identify the deviation. Then, in order to access the two-body Husimi measure, we look at the second derivative at $\varepsilon = 0$ instead of the first derivative.

Let us detail the argument. Let $b \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{R}_+)$ be a non-negative function on the phase space and introduce its coherent state quantization

$$B_\hbar := \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} b(x,p)\, P_{x,p}^\hbar \,\mathrm{d}x\,\mathrm{d}p,$$

where we recall that $P_{x,p}^\hbar = |f_{x,p}^\hbar\rangle\,\langle f_{x,p}^\hbar|$ is the orthogonal projection onto $f_{x,p}^\hbar$. We then consider the operator

$$B_{N,\hbar} := \sum_{j=1}^N (B_\hbar)_j \tag{B.48}$$

in the N-particle space. Note that $B_\hbar$ is a bounded self-adjoint operator with

$$0 \le B_\hbar \le \|b\|_{L^\infty(\mathbb{R}^{2d})}\hbar^d \tag{B.49}$$

due to the coherent state representation (B.39) and that it is trace-class with

$$\mathrm{Tr}(B_\hbar) \le \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} b(x,p)\,\mathrm{d}x\,\mathrm{d}p. \tag{B.50}$$

In particular $B_{N,\hbar}$ is bounded uniformly in N, with

$$\|B_{N,\hbar}\|_{\mathcal{B}(\bigwedge^N L^2(\mathbb{R}^3))} \le \min\big(N\hbar^d\|b\|_{L^\infty(\mathbb{R}^{2d})}, (2\pi)^{-d}\|b\|_{L^1(\mathbb{R}^{2d})}\big).$$

This is because

$$\Big\|\sum_{j=1}^N C_j\Big\|_{\mathcal{B}(\bigwedge^N L^2(\mathbb{R}^3))} \le \|C\|_{\mathfrak{S}^1(L^2(\mathbb{R}^3))} \tag{B.51}$$

for any trace class operator C. In the sequel we will just denote by $\|\cdot\| = \|\cdot\|_{\mathcal{B}(\mathfrak{H})}$ the operator norm and omit the underlying Hilbert space $\mathfrak{H}$ which could be $\bigwedge^N L^2(\mathbb{R}^3)$ or $L^2(\mathbb{R}^3)$. We introduce the perturbed Hamiltonian

$$H_{N,\hbar}(\varepsilon) := H_{N,\hbar} + \varepsilon B_{N,\hbar},$$

[1] After inspection one sees that the argument used in [53] works under the condition that $\widehat{w}(p) \ge a|p|^{-a}$ for some $a > 0$ for large p. Not all interaction potentials can therefore be covered.

for $\varepsilon \in \mathbb{R}$. The perturbation is uniformly bounded, hence will not affect the limit $N \to \infty$ for fixed ε. More precisely, let us call

$$\Gamma_{N,\hbar,\beta}(\varepsilon) := \frac{e^{-\beta H_{N,\hbar}(\varepsilon)}}{\operatorname{Tr} e^{-\beta H_{N,\hbar}(\varepsilon)}}$$

the associated Gibbs state and

$$F_{N,\hbar,\beta}(\varepsilon) := -\frac{\log \operatorname{Tr}(e^{-\beta H_{N,\hbar}(\varepsilon)})}{\beta}$$

the corresponding free energy. Everywhere we assume that $\hbar N^{1/d} \to \rho$ and $\beta > 0$ is fixed. By plugging $\Gamma_{N,\hbar,\beta}(\varepsilon)$ into the variational principle at $\varepsilon = 0$ and conversely, we obtain immediately that

$$\begin{aligned} F_{N,\hbar,\beta}(0) + \frac{\varepsilon}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} b\, m^{(1)}_{f,\Gamma_{N,\hbar,\beta}(\varepsilon)} \\ \leq F_{N,\hbar,\beta}(\varepsilon) \leq F_{N,\hbar,\beta}(0) + \frac{\varepsilon}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} b\, m^{(1)}_{f,\Gamma_{N,\hbar,\beta}(0)}. \end{aligned} \tag{B.52}$$

We have used here that $\operatorname{Tr}(B_\hbar \Gamma^{(1)}) = (2\pi)^{-d} \iint_{\mathbb{R}^{2d}} b\, m^{(1)}_{f,\Gamma}$ for all states Γ. Since $0 \leq m^{(1)}_{f,\Gamma} \leq 1$, this proves that

$$F_{N,\hbar,\beta}(\varepsilon) = \mathcal{E}^{N,\hbar}_{\rm Can}(\Gamma_{N,\hbar,\beta}(\varepsilon)) = e^{\beta}_{\rm Can}(\hbar, N) + O(\varepsilon)$$

where $O(\varepsilon)$ is even uniform in N. Hence from the analysis in the previous section, we deduce immediately that

$$m^{(1)}_{\Gamma_{N,\hbar,\beta}(\varepsilon)} \longrightarrow m_0$$

strongly in $L^1(\mathbb{R}^{2d})$ for any fixed ε. Going back to (B.52) we infer that

$$F_{N,\hbar,\beta}(\varepsilon) = F_{N,\hbar,\beta}(0) + \frac{\varepsilon}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} b m_0 + o(1).$$

A different way to state the same limit is

$$f_N(\varepsilon) := \frac{\operatorname{Tr} e^{-\beta H_{N,\hbar} - \beta\varepsilon B_{N,\hbar}}}{\operatorname{Tr} e^{-\beta H_{N,\hbar}}} \longrightarrow \exp\Big(-\frac{\varepsilon\beta}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} b m_0\Big). \tag{B.53}$$

It turns out that the so-defined function f_N is C^∞ on $\mathbb{R}$ with all its derivatives locally uniformly bounded in N. This follows from the following general fact.

Lemma B.14. *Let A be a self-adjoint operator such that $\operatorname{Tr}(e^A) < \infty$ and let B be a bounded self-adjoint operator, on a Hilbert space $\mathfrak{H}$. Then the function*

$$\varepsilon \in \mathbb{R} \mapsto \frac{\operatorname{Tr}(e^{A+\varepsilon B})}{\operatorname{Tr}(e^A)}$$

is C^∞ and its derivatives are bounded by

$$\left|\frac{\mathrm{d}^k}{\mathrm{d}\varepsilon^k}\frac{\mathrm{Tr}(e^{A+\varepsilon B})}{\mathrm{Tr}(e^A)}\right| \le \|B\|^k \frac{\mathrm{Tr}(e^{A+\varepsilon B})}{\mathrm{Tr}(e^A)} \le \|B\|^k e^{|\varepsilon|\|B\|}$$

for $k \ge 0$.

Proof. Note that $\mathrm{Tr}(e^{A+\varepsilon B}) \le e^{\varepsilon\|B\|}\,\mathrm{Tr}(e^A)$ since $A+\varepsilon B \le A + |\varepsilon|\|B\|$. We have for the first derivative

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\frac{\mathrm{Tr}(e^{A+\varepsilon B})}{\mathrm{Tr}(e^A)} = \frac{\mathrm{Tr}(Be^{A+\varepsilon B})}{\mathrm{Tr}(e^A)}$$

which is then clearly bounded by $\|B\|$. The second derivative is given by Duhamel's formula

$$\frac{\mathrm{d}^2}{\mathrm{d}\varepsilon^2}\frac{\mathrm{Tr}(e^{A+\varepsilon B})}{\mathrm{Tr}(e^A)} = \int_0^1 \frac{\mathrm{Tr}(Be^{t(A+\varepsilon B)}Be^{(1-t)(A+\varepsilon B)})}{\mathrm{Tr}(e^A)}\,\mathrm{d}t \tag{B.54}$$

and we have by Hölder's inequality in Schatten spaces

$$\begin{aligned}|\mathrm{Tr}(Be^{t(A+\varepsilon B)}Be^{(1-t)(A+\varepsilon B)})| &\le \|B\|^2\|e^{t(A+\varepsilon B)}\|_{\mathfrak{S}^{\frac{1}{t}}}\|e^{(1-t)(A+\varepsilon B)}\|_{\mathfrak{S}^{\frac{1}{1-t}}}\\ &= \|B\|^2\,\mathrm{Tr}(e^{A+\varepsilon B}) \le \|B\|^2 e^{|\varepsilon|\|B\|}\,\mathrm{Tr}(e^A),\end{aligned}$$

as claimed. The argument is the same for the higher order derivatives. The function is indeed real-analytic on $\mathbb{R}$ but this fact is not needed in our argument. □

Since $B_{N,\hbar}$ is bounded uniformly in N and $\hbar$, we conclude from the lemma that f_N is bounded in $W^{k,\infty}_{\mathrm{loc}}$ for all k. This implies that $f_N^{(k)}$ converges locally uniformly to the kth derivative of the right side of (B.53) for all k. In particular, we have

$$f_N''(0) \longrightarrow \left(\frac{\beta}{(2\pi)^d}\iint_{\mathbb{R}^{2d}} bm_0\right)^2. \tag{B.55}$$

On the other hand, we can compute the second derivative $f_N''(0)$ explicitly, using (B.54):

$$f_N''(0) = \beta^2\int_0^1 \frac{\mathrm{Tr}(B_{N,\hbar}\,e^{-t\beta H_{N,\hbar}}B_{N,\hbar}\,e^{-(1-t)\beta H_{N,\hbar}})}{\mathrm{Tr}(e^{-\beta H_{N,\hbar}})}\,\mathrm{d}t. \tag{B.56}$$

We claim that this indeed behaves as

$$f_N''(0) = \frac{\beta^2}{(2\pi)^{2d}}\iint_{\mathbb{R}^{4d}} b\otimes b\, m^{(2)}_{f,\Gamma_{N,\hbar,\beta}} + o(1) \tag{B.57}$$

and first explain why this is useful before justifying (B.57). From the weak convergence of $m^{(2)}_{f,\Gamma_{N,\hbar,\beta}}$ mentioned in the previous section, we obtain

$$\lim_{\substack{N\to\infty\\ N\hbar^d\to\rho}} f_N''(0) = \frac{\beta^2}{(2\pi)^{2d}}\int_{\mathcal{S}}\left(\int_{\mathbb{R}^{2d}} bm\right)^2\mathrm{d}\mathcal{P} \tag{B.58}$$

with the de Finetti measure $\mathcal{P}$. Comparing (B.55) with (B.58) and using $m_0 = \int_{\mathcal{S}} m \, \mathrm{d}\mathcal{P}$, we conclude that

$$\int_{\mathcal{S}} \Big(\int_{\mathbb{R}^{2d}} bm \Big)^2 \mathrm{d}\mathcal{P}(m) = \Big(\int_{\mathcal{S}} \int_{\mathbb{R}^{2d}} bm \, \mathrm{d}\mathcal{P}(m) \Big)^2$$

for every non-negative $b \in C_c^\infty(\mathbb{R}^{2d})$. This proves that $\mathcal{P} = \delta_{m_0}$ as desired. The limits (B.16) and (B.17) then follow for all $k \geq 2$. Therefore, it only remains to prove (B.57).

The idea of the proof of (B.57) is simple. Since we are in a semi-classical regime, the order of the operators in the trace (B.56) should not matter. If we put the two $B_{N,\hbar}$ together, we obtain after a calculation

$$\mathrm{Tr}\big((B_{N,\hbar})^2 \Gamma_{N,\hbar,\beta}\big) = \mathrm{Tr}\big((B_\hbar)^2 \Gamma^{(1)}_{N,\hbar}\big) + \frac{1}{(2\pi)^{2d}} \iint_{\mathbb{R}^{4d}} b \otimes b \, m^{(2)}_{f,\Gamma_{N,\hbar,\beta}}.$$

The first term tends to zero since

$$\mathrm{Tr}\big((B_\hbar)^2 \Gamma^{(1)}_{N,\hbar}\big) \leq N \|B_\hbar\|^2 \leq \|b\|^2_{L^\infty(\mathbb{R}^{2d})} N \hbar^{2d},$$

whereas the second term converges to $(2\pi)^{-2d} \int_{\mathcal{S}} \big(\iint_{\mathbb{R}^{2d}} bm \big)^2 d\mathcal{P}(m)$ due to the weak convergence of $m^{(2)}_{f,\Gamma_{N,\hbar,\beta}}$. Therefore we have to compare $f_N''(0)$ with $\mathrm{Tr}(B_{N,\hbar})^2 \Gamma_{N,\hbar,\beta}$.

In [34], it is proven that the function

$$t \mapsto \mathrm{Tr}\big(B_{N,\hbar} \, e^{-t\beta H_{N,\hbar}} B_{N,\hbar} \, e^{-(1-t)\beta H_{N,\hbar}}\big)$$

is convex on $[0,1]$, non-increasing on $[0,1/2]$ and non-decreasing on $[1/2,1]$. Using that the function is minimal at $t = 1/2$ and above its tangent at $t = 0$ provides the bound

$$\begin{aligned}
&\mathrm{Tr}\big(B_{N,\hbar} \, e^{-t\beta H_{N,\hbar}} B_{N,\hbar} \, e^{-(1-t)\beta H_{N,\hbar}}\big) \\
&\qquad \geq \mathrm{Tr}\big(B_{N,\hbar} \, e^{-\frac{\beta}{2} H_{N,\hbar}} B_{N,\hbar} \, e^{-\frac{\beta}{2} H_{N,\hbar}}\big) \\
&\qquad \geq \mathrm{Tr}\big((B_{N,\hbar})^2 e^{-\beta H_{N,\hbar}}\big) + \frac{\beta}{4} \mathrm{Tr}\big(\big[[H_{N,\hbar}, B_{N,\hbar}], B_{N,\hbar}\big] \, e^{-\beta H_{N,\hbar}}\big)
\end{aligned}$$

for all $t \in [0;1]$, see [34]. Inserting in (B.56), we find that

$$f_N''(0) \geq \beta^2 \, \mathrm{Tr}\big((B_{N,\hbar})^2 \Gamma_{N,\hbar,\beta}\big) + \frac{\beta^3}{4} \mathrm{Tr}\big(\big[[H_{N,\hbar}, B_{N,\hbar}], B_{N,\hbar}\big] \, \Gamma_{N,\hbar,\beta}\big). \tag{B.59}$$

Hence (B.57) readily follows from the following result.

Lemma B.15 (Convergence of the double commutator). *With $B_{N,\hbar}$ defined as in (B.48), we have*

$$\lim_{\substack{N\to\infty \\ N\hbar^d \to \rho}} \mathrm{Tr}\big(\big[[H_{N,\hbar}, B_{N,\hbar}], B_{N,\hbar}\big] \, \Gamma_{N,\hbar,\beta}\big) = 0. \tag{B.60}$$

Proof. We have

$$\begin{aligned}\big[[H_{N,\hbar},B_{N,\hbar}],B_{N,\hbar}\big]\\ &=\sum_{j=1}^N\big[[H_{1,\hbar},B_\hbar],B_\hbar\big]_j+\frac{1}{N}\sum_{1\le j\neq k\le N}\big[[w_{jk},(B_\hbar)_j],(B_\hbar)_j+(B_\hbar)_k\big]\end{aligned}\tag{B.61}$$

with $H_{1,\hbar}=|i\hbar\nabla+A|^2+V$ the one-particle operator and w_{jk} the multiplication operator by $w_N(x_j-x_k)$. The commutators have been used to dramatically reduce the number of terms, but will not play any role anymore. We will estimate separately the terms $(B_\hbar H_{1,\hbar}B_\hbar)_j$, $(H_{1,\hbar}B_\hbar^2)_j$, $w_{jk}(B_\hbar)_j(B_\hbar)_{j'}$ and $(B_\hbar)_j w_{jk}(B_\hbar)_{j'}$ with $j'\in\{k,j\}$.

First we deal with the kinetic energy. For instance we can bound, by Hölder's inequality in Schatten spaces,

$$\begin{aligned}&\big\|B_\hbar(-\hbar^2\Delta)B_\hbar\big\|_{\mathfrak{S}^1}+\big\|(-\hbar^2\Delta)(B_\hbar)^2\big\|_{\mathfrak{S}^1}\\ &\qquad\le 2\|B_\hbar\|\big\|B_\hbar\big\|_{\mathfrak{S}^1}^{\frac12}\big\|(-\hbar^2\Delta)B_\hbar^{\frac12}\big\|_{\mathfrak{S}^2}\le\frac{C}{N}\big\|(-\hbar^2\Delta)B_\hbar^{\frac12}\big\|_{\mathfrak{S}^2}.\end{aligned}$$

We have used here our estimates (B.49) and (B.50) on the norm and trace of the non-negative operator $B_\hbar$. The last Hilbert-Schmidt norm is equal to

$$\begin{aligned}\big\|(-\hbar^2\Delta)B_\hbar^{\frac12}\big\|_{\mathfrak{S}^2}^2&=\mathrm{Tr}\big((-\hbar^2\Delta)B_\hbar(-\hbar^2\Delta)\big)\\ &=\frac{1}{(2\pi)^d}\iint_{\mathbb{R}^{2d}}b(x,p)\|\hbar^2\Delta f_{x,p}^\hbar\|^2\,\mathrm{d}x\,\mathrm{d}p.\end{aligned}$$

Using that

$$\begin{aligned}\hbar^2\Delta f_{x,p}^\hbar(y)&=\hbar\,\hbar^{-d/4}(\Delta f)\Big(\frac{x-y}{\sqrt{\hbar}}\Big)e^{ip\cdot y/\hbar}-|p|^2f_{x,p}^\hbar(y)\\ &\quad+2i\sqrt{\hbar}\,\hbar^{-d/4}p\cdot(\nabla f)\Big(\frac{x-y}{\sqrt{\hbar}}\Big)e^{ip\cdot y/\hbar},\end{aligned}$$

we find that

$$\big\|(-\hbar^2\Delta)B_\hbar^{\frac12}\big\|_{\mathfrak{S}^2}\le C\iint_{\mathbb{R}^{2d}}(|p|^4+\hbar|p|^2+\hbar^2)b(x,p)\,\mathrm{d}x\,\mathrm{d}p.$$

This is uniformly bounded since b has a compact support in the phase space. Using (B.51), we conclude as we wanted that

$$\mathrm{Tr}\Big(\Gamma_{N,\hbar,\beta}\sum_{j=1}^N\big[[-\hbar^2\Delta,B_\hbar],B_\hbar\big]_j\Big)=O(N^{-1}).$$

For the potential term we have to use more information on the state $\Gamma_{N,\hbar,\beta}$. We first estimate

$$\mathrm{Tr}\big(\Gamma_{N,\hbar,\beta}^{(1)}VB_\hbar^2\big)\le\|B_\hbar\|^{\frac32}\big\|(\Gamma_{N,\hbar,\beta}^{(1)})^{\frac12}|V|^{\frac12}\big\|_{\mathfrak{S}^2}\big\||V|^{\frac12}B_\hbar^{\frac12}\big\|_{\mathfrak{S}^2}.$$

Using the Lieb-Thirring inequality for $V_- \in L^{1+d/2}(\mathbb{R}^3)$ as in (B.38) and that the energy is $O(N)$ for V_+, we see that

$$\big\|(\Gamma^{(1)}_{N,\hbar,\beta})^{1/2}|V|^{1/2}\big\|^2_{\mathfrak{S}^2} = \operatorname{Tr}\Gamma^{(1)}_{N,\hbar,\beta}|V| = O(N).$$

Hence we can deduce that

$$\operatorname{Tr}\big(\Gamma^{(1)}_{N,\hbar,\beta} V B_\hbar^2\big) \leq \frac{C}{N}\big\||V|^{\frac12}B_\hbar^{\frac12}\big\|.$$

Like for the kinetic energy, we compute the Hilbert-Schmidt norm

$$\begin{aligned}
\big\||V|^{\frac12}B_\hbar^{\frac12}\big\|^2_{\mathfrak{S}^2} &= \operatorname{Tr}|V|^{\frac12}B_\hbar|V|^{\frac12} \\
&= \frac{1}{(2\pi)^d}\iint_{\mathbb{R}^d\times\mathbb{R}^d} b(x,p)\big\||V|^{\frac12}f^\hbar_{x,p}\big\|^2_{L^2(\mathbb{R}^d)}\,\mathrm{d}x\,\mathrm{d}p \\
&= \frac{1}{(2\pi)^d}\iint_{\mathbb{R}^{2d}} b(x,p)\;|V| * |f^\hbar_{0,0}|^2(x)\,\mathrm{d}x\,\mathrm{d}p \\
&\leq C\int_{B_R}|V(x)|\,\mathrm{d}x
\end{aligned} \tag{B.62}$$

where B_R is a fixed large ball, chosen large enough such that $\operatorname{supp}(b) \subset B_{R-1}$. We are using here that $f^\hbar_{0,0}$ has compact support, hence $\operatorname{supp}(f^\hbar_{0,0}) \subset B_1$, for $\hbar$ small enough. Since $V \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ by assumption, this proves that

$$\operatorname{Tr}\big(\Gamma^{(1)}_{N,\hbar,\beta} V B_\hbar^2\big) = O(N^{-1}).$$

The argument is similar for $\operatorname{Tr}(\Gamma^{(1)}_{N,\hbar,\beta}B_\hbar^2 V)$. Finally, we also have

$$\operatorname{Tr}\big(\Gamma^{(1)}_{N,\hbar,\beta}B_\hbar V B_\hbar\big) \leq \|B_\hbar\|\big\|B_\hbar^{\frac12}|V|^{\frac12}\big\|^2_{\mathfrak{S}^2} = O(N^{-1}) \tag{B.63}$$

by (B.62). This concludes the proof that the potential terms tend to 0. The argument is exactly the same for $|A|^2$. For $i\hbar\nabla\cdot A + A\cdot i\hbar\nabla$, we argue similarly, using that

$$\big\||A|B_\hbar^{\frac12}\big\|_{\mathfrak{S}^2} + \big\|A\cdot(i\hbar\nabla)B_\hbar^{\frac12}\big\|_{\mathfrak{S}^2} \leq C\int_{B_R}|A|$$

and

$$\Big\||i\hbar\nabla|\sqrt{\Gamma^{(1)}_{N,\hbar,\beta}}\Big\|^2_{\mathfrak{S}^2} = \operatorname{Tr}(-\hbar^2\Delta)\Gamma^{(1)}_{N,\hbar,\beta} = O(N).$$

Let us finally turn to the interaction. First we look at

$$\operatorname{Tr}\Big(\Gamma_{N,\hbar,\beta}\frac1N\sum_{1\leq j\neq k\leq N}(B_\hbar)_j w_{jk}(B_\hbar)_k\Big) = (N-1)\operatorname{Tr}\big(\Gamma_{N,\hbar,\beta}(B_\hbar)_1 w_{12}(B_\hbar)_2\big)$$

and use the Cauchy-Schwarz inequality to estimate

$$\pm(B_\hbar)_1 w_{12}(B_\hbar)_2 \leq (B_\hbar)_1|w_{12}|(B_\hbar)_1 + (B_\hbar)_2|w_{12}|(B_\hbar)_2.$$

We look for instance at

$$(N-1)\operatorname{Tr}\big(\Gamma_{N,\hbar,\beta}(B_\hbar)_2 w_{12}(B_\hbar)_2\big) = \operatorname{Tr}\Big(\Gamma_{N,\hbar,\beta}\sum_{j=2}^N (B_\hbar)_j w_{1j}(B_\hbar)_j\Big).$$

For fixed x_1, the operator $\sum_{j=2}^N (B_\hbar)_j w_{1j}(B_\hbar)_j$ (acting on the remaining $N-1$ variables) is estimated as in (B.51) by

$$\Big\|\sum_{j=2}^N (B_\hbar)_j w_{1j}(B_\hbar)_j\Big\| \le \big\|B_\hbar |w_N(x_1 - \,\cdot\,)| B_\hbar\big\|_{\mathfrak{S}^1} \le \frac{C}{N}\sup_{x_1\in\mathbb{R}^d}\int_{B(x_1,R)}|w_N|.$$

When $\eta > 0$ the supremum can be bounded by $\int_{\mathbb{R}^d}|w_N| = \int_{\mathbb{R}^d}|w|$, since we assume that $w \in L^1(\mathbb{R}^d)$ in this case. When $\eta = 0$ (hence $w_N = w$) this can be controlled by

$$\sup_{x_1\in\mathbb{R}^d}\int_{B(x_1,R)}|w| \le |B_R|\|w_2\|_{L^\infty(\mathbb{R}^d)} + |B_R|^{1+\frac{2}{d}}\|w_1\|_{L^{1+\frac{d}{2}}(\mathbb{R}^d)}$$

since $w = w_1 + w_2 \in L^{1+d/2} + L^\infty(\mathbb{R}^d)$. In all cases, we have proved that

$$\operatorname{Tr}\Big(\Gamma_{N,\hbar,\beta}\frac{1}{N}\sum_{1\le j\neq k\le N}(B_\hbar)_j w_{jk}((B_\hbar)_j + (B_\hbar)_k)\Big) = O(N^{-1}).$$

It then remains to look at

$$\begin{aligned}
&\big|(N-1)\operatorname{Tr}\big(\Gamma_{N,\hbar,\beta}(B_\hbar)_{j'}(B_\hbar)_2 w_{12}\big)\big| \\
&\qquad \le (N-1)\sqrt{\operatorname{Tr}\big(\Gamma_{N,\hbar,\beta}(B_\hbar)_{j'}(B_\hbar)_2|w_{12}|(B_\hbar)_2(B_\hbar)_{j'}\big)}\sqrt{\operatorname{Tr}(\Gamma_{N,\hbar,\beta}|w_{12}|)},
\end{aligned}$$

where $j' \in \{1,2\}$. The first term is estimated as before by

$$\operatorname{Tr}\big(\Gamma_{N,\hbar,\beta}(B_\hbar)_{j'}(B_\hbar)_2|w_{12}|(B_\hbar)_2(B_\hbar)_{j'}\big) \le \frac{C}{N^3}\sup_{x\in\mathbb{R}^d}\int_{B(x,R)}|w_N|.$$

The supremum is uniformly bounded. Hence

$$\big|(N-1)\operatorname{Tr}\big(\Gamma_{N,\hbar,\beta}(B_\hbar)_{j'}(B_\hbar)_2 w_{12}\big)\big| \le \frac{C}{N^{1/2}}\sqrt{\operatorname{Tr}(\Gamma_{N,\hbar,\beta}|w_{12}|)}. \tag{B.64}$$

The estimate on $\operatorname{Tr}(\Gamma_{N,\hbar,\beta}|w_{12}|)$ depends on the value of η. If $\eta = 0$, then $w_N = w$ and we have $\operatorname{Tr}(\Gamma_{N,\hbar,\beta}|w_{12}|) = O(1)$ by the Lieb-Thirring inequality. If $\eta > 1/d$, we have assumed that $w \ge 0$, hence $\operatorname{Tr}(\Gamma_{N,\hbar,\beta}|w_{12}|) = \operatorname{Tr}(\Gamma_{N,\hbar,\beta}w_{12})$ is uniformly bounded since this term appears in the energy. Finally, when $0 < \eta < 1/d$, the Lieb-Thirring inequality implies

$$\operatorname{Tr}(\Gamma_{N,\hbar,\beta}|w_{12}|) \le C\|w_N\|_{L^{1+d/2}(\mathbb{R}^d)} = CN^{d\eta\frac{d/2}{1+d/2}}\|w\|_{L^{1+d/2}(\mathbb{R}^d)}.$$

When inserted in (B.64), we obtain an error of the order $N^{-\frac{1}{2}+\frac{d\eta}{2}\frac{1}{1+d/2}} \to 0$. This concludes the proof of Lemma B.15. □

At this point we have finished the proof of Theorems B.2 and B.8 for the exact N-particle Gibbs states $\Gamma_{N,\hbar,\beta}$. It is possible to handle approximate Gibbs states using the relative entropy and Pinsker's inequality as we did for the one-particle Husimi functions. Indeed, consider a sequence of states Γ_N such that

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

We can write

$$\mathcal{E}_{\mathrm{Can}}^{N,\hbar}(\Gamma_N) - e_{\mathrm{Can}}^{\beta}(\hbar, N) = \frac{1}{\beta}\,\mathcal{H}(\Gamma_N, \Gamma_{N,\hbar,\beta})$$

where $\mathcal{H}(A,B) = \operatorname{Tr} A(\log A - \log B)$ if the relative entropy. From the quantum Pinsker inequality $\mathcal{H}(A,B) \geq \|A-B\|_{\mathfrak{S}^1}^2/2$ we infer that

$$\operatorname{Tr}|\Gamma_N - \Gamma_{N,\hbar,\beta}| \longrightarrow 0$$

in trace norm. Since $\|m_{f,\Gamma}^{(k)}\|_{L^\infty(\mathbb{R}^{2dk})} \leq \operatorname{Tr}|\Gamma|$ by [18, Eq. (1.15)], we conclude that

$$\|m_{f,\Gamma_N}^{(k)} - m_{f,\Gamma_{N,\hbar,\beta}}^{(k)}\|_{L^\infty(\mathbb{R}^{2dk})} \longrightarrow 0.$$

Therefore $m_{f,\Gamma_N}^{(k)}$ has the same weak limit as the exact Gibbs state. The proof of Theorems B.2 and B.8 is now complete.

B.6 Proof of Theorem B.1: Study of the semiclassical functional

This section is devoted to the proof of Theorem B.1 and some auxiliary results on the semiclassical functional. We begin our analysis with the free particle case ($w = 0$) and then generalize to systems with pair interaction. We recall that the magnetic potential does not affect the energy, only the minimizer, and can be removed by a change of variables so we do not consider it here. For this section and for $\rho > 0$ we denote by

$$S_{\mathrm{Vla}}(\rho) = \left\{ m \in L^1(\mathbb{R}^{2d}) \,\middle|\, 0 \leq m \leq 1,\ \tfrac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} m = \rho \right\}.$$

the set of admissible semi-classical measures.

B.6.1 The free gas

Proposition B.16 (Minimizing the free semi-classical energy). *Suppose that $w = 0$, and that $V_+ \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ satisfies $\int_{\mathbb{R}^d} e^{-\beta V_+(x)}\,\mathrm{d}x < \infty$ for some $\beta > 0$ and $V_- \in L^{d/2}(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$. Fix $\rho > 0$ and define $m_0 \in S_{\mathrm{Vla}}(\rho)$ by*

$$m_0(x,p) := \frac{1}{1 + e^{\beta(p^2 + V(x) - \mu)}},$$

where μ is the unique chemical potential such that

$$\frac{1}{(2\pi)^d}\iint_{\mathbb{R}^{2d}} m_0(x,p)\,\mathrm{d}x\,\mathrm{d}p = \rho.$$

Then

$$\begin{aligned} e^{\beta,0}_{\mathrm{Vla}}(\rho) &= \mathcal{E}^{\beta,\rho,0}_{\mathrm{Vla}}(m_0) \\ &= -\frac{1}{(2\pi)^d\beta}\int_{\mathbb{R}^{2d}} \log\left(1+e^{-\beta(p^2+V(x)-\mu)}\right)\mathrm{d}x\,\mathrm{d}p + \mu\rho. \end{aligned} \tag{B.65}$$

Proof. The map

$$\begin{aligned} R:\ \ &\mathbb{R} \longrightarrow \mathbb{R} \\ &\mu \longmapsto (2\pi)^{-d}\iint_{\mathbb{R}^{2d}} m_0(x,p)\,\mathrm{d}x\,\mathrm{d}p \end{aligned}$$

is well-defined on $\mathbb{R}$, using that

$$\frac{1}{1+e^{\beta(p^2+V(x)-\mu)}} \leq \frac{\max(1,e^{\beta\mu})}{1+e^{\beta(p^2+V(x))}}$$

which is integrable under our conditions on V, by the remarks after Theorem B.1. In addition, R is increasing and continuous with

$$\lim_{\mu\to-\infty} R(\mu) = 0, \qquad \lim_{\mu\to+\infty} R(\mu) = +\infty.$$

Therefore we can always find μ so that the density of m_0 equals the given ρ. Note then that

$$1 - m_0(x,p) = e^{\beta(p^2+V(x)-\mu)}m_0(x,p) = \frac{1}{1+e^{-\beta(p^2+V(x)-\mu)}},$$

so that

$$\begin{aligned} \mathcal{E}^{\beta,\rho,0}_{\mathrm{Vla}}(m_0) &= \frac{1}{(2\pi)^d\beta}\int_{\mathbb{R}^{2d}} \Big(\beta(p^2+V(x)-\mu)m_0 + m_0\log m_0 \\ &\qquad\qquad - m_0\log\left(e^{\beta(p^2+V(x)-\mu)}m_0\right)\Big)\,\mathrm{d}x\,\mathrm{d}p \\ &\quad + \frac{1}{(2\pi)^d\beta}\int_{\mathbb{R}^{2d}} \left(\log(1-m_0)+\beta\mu\,m_0\right)\,\mathrm{d}x\,\mathrm{d}p \\ &= -\frac{1}{(2\pi)^d\beta}\int_{\mathbb{R}^{2d}} \log(1+e^{-\beta(p^2+V(x)-\mu)})\,\mathrm{d}x\,\mathrm{d}p + \mu\rho, \end{aligned}$$

showing the second equality in (B.65). That m_0 is the minimizer follows from the fact that the free energy is strictly convex. For instance, for any other $m \in S_{\mathrm{Vla}}(\rho)$, since the function $s(t) = t\log t + (1-t)\log(1-t)$ is convex on $(0,1)$ with derivative $s'(t) = \log(\frac{t}{1-t})$, we have pointwise

$$\begin{aligned} s(m) &\geq s(m_0) + s'(m_0)(m-m_0) \\ &= -\beta(p^2+V(x)-\mu)m + \beta(p^2+V(x)-\mu)m_0 + s(m_0), \end{aligned} \tag{B.66}$$

replacing m_0 by its expression implies that $\mathcal{E}^{\beta,\rho,0}_{\mathrm{Vla}}(m) \geq \mathcal{E}^{\beta,\rho,0}_{\mathrm{Vla}}(m_0)$. That m_0 is the unique minimizer follows from the fact that $\mathcal{E}^{\beta,\rho,0}_{\mathrm{Vla}}$ is a strictly convex functional. □

Remark B.17. *For an arbitrary domain $\Omega \subseteq \mathbb{R}^{2d}$, we have by the very same arguments that*

$$\min_{\substack{m \in L^1(\Omega) \\ 0 \le m \le 1}} \left\{ \frac{1}{(2\pi)^d} \int_\Omega \big((p^2 + V(x)) m(x,p) \,\mathrm{d}x + \frac{1}{\beta} s(m(x,p)) \big) \,\mathrm{d}x \,\mathrm{d}p \right\} = -\frac{1}{(2\pi)^d \beta} \int_\Omega \log\big(1 + e^{-\beta(p^2+V(x))}\big) \,\mathrm{d}x \,\mathrm{d}p.$$

with the unique minimizer $\widetilde{m_0}(x,p) = (1 + e^{\beta(p^2+V(x))})^{-1}$ and no chemical potential since we have dropped the mass constraint.

B.6.2 The interacting gas

We now deal with the interacting case. When $w \neq 0$, to retrieve the existence of minimizers as well as their expression, we need to use compactness techniques and compute the Euler-Lagrange equation. We divide the proof in several lemmas. We start by proving the semi-continuity of the functional in Lemma B.18 and then prove the existence of minimizers on $S_{\mathrm{Vla}}(\rho)$ in Lemma B.19. To obtain the form of the minimizers we compute the Euler-Lagrange equation but because the entropy s is not differentiable in 0 and 1 we first need to prove in Lemma B.20 that minimizers cannot be equal to 0 nor 1 in sets of non zero measure. The proof of Theorem B.1 is given at the end of this subsection.

Lemma B.18. *Fix $\rho, \beta_0 > 0$. Suppose that $w = 0$, and that $V_+ \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$, $V_- \in L^{d/2}(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ satisfies $\int_{\mathbb{R}^d} e^{-\beta_0 V_+(x)} \,\mathrm{d}x < \infty$. Then for all $\beta > \beta_0$, $\mathcal{E}^{\beta,\rho,0}_{\mathrm{Vla}}$ is L^1-strongly lower semi-continuous on $S_{\mathrm{Vla}}(\rho)$.*

Proof. We have to show that for any $C_0 \in \mathbb{R}$

$$\mathcal{L}(C_0) := \left\{ m \in S_{\mathrm{Vla}}(\rho) \,\middle|\, \mathcal{E}^{\beta,\rho,0}_{\mathrm{Vla}}(m) \le C_0 \right\}$$

is closed with respect to the L^1-norm on $S_{\mathrm{Vla}}(\rho)$. Let $(m_n) \subseteq \mathcal{L}(C_0)$ be a sequence converging towards some $m \in L^1(\mathbb{R}^d)$ with respect to the L^1-norm. By the L^1 convergence we immediately have $\frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} m = \rho$, we can also extract a subsequence converging almost everywhere and obtain $0 \le m \le 1$. Applying Remark B.17 with $\Omega = \{|x| + |y| \ge R\}$, we have for any $R > 0$ that

$$\frac{1}{(2\pi)^d} \iint_{|x|+|p| \ge R} (p^2 + V(x)) m_n(x,p) + \frac{1}{\beta} s(m_n(x,p)) \,\mathrm{d}x \,\mathrm{d}p \ge -\frac{1}{\beta} \iint_{|x|+|p| \ge R} \log\big(1 + e^{-\beta(p^2+V(x))}\big) \,\mathrm{d}x \,\mathrm{d}p = o_R(1). \tag{B.67}$$

Now we use that (m_n) is bounded in $L^\infty(\mathbb{R}^{2d})$ to obtain that $m_n \to m$ in $L^p(\mathbb{R}^{2d})$ for all $1 \le p < \infty$. By Fatou's lemma and dominated convergence we obtain

$$\liminf_{n\to\infty} \iint_{|x|+|p|\le R} (p^2 + V_+(x)) m_n(x,p)\,\mathrm{d}x\,\mathrm{d}p \geq \iint_{|x|+|p|\le R} (p^2 + V_+(x)) m(x,p)\,\mathrm{d}x\,\mathrm{d}p,$$

$$\iint_{|x|+|p|\le R} V_-(x) m_n(x,p)\,\mathrm{d}x\,\mathrm{d}p \underset{n\to\infty}{\longrightarrow} \iint_{|x|+|p|\le R} V_-(x) m(x,p)\,\mathrm{d}x\,\mathrm{d}p.$$

It remains to deal with the entropy term: by continuity of s and by dominated convergence we have

$$\iint_{|x|+|p|\le R} s(m_n(x,p))\,\mathrm{d}x\,\mathrm{d}p \underset{n\to\infty}{\longrightarrow} \iint_{|x|+|p|\le R} s(m(x,p))\,\mathrm{d}x\,\mathrm{d}p.$$

All in all we obtain

$$\begin{aligned}
C_0 &\geq \liminf_{n\to\infty} \mathcal{E}^{\beta,\rho,0}_{\mathrm{Vla}}(m_n) \\
&\geq \frac{1}{(2\pi)^d} \iint_{|x|+|p|\le R} (p^2 + V(x)) m(x,p)\,\mathrm{d}x\,\mathrm{d}p \\
&\quad + \frac{1}{\beta} \iint_{|x|+|p|\le R} s(m(x,p))\,\mathrm{d}x\,\mathrm{d}p + o(R) \\
&\geq \frac{1}{(2\pi)^d} \iint_{|x|+|p|\le R} (p^2 + V_+(x)) m(x,p)\,\mathrm{d}x\,\mathrm{d}p + o(R) \\
&\quad - \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} V_-(x) m(x,p)\,\mathrm{d}x\,\mathrm{d}p + \frac{1}{\beta} \iint_{\mathbb{R}^{2d}} s(m(x,p))\,\mathrm{d}x\,\mathrm{d}p.
\end{aligned}$$

Finally, we use the monotone convergence theorem and let R tend to ∞ to obtain $\mathcal{E}^{\beta,\rho,0}_{\mathrm{Vla}}(m) \le C_0$. □

Lemma B.19. *Fix $\rho, \beta_0 > 0$. Suppose that $w \in L^{1+d/2}(\mathbb{R}^d) + L^\infty_\varepsilon(\mathbb{R}^d) + \mathbb{R}_+\delta_0$, $V_+ \in L^1_{\mathrm{loc}}(\mathbb{R}^d), V_- \in L^{1+d/2}(\mathbb{R}^d)$ satisfies $\int_{\mathbb{R}^d} e^{-\beta_0 V_+(x)}\,\mathrm{d}x < \infty$ and $V_+(x) \to \infty$ as $|x| \to \infty$. Then for all $\beta > \beta_0$, $\mathcal{E}^{\beta,\rho}_{\mathrm{Vla}}$ is bounded below and has a minimizer m_0 in $S_{\mathrm{Vla}}(\rho)$.*

Proof. Let $(m_n) \subseteq S_{\mathrm{Vla}}(\rho)$ be a minimizing sequence, i.e. $\mathcal{E}^{\beta,\rho}_{\mathrm{Vla}}(m_n) \to e^{\beta}_{\mathrm{Vla}}(\rho)$ as $n \to \infty$. Since (m_n) is bounded in both $L^1(\mathbb{R}^{2d})$ and $L^\infty(\mathbb{R}^{2d})$, one can verify that up to extraction the sequence has a weak limit $m_0 \in L^1(\mathbb{R}^{2d}) \cap L^\infty(\mathbb{R}^{2d})$ satisfying

$$\int_{\mathbb{R}^{2d}} m_n(x,p)\varphi(x,p)\,\mathrm{d}x\,\mathrm{d}p \to \int_{\mathbb{R}^{2d}} m_0(x,p)\varphi(x,p)\,\mathrm{d}x\,\mathrm{d}p \tag{B.68}$$

for any $\varphi \in L^1(\mathbb{R}^{2d}) + L^\infty_\varepsilon(\mathbb{R}^{2d})$. Moreover, the weak limit m_0 satisfies $0 \le m_0 \le 1$ and $\int_{\mathbb{R}^{2d}} m_0 \le \rho(2\pi)^d$. Note that we do not have pointwise convergence a priori.

Let us prove that m_0 is a minimizer of $\mathcal{E}^{\beta,\rho}_{\rm Vla}$ in $S_{\rm Vla}(\rho)$. Our first step is to show the tightness of the sequence of probability measures (m_n) to obtain $\int_{\mathbb{R}^{2d}} m_0 = (2\pi)^d\rho$, then we argue that $m_0 \in S_{\rm Vla}(\rho)$ and minimizes $\mathcal{E}^{\beta,\rho}_{\rm Vla}$ using weak lower-semicontinuity.

We start out by bounding the interaction term using some of the kinetic energy. Let $\varepsilon > 0$ and let us write $w = w_1 + w_2 + a\delta_0$ with $w_1 \in L^{1+d/2}(\mathbb{R}^d)$, $\|w_2\|_{L^\infty(\mathbb{R}^d)} < \varepsilon$ and $a \geq 0$. We use Young's inequality to bound the interaction term

$$\begin{aligned}\int_{\mathbb{R}^d} w * \rho_{m_n}\rho_{m_n} &\geq \|w_1\|_{L^{1+d/2}(\mathbb{R}^d)}\|\rho_{m_n}\|_{L^{1+2/d}(\mathbb{R}^d)}\|\rho_{m_n}\|_{L^1(\mathbb{R}^d)} \\ &\quad + \|w_2\|_{L^\infty(\mathbb{R}^d)}\|\rho_{m_n}\|^2_{L^1(\mathbb{R}^d)} \\ &\geq C\varepsilon \iint_{\mathbb{R}^{2d}} p^2 m_n(x,p)\,\mathrm{d}x\,\mathrm{d}p - C. \end{aligned}\tag{B.69}$$

In the last inequality we have used the well-known fact [38] that

$$\begin{aligned}\int_{\mathbb{R}^d} p^2 m(x,p)\,\mathrm{d}p &\geq \inf_{\substack{0\leq \widetilde{m}\leq 1 \\ \int \widetilde{m} = (2\pi)^d \rho_m(x)}} \int_{\mathbb{R}^d} p^2 \widetilde{m}(p)\,\mathrm{d}p \\ &= (2\pi)^d c_{\rm TF}\frac{d}{d+2}\rho_m(x)^{1+2/d}, \end{aligned}\tag{B.70}$$

which gives the Lieb-Thirring inequality for classical measures on phase space. Similarly we have

$$\int_{\mathbb{R}^d} V_-(x)\rho_{m_n}(x)\,\mathrm{d}x \leq C\Big(\varepsilon^{-d/2}\|V_-\|^{1+d/2}_{L^{1+d/2}(\mathbb{R}^d)} + \varepsilon\|\rho_{m_n}\|^{1+2/d}_{L^{1+2/d}(\mathbb{R}^d)}\Big). \tag{B.71}$$

Now using Proposition B.16, (B.70), (B.69) and (B.71), denoting $\alpha = (\beta-\beta_0)/(2\beta)$ we have

$$\begin{aligned} C \geq \mathcal{E}^{\beta,\rho}_{\rm Vla}(m_n) &\geq \frac{\alpha}{(2\pi)^d}\iint_{\mathbb{R}^{2d}} (p^2 + V(x))m_n + \frac{1}{2\rho}\int_{\mathbb{R}^d}(w*\rho_{m_n})\rho_{m_n} \\ &\quad + \frac{1}{2}e^{\beta(1-\alpha),0}_{\rm Vla}(\rho) \\ &\geq \frac{\alpha - C\varepsilon}{(2\pi)^d}\iint_{\mathbb{R}^{2d}}(p^2+V_+(x))m_n - C \end{aligned}\tag{B.72}$$

Note that by construction, $\beta(1-\alpha) > \beta_0$. Taking $\varepsilon > 0$ sufficiently small but positive, the above inequality shows the tightness condition

$$\iint_{\mathbb{R}^{2d}} (p^2 + V_+(x))m_n(x,p)\,\mathrm{d}x\,\mathrm{d}p \leq C. \tag{B.73}$$

Therefore $\iint_{\mathbb{R}^{2d}} m_0 = (2\pi)^d\rho$.

Now we prove that $\liminf_{n\to\infty}\mathcal{E}^{\beta,\rho}_{\rm Vla}(m_n) \geq \mathcal{E}^{\beta,\rho}_{\rm Vla}(m_0)$. From the tightness condition it is easy to verify that $\rho_{m_n} \rightharpoonup \rho_{m_0}$ and that

$$\int_{\mathbb{R}^d}(w - a\delta_0) * \rho_{m_n}\rho_{m_n} \to \int_{\mathbb{R}^d}(w-a\delta_0)*\rho_{m_0}\rho_{m_0}.$$

To finish, we deal with the delta part of the interaction as well as the entropy part. We use that a continuous convex function is always weakly lower semi-continuous. We obain

$$a\int_{\mathbb{R}^d}\rho_{m_0}^2=\int_{\mathbb{R}^d}\lim_{n\to\infty}\rho_{m_n}^2\leq\lim_{n\to\infty}\int_{\mathbb{R}^d}\rho_{m_n}^2,$$
$$\int_{\mathbb{R}^d}s(m_0)=\int_{\mathbb{R}^d}\lim_{n\to\infty}s(m_n)\leq\liminf_{n\to\infty}\int_{\mathbb{R}^d}s(m_n).$$

□

Lemma B.20. *Fix $\rho,\beta_0>0$. Suppose that $w\in L^{1+d/2}(\mathbb{R}^d)+L^\infty_\varepsilon(\mathbb{R}^d)+\mathbb{R}_+\delta_0$, $V_+\in L^1_{\text{loc}}(\mathbb{R}^d), V_-\in L^{1+d/2}(\mathbb{R}^d)$ satisfies $\int_{\mathbb{R}^d}e^{-\beta_0V_+(x)}\,\mathrm{d}x<\infty$ and $V_+(x)\to\infty$ as $|x|\to\infty$. Then any minimizer $m_0\in S_{\text{Vla}}(\rho)$ of $\mathcal{E}^{\beta,\rho}_{\text{Vla}}$ satisfies*

$$0<m(x,p)<1,\qquad \textit{for } (x,p)\in\mathbb{R}^{2d} \textit{ almost everywhere.}$$

Proof. Define $\Omega_1:=\{m_0=1\}$ and $\Omega_0:=\{m_0=0\}$. Our goal is to prove that Ω_1 and Ω_0 have 0 measure. To this end, we will first show that $|\Omega_1||\Omega_0|=0$. Then we use that at least one of them is a null set to prove that so is the other one. Let us first assume neither of them are null sets. Let $r>0$, $0<\lambda<\frac{1}{2}$ and for almost every $(\xi_1,\xi_2)\in\Omega_1\times\Omega_0$ define

$$\varphi_1=\lambda\mathbb{1}_{B(\xi_1,r)\cap\Omega_1},\qquad \varphi_2=\lambda\mathbb{1}_{B(\xi_2,r')\cap\Omega_0},$$

where $r':=\min\{s\geq 0\,|\,|B(\xi_2,s)\cap\Omega_0|=|B(\xi_1,r)\cap\Omega_1|\}$. We will use the notation $v(r)=|B(\xi_1,r)\cap\Omega_1|$. Note that by Lebesgue's density theorem, for almost every $(\xi_1,\xi_2)\in\Omega_1\times\Omega_0$ we have $v(r)>0$ and $r'<\infty$. In order to obtain a contradiction, we will use $m_0-\varphi_1+\varphi_2\in S_{\text{Vla}}(\rho)$ as a trial state and that m_0 is a minimizer of $\mathcal{E}^{\beta,\rho}_{\text{Vla}}$. Let us estimate the entropy, using that $s(0)=s(1)=0$ and $s(t)=s(1-t)$, we obtain

$$\begin{aligned}\iint_{\mathbb{R}^{2d}}s(m_0-\varphi_1+\varphi_2)&=\iint_{\mathbb{R}^{2d}}s(m_0)+s(\varphi_1)+s(\varphi_2)\\&=2s(\lambda)v(r)+\iint_{\mathbb{R}^{2d}}s(m_0).\end{aligned}$$

It remains to estimate the contribution to the interaction energy, we have

$$\begin{aligned}\int_{\mathbb{R}^d}\rho_{m_0-\varphi_1+\varphi_2}w*\rho_{m_0-\varphi_1+\varphi_2}&=\int_{\mathbb{R}^d}\rho_{m_0}w*\rho_{m_0}+2\int_{\mathbb{R}^d}\rho_{\varphi_2-\varphi_1}w*\rho_{m_0}\\&\quad+\int_{\mathbb{R}^d}\rho_{\varphi_2-\varphi_1}w*\rho_{\varphi_2-\varphi_1}.\end{aligned}$$

Let $\varepsilon > 0$ and let us write $w = w_1 + w_2 + a\delta_0$ with $w_1 \in L^{1+d/2}(\mathbb{R}^d)$, $\|w_2\|_{L^\infty(\mathbb{R}^d)} < \varepsilon$ and $a \geq 0$. We first use Young's inequality to bound the last term

$$\begin{aligned}
&\int_{\mathbb{R}^d} w * (\rho_{\varphi_2} - \rho_{\varphi_1})(\rho_{\varphi_2} - \rho_{\varphi_1}) \\
&\qquad \leq \|w_1\|_{L^{1+d/2}(\mathbb{R}^d)} \|\rho_{\varphi_2} - \rho_{\varphi_1}\|_{L^1(\mathbb{R}^d)} \|\rho_{\varphi_2} - \rho_{\varphi_1}\|_{L^{1+2/d}(\mathbb{R}^d)} \\
&\qquad\quad + \|w_2\|_{L^\infty_\varepsilon(\mathbb{R}^d)} \|\rho_{\varphi_2} - \rho_{\varphi_1}\|^2_{L^1(\mathbb{R}^d)} + a\|\rho_{\varphi_2} - \rho_{\varphi_1}\|^2_{L^2(\mathbb{R}^d)} \\
&\qquad \leq C\lambda^2 \big(\|w\|_{L^{1+d/2}(\mathbb{R}^d)} v(r)^{1+\frac{d}{d+2}} + \|w_2\|_{L^\infty_\varepsilon(\mathbb{R}^d)} v(r)^2 + av(r)\big).
\end{aligned}$$

Next and similarly we estimate the second term (minus the delta interaction)

$$\begin{aligned}
&\int_{\mathbb{R}^d} (w_1 + w_2) * \rho_{m_0}(\rho_{\varphi_2} - \rho_{\varphi_1}) \\
&\quad \leq \|w_1\|_{L^{1+d/2}(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^{1+2/d}(\mathbb{R}^d)} \|\rho_{\varphi_2} - \rho_{\varphi_1}\|_{L^1(\mathbb{R}^d)} \\
&\quad\quad + \|w_2\|_{L^\infty_\varepsilon(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^1(\mathbb{R}^d)} \|\rho_{\varphi_2} - \rho_{\varphi_1}\|_{L^1(\mathbb{R}^d)} \\
&\quad \leq C\lambda\big(\|w_1\|_{L^{1+d/2}(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^{1+2/d}(\mathbb{R}^d)} + \|w_2\|_{L^\infty_\varepsilon(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^1(\mathbb{R}^d)}\big) v(r).
\end{aligned}$$

Since m_0 is a minimizer, these estimates imply that

$$\begin{aligned}
\mathcal{E}^{\beta,\rho}_{\mathrm{Vla}}(m_0) &\leq \mathcal{E}^{\beta,\rho}_{\mathrm{Vla}}(m_0 - \varphi_1 + \varphi_2) \\
&\leq \mathcal{E}^{\beta,\rho}_{\mathrm{Vla}}(m_0) + \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} (p^2 + V(x) + a\rho_{m_0})(\varphi_2 - \varphi_1) \\
&\quad + C\lambda^2 \big(\|w\|_{L^{1+d/2}(\mathbb{R}^d)} v(r)^{1+\frac{d}{d+2}} + \|w_2\|_{L^\infty_\varepsilon(\mathbb{R}^d)} v(r)^2 + av(r)\big) \\
&\quad + C\lambda\big(\|w_1\|_{L^{1+d/2}(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^{1+2/d}(\mathbb{R}^d)} \\
&\qquad\qquad + \|w_2\|_{L^\infty_\varepsilon(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^1(\mathbb{R}^d)} \big) v(r) + \frac{2s(\lambda)}{(2\pi)^d \beta} v(r).
\end{aligned}$$

Now we divide the last inequality by $v(r)$ and we let r tend to zero and use the Lebesgue differentiation theorem (and the Lebesgue density theorem), to obtain that for almost all $(\xi_1, \xi_2) \in \Omega_1 \times \Omega_0$

$$\begin{aligned}
-\frac{2s(\lambda)}{\lambda\beta} \leq &\; - p_1^2 - V(x_1) - a\rho_{m_0}(x_1) + p_2^2 + V(x_2) + a\rho_{m_0}(x_2) \\
&+ C \|w\|_{L^{1+d/2}(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^{1+2/d}(\mathbb{R}^d)}.
\end{aligned}$$

Now letting λ tend to zero, we have that for almost all $(\xi_1, \xi_2) \in \Omega_1 \times \Omega_0$, $p_2^2 + V(x_2) + a\rho_{m_0}(x_2) - p_1^2 - V(x_1) - a\rho_{m_0}(x_1) = \infty$ which, since $V \in L^{1+d/2}_{\mathrm{loc}}(\mathbb{R}^d)$ and $\rho_{m_0} \in L^{1+2/d}_{\mathrm{loc}}(\mathbb{R}^d)$, implies that $|\Omega_1 \times \Omega_0| = 0$. Therefore, at least one of them is a null set, we will treat the case where $|\Omega_0| = 0$ and $|\Omega_1| \neq 0$, the other one can be dealt with similarly. Because m has finite mass we can find $\varepsilon > 0$ such that $\Omega_{2,\varepsilon} := \{1 - \varepsilon \leq m(x,p) \leq 1 - \varepsilon/2\}$ is not a null set. Defining φ_1 and φ_2 (replacing

Ω_0 by $\Omega_{2,\varepsilon}$) as before and doing the same computations we obtain that for almost all $(\xi_1, \xi_2) \in \Omega_1 \times \Omega_{2,\varepsilon}$

$$-\frac{s(\lambda)}{\lambda\beta} \leq -p_1^2 - V(x_1) - a\rho_{m_0}(x_1) + p_2^2 + V(x_2) + a\rho_{m_0}(x_2) \\ + \frac{s(m(\xi_2)-\lambda) - s(m(\xi_2))}{\lambda} + C\, \|w\|_{L^{1+d/2}(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^{1+2/d}(\mathbb{R}^d)}\,.$$

Because s is continuously differentiable on $[1-2\varepsilon, 1-\varepsilon/2]$, the difference quotient above is bounded uniformly in $\xi_2 \in \Omega_{2,\varepsilon}$ and $\lambda > 0$ small enough. Letting λ tend to zero, we end up with the same contradiction as before showing that Ω_1 is a null set. □

Proof of Theorem B.1. We assume $A = 0$ without loss of generality, since it can be removed by a change of variable.

We will first show that the expression (B.5) of the minimizers is correct by computing the Euler-Lagrange equation associated with any such minimizer m_0. This gives automatically the expression of the minimum energy (B.6). We conclude, in the case $\widehat{w} \geq 0$, by showing that the chemical potential μ is given by (B.8).

Let $\varepsilon > 0$ small enough and $\varphi \in L^1 \cap L^\infty(\{\varepsilon < m_0 < 1-\varepsilon\})$ such that $\iint_{\mathbb{R}^{2d}} \varphi(x,p)\,\mathrm{d}x\,\mathrm{d}p = (2\pi)^d\rho$. For $\delta = \frac{\varepsilon}{1+\|\varphi\|_\infty}$ we have

$$m_t := \frac{m_0 + t\varphi}{1+t} \in S_{\mathrm{Vla}}(\rho)$$

for all $t \in (-\delta, \delta)$. Since m_0 is a minimizer, we must have $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}^\beta_{\mathrm{Vla}}(m_t)|_{t=0} = 0$. Using that $\frac{\mathrm{d}}{\mathrm{d}t}m_t = (\varphi - m_0)(1+t)^{-2}$ and $s'(t) = \log(\frac{t}{1-t})$ we obtain

$$\iint_{\mathbb{R}^{2d}} \Big(p^2 + V(x) + \frac{1}{\rho} w * \rho_{m_0}(x) + \frac{1}{\beta}\log\Big(\frac{m_0(x,p)}{1-m_0(x,p)}\Big)\Big)\varphi(x,p)\,\mathrm{d}x\,\mathrm{d}p \\ = \iint_{\mathbb{R}^{2d}} \Big(p^2 + V(x) + \frac{1}{\rho} w * \rho_{m_0}(x) \\ + \frac{1}{\beta}\log\Big(\frac{m_0(x,p)}{1-m_0(x,p)}\Big)\Big)m_0(x,p)\,\mathrm{d}x\,\mathrm{d}p.$$

Denoting the right hand side by $(2\pi)^d\mu_{\mathrm{Vla}}(\rho)\rho$, we have shown for any φ verifying the above conditions that

$$\iint_{\{\varepsilon<m<1-\varepsilon\}} \Big(p^2 + V(x) + \frac{1}{\rho} w * \rho_{m_0}(x) \\ + \frac{1}{\beta}\log(\frac{m_0(x,p)}{1-m_0(x,p)}) - \mu_{\mathrm{Vla}}(\rho)\Big)\varphi(x,p)\,\mathrm{d}x\,\mathrm{d}p = 0.$$

This is enough for the left factor in the integrand above to be zero almost everywhere on $\{\varepsilon < m_0 < 1-\varepsilon\}$. But ε can be taken arbitrary small and by Lemma B.20 we have $\bigcup_{\varepsilon>0}\{\varepsilon < m_0 < 1-\varepsilon\} = \{0 < m_0 < 1\} = \mathbb{R}^{2d}$ almost everywhere, from which we obtain (B.5).

That $\rho_{m_0} \in L^2(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ follows from Lemma B.13 and the fact that m_0 satisfies (B.5).

It remains to prove (B.8) when it is assumed that $\widehat{w} \geq 0$. This is a classical argument and we only sketch it, we refer to [41] for further details. First note that the assumption $\widehat{w} \geq 0$ ensures the convexity of $\mathcal{E}_{\text{Vla}}^{\beta,\rho}$, hence for $\rho' > 0$, $F_{\text{Vla}}^{\beta}(\rho', \rho)$ is the minimum of a convex function under a linear constraint, it is therefore convex. This implies that, for $\rho' > 0$, the function $F_{\text{Vla}}^{\beta}(\cdot, \rho')$ is continuous on $\mathbb{R}_+$ and continuously differentiable except maybe in a countable number of values of ρ. We first show that

$$\mathbb{R}_+^* \ni \rho \mapsto \mu(\rho) \in \mathbb{R}$$

defines a bijection, where $\mu(\rho)$, defined in (B.5), is the Lagrange multiplier associated to the constraint ρ. Consider, for $\mu \in \mathbb{R}$, the unconstrained minimization problem

$$\inf_{0\leq m\leq 1} \mathcal{E}_{\text{Vla}}^{\beta,\rho'}(m) - \frac{\mu}{(2\pi)^d}\iint_{\mathbb{R}^{2d}} m = \inf_{\rho\geq 0} F_{\text{Vla}}^{\beta}(\rho,\rho') - \mu\rho. \tag{B.74}$$

This yields a minimizer m^μ and hence a density $\rho(\mu) := (2\pi)^{-d}\iint m^\mu$, see Remark B.17. The expression of m^μ can be computed through the Euler-Lagrange equation,

$$m^\mu = \frac{1}{1 + e^{\beta(p^2 + V + \rho'^{-1}\rho_{m^\mu} * w - \mu)}}$$

From (B.74), the density m^μ must also satisfy $\mathcal{E}_{\text{Vla}}^{\beta,\rho'}(m^\mu) = F_{\text{Vla}}^{\beta}(\rho(\mu), \rho')$ and since $\widehat{w} \geq 0$, we conclude that m^μ is also the unique solution of this equation and must satisfy (B.5) where $\mu(\rho)$ appears. By identification, $\mu = \mu(\rho)$ is the Lagrange multiplier associated to the minimization problem at density ρ. This proves the bijective correspondance between $\mu(\rho)$ and ρ.

Finally, if $F_{\text{Vla}}^{\beta}(\cdot, \rho')$ is differentiable in some ρ_0, the above discussion shows (B.8) for $\rho = \rho_0$. But because of the one-to-one correspondance between μ and ρ, $\partial_\rho F_{\text{Vla}}^{\beta}$ cannot be discontinuous, this concludes the proof. $\square$

Acknowledgement

We thank Robert Seiringer for useful comments. This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement MDFT No 725528 of M.L.). This work was started when P.S.M. was a visiting student at the University Paris-Dauphine. P.S.M. was partially supported by the Sapere Aude grant DFF–4181-00221 from the Independent Research Fund Denmark.

References

[1] G. L. Aki, P. A. Markowich, and C. Sparber. *Classical limit for semirelativistic Hartree systems. J. Math. Phys.*, **49**(10):102110, 10, 2008. ISSN 0022-2488. doi:10.1063/1.3000059.

[2] V. Bach, S. Breteaux, S. Petrat, P. Pickl, and T. Tzaneteas. *Kinetic energy estimates for the accuracy of the time-dependent Hartree-Fock approximation with Coulomb interaction. J. Math. Pures Appl.*, **105**(1):1–30, 2016. ISSN 0021-7824. doi:https://doi.org/10.1016/j.matpur.2015.09.003.

[3] V. Bach, E. H. Lieb, and J. P. Solovej. *Generalized Hartree-Fock theory and the Hubbard model. J. Statist. Phys.*, **76**(1-2):3–89, 1994. ISSN 0022-4715.

[4] C. Bardos, F. Golse, A. D. Gottlieb, and N. J. Mauser. *Mean field dynamics of fermions and the time-dependent Hartree-Fock equation. J. Math. Pures Appl. (9)*, **82**(6):665–683, 2003. ISSN 0021-7824. doi:10.1016/S0021-7824(03)00023-0.

[5] M. Barranco and J.-R. Buchler. *Equation of state of hot, dense stellar matter: Finite temperature nuclear Thomas-Fermi approach. Phys. Rev. C*, **24**:1191–1202, 1981. doi:10.1103/PhysRevC.24.1191.

[6] N. Benedikter, V. Jaksic, M. Porta, C. Saffirio, and B. Schlein. *Mean-field evolution of fermionic mixed states. Comm. Pure Appl. Math.*, **69**(12):2250–2303, 2016.

[7] N. Benedikter, P. Nam, M. Porta, B. Schlein, and R. Seiringer. *Optimal Upper Bound for the Correlation Energy of a Fermi Gas in the Mean-Field Regime. Communications in Mathematical Physics*, 2019. ISSN 1432-0916. doi:10.1007/s00220-019-03505-5.

[8] N. Benedikter, M. Porta, C. Saffirio, and B. Schlein. *From the Hartree dynamics to the Vlasov equation. Arch. Ration. Mech. Anal.*, **221**(1):273–334, 2016. ISSN 0003-9527. doi:10.1007/s00205-015-0961-z.

[9] N. Benedikter, M. Porta, and B. Schlein. *Mean-field dynamics of fermions with relativistic dispersion. J. Math. Phys.*, **55**(2):021901, 10, 2014. ISSN 0022-2488. doi:10.1063/1.4863349.

[10] N. Benedikter, M. Porta, and B. Schlein. *Mean-Field Evolution of Fermionic Systems. Comm. Math. Phys.*, **331**(3):1087–1131, 2014. ISSN 0010-3616. doi:10.1007/s00220-014-2031-z.

[11] L. G. Brown and H. Kosaki. *Jensen's inequality in semi-finite von Neumann algebras. J. Operator Theory*, **23**(1):3–19, 1990. ISSN 0379-4024.

[12] K. A. Brueckner, J. R. Buchler, S. Jorna, and R. J. Lombard. *Statistical Theory of Nuclei. Phys. Rev.*, **171**:1188–1195, 1968. doi:10.1103/PhysRev.171.1188.

[13] R. D. Cowan and J. Ashkin. *Extension of the Thomas-Fermi-Dirac Statistical Theory of the Atom to Finite Temperatures. Phys. Rev.*, **105**:144–157, 1957. doi:10.1103/PhysRev.105.144.

[14] H. L. Cycon, R. G. Froese, W. Kirsch, and B. Simon. *Schrödinger operators with application to quantum mechanics and global geometry.* Texts and Monographs in Physics. Springer-Verlag, Berlin, study edition, 1987. ISBN 3-540-16758-7.

[15] E. Dietler, S. Rademacher, and B. Schlein. *From Hartree dynamics to the relativistic Vlasov equation. J. Stat. Phys.*, **172**(2):398–433, 2018. ISSN 0022-4715. doi:10.1007/

s10955-018-1973-5.

[16] A. Elgart, L. Erdős, B. Schlein, and H.-T. Yau. *Nonlinear Hartree equation as the mean field limit of weakly coupled fermions. J. Math. Pures Appl.*, **83**(10):1241–1273, 2004. ISSN 0021-7824.

[17] R. P. Feynman, N. Metropolis, and E. Teller. *Equations of State of Elements Based on the Generalized Fermi-Thomas Theory. Phys. Rev.*, **75**:1561–1573, 1949. doi:10.1103/PhysRev.75.1561.

[18] S. Fournais, M. Lewin, and J. P. Solovej. *The semi-classical limit of large fermionic systems. Calc. Var. Partial Differ. Equ.*, pages 57–105, 2018. doi:10.1007/s00526-018-1374-2.

[19] J. Fröhlich and A. Knowles. *A microscopic derivation of the time-dependent Hartree-Fock equation with Coulomb two-body interaction. J. Stat. Phys.*, **145**(1):23–50, 2011. ISSN 0022-4715. doi:10.1007/s10955-011-0311-y.

[20] J. J. Gilvarry and G. H. Peebles. *Solutions of the Temperature-Perturbed Thomas-Fermi Equation. Phys. Rev.*, **99**:550–552, 1955. doi:10.1103/PhysRev.99.550.

[21] S. Giorgini, L. P. Pitaevskii, and S. Stringari. *Theory of ultracold atomic Fermi gases. Rev. Mod. Phys.*, **80**:1215–1274, 2008. doi:10.1103/RevModPhys.80.1215.

[22] F. Golse, C. Mouhot, and T. Paul. *On the Mean Field and Classical Limits of Quantum Mechanics. Comm. Math. Phys.*, **343**(1):165–205, 2016. ISSN 1432-0916. doi:10.1007/s00220-015-2485-7.

[23] F. Golse and T. Paul. *The Schrödinger equation in the mean-field and semiclassical regime. Arch. Ration. Mech. Anal.*, **223**(1):57–94, 2017. ISSN 0003-9527. doi:10.1007/s00205-016-1031-x.

[24] A. D. Gottlieb. *Examples of bosonic de Finetti states over finite dimensional Hilbert spaces. J. Stat. Phys.*, **121**(3-4):497–509, 2005. ISSN 0022-4715. doi:10.1007/s10955-005-7005-2.

[25] A. Grabsch, S. N. Majumdar, G. Schehr, and C. Texier. *Fluctuations of observables for free fermions in a harmonic trap at finite temperature. SciPost Phys.*, **4**:14, 2018. doi:10.21468/SciPostPhys.4.3.014.

[26] C. Hainzl, M. Porta, and F. Rexze. *On the correlation energy of the mean-field Fermi gas. ArXiv e-prints*, arXiv:1806.11411, 2018.

[27] B. Hauksson and J. Yngvason. *Asymptotic Exactness of Magnetic Thomas–Fermi Theory at Nonzero Temperature. Journal of Statistical Physics*, **116**(1):523–546, 2004. ISSN 1572-9613. doi:10.1023/B:JOSS.0000037223.74597.4e.

[28] P. Hertel, H. Narnhofer, and W. Thirring. *Thermodynamic functions for fermions with gravostatic and electrostatic interactions. Comm. Math. Phys.*, **28**(2):159–176, 1972. ISSN 0010-3616. doi:10.1007/BF01645513.

[29] P. Hertel and W. Thirring. *Free energy of gravitating fermions. Comm. Math. Phys.*, **24**(1):22–36, 1971. ISSN 0010-3616. doi:10.1007/BF01907031.

[30] R. Latter. *Temperature Behavior of the Thomas-Fermi Statistical Model for Atoms. Phys. Rev.*, **99**:1854–1870, 1955. doi:10.1103/PhysRev.99.1854.

[31] M. Lewin, P. Nam, and N. Rougerie. *Bose Gases at Positive Temperature and Non-Linear Gibbs Measures.* In *Proceedings of the International Congress of Mathematical*

Physics. 2015. ArXiv e-prints.

[32] M. Lewin, P. T. Nam, and N. Rougerie. *Derivation of Hartree's theory for generic mean-field Bose systems. Adv. Math.*, **254**:570–621, 2014. doi:10.1016/j.aim.2013.12.010.

[33] M. Lewin, P. T. Nam, and N. Rougerie. *Derivation of nonlinear Gibbs measures from many-body quantum mechanics. J. Éc. polytech. Math.*, **2**:65–115, 2015. doi:10.5802/jep.18.

[34] M. Lewin, P. T. Nam, and N. Rougerie. *Classical field theory limit of 2D many-body quantum Gibbs states. ArXiv e-prints*, 2018.

[35] M. Lewin, P. T. Nam, and N. Rougerie. *Gibbs measures based on 1D (an)harmonic oscillators as mean-field limits. J. Math. Phys.*, **59**:041901, 2018. doi:10.1063/1.5026963.

[36] M. Lewin, P. T. Nam, and N. Rougerie. *The interacting 2D Bose gas and nonlinear Gibbs measures.* In B. S. Giuseppe Genovese and V. Sohinger, editors, *Gibbs measures for nonlinear dispersive equations.* 2018. Oberwolfach mini-workshop.

[37] M. Lewin, P. T. Nam, S. Serfaty, and J. P. Solovej. *Bogoliubov spectrum of interacting Bose gases. Comm. Pure Appl. Math.*, **68**(3):413–471, 2015. doi:10.1002/cpa.21519.

[38] E. H. Lieb and M. Loss. *Analysis*, volume 14 of *Graduate Studies in Mathematics.* American Mathematical Society, Providence, RI, 2nd edition, 2001. ISBN 0-8218-2783-9.

[39] E. H. Lieb, R. Seiringer, and J. P. Solovej. *Ground-state energy of the low-density Fermi gas. Phys. Rev. A*, **71**:053605, 2005.

[40] E. H. Lieb and B. Simon. *The Hartree-Fock theory for Coulomb systems. Commun. Math. Phys.*, **53**(3):185–194, 1977. ISSN 0010-3616.

[41] E. H. Lieb and B. Simon. *The Thomas-Fermi theory of atoms, molecules and solids. Adv. Math.*, **23**(1):22–116, 1977. ISSN 0001-8708.

[42] E. H. Lieb and W. E. Thirring. *Bound on kinetic energy of fermions which proves stability of matter. Phys. Rev. Lett.*, **35**:687–689, 1975.

[43] E. H. Lieb and W. E. Thirring. *Inequalities for the moments of the eigenvalues of the Schrödinger hamiltonian and their relation to Sobolev inequalities*, pages 269–303. Studies in Mathematical Physics. Princeton University Press, 1976.

[44] E. H. Lieb and W. E. Thirring. *Gravitational collapse in quantum mechanics with relativistic kinetic energy. Ann. Physics*, **155**(2):494–512, 1984. ISSN 0003-4916.

[45] E. H. Lieb and H.-T. Yau. *The Chandrasekhar theory of stellar collapse as the limit of quantum mechanics. Commun. Math. Phys.*, **112**(1):147–174, 1987. ISSN 0010-3616.

[46] P. Madsen. *In preparation.* Ph.D. thesis, Aarhus University, 2019.

[47] N. H. March. *Equations of State of Elements from the Thomas-Fermi Theory II: Case of Incomplete Degeneracy. Proc. Phys. Soc.*, **68**(12):1145, 1955.

[48] R. E. Marshak and H. A. Bethe. *The Generalized Thomas-Fermi Method as Applied to Stars. Astrophys. J.*, **91**:239, 1940. doi:10.1086/144159.

[49] J. Messer. *Nonmonotonicity of the mass distribution and existence of the gravitational phase transition. Phys. Lett. A*, **83**(6):304–306, 1981. ISSN 0375-9601. doi:10.1016/0375-9601(81)90991-9.

[50] J. Messer. *On the gravitational phase transition in the Thomas-Fermi model. J. Math.*

Phys., **22**(12):2910–2917, 1981. ISSN 0022-2488. doi:10.1063/1.525172.

[51] J. Messer. *Temperature dependent Thomas-Fermi theory*, volume 147 of *Lecture Notes in Physics*. Springer-Verlag, Berlin-New York, 1981. ISBN 3-540-10875-0.

[52] H. Narnhofer and G. Sewell. *Vlasov hydrodynamics of a quantum mechanical model. Comm. Math. Phys.*, **79**(1):9–24, 1981. ISSN 0010-3616. doi:10.1007/BF01208282.

[53] H. Narnhofer and W. Thirring. *Asymptotic exactness of finite temperature Thomas-Fermi theory. Ann. Phys.*, **134**(1):128 – 140, 1981. ISSN 0003-4916. doi:10.1016/0003-4916(81)90008-7.

[54] S. Petrat and P. Pickl. *A new method and a new scaling for deriving fermionic mean-field dynamics. Math. Phys. Anal. Geom.*, **19**(1):Art. 3, 51, 2016. ISSN 1385-0172. doi:10.1007/s11040-016-9204-2.

[55] M. Reed and B. Simon. *Methods of Modern Mathematical Physics. I. Functional analysis.* Academic Press, 1972.

[56] D. W. Robinson. *The thermodynamic pressure in quantum statistical mechanics.* Springer-Verlag, Berlin-New York, 1971. Lecture Notes in Physics, Vol. 9.

[57] N. Rougerie. *De Finetti theorems, mean-field limits and Bose-Einstein condensation. ArXiv e-prints*, 2015.

[58] D. Ruelle. *Statistical mechanics. Rigorous results.* Singapore: World Scientific. London: Imperial College Press, 1999. ISBN 9789810238629.

[59] K. Schönhammer. *Deviations from Wick's theorem in the canonical ensemble. Phys. Rev. A*, **96**:012102, 2017. doi:10.1103/PhysRevA.96.012102.

[60] R. Seiringer. *The thermodynamic pressure of a dilute Fermi gas. Comm. Math. Phys.*, **261**(3):729–757, 2006. ISSN 0010-3616. doi:10.1007/s00220-005-1433-3.

[61] B. Simon. *The classical limit of quantum partition functions. Comm. Math. Phys.*, **71**(3):247–276, 1980.

[62] H. Spohn. *On the Vlasov hierarchy. Math. Methods Appl. Sci.*, **3**(4):445–455, 1981. ISSN 0170-4214. doi:10.1002/mma.1670030131.

[63] W. E. Thirring. *Quantum Mathematical Physics - Atoms, Molecules and Large Systems.* Springer, Second Edition 2002. ISBN 9783540430780.

[64] A. Triay. *In preparation.* Ph.D. thesis, University of Paris-Dauphine, 2019.

Supplement B

Thermodynamic limits

In this chapter, I collect and prove a few useful results that were applied in Paper B, some of them without reference. The contents of the following *cannot* be considered new results. However, since I do not know any good references for the precise results that we need, I have decided to include them here for completeness. The main purpose of the following is to provide a proof of the existence of the thermodynamic limit for a system of non-interacting fermions in cubes, with periodic boundary conditions and at positive temperature. In order to provide an expression for the free energy in the limit, I will also need to consider the thermodynamic limit in the grand canonical model, where many expressions are explicitly computable. Proposition BB.16 below is used in the proof of Proposition B.9 in Paper B.

Along the way, I also recall a few useful results on the anti-symmetrization of general quantum states in the canonical model. Corollaries BB.7 and BB.8 below are also used in the proof of Proposition B.9 in Paper B.

Parts of the calculations in this chapter were carried out in cooperation with Mathieu Lewin and Arnaud Triay during my stay at Université Paris-Dauphine. The results contained here can also be found in [7].

BB.1 The grand canonical model

Even though we are primarily interested in canonical models, where the number of particles is conserved, it is convenient to also introduce corresponding grand canonical models, which is the content of this section. Most of the definitions and basic facts below can also be found e.g. in the more comprehensive works [1, 3].

Let $\mathcal{H}$ be any separable Hilbert space (think of $\mathcal{H} = L^2(\Lambda)$ for some domain $\Lambda \subseteq \mathbb{R}^d$), and denote by $\mathcal{H}^n := \bigwedge^n \mathcal{H}$ the n-fold anti-symmetric tensor product of $\mathcal{H}$, with the convention that $\bigwedge^0 \mathcal{H} = \mathbb{C}$. The fermionic (or anti-symmetric) Fock space over $\mathcal{H}$ is then defined by

$$\mathcal{F} = \mathcal{F}_a(\mathcal{H}) = \bigoplus_{n\geq 0} \mathcal{H}^n.$$

Let $\beta > 0$ and suppose that H is a self-adjoint operator on $\mathcal{H}$ satisfying $\operatorname{Tr} e^{-\beta H} < \infty$. Then the second quantization of H is defined by

$$\mathrm{d}\Gamma(H) = \mathbb{H} := 0 \oplus \bigoplus_{n\geq 1} \sum_{j=1}^{n} H_j, \tag{BB.1}$$

where H_j acts on the j^{th} component of $\mathcal{H}^n$. Introducing the number operator $\mathcal{N} := \mathrm{d}\Gamma(1)$, the grand canonical free energy functional at inverse temperature β and chemical potential $\mu \in \mathbb{R}$ is defined by

$$\mathcal{E}^{\beta}_{\mathrm{GC}}(\Gamma) := \operatorname{Tr}\, \mathrm{d}\Gamma(H-\mu)\Gamma + \frac{1}{\beta}\operatorname{Tr}\Gamma\log\Gamma = \operatorname{Tr}(\,\mathrm{d}\Gamma(H) - \mu\mathcal{N}) + \frac{1}{\beta}\operatorname{Tr}\Gamma\log\Gamma \tag{BB.2}$$

on the set of grand canonical states

$$S_{\mathrm{GC}} = \{\Gamma \in \mathfrak{S}_1(\mathcal{F}) \mid 0 \leq \Gamma, \operatorname{Tr}\Gamma = 1\}.$$

The energy functional has minimum energy

$$e^{\beta}_{\mathrm{GC}}(\mu) := \inf_{\Gamma\in S_{\mathrm{GC}}} \mathcal{E}^{\beta}_{\mathrm{GC}}(\Gamma) = -\frac{1}{\beta}\log\operatorname{Tr} e^{-\beta(\,\mathrm{d}\Gamma(H)-\mu\mathcal{N})},$$

which is achieved uniquely by the Gibbs state $\Gamma_0 := Z^{-1}e^{-\beta(\,\mathrm{d}\Gamma(H)-\mu\mathcal{N})}$, where Z is the grand canonical partition function

$$Z = \operatorname{Tr}_{\mathcal{F}} e^{-\beta(\,\mathrm{d}\Gamma(H)-\mu\mathcal{N})} = \sum_{n\geq 1}\operatorname{Tr}_{\mathcal{H}^n} e^{-\beta(\sum_{j=1}^{n} H_j - \mu n)}.$$

Minimizers of functionals of the form (BB.2), with H being a one-body operator, are also called *quasi-free* states.

For $\psi_1 \in \mathcal{H}^{N_1}$ and $\psi_2 \in \mathcal{H}^{N_2}$ the anti-symmetric tensor product $\psi_1 \wedge \psi_2 \in \mathcal{H}^{N_1+N_2}$ is defined by

$$\psi_1 \wedge \psi_2 = \frac{\sqrt{(N_1+N_2)!}}{\sqrt{N_1! N_2!}} \sum_{\sigma\in\mathcal{S}_{N_1+N_2}} \operatorname{sgn}(\sigma) P_\sigma(\psi_1 \otimes \psi_2),$$

where $\mathcal{S}_{N_1+N_2}$ is the symmetric group, and P_σ for $\sigma \in \mathcal{S}_N$ is the permuation operator on $\bigotimes^N \mathcal{H}$ acting on pure tensors by

$$P_\sigma(u_1 \otimes \cdots \otimes u_N) = u_{\sigma(1)} \otimes \cdots \otimes u_{\sigma(N)} \tag{BB.3}$$

for any set of vectors $u_1, \dots u_N \in \mathcal{H}$. Given a vector $f \in \mathcal{H}$, the fermionic creation operator is defined on N-particles sectors $a^\dagger(f) : \mathcal{H}^N \to \mathcal{H}^{N+1}$ by

$$a^\dagger(f)\psi := f \wedge \psi,$$

and the annihilation operator $a(f) : \mathcal{H}^N \to \mathcal{H}^{N-1}$ by $a(f)\mathcal{H}^0 = \{0\}$ for $N = 0$, and through the relation

$$\langle \psi_{N-1}, a(f)\psi_N \rangle = \langle a^\dagger(f)\psi_{N-1}, \psi_N \rangle$$

for $N \geq 1$, where $\psi_{N-1} \in \mathcal{H}^{N-1}$ and $\psi_N \in \mathcal{H}^N$. In the anti-symmetric case, these operators extend to bounded operators on the whole Fock space $\mathcal{F}$, with $\|a^\dagger(f)\| = \|a(f)\| = \|f\|$, and they satisfy the canonical anti-commutation relations

$$\begin{cases} a(f)a^\dagger(g) + a^\dagger(g)a(f) = \langle f, g \rangle \mathbb{1}, \\ a^\dagger(f)a^\dagger(g) + a^\dagger(g)a^\dagger(f) = 0, \\ a(f)a(g) + a(g)a(f) = 0. \end{cases} \tag{BB.4}$$

Using the creation and annihilation operators, one can also define the k-body reduced density matrices $\Gamma^{(k)} : \mathcal{H}^k \to \mathcal{H}^k$ of a grand canonical state $\Gamma \in S_{\mathrm{GC}}$ by the relation

$$\left\langle u_1 \wedge \cdots \wedge u_k, \Gamma^{(k)} v_1 \wedge \cdots \wedge v_k \right\rangle = \mathrm{Tr}_{\mathcal{F}}\big(\Gamma a^\dagger(v_1) \cdots a^\dagger(v_k) a(u_k) \cdots a(u_1)\big). \tag{BB.5}$$

We always have $\Gamma^{(k)} \geq 0$, but $\Gamma^{(k)}$ need not be a trace-class operator [3], since

$$\mathrm{Tr}_{\mathcal{H}^k} \Gamma^{(k)} = \mathrm{Tr}_{\mathcal{F}}\left(\binom{\mathcal{N}}{k} \Gamma \right) \tag{BB.6}$$

is not finite for all $\Gamma \in S_{\mathrm{GC}}$.

BB.1.1 The grand canonical Gibbs state

Here I will introduce a unitary operator of the anti-symmetric Fock space that is very useful for calculations. Suppose that (u_i) is an orthonormal basis of the Hilbert space $\mathcal{H}$. We will use that the anti-symmetric Fock space generated by a single vector u is $\mathcal{F}_a(\mathbb{C}u) = \mathbb{C} \oplus \mathbb{C}u$, and that $\mathcal{F}_a(\mathcal{H}_1 \oplus \mathcal{H}_2) \simeq \mathcal{F}_a(\mathcal{H}_1) \otimes \mathcal{F}_a(\mathcal{H}_2)$, such that

$$\mathcal{F}_a(\mathcal{H}) \simeq \bigotimes_{i \geq 1} \mathcal{F}_a(\mathbb{C}u_i) = \bigotimes_{i \geq 1} \mathbb{C}^2.$$

Here the infinite tensor product on the right hand side should be interpreted as the closure of the linear span of vectors of the form $\otimes_{i \geq 1} v_i$ with $v_i = (1, 0)$ for all but finitely many i, with respect to the inner product $\langle \otimes_i v_i, \otimes_i w_i \rangle = \prod_i \langle v_i, w_i \rangle_{\mathbb{C}^2}$. More precisely, the isomorphism above is given by the operator defined on the canonical basis of $\mathcal{F}_a(\mathcal{H})$ by

$$\begin{aligned} \mathcal{U} : \mathcal{F}_a(\mathcal{H}) &\longrightarrow \bigotimes_{i \geq 1} \mathbb{C}^2 \\ u_{i_1} \wedge \cdots \wedge u_{i_k} &\longmapsto \bigotimes_{i \geq 1} \begin{pmatrix} 1 - \prod_{p=1}^k (1 - \delta_{i, i_p}) \\ \prod_{p=1}^k (1 - \delta_{i, i_p}) \end{pmatrix}, \end{aligned}$$

where $\delta_{i,k}$ is the Kronecker delta. In other words, $\mathcal{U}(u_{i_1} \wedge \cdots \wedge u_{i_k})$ has a $(0,1)$ in the j^{th} component if and only if $i_p = j$ for some p, and a $(1,0)$ in the j^{th} component otherwise.

Denoting $a_k := a(u_k)$ and $a_k^\dagger := a^\dagger(u_k)$, the creation and annihilation operators in this representation of the Fock space become

$$\mathcal{U}a_k\mathcal{U}^* = \bigotimes_{i\geq 1} \begin{pmatrix} 1-\delta_{i,k} & \delta_{i,k} \\ 0 & 1-\delta_{i,k} \end{pmatrix}, \qquad \mathcal{U}a_k^\dagger\mathcal{U}^* = \bigotimes_{i\geq 1} \begin{pmatrix} 1-\delta_{i,k} & 0 \\ \delta_{i,k} & 1-\delta_{i,k} \end{pmatrix}.$$

Furthermore,

$$\mathcal{U}a_k^\dagger a_k\mathcal{U}^* = \bigotimes_{i\geq 1} \begin{pmatrix} 1-\delta_{i,k} & 0 \\ 0 & 1 \end{pmatrix}, \tag{BB.7}$$

and for $j \neq k$,

$$\mathcal{U}a_j^\dagger a_k\mathcal{U}^* = \bigotimes_{i\geq 1} \begin{pmatrix} 1-\delta_{i,j}-\delta_{i,k} & \delta_{i,k} \\ \delta_{i,j} & 1-\delta_{i,j}-\delta_{i,k} \end{pmatrix}. \tag{BB.8}$$

Proposition BB.1. *Let $\Gamma_0 = Z^{-1}e^{-\beta(\,\mathrm{d}\Gamma(H-\mu))}$ be the Gibbs state corresponding to the Hamiltonian H at chemical potential μ. Then*

(1) The grand canonical minimal free energy satisfies

$$e^\beta_{\mathrm{GC}}(\mu) = -\frac{1}{\beta}\log \mathrm{Tr}_{\mathcal{F}}\, e^{-\beta(\,\mathrm{d}\Gamma(H)-\mu\mathcal{N})} = -\frac{1}{\beta}\,\mathrm{Tr}_{\mathcal{H}}\log\big(1+e^{-\beta(H-\mu)}\big).$$

(2) The 1-body reduced density matrix of Γ_0 is given by

$$\Gamma_0^{(1)} = \frac{1}{1+e^{\beta(H-\mu)}}.$$

(3) The entropy of Γ_0 is given by

$$\mathrm{Tr}_{\mathcal{F}}\,\Gamma_0\log\Gamma_0 = \mathrm{Tr}_{\mathcal{H}}\big(\Gamma_0^{(1)}\log\Gamma_0^{(1)} + \big(1-\Gamma_0^{(1)}\big)\log\big(1-\Gamma_0^{(1)}\big)\big).$$

(4) Γ_0 maximizes the entropy fixed $\Gamma_0^{(1)}$, i.e., if $\Gamma \in S_{\mathrm{GC}}$ is any grand canonical state with $\Gamma^{(1)} = \Gamma_0^{(1)}$, then

$$\mathrm{Tr}_{\mathcal{F}}\,\Gamma\log\Gamma \geq \mathrm{Tr}_{\mathcal{F}}\,\Gamma_0\log\Gamma_0.$$

Proof. By absorbing β and μ into H, we can assume that $\beta = 1$ and $\mu = 0$. Because e^{-H} is trace class, we can write $H = \sum_i h_i|u_i\rangle\langle u_i|$, where (u_i) is an orthonormal basis of $\mathcal{H}$, and hence the second quantization of H can be written $\mathrm{d}\Gamma(H) = \sum_i h_i a_i^\dagger a_i$. It follows easily from the canonical anti-commutation relations (BB.4) that $(a_i^\dagger a_i)$ is a family of commuting projections, so

$$e^{-\,\mathrm{d}\Gamma(H)} = \prod_{i\geq 1} e^{-h_i a_i^\dagger a_i} = \prod_{i\geq 1}((1 - a_i^\dagger a_i) + e^{-h_i} a_i^\dagger a_i).$$

Combining this with (BB.7), we have

$$\begin{aligned}
&\mathcal{U} e^{-\,\mathrm{d}\Gamma(H)} \mathcal{U}^* \\
&\quad = \prod_{i\geq 1}\Bigg(\bigotimes_{j\geq 1}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} - \bigotimes_{j\geq 1}\begin{pmatrix}1-\delta_{i,j} & 0\\ 0 & 1\end{pmatrix} + e^{-h_i}\bigotimes_{j\geq 1}\begin{pmatrix}1-\delta_{i,j} & 0\\ 0 & 1\end{pmatrix}\Bigg) \\
&\quad = \prod_{i\geq 1}\Bigg(\bigotimes_{j\geq 1}\begin{pmatrix}1 & 0\\ 0 & 1-\delta_{i,j}\end{pmatrix} + \bigotimes_{j\geq 1}\begin{pmatrix}1-\delta_{i,j} & 0\\ 0 & 1+\delta_{i,j}(e^{-h_i}-1)\end{pmatrix}\Bigg) \\
&\quad = \prod_{i\geq 1}\Bigg(\bigotimes_{j\geq 1}\begin{pmatrix}1 & 0\\ 0 & 1+\delta_{i,j}(e^{-h_i}-1)\end{pmatrix}\Bigg) = \bigotimes_{i\geq 1}\begin{pmatrix}1 & 0\\ 0 & e^{-h_i}\end{pmatrix}.
\end{aligned}$$

This implies $Z = \operatorname{Tr} e^{-\,\mathrm{d}\Gamma(H)} = \prod_{i\geq 1}(1 + e^{-h_i})$, and hence

$$\log Z = \log \operatorname{Tr} e^{-\,\mathrm{d}\Gamma(H)} = \sum_{i\geq 1}\log(1 + e^{-h_i}) = \operatorname{Tr}\log(1 + e^{-H}), \tag{BB.9}$$

showing that *(1)* holds. Furthermore, denoting $Z_i = 1 + e^{-h_i}$, we can now write

$$\mathcal{U}\Gamma_0\mathcal{U}^* = \bigotimes_{i\geq 1}\frac{1}{Z_i}\begin{pmatrix}1 & 0\\ 0 & e^{-h_i}\end{pmatrix},$$

so using (BB.8), we conclude that $\Gamma_0 a_j^\dagger a_k = 0$ whenever $j \neq k$. Also applying (BB.7), we calculate

$$\begin{aligned}
\langle u_j, \Gamma_0^{(1)} u_k\rangle = \operatorname{Tr}(\Gamma_0 a_j^\dagger a_k) &= \delta_{j,k}\operatorname{Tr}\Bigg(\bigotimes_{i\geq 1}\frac{1}{Z_i}\begin{pmatrix}1-\delta_{i,k} & 0\\ 0 & e^{-h_i}\end{pmatrix}\Bigg) \\
&= \frac{e^{-h_k}}{1+e^{-h_k}}\delta_{j,k},
\end{aligned}$$

showing *(2)*. Now noting that $1 - \Gamma_0^{(1)} = \frac{e^H}{1+e^H}$, we calculate

$$\begin{aligned}
\operatorname{Tr}\,\mathrm{d}\Gamma(H)\Gamma_0 &= \operatorname{Tr} H\Gamma_0^{(1)} + \operatorname{Tr}\Gamma_0^{(1)}\log\Gamma_0^{(1)} - \operatorname{Tr}\Gamma_0^{(1)}\log\Gamma_0^{(1)} \\
&= \operatorname{Tr}\Gamma_0^{(1)}\big(\log e^H + \log\frac{1}{1+e^H}\big) - \operatorname{Tr}\Gamma_0^{(1)}\log\Gamma_0^{(1)} \\
&= \operatorname{Tr}\Gamma_0^{(1)}\log\big(1-\Gamma_0^{(1)}\big) - \operatorname{Tr}\Gamma_0^{(1)}\log\Gamma_0^{(1)},
\end{aligned}$$

so using (BB.9),

$$\begin{aligned}\operatorname{Tr}\Gamma_0\log\Gamma_0 &= \operatorname{Tr}\Gamma_0\log\frac{e^{-\,\mathrm{d}\Gamma(H)}}{Z} = -\operatorname{Tr}\,\mathrm{d}\Gamma(H)\Gamma_0 - \log Z\\ &= \operatorname{Tr}\Gamma_0^{(1)}\log\Gamma_0^{(1)} - \operatorname{Tr}\Gamma_0^{(1)}\log\big(1-\Gamma_0^{(1)}\big) + \operatorname{Tr}\log\big(1-\Gamma_0^{(1)}\big)\\ &= \operatorname{Tr}\big(\Gamma_0^{(1)}\log\Gamma_0^{(1)} + \big(1-\Gamma_0^{(1)}\big)\log\big(1-\Gamma_0^{(1)}\big)\big),\end{aligned}$$

which is *(3)*. Finally, to obtain *(4)*, we simply use that Γ_0 minimizes the grand canonical energy functional, so if Γ is any other state with the same 1-body reduced density matrix $\Gamma^{(1)} = \Gamma_0^{(1)}$, we have

$$\operatorname{Tr}\Gamma\log\Gamma = \mathcal{E}_{\mathrm{GC}}(\Gamma) - \operatorname{Tr}H\Gamma^{(1)} \geq \mathcal{E}_{\mathrm{GC}}(\Gamma_0) - \operatorname{Tr}H\Gamma_0^{(1)} = \operatorname{Tr}\Gamma_0\log\Gamma_0.$$

□

Proposition BB.2. *For any grand canonical fermionic state* $\Gamma \in S_{\mathrm{GC}}$ *with* $\operatorname{Tr}\Gamma^{(1)} = \operatorname{Tr}\mathcal{N}\Gamma < \infty$*, we have the bound*

$$\operatorname{Tr}_{\mathcal{F}}\Gamma\log\Gamma \geq \operatorname{Tr}_{\mathcal{H}}\big(\Gamma^{(1)}\log\Gamma^{(1)} + \big(1-\Gamma^{(1)}\big)\log\big(1-\Gamma^{(1)}\big)\big).$$

Proof. The basic idea of the proof is to use $\Gamma^{(1)}$ to construct a quasi-free state (on a possibly smaller Hilbert space) with entropy equal to the right hans side above, and then apply Proposition BB.1. By the spectral theorem we can write $\Gamma = \sum_{j\geq 1}\lambda_j|\Psi_j\rangle\langle\Psi_j|$, where (Ψ_j) is an orthonormal basis of the Fock space $\mathcal{F}_a(\mathcal{H})$, and the eigenvalues λ_j satisfy $0 \leq \lambda_j \leq 1$ and $\sum_j \lambda_j = 1$. Similarly, since the one body density matrix also satisfies $0 \leq \Gamma^{(1)} \leq \mathbb{1}$, we can write $\Gamma^{(1)} = \sum_{j\geq 1}\mu_j|\varphi_j\rangle\langle\varphi_j|$ with $0 \leq \mu_j \leq 1$ and $\sum_j \mu_j = \operatorname{Tr}\Gamma^{(1)}$, and with (φ_j) being a basis of the Hilbert space $\mathcal{H}$. We will construct a quasi-free state whose one particle density matrix has spectrum $\{\mu_j \mid 0 < \mu_j < 1\}$, so we order the eigenvalues μ_j such that $\mu_j = 1$ for $1 \leq j \leq k$.

Fixing for the moment a $j_0 \leq k$ and recalling the notation $a_j := a(\varphi_j)$, $a_j^\dagger := a^\dagger(\varphi_j)$, we have by definition of $\Gamma^{(1)}$ that

$$\sum_{j\geq 1}\lambda_j\langle\Psi_j, a_{j_0}^\dagger a_{j_0}\Psi_j\rangle = \operatorname{Tr}(\Gamma a_{j_0}^\dagger a_{j_0}) = \langle\varphi_{j_0}, \Gamma^{(1)}\varphi_{j_0}\rangle = 1,$$

so since $\operatorname{Tr}\Gamma = 1$, we must have $\langle\Psi_j, a_{j_0}^\dagger a_{j_0}\Psi_j\rangle = 1$ for all j such that $\lambda_j \neq 0$, implying for these j that $\Psi_j = a_{j_0}^\dagger a_{j_0}\Psi_j$. Thus, using the canonical anticommutation relations, we can write $\Psi_j = a_1^\dagger\cdots a_k^\dagger a_k\cdots a_1\Psi_j = a_1^\dagger\cdots a_k^\dagger\widetilde{\Psi}_j$, where the vectors $\widetilde{\Psi}_j := a_k\cdots a_1\Psi_j$ are orthonormal and can be regarded as vectors in the smaller Fock space $\mathcal{F}_a((\operatorname{span}(\varphi_1,\ldots,\varphi_k))^\perp)$ generated by the orthogonal complement of $\varphi_1,\ldots,\varphi_k$.

On the other hand, supposing that $\mu_{j_0} = 0$, then we obtain as above

$$\sum_{j\geq 1} \lambda_j \langle \Psi_j, a_{j_0}^\dagger a_{j_0} \Psi_j \rangle = \operatorname{Tr}(\Gamma a_{j_0}^\dagger a_{j_0}) = \langle \varphi_{j_0}, \Gamma^{(1)} \varphi_{j_0} \rangle = 0,$$

implying that $a_{j_0}\Psi_j = 0$, and hence also $a_{j_0}\widetilde{\Psi}_j = 0$ for all j with $\lambda_j \neq 0$. This means that $\widetilde{\Psi}_j$ does not see any of the kernel of $\Gamma^{(1)}$, so if we define the smaller Hilbert space $\widetilde{\mathcal{H}} := (\operatorname{span}(\varphi_1, \ldots, \varphi_k) \cup \ker \Gamma^{(1)})^\perp \subseteq \mathcal{H}$, and a state

$$\widetilde{\Gamma} := \sum_{\lambda_j \neq 0} \lambda_j |\widetilde{\Psi}_j\rangle\langle\widetilde{\Psi}_j|$$

on the Fock space $\mathcal{F}_a(\widetilde{\mathcal{H}})$, then $\widetilde{\Gamma}$ has the same entropy as Γ, and the one-body density matrix of $\widetilde{\Gamma}$ is by construction

$$\widetilde{\Gamma}^{(1)} = \sum_{0<\mu_j<1} \mu_j |\varphi_j\rangle\langle\varphi_j|.$$

At this point, we can define a self-adjoint operator H on $\widetilde{\mathcal{H}}$ by

$$H := \log \frac{1 - \widetilde{\Gamma}^{(1)}}{\widetilde{\Gamma}^{(1)}} = \sum_{0<\mu_j<1} \log \frac{1-\mu_j}{\mu_j} |\varphi_j\rangle\langle\varphi_j|.$$

Then by Proposition BB.1 the quasi-free state on $\mathcal{F}_a(\widetilde{\mathcal{H}})$ generated by H has the same one body density matrix as $\widetilde{\Gamma}$, and we conlude that

$$\begin{aligned} \operatorname{Tr}\Gamma\log\Gamma = \operatorname{Tr}\widetilde{\Gamma}\log\widetilde{\Gamma} &\geq \operatorname{Tr}\big(\widetilde{\Gamma}^{(1)}\log\widetilde{\Gamma}^{(1)} + \big(1-\widetilde{\Gamma}^{(1)}\big)\log\big(1-\widetilde{\Gamma}^{(1)}\big)\big) \\ &= \operatorname{Tr}\big(\Gamma^{(1)}\log\Gamma^{(1)} + \big(1-\Gamma^{(1)}\big)\log\big(1-\Gamma^{(1)}\big)\big), \end{aligned}$$

finishing the proof. □

BB.1.2 The grand canonical thermodynamic limit

Definition BB.3 (η-regularity). A subset $\Lambda \subseteq \mathbb{R}^d$ is said to have η-regular boundary if there exists a $t_0 > 0$ such that for all $t \in [0, t_0)$ we have

$$|\{x \in \mathbb{R}^d \mid d(x, \partial\Lambda) \leq |\Lambda|^{\frac{1}{d}} t\}| \leq |\Lambda|\eta(t),$$

where $\eta : [0, t_0) \to \mathbb{R}_+$ is a continuous function with $\eta(0) = 0$.

Proposition BB.4. *Let $\Lambda_n \subseteq \mathbb{R}^d$ be a sequence of bounded, connected domains with $|\Lambda_n| \to \infty$, and suppose furthermore that Λ_n has η-regular boundary, where η is independent of n. Denoting by*

$$e_{\mathrm{GC}}^\beta(\Lambda_n, \mu) = -\frac{1}{\beta}\operatorname{Tr}\log\big(1 + e^{-\beta(-\Delta^{\Lambda_n} - \mu)}\big)$$

the corresponding grand canonical free energy at chemical potential μ*, then we have for any* $\mu \in \mathbb{R}$ *in the thermodynamic limit*

$$f_{\mathrm{GC}}(\beta,\mu) := \lim_{n\to\infty} \frac{1}{|\Lambda_n|} e^{\beta}_{\mathrm{GC}}(\Lambda_n,\mu) = -\frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^d} \log\bigl(1 + e^{-\beta(p^2-\mu)}\bigr)\,\mathrm{d}p$$

independently of the sequence (Λ_n)*.*

Proof. The proof is done using Dirichlet-Neumann bracketing. For the duration of the proof we will for any set $\Lambda \subseteq \mathbb{R}^d$ denote by $-\Delta_{\mathrm{D}}^{\Lambda}$ the Dirichlet Laplacian on Λ, and by $-\Delta_{\mathrm{N}}^{\Lambda}$ the Neumann Laplacian on Λ. Decompose $\mathbb{R}^d$ into a union of cubes C_j of side length $\ell > 0$. To provide an upper bound on $e^{\beta}_{\mathrm{GC}}(\Lambda_n,\mu)$ we will approximate Λ_n from the inside by a union of cubes and consider the Dirichlet Laplacian on each cube. For the corresponsing lower bound, we will instead approximate Λ_n from the outside and use the Neumann Laplacian. Recall (e.g. from [5, Sec. XIII.15]) that for any $\Lambda \supseteq \widetilde{\Lambda}$ we have

$$-\Delta_{\mathrm{N}}^{\Lambda} \le -\Delta_{\mathrm{D}}^{\Lambda} \le -\Delta_{\mathrm{D}}^{\widetilde{\Lambda}},$$

and if Λ_1 and Λ_2 are disjoint open sets, then $-\Delta_{\mathrm{D/N}}^{\Lambda_1\cup\Lambda_2} = -\Delta_{\mathrm{D/N}}^{\Lambda_1} \oplus -\Delta_{\mathrm{D/N}}^{\Lambda_2}$.

Define

$$\widetilde{\Lambda}_n := \bigcup_{C_j \subseteq \Lambda_n} C_j \subseteq \Lambda_n$$

to be the union of all the cubes C_j completely contained in Λ_n, and note that if $x \in C_j \cap \Lambda_n$ is any point, with C_j intersecting the boundary of Λ_n (that is, $C_j \cap \Lambda_n^c \neq \emptyset$), then $d(x,\partial\Lambda_n) \le \operatorname{diam} C_j = \sqrt{d}\ell$. Thus, using the η-regularity of Λ_n, we estimate

$$\begin{aligned} |\widetilde{\Lambda}_n| &= |\Lambda_n| - \sum_{C_j\cap\Lambda_n^c\neq\emptyset} |C_j \cap \Lambda_n| \ge |\Lambda_n| - |\{x \mid d(x,\partial\Lambda_n) \le \sqrt{d}\ell\}| \\ &\ge |\Lambda_n|(1 - \eta(\sqrt{d}\ell|\Lambda_n|^{-\frac{1}{d}})), \end{aligned} \tag{BB.10}$$

so $|\widetilde{\Lambda}_n|$ is comparable to $|\Lambda_n|$ in the $n \to \infty$ limit, for any fixed $\ell > 0$. Note also that $\widetilde{\Lambda}_n$ consists of exactly $K_n = |\widetilde{\Lambda}_n|/|C_j|$ cubes. Since the eigenvalues of $-\Delta_{\mathrm{D}}^{C_j}$ are explicitly determined (e.g. using formula (114) in [5]) by the numbers $\frac{\pi^2}{\ell^2}n^2$ for $n \in \mathbb{N}^d$, we have for each cube

$$-\operatorname{Tr}\log\bigl(1 + e^{-\beta(-\Delta_{\mathrm{D}}^{C_j}-\mu)}\bigr) = \sum_{n\in(\frac{\pi}{\ell}\mathbb{N})^d} -\log\bigl(1 + e^{-\beta(n^2-\mu)}\bigr),$$

where, since $t \to -\log(1+e^{-\beta t})$ is increasing, the sum can be recognised as an upper Riemann sum for the integral $-\log\left(1 + e^{-\beta(p^2-\mu)}\right)$ on the set $\{p \in \mathbb{R}^d \mid p_i \ge \frac{1}{\ell}\}$.

Hence we obtain by operator monotonicity of the function $t \to -\log(1+e^{-\beta t})$,

$$\begin{aligned}\frac{1}{|\Lambda_n|}e^{\beta}_{\mathrm{GC}}(\Lambda_n,\mu) \le \frac{1}{|\Lambda_n|}e^{\beta}_{\mathrm{GC}}(\widetilde{\Lambda}_n,\mu) &= -\frac{K_n}{|\Lambda_n|\beta}\operatorname{Tr}\log\bigl(1+e^{-\beta(-\Delta_{\mathrm{D}}^{C_j}-\mu)}\bigr)\\ &\le -\frac{K_n}{|\Lambda_n|}\frac{\ell^d}{\pi^d\beta}\int_{p_i\ge\frac{1}{\ell}}\log\bigl(1+e^{-\beta(p^2-\mu)}\bigr)\,\mathrm{d}p.\end{aligned}$$

Since $K_n\ell^d = |\widetilde{\Lambda}_n| \sim |\Lambda_n|$, we can take first $n\to\infty$ while keeping ℓ fixed, and then take $\ell\to\infty$ to obtain on the right hand side

$$\frac{1}{\pi^d\beta}\int_{p_i\ge 0}\log\bigl(1+e^{-\beta(p^2-\mu)}\bigr)\,\mathrm{d}p = \frac{1}{(2\pi)^d\beta}\int_{\mathbb{R}^d}\log\bigl(1+e^{-\beta(p^2-\mu)}\bigr)\,\mathrm{d}p,$$

which concludes the proof of the upper bound.

For the lower bound we instead define

$$\widetilde{\Lambda}_n := \bigcup_{C_j\cap\Lambda_n\neq\emptyset} C_j \supseteq \Lambda_n,$$

a union of $K_n = |\Lambda_n|/|C_j|$ cubes of side length $\ell>0$. Exactly as before, we have by the η-regularity

$$\begin{aligned}|\widetilde{\Lambda}_n| &\le |\Lambda_n| + \sum_{C_j\cap\Lambda_n\neq\emptyset}|C_j\cap\Lambda_n^c| \le |\Lambda_n| + |\{x \mid d(x,\partial\Lambda_n)\le\sqrt{d}\ell\}|\\ &\le |\Lambda_n|(1+\eta(\sqrt{d}\ell|\Lambda_n|^{-\frac{1}{d}})),\end{aligned} \tag{BB.11}$$

so $\widetilde{\Lambda}_n$ is again a good approximation of Λ_n. The eigenvalues of the Neumann Laplacian in a cube are the same as for the Dirichlet Laplacian, except that they are indexed by $n\in\mathbb{N}_0^d$ instead of $\mathbb{N}^d$. Thus we have in the same way as before

$$-\operatorname{Tr}\log\bigl(1+e^{-\beta(-\Delta_{\mathrm{N}}^{C_j}-\mu)}\bigr) = \sum_{n\in(\frac{\pi}{\ell}\mathbb{N}_0)^d} -\log\bigl(1+e^{-\beta(n^2-\mu)}\bigr),$$

so this time recognising the right hand side as a lower Riemann sum for the integral of $-\log\left(1+e^{-\beta(p^2-\mu)}\right)$ on the set $\{p\in\mathbb{R}^d \mid p_i \ge -\frac{1}{\ell}\}$,

$$\begin{aligned}\frac{1}{|\Lambda_n|}e^{\beta}_{\mathrm{GC}}(\Lambda_n,\mu) \ge \frac{1}{|\Lambda_n|}e^{\beta}_{\mathrm{GC}}(\widetilde{\Lambda}_n,\mu) &= -\frac{K_n}{|\Lambda_n|\beta}\operatorname{Tr}\log\bigl(1+e^{-\beta(-\Delta_{\mathrm{N}}^{C_j}-\mu)}\bigr)\\ &\ge -\frac{K_n}{|\Lambda_n|}\frac{\ell^d}{\pi^d\beta}\int_{p_i\ge-\frac{1}{\ell}}\log\bigl(1+e^{-\beta(p^2-\mu)}\bigr)\,\mathrm{d}p.\end{aligned}$$

First taking $n\to\infty$ followed by $\ell\to\infty$ finishes the proof. □

BB.2 The canonical model

Let H be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$, and consider the operator

$$H_N := \sum_{i=1}^{N} H_i,$$

acting on $\mathcal{H}^N = \bigwedge^N \mathcal{H}$. The N-particle fermionic free energy functional at inverse temperature $\beta > 0$ is defined by

$$\mathcal{E}^{\beta}_{\text{Can}}(\Gamma) := \operatorname{Tr} H_N \Gamma + \frac{1}{\beta} \operatorname{Tr} \Gamma \log \Gamma$$

on the set of N-body fermionic states

$$S^N_{\text{Can}} := \{\Gamma \in \mathfrak{S}_1(\mathcal{H}^N) \mid 0 \leq \Gamma \leq \mathbb{1}, \operatorname{Tr} \Gamma = 1\}.$$

As in the grand canonical case, the minimal free energy is

$$e^{\beta}_{\text{Can}}(N) := \inf_{\Gamma \in S^N_{\text{Can}}} \big(\operatorname{Tr} H_N \Gamma + \frac{1}{\beta} \operatorname{Tr} \Gamma \log \Gamma\big) = -\frac{1}{\beta} \log \operatorname{Tr} e^{-\beta H_N},$$

where the infimum is achieved uniquely when Γ is the Gibbs state

$$\Gamma_N := \frac{1}{Z_N} e^{-\beta H_N}, \tag{BB.12}$$

where $Z_N = \operatorname{Tr} e^{-\beta H_N}$ is the partition function, ensuring that $\operatorname{Tr} \Gamma_N = 1$. Since any canonical state Γ is automatically also a grand canonical state on the Fock space $\mathcal{F}_a(\mathcal{H})$, we can define the k-particle reduced density matrices as in (BB.5). However, we can also define the k-particle density matrix using partial traces $\Gamma^{(k)} := \frac{N!}{(N-k)!} \operatorname{Tr}_{k+1\to N} \Gamma$, or, by duality, as the unique operator $\Gamma^{(k)} \in \mathfrak{S}_1(\mathcal{H}^k)$ satisfying

$$\operatorname{Tr} A\Gamma^{(k)} = \frac{N!}{(N-k)!} \operatorname{Tr}(A \otimes \mathbb{1}_{N-k})\Gamma$$

for all bounded operators $A \in \mathcal{B}(\mathcal{H}^k)$.

BB.2.1 Anti-symmetrization of states

In the following, we recall the anti-symmetrization of two canonical fermionic states living in orthogonal subspaces of the same Hilbert space, as well as some useful properties. Let $\mathcal{H}$ be a separable Hilbert space. Using the permutation operators P_σ defined in (BB.3), we define the projection $\Pi : \bigotimes^N \mathcal{H} \to \bigwedge^N \mathcal{H}$ onto the fermionic subspace by

$$\Pi = \frac{1}{N!} \sum_{\sigma \in \mathcal{S}_N} \operatorname{sgn}(\sigma) P_\sigma.$$

Let $N = N_1 + N_2$ and $\Psi_i \in \bigwedge^{N_i}\mathcal{H}$ for $i = 1, 2$, and recall the anti-symmetrization of the two wave functions Ψ_1 and Ψ_2

$$\Psi_1 \wedge \Psi_2 = \Big(\frac{(N_1+N_2)!}{N_1!N_2!}\Big)^{\frac{1}{2}}\,\Pi(\Psi_1 \otimes \Psi_2).$$

We want to carry this anti-symmetrization procedure over to general fermionic states. Beginning with pure states, notice that

$$\Pi\,|\Psi_1 \otimes \Psi_2\rangle\,\langle\Psi_1 \otimes \Psi_2|\,\Pi = \frac{N_1!N_2!}{(N_1+N_2)!}\,|\Psi_1 \wedge \Psi_2\rangle\,\langle\Psi_1 \wedge \Psi_2|\,. \tag{BB.13}$$

Based on this we make the following definition.

Definition BB.5. For $i \in \{1, 2\}$, let $N_i \geq 1$ and Γ_i be a fermionic state on $\bigwedge^{N_i}\mathcal{H}$. We define the anti-symmetrization of the two states to be

$$\Gamma_1 \wedge \Gamma_2 := \frac{(N_1+N_2)!}{N_1!N_2!}\Pi(\Gamma_1 \otimes \Gamma_2)\Pi. \tag{BB.14}$$

We may write $\Gamma_1 = \sum_k \mu_k\,|\psi_k\rangle\,\langle\psi_k|$ with $\psi_k \in \bigwedge^{N_1}\mathcal{H}$ being an orthonormal basis of $\bigwedge^{N_1}\mathcal{H}$, and similarly $\Gamma_2 = \sum_j \lambda_j\,|\varphi_j\rangle\,\langle\varphi_j|$. Then by (BB.13) it follows that

$$\Gamma_1 \wedge \Gamma_2 = \sum_{k,j}\mu_k\lambda_j\,|\psi_k \wedge \varphi_j\rangle\,\langle\psi_k \wedge \varphi_j|\,. \tag{BB.15}$$

Generally, $\Gamma_1 \wedge \Gamma_2$ need not be a state, in the sense that $\operatorname{Tr}\Gamma_1 \wedge \Gamma_2 = 1$ does not necessarily hold (because $\varphi_j \wedge \psi_k$ may not be normalized). However, when Γ_1 and Γ_2 live on different (orthogonal) subspaces of the Hilbert space $\mathcal{H}$, then $\Gamma_1 \wedge \Gamma_2$ is a fermionic $N_1 + N_2$-body state, as the following lemma demonstrates, among other things.

Lemma BB.6 (One- and two-body densities). *For $i \in \{1, 2\}$, let $N_i \geq 1$ and Q_i orthogonal projections on $\mathcal{H}$ satisfying $Q_1Q_2 = 0$. Let Γ_i be a fermionic state on $\bigwedge^{N_i} Q_i\mathcal{H}$. Then the one-body reduced density matrix of $\Gamma_1 \wedge \Gamma_2$ is*

$$(\Gamma_1 \wedge \Gamma_2)^{(1)} = \Gamma_1^{(1)} + \Gamma_2^{(1)}. \tag{BB.16}$$

In particular, $\Gamma_1 \wedge \Gamma_2$ is a state on $\bigwedge^{N_1+N_2}\mathcal{H}$. Moreover, for any $W \in \mathcal{B}(\mathcal{H} \wedge \mathcal{H})$ such that $[W, Q_i \otimes Q_j] = 0$ for $i, j \in \{1, 2\}$ we have

$$\operatorname{Tr} W(\Gamma_1 \wedge \Gamma_2)^{(2)} = \operatorname{Tr} W\big(\Gamma_1^{(2)} + \Gamma_2^{(2)} + \Gamma_1^{(1)} \otimes \Gamma_2^{(1)} + \Gamma_2^{(1)} \otimes \Gamma_1^{(1)}\big). \tag{BB.17}$$

Proof. Because of (BB.15), it is enough to show (BB.16) and (BB.17) for pure states $\Gamma_i = |\Psi_i\rangle\langle\Psi_i|$. Suppose that $A \in \mathcal{B}(\mathcal{H})$ and denote $N = N_1+N_2$ and $A_1 = A \otimes \mathbb{1}_{N-1}$. By definition of the anti-symmetrization $\Gamma_1 \wedge \Gamma_2$ we have

$$\begin{aligned}\operatorname{Tr} A_1\Gamma_1 \wedge \Gamma_2 &= \big\langle\Psi_1 \wedge \Psi_2, A_1\Psi_1 \wedge \Psi_2\big\rangle \\ &= \frac{1}{N_1!N_2!N!}\sum_{\sigma,\tau\in\mathcal{S}_N}\operatorname{sgn}(\sigma\tau)\big\langle P_\sigma(\Psi_1 \otimes \Psi_2), A_1P_\tau(\Psi_1 \otimes \Psi_2)\big\rangle,\end{aligned} \tag{BB.18}$$

where, since $P_1 P_2 = 0$, each term

$$\begin{aligned}&\big\langle P_\sigma(\Psi_1 \otimes \Psi_2), A_1 P_\tau(\Psi_1 \otimes \Psi_2)\big\rangle \\ &\qquad = \big\langle P_\sigma(Q_1^{\otimes N_1} \otimes Q_2^{\otimes N_2})(\Psi_1 \otimes \Psi_2), A_1 P_\tau(Q_1^{\otimes N_1} \otimes Q_2^{\otimes N_2})(\Psi_1 \otimes \Psi_2)\big\rangle\end{aligned}$$

can be non-zero only if σ and τ satisfy the conditions

$$\begin{aligned}\tau(\{1,\dots N_1\}) &\subseteq \sigma(\{1,\dots,N_1\}) \cup \{1\},\\ \tau(\{N_1+1,\dots,N\}) &\subseteq \sigma(\{N_1+1,\dots,N\}) \cup \{1\},\end{aligned}$$

which are equivalent to $\tau(\{1,\dots N_1\}) = \sigma(\{1,\dots,N_1\})$. With σ fixed, there are exactly $N_1!N_2!$ permutations τ satisfying this. If τ is one of these, we can write $\tau = \sigma\tilde{\sigma}$ for a unique permutation $\tilde{\sigma}$ with $\tilde{\sigma}(\{1,\dots,N_1\}) = \{1,\dots,N_1\}$ and $\operatorname{sgn}(\tilde{\sigma}) = \operatorname{sgn}(\sigma\tau)$. Then by anti-symmetry we have $P_\tau \Psi_1 \otimes \Psi_2 = P_\sigma P_{\tilde{\sigma}} \Psi_1 \otimes \Psi_2 = \operatorname{sgn}(\tilde{\sigma}) P_\sigma \Psi_1 \otimes \Psi_2$, so continuing from (BB.18),

$$\operatorname{Tr} A_1 \Gamma_1 \wedge \Gamma_2 = \frac{1}{N!} \sum_{\sigma \in \mathcal{S}_N} \big\langle P_\sigma(\Psi_1 \otimes \Psi_2), A_1 P_\sigma(\Psi_1 \otimes \Psi_2)\big\rangle.$$

Now, if for instance $\sigma^{-1}(1) \in \{1,\dots,N_1\}$, then

$$\begin{aligned}\big\langle P_\sigma(\Psi_1 \otimes \Psi_2), A_1 P_\sigma(\Psi_1 \otimes \Psi_2)\big\rangle &= \big\langle P_\sigma(\Psi_1 \otimes \Psi_2), P_\sigma A_{\sigma^{-1}(1)}(\Psi_1 \otimes \Psi_2)\big\rangle \\ &= \big\langle \Psi_1, A_1 \Psi_1\big\rangle = \operatorname{Tr} A_1 \Gamma_1,\end{aligned}$$

and similarly if $\sigma^{-1}(1) \in \{N_1+1,\dots,N\}$, so finally we have

$$\begin{aligned}\operatorname{Tr} A_1 (\Gamma_1 \wedge \Gamma_2)^{(1)} &= \frac{1}{(N-1)!} \sum_{\sigma \in \mathcal{S}_N} \big\langle P_\sigma(\Psi_1 \otimes \Psi_2), A_1 P_\sigma(\Psi_1 \otimes \Psi_2)\big\rangle \\ &= N_1 \operatorname{Tr} A_1 \Gamma_1 + N_2 \operatorname{Tr} A_1 \Gamma_2 = \operatorname{Tr} A_1 \Gamma_1^{(1)} + \operatorname{Tr} A_1 \Gamma_2^{(1)}.\end{aligned}$$

Consider now an interaction $W \in \mathcal{B}(\mathcal{H} \wedge \mathcal{H})$ with $[W, Q_i \otimes Q_j] = 0$ for $i,j \in \{1,2\}$. Expanding as in (BB.18), we have

$$\operatorname{Tr} W_{1,2} \Gamma_1 \wedge \Gamma_2 = \frac{1}{N_1!N_2!N!} \sum_{\sigma,\tau \in \mathcal{S}_N} \operatorname{sgn}(\sigma\tau) \big\langle P_\sigma(\Psi_1 \otimes \Psi_2), W_{1,2} P_\tau(\Psi_1 \otimes \Psi_2)\big\rangle,$$

where $W_{1,2} = W \otimes \mathbb{1}_{N-2}$. Since W commutes with the projections $Q_i \otimes Q_j$, the permutations σ and τ must satisfy the same condition $\tau(\{1,\dots N_1\}) = \sigma(\{1,\dots,N_1\})$ as before, in order for the corresponding term in the sum above to be non-zero. Now, if for instance $\sigma^{-1}(1), \sigma^{-1}(2) \in \{1,\dots,N_1\}$, then

$$\operatorname{sgn}(\sigma\tau) \big\langle P_\sigma(\Psi_1 \otimes \Psi_2), W_{1,2} P_\tau(\Psi_1 \otimes \Psi_2)\big\rangle = \frac{1}{N_1(N_1-1)} \operatorname{Tr} W \Gamma_1^{(2)}.$$

Similiarly, if $\sigma^{-1}(1) \in \{1,\ldots,N_1\}$ and $\sigma^{-1}(2) \in \{N_1+1,\ldots,N\}$, we have

$$\operatorname{sgn}(\sigma\tau)\big\langle P_\sigma(\Psi_1 \otimes \Psi_2), W_{1,2}P_\tau(\Psi_1 \otimes \Psi_2)\big\rangle = \frac{1}{N_1N_2}\operatorname{Tr} W\Gamma_1^{(1)} \otimes \Gamma_2^{(1)}.$$

Hence, collecting terms and counting permutations, we conclude

$$\begin{aligned}\operatorname{Tr} W(\Gamma_1 \wedge \Gamma_2)^{(2)} &= N(N-1)\operatorname{Tr} W_{1,2}\Gamma_1 \wedge \Gamma_2 \\ &= \operatorname{Tr} W\big(\Gamma_1^{(2)} + \Gamma_2^{(2)} + \Gamma_1^{(1)} \otimes \Gamma_2^{(1)} + \Gamma_2^{(1)} \otimes \Gamma_1^{(1)}\big).\end{aligned}$$

□

The two following corollaries are used without reference in the proof of Proposition B.9 in Paper B.

Corollary BB.7. *In particular, if $\mathcal{H} = L^2(\mathbb{R}^d)$ we have*

$$\rho^{(2)}_{\Gamma_1\wedge\Gamma_2}(x,y) = \rho^{(2)}_{\Gamma_1}(x,y) + \rho^{(2)}_{\Gamma_2}(x,y) + \rho^{(1)}_{\Gamma_1}(x)\rho^{(1)}_{\Gamma_2}(y) + \rho^{(1)}_{\Gamma_2}(x)\rho^{(1)}_{\Gamma_1}(y).$$

Corollary BB.8 (Additivity of entropy and kinetic energy). *Denoting by $H_{\Lambda,N} = \sum_{i=1}^N -\Delta_i^\Lambda$ the N-body Laplacian on Λ (with Dirichlet boundary conditions), and let Γ_i be an N_i-body fermionic state on Λ_i, $i = 1,2$, where $\Lambda = \Lambda_1 \cup \Lambda_2$ is a disjoint union. Then the anti-symmetrization of Γ_1 and Γ_2 satisfies*

$$\operatorname{Tr}(\Gamma_1 \wedge \Gamma_2)\log(\Gamma_1 \wedge \Gamma_2) = \operatorname{Tr}\Gamma_1\log\Gamma_1 + \operatorname{Tr}\Gamma_2\log\Gamma_2, \tag{BB.19}$$

and

$$\operatorname{Tr} H_{\Lambda,N_1+N_2}\Gamma_1 \wedge \Gamma_2 = \operatorname{Tr} H_{\Lambda_1,N_1}\Gamma_1 + \operatorname{Tr} H_{\Lambda_2,N_2}\Gamma_2. \tag{BB.20}$$

Proof. Using (BB.15) along with the spectral theorem it is obvious that (BB.19) holds, and (BB.20) follows directly from (BB.16). □

BB.2.2 The canonical thermodynamic limit

Given an open, connected subset $\Lambda \subseteq \mathbb{R}^d$, we denote by $-\Delta^\Lambda$ the Dirichlet Laplacian on $L^2(\Lambda)$, and

$$H_{\Lambda,N} = \sum_{i=1}^N -\Delta_i^\Lambda,$$

acting on the Hilbert space $\mathcal{H} = \bigwedge^N L^2(\Lambda)$. In this subsection, the existence of the thermodynamic limit of the canonical free energy is proved for general sequences of domains (Λ_N) with $|\Lambda_N| \to \infty$ and $N/|\Lambda_N| \to \rho$ for any density $\rho > 0$. Recall the notion of η-regularity from Definition BB.3.

Theorem BB.9. *Let $\rho, \beta > 0$ and $\Lambda_N \subseteq \mathbb{R}^d$ a sequence of bounded, connected sets such that $|\Lambda_N| \to \infty$ and $N/|\Lambda_N| \to \rho$ as N tends to infinity, and suppose furthermore that Λ_N has η-regular boundary, where η is independent of N. Then the thermodynamic limit*

$$f_{\mathrm{Can}}(\beta, \rho) := \lim_{N\to\infty} \frac{1}{|\Lambda_N|} e^{\beta}_{\mathrm{Can}}(\Lambda_N, N) = \lim_{N\to\infty} -\frac{1}{|\Lambda_N|\beta} \log \operatorname{Tr} e^{-\beta H_{\Lambda_N,N}} \tag{BB.21}$$

exists, and is independent of the sequence (Λ_N).

Remark BB.10 (Periodic boundary conditions). *With the existence of the thermodynamic limit established for the Dirichlet Laplacian, it is not difficult to generalize to the Laplacian on cubes with* periodic *boundary conditions. Denoting by $e^{\beta,\mathrm{per}}_{\mathrm{Can}}(\Lambda(L), N)$ the free energy for the periodic Laplacian in a cube $\Lambda(L) = (-L/2, L/2)^d$, it is clear that*

$$e^{\beta,\mathrm{per}}_{\mathrm{Can}}(\Lambda(L), N) \le e^{\beta}_{\mathrm{Can}}(\Lambda(L), N),$$

since any state on $\Lambda(L)$ satisfying Dirichlet boundary conditions also automatically satisfies periodic boundary conditions.

On the other hand, following steps 1 and 2 in the proof of Proposition B.9 in Paper B (but neglecting correlations) yields for any $\ell > 0$ an N-body Dirichlet trial state Γ on $\Lambda(L+\ell)$ satisfying

$$\operatorname{Tr}\big(-\Delta^{\Lambda(L+\ell)}\big)\Gamma + \frac{1}{\beta}\operatorname{Tr}\Gamma\log\Gamma \le e^{\beta,\mathrm{per}}_{\mathrm{Can}}(\Lambda(L), N) + C\frac{N}{\ell^2}.$$

for some constant $C > 0$. Taking $1 \ll \ell \ll L$, we conclude that the thermodynamic limit with periodic boundary conditions is the same as with Dirichlet conditions,

$$\lim_{\substack{N\to\infty \\ NL^{-d}\to\rho}} \frac{1}{L^d} e^{\beta,\mathrm{per}}_{\mathrm{Can}}(\Lambda(L), N) = f_{\mathrm{Can}}(\beta, \rho).$$

To prove Theorem BB.9, we follow ideas from [2, 4] based on sub-additivity of the canonical free energy. The existence will be proved first for a special sequence of cubes, and afterwards it will be generalized to arbitrary sequences of domains. We start out by making some introductory observations on the free energy

Lemma BB.11 (Basic properties of the free energy). *We have the following basic properties of the canonical free energy:*

(1) The free energy is monotone in the sense that

$$e^{\beta}_{\mathrm{Can}}(\Lambda_1, N) \ge e^{\beta}_{\mathrm{Can}}(\Lambda_2, N)$$

whenever $\Lambda_1 \subseteq \Lambda_2$.

(2) *Suppose that Λ_1 and Λ_2 are disjoint subsets of $\mathbb{R}^d$, $\beta > 0$, and N_1, N_2 are positive integers. Then the free energy is sub-additive in the sense that*

$$e^\beta_{\mathrm{Can}}(\Lambda_1 \cup \Lambda_2, N_1 + N_2) \le e^\beta_{\mathrm{Can}}(\Lambda_1, N_1) + e^\beta_{\mathrm{Can}}(\Lambda_2, N_2).$$

(3) *Finally, for any $\rho \ge 0$ and $\mu \in \mathbb{R}$ we can bound the free energy from below by*

$$\liminf_{\substack{N\to\infty \\ N|\Lambda_N|^{-1}\to\rho}} \frac{1}{|\Lambda_N|} e^\beta_{\mathrm{Can}}(\Lambda_N, N) \ge -\frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^d} \log\bigl(1 + e^{-\beta(p^2-\mu)}\bigr)\,\mathrm{d}p + \mu\rho.$$

Proof. (1). This is trivial since any N-particle state on the domain Λ_1 is also an N-particle state on Λ_2.

(2). Denote by Γ_1 and Γ_2 the Gibbs states on Λ_1 and Λ_2, respectively, and consider the anti-symmetrization $\Gamma := \Gamma_1 \wedge \Gamma_2$, which is a suitable trial state on $\Lambda := \Lambda_1 \cup \Lambda_2$. Since both the kinetic energy and the entropy behave additively under anti-symmetrization by Corollary BB.8, we obtain with $N := N_1 + N_2$,

$$\begin{aligned} e^\beta_{\mathrm{Can}}(\Lambda, N) &\le \operatorname{Tr} H_{\Lambda,N}\Gamma + \frac{1}{\beta}\operatorname{Tr}\Gamma\log\Gamma \\ &= \operatorname{Tr} H_{\Lambda_1,N_1}\Gamma_1 + \frac{1}{\beta}\operatorname{Tr}\Gamma_1\log\Gamma_1 + \operatorname{Tr} H_{\Lambda_2,N_2}\Gamma_2 + \frac{1}{\beta}\operatorname{Tr}\Gamma_2\log\Gamma_2 \\ &= e^\beta_{\mathrm{Can}}(\Lambda_1, N_1) + e^\beta_{\mathrm{Can}}(\Lambda_2, N_2). \end{aligned}$$

(3). Since any N-particle fermionic state is automatically also a state on anti-symmetric Fock space, we can always bound the canonical free energy from below by the grand canonical energy. More precisely, for any $\mu \in \mathbb{R}$

$$\begin{aligned} e^\beta_{\mathrm{Can}}(\Lambda, N) &= \inf_{\Gamma\in S^N_{\mathrm{Can}}} \Bigl(\operatorname{Tr} H_{\Lambda,N}\Gamma + \frac{1}{\beta}\operatorname{Tr}\Gamma\log\Gamma\Bigr) \\ &= \inf_{\Gamma\in S^N_{\mathrm{Can}}} \Bigl(\operatorname{Tr}\sum_{i=1}^N(-\Delta^\Lambda_i - \mu)\Gamma + \frac{1}{\beta}\Gamma\log\Gamma\Bigr) + \mu N \\ &\ge e^\beta_{\mathrm{GC}}(\Lambda, \mu) + \mu N, \end{aligned}$$

so utilizing the thermodynamic limit of the grand canonical free energy Proposition BB.4,

$$\liminf_{\substack{N\to\infty \\ N|\Lambda_N|^{-1}\to\rho}} \frac{1}{|\Lambda_N|} e^\beta_{\mathrm{Can}}(\Lambda_N, N) \ge -\frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^d} \log\bigl(1 + e^{-\beta(p^2-\mu)}\bigr)\,\mathrm{d}p + \mu\rho.$$

□

Lemma BB.12. *If Λ is a disjoint union of k identical cubes, then for any $N \ge k$, we have the upper bound*

$$e^\beta_{\mathrm{Can}}(\Lambda, N) \le C_d \frac{N^{1+\frac{2}{d}}}{|\Lambda|^{\frac{2}{d}}}. \tag{BB.22}$$

Proof. We prove first that the bound holds for any single cube and then generalize to unions of cubes. Suppose that $\Lambda = (0,L)^d$. We will construct a trial state for the variational problem by splitting Λ into at least N smaller cubes and placing a single particle in N of these cubes. Defining $\ell = L\lceil N^{\frac{1}{d}}\rceil^{-1}$, we can split Λ into exactly $(L\ell^{-1})^d = \lceil N^{\frac{1}{d}}\rceil^d \geq N$ smaller cubes of side length ℓ. Let $u \in C^\infty((0,1)^d)$ be any L^2-normalized function on the unit cube satisfying Dirichlet boundary conditions, and define for $n \in \mathbb{Z}^d$ a function $u_n^\ell(x) = \ell^{-\frac{d}{2}} u(\frac{x-n}{\ell})$ on the cube $\Lambda_n := (0,\ell)^d + n\ell$. By choosing N different indices $n_1, \ldots, n_N \in \mathbb{Z}^d$ with $\Lambda_{n_i} \subseteq \Lambda$, we can define a normalized N-body wave function by

$$\Psi := u_{n_1}^\ell \wedge \cdots \wedge u_{n_N}^\ell$$

on the union of cubes $\bigcup_i \Lambda_{n_i}$, and extend it by zero to the rest of Λ. Since Ψ is a pure state, and using the additivity of kinetic energy Corollary BB.8, we calculate

$$\begin{aligned} e_{\mathrm{Can}}^\beta(\Lambda, N) &\leq \langle \Psi, H_{\Lambda,N}\Psi \rangle = N \int_{(0,\ell)^d} |\nabla u_0^\ell(x)|^2 \,\mathrm{d}x \\ &= \frac{N}{\ell^2} \int_{(0,1)^d} |\nabla u(x)|^2 \,\mathrm{d}x \leq \frac{2N^{1+\frac{d}{2}}}{L^2} \int_{(0,1)^d} |\nabla u(x)|^2 \,\mathrm{d}x, \end{aligned}$$

showing that (BB.22) holds when Λ is just a single cube.

Suppose now that $\Lambda = \bigcup_{i=1}^k \Lambda_i$ is a union of cubes. Since $N \geq k$, we can write $N = N_k k + r_k$, where $N_k \geq 1$ and $0 \leq r_k < k$. Then we can define integers $\widetilde{N}_i \in \{N_k, N_k+1\}$ such that $N = \widetilde{N}_1 + \cdots + \widetilde{N}_k$, and because $|\Lambda| = k|\Lambda_i|$, we have

$$\frac{\widetilde{N}_i}{|\Lambda_i|} \leq \frac{(N_k+1)k}{k|\Lambda_i|} \leq \frac{2N}{|\Lambda|}.$$

Thus, using sub-additivity,

$$\begin{aligned} e_{\mathrm{Can}}^\beta(\Lambda, N) &\leq \sum_{i=1}^k e_{\mathrm{Can}}^\beta(\Lambda_i, \widetilde{N}_i) \leq \sum_{i=1}^k C_d \frac{\widetilde{N}_i^{1+\frac{2}{d}}}{|\Lambda_i|^{\frac{2}{d}}} \\ &\leq \sum_{i=1}^k C_d \widetilde{N}_i \Big(\frac{2N}{|\Lambda|}\Big)^{\frac{2}{d}} = 2^{\frac{2}{d}} C_d \frac{N^{1+\frac{2}{d}}}{|\Lambda|^{\frac{2}{d}}}, \end{aligned}$$

concluding the proof. □

We now prove Theorem BB.9 in the case of a special sequence of cubes.

Proposition BB.13. *Let $\rho, \beta > 0$ and consider the sequence of cubes Λ_n with side lengths $L_n = 2^n \rho^{-1/d}$. Then the limit*

$$f_{\mathrm{Can}}(\beta, \rho) := \lim_{n\to\infty} \frac{1}{L_n^d} e_{\mathrm{Can}}^\beta(\Lambda_n, 2^{dn})$$

exists.

Proof. The idea is simply to argue that the sequence on the right hand side above is decreasing and bounded from below. Dividing Λ_n into 2^d smaller cubes of side length $\frac{1}{2}L_n = L_{n-1}$, and putting $2^{d(n-1)}$ particles in each of these cubes, we obtain by sub-additivity and translation invariance

$$\begin{aligned}\frac{1}{L_n^d}e^{\beta}_{\mathrm{Can}}(\Lambda_n, 2^{dn}) &\leq \frac{1}{L_n^d}2^d e^{\beta}_{\mathrm{Can}}\big(\Lambda_{n-1}, 2^{d(n-1)}\big)\\ &= \frac{1}{L_{n-1}^d}e^{\beta}_{\mathrm{Can}}\big(\Lambda_{n-1}, 2^{d(n-1)}\big).\end{aligned}$$

Noting that $\frac{1}{L_n^d}e^{\beta}_{\mathrm{Can}}(\Lambda_n, 2^{dn})$ is bounded from below by Lemma BB.11 finishes the proof. $\square$

Proof of Theorem BB.9.. Fix $\beta, \rho > 0$ along with a positive integer $n \in \mathbb{N}$, and suppose that we have a sequence of domains (Λ_N) as in the theorem. Split $\mathbb{R}^d$ into a union of cubes C_j, all of side length $\ell_n = 2^n\rho^{-1/d}$. An upper bound to $e^{\beta}_{\mathrm{Can}}(\Lambda_N, N)$ will be given by approximating Λ_N from the inside using the cubes C_j, and a lower bound will be obtained by approximating from the outside, see Fig. BB.1. Let us consider the upper bound first.

We define as in the proof of Proposition BB.4

$$\widetilde{\Lambda}_N = \bigcup_{C_j \subseteq \Lambda_N} C_j \subseteq \Lambda_N,$$

and recall that by regularity we have the estimate (BB.10), that is,

$$|\widetilde{\Lambda}_N| \geq |\Lambda_N|(1 - \eta(\sqrt{d}\ell_n|\Lambda_N|^{-\frac{1}{d}})).$$

Note that $\widetilde{\Lambda}_N$ consists of exactly $K_N = |\widetilde{\Lambda}_N|/|C_j|$ cubes, and that $N/K_N \to 2^{dn}$ as $N \to \infty$. Fix now any $0 < \varepsilon < 1$ and put 2^{dn} particles each in $K_N - \lfloor \varepsilon K_N \rfloor$ of the cubes in $\widetilde{\Lambda}_N$. Place the $\widetilde{N} := N - (K_N - \lfloor \varepsilon K_N \rfloor)2^{dn}$ remaining particles in the union $\Lambda_N^{\varepsilon} = \bigcup_{\lfloor \varepsilon K_N \rfloor} C_j$ of the last $\lfloor \varepsilon K_N \rfloor$ cubes, and note that $\widetilde{N} \geq \lfloor \varepsilon K_N \rfloor$ for N large enough (so that we can apply Lemma BB.12), and that $\widetilde{N}/N \to \varepsilon$. We obtain by monotonicity and sub-additivity of the free energy

$$\begin{aligned}\frac{e^{\beta}_{\mathrm{Can}}(\Lambda_N, N)}{|\Lambda_N|} &\leq \frac{e^{\beta}_{\mathrm{Can}}(\widetilde{\Lambda}_N, N)}{|\Lambda_N|}\\ &\leq (K_N - \lfloor \varepsilon K_N \rfloor)\frac{e^{\beta}_{\mathrm{Can}}(C_j, 2^{dn})}{|\Lambda_N|} + \frac{e^{\beta}_{\mathrm{Can}}(\Lambda_N^{\varepsilon}, \widetilde{N})}{|\Lambda_N|}\\ &\leq \frac{|\widetilde{\Lambda}_N| - \lfloor \varepsilon K_N \rfloor |C_j|}{|\Lambda_N|}\frac{e^{\beta}_{\mathrm{Can}}(C_j, 2^{dn})}{|C_j|} + \omega_d\frac{\widetilde{N}^{1+\frac{2}{d}}}{|\Lambda_N|(\lfloor \varepsilon K_N \rfloor |C_j|)^{\frac{2}{d}}},\end{aligned}$$

where the last inequality uses the upper bound in Lemma BB.11. First taking N to infinity yields

$$\limsup_{N\to\infty}\frac{1}{|\Lambda_N|}e^{\beta}_{\mathrm{Can}}(\Lambda_N, N) \leq (1-\varepsilon)\frac{1}{|C_j|}e^{\beta}_{\mathrm{Can}}(C_j, 2^{dn}) + \varepsilon\omega_d\rho^{1+\frac{2}{d}},$$

so afterwards taking $\varepsilon \to 0$ and $n \to \infty$ using Proposition BB.13, we conclude the upper bound

$$\limsup_{N\to\infty} \frac{1}{|\Lambda_N|} e^{\beta}_{\mathrm{Can}}(\Lambda_N, N) \leq f_{\mathrm{Can}}(\beta, \rho).$$

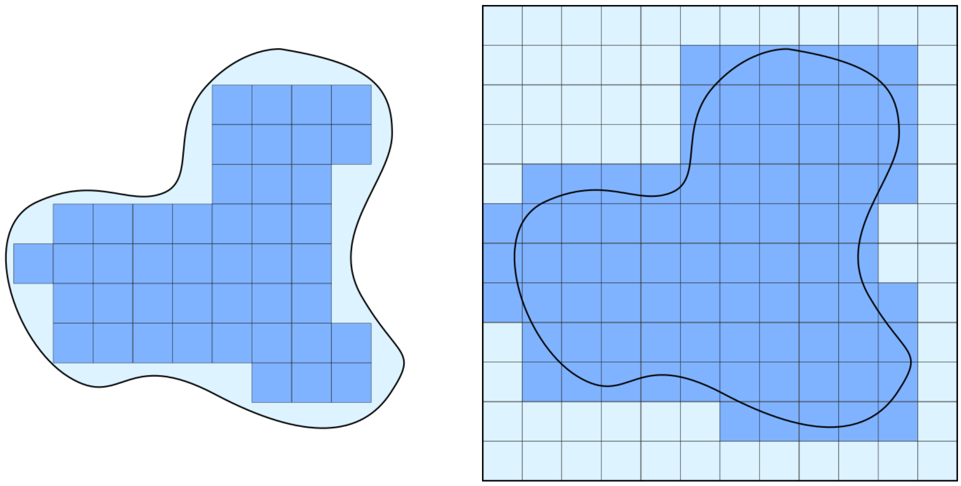

Figure BB.1: Strategy for proving lower and upper bounds on the free energy. On the left, for the lower bound, a set Λ_N approximated from the inside by a union of cubes. On the right, for the upper bound, Λ_N is placed in a large cube and approximated from the outside by smaller cubes.

For the lower bound, the general idea is the same, but Λ_N will instead be approximated from the outside by a union of cubes, that is, we now define

$$\widetilde{\Lambda}_N = \bigcup_{C_j \cap \Lambda_N \neq \emptyset} C_j \supseteq \Lambda_N$$

as in the proof of Proposition BB.4. Again we have the estimate (BB.11), i.e.

$$|\widetilde{\Lambda}_N| \leq |\Lambda_N|(1 + \eta(\sqrt{d}\ell_n|\Lambda_N|^{-\frac{1}{d}})).$$

By the connectedness and η-regularity of Λ_N, it follows from [2, Lemma 1] that the volume of the smallest cube containing Λ_N is of order $|\Lambda_N|$. By possibly translating and enlarging this cube a little, we can choose a cube C'_N containing $\widetilde{\Lambda}_N$ such that C'_N is a union of a number of the smaller cubes C_j for some $k_N \geq n$, and such that for some $\alpha > 2$,

$$2|\widetilde{\Lambda}_N| \leq |C'_N| \leq \alpha|\Lambda_N|. \tag{BB.23}$$

Then C'_N has volume $2^{dk_N}\rho^{-1}$ for some $k_N \geq n$, and $C'_N \setminus \widetilde{\Lambda}_N$ is a union of exactly $K_N := \frac{|C'_N \setminus \widetilde{\Lambda}_N|}{|C_j|}$ cubes. We will now put N particles in $\widetilde{\Lambda}_N$ and approximately 2^{dn} particles in each of the cubes in $C'_N \setminus \widetilde{\Lambda}_N$, such that there are exactly 2^{dk_N} particles in C'_N in total. More precisely, we again fix $0 < \varepsilon < 1$ and place 2^{dn} particles each in $K_N - \lfloor \varepsilon K_N \rfloor$ of the cubes of $C'_N \setminus \widetilde{\Lambda}_N$, and $\widetilde{N} := 2^{dk_N} - N - (K_N - \lfloor \varepsilon K_N \rfloor) 2^{dn}$ particles in the union Λ_N^ε of the remaining $\lfloor \varepsilon K_N \rfloor$ cubes of $C'_N \setminus \widetilde{\Lambda}_N$.

Before we proceed, let us argue that this number $\widetilde{N}$ is at least $\lfloor \varepsilon K_N \rfloor$ when N is large enough (so that Lemma BB.12 is applicable). To see this, note by definition of K_N and (BB.23) that

$$K_N 2^{dn} = |C'_N \setminus \widetilde{\Lambda}_N| \rho \geq |\widetilde{\Lambda}_N| \rho,$$

and since $N/|\widetilde{\Lambda}_N| \to \rho$, we have for any $\delta > 0$ and N large enough that

$$N - |\widetilde{\Lambda}_N| \rho \leq \delta |\widetilde{\Lambda}_N| \rho \leq \delta K_N 2^{dn}.$$

Thus, using that

$$2^{dk_N} - N - K_N 2^{dn} = |C'_N| \rho - N - |C'_N \setminus \widetilde{\Lambda}_N| \rho = |\widetilde{\Lambda}_N| \rho - N,$$

we easily obtain

$$\widetilde{N} = |\widetilde{\Lambda}_N| \rho - N + \lfloor \varepsilon K_N \rfloor 2^{dn} \geq \lfloor \varepsilon K_N \rfloor 2^{dn} - \delta K_N 2^{dn},$$

which is greater than $\lfloor \varepsilon K_N \rfloor$ if we choose $\delta \leq \varepsilon(1 - 2^{-dn})$.

Now, as before, we obtain by sub-additivity

$$\begin{aligned} e^\beta_{\mathrm{Can}}(C'_N, 2^{dk_N}) \leq e^\beta_{\mathrm{Can}}(\Lambda_N, N) & \\ + (K_N - \lfloor \varepsilon K_N \rfloor) e^\beta_{\mathrm{Can}}(C_j, 2^{dn}) &+ e^\beta_{\mathrm{Can}}(\Lambda_N^\varepsilon, \widetilde{N}). \end{aligned} \tag{BB.24}$$

We have by definition of K_N

$$\frac{K_N - \lfloor \varepsilon K_N \rfloor}{|\Lambda_N|} e^\beta_{\mathrm{Can}}(C_j, 2^{dn}) = (1 - \varepsilon) \frac{|C'_N \setminus \widetilde{\Lambda}_N|}{|\Lambda_N|} \frac{e^\beta_{\mathrm{Can}}(C_j, 2^{dn})}{|C_j|} + o(1)$$

so using that $e^\beta_{\mathrm{Can}}(C'_N, 2^{dk_N}) \geq f_{\mathrm{Can}}(\beta, \rho) |C'_N|$ (which follows from the proof of Proposition BB.13) and continuing from (BB.24), we obtain

$$\begin{aligned} \frac{e^\beta_{\mathrm{Can}}(\Lambda_N, N)}{|\Lambda_N|} &\geq \frac{|C'_N|}{|\Lambda_N|} f_{\mathrm{Can}}(\beta, \rho) - \frac{e^\beta_{\mathrm{Can}}(\Lambda_N^\varepsilon, \widetilde{N})}{|\Lambda_N|} \\ &\quad - (1 - \varepsilon) \frac{|C'_N \setminus \widetilde{\Lambda}_N|}{|\Lambda_N|} \frac{e^\beta_{\mathrm{Can}}(C_j, 2^{dn})}{|C_j|} \\ &= \frac{|\widetilde{\Lambda}_N|}{|\Lambda_N|} f_{\mathrm{Can}}(\beta, \rho) - \frac{e^\beta_{\mathrm{Can}}(\Lambda_N^\varepsilon, \widetilde{N})}{|\Lambda_N|} \\ &\quad + \frac{|C'_N \setminus \widetilde{\Lambda}_N|}{|\Lambda_N|} \Big(f_{\mathrm{Can}}(\beta, \rho) - (1 - \varepsilon) \frac{e^\beta_{\mathrm{Can}}(C_j, 2^{dn})}{|C_j|} \Big). \end{aligned}$$

Let us estimate the second term above. Since

$$\frac{\widetilde{N}}{N} = \frac{\lfloor \varepsilon K_N \rfloor 2^{dn}}{N} + o(1) = \varepsilon \frac{|C'_N \setminus \widetilde{\Lambda}_N| \rho}{N} + o(1) \leq \varepsilon \alpha \frac{|\Lambda_N| \rho}{N} + o(1),$$

and
$$\frac{|\Lambda_N^\varepsilon|}{N} = \frac{\lfloor \varepsilon K_N \rfloor |C_j|}{N} \geq \varepsilon \frac{|\Lambda_N|}{N} - \frac{|C_j|}{N} \to \frac{\varepsilon}{\rho},$$
we have by the upper bound in Lemma BB.12 that
$$\limsup_{N\to\infty} \frac{e^\beta_{\mathrm{Can}}(\Lambda_N^\varepsilon, \widetilde{N})}{|\Lambda|_N} \leq \limsup_{N\to\infty} \omega_d \frac{\widetilde{N}^{1+\frac{2}{d}}}{|\Lambda_N||\Lambda_N^\varepsilon|^{\frac{2}{d}}} \leq \varepsilon w_d \alpha^{1+\frac{2}{d}} \rho^{1+\frac{2}{d}}.$$

Hence, because $\frac{|C'_N \setminus \widetilde{\Lambda}_N|}{|\Lambda_N|}$ is bounded, we obtain for some constant $c \in \mathbb{R}$ that
$$\begin{aligned}\liminf_{N\to\infty} \frac{e^\beta_{\mathrm{Can}}(\Lambda_N, N)}{|\Lambda_N|} \geq{}& f_{\mathrm{Can}}(\beta,\rho) - \varepsilon w_d \alpha^{1+\frac{2}{d}} \rho^{1+\frac{2}{d}} \\ &+ c\Big(f_{\mathrm{Can}}(\beta,\rho) - (1-\varepsilon)\frac{e^\beta_{\mathrm{Can}}(C_j, 2^{dn})}{|C_j|}\Big).\end{aligned}$$

Finally, taking $n \to \infty$ and $\varepsilon \to 0$ yields the desired bound, finishing the proof. ☐

Lemma BB.14 (Properties of f_{Can}). *Let $\beta > 0$.*

(1) $f_{\mathrm{Can}}(\beta, \cdot\,)$ is continuous at $\rho = 0$, with $f_{\mathrm{Can}}(\beta, 0) = 0$.

(2) $f_{\mathrm{Can}}(\beta, \cdot\,)$ is convex (and hence also continuous) in $\rho \in \mathbb{R}_+$.

(3) Fix a domain $\Lambda_0 \subseteq \mathbb{R}^d$ and consider sequences of the type $\Lambda_N = L_N \Lambda_0$, where (L_N) is a sequence of positive numbers. Then the convergence in the thermodynamic limit (BB.21) for fixed Λ_0 is locally uniform in the density $\rho = \lim_{N\to\infty} \frac{N}{L_N^d |\Lambda_0|}$.

Proof. (1). We will argue both that the thermodynamic limit is
$$\lim_{\substack{N\to\infty \\ N|\Lambda_N|^{-1}\to 0}} \frac{1}{|\Lambda_N|} e^\beta_{\mathrm{Can}}(\Lambda_N, N) = 0,$$

and that $\lim_{\rho\to 0} f_{\mathrm{Can}}(\beta,\rho) = 0$. Because of the lower bound on the free energy from Lemma BB.11, we have for any $\mu \in \mathbb{R}$ and non-negative ρ that
$$\begin{aligned}\liminf_{\substack{N\to\infty \\ N|\Lambda_N|^{-1}\to \rho}} \frac{e^\beta_{\mathrm{Can}}(\Lambda_N, N)}{|\Lambda_N|} &\geq -\frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^d} \log\big(1 + e^{-\beta(p^2-\mu)}\big)\, \mathrm{d}p + \mu\rho \\ &\geq -\frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^d} e^{-\beta(p^2-\mu)}\, \mathrm{d}p + \mu\rho = -C_\beta e^{\beta\mu} + \mu\rho.\end{aligned}$$

Hence, for $\rho = 0$, we simply take $\mu \to -\infty$ to obtain
$$\liminf_{\substack{N\to\infty \\ N|\Lambda_N|^{-1}\to 0}} \frac{e^\beta_{\mathrm{Can}}(\Lambda_N, N)}{|\Lambda_N|} \geq 0.$$

On the other hand, choosing $\mu = \frac{1}{\beta}\log\rho$ in the case $\rho > 0$, we have

$$f_{\text{Can}}(\beta,\rho) \geq -C_\beta\rho + \frac{1}{\beta}\rho\log\rho \xrightarrow{\rho\to 0} 0.$$

Taking the thermodynamic limit along a sequence of cubes, the two corresponding upper bounds follow from the upper bound on the free energy in Lemma BB.12.

(2). Let $\rho_1,\rho_2 > 0$ and $0 < t < 1$ be arbitrary, and put $\rho = t\rho_1 + (1-t)\rho_2$. Suppose further that Λ_N is a sequence of boxes such that the assumptions of Theorem BB.9 are satisfied. Cut each box into two smaller boxes $\Lambda_N^{(1)}$ and $\Lambda_N^{(2)}$ such that $|\Lambda_N^{(1)}| = t|\Lambda_N|$ and $|\Lambda_N^{(2)}| = (1-t)|\Lambda_N|$. Putting respectively $N_1 := \lfloor t|\Lambda_N|\rho_1\rfloor$ and $N_2 := \lfloor (1-t)|\Lambda_N|\rho_2\rfloor$ in each box we have that $N_i|\Lambda_N^{(i)}| \to \rho_i$ as N tends to infinity, so by sub-additivity,

$$\begin{aligned} f_{\text{Can}}(\beta,\rho) &= \lim_{N\to\infty}\frac{1}{|\Lambda_N|}e^\beta_{\text{Can}}(\Lambda_N,N) \\ &\leq \lim_{N\to\infty} t\frac{1}{|\Lambda_N^{(1)}|}e^\beta_{\text{Can}}(\Lambda_N^{(1)},N_1) + (1-t)\frac{1}{|\Lambda_N^{(2)}|}e^\beta_{\text{Can}}(\Lambda_N^{(2)},N_2) \\ &= t f_{\text{Can}}(\beta,\rho_1) + (1-t) f_{\text{Can}}(\beta,\rho_2), \end{aligned}$$

showing convexity.

(3). The uniform convergence in ρ for this particular type of sequences follows from a simple change of variables along with an elementary fact. Given a $\rho > 0$ we denote $\Lambda_\rho = (\frac{N}{\rho|\Lambda_0|})^{\frac{1}{d}}\Lambda_0$ and by changing variables,

$$\begin{aligned} e^\beta_{\text{Can}}(\rho,N) &:= \frac{1}{|\Lambda_\rho|}e^\beta_{\text{Can}}(\Lambda_\rho,N) = -\frac{\rho}{N\beta}\log\operatorname{Tr} e^{-\beta\sum_{i=1}^N -\Delta_i^{\Lambda_\rho}} \\ &= -\frac{\rho}{N\beta}\log\operatorname{Tr} e^{-\beta\sum_{i=1}^N -(\frac{\rho|\Lambda_0|}{N})^{\frac{2}{d}}\Delta_i^{\Lambda_0}}. \end{aligned}$$

This means with $\rho_N := \frac{N}{|\Lambda_N|} = \frac{N}{L_N^d|\Lambda_0|}$ that we can write

$$f_{\text{Can}}(\beta,\rho) = \lim_{N\to\infty}\frac{1}{|\Lambda_N|}e^\beta_{\text{Can}}(\Lambda_N,N) = \lim_{N\to\infty} e^\beta_{\text{Can}}(\rho_N,N).$$

We can now to conclude that the convergence is locally uniform in ρ by applying the following elementary fact, which is easily shown by contradiction:

- Suppose that X is any locally compact metric space, and let (g_n) be a sequence of functions on X with values in a metric space Y. If there exists a continuous function g on X satisfying that $g_n(x_n) \to g(x)$ for any convergent sequence x_n in X with limit point x, then g_n converges to g locally uniformly on X.

□

Proposition BB.15 (Equivalence of ensembles). *Let $\beta, \rho > 0$ be any positive numbers and define $\mu(\rho)$ to be the unique solution to the equation*

$$\rho = \frac{\partial}{\partial\mu} f_{\mathrm{GC}}(\beta, \mu(\rho)) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{1}{1 + e^{\beta(p^2 - \mu(\rho))}} \,\mathrm{d}p. \tag{BB.25}$$

Then we have

$$\begin{aligned} f_{\mathrm{Can}}(\beta, \rho) &= \lim_{\substack{N\to\infty \\ N|\Lambda_N|^{-1}\to\rho}} e^{\beta}_{\mathrm{GC}}(\Lambda_N, \mu(\rho)) + \mu(\rho)\frac{N}{|\Lambda_N|} \\ &= -\frac{1}{(2\pi)^d\beta} \int_{\mathbb{R}^d} \log\bigl(1 + e^{-\beta(p^2 - \mu(\rho))}\bigr) \,\mathrm{d}p + \mu(\rho)\rho. \end{aligned} \tag{BB.26}$$

Proof. Because of Lemma BB.11 we only need to give an upper bound on $f_{\mathrm{Can}}(\beta, \rho)$. For this I will follow the idea of [6], using the fact that $f_{\mathrm{Can}}(\beta, \cdot\,)$ is its own double Legendre transform due to convexity. Thus we introduce the Legendre transform of $f_{\mathrm{Can}}(\beta, \cdot\,)$,

$$f^*_{\mathrm{Can}}(\beta, \mu) := \sup_{0\le\rho<\infty} (\mu\rho - f_{\mathrm{Can}}(\beta, \rho)), \qquad \mu \in \mathbb{R}. \tag{BB.27}$$

If we can bound the grand canonical free energy from below using this function, i.e. if

$$f_{\mathrm{GC}}(\beta, \mu) := \lim_{N\to\infty} \frac{1}{|\Lambda_N|} e^{\beta}_{\mathrm{GC}}(\Lambda_N, \mu) \ge -f^*_{\mathrm{Can}}(\beta, \mu), \tag{BB.28}$$

then we have the following series of inequalities, using the already established lower bound on $f_{\mathrm{Can}}(\beta, \rho)$,

$$f_{\mathrm{Can}}(\beta, \rho) \ge \sup_{\mu\in\mathbb{R}} (f_{\mathrm{GC}}(\beta, \mu) + \mu\rho) \ge \sup_{\mu\in\mathbb{R}} (\mu\rho - f^*_{\mathrm{Can}}(\beta, \mu)) = f_{\mathrm{Can}}(\beta, \rho).$$

From this we conclude that (BB.26) holds when μ satisfies the equation

$$\rho = \frac{\partial}{\partial\mu} f_{\mathrm{GC}}(\beta, \mu) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{1}{1 + e^{\beta(p^2 - \mu)}} \,\mathrm{d}p.$$

The rest of the proof is thus devoted to proving (BB.28). Since the thermodynamic limit is independent of the sequence of domains, we can fix a sequence of the form $\Lambda_N = L_N \Lambda_0$, where $\Lambda_0 \subseteq \mathbb{R}^d$ is some basis domain, and L_N is a sequence of positive integers with $\frac{N}{L_N^d |\Lambda_0|} \to \rho$. Recall that the grand canonical free energy is given by

$$e^{\beta}_{\mathrm{GC}}(\Lambda_N, \mu) = -\frac{1}{\beta} \log\Bigl(\sum_{n\ge 0} \operatorname{Tr} e^{-\beta(H_{\Lambda_N, n} - \mu n)}\Bigr).$$

We will fix a number $C > 0$ and estimate the terms with $n \le C|\Lambda_N|$ and $n > C|\Lambda_N|$ separately, starting with the low n terms.

Because of the locally uniform convergence of Lemma BB.14, and by continuity of the thermodynamic limit we can pick N large enough such that for $n \leq C|\Lambda_N|$, we have for some arbitrary $\varepsilon > 0$,

$$-\frac{1}{\beta}\log \operatorname{Tr} e^{-\beta H_{\Lambda_N,n}} = e^{\beta}_{\mathrm{Can}}(\Lambda_N, n) \geq |\Lambda_N|(f_{\mathrm{Can}}(\beta, n|\Lambda_N|^{-1}) - \varepsilon).$$

This means that

$$\begin{aligned}\sum_{n\leq C|\Lambda_N|} \operatorname{Tr} e^{-\beta(H_{\Lambda_N,n}-\mu n)} &\leq \sum_{n\leq C|\Lambda_N|} e^{\beta|\Lambda_N|(\mu n|\Lambda_N|^{-1} - f_{\mathrm{Can}}(\beta,n|\Lambda_N|^{-1})+\varepsilon)} \\ &\leq \sum_{n\leq C|\Lambda_N|} e^{\beta|\Lambda_N|(f^*_{\mathrm{Can}}(\beta,\mu)+\varepsilon)} \\ &\leq C|\Lambda_N| e^{\beta|\Lambda_N|(f^*_{\mathrm{Can}}(\beta,\mu)+\varepsilon)}. \end{aligned} \tag{BB.29}$$

For the terms with $n > C|\Lambda_N|$, we will take advantage of the fact that the kinetic energy grows faster than n, by the Lieb-Thirring inequality:

$$H_{\Lambda_N,n}\Gamma \geq C_{\mathrm{LT}}\frac{n^{1+\frac{2}{d}}}{|\Lambda_N|^{\frac{2}{d}}},$$

for any n-particle fermionic state Γ. Using this, we get the estimate

$$\begin{aligned}-\frac{1}{\beta}\log \operatorname{Tr} e^{-\beta H_{\Lambda_N,n}} &= \min_{\Gamma}\big(\operatorname{Tr} H_{\Lambda_N,n}\Gamma + \frac{1}{\beta}\operatorname{Tr}\Gamma\log\Gamma\big) \\ &\geq \frac{1}{2}C_{\mathrm{LT}}\frac{n^{1+\frac{2}{d}}}{|\Lambda_N|^{\frac{2}{d}}} - \frac{1}{\beta}\log \operatorname{Tr} e^{-\frac{\beta}{2}H_{\Lambda_N,n}},\end{aligned}$$

where, by choosing N large enough, we can bound the last term by

$$-\frac{1}{\beta}\log \operatorname{Tr} e^{-\frac{\beta}{2}H_{\Lambda_N,n}} \geq \frac{1}{2}e^{\beta/2}_{\mathrm{GC}}(\Lambda_N, 2\mu) + \mu n \geq \frac{|\Lambda_N|}{2}(f_{\mathrm{GC}}(\beta/2, 2\mu) - \varepsilon) + \mu n.$$

Thus, since f_{GC} is negative, we obtain for $n > C|\Lambda_N|$,

$$\begin{aligned}\operatorname{Tr} e^{-\beta H_{\Lambda_N,n}} &\leq e^{-\beta\mu n}e^{-\frac{\beta}{2}\left(C_{\mathrm{LT}}n^{1+\frac{2}{d}}|\Lambda_N|^{-\frac{2}{d}}+|\Lambda_N|(f_{\mathrm{GC}}(\beta/2,2\mu)-\varepsilon)\right)} \\ &\leq e^{-\beta\mu n}e^{-\frac{\beta}{2}n\left(C_{\mathrm{LT}}C^{\frac{2}{d}}+C^{-1}(f_{\mathrm{GC}}(\beta/2,2\mu)-\varepsilon)\right)}.\end{aligned}$$

Hence, choosing C sufficiently large (independently on N) to make the exponents above as negative as we want, the contribution from the terms with $n > C|\Lambda_N|$ can be bounded by, say,

$$\sum_{n>C|\Lambda_N|} \operatorname{Tr} e^{-\beta(H_{\Lambda_N,n}-\mu n)} \leq \sum_{n>C|\Lambda_N|}\left(\frac{1}{2}\right)^n,$$

which becomes small when N tends to infinity. Combining with (BB.29), we conclude for large N that

$$\begin{aligned}\frac{1}{|\Lambda_N|}e^{\beta}_{\mathrm{GC}}(\Lambda_N,\mu) &\geq -\frac{1}{\beta|\Lambda_N|}\log(C|\Lambda_N|e^{\beta|\Lambda_N|(f^*_{\mathrm{Can}}(\beta,\mu)+\varepsilon)}+o(1)) \\ &= -\frac{\log(C|\Lambda_N|)}{\beta|\Lambda_N|} - f^*_{\mathrm{Can}}(\beta,\mu) - \varepsilon + o(1).\end{aligned}$$

Since ε is arbitrary, taking N to infinity shows that (BB.28) holds, finishing the proof. □

Finally, combining Remark BB.10, Lemma BB.14, and Proposition BB.15 we immediately obtain the following result, which (up to a rescaling) is used in the proof of Proposition B.9 (the construction of trial states for the upper energy bound in Paper B):

Proposition BB.16. *Let $\beta,\rho > 0$, and denote for $L > 0$ the cube $\Lambda(L) = \left(-\frac{L}{2},\frac{L}{2}\right)^d$. Then, locally uniformly in the density ρ, the thermodynamic limit for cubes with periodic boundary conditions is*

$$\lim_{\substack{N\to\infty \\ NL^{-d}\to\rho}} \frac{1}{L^d}e^{\beta,\mathrm{per}}_{\mathrm{Can}}(\Lambda(L),N) = -\frac{1}{(2\pi)^d\beta}\int_{\mathbb{R}^d}\log\left(1+e^{-\beta(p^2-\mu(\rho))}\right)\mathrm{d}p + \mu(\rho)\rho,$$

where $\mu(\rho)$ is the unique solution to the equation (BB.25).

References

[1] V. Bach, E. H. Lieb, and J. P. Solovej. *Generalized Hartree-Fock theory and the Hubbard model. J. Statist. Phys.*, **76**(1-2):3–89, 1994. ISSN 0022-4715.

[2] M. E. Fisher. *The free energy of a macroscopic system. Arch. Ration. Mech. Anal.*, **17**:377–410, 1964. ISSN 0003-9527.

[3] M. Lewin. *Geometric methods for nonlinear many-body quantum systems. J. Funct. Anal.*, **260**:3535–3595, 2011. doi:10.1016/j.jfa.2010.11.017.

[4] M. Lewin, E. H. Lieb, and R. Seiringer. *Statistical Mechanics of the Uniform Electron Gas. J. Éc. polytech. Math.*, **5**:79–116, 2018. doi:10.5802/jep.64.

[5] M. Reed and B. Simon. *Methods of Modern Mathematical Physics. IV. Analysis of operators.* Academic Press, New York, 1978. ISBN 0-12-585004-2.

[6] D. Ruelle. *Statistical mechanics. Rigorous results.* Singapore: World Scientific. London: Imperial College Press, 1999. ISBN 9789810238629.

[7] A. Triay. *In preparation.* Ph.D. thesis, University of Paris-Dauphine, 2019.