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SEMI-CLASSICAL LIMIT OF LARGE FERMIONIC SYSTEMS AT POSITIVE TEMPERATURE

MATHIEU LEWIN, PETER S. MADSEN, AND ARNAUD TRIAY

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.

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In this article we study mean-field-type limits for a system of N fermions at temperature T>0 in a fixed confining potential. We assume that the interaction has an intensity of the order 1/N and that there is an effective semi-classical parameter $\hbar=N^{-1/d}$ where d is the space dimension. In the limit we obtain the nonlinear Thomas-Fermi problem at the corresponding temperature T>0. This paper is an extension of a recent work [16] 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 [15, 18, 22, 11]. It has also played an important role in astrophysics, where the very high pressure encountered in the core of neutron stars and white dwarfs makes it valuable for all kinds of elements of the periodic table [40, 39, 10, 4]. 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 [19].

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In the regime considered in this paper, a mean-field scaling is coupled to a semi-classical limit. This creates some mathematical difficulties. Before [16], this limit has been rigorously considered at T=0 for atoms by Lieb and Simon in [33, 32] and for pseudo-relativistic stars by Lieb, Thirring and Yau in [36, 37]. Upper and lower bounds on the next order correction have recently been derived in [21, 6], for particles evolving on the torus. There are several mathematical works on the time-dependent setting [41, 49, 3, 14, 17, 8, 5, 1, 42, 7, 13], in which the Schrödinger dynamics has been proved to converge to the Vlasov time-dependent 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 [31] at T=0 and in [47] at T>0.

The mean-field limit at positive temperature for fermions is completely different from the bosonic case. It was proved in [24] 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 [29]. 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 [20, 25, 27, 28, 26, 45]. Without statistics (boltzons), the temperature does affect the leading order of the energy [23], and the same happens for fermions, as we will demonstrate.

Our method for studying the Fermi gas in the coupled mean-field/semiclassical limit relies on previous techniques introduced in [16]. 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 5 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 [16] based on the classical de Finetti theorem for fermions.

The article is organized as follows. In the next section we introduce both the N-particle quantum Hamiltonian and the positive-temperature Thomas-Fermi theory which is obtained in the limit. We then state our main theorems, Theorem 2 and Theorem 7. As an intermediate result for the upper bound, we show in Section 2 how to approximate a classical density by an N body quantum state. In Section 3, we use this trial state and some known results about the free Fermi gas at positive temperature to prove our main result in the non-interacting case. The interacting case is dealt with in Section 4. Finally, in Section 5 we study the Gibbs state and the minimizers of the Thomas-Fermi functional at positive temperature (Theorem 1).

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1. Models and main results

1.1. The Vlasov and Thomas-Fermi functionals at T > 0. For a given density $\rho > 0$ and an inverse temperature $\beta > 0$, the Vlasov functional at positive temperature is given by

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

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

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

is the spatial density of particles. Here m is a positive measure on the phase space $\mathbb{R}^d \times \mathbb{R}^d$, with the convention

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

and which is assumed to satisfy Pauli's principle $0 \le m \le 1$. 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. We denote the Vlasov minimum free energy by

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

$$\min_{\substack{0 \le m(p) \le 1 \\ (2\pi)^{-d} \int_{\mathbb{R}^d} m(p) \, \mathrm{d}p = \nu}} \left(\frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} |p + A|^2 m(p) \, \mathrm{d}p + \frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^d} s(m(p)) \, \mathrm{d}p \right)$$

$$= -\frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^d} \log \left(1 + e^{-\beta \left(p^2 - \mu_{\mathrm{FG}}(\beta, \nu) \right)} \right) \, \mathrm{d}p + \mu_{\mathrm{FG}}(\beta, \nu) \, \nu$$

where $\mu_{FG}(\beta, \nu)$ is the unique solution to the implicit equation

$$\frac{1}{(2\pi)^d} \int_{\mathbb{D}^d} \frac{1}{1 + e^{\beta(p^2 - \mu_{FG}(\beta, \nu))}} \, \mathrm{d}p = \nu$$

and with the unique corresponding minimizer

$$m_{\nu,A}(p) = \frac{1}{1 + e^{\beta(|p+A|^2 - \mu_{\text{FG}}(\beta,\nu))}}$$

This is the uniform Fermi gas at density $\nu > 0$. For later purposes we introduce the free energy of the Fermi gas

$$F_{\beta}(\nu) := -\frac{1}{(2\pi)^{d}\beta} \int_{\mathbb{R}^{d}} \log\left(1 + e^{-\beta(p^{2} - \mu_{\text{FG}}(\beta, \nu))}\right) dp + \mu_{\text{FG}}(\beta, \nu) \nu.$$
 (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, which leads to the Thomas-Fermi minimization problem at positive temperature $T=1/\beta$

$$e_{\text{Vla}}^{\beta}(\rho) = \min_{\substack{\nu \in L^{1}(\mathbb{R}^{d}, \mathbb{R}_{+}) \\ \int_{\mathbb{R}^{d}} \nu(x) \, \mathrm{d}x = \rho}} \left\{ \int_{\mathbb{R}^{d}} F_{\beta}(\nu(x)) \, \mathrm{d}x + \int_{\mathbb{R}^{d}} V(x)\nu(x) \, \mathrm{d}x$$

The Vlasov minimization (2) on phase space will be more tractable and we will almost never use the Thomas-Fermi formulation (4) of the problem.

Now we discuss the existence of a unique Vlasov minimizer for (2), under appropriate assumptions on V, A, w. We use everywhere the notation $V_{\pm} = \max(\pm V, 0)$ for the positive and negative parts of V, which are both positive functions by definition.

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

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

Then, for all $\beta > \beta_0$, there are minimizers for the Vlasov problem (2). Any minimizer m_0 solves the nonlinear equation

$$m_0(x,p) = \frac{1}{1 + \exp\left(\beta(|p + A(x)|^2 + V(x) + \rho^{-1}w * \rho_{m_0}(x) - \mu)\right)}, \quad (5)$$

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

$$e_{\text{Vla}}^{\beta}(\rho) = -\frac{1}{(2\pi)^{d} \beta} \iint_{\mathbb{R}^{2d}} \log \left(1 + e^{-\beta \left(|p|^{2} + V(x) + \rho^{-1} w * \rho_{m_{0}}(x) - \mu \right)} \right) dx dp + \mu \rho - \frac{1}{2\rho} \iint_{\mathbb{R}^{2d}} w(x - y) \rho_{m_{0}}(x) \rho_{m_{0}}(y) dx dy.$$
 (6)

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

$$F_{\mathrm{Vla}}^{\beta}(\rho, \rho') := \inf_{\substack{0 \le m \le 1 \\ (2\pi)^{-d} \iint_{\mathbb{R}^{2d}} m = \rho}} \mathcal{E}_{\mathrm{Vla}}^{\beta, \rho'}(m). \tag{7}$$

Then, for any $\rho' > 0$, $F_{Vla}^{\beta}(\cdot, \rho')$ is C^1 on \mathbb{R}_+ and the multiplier appearing in (5) is given by

$$\mu = \frac{\partial F_{\text{Vla}}^{\beta}}{\partial \rho} (\rho, \rho') |_{\rho' = \rho}.$$
 (8)

The proof of Theorem 1 is classical and given for completeness in Section 5. Note that the magnetic potential A has only a trivial effect on the minimization problem. The minimizers for a given A are exactly equal to the $m_0(x, p + A)$ with m_0 a minimizer for $A \equiv 0$. The value of the minimal energy, the density ρ_{m_0} and the Lagrange multiplier μ are unchanged under this transformation.

The two conditions $e^{-\beta V_+} \in L^1(\mathbb{R}^d)$ and $V_- \in L^{d/2}(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ have been chosen to ensure that the minimizer has a finite total mass and a finite total energy. This is because

$$\iint_{\mathbb{R}^{2d}} \frac{1}{1 + e^{\beta(p^2 + V_+ - V_-)}} \le \iint_{\mathbb{R}^{2d}} e^{-\beta(p^2/2 + V_+)} + |\{p^2 \le 2V_-\}| \\
\le C \int_{\mathbb{R}^d} \left(\beta^{-\frac{d}{2}} e^{-\beta V_+} + V_-^{\frac{d}{2}}\right) \tag{9}$$

and, similarly,

$$\iint_{\mathbb{R}^{2d}} \log \left(1 + e^{-\beta(p^2 + V_+ - V_-)} \right) dx dp$$

$$\leq \iint_{\mathbb{R}^{2d}} e^{-\beta(p^2 / 2 + V_+)} + C \iint_{\{p^2 \leq 2V_-\}} (1 + \beta V_-)$$

$$\leq C \int_{\mathbb{R}^d} \left(\beta^{-\frac{d}{2}} e^{-\beta V_+} + V_-^{\frac{d}{2}} + \beta V_-^{1 + \frac{d}{2}} \right).$$

- 1.2. 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. (1) introduced in the previous section.
- 1.2.1. 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

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

$$|A|^2, w \in L^{1+\frac{d}{2}}\left(\mathbb{R}^d\right) + L_{\varepsilon}^{\infty}\left(\mathbb{R}^d\right)$$

and that w is an even function. We also assume that the electric potential $V \in L^{1+d/2}_{loc}(\mathbb{R}^d)$ is confining, that is, $V(x) \to \infty$ when $|x| \to \infty$, and that the divergence is so fast that $\int e^{-\beta_0 V_+(x)} dx < \infty$ for some $\beta_0 > 0$. Note that this implies that V_- has a compact support, hence in particular

 $V_- \in L^{d/2}(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$. At inverse temperature $\beta > \beta_0$, the canonical free energy is given by the functional

$$\mathcal{E}_{\operatorname{Can}}^{N,\hbar}(\Gamma) = \operatorname{Tr}(H_{N,\hbar}\Gamma) + \frac{1}{\beta}\operatorname{Tr}(\Gamma\log\Gamma), \tag{11}$$

defined for all fermionic quantum states $\Gamma = \Gamma^* \geq 0$ with $\text{Tr}(\Gamma) = 1$. The minimum over all Γ is uniquely attained at the Gibbs state

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

where $Z = \text{Tr } e^{-\beta H_{N,\hbar}}$, which leads to the minimum free energy

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

Our main result is the following.

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

$$\lim_{\substack{N \to \infty \\ \hbar^d N \to \rho}} \hbar^d e_{\operatorname{Can}}^{\beta}(\hbar, N) = e_{\operatorname{Vla}}^{\beta}(\rho).$$
 (12)

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

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

then for all $k \geq 1$ we have in the same limit

$$\int_{\mathbb{R}^{2dk}} m_{f,\Gamma_N}^{(k)} \varphi \to \int_{\mathbb{R}^{2dk}} m_0^{\otimes k} \varphi \tag{13}$$

for all $\varphi \in L^1(\mathbb{R}^{2dk}) + L^{\infty}(\mathbb{R}^{2dk})$, where $m_{f,\Gamma_N}^{(k)}$ is the k-particle Husimi function of Γ_N and m_0 is the unique minimizer of the Vlasov functional in Eq. (5). Similarly, if we denote by $\mathcal{W}_{\Gamma_N}^{(k)}$ the k-particle Wigner measure of Γ_N , we also have,

$$\int_{\mathbb{R}^{2dk}} \mathcal{W}_{\Gamma_N}^{(k)} \varphi \to \int_{\mathbb{R}^{2dk}} m_0^{\otimes k} \varphi, \tag{14}$$

for all φ satisfying $\partial_{x_1}^{\alpha_1}...\partial_{x_k}^{\alpha_k}\partial_{p_1}^{\beta_1}...\partial_{p_k}^{\beta_k}\varphi \in L^{\infty}(\mathbb{R}^{2dk})$, where $\max(\alpha_j,\beta_j) \leq 1$. Finally, the one particle density of Γ_N satisfies the following convergence

$$m_{f,\Gamma_N}^{(1)} \longrightarrow m_0 \text{ strongly in } L^1(\mathbb{R}^{2d}),$$
 (15)

$$\rho_{m_{f,\Gamma_N}^{(1)}} \longrightarrow \rho_{m_0} \text{ strongly in } L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d), \tag{16}$$

moreover, we have

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

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 [16]. These are some natural semiclassical measures that can be associated with Γ_N in the k-particle phase space \mathbb{R}^{2dk} . We will recall their definition in the proof later

in Section 4.3. The convergence of states as in (13) and (14) actually follows rather easily from the theory developed in [16] and most of this article will be dedicated to the proof of the limit (12).

Remark 3. For simplicity we work with a confining potential V but Theorems 1 and 2 hold the same when \mathbb{R}^d is replaced by a bounded domain Ω with any boundary conditions.

Remark 4. Our lower bound relies on the strong assumption that $\widehat{w} \geq 0$, but the upper bound does not. It is classical that a positive Fourier transform allows to easily bound the interaction from below by a one-body potential, see Eq. (39) below.

Remark 5. Without the assumption $\widehat{w} \geq 0$, the Vlasov functional $\mathcal{E}_{Vla}^{\beta,\rho}$ can have several minimizers and the limit in Eq. (13) is believed to be an average over the set of minimizers of $\mathcal{E}_{Vla}^{\beta,\rho}$. Namely there exists a so called de Finetti measure \mathcal{P} [16], concentrated on the set of minimizers for e_{Vla}^{β} , such that

$$m_{f,\Gamma_N}^{(k)} \rightharpoonup \int m^{\otimes k} \mathrm{d}\mathcal{P}(m),$$

in the sense defined in Theorem 2. We conjecture the following Fatou-type inequality on the entropy

$$\liminf_{\substack{N \to \infty \\ h^d N \to \rho}} \hbar^d \operatorname{Tr} \Gamma_N \log \Gamma_N \ge \int \left(\int_{\mathbb{R}^{2d}} s(m) \right) d\mathcal{P}(m) \tag{17}$$

for general sequences (Γ_N) with de Finetti measure \mathcal{P} . Should this inequality be true, we could remove the assumption $\widehat{w} \geq 0$ in Theorem 2. In fact, in our proof we show that the above inequality holds when the right-hand side is replaced by

$$\int_{\mathbb{R}^{2d}} s\left(\int m \,\mathrm{d}\mathcal{P}(m)\right).$$

When there is a unique minimizer, the two coincide.

Example 6 (Large atoms in a strong harmonic potential). The Hamiltonian in Eq. (10) can describe a large atom in a strong harmonic potential. Indeed, consider N electrons in a harmonic trap and interacting with a nucleus of charge Z. In the Born-Oppenheimer approximation, the N electrons are described by the Hamiltonian

$$\sum_{j=1}^{N} -\Delta_{x_j} + \omega^2 |x_j|^2 - \frac{Z}{|x_j|} + \sum_{j \le k} \frac{1}{|x_j - x_k|}.$$

Scaling length in the manner $x_j = N^{-1/2}x_j'$ we see that this Hamiltonian is unitarily equivalent to

$$N^{4/3} \left(\sum_{j=1}^{N} -N^{-\frac{2}{3}} \Delta_{x_j} + \left(\omega N^{-1} \right)^2 |x_j|^2 - \frac{ZN^{-1}}{|x_j|} + \frac{1}{N} \sum_{j < k} \frac{1}{|x_j - x_k|} \right).$$

Hence taking Z proportional to N and ω proportional to N, we obtain the Hamiltonian of Eq. (10) with d=3, A=0, $V(x)=|x|^2$ and $w(x)=|x|^{-1}$. In the limit we find the positive-temperature Thomas-Fermi model for an

atom in a harmonic trap, which has stimulated many works in the Physics literature [15, 18, 22, 11].

1.2.2. 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

$$w_N(x) := N^{d\eta} w(N^{\eta} x) \tag{18}$$

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 [31] for the ground state and [47] 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 7 (Dilute limit). Let $\beta_0, \rho > 0$. We assume that $V \in L^{1+d/2}_{loc}(\mathbb{R}^d)$ is such that $V(x) \to \infty$ at infinity and that $\int e^{-\beta_0 V_+(x)} dx < \infty$. Furthermore, assume that $|A|^2 \in L^{1+d/2}(\mathbb{R}^d) + L^{\infty}_{\varepsilon}(\mathbb{R}^d)$ and $w \in L^1(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ is even.

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

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

where $e_{\text{Can}}^{\beta,(\int_{\mathbb{R}^d} w)\delta_0}(\rho)$ is the minimum of the Vlasov energy with interaction potential $(\int_{\mathbb{R}^d} w)\delta_0$.

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

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

where $e_{\text{Can}}^{\beta,0}(\rho)$ is the minimum of the Vlasov energy without interaction potential.

In both cases, we have the same convergence of approximate Gibbs states as in Theorem 2.

The proof of Theorem 7 is given in Section 4.

2. Contruction 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 [47] where the thermodynamic limit of non-zero spin interacting fermions were studied in the grand-canonical picture. In particular we will make use of [47, Lemma 2]. Precisely we prove the following proposition.

Proposition 8 (Canonical trial states). Let $\rho_0 \in C_c^{\infty}(\mathbb{R}^d)$ be such that $\int_{\mathbb{R}^d} \rho_0 = 1$. Assume $|A|^2 \in L^{1+d/2}(\mathbb{R}^d)$, $w \in L^1(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$. If $\eta d > 1$, we assume w to be compactly supported. Then, there is a sequence of canonical states Γ_N on $\bigwedge_{i=1}^N L^2(\mathbb{R}^d)$ satisfying

$$\hbar^{d} \left(\operatorname{Tr} \sum_{i=1}^{N} (i\hbar \nabla + A)^{2} \Gamma_{N} + \operatorname{Tr} \Gamma_{N} \log \Gamma_{N} \right) \underset{h \stackrel{N \to \infty}{\to \infty}}{\longrightarrow} \int_{\mathbb{R}^{d}} F_{\beta}(\rho_{0}), \tag{19}$$

$$\left\| \frac{1}{N} \rho_{\Gamma_N}^{(1)} - \rho_0 \right\|_{L^1(\mathbb{R}^d)} \underset{h^d N \to 1}{\longrightarrow} 0 \tag{20}$$

and

$$\frac{\hbar^{d}}{N} \int_{\mathbb{R}^{2d}} w_{N}(x-y) \rho_{\Gamma_{N}}^{(2)}(x,y) dx dy \xrightarrow[\hbar^{d}N\to 1]{N\to\infty} \begin{cases}
\int_{\mathbb{R}^{d}} (w*\rho_{0}) \rho_{0} & \text{if } \eta = 0 \\
\left(\int_{\mathbb{R}^{d}} w\right) \int_{\mathbb{R}^{d}} \rho_{0}^{2} & \text{if } 0 < d\eta < 1 \\
0 & \text{if } d\eta > 1, d \ge 3.
\end{cases} \tag{21}$$

Furthermore, we can take $\rho_{\Gamma_N}^{(1)}$ to be supported in a compact set which is independent of N and uniformly bounded in $L^{\infty}(\mathbb{R}^d)$ so that the convergence (20) 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 and then do the thermodynamic limit in these cubes. This choice allows us to control the one-body density, which will be almost constant in these boxes. Without loss of generality, we will write the proof for A = 0. The proof is the same for $A \neq 0$.

Step 1. Definition of the trial state. Let $\rho_0 \in C_c^{\infty}(\mathbb{R}^d)$ and take R > 0 such that supp $\rho_0 \subset [-R/2, R/2)^d =: C_R$. Divide C_R in small cubes of size $\ell > 0$, $C_R \subset \bigcup_{z \in B_{\infty}(R\ell^{-1}) \cap \mathbb{Z}^d} \Lambda_z$ with $\Lambda_z := z\ell + [-\ell/2, \ell/2)^d$. We will take later $1 \gg \ell \gg \hbar$. For all z define $N_z := \lfloor \hbar^d \ell^d \min_{\Lambda_z} \rho_0 \rfloor$ so that $\sum_z N_z \leq N$. For $0 < \varepsilon < \ell/4$ and for all z, define the box

$$\widetilde{\Lambda}_z := z\ell + \left[-\frac{\ell - \varepsilon}{2}, \frac{\ell - \varepsilon}{2} \right)^d \subset \Lambda_z$$

and denote by

$$\widetilde{\Gamma}_{z} = \frac{e^{-\beta \left(\sum_{i=1}^{N_{z}} - \hbar^{2} \Delta_{i}^{\text{per}}\right)}}{Z_{z}} = \sum_{k \in \mathcal{P}_{N_{z}}(\mathbb{Z}^{d})} \lambda_{k} \left| e_{k_{1}} \wedge \cdots \wedge e_{k_{N_{z}}} \right\rangle \left\langle e_{k_{1}} \wedge \cdots \wedge e_{k_{N_{z}}} \right|$$

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 subset 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 Λ_z and λ_k the eigenvalues of $\widetilde{\Gamma}_z$ associated with $e_k = e_{k_1} \wedge ... \wedge e_{k_{N_z}}$. 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 $\chi_{\varepsilon} = \varepsilon^{-d} \chi(\varepsilon^{-1})$ and define for $j \in \mathbb{Z}^d$

 $f_j := e_j \sqrt{\mathbb{1}_{\widetilde{\Lambda}_z} * \chi_{\varepsilon}}.$

Note that

$$\int_{\Lambda_z} f_j \overline{f_k} = \int e_j \overline{e_k} \left(\mathbb{1}_{\widetilde{\Lambda}_z} * \chi_{\varepsilon} \right) = \int \int_{\widetilde{\Lambda}_z} e_j(x) \overline{e_k}(x) \chi_{\varepsilon}(y - x) \mathrm{d}y \mathrm{d}x$$
$$= \int_{\widetilde{\Lambda}_z} e_j \overline{e_k} \int_{\mathbb{R}^d} \chi = \delta_{j,k}.$$

Hence the family $(f_j)_j$ is still orthonormal and one can check that it satisfies $f_j \equiv e_j$ in $[-(\ell-2\varepsilon)/2, (\ell-2\varepsilon)/2)^d$ and as well as the Dirichlet boundary condition on Λ_z . Besides from having a state satisfying the Dirichlet boundary condition, we also want to add correlations in order to deal with the $d\eta > 1$ case. Let $\varphi \in C_c^{\infty}(\mathbb{R}^d)$ such that $\varphi \equiv 1$ in B(0,1) and $\varphi \leq 1$ almost everywhere and for s > 0 denote $\varphi_s = \varphi(s^{-1}\cdot)$. Following [47], we define the correlation function $F(x_1, ..., x_{N_z}) = \prod_{i < j} \varphi_s(x_i - x_j)$ and the state

$$\Gamma_z = \sum_{k \in \mathcal{P}_{N_z}(\mathbb{Z}^d)} \lambda_k Z_k^{-1} \left| F f_{k_1} \wedge \dots \wedge f_{k_{N_z}} \right\rangle \left\langle F f_{k_1} \wedge \dots \wedge f_{k_{N_z}} \right|,$$

where $Z_k = \|Ff_{k_1} \wedge ... \wedge f_{k_{N_z}}\|_{L^2(\Lambda_z^{N_z})}^2$ are normalization factors. Now consider the state

$$\Gamma := \bigwedge_{z} \Gamma_{z}.$$

We will show that Γ satisfies the three limits Eq. (19), (20) and (21). 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.

$$s \ll \hbar \ll \varepsilon \ll \ell \ll N^{-\eta}$$
 and $s\ell \ll \hbar^2$.

One could in fact take $\Gamma_{F=1}$ (removing the factor F, see below) and remove the dependence in s. In the case $\eta d > 1$, the convergence holds in the regime

$$N^{-\eta} \ll s \ll \hbar \ll \varepsilon \ll \ell$$
 and $s\ell \ll \hbar^2$.

Step 2. Verification of (19). 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 $X = (\sqrt{\mathbb{1}_{\tilde{\Lambda}_z} * \chi_{\varepsilon}})^{\otimes N_z}$ so that $\Psi_k^z := f_{k_1} \wedge ... \wedge f_{k_{N_z}} = X e_{k_1} \wedge ... \wedge e_{k_{N_z}}$ (we will omit the superscript z when there is no ambiguity) and denote $\nabla, -\Delta$ the gradient and the Laplacian for all coordinates $x_1, ..., x_{N_z}$ in the box Λ_z with Dirichlet boundary condition, we can check that

$$\nabla \left(FX e_{k_1} \wedge \ldots \wedge e_{k_{N_z}} \right) = \left(X \nabla F + F \nabla X + i FX \sum_{j=1}^{N_z} \frac{2\pi k_j}{\ell - \varepsilon} \right) e_{k_1} \wedge \ldots \wedge e_{k_{N_z}}.$$

Hence,

$$\operatorname{Tr}(-\Delta)\Gamma_z = \sum_{k \in \mathcal{P}_{N_z}(\mathbb{Z}^d)} \frac{\lambda_k}{Z_k} \left(\varepsilon_k + \| (X\nabla F + F\nabla X) e_{k_1} \wedge \ldots \wedge e_{k_{N_z}} \|_{L^2(\Lambda_z^{N_z})}^2 \right)$$

where

$$\varepsilon_k := \left| 2\pi (\ell - \varepsilon)^{-1} \sum_{j=1}^{N_z} k_j \right|^2$$

is the eigenvalue of $-\Delta^{\mathrm{per}}$ associated with the eigenfunction e_k . Note that $\lambda_k \propto e^{-\beta\hbar^2\varepsilon_k}$. We will show that $\sum_k \lambda_k Z_k^{-1}\varepsilon_k \simeq \sum_k \lambda_k \varepsilon_k = \mathrm{Tr}(-\Delta^{\mathrm{per}})\widetilde{\Gamma}$ 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 $a_1,...,a_p>0$ we have

$$1 \ge \prod_{n=1}^{p} (1 - a_n) \ge 1 - \sum_{n=1}^{p} a_n.$$
 (22)

Hence,

$$Z_{k} = \int_{\Lambda_{z}^{N_{z}}} \prod_{1 \leq n < m \leq N_{z}} \varphi_{s}(x_{n} - x_{m})^{2} |\Psi_{k}|^{2} dX$$

$$\geq 1 - \int_{\Lambda_{z}^{N_{z}}} \sum_{1 \leq n < m \leq N_{z}} (1 - \varphi_{s}(x_{n} - x_{m})^{2}) |\Psi_{k}|^{2} dX$$

$$\geq 1 - \int_{\Lambda_{z}^{2}} (1 - \varphi_{s}(x_{1} - x_{2})^{2}) \rho_{\Psi_{k}}^{(1)}(x_{1}) \rho_{\Psi_{k}}^{(1)}(x_{2}) dx_{1} dx_{2}$$

$$\geq 1 - C s^{d} \ell^{d} \hbar^{-2d}, \qquad (23)$$

where we used that $\rho_{\Psi_k}^{(2)}(x,y) \leq \rho_{\Psi_k}^{(1)}(x)\rho_{\Psi_k}^{(1)}(y)$ because Ψ_k is a Slater determinant, and that $\rho_{\Psi_k}^{(1)} = N_z \ell^{-d} \mathbb{1}_{\widetilde{\Lambda}_z} * \chi_{\varepsilon} \leq C \hbar^{-d}$.

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

$$\|\nabla F\Psi_k\|_{L^2(\Lambda_z^{N_z})}^2 \le C \int_{\Lambda_z^{3d}} |\nabla \varphi_s(x_1 - x_2)| |\nabla \varphi_s(x_1 - x_3)| \times \\ \times \rho_{\Psi_k}^{(1)}(x_1) \rho_{\Psi_k}^{(1)}(x_2) \rho_{\Psi_k}^{(1)}(x_3) dx_1 dx_2 dx_3 \\ + C \int_{\Lambda_z^{2d}} |\nabla \varphi_s(x_1 - x_2)|^2 \rho_{\Psi_k}^{(1)}(x_1) \rho_{\Psi_k}^{(1)}(x_2) dx_1 dx_2 \\ \le C s^{-2} \left(s^{2d} \ell^d \hbar^{-3d} + s^d \ell^d \hbar^{-2d} \right).$$

Now we turn to the ∇X part. We have

$$\nabla_{x_1} X(x_1, ..., x_{N_z}) = \frac{\nabla \sqrt{\mathbb{1}_{\widetilde{\Lambda}_z} * \chi_{\varepsilon}}(x_1)}{\sqrt{\mathbb{1}_{\widetilde{\Lambda}_z} * \chi_{\varepsilon}(x_1)}} X(x_1, ..., x_{N_z})$$

and

$$\begin{split} \int_{\Lambda_z^{N_z}} |\nabla X|^2 |e_{k_1} \wedge \ldots \wedge e_{k_{N_z}}|^2 &= \int_{\Lambda_z^{N_z}} \sum_{j=1}^{N_z} \left| \frac{\nabla \sqrt{\mathbbm{1}_{\widetilde{\Lambda}_z} * \chi_{\varepsilon}}(x_1)}{\sqrt{\mathbbm{1}_{\widetilde{\Lambda}_z} * \chi_{\varepsilon}}(x_1)} \right|^2 |\Psi_k|^2 \\ &= \int_{\Lambda_z} \left| \frac{\nabla \sqrt{\mathbbm{1}_{\widetilde{\Lambda}_z} * \chi_{\varepsilon}}(x_1)}{\sqrt{\mathbbm{1}_{\widetilde{\Lambda}_z} * \chi_{\varepsilon}}(x_1)} \right|^2 \rho_{\Psi_k}^{(1)} \\ &\leq C \int_{\Lambda_z} \left| \nabla \sqrt{\mathbbm{1}_{\widetilde{\Lambda}_z} * \chi_{\varepsilon}}(x_1) \right|^2 N_z \ell^{-d} \\ &\leq C N_z \ell^{-d} \int_{\Lambda_z} \int |\nabla \sqrt{\chi_{\varepsilon}}|^2 \leq C \ell^d \hbar^{-d} \varepsilon^{-2}, \end{split}$$

where we used the pointwise bound $\left|\nabla\sqrt{\mathbb{1}_{\widetilde{\Lambda}_z}*\chi_{\varepsilon}}(x_1)\right|^2 \leq \int |\nabla\sqrt{\chi_{\varepsilon}}|^2$. Since X and F are both bounded by 1 we obtain

$$\operatorname{Tr}(-\Delta)\Gamma_z = \operatorname{Tr}(-\Delta^{\operatorname{per}})\widetilde{\Gamma}_z + \mathcal{O}\bigg(\frac{s^{2(d-1)}\ell^d\hbar^{-3d} + s^{d-2}\ell^d\hbar^{-2d} + \ell^d\hbar^{-d}\varepsilon^{-2}}{1 - Cs^d\ell^d\hbar^{-2d}} + N_z^{1+2/d}s^d\ell^d\hbar^{-2d}\bigg).$$

We proceed with estimating the entropy of Γ_z . Thanks to [47, Lemma 2] we have

$$\operatorname{Tr} \Gamma_z \log \Gamma_z \leq \operatorname{Tr} \widetilde{\Gamma}_z \log \widetilde{\Gamma}_z - \log \min_k Z_k$$
$$= \operatorname{Tr} \widetilde{\Gamma}_z \log \widetilde{\Gamma}_z + \mathcal{O}\left(s^d \ell^d \hbar^{-2d}\right),$$

where we used the estimate (23) on Z_k . Combining the last two estimates gives

$$\begin{split} \operatorname{Tr}(-\hbar^2\Delta)\Gamma + \operatorname{Tr}\Gamma\log\Gamma \\ &= \sum_z \operatorname{Tr}(-\hbar^2\Delta)\Gamma_z + \operatorname{Tr}\Gamma\log\Gamma_z \\ &\leq \sum_z e_{\operatorname{Can}}^{\beta,\operatorname{per}}(\widetilde{\Lambda}_z,\hbar,N_z) + \ell^{-d}\mathcal{O}\left(s^d\ell^d\hbar^{-2d}\right) + \mathcal{O}\left((\hbar^{-d}\ell^d)^{1+2/d}s^d\ell^d\hbar^{-2d}\right) \\ &+ \hbar^2\ell^{-d}\mathcal{O}\left(\frac{s^{2(d-1)}\ell^d\hbar^{-3d} + s^{d-2}\ell^d\hbar^{-2d} + \ell^d\hbar^{-d}\varepsilon^{-2}}{1 - Cs^d\ell^d\hbar^{-2d}}\right), \end{split}$$

where we used that $N_z \leq \|\rho_0\|_{L^{\infty}(\mathbb{R}^d)} \hbar^{-d} \ell^d$. It is a known fact [44, 46] (see also [38, 51] for more details) that

$$e_{\operatorname{Can}}^{\beta,\operatorname{per}}(\widetilde{\Lambda}_z,\hbar,N_z) = \hbar^{-d}\ell^d F_{\beta}(N_z/(\hbar^{-d}\ell^d)) + o(\hbar^{-d}\ell^d)$$
 (24)

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

$$\begin{split} &\hbar^d \big(\operatorname{Tr}(-\hbar^2 \Delta) \Gamma + \operatorname{Tr} \Gamma \log \Gamma \big) \leq \ell^d \sum_{z \in \mathbb{Z}^d} F_{\beta}(\rho(z)) + o(1) + \mathcal{O}(\varepsilon/\ell) \\ &+ \mathcal{O}\left((s\ell/\hbar^2)^d \ell^2 \right) + \mathcal{O}\left(s/\hbar \right)^d + \mathcal{O}\left(\frac{(s/\hbar)^{2(d-1)} + (s/\hbar)^{d-2} + (\hbar/\varepsilon)^2}{1 - C(s\ell/\hbar^2)^d} \right). \end{split}$$

If $s \ll \hbar \ll \varepsilon \ll \ell$ with the extra condition that $s\ell \ll \hbar^2$ we obtain the upper bound in (19) 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 (20). Let us recall that $\Gamma_{F=1}$ is the uncorrelated version of the trial state (which corresponds to taking $\varphi \equiv 1$) and that we denote by $\rho_{F=1}^{(k)}$ its k-particle density, for $k \geq 1$. From (22) and using that $\Gamma_{F=1}$ is a sum of Slater determinants we have

$$N^{-1} \| \rho_{\Gamma}^{(1)} - \rho_{F=1}^{(1)} \|_{L^{1}(\mathbb{R}^{d})}$$

$$\leq N^{-1} \sum_{z \in \mathbb{Z}^{d}} \sum_{k \in \mathcal{P}_{N_{z}}(\mathbb{Z}^{d})} \lambda_{k}^{z} \iint_{\mathbb{R}^{2d}} (1 - \varphi_{s}(x_{1} - x_{2})^{2}) \rho_{\Psi_{k}^{z}}^{(2)}(x_{1}, x_{2}) dx_{1} dx_{2}$$

$$\leq CN^{-1} \sum_{z \in \mathbb{Z}^{d}} \iint_{\Lambda_{z}^{2}} (1 - \varphi_{s}(x_{1} - x_{2})^{2}) N_{z}^{2} \ell^{-2d} dx_{1} dx_{2}$$

$$\leq CN^{-1} \sum_{z \in \mathbb{Z}^{d}} s^{d} \ell^{d} N_{z}^{2} \ell^{-2d}$$

$$\leq C(s/\hbar)^{d}.$$

We also used that $\rho_{\Psi_k^z}^{(2)} \leq \rho_{\Psi_k^z}^{(1)} \otimes \rho_{\Psi_k^z}^{(1)} \leq \|\rho_0\|_{L^{\infty}(\mathbb{R}^d)} N_z^2 \ell^{-2d}$. Finally, denoting by $\Gamma_{z,F=1}$ the uncorrelated version of Γ_z and by $\rho_{z,F=1}^{(1)}$ its one-body density we have

$$||N^{-1}\rho_{F=1}^{(1)} - \rho_0||_{L^1(\mathbb{R}^d)} \leq \sum_{z} ||N^{-1}\rho_{z,F=1}^{(1)} - \rho_0 \mathbb{1}_{\Lambda_z}||_{L^1(\mathbb{R}^d)}$$

$$\leq C \sum_{z} \left(||\nabla \rho_0||_{L^{\infty}(\mathbb{R}^d)} \ell^{d+1} + ||\rho_0||_{L^{\infty}(\mathbb{R}^d)} \ell^{d-1} \varepsilon \right)$$

$$\leq C(\ell + \varepsilon/\ell).$$

We have used that in $z\ell + [-(\ell - 2\varepsilon)/2, (\ell - 2\varepsilon)/2)^d$,

$$N^{-1}\rho_{z,F=1}^{(1)} = N^{-1}\ell^{-d}\lfloor \hbar^{-d}\ell^{d} \min_{\Lambda_{z}} \rho_{0} \rfloor = \rho_{0} + \mathcal{O}(\hbar^{d}\ell^{d}) + \mathcal{O}(\|\nabla\rho_{0}\|_{L^{\infty}(\mathbb{R}^{d})}\ell)$$

and that

$$||N^{-1}\rho_{z,F=1}^{(1)} - \rho_0 \mathbb{1}_{\Lambda_z}||_{L^{\infty}(\Lambda_z)} \le C||\rho_0||_{L^{\infty}(\mathbb{R}^d)}.$$

Under the stated conditions on \hbar, ℓ, s and ε we have $N^{-1}\rho_{\Gamma}^{(1)} \to \rho_0$ in $L^1(\mathbb{R}^d)$.

Step 4. Verification of (21). Let us first turn to the case $0 \le \eta d < 1$. Note that

$$\rho_{\Gamma}^{(2)} = \sum_{z \in \mathbb{Z}^d} \rho_{\Gamma_z}^{(2)} + \sum_{z \neq z'} \rho_{\Gamma_z}^{(1)} \otimes \rho_{\Gamma_{z'}}^{(1)}
= \rho_{\Gamma}^{(1)} \otimes \rho_{\Gamma}^{(1)} + \sum_{z \in \mathbb{Z}^d} \rho_{\Gamma_z}^{(2)} - \rho_{\Gamma_z}^{(1)} \otimes \rho_{\Gamma_z}^{(1)}.$$
(25)

The second term above is negligible in our regime. Indeed, using the triangle inequality, the Lieb-Thirring inequality [34, 35] and Young's inequality we obtain

$$N^{-2} \left| \sum_{z \in \mathbb{Z}^d} \int_{\mathbb{R}^d} w_N(x - y) \left(\rho_{\Gamma_z}^{(2)} - \rho_{\Gamma_z}^{(1)} \otimes \rho_{\Gamma_z}^{(1)} \right) \right|$$

$$\leq CN^{-2} \|w_N\|_{L^{1+d/2}(\mathbb{R}^d)} \sum_{z \in \mathbb{Z}^d} \left\{ \|\rho_{\Gamma_z}^{(1)}\|_{L^{1+2/d}(\mathbb{R}^d)} \|\rho_{\Gamma_z}^{(1)}\|_{L^1(\mathbb{R}^d)} + N_z^2 \left(\frac{\operatorname{Tr} \Gamma_z \left(\sum_{j=1}^{N_z} - \Delta_{z_j} \right)}{N_z^{1+2/d}} \right)^{\frac{1}{1+2/d}} \right\}$$

$$\leq CN^{-2} N^{d\eta} \frac{d}{d+2} \sum_{z \in \mathbb{Z}^d} N_z^2 \ell^{-\frac{2}{1+2/d}}$$

$$\leq C(N^{\eta} \ell)^d \ell^{d(1 - \frac{1}{d+2})}$$

where we used that $\rho_{\Gamma_z}^{(1)} \leq CN_z\ell^{-d} \leq C\|\rho_0\|_{L^\infty(\mathbb{R}^d)}\hbar^{-d}$ almost everywhere and the estimate on the kinetic energy of Γ_z computed before. Hence, if $N^{-1}\rho_{\Gamma}^{(1)} \to \rho_0$ in $L^1(\mathbb{R}^d)$ and if $\ell = o(N^{-\eta})$, since both $N^{-1}\rho_{\Gamma}^{(1)}$ and ρ_0 are bounded (uniformly in N) in $L^\infty(\mathbb{R}^d)$, by (25) and the use of Young's inequality we obtain (21) for $0 \leq \eta d \leq 1$.

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.

3. Proof of Theorem 2 in the non-interacting case $w \equiv 0$

In this section we prove the convergence (12) of the free energy in Theorem 2 in the case where the interaction is dropped, that is $w \equiv 0$. We study the interacting case later in Section 4. The convergence of states will be discussed in Section 4.3.

The non-interacting case is well understood since the Hamiltonian is quadratic in creation and annihilation operators in the grand canonical picture. The minimizers are known to be the so-called quasi-free states [2]. 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 8 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 [50].

Lemma 9 (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

$$\min_{\substack{0 \leq \gamma \leq 1 \\ \gamma \in \mathfrak{S}_{1}(\mathfrak{H})}} \left(\operatorname{Tr} H \gamma + \frac{1}{\beta} \operatorname{Tr} s \left(\gamma \right) \right) = -\frac{1}{\beta} \operatorname{Tr} \log \left(1 + e^{-\beta H} \right),$$

with the unique minimizer being $\gamma_0 = \frac{1}{1+e^{\beta H}}$.

With Lemma 9 at hand we are able to provide the

Proof of Theorem 2 in the non-interacting case. Suppose that w=0. We start out by proving the upper bound on the energy, using the trial states constructed in the previous section. Let $\rho > 0$ and $0 \le \nu \in C_c^{\infty}(\mathbb{R}^d)$ with $\int_{\mathbb{R}^d} \nu(x) dx = \rho$. By Proposition 8 we then have a sequence (Γ_N) of canonical N-particle states satisfying

$$\hbar^{d} \operatorname{Tr} \left(\sum_{j=1}^{N} |i\hbar \nabla_{x_{j}} + A(x_{j})|^{2} \Gamma_{N} \right) + \frac{\hbar^{d}}{\beta} \operatorname{Tr} \Gamma_{N} \log \Gamma_{N} \to \int_{\mathbb{R}^{d}} F_{\beta} \left(\nu \left(x \right) \right) dx.$$

The one-particle densities $\hbar^d \rho_{\Gamma_N}^{(1)}$ converge to ν strongly in $L^1(\mathbb{R}^d)$ and are uniformly bounded in $L^{\infty}(\mathbb{R}^d)$. Hence they converge strongly in all $L^p(\mathbb{R}^d)$ for $p \in [1, \infty)$. Since $V \in L^{1+d/2}_{loc}(\mathbb{R}^d)$ and $\rho_{\Gamma_N}^{(1)}$ are, by construction, supported in a fixed compact set, we have

$$\hbar^{d} \operatorname{Tr} V(x) \Gamma_{N}^{(1)} = \hbar^{d} \int_{\mathbb{R}^{d}} V(x) \rho_{\Gamma_{N}}^{(1)}(x) dx \to \int_{\mathbb{R}^{d}} V(x) \nu(x) dx.$$

This means that

$$\hbar^{d} e_{\operatorname{Can}}^{\beta}\left(\hbar, N\right) \leq \hbar^{d} \mathcal{E}_{\operatorname{Can}}^{N, \hbar}\left(\Gamma_{N}\right) \to \int_{\mathbb{R}^{d}} F_{\beta}\left(\nu\left(x\right)\right) \, \mathrm{d}x + \int_{\mathbb{R}^{d}} V\left(x\right) \nu\left(x\right) \, \mathrm{d}x,$$

and, since ν is arbitrary, we have shown that

$$\limsup_{\substack{N \to \infty \\ \hbar^d N \to \rho}} \hbar^d e_{\operatorname{Can}}^{\beta} \left(\hbar, N \right) \le e_{\operatorname{Vla}}^{\beta} \left(\rho \right).$$

To prove the lower bound, we use the following bound [2, 50] on the entropy

$$\operatorname{Tr} \Gamma \log \Gamma \geq \operatorname{Tr} \left(\Gamma^{(1)} \log \Gamma^{(1)} + \left(1 - \Gamma^{(1)} \right) \log \left(1 - \Gamma^{(1)} \right) \right) = \operatorname{Tr} s \left(\Gamma^{(1)} \right)$$

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 9 above, we have for any $\mu \in \mathbb{R}$ and any N-body state Γ

$$\mathcal{E}_{\operatorname{Can}}^{N,\hbar}(\Gamma) \ge \operatorname{Tr}\left(|i\hbar\nabla + A(x)|^2 + V(x) - \mu\right)\Gamma^{(1)} + \frac{1}{\beta}\operatorname{Tr}s\left(\Gamma^{(1)}\right) + \mu N$$
$$\ge -\frac{1}{\beta}\operatorname{Tr}\log\left(1 + e^{-\beta\left(|i\hbar\nabla + A(x)|^2 + V(x) - \mu\right)}\right) + \mu N.$$

Thus, we are left to using the known semi-classical convergence (whose proof is recalled below in Proposition 10)

$$\lim_{\hbar \to 0} \inf -\frac{\hbar^d}{\beta} \operatorname{Tr} \log \left(1 + e^{-\beta \left(|i\hbar\nabla + A(x)|^2 + V(x) - \mu \right)} \right)
\geq -\frac{1}{(2\pi)^d \beta} \iint_{\mathbb{R}^{2d}} \log \left(1 + e^{-\beta \left(p^2 + V(x) - \mu \right)} \right) dx dp, \quad (26)$$

and to take $\mu = \mu_{\text{Vla}}(\rho)$. Recognizing the expression of the Vlasov free energy on the right-hand side we appeal to Theorem 1 and immediately obtain

$$\liminf_{\substack{N \to \infty \\ \hbar^d N \to \rho}} \hbar^d e_{\operatorname{Can}}^{\beta}\left(\hbar, N\right) \ge e_{\operatorname{Vla}}^{\beta}\left(\rho\right),$$

concluding the proof of (12) in the non-interacting case.

In (26) we have used the following well-known fact, which we prove for completeness.

Proposition 10 (Semi-classical limit). Let $\beta_0 > 0$, we assume that $|A|^2 \in L^{1+d/2}(\mathbb{R}^d) + L_{\varepsilon}^{\infty}(\mathbb{R}^d)$, $V \in L_{\text{loc}}^{1+d/2}(\mathbb{R}^d)$ is such that $V(x) \to \infty$ at infinity and that $\int e^{-\beta_0 V_+(x)} dx < \infty$. Then for any chemical potential $\mu \in \mathbb{R}$ and all $\beta > \beta_0$,

$$\limsup_{\hbar \to 0} \frac{\hbar^d}{\beta} \operatorname{Tr} \log \left(1 + e^{-\beta \left((|i\hbar \nabla + A|^2 + V - \mu) \right)} \right)$$

$$\leq \frac{1}{(2\pi)^d \beta} \iint_{\mathbb{R}^{2d}} \log \left(1 + e^{-\beta \left(p^2 + V(x) - \mu \right)} \right) dx dp. \quad (27)$$

This result is known [50] and the proof we provide here is essentially the one in [48], where however the von Neumann entropy $x \log(x)$ was used instead of the Fermi-Dirac entropy $x \log(x) + (1-x) \log(1-x)$. In fact, Theorem 2 shows that the inequality (27) is indeed an equality.

Proof of Proposition 10. 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 $\chi^2 + \eta^2 = 1$, supp $\chi \subseteq B(0,1)$ and supp $\eta \subseteq B(0,\frac{1}{2})^c$. For R>0, denote $\chi_R=\chi\left(\frac{\cdot}{R}\right)$ and $\eta_R=\eta\left(\frac{\cdot}{R}\right)$. Let $H_\hbar=|i\hbar\nabla+A|^2+V$ and take $\gamma^\hbar=\frac{1}{1+e^{\beta H_\hbar}}$ as in Lemma 9. By the IMS localization formula we have

$$\operatorname{Tr} H_{\hbar} \gamma^{\hbar} = \operatorname{Tr} \left(H_{\hbar} \chi_R \gamma^{\hbar} \chi_R \right) + \operatorname{Tr} \left(H_{\hbar} \eta_R \gamma^{\hbar} \eta_R \right) - \hbar^2 \operatorname{Tr} \left(|\nabla \chi_R|^2 + |\nabla \eta_R|^2 \right) \gamma^{\hbar}, \tag{28}$$

and using the convexity of s and [9, Theorem 14],

$$\operatorname{Tr} s\left(\gamma^{\hbar}\right) = \operatorname{Tr} \chi_{R} s\left(\gamma^{\hbar}\right) \chi_{R} + \operatorname{Tr} \eta_{R} s\left(\gamma^{\hbar}\right) \eta_{R}$$

$$\geq \operatorname{Tr} s\left(\chi_{R} \gamma^{\hbar} \chi_{R}\right) + \operatorname{Tr} s\left(\eta_{R} \gamma^{\hbar} \eta_{R}\right). \tag{29}$$

We first deal with the localization outside the ball. The operators we consider in $B\left(0,\frac{R}{2}\right)^c$ are the ones with Dirichlet boundary condition. We obtain by Lemma 9 that the remainder terms are bounded by

$$\operatorname{Tr}\left(H_{\hbar}\eta_{R}\gamma^{\hbar}\eta_{R}\right) + \frac{1}{\beta}\operatorname{Tr}s\left(\eta_{R}\gamma^{\hbar}\eta_{R}\right)$$

$$\geq -\frac{1}{\beta}\operatorname{Tr}_{L^{2}(B\left(0,\frac{R}{2}\right)^{c})}\log\left(1 + e^{-\beta\left(|i\hbar\nabla + A|^{2} + V - C\right)}\right)$$

$$\geq -\frac{C}{\beta}\operatorname{Tr}_{L^{2}(B\left(0,\frac{R}{2}\right)^{c})}e^{-\beta\left(|i\hbar\nabla + A|^{2} + V\right)}$$

$$\geq -\frac{C}{\beta}\operatorname{Tr}_{L^{2}(B\left(0,\frac{R}{2}\right)^{c})}e^{-\beta\left(-\hbar^{2}\Delta^{D} + V\right)}$$

$$\geq -\frac{C}{\beta}\operatorname{Tr}_{L^{2}(\mathbb{R}^{d})}e^{-\beta\left(-\hbar^{2}\Delta + (1-\alpha)V + \alpha\inf_{B(0,R)^{c}}V\right)}$$

$$\geq -\frac{Ce^{-\alpha\inf_{B(0,R)^{c}}V}}{(2\pi\hbar)^{d}}\iint_{\mathbb{R}^{2d}}e^{-\beta\left(p^{2} + (1-\alpha)V(x)\right)}dxdp, \tag{32}$$

where $\alpha > 0$ is such that $\beta(1 - \alpha) > \beta_0$. The inequality (30) comes from the diamagnetic inequality [12] and (31) is obtained by the min-max characterization of the eigenvalues. The last inequality follows from Golden-Thompson's formula [43, Theorem VIII.30].

The error term in the IMS formula can be estimated by

$$-\operatorname{Tr}\left(\left|\nabla\chi_{R}\right|^{2}+\left|\nabla\eta_{R}\right|^{2}\right)\gamma^{\hbar} \geq -\frac{C}{R}\operatorname{Tr}\gamma^{\hbar}$$

$$\geq -\frac{C}{R}\operatorname{Tr}e^{-\beta H_{\hbar}}$$

$$\geq -\frac{C}{R\left(2\pi\hbar\right)^{d}}\iint_{\mathbb{R}^{2d}}e^{-\beta\left(p^{2}+V(x)\right)}\,\mathrm{d}x\,\mathrm{d}p, \quad (33)$$

where we used again the diamagnetic and Golden-Thompson inequalities.

Next we derive a bound on the densities $\rho_{\gamma_R^{\hbar}}$, where $\gamma_R^{\bar{\hbar}} = \chi_R \gamma^{\bar{\hbar}} \chi_R$, using the Lieb-Thirring inequality [34, 35]. Combining (28), (29), (32) and (33) we have shown

$$\operatorname{Tr} H_{\hbar} \gamma_{R}^{\hbar} + \frac{1}{\beta} \operatorname{Tr} s \left(\gamma_{R}^{\hbar} \right) - \frac{\varepsilon \left(R \right)}{\hbar^{d}} \leq \operatorname{Tr} H_{\hbar} \gamma^{\hbar} + \frac{1}{\beta} \operatorname{Tr} s \left(\gamma^{\hbar} \right)$$
$$= -\frac{1}{\beta} \operatorname{Tr} \log \left(1 + e^{-\beta H_{\hbar}} \right) \leq 0 \quad (34)$$

where $\varepsilon(R) \to 0$ when $R \to \infty$. By Lemma 9 we have

$$\operatorname{Tr} H_{\hbar} \gamma_{R}^{\hbar} + \frac{1}{\beta} \operatorname{Tr} s \left(\gamma_{R}^{\hbar} \right) \geq \frac{1}{2} \operatorname{Tr} \left(-\hbar^{2} \Delta \right) \gamma_{R}^{\hbar}$$
$$- \frac{1}{\beta} \operatorname{Tr} \log \left(1 + e^{-\beta \left(|i\hbar \nabla + A|^{2}/2 + V \right)} \right) - \frac{C}{\hbar^{d}}$$

where, as in (32),

$$\operatorname{Tr} \log \left(1 + e^{-\beta \left(|i\hbar\nabla + A|^2/2 + V \right)} \right) \le \frac{Ce^{-\alpha \inf V}}{\left(2\pi\hbar \right)^d} \iint_{\mathbb{R}^{2d}} e^{-\beta \left(p^2/2 + (1-\alpha)V(x) \right)} \, \mathrm{d}x \, \mathrm{d}p.$$

This implies the following bound on the kinetic energy

$$\operatorname{Tr}\left(-\hbar^2\Delta\right)\gamma_R^{\hbar} \le \frac{C}{\hbar^d}.\tag{35}$$

By the Lieb-Thirring inequality, we obtain

$$\int_{\mathbb{D}^d} \rho_{\gamma_R^{\hbar}}(x)^{1+\frac{2}{d}} \, \mathrm{d}x \le C \, \mathrm{Tr}\left(-\Delta \gamma_R^{\hbar}\right) \le \frac{1}{\hbar^{d+2}} C. \tag{36}$$

We return to the estimate on the localized terms in (28) and (29), using coherent states. Let $f \in C_c^{\infty}(\mathbb{R}^d)$ be a real-valued and even function, and consider the coherent state $f_{x,p}^{\hbar}(y) = \hbar^{-\frac{d}{4}} f(\hbar^{-\frac{1}{2}}(y-x)) e^{i\frac{p\cdot y}{\hbar}}$. The projections $|f_{x,p}^{\hbar}\rangle \langle f_{x,p}^{\hbar}|$ give rise to a resolution of the identity on $L^2(\mathbb{R}^d)$:

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

Using this in combination with Jensen's inequality and the spectral theorem, we obtain

$$\operatorname{Tr} s\left(\chi_{R} \gamma^{\hbar} \chi_{R}\right) = \frac{1}{(2\pi\hbar)^{d}} \iint_{\mathbb{R}^{2d}} \left\langle f_{x,p}^{\hbar}, s\left(\gamma_{R}^{\hbar}\right) f_{x,p}^{\hbar} \right\rangle dx dp$$

$$\geq \frac{1}{(2\pi\hbar)^{d}} \iint_{\mathbb{R}^{2d}} s\left(\left\langle f_{x,p}^{\hbar}, \gamma_{R}^{\hbar} f_{x,p}^{\hbar} \right\rangle\right) dx dp. \tag{37}$$

On the other hand, applying [16, Corollary 2.5] we have

$$\operatorname{Tr} H_{\hbar} \chi_{R} \gamma^{\hbar} \chi_{R}$$

$$= \frac{1}{(2\pi\hbar)^{d}} \iint_{\mathbb{R}^{2d}} \left\langle f_{x,p}^{\hbar}, H_{\hbar} \gamma_{R}^{\hbar} f_{x,p}^{\hbar} \right\rangle dx dp$$

$$= \frac{1}{(2\pi\hbar)^{d}} \iint_{\mathbb{R}^{2d}} \left(|p+A|^{2} + V(x) \right) \left\langle f_{x,p}^{\hbar}, \gamma_{R}^{\hbar} f_{x,p}^{\hbar} \right\rangle dx dp$$

$$+ \int_{\mathbb{R}^{d}} \rho_{\gamma_{R}^{\hbar}} \left(A^{2} - A^{2} * \left| f^{\hbar} \right|^{2} \right) - 2\Re \operatorname{Tr} \left(A - A * \left| f^{\hbar} \right|^{2} \right) \cdot i\hbar \nabla \gamma_{R}^{\hbar}$$

$$- \hbar \int_{\mathbb{R}^{d}} |\nabla f|^{2} + \int_{\mathbb{R}^{d}} \rho_{\gamma_{R}^{\hbar}} \left(V - V * \left| f^{\hbar} \right|^{2} \right)$$
(38)

Since $\hbar^d \rho_{\gamma_R^\hbar}$ is supported in B(0,R) and is uniformly bounded in $L^{1+2/d}\left(\mathbb{R}^d\right)$ by (36), and $V*\left|f^\hbar\right|^2$ converges to V locally in $L^{1+d/2}\left(\mathbb{R}^d\right)$. The same argument applied to A and $|A|^2$ combined with Hölder's inequality, the Lieb-Thirring inequality and (35) shows that the remainder terms above are $o\left(\hbar^{-d}\right)$. At last, combining (34), (37) and (38) as well as a simple adaptation of Proposition 14 to finite domains (Remark 15) yields

$$\begin{split} \limsup_{\hbar \to 0} \hbar^d \operatorname{Tr} \log \left(1 + e^{-\beta \left(|i\hbar \nabla + A|^2 + V \right)} \right) \\ & \leq \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} \log \left(1 + e^{-\beta \left(p^2 + V(x) \right)} \right) \, \mathrm{d}x \, \mathrm{d}p + \varepsilon \left(R \right), \end{split}$$

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 10 (possibly unbounded below). For K > 0, we take the cut off potential $V_K = V \mathbb{1}_{\{V \ge -K\}}$ and for any $0 < \varepsilon < 1$ we obtain using Lemma 9

$$-\frac{1}{\beta}\operatorname{Tr}\log\left(1+e^{-\beta\left(|i\hbar\nabla+A|^{2}+V\right)}\right)$$

$$\geq \min_{0\leq\gamma\leq1}\left(\operatorname{Tr}\left((1-\varepsilon)|i\hbar\nabla+A|^{2}+V_{K}\right)\gamma+\frac{1}{\beta}\operatorname{Tr}s\left(\gamma\right)\right)$$

$$+\min_{0\leq\gamma\leq1}\operatorname{Tr}\left(\varepsilon|i\hbar\nabla+A|^{2}+V-V_{K}\right)\gamma$$

$$=-\frac{1}{\beta}\operatorname{Tr}\log\left(1+e^{-\beta\left((1-\varepsilon)|i\hbar\nabla+A|^{2}+V_{K}\right)}\right)$$

$$-\operatorname{Tr}\left(\varepsilon|i\hbar\nabla+A|^{2}+V-V_{K}\right).$$

Applying the Lieb-Thirring inequality, we obtain

$$\operatorname{Tr}\left(\varepsilon|i\hbar\nabla + A|^2 + V - V_K\right)_{-} \le C\hbar^{-d}\varepsilon^{-d/2} \int_{\mathbb{R}^d} (V - V_K)_{-}^{1+d/2} \, \mathrm{d}x.$$

This means that for any K and ε

$$\limsup_{\hbar \to 0} \hbar^{d} \operatorname{Tr} \log \left(1 + e^{-\beta \left(|i\hbar \nabla + A|^{2} + V \right)} \right) \\
\leq \frac{1}{(2\pi)^{d}} \iint_{\mathbb{R}^{2d}} \log \left(1 + e^{-\beta \left((1-\varepsilon)p^{2} + V_{K}(x) \right)} \right) dx dp \\
+ \varepsilon^{-d/2} C \int_{\mathbb{R}^{d}} (V - V_{K})_{-}^{1+d/2} dx.$$

First taking $K \to \infty$ and afterwards $\varepsilon \to 0$, the result follows using the monotone convergence theorem.

4. Proof of Theorem 2 in the general case

In this section we deal with the interacting case $w \neq 0$. We first focus on the proof of Theorem 2 (mean-field limit) before proving Theorem 7 (dilute limit).

4.1. Convergence of the energy in the mean-field limit $\eta = 0$. Here we prove (12) in the case of general $w \in L^{1+d/2}(\mathbb{R}^d) + L_{\varepsilon}^{\infty}(\mathbb{R}^d)$. The upper bound on the canonical energy follows immediately from the trial states constructed in Proposition 8, so we concentrate on proving the lower bound. This is the content of the following proposition.

Proposition 11. Let $\beta_0, \rho > 0$, $V \in L^{1+d/2}_{loc}(\mathbb{R}^d)$ such that $V(x) \to \infty$ when $|x| \to \infty$ and $\int e^{-\beta_0 V_+(x)} dx < \infty$. Furthermore, let $|A|^2, w \in L^{1+d/2}(\mathbb{R}^d) + L^{\infty}_{\varepsilon}(\mathbb{R}^d)$, w be even and satisfy $\widehat{w} \ge 0$. Then we have

$$\lim_{\substack{N \to \infty \\ \hbar^d N \to \rho}} \hbar^d e_{\operatorname{Can}}^{\beta}(\hbar, N) \ge e_{\operatorname{Vla}}^{\beta}(\rho).$$

Proof. The main idea of the proof is to replace w by an effective one-body potential, and then use the lower bound in the non-interacting case.

We begin by regularizing the interaction potential: let $\varphi \in C_c^{\infty}(\mathbb{R}^d)$ even and real-valued, define $\chi = \varphi * \varphi$ and $w_{\varepsilon} = w * \chi_{\varepsilon}$ with $\chi_{\varepsilon} = \varepsilon^{-d} \chi(\varepsilon^{-1})$

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 [16, Lemma 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 $0 \le \widehat{w} \in L^1(\mathbb{R}^d)$, it is classical that we can bound w from below by a one-body potential, see, e.g., [16, Lem. 3.6]. More precisely, we have for all $x_1, \ldots, x_N \in \mathbb{R}^d$ and $\varphi \in C_c^{\infty}(\mathbb{R}^d)$

$$\int_{\mathbb{R}^d} \widehat{w} \left| \sum_{i=1}^N \widehat{\delta_{x_i}} - \varphi \right|^2 \ge 0,$$

which after expanding is the same as

$$\sum_{1 \le i < j \le N} w(x_i - x_j) \ge \sum_{i=1}^N w * \varphi(x_i) - \frac{1}{2} \int_{\mathbb{R}^d} (\varphi * w) \varphi - \frac{N}{2} w(0). \tag{39}$$

Let m_0 be the minimizer of the semiclassical problem with density ρ , whose existence is guaranteed by Theorem 1. For any N-body trial state Γ we obtain from (39)

$$\operatorname{Tr} H_{N,\hbar}\Gamma \ge \operatorname{Tr} \left((i\hbar \nabla + A(x))^2 + V(x) + \rho^{-1} w * \rho_{m_0}(x) \right) \Gamma^{(1)} - \frac{N}{2\rho^2} \int_{\mathbb{R}^d} (\rho_{m_0} * w) \rho_{m_0} - \frac{1}{2} w(0),$$

where $\Gamma^{(1)}$ is the 1-particle reduced density matrix of Γ . Let $\mu_{\text{Vla}}(\rho)$ be the chemical potential corresponding to the minimizer m_0 and define $V^{\text{eff}} = V + \rho^{-1}w * \rho_{m_0}(x) - \mu_{\text{Vla}}(\rho)$. Denoting by $e_{\text{Can}}^{\beta,\text{eff}}(\hbar, N)$ the minimum of the canonical energy with potential V^{eff} and with no interaction, we obtain using the convergence shown for the non-interacting case in Section 3,

$$\hbar^{d} e_{\operatorname{Can}}^{\beta}(\hbar, N) \geq \hbar^{d} e_{\operatorname{Can}}^{\beta, \operatorname{eff}}(\hbar, N) - \frac{\hbar^{d} N}{2\rho^{2}} \int_{\mathbb{R}^{d}} (\rho_{m_{0}} * w) \rho_{m_{0}} + \mu_{\operatorname{Vla}}(\rho) \hbar^{d} N$$

$$\xrightarrow[N \to \infty]{} -\frac{1}{\beta(2\pi)^{d}} \iint_{\mathbb{R}^{2d}} \log(1 + e^{-\beta(p^{2} + V^{\operatorname{eff}}(x))}) \, \mathrm{d}x \, \mathrm{d}p$$

$$-\frac{1}{2\rho} \int_{\mathbb{R}^{d}} (\rho_{m_{0}} * w) \rho_{m_{0}} + \mu_{\operatorname{Vla}}(\rho) \rho$$

$$= e_{\operatorname{Vla}}^{\beta}(\rho),$$

where the last equality is due to Theorem 1. This concludes the proof of the convergence of energy in Theorem 2. \Box

4.2. Convergence of the energy in the dilute limit $\eta > 0$. Here we prove the convergence of the energy in Theorem 7 where $\eta > 0$. We first state a lemma about the regularity of the minimizers of (4) when the interaction has a Dirac component. It will be needed in the proof of the convergence of the energy in Theorem 7 below.

Lemma 12. Let $\beta, a, \rho > 0$, let A, V satisfy the assumptions of Theorem 1, let $w = a\delta_0$ for some a > 0. If $m \in L^1(\mathbb{R}^{2d})$ satisfies the non-linear equation (5), then $\rho_m \in L^{1+d/2}(\mathbb{R}^d)$.

Proof. For simplicity and without loss of generality, we assume that $a = \rho = 1$, $\mu = 0$ and we take $w = \delta_0$ and A = 0. Since $\rho_m \in L^1(\mathbb{R}^d)$, it is sufficient to show that $\rho_m \mathbb{1}_{\{\rho_m(x) \geq 1\}}$ is in $L^{1+d/2}(\mathbb{R}^d)$. Recalling that m satisfies the equation

$$m(x,p) = \frac{1}{1 + e^{\beta(p^2 + V(x) + \rho_m(x))}},$$
 (40)

we immediately have

$$\rho_m(x) \le \frac{e^{-\beta(V(x) + \rho_m(x))}}{(2\pi)^d} \int_{\mathbb{R}^d} e^{-\beta p^2} \, \mathrm{d}p = C_{d,\beta} e^{-\beta(V(x) + \rho_m(x))},$$

implying that

$$\rho_m(x)e^{\beta\rho_m(x)} \le C_{d,\beta}e^{\beta V_-(x)}.$$

Hence

$$\rho_m \mathbb{1}_{\{\rho_m \ge 1\}} \le (V_- + \log C_{d,\beta}) \mathbb{1}_{\{\rho_m \ge 1\}} \in L^{1 + \frac{d}{2}}(\mathbb{R}^d),$$

since $V_{-} \in L^{1+\frac{d}{2}}\left(\mathbb{R}^{d}\right)$ and $\{\rho_{m} \geq 1\}$ has finite measure by Markov's inequality.

Remark 13. If w = 0 then ρ_m behaves like $V_-^{d/2}$, it can be seen by doing the same computation as in (9). Therefore, without other assumptions than $w \in L^{1+\frac{d}{2}}(\mathbb{R}^d)$, we cannot expect more from ρ_m .

4.2.1. Case $0 < \eta < 1/d$. We assume that $0 < d\eta < 1$ and take $w \in L^1(\mathbb{R}^d)$ with $0 \le \widehat{w} \in L^1(\mathbb{R}^d)$. Take $w_N = N^{d\eta}w(N^{\eta}\cdot)$ and consider the canonical model with this interaction. Denoting $a = \int_{\mathbb{R}^d} w(x) dx$, Proposition 8 implies that

$$\limsup_{\substack{N \to \infty \\ \hbar^d N \to \rho}} \hbar^d e_{\operatorname{Can}}^{\beta} \left(N, \hbar \right) \le e_{\operatorname{Vla}}^{\beta, w = a\delta_0} \left(\rho \right).$$

To show the lower bound, we follow the argument of Proposition 11. 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 (39) with $\varphi = \frac{N}{\rho} \rho_{m_0}$, we obtain

$$\operatorname{Tr} H_{N,\hbar} \Gamma_{N} \geq \operatorname{Tr} \left((i\hbar \nabla + A)^{2} + V^{\text{eff}} \right) \Gamma_{N}^{(1)} + \frac{1}{\rho} \operatorname{Tr} \left(w_{N} * \rho_{m_{0}} - a\rho_{m_{0}} \right) \Gamma_{N}^{(1)} - \frac{N}{2\rho^{2}} \int_{\mathbb{R}^{d}} \left(\rho_{m_{0}} * w_{N} \right) \rho_{m_{0}} + \mu_{\text{Vla}}^{w=a\delta_{0}} \left(\rho \right) N + o \left(\hbar^{-d} \right), \tag{41}$$

where $V^{\rm eff} = V + \frac{a}{\rho} \rho_{m_0} - \mu_{\rm Vla}^{w=a\delta_0}(\rho)$. Here, by Hölder's inequality, we have

$$\hbar^d \operatorname{Tr}(w_N * \rho_{m_0} - a \rho_{m_0}) \Gamma_N^{(1)}$$

$$= \hbar^{d} \int_{\mathbb{R}^{d}} (w_{N} * \rho_{m_{0}} - a\rho_{m_{0}}) \rho_{\Gamma_{N}^{(1)}}$$

$$\leq \left\| \hbar^{d} \rho_{\Gamma_{N}^{(1)}} \right\|_{L^{1+2/d}(\mathbb{R}^{d})} \|w_{N} * \rho_{m_{0}} - a\rho_{m_{0}}\|_{L^{1+d/2}(\mathbb{R}^{d})},$$

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 12. Finally we have,

$$\int_{\mathbb{R}^d} \left(\rho_{m_0} * w_N \right) \rho_{m_0} \longrightarrow a \int_{\mathbb{R}^d} \rho_{m_0}^2.$$

Hence, continuing from (41), we conclude that

$$\lim_{\substack{N \to \infty \\ \hbar^d N \to \rho}} \hbar^d e_{\operatorname{Can}}^{\beta} \left(N, \hbar \right) \ge -\frac{1}{\left(2\pi \right)^d \beta} \iint_{\mathbb{R}^{2d}} \log \left(1 + e^{-\beta \left(p^2 + V^{\operatorname{eff}}(x) \right)} \right) \, \mathrm{d}x \, \mathrm{d}p \\
+ \mu_{\operatorname{Vla}}^{w = a\delta_0} \left(\rho \right) \rho - \frac{a}{2\rho} \int_{\mathbb{R}^d} \rho_{m_0}^2 \\
= e_{\operatorname{Vla}}^{\beta, w = a\delta_0} \left(\rho \right).$$

4.2.2. 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

$$\liminf_{\substack{N \to \infty \\ \hbar^d N \to \rho}} \hbar^d e_{\operatorname{Can}}^{\beta} \left(N, \hbar \right) \geq \liminf_{\substack{N \to \infty \\ \hbar^d N \to \rho}} \hbar^d e_{\operatorname{Can}}^{\beta, w = 0} \left(N, \hbar \right) = e_{\operatorname{Vla}}^{\beta, w = 0} \left(\rho \right).$$

On the other hand, it follows from Proposition 8 that we also have the corresponding upper bound, so

$$\lim_{\substack{N \to \infty \\ \hbar^d N \to \rho}} \hbar^d e_{\operatorname{Can}}^{\beta} \left(N, \hbar \right) = e_{\operatorname{Vla}}^{\beta, w = 0} \left(\rho \right).$$

This finishes the proof of the convergence of the energy in the dilute limit.

- 4.3. Convergence of states. Without loss of generality, we take again $\rho = 1$.
- 4.3.1. Convergence of the k-particle Husimi and Wigner measures. The proof of the limits (13) and (14) in the case $\widehat{w} \geq 0$ is a corollary of the proof of [16, Theorem 2.7] and that $\mathcal{E}_{\text{Vla}}^{\beta,\rho}$ has a unique minimizer. In particular, the limiting measures do not depend on the coherent state function f. We start by briefly recalling the definitions and then we sketch the proof of the convergence of states.

For $f \in L^2(\mathbb{R}^d)$ a normalized, real-valued function and $(x,p) \in \mathbb{R}^{2d}$, $\hbar > 0$, we define $f_{x,p}^{\hbar}(y) = \hbar^{-d/4} f((x-y)/\hbar^{1/2}) e^{ip \cdot y/\hbar}$ and denote by $P_{x,p}^{\hbar} = |f_{x,p}^{\hbar}\rangle \langle f_{x,p}^{\hbar}|$ the orthogonal projection onto $f_{x,p}^{\hbar}$. For $k \geq 1$, we introduce the k-particle Husimi measure of a state Γ

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

for $x_1, p_1, ..., x_k, p_k \in \mathbb{R}^{2dk}$. We also recall the definition of the Wigner measure,

$$\mathcal{W}_{\Gamma}^{(k)}(x_1,...,p_k) = \int_{\mathbb{R}^{dk}} \int_{\mathbb{R}^{d(N-k)}} e^{-i\sum_{\ell=1}^k p_{\ell} \cdot y_{\ell}} \times \times \Gamma(x_1 + \hbar y_1/2,...,x_k + \hbar y_k/2, z_{k+1},...,z_N) \, dy_1...dy_k dz_{k+1}...dz_N,$$

for $x_1, p_1, ..., x_k, p_k \in \mathbb{R}^{2dk}$, where $\Gamma(\cdot, \cdot)$ is the kernel of the operator Γ . The rest of the proof is the same as in [16] and we just outline it. Using [16, 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 $\mathcal{B} = \{\mu \in L^1(\mathbb{R}^{2d}), 0 \leq \mu \leq 1, \int_{\mathbb{R}^{2d}} \mu \leq \rho\}$ such that, up to a subsequence, we have

$$\int_{\mathbb{R}^{2dk}} m_{f,\Gamma_N}^{(k)} \varphi \to \int_{\mathcal{B}} \left(\int_{\mathbb{R}^{2dk}} m^{\otimes k} \varphi \right) d\mathcal{P}(m),$$

for any $\varphi \in L^1(\mathbb{R}^{2dk}) + L^{\infty}(\mathbb{R}^{2dk})$ and similarly for the Wigner measures. We begin with the case $\eta = 0$. Using coherent states, the tightness of $(m_{f,\Gamma_N}^{(1)})_N$ and a finite volume approximation we obtain

$$\lim_{\substack{N_j \to \infty \\ \hbar^d N_j \to \rho}} \hbar^d e_{\operatorname{Can}}^{\beta}(\hbar, N_j) \ge \frac{1}{(2\pi)^d} \int_{\mathcal{B}} \left(\int_{\mathbb{R}^{2dk}} (p^2 + V(x)) m(x, p) \right) d\mathcal{P}(m) + \frac{1}{2} \int_{\mathcal{B}} \left(\int_{\mathbb{R}^{2dk}} (w * \rho_m) \rho_m \right) d\mathcal{P}(m) + \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} s \left(\int_{\mathcal{B}} m \, d\mathcal{P}(m) \right). \tag{42}$$

The lower semi-continuity of the entropy term can be justified as in the proof of Lemma 17. The case $0 < \eta < 1/d$ can be adapted using (39) 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.

Then, because V is confining, one can show that the de Finettti measure \mathcal{P} is supported on $\mathcal{S} = \{\mu \in L^1(\mathbb{R}^{2d}), 0 \leq \mu \leq 1, \int_{\mathbb{R}^{2d}} \mu = \rho\}$. If we denote $\overline{m} = \int_{\mathcal{S}} m \, d\mathcal{P}(m)$, the right side of (42) is not exactly $\mathcal{E}_{\operatorname{Can}}(\overline{m})$ because of the interaction term. In the case $0 \leq \eta < 1/d$ we assumed $\widehat{w} \geq 0$, hence the following inequality follows from convexity:

$$\int_{\mathcal{S}} \left(\int_{\mathbb{R}^{2dk}} w * \rho_m \rho_m \right) d\mathcal{P}(m) \ge \int_{\mathbb{R}^{2d}} w * \rho_{\overline{m}} \rho_{\overline{m}}.$$

The case $1/d < \eta$ is immediate since assumed $w \ge 0$ and the limiting energy has no interaction term. Gathering the above inequalties we have

$$\lim_{\substack{N_j \to \infty \\ \hbar^d N_j \to \rho}} \hbar^d e_{\operatorname{Can}}^{\beta}(\hbar, N_j) \ge \mathcal{E}_{\operatorname{Vla}}^{\beta, \rho, \bullet}(\overline{m}) \ge e_{\operatorname{Vla}}^{\beta, \bullet}(\rho),$$

where $\mathcal{E}_{\mathrm{Vla}}^{\beta,\rho,\bullet}$ and $e_{\mathrm{Vla}}^{\beta,\bullet}(\rho)$ 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, the equality in this series of inequalities forces \mathcal{P} to be supported on the set of minimizers of $\mathcal{E}_{\mathrm{Vla}}^{\beta,\rho,\bullet}$. In our case, it is the singleton $\{m_0\}$. And since this limit does not depend on the subsequence we have taken, we conclude that the whole sequence converges.

4.3.2. Convergence of the 1-particle Husimi measure and spatial density. The convergence in $L^1(\mathbb{R}^d)$ of $m_{f,\Gamma_N}^{(1)}$ comes from the fact that $\mathcal{E}_{\text{Vla}}^{\beta,\rho}$ has good coercive properties. For simplicity we take A=0 in the following. Using Eq. (39) with $\varphi=N\rho_{m_0}$ as well as [16, Lemma 2.4] with a finite volume approximation such as what has been done in the proof of Proposition 10,

one obtains that

$$\hbar^{d} e_{\operatorname{Can}}^{\beta}(\hbar, N) \geq \frac{1}{(2\pi)^{d}} \iint_{\mathbb{R}^{2d}} \left(p^{2} + V(x) + \frac{1}{2\rho} w_{N} * \rho_{m_{0}}(x) \right) m_{f, \Gamma_{N}}^{(1)}(x, p) dx dp
+ \frac{1}{(2\pi)^{d}\beta} \iint_{\mathbb{R}^{2d}} s(m_{f, \Gamma_{N}}^{(1)}) + o(1)
= e_{\operatorname{Vla}}^{\beta, \bullet}(\rho) + \frac{1}{(2\pi)^{d}\beta} \iint_{\mathbb{R}^{2d}} (s(m_{f, \Gamma_{N}}^{(1)}) - s(m_{0})) + o(1)$$
(43)

As before we denote by $e_{\text{Vla}}^{\beta,\bullet}(\rho)$ the appropriate limiting energy, depending on the choice of η . Recall that in the case $\eta > 1/d$, the interaction potential is assumed to be non negative, so the interaction term is just dropped. We now focus on the second term in (43). Let us remark that

$$s(m_{f,\Gamma_N}^{(1)}) - s(m_0)$$

$$= m_{f,\Gamma_N}^{(1)} \log \left(\frac{m_{f,\Gamma_N}^{(1)}}{m_0}\right) + (1 - m_{f,\Gamma_N}^{(1)}) \log \left(\frac{1 - m_{f,\Gamma_N}^{(1)}}{1 - m_0}\right)$$

$$+ (m_0 - m_{f,\Gamma_N}^{(1)}) \log \left(\frac{1 - m_0}{m_0}\right)$$

$$\geq m_0 \log \left(\frac{m_{f,\Gamma_N}^{(1)}}{m_0}\right) + \beta(m_0 - m_{f,\Gamma_N}^{(1)}) \left(p^2 + V + \frac{1}{\rho} w_N * \rho_{m_0} - \mu + \beta^{-1}\right),$$

where we used the expression of m_0 (5) and the pointwise inequality $x \log(x/y) + (y-x) \ge 0$ for any x, y > 0. Integrating over x and p, we obtain on the right side the sum of the relative von Neumann entropy of $m_{f,\Gamma_N}^{(1)}$ and m_0 , and a term which tends to zero, due to the weak convergence we have proven. By Pinsker's inequality and (43) we obtain

$$h^d e_{\text{Can}}^{\beta}(\hbar, N) - e_{\text{Vla}}^{\beta, \bullet}(\rho) \ge \frac{1}{2(2\pi)^d \beta} \left(\int_{\mathbb{R}^{2d}} |m_{f, \Gamma_N}^{(1)} - m_0| \right)^2 + o(1).$$

The convergence of the energies gives the strong convergence in $L^1(\mathbb{R}^{2d})$ of $m_{f,\Gamma_N}^{(1)}$ towards the Vlasov minimizer m_0 . This automatically gives that $\rho_{m_{f,\Gamma_N}^{(1)}} \to \rho_{m_0}$ in $L^1(\mathbb{R}^d)$. The convergence in $L^{1+2/d}(\mathbb{R}^d)$ follows from the (classical) Lieb-Thirring inequality

$$\|\rho_m\|_{L^{1+d/2}(\mathbb{R}^d)} \le C\|m\|_{L^1(\mathbb{R}^{2d},p^2dxdp)}^{\frac{d}{d+2}}\|m\|_{L^{\infty}(\mathbb{R}^{2d})}^{\frac{2}{d+2}}$$

for any m in $L^1(\mathbb{R}^{2d})$.

Finally, by the Lieb-Thirring inequality $\hbar^d \rho_{\Gamma_N}^{(1)}$ is bounded in $L^1(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$, hence this sequence is weakly precompact in those spaces. On the other hand, for any $\varphi \in C_c^{\infty}(\mathbb{R}^d)$ we have by [16, Lemma 2.4]

$$\int_{\mathbb{R}^d} \rho_{m_{f,\Gamma_N}^{(1)}} \varphi = \int_{\mathbb{R}^d} \hbar^d \rho_{\Gamma_N}^{(1)} \varphi * |f^{\hbar}|^2$$

and let $\tilde{\rho}$ be an accumulation point for $\hbar^d \rho_{\Gamma_N}^{(1)}$, by passing to the limit in both sides we obtain

$$\int_{\mathbb{R}^d} \rho_{m_0} \varphi = \int_{\mathbb{R}^d} \widetilde{\rho} \varphi.$$

The test function φ being arbitrary, we conclude that $\hbar^d \rho_{\Gamma_N}^{(1)}$ has a single accumulation point and therefore converges weakly in $L^1(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ towards ρ_{m_0} .

5. Proof of Theorem 1: Study of the semiclassical functional

This section is devoted to the proof of Theorem 1 and some auxiliary results on the semiclassical functional. We begin our analysis with the free particle case (w=0) and then generalize to systems with pair interaction. We recall that the magnetic potential does not affect the energy, only the minimizer, and can be removed by a change of variables so we do not consider it here. For this section and for $\rho > 0$ we denote by

$$S_{\text{Vla}}(\rho) = \left\{ m \in L^1(\mathbb{R}^{2d}) \mid 0 \le m \le 1, \ \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} m = \rho \right\}.$$

the set of admissible semi-classical measures.

5.1. The free gas.

Proposition 14 (Minimizing the free semi-classical energy). Suppose that w = 0, and that $V_+ \in L^1_{loc}(\mathbb{R}^d)$ satisfies $\int_{\mathbb{R}^d} e^{-\beta V_+(x)} dx < \infty$ for some $\beta > 0$ and $V_- \in L^{d/2}(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$. Fix $\rho > 0$ and define $m_0 \in S_{Vla}(\rho)$ by

$$m_0(x,p) := \frac{1}{1 + e^{\beta(p^2 + V(x) - \mu)}},$$

where μ is the unique chemical potential such that

$$\frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} m_0(x, p) \, dx \, dp = \rho.$$

Then

$$e_{\text{Vla}}^{\beta,w=0}(\rho) = \mathcal{E}_{\text{Vla}}^{\beta,\rho,w=0}(m_0)$$

$$= -\frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^{2d}} \log\left(1 + e^{-\beta(p^2 + V(x) - \mu)}\right) dx dp + \mu\rho. \tag{44}$$

Proof. The map

$$R := \mu \mapsto (2\pi)^{-d} \iint_{\mathbb{R}^{2d}} m_0(x, p) \, dx \, dp$$

is well-defined on \mathbb{R} , using that

$$\frac{1}{1 + e^{\beta(p^2 + V(x) - \mu)}} \le \frac{\max(1, e^{\beta\mu})}{1 + e^{\beta(p^2 + V(x))}}$$

which is integrable under our conditions on V, by the remarks after Theorem 1. In addition, R is increasing and continuous with

$$\lim_{\mu \to -\infty} R(\mu) = 0, \qquad \lim_{\mu \to +\infty} R(\mu) = +\infty.$$

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

$$\mathcal{E}_{\text{Vla}}^{\beta,\rho,w=0}(m_0) = \frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^{2d}} \left\{ \beta \left(p^2 + V(x) - \mu \right) m_0 + m_0 \log m_0 - m_0 \log \left(e^{\beta \left(p^2 + V(x) - \mu \right)} m_0 \right) \right\} dx dp + \frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^{2d}} \left(\log \left(1 - m_0 \right) + \beta \mu m_0 \right) dx dp = -\frac{1}{(2\pi)^d \beta} \int_{\mathbb{R}^{2d}} \log \left(1 + e^{-\beta \left(p^2 + V(x) - \mu \right)} \right) dx dp + \mu \rho,$$

showing the second equality in (44). That m_0 is the minimizer follows from the fact that the free energy is strictly convex. For instance, for any other $m \in S_{\text{Vla}}(\rho)$, since the function $s(t) = t \log t + (1-t) \log (1-t)$ is convex on (0,1) with derivative $s'(t) = \log \left(\frac{t}{1-t}\right)$, we have pointwise

$$s(m) \ge s(m_0) + s'(m_0)(m - m_0)$$

= $-\beta (p^2 + V(x) - \mu) m + \beta (p^2 + V(x) - \mu) m_0 + s(m_0),$ (45)

replacing m_0 by its expression implies that $\mathcal{E}_{\text{Vla}}^{\beta,\rho,w=0}(m) \geq \mathcal{E}_{\text{Vla}}^{\beta,\rho,w=0}(m_0)$. That m_0 is the unique minimizer follows from the fact that $\mathcal{E}_{\text{Vla}}^{\beta,\rho,w=0}$ is a strictly convex functional.

Remark 15. For an arbitrary domain $\Omega \subseteq \mathbb{R}^{2d}$, we have by the very same arguments that

$$\begin{split} \min_{\substack{m \in L^{1}(\Omega) \\ 0 \leq m \leq 1}} \left\{ \frac{1}{(2\pi)^{d}} \int_{\Omega} \left(\left(p^{2} + V\left(x \right) \right) m\left(x, p \right) \, \mathrm{d}x + \frac{1}{\beta} s\left(m\left(x, p \right) \right) \right) \mathrm{d}x \, \mathrm{d}p \right\} \\ &= -\frac{1}{(2\pi)^{d} \beta} \int_{\Omega} \log \left(1 + e^{-\beta \left(p^{2} + V\left(x \right) \right)} \right) \, \mathrm{d}x \, \mathrm{d}p. \end{split}$$

with the unique minimizer $\widetilde{m_0}(x,p) = (1 + e^{\beta(p^2 + V(x))})^{-1}$ and no chemical potential since we have dropped the mass constraint.

5.2. The interacting gas. We now deal with the interacting case. When $w \neq 0$, to retrieve the existence of minimizers as well as their expression, we need to use compactness techniques and compute the Euler-Lagrange equation. We divide the proof in several lemmas. We start by proving the semi-continuity of the functional in Lemma 16 and then prove the existence of minimizers on $S_{\text{Vla}}(\rho)$ in Lemma 17. 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 18 that minimizers cannot be equal to 0 nor 1 in sets of non zero measure. The proof of Theorem 1 is given at the end of this subsection.

Lemma 16. Fix $\rho, \beta_0 > 0$. Suppose that w = 0, and that $V_+ \in L^1_{loc}(\mathbb{R}^d)$, $V_- \in L^{d/2}(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ satisfies $\int_{\mathbb{R}^d} e^{-\beta_0 V_+(x)} dx < \infty$. Then for all $\beta > \beta_0$, $\mathcal{E}_{Vla}^{\beta,\rho,w=0}$ is L^1 -strongly lower semi-continuous on $S_{Vla}(\rho)$.

Proof. We have to show that for any $C_0 \in \mathbb{R}$

$$\mathcal{L}(C_0) := \left\{ m \in S_{\text{Vla}}(\rho) \mid \mathcal{E}_{\text{Vla}}^{\beta,\rho,w=0}(m) \le C_0 \right\}$$

is closed with respect to the L^1 -norm on $S_{\text{Vla}}(\rho)$. Let $(m_n) \subseteq \mathcal{L}(C_0)$ be a sequence converging towards some $m \in L^1(\mathbb{R}^d)$ with respect to the L^1 -norm. By the L^1 convergence we immediately have $\frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} m = \rho$, we can also extract a subsequence converging almost everywhere and obtain $0 \le m \le 1$. Applying Remark 15 with $\Omega = \{|x| + |y| \ge R\}$, we have for any R > 0 that

$$\frac{1}{(2\pi)^{d}} \iint_{|x|+|p| \ge R} (p^{2} + V(x)) m_{n}(x,p) + \frac{1}{\beta} s(m_{n}(x,p)) dx dp$$

$$\ge -\frac{1}{\beta} \iint_{|x|+|p| > R} \log \left(1 + e^{-\beta(p^{2}+V(x))}\right) dx dp = o_{R}(1). \tag{46}$$

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

$$\lim_{n \to \infty} \iint_{|x|+|p| \le R} \left(p^2 + V_+(x) \right) m_n(x,p) \, \mathrm{d}x \, \mathrm{d}p$$

$$\ge \iint_{|x|+|p| \le R} \left(p^2 + V_+(x) \right) m(x,p) \, \mathrm{d}x \, \mathrm{d}p,$$

$$\iint_{|x|+|p| \le R} V_-(x) m_n(x,p) \, \mathrm{d}x \, \mathrm{d}p \xrightarrow[n \to \infty]{} \iint_{|x|+|p| \le R} V_-(x) m(x,p) \, \mathrm{d}x \, \mathrm{d}p.$$

It remains to deal with the entropy term: by continuity of s and by dominated convergence we have

$$\iint_{|x|+|p| \le R} s\left(m_n\left(x,p\right)\right) \, \mathrm{d}x \, \mathrm{d}p \underset{n \to \infty}{\longrightarrow} \iint_{|x|+|p| \le R} s\left(m\left(x,p\right)\right) \, \mathrm{d}x \, \mathrm{d}p.$$

All in all we obtain

$$C_{0} \geq \liminf_{n \to \infty} \mathcal{E}_{\text{Vla}}^{\beta,\rho,w=0}(m_{n})$$

$$\geq \frac{1}{(2\pi)^{d}} \iint_{|x|+|p|\leq R} (p^{2}+V(x)) m(x,p) dx dp$$

$$+ \frac{1}{\beta} \iint_{|x|+|p|\leq R} s(m(x,p)) dx dp + o(R)$$

$$\geq \frac{1}{(2\pi)^{d}} \iint_{|x|+|p|\leq R} (p^{2}+V_{+}(x)) m(x,p) dx dp + o(R)$$

$$- \frac{1}{(2\pi)^{d}} \iint_{\mathbb{R}^{2d}} V_{-}(x) m(x,p) dx dp + \frac{1}{\beta} \iint_{\mathbb{R}^{2d}} s(m(x,p)) dx dp.$$

Finally, we use the monotone convergence theorem and let R tend to ∞ to obtain $\mathcal{E}_{\text{Vla}}^{\beta,\rho,w=0}\left(m\right)\leq C_{0}$.

Lemma 17. Fix $\rho, \beta_0 > 0$. Suppose that $w \in L^{1+d/2}(\mathbb{R}^d) + L_{\varepsilon}^{\infty}(\mathbb{R}^d) + \mathbb{R}_{+}\delta_0$, $V_{+} \in L^{1}_{loc}(\mathbb{R}^d)$, $V_{-} \in L^{1+d/2}(\mathbb{R}^d)$ satisfies $\int_{\mathbb{R}^d} e^{-\beta_0 V_{+}(x)} dx < \infty$ and $V_{+}(x) \to \infty$ as $|x| \to \infty$. Then for all $\beta > \beta_0$, $\mathcal{E}_{Vla}^{\beta,\rho}$ is bounded below and has a minimizer m_0 in $S_{Vla}(\rho)$.

Proof. Let $(m_n) \subseteq S_{\text{Vla}}(\rho)$ be a minimizing sequence, i.e. $\mathcal{E}_{\text{Vla}}^{\beta,\rho}(m_n) \to e_{\text{Vla}}^{\beta}(\rho)$ 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

$$\int_{\mathbb{R}^{2d}} m_n(x, p) \varphi(x, p) \, dx \, dp \to \int_{\mathbb{R}^{2d}} m_0(x, p) \varphi(x, p) \, dx \, dp \qquad (47)$$

for any $\varphi \in L^1(\mathbb{R}^{2d}) + L_{\varepsilon}^{\infty}(\mathbb{R}^{2d})$. Moreover, the weak limit m_0 satisfies $0 \leq m_0 \leq 1$ and $\int_{\mathbb{R}^{2d}} m_0 \leq \rho (2\pi)^d$. Note that we do not have pointwise convergence a priori. Let us prove that m_0 is a minimizer of $\mathcal{E}_{\text{Vla}}^{\beta,\rho}$ in $S_{\text{Vla}}(\rho)$. Our first step is to show the tightness of the sequence of probability measures (m_n) to obtain $\int_{\mathbb{R}^{2d}} m_0 = (2\pi)^d \rho$, then we argue that $m_0 \in S_{\text{Vla}}(\rho)$ and minimizes $\mathcal{E}_{\text{Vla}}^{\beta,\rho}$ using weak lower-semicontinuity.

We start out by bounding the interaction term using some of the kinetic energy. Let $\varepsilon > 0$ and let us write $w = w_1 + w_2 + a\delta_0$ with $w_1 \in L^{1+d/2}(\mathbb{R}^d)$, $\|w_2\|_{L^{\infty}(\mathbb{R}^d)} < \varepsilon$ and $a \geq 0$. We use Young's inequality to bound the interaction term

$$\int_{\mathbb{R}^{d}} w * \rho_{m_{n}} \rho_{m_{n}} \geq ||w_{1}||_{L^{1+d/2}(\mathbb{R}^{d})} ||\rho_{m_{n}}||_{L^{1+2/d}(\mathbb{R}^{d})} ||\rho_{m_{n}}||_{L^{1}(\mathbb{R}^{d})} + ||w_{2}||_{L^{\infty}(\mathbb{R}^{d})} ||\rho_{m_{n}}||_{L^{1}(\mathbb{R}^{d})}^{2}$$

$$\geq C\varepsilon \iint_{\mathbb{R}^{2d}} p^{2} m_{n}(x, p) \, dx \, dp - C. \tag{48}$$

In the last inequality we have used the well-known fact [30] that

$$\int_{\mathbb{R}^{d}} p^{2} m(x, p) dp \ge \inf_{\substack{0 \le \widetilde{m} \le 1 \\ \int \widetilde{m} = (2\pi)^{d} \rho_{m}(x)}} \int_{\mathbb{R}^{d}} p^{2} \widetilde{m}(p) dp$$

$$= (2\pi)^{d} c_{\text{TF}} \frac{d}{d+2} \rho_{m}(x)^{1+2/d}, \tag{49}$$

which gives the Lieb-Thirring inequality for classical measures on phase space. Similarly we have

$$\int_{\mathbb{R}^d} V_{-}(x) \rho_{m_n}(x) dx \le C \left(\varepsilon^{-d/2} \|V_{-}\|_{L^{1+d/2}(\mathbb{R}^d)}^{1+d/2} + \varepsilon \|\rho_{m_n}\|_{L^{1+2/d}(\mathbb{R}^d)}^{1+2/d} \right).$$
 (50)

Now using Proposition 14, (49), (48) and (50), denoting $\alpha = (\beta - \beta_0)/(2\beta)$ we have

$$C \geq \mathcal{E}_{\mathrm{Vla}}^{\beta,\rho}(m_n) \geq \frac{\alpha}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} \left(p^2 + V(x) \right) m_n + \frac{1}{2\rho} \iint_{\mathbb{R}^d} \left(w * \rho_{m_n} \right) \rho_{m_n}$$

$$+ \frac{1}{2} e_{\mathrm{Vla}}^{\beta(1-\alpha),w=0}(\rho)$$

$$\geq \frac{\alpha - C\varepsilon}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} \left(p^2 + V_+(x) \right) m_n - C$$

$$(51)$$

Note that by construction, $\beta(1-\alpha) > \beta_0$. Taking $\varepsilon > 0$ sufficiently small but positive, the above inequality shows the tightness condition

$$\iint_{\mathbb{R}^{2d}} \left(p^2 + V_+(x) \right) m_n(x, p) \, \mathrm{d}x \, \mathrm{d}p \le C. \tag{52}$$

Therefore $\iint_{\mathbb{R}^{2d}} m_0 = (2\pi)^d \rho$.

Now we prove that $\liminf_{n\to\infty} \mathcal{E}_{\mathrm{Vla}}^{\beta,\rho}(m_n) \geq \mathcal{E}_{\mathrm{Vla}}^{\beta,\rho}(m_0)$. From the tightness condition it is easy to verify that $\rho_{m_n} \rightharpoonup \rho_{m_0}$ and that

$$\int_{\mathbb{R}^d} (w - a\delta_0) * \rho_{m_n} \rho_{m_n} \to \int_{\mathbb{R}^d} (w - a\delta_0) * \rho_{m_0} \rho_{m_0}.$$

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 obtain

$$a \int_{\mathbb{R}^d} \rho_{m_0}^2 = \int_{\mathbb{R}^d} \lim_{n \to \infty} \rho_{m_n}^2 \le \lim_{n \to \infty} \int_{\mathbb{R}^d} \rho_{m_n}^2,$$
$$\int_{\mathbb{R}^d} s(m_0) = \int_{\mathbb{R}^d} \lim_{n \to \infty} s(m_n) \le \liminf_{n \to \infty} \int_{\mathbb{R}^d} s(m_n).$$

Lemma 18. Fix $\rho, \beta_0 > 0$. Suppose that $w \in L^{1+d/2}(\mathbb{R}^d) + L_{\varepsilon}^{\infty}(\mathbb{R}^d) + \mathbb{R}_{\varepsilon}^{\infty}(\mathbb{R}^d) + \mathbb{R}_{\varepsilon}^{\infty}(\mathbb{R}^d)$, $V_+ \in L^1_{loc}(\mathbb{R}^d)$, $V_- \in L^{1+d/2}(\mathbb{R}^d)$ satisfies $\int_{\mathbb{R}^d} e^{-\beta_0 V_+(x)} dx < \infty$ and $V_+(x) \to \infty$ as $|x| \to \infty$. Then any minimizer $m_0 \in S_{Vla}(\rho)$ of $\mathcal{E}_{Vla}^{\beta,\rho}$ satisfies

$$0 < m(x, p) < 1$$
 for $(x, p) \in \mathbb{R}^{2d}$ 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 then 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

$$\varphi_1 = \lambda \mathbb{1}_{B(\xi_1, r) \cap \Omega_1}, \quad \varphi_2 = \lambda \mathbb{1}_{B(\xi_2, r') \cap \Omega_0},$$

where $r' := \min\{s \geq 0 \mid |B(\xi_2, s) \cap \Omega_0| = |B(\xi_1, r) \cap \Omega_1|\}$. We will use the notation $v(r) = |B(\xi_1, r) \cap \Omega_1|$. Note that by Lebesgue's density theorem, for almost every $(\xi_1, \xi_2) \in \Omega_1 \times \Omega_0$ we have v(r) > 0 and $r' < \infty$. The idea is to consider the function $m_0 - \varphi_1 + \varphi_2 \in S_{\text{Vla}}(\rho)$ and use the fact that m_0 is a minimizer of $\mathcal{E}_{\text{Vla}}^{\beta,\rho}$ to obtain a contradiction. Let us estimate the entropy, using that s(0) = s(1) = 0 and s(t) = s(1-t), we obtain

$$\iint_{\mathbb{R}^{2d}} s \left(m_0 - \varphi_1 + \varphi_2 \right) = \iint_{\mathbb{R}^{2d}} s \left(m_0 \right) + s(\varphi_1) + s(\varphi_2)$$
$$= 2s \left(\lambda \right) v(r) + \iint_{\mathbb{R}^{2d}} s \left(m_0 \right).$$

It remains to estimate the contribution of this small perturbation to interaction energy, we have

$$\int_{\mathbb{R}^d} \rho_{m_0 - \varphi_1 + \varphi_2} w * \rho_{m_0 - \varphi_1 + \varphi_2} = \int_{\mathbb{R}^d} \rho_{m_0} w * \rho_{m_0} + 2 \int_{\mathbb{R}^d} \rho_{\varphi_2 - \varphi_1} w * \rho_{m_0} + \int_{\mathbb{R}^d} \rho_{\varphi_2 - \varphi_1} w * \rho_{\varphi_2 - \varphi_1}.$$

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

$$\int_{\mathbb{R}^{d}} w * (\rho_{\varphi_{2}} - \rho_{\varphi_{1}}) (\rho_{\varphi_{2}} - \rho_{\varphi_{1}})
\leq \|w_{1}\|_{L^{1+d/2}(\mathbb{R}^{d})} \|\rho_{\varphi_{2}} - \rho_{\varphi_{1}}\|_{L^{1}(\mathbb{R}^{d})} \|\rho_{\varphi_{2}} - \rho_{\varphi_{1}}\|_{L^{1+2/d}(\mathbb{R}^{d})}
+ \|w_{2}\|_{L_{\varepsilon}^{\infty}(\mathbb{R}^{d})} \|\rho_{\varphi_{2}} - \rho_{\varphi_{1}}\|_{L^{1}(\mathbb{R}^{d})}^{2} + a\|\rho_{\varphi_{2}} - \rho_{\varphi_{1}}\|_{L^{2}(\mathbb{R}^{d})}^{2}
\leq C\lambda^{2} \left(\|w\|_{L^{1+d/2}(\mathbb{R}^{d})} v(r)^{1+\frac{d}{d+2}} + \|w_{2}\|_{L_{\varepsilon}^{\infty}(\mathbb{R}^{d})} v(r)^{2} + av(r) \right).$$

Next and similarly we estimate the second term (minus the delta interaction)

$$\int_{\mathbb{R}^{d}} (w_{1} + w_{2}) * \rho_{m_{0}} (\rho_{\varphi_{2}} - \rho_{\varphi_{1}})
\leq ||w_{1}||_{L^{1+d/2}(\mathbb{R}^{d})} ||\rho_{m_{0}}||_{L^{1+2/d}(\mathbb{R}^{d})} ||\rho_{\varphi_{2}} - \rho_{\varphi_{1}}||_{L^{1}(\mathbb{R}^{d})}
+ ||w_{2}||_{L_{\varepsilon}^{\infty}(\mathbb{R}^{d})} ||\rho_{m_{0}}||_{L^{1}(\mathbb{R}^{d})} ||\rho_{\varphi_{2}} - \rho_{\varphi_{1}}||_{L^{1}(\mathbb{R}^{d})}
\leq C\lambda(||w_{1}||_{L^{1+d/2}(\mathbb{R}^{d})} ||\rho_{m_{0}}||_{L^{1+2/d}(\mathbb{R}^{d})} + ||w_{2}||_{L_{\varepsilon}^{\infty}(\mathbb{R}^{d})} ||\rho_{m_{0}}||_{L^{1}(\mathbb{R}^{d})})v(r).$$

Since m_0 is a minimizer, these estimates imply that

$$\mathcal{E}_{\text{Vla}}^{\beta,\rho}(m_0) \leq \mathcal{E}_{\text{Vla}}^{\beta,\rho}(m_0 - \varphi_1 + \varphi_2)
\leq \mathcal{E}_{\text{Vla}}^{\beta,\rho}(m_0) + \frac{1}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} \left(p^2 + V(x) + a\rho_{m_0} \right) (\varphi_2 - \varphi_1)
+ C\lambda^2 \left(\|w\|_{L^{1+d/2}(\mathbb{R}^d)} v(r)^{1+\frac{d}{d+2}} + \|w_2\|_{L_{\varepsilon}^{\infty}(\mathbb{R}^d)} v(r)^2 + av(r) \right)
+ C\lambda \left(\|w_1\|_{L^{1+d/2}(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^{1+2/d}(\mathbb{R}^d)}
+ \|w_2\|_{L_{\varepsilon}^{\infty}(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^1(\mathbb{R}^d)} \right) v(r) + \frac{2s(\lambda)}{(2\pi)^d \beta} v(r).$$

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 $(\xi_1, \xi_2) \in \Omega_1 \times \Omega_0$

$$-\frac{2s(\lambda)}{\lambda\beta} \le -p_1^2 - V(x_1) - a\rho_{m_0}(x_1) + p_2^2 + V(x_2) + a\rho_{m_0}(x_2) + C \|w\|_{L^{1+d/2}(\mathbb{R}^d)} \|\rho_{m_0}\|_{L^{1+2/d}(\mathbb{R}^d)}.$$

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 $V \in L^{1+d/2}_{loc}(\mathbb{R}^d)$ and $\rho_{m_0} \in L^{1+2/d}_{loc}(\mathbb{R}^d)$, 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 1. We assume A=0 without loss of generality, since it can be removed by a change of variable.

We will first show that the expression (5) of the minimizers is correct by computing the Euler-Lagrange equation associated with any such minimizer m_0 . This gives automatically the expression of the minimum energy (6). We conclude, in the case $\widehat{w} \geq 0$, by showing that the chemical potential μ is given by (8).

Let $\varepsilon > 0$ small enough and $\varphi \in L^1 \cap L^\infty(\{\varepsilon < m < 1 - \varepsilon\})$ such that $\iint \varphi = (2\pi)^d \rho$. For $\delta = \frac{\varepsilon}{1+\|\varphi\|_\infty}$ we have $m_t := \frac{m_0+t\varphi}{1+t} \in S_{\text{Vla}}(\rho)$ for all $t \in (-\delta, \delta)$. Since m_0 is a minimizer, we must have $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_{\mathrm{Vla}}^\beta(m_t)_{|t=0} = 0$. 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

$$\iint_{\mathbb{R}^{2d}} \left(p^2 + V(x) + \frac{1}{\rho} w * \rho_{m_0}(x) + \frac{1}{\beta} \log \left(\frac{m_0(x, p)}{1 - m_0(x, p)} \right) \right) \varphi(x, p) \, dx \, dp$$

$$= \iint_{\mathbb{R}^{2d}} \left(p^2 + V(x) + \frac{1}{\rho} w * \rho_{m_0}(x) + \frac{1}{\beta} \log \left(\frac{m_0(x, p)}{1 - m_0(x, p)} \right) \right) m_0(x, p) \, dx \, dp. \tag{53}$$

Denoting the right hand side by $(2\pi)^d \mu_{\text{Vla}}(\rho) \rho$, we have shown for any φ verifying the above conditions that

$$\iint_{\{\varepsilon < m < 1 - \varepsilon\}} \left(p^2 + V(x) + \frac{1}{\rho} w * \rho_{m_0}(x) + \frac{1}{\beta} \log \left(\frac{m_0(x, p)}{1 - m_0(x, p)} \right) - \mu_{\text{Vla}}(\rho) \right) \varphi(x, p) \, dx \, dp = 0.$$

This is enough for the left factor in the integrand above to be zero almost everywhere on $\{\varepsilon < m < 1 - \varepsilon\}$. But ε can be taken arbitrary small and by Lemma 18 we have $\bigcup_{\varepsilon>0} \{\varepsilon < m < 1 - \varepsilon\} = \{0 < m < 1\} = \mathbb{R}^{2d}$ almost everywhere, from which we obtain (5).

That $\rho_{m_0} \in L^2(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$ follows from Lemma 12 and the fact that m_0 satisfies (5).

It remains to prove (8) when it is assumed that $\widehat{w} \geq 0$. This is a classical argument and we only sketch it, we refer to [33] for further details. First

note that the assumption $\widehat{w} \geq 0$ ensures the convexity of $\mathcal{E}_{\mathrm{Vla}}^{\beta,\rho}$, hence for $\rho' > 0$, $F_{\mathrm{Vla}}^{\beta}(\rho',\rho)$ is the minimum of a convex function under a linear constraint, it is therefore convex. This implies that, for $\rho' > 0$, the function $F_{\mathrm{Vla}}^{\beta}(\cdot,\rho')$ is continuous on \mathbb{R}_+ and continuously differentiable except maybe in a countable number of values of ρ . We first show that

$$\mathbb{R}_+^* \ni \rho \mapsto \mu(\rho) \in \mathbb{R}$$

defines a bijection, where $\mu(\rho)$, defined in (5), is the Lagrange multiplier associated to the constraint ρ . Consider, for $\mu \in \mathbb{R}$, the unconstrained minimization problem

$$\inf_{0 \le m \le 1} \mathcal{E}_{\text{Vla}}^{\beta, \rho'}(m) - \frac{\mu}{(2\pi)^d} \iint_{\mathbb{R}^{2d}} m = \inf_{\rho \ge 0} F_{\text{Vla}}^{\beta}(\rho, \rho') - \mu \rho. \tag{54}$$

This yields a minimizer m^{μ} and hence a density $\rho(\mu) := (2\pi)^{-d} \iint m^{\mu}$, see Remark 15. 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 (54), the density m^{μ} must also satisfy $\mathcal{E}_{\mathrm{Vla}}^{\beta,\rho'}(m^{\mu}) = F_{\mathrm{Vla}}^{\beta}(\rho(\mu),\rho')$ and since $\widehat{w} \geq 0$, we conclude that m^{μ} is also the unique solution of this equation and must satisfy (5) where $\mu(\rho)$ appears. By identification, $\mu = \mu(\rho)$ is the Lagrange multiplier associated to the minimization problem at density ρ . This proves the bijective correspondance between $\mu(\rho)$ and ρ .

Finally, if $F_{\text{Vla}}^{\beta}(\cdot, \rho')$ is differentiable in some ρ_0 , the above discussion shows (8) for $\rho = \rho_0$. But because of the one-to-one correspondence between μ and ρ , $\partial_{\rho}F_{\text{Vla}}^{\beta}$ cannot be discontinuous, this concludes the proof.

References

- [1] 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., in press (2015).
- [2] V. Bach, E. H. Lieb, and J. P. Solovej, Generalized Hartree-Fock theory and the Hubbard model, J. Statist. Phys., 76 (1994), pp. 3–89.
- [3] 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 (2003), pp. 665–683.
- [4] M. Barranco and J.-R. Buchler, Equation of state of hot, dense stellar matter: Finite temperature nuclear thomas-fermi approach, Phys. Rev. C, 24 (1981), pp. 1191– 1202.
- [5] N. BENEDIKTER, V. JAKSIC, M. PORTA, C. SAFFIRIO, AND B. SCHLEIN, Mean-field Evolution of Fermionic Mixed States, Comm. Pure Appl. Math., 69 (2016), pp. 2250– 2303.
- [6] 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, ArXiv e-prints, (2018), p. arXiv:1809.01902.
- [7] N. BENEDIKTER, M. PORTA, C. SAFFIRIO, AND B. SCHLEIN, From the Hartree dynamics to the Vlasov equation, Arch. Ration. Mech. Anal., 221 (2016), pp. 273– 334.
- [8] N. Benedikter, M. Porta, and B. Schlein, Mean-field evolution of fermionic systems, Comm. Math. Phys., 331 (2014), pp. 1087–1131.

- [9] L. G. Brown and H. Kosaki, Jensen's inequality in semi-finite von Neumann algebras, J. Operator Theory, 23 (1990), pp. 3-19.
- [10] K. A. BRUECKNER, J. R. BUCHLER, S. JORNA, AND R. J. LOMBARD, Statistical theory of nuclei, Phys. Rev., 171 (1968), pp. 1188–1195.
- [11] R. D. COWAN AND J. ASHKIN, Extension of the Thomas-Fermi-Dirac statistical theory of the atom to finite temperatures, Phys. Rev., 105 (1957), pp. 144–157.
- [12] 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 ed., 1987.
- [13] E. Dietler, S. Rademacher, and B. Schlein, From Hartree dynamics to the relativistic Vlasov equation, J. Stat. Phys., 172 (2018), pp. 398–433.
- [14] 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 (2004), pp. 1241–1273.
- [15] R. P. FEYNMAN, N. METROPOLIS, AND E. TELLER, Equations of state of elements based on the generalized Fermi-Thomas theory, Phys. Rev., 75 (1949), pp. 1561–1573.
- [16] S. Fournais, M. Lewin, and J. P. Solovej, *The semi-classical limit of large fermionic systems*, Calc. Var. Partial Differ. Equ., (2018), pp. 57–105.
- [17] J. FRÖHLICH AND A. KNOWLES, A microscopic derivation of the time-dependent Hartree-Fock equation with Coulomb two-body interaction, J. Stat. Phys., 145 (2011), pp. 23–50.
- [18] J. J. Gilvarry and G. H. Peebles, Solutions of the temperature-perturbed Thomas-Fermi equation, Phys. Rev., 99 (1955), pp. 550–552.
- [19] S. GIORGINI, L. P. PITAEVSKII, AND S. STRINGARI, Theory of ultracold atomic Fermi gases, Rev. Mod. Phys., 80 (2008), pp. 1215–1274.
- [20] A. D. Gottlieb, Examples of bosonic de Finetti states over finite dimensional Hilbert spaces, J. Stat. Phys., 121 (2005), pp. 497–509.
- [21] C. Hainzl, M. Porta, and F. Rexze, On the correlation energy of the mean-field Fermi gas, ArXiv e-prints, (2018), p. arXiv:1806.11411.
- [22] R. LATTER, Temperature behavior of the Thomas-Fermi statistical model for atoms, Phys. Rev., 99 (1955), pp. 1854–1870.
- [23] 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.
- [24] M. Lewin, P. T. Nam, and N. Rougerie, Derivation of Hartree's theory for generic mean-field Bose systems, Adv. Math., 254 (2014), pp. 570–621.
- [25] _____, Derivation of nonlinear Gibbs measures from many-body quantum mechanics, J. Éc. polytech. Math., 2 (2015), pp. 65–115.
- [26] ——, Classical field theory limit of 2D many-body quantum Gibbs states, ArXiv e-prints, (2018).
- [27] ——, Gibbs measures based on 1D (an)harmonic oscillators as mean-field limits, J. Math. Phys., 59 (2018), p. 041901.
- [28] ——, The interacting 2D Bose gas and nonlinear Gibbs measures, in Gibbs measures for nonlinear dispersive equations, B. S. Giuseppe Genovese and V. Sohinger, eds., 2018. Oberwolfach mini-workshop.
- [29] M. Lewin, P. T. Nam, S. Serfaty, and J. P. Solovej, *Bogoliubov spectrum of interacting Bose gases*, Comm. Pure Appl. Math., 68 (2015), pp. 413–471.
- [30] E. H. LIEB AND M. Loss, Analysis, vol. 14 of Graduate Studies in Mathematics, American Mathematical Society, Providence, RI, 2nd ed., 2001.
- [31] E. H. LIEB, R. SEIRINGER, AND J. P. SOLOVEJ, Ground-state energy of the lowdensity Fermi gas, Phys. Rev. A, 71 (2005), p. 053605.
- [32] E. H. LIEB AND B. SIMON, *The Hartree-Fock theory for Coulomb systems*, Commun. Math. Phys., 53 (1977), pp. 185–194.
- [33] —, The Thomas-Fermi theory of atoms, molecules and solids, Adv. Math., 23 (1977), pp. 22–116.
- [34] E. H. LIEB AND W. E. THIRRING, Bound on kinetic energy of fermions which proves stability of matter, Phys. Rev. Lett., 35 (1975), pp. 687–689.

- [35] —, Inequalities for the moments of the eigenvalues of the Schrödinger hamiltonian and their relation to Sobolev inequalities, Studies in Mathematical Physics, Princeton University Press, 1976, pp. 269–303.
- [36] ——, Gravitational collapse in quantum mechanics with relativistic kinetic energy, Ann. Physics, 155 (1984), pp. 494–512.
- [37] E. H. LIEB AND H.-T. YAU, The Chandrasekhar theory of stellar collapse as the limit of quantum mechanics, Commun. Math. Phys., 112 (1987), pp. 147–174.
- [38] P. S. Madsen, In preparation, PhD thesis, Aarhus University, 2019.
- [39] N. H. March, Equations of State of Elements from the Thomas-Fermi Theory II: Case of Incomplete Degeneracy, Proc. Phys. Soc., 68 (1955), p. 1145.
- [40] R. E. MARSHAK AND H. A. BETHE, The Generalized Thomas-Fermi Method as Applied to Stars., Astrophys. J., 91 (1940), p. 239.
- [41] H. NARNHOFER AND G. SEWELL, Vlasov hydrodynamics of a quantum mechanical model, Comm. Math. Phys., 79 (1981), pp. 9-24.
- [42] S. Petrat and P. Pickl, A new method and a new scaling for deriving fermionic mean-field dynamics, Math. Phys. Anal. Geom., 19 (2016), pp. Art. 3, 51.
- [43] M. REED AND B. SIMON, Methods of Modern Mathematical Physics. I. Functional analysis, Academic Press, 1972.
- [44] D. W. Robinson, The thermodynamic pressure in quantum statistical mechanics, Springer-Verlag, Berlin-New York, 1971. Lecture Notes in Physics, Vol. 9.
- [45] N. ROUGERIE, De Finetti theorems, mean-field limits and Bose-Einstein condensation, ArXiv e-prints, (2015).
- [46] D. RUELLE, Statistical mechanics. Rigorous results, Singapore: World Scientific. London: Imperial College Press, 1999.
- [47] R. SEIRINGER, The thermodynamic pressure of a dilute Fermi gas, Comm. Math. Phys., 261 (2006), pp. 729–757.
- [48] B. Simon, The classical limit of quantum partition functions, Comm. Math. Phys., 71 (1980), pp. 247–276.
- [49] H. Spohn, On the Vlasov hierarchy, Math. Methods Appl. Sci., 3 (1981), pp. 445-455.
- [50] W. E. Thirring, Quantum Mathematical Physics, vol. Atoms, Molecules and Large Systems, Springer, Second Edition 2002.
- [51] A. Triay, In preparation, PhD thesis, University of Paris-Dauphine, 2019.

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