A PROBLEM OF MOMENT REALIZABILITY IN QUANTUM STATISTICAL PHYSICS

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Abstract. This work is a generalization of the results previously obtained in [17] in a one-dimensional setting: we revisit the problem of the minimization of the quantum free energy (entropy + energy) under local constraints (moments) and prove the existence of minimizers in various configurations. While [17] addressed the 1D case on bounded domains, we treat in the present paper the multi-dimensional case as well as unbounded domains and non-linear interactions as Hartree/Hartree-Fock. Moreover, whereas [17] dealt with the first moment only, namely the charge density, we extend the results to the second moment, the current density.

1. Introduction

The problem of moment realizability in the quantum framework that we analyze in this paper is an essential ingredient of the recent theory developed by Degond and Ringhofer [9], see also [6, 8], on the derivation of quantum hydrodynamics models from first principles. Their approach consists in transposing Levermore's [15] moment closure strategy by entropy minimization to the quantum picture. Roughly speaking, starting from the quantum Liouville equation for a density operator ϱ, they obtain an unclosed cascade of equations on moments of ϱ that is closed by a minimization of the quantum free energy. In doing so, many different models can be obtained depending on the configuration or the chosen asymptotics: Quantum Drift-Diffusion, Quantum Energy-Transport, or also Quantum Navier-Stokes, see [3, 4, 5, 6, 7, 8, 12, 13] for more precisions.

The mathematical justification of this theory based on entropy minimization has yet to be done. The first step towards this goal is the analysis of the quantum moment problem that we started in [17] and pursue in this paper. The classical version of the moment realizability problem with applications to kinetic equations is well-known: in the case of three moments (density, current and energy), the associated local equilibria are the classical Maxwellian and the obtained hydrodynamic model is the Euler equation ; for higher moments, the question of moment realizability was investigated in [14]. In the quantum setting, physical situations involving minimization of the free energy have already been widely addressed in the literature, particularly for the study of the stability of matter, see for instance [16, 10, 11] and the references therein. While the latter models involve *global* constraints, for instance the total number of particles in the system, the moment problem we consider here involves *local* constraints. In other words, focusing on the first moment only, i.e. the density $n(x)$, we fix the local value of the density at a physical point x rather than the total number of particles. This has several consequences. First of all, the minimization problem, in particular the characterization of the minimizer, becomes considerably more difficult in that the Lagrange parameters associated to the constraints are not constant functions any longer as in the case of global constraints but functions of the position. Devising an appropriate equation for such Lagrange parameters and characterizing their regularity is a delicate task that has found partial answers in a one-dimensional setting only, see [17]. The question of the characterization for the multi-dimensional case is an open problem. The second consequence is that when prescribing local constraints, which are therefore stronger than global constraints, some additional information is added into the minimization problem. As we will see below, this allows us to show that, in some configurations, the free energy admits minimizers under local constraints, while it does not under global constraints (the free energy is not bounded from below in such a case while it is for local constraints, see [11, 16]). The problem we have in mind is the minimization of a quantum free energy involving a Von Neumann entropy term (or also called Boltzmann entropy) of the form $\mathrm{Tr}(\varrho \log \varrho)$ for a density operator ϱ. The consequence of Theorems 2.1 and 4.3 proved in this article is the proper definition of the *quantum Maxwellian* used in [3, 4, 7, 12].

The results we present in this paper generalize that of [17] in various aspects: not only we treat multi-dimensional problems, while [17] addresses the one-dimensional case only, but we also extend our previous results to unbounded domains. Besides, the theory of Degond and Ringhofer essentially considers the three first moments, namely the density, the current and the energy. We are able to treat the density and current constraints only and this is a consequence of the compactness method we are using for the proofs. There is enough compactness to tackle the first two constraints, but not enough for the last one, the energy. Moreover, non-linear systems as Hartree or Hartree-Fock systems are also considered. Our results concern the *existence* (and uniqueness) of minimizers, and not their *characterization*. As previously mentioned, the analysis of the Lagrange parameters is difficult and so far only a one-dimensional theory is available, see [17].

The paper is structured as follows: in section 2, we introduce the mathematical framework and state our main result in Theorem 2.1. For the sake of clarity of the exposition, we present here the most significant result, leaving the most general cases as extensions. Theorem 2.1 provides existence and uniqueness of minimizers in $\mathbb{R}^d$, $d \geq 1$, for the quantum free energy with Boltzmann (or Fermi-Dirac) entropy under a local constraint of density. The proof of the theorem is carried out in section 3. The extensions of Theorem 2.1 are presented in section 4: we treat more general entropies, bounded domains, non-linear interactions as Hartree/Hartree-Fock and finally the second order constraint.

2. **Setting of the problem and main result**

As described in the introduction, for a given temperature $T > 0$, we will consider the problem of minimizing a free energy functional defined on density matrices by

$$F(\varrho) = E(\varrho) + TS(\varrho)$$

under the constraint that the density of charge n_ϱ associated to ϱ is a given function $n(x)$. Before stating our main theorem, we successively define the functional framework for density matrices, the energy functional $E(\varrho)$ and the entropy functional $S(\varrho)$.

Let us define the following space of operators on $L^2(\mathbb{R}^d)$, $d \in \mathbb{N}$:

$$\mathcal{E} = \left\{ \varrho \in \mathcal{J}_1,\ \varrho = \varrho^* \text{ and } \sqrt{-\Delta}|\varrho|\sqrt{-\Delta} \in \mathcal{J}_1 \right\},$$

where $\mathcal{J}_1$ denotes the space of trace-class operators. This space $\mathcal{E}$ is a Banach space endowed with the norm

$$\|\varrho\|_{\mathcal{E}} = \operatorname{Tr}|\varrho| + \operatorname{Tr}(\sqrt{-\Delta}|\varrho|\sqrt{-\Delta}).$$

The energy space will be the following closed convex subspace of $\mathcal{E}$:

$$\mathcal{E}_+ = \{\varrho \in \mathcal{E} :\ 0 \leq \varrho \leq 1\}.$$

Consider now a density matrix $\varrho \in \mathcal{E}_+$, with the spectral decomposition

$$\varrho = \sum_{i \in \mathbb{N}^*} \lambda_i \left|\psi_i\right\rangle \left\langle\psi_i\right|,$$

the density of charge n_ϱ associated to ϱ is defined by

$$n_\varrho = \sum_{i \in \mathbb{N}^*} \lambda_i |\psi_i|^2. \tag{2.1}$$

It can also be characterized by the weak formulation

$$\int_{\mathbb{R}^d} n_\varrho\, \phi\, dx = \operatorname{Tr}(\varrho\phi), \qquad \forall \phi \in L^\infty(\mathbb{R}^d), \tag{2.2}$$

where, in the right-hand side, ϕ means the operator of multiplication by ϕ.

The kinetic energy of a density matrix reads

$$E(\varrho) = \operatorname{Tr}(\sqrt{-\Delta}\varrho\sqrt{-\Delta}) = \sum_{i \in \mathbb{N}^*} \lambda_i \|\nabla\psi_i\|_{L^2}^2 \tag{2.3}$$

and its entropy is defined by

$$S(\varrho) = \operatorname{Tr}\left(\beta(\varrho)\right), \tag{2.4}$$

where β is either the Boltzmann entropy $\beta(\varrho) = \varrho \log \varrho$ or the Fermi-Dirac entropy $\beta(\varrho) = \varrho \log \varrho + (1-\varrho)\log(1-\varrho)$; we will set

$$\beta(\varrho) = \varrho \log \varrho + \varepsilon(1-\varrho)\log(1-\varrho), \qquad \text{with } \varepsilon \in \{0, 1\}. \tag{2.5}$$

More general models will be treated as extensions in Section 4, where non linear energies as well as other entropies are considered.

Let us now discuss our assumptions on the given density $n(x) \geq 0$. Since $\operatorname{Tr}\varrho = \int n_\varrho(x)dx$, in order to deal with density matrices of trace one, we will assume that $\int n(x)dx = 1$. Moreover, from the definitions (2.1) and (2.3), and using the Cauchy-Schwarz inequality, one obtains

$$\|\nabla\sqrt{n_\varrho}\|_{L^2}^2 \leq E(\varrho).$$

We will thus also assume that $\sqrt{n}$ belongs to $H^1(\mathbb{R}^d)$. Nevertheless, these assumptions on n are still not sufficient. Indeed, there exist density matrices of finite energy $\varrho \in \mathcal{E}_+$ with entropy $S(\varrho)$ equal to $-\infty$. Hence, without additional assumption on the density n, our constrained minimization problem may be ill-posed. To avoid this problem, it will be sufficient to assume that $n \log n$ belongs to $L^1(\mathbb{R}^d)$. Indeed, the following crucial inequality is proved in [10]:

$$E(\varrho) + \sum_{i \in \mathbb{N}^*} \lambda_i \log \lambda_i \geq \int_{\mathbb{R}^d} n_\varrho(x) \log n_\varrho(x) dx + \frac{d}{2}\log(4\pi) \int_{\mathbb{R}^d} n_\varrho(x) dx. \tag{2.6}$$

This inequality, which can be seen as a logarithmic Sobolev inequality for systems, ensures that $S(\varrho) = \sum_{i\in\mathbb{N}^*} \beta(\lambda_i)$ is bounded from below as soon as $n_\rho \log n_\varrho$ belongs to L^1 (note that, as $\lambda \to 0$, we have $\beta(\lambda) \sim \lambda \log \lambda$).

Our main result is the following theorem.

Theorem 2.1. *Consider a density $n(x) \geq 0$ defined a.e. on $\mathbb{R}^d$ such that*

$$\int_{\mathbb{R}^d} n(x)dx = 1, \qquad n \log n \in L^1(\mathbb{R}^d), \qquad \sqrt{n} \in H^1(\mathbb{R}^d). \tag{2.7}$$

Then the following minimization problem with constraint:

$$\min F(\varrho) \text{ for } \varrho \in \mathcal{E}_+ \text{ such that } n_\varrho = n \tag{2.8}$$

where

$$F(\varrho) = E(\varrho) + TS(\varrho), \qquad T > 0, \tag{2.9}$$

E, S being defined by (2.3), (2.4), (2.5), *is attained for a unique density operator.*

Theorem 2.1 is extended in section 4 to more general frameworks: other types of entropies (like $\mathcal{C}^1$), bounded domains, non-linear interactions and the current density constraint. Let us point out that the hypothesis that $n \log n \in L^1(\mathbb{R}^d)$ is crucial for the theorem. Indeed, when the constraint is global, i.e. when only $\int ndx$ is prescribed, the problem is known to be ill-posed in the sense that the functional does not admit any minimizer since it is not bounded from below [16]. It is the fact that n is prescribed locally that allows us to assume that $n \log n \in L^1(\mathbb{R}^d)$ and then to bound the free energy from below and prove the existence of minimizers.

The proof essentially relies on compactness arguments. The main difference with the method of [17] is the fact that since the problem is now posed on an unbounded domain, the Laplacian $-\Delta$ does not have a compact resolvent anymore. This compactness property of the resolvent was extensively used in [17] to prove for instance the continuity of the entropy term. Here, the absence of compactness is compensated by the fact that we prescribe $n \log n \in L^1(\mathbb{R}^d)$, and together with the logarithmic Sobolev inequality proved in (2.6) coupled to a Jensen inequality from [2], this allows us to obtain that the entropy is continuous.

3. **Compactness of minimizing sequences**

This section is devoted to the proof of our main Theorem 2.1. We denote

$$\mathcal{A} = \{\varrho \in \mathcal{E}_+ \text{ such that } n_\varrho = n\}.$$

Step 1: $\mathcal{A}$ is not empty. Consider the L^2 projector on $\sqrt{n}$ defined by

$$\sigma = \left|\sqrt{n}\right\rangle \left\langle\sqrt{n}\right|.$$

We have

$$n_\sigma = n, \quad E(\sigma) = \left\|\nabla\sqrt{n}\right\|^2_{L^2} < +\infty,$$

thus $\sigma \in \mathcal{A}$. This proves that the set $\mathcal{A}$ is not empty.

Step 2: the free energy F is bounded from below on $\mathcal{A}$. The following inequality is proved in [10] after an optimization of the logarithmic Sobolev inequality (2.6) under a scaling preserving the L^2 norm: for all ϱ, we have

$$\int_{\mathbb{R}^d} n_\varrho \log n_\varrho dx \leq \sum_{i\in\mathbb{N}^*} \lambda_i \log \lambda_i + \frac{d}{2} \log\left(\frac{e}{2\pi d} \frac{E(\varrho)}{\mathrm{Tr}(\varrho)} \right) \mathrm{Tr}(\varrho), \tag{3.1}$$

where $(\lambda_i)_{i\in\mathbb{N}^*}$ denotes the nonincreasing sequence of eigenvalues of ϱ. Therefore, since by assumption we have $n \log n \in L^1$ and $\int n(x)dx = 1$, we deduce that, for all $\varrho \in \mathcal{A}$, we have

$$\sum_{i\in\mathbb{N}^*} \lambda_i \log \lambda_i \geq -C(n) - \frac{d}{2} \log\left(E(\varrho)\right), \tag{3.2}$$

where the constant $C(n) \geq 0$ only depends on n.

Let us bound the second part of the entropy in the case $\varepsilon = 1$ in (2.5): the term $\sum_{i\in\mathbb{N}^*}(1-\lambda_i)\log(1-\lambda_i)$. For all $\lambda \in (0,1]$, one has

$$-\lambda \leq (1-\lambda)\log(1-\lambda) \leq 0,$$

thus

$$\sum_{i\in\mathbb{N}^*}(1-\lambda_i)\log(1-\lambda_i) \geq -\mathrm{Tr}(\varrho). \tag{3.3}$$

Hence, from (3.2) and (3.3), one deduces that for all $\varrho \in \mathcal{A}$, we have

$$\begin{aligned} F(\varrho) &= E(\varrho) + TS(\varrho) \geq E(\varrho) - TC(n) - \frac{dT}{2} \log\left(E(\varrho)\right) - \varepsilon T \\ &\geq \min_{e\in\mathbb{R}_+^*} \left(e - TC(n) - \frac{dT}{2} \log\left(e\right) - \varepsilon T \right) =: -C'(n). \end{aligned} \tag{3.4}$$

The free energy is thus bounded from below on $\mathcal{A}$.

From Step 1 and Step 2, the infimum of F on $\mathcal{A}$ is well-defined and is not $-\infty$. From now on, we consider a minimizing sequence $(\varrho_k)_{k\in\mathbb{N}}$, i.e. a sequence satisfying $\varrho_k \in \mathcal{A}$ and

$$\lim_{k\to+\infty} F(\varrho_k) = \inf_{\varrho\in\mathcal{A}} F(\varrho). \tag{3.5}$$

Step 3: uniform bound and first convergence result. Let us prove that the minimizing sequence $(\varrho_k)_{k\in\mathbb{N}}$ is bounded in $\mathcal{E}$. Since $\varrho_k \in \mathcal{A}$, we already have

$$\|\varrho_k\|_{\mathcal{J}_1} = \mathrm{Tr}(\varrho_k) = \int_{\mathbb{R}^d} n(x)dx < +\infty.$$

Moreover, from (3.5), we have

$$\sup_{k\in\mathbb{N}^*} F(\varrho_k) < +\infty.$$

Hence, the inequality (3.4) yields

$$\sup_{k\in\mathbb{N}^*} E(\varrho_k) < +\infty.$$

We have then

$$\sup_{k\in\mathbb{N}^*} \|\varrho_k\|_{\mathcal{E}} < +\infty.$$

Since $(\varrho_k)_{k\in\mathbb{N}}$ is a bounded sequence of $\mathcal{E}$, and following for instance the arguments of [17], there exists $\varrho \in \mathcal{E}_+$ such that, up to an extraction of a subsequence, ϱ_k and $(1-\Delta)^{1/2}\varrho_k(1-\Delta)^{1/2}$ converge in the $\mathcal{J}_1$ weak-$*$ topology respectively to ϱ and

$(1-\Delta)^{1/2}\varrho(1-\Delta)^{1/2}$ as $k\to+\infty$. This means that, for all compact operator K on $L^2(\mathbb{R}^d)$ we have

$$\mathrm{Tr}(K\varrho_k)\to\mathrm{Tr}(K\varrho),\quad \mathrm{Tr}(K(1-\Delta)^{1/2}\varrho_k(1-\Delta)^{1/2})\to\mathrm{Tr}(K(1-\Delta)^{1/2}\varrho(1-\Delta)^{1/2}) \tag{3.6}$$

as $k\to+\infty$. Moreover, we have

$$\mathrm{Tr}(1-\Delta)^{1/2}\varrho(1-\Delta)^{1/2})\le\liminf_{k\to+\infty}\mathrm{Tr}((1-\Delta)^{1/2}\varrho_k(1-\Delta)^{1/2}). \tag{3.7}$$

Step 4: ϱ satisfies the constraint. Let us prove the convergence of ϱ_k in the weak $\mathcal{J}_1$ topology, i.e. that for all bounded operator $\sigma\in\mathcal{L}(L^2(\mathbb{R}^d))$,

$$\mathrm{Tr}(\sigma\varrho_k)\to\mathrm{Tr}(\sigma\varrho)\text{ as }k\to+\infty. \tag{3.8}$$

To show that no loss of mass occurs at the infinity, we will use in a crucial way the fact that the density of ϱ_k is a fixed L^1 function $n(x)$.

Let us introduce a truncation function χ with values in $[0,1]$, such that $\chi\equiv 1$ on the centered ball of radius 1 and $\chi\equiv 0$ outside the centered ball or radius 2. We denote $\chi_R(x)=\chi(x/R)$. Identifying the function χ_R and the operator of multiplication by χ_R, we write

$$\begin{aligned}\mathrm{Tr}(\sigma\varrho_k) &= \mathrm{Tr}(\sigma\chi_R\varrho_k)+\mathrm{Tr}(\sigma(1-\chi_R)\varrho_k)\\ &= \mathrm{Tr}((1-\Delta)^{-1/2}\sigma\chi_R(1-\Delta)^{-1/2}(1-\Delta)^{1/2}\varrho_k(1-\Delta)^{1/2})\\ &\quad+\mathrm{Tr}(\sigma(1-\chi_R)\varrho_k)\end{aligned} \tag{3.9}$$

From Sobolev embeddings on compact domains, one deduces that, for all $R>0$, the operator $\chi_R(1-\Delta)^{-1/2}$ is compact on $L^2(\mathbb{R}^d)$. Moreover, the operators $(1-\Delta)^{-1/2}$ and σ are bounded. Hence, by composition, the operator $K=(1-\Delta)^{-1/2}\sigma\chi_R(1-\Delta)^{-1/2}$ is compact and (3.6) yields, for all $R>0$,

$$\begin{aligned}&\lim_{k\to+\infty}\mathrm{Tr}((1-\Delta)^{-1/2}\sigma\chi_R(1-\Delta)^{-1/2}(1-\Delta)^{1/2}\varrho_k(1-\Delta)^{1/2})=\\ &\qquad=\mathrm{Tr}((1-\Delta)^{-1/2}\sigma\chi_R(1-\Delta)^{-1/2}(1-\Delta)^{1/2}\varrho(1-\Delta)^{1/2})=\mathrm{Tr}(\sigma\chi_R\varrho).\end{aligned} \tag{3.10}$$

Consider now the last term in (3.9) and let us show that no mass can be lost at the infinity. Denote by $\underline{\sigma}(x,y)$ the integral kernel of σ and by $(\lambda_{k,i},\psi_{k,i})_{i\in\mathbb{N}^*}$ the spectral elements of ϱ_k. Notice that $\underline{\sigma}\in L^2(\mathbb{R}^3\times\mathbb{R}^3)$. By using Cauchy-Schwarz inequalities, we get

$$\begin{aligned}\mathrm{Tr}(\sigma(1-\chi_R)\varrho_k) &= \sum_{i\in\mathbb{N}^*}\lambda_{k,i}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\underline{\sigma}(x,y)(1-\chi_R(y))\psi_{k,i}(y)\overline{\psi_{k,i}}(x)dxdy\\ &\le \sum_{i\in\mathbb{N}^*}\lambda_{k,i}\|\underline{\sigma}\|_{L^2}\|(1-\chi_R)\psi_{k,i}\|_{L^2}\|\psi_{k,i}\|_{L^2}\\ &\le \|\underline{\sigma}\|_{L^2}\left(\sum_{i\in\mathbb{N}^*}\lambda_{k,i}\right)^{1/2}\left(\sum_{i\in\mathbb{N}^*}\lambda_{k,i}\int_{\mathbb{R}^3}(1-\chi_R(x))|\psi_{k,i}(x)|^2dx\right)^{1/2}\\ &= \|\underline{\sigma}\|_{L^2}\left(\int_{\mathbb{R}^3}(1-\chi_R(x))n(x)dx\right)^{1/2}\end{aligned}$$

where we used that $\varrho_k\in\mathcal{A}$, i.e. that $\mathrm{Tr}(\varrho_k)=1$ and that $n_\varrho=n$. From this last estimate and by dominated convergence, since n belongs to L^1, one deduces that

$$\lim_{R\to+\infty}\sup_{k\in\mathbb{N}}\mathrm{Tr}(\sigma(1-\chi_R)\varrho_k)=0. \tag{3.11}$$

Finally, (3.9), (3.10) and (3.11) yield (3.8). This implies in particular that $n_\varrho = n$. To see this fact, use the characterization (2.2) of n_ϱ and choose σ as the multiplication operator by the function ϕ in (3.8). This means that ϱ belongs to $\mathcal{A}$.

Step 5: strong convergence of ϱ_k. From the previous step, we know that ϱ_k converges to ϱ weakly in $\mathcal{J}_1$, which implies the weak operator convergence. Moreover, since these operators are positive, we have the convergence of the norms:

$$\|\varrho_k\|_{\mathcal{J}_1} = \mathrm{Tr}(\varrho_k) = 1 = \mathrm{Tr}(\varrho) = \|\varrho\|_{\mathcal{J}_1}.$$

Hence, the following lemma from [19] shows that the convergence holds in the strong $\mathcal{J}_1$ topology:

$$\lim_{k\to+\infty} \|\varrho_k - \varrho\|_{\mathcal{J}_1} = 0. \tag{3.12}$$

Lemma 3.1 (Theorem 2.21 and addendum H of [19])**.** *Suppose that $A_k \to A$ weakly in the sense of operators and that $\|A_k\|_{\mathcal{J}_1} \to \|A\|_{\mathcal{J}_1}$. Then $\|A_k - A\|_{\mathcal{J}_1} \to 0$.*

We will now prove the convergence of the entropy:

$$\mathrm{Tr}(\beta(\varrho)) = \lim_{k\to+\infty} \mathrm{Tr}(\beta(\varrho_k)). \tag{3.13}$$

Note that this result cannot be simply deduced by weak convergence and semicontinuity, since β is negative. Let us decompose the entropy into the sum of a singular and a regular (near 0) part:

$$\beta = \beta_s + \beta_r \quad \text{with} \quad \beta_s(\lambda) = \lambda\log\lambda - \lambda, \quad \beta_r(\lambda) = \lambda + \varepsilon(1-\lambda)\log(1-\lambda).$$

From the $\mathcal{J}_1$ convergence of ϱ_k, it is easy to prove the convergence of the regular part:

$$\mathrm{Tr}(\beta_r(\varrho)) = \lim_{k\to+\infty} \mathrm{Tr}(\beta_r(\varrho_k)), \tag{3.14}$$

by combining two facts. First, the convergence of ϱ_k to ϱ in the $\mathcal{J}_1$ norm implies the convergence of the eigenvalues, see Lemma A.2 in [17]: if we denote by $(\lambda_{k,i}, \psi_{k,i})_{i\in\mathbb{N}^*}$ the nonincreasing sequence of eigenvalues and the associated eigenfunctions of ϱ_k, and by $(\lambda_i, \psi_i)_{i\in\mathbb{N}^*}$ the (nonincreasing) eigenvalues and eigenfunctions of ϱ, we have

$$\forall i \in \mathbb{N}^*, \qquad \lambda_{k,i} \to \lambda_i. \tag{3.15}$$

Since the function β_r is continuous, this implies that

$$\forall N \in \mathbb{N}^*, \quad \lim_{k\to+\infty} \sum_{i<N} |\beta_r(\lambda_{k,i}) - \beta_r(\lambda_i)| = 0. \tag{3.16}$$

Second, we have the bound

$$|\beta_r(\lambda)| \le C|\lambda|. \tag{3.17}$$

From (3.15) and from $\sum_{i\in\mathbb{N}^*} \lambda_{k,i} = \sum_{i\in\mathbb{N}^*} \lambda_i = 1$, one deduces that

$$\lim_{N\to+\infty} \sup_{k\in\mathbb{N}^*} \sum_{i\ge N} \lambda_{k,i} = 0 \quad \text{and} \quad \lim_{N\to+\infty} \sum_{i\ge N} \lambda_i = 0,$$

which implies, by (3.17), that

$$\lim_{N\to+\infty} \sup_{k\in\mathbb{N}^*} \sum_{i\ge N} |\beta_r(\lambda_{k,i})| = 0 \quad \text{and} \quad \lim_{N\to+\infty} \sum_{i\ge N} |\beta_r(\lambda_i)| = 0. \tag{3.18}$$

By combining (3.16) and (3.18), one gets (3.14).

Step 6: convergence of the entropy, part 1. In the next two steps, we prove the convergence of the singular part:

$$\mathrm{Tr}(\beta_s(\varrho)) = \lim_{k\to+\infty} \mathrm{Tr}(\beta_s(\varrho_k)) \tag{3.19}$$

where we recall that $\beta_s(\lambda) = \lambda\log\lambda - \lambda$. We shall use a truncation method inspired from [11]. Let us introduce two truncation functions χ and ξ with values in $[0,1]$, such that $\chi^2+\xi^2 = 1$, $\chi \equiv 1$ on the centered ball of radius 1 and $\chi \equiv 0$ outside the centered ball or radius 2. We denote $\chi_R(x) = \chi(x/R)$ and $\xi_R(x) = \xi(x/R)$ for $R \geq 1$. We will use the following "Jensen inequality for traces", taken from [2]:

Lemma 3.2 ([2])**.** *Let β be a continuous and convex function defined on $[0,1]$ with $\beta(0) = 0$. Let $\varrho \in \mathcal{E}_+$ and let X be a self-adjoint operator on $L^2(\mathbb{R}^d)$ such that $X^2 \leq 1$. Then we have*

$$\mathrm{Tr}(\beta(X\varrho X)) \leq \mathrm{Tr}(X\beta(\varrho)X).$$

Applying this lemma yields

$$\mathrm{Tr}(\beta_s(\chi_R\,\varrho_k\,\chi_R)) + \mathrm{Tr}(\beta_s(\xi_R\,\varrho_k\,\xi_R)) \leq \mathrm{Tr}(\beta_s(\varrho_k)). \tag{3.20}$$

We will pass to the limit separately in the two terms of the left-hand side. For clarity, we divide the proof of (3.13) into two steps. In this step, we treat the term $\mathrm{Tr}(\beta_s(\chi_R\,\varrho_k\,\chi_R))$, R being fixed. In Step 7 we treat the other term $\mathrm{Tr}(\beta_s(\xi_R\,\varrho_k\,\xi_R))$ and we conclude.

Denote $\widetilde{\varrho}_k = \chi_R\,\varrho_k\,\chi_R$ and $\widetilde{\varrho} = \chi_R\,\varrho\,\chi_R$. For all $\eta > 0$, we decompose

$$\beta_s(\lambda) = \beta_s^0(\lambda) + \beta_s^1(\lambda) = (\beta_s \circ \mathbb{1}_{\lambda>\eta})(\lambda) + (\beta_s \circ \mathbb{1}_{\lambda\leq\eta})(\lambda). \tag{3.21}$$

and denote respectively by $(\widetilde{\lambda}_{k,i})_{i\in\mathbb{N}^*}$ and $(\widetilde{\lambda}_i)_{i\in\mathbb{N}^*}$ the nonincreasing sequences of eigenvalues of $\widetilde{\varrho}_k$ and $\widetilde{\varrho}$. Since the operator of multiplication by χ_R is bounded on $L^2(\mathbb{R}^d)$, the strong $\mathcal{J}_1$ convergence (3.12) proved in Step 5 implies that

$$\|\widetilde{\varrho}_k - \widetilde{\varrho}\|_{\mathcal{J}_1} = \|\chi_R(\varrho_k - \varrho)\chi_R\|_{\mathcal{J}_1} \to 0 \quad \text{as } k \to +\infty. \tag{3.22}$$

As seen above, the convergence in $\mathcal{J}_1$ implies the convergence of eigenvalues, thus

$$\forall i \in \mathbb{N}^*, \quad \lim_{k\to+\infty} \widetilde{\lambda}_{k,i} = \widetilde{\lambda}_i. \tag{3.23}$$

Hence, for all $\eta > 0$, we have

$$\mathrm{Tr}(\beta_s^0(\widetilde{\varrho}_k)) = \sum_{\widetilde{\lambda}_{k,i}>\eta} \beta_s(\widetilde{\lambda}_{k,i}) \to \sum_{\widetilde{\lambda}_i>\eta} \beta_s(\widetilde{\lambda}_i) = \mathrm{Tr}(\beta_s^0(\widetilde{\varrho})), \tag{3.24}$$

as $k \to +\infty$, both sums being finite.

We now claim that, for all R,

$$\lim_{\eta\to 0}\sup_{k\in\mathbb{N}^*} |\mathrm{Tr}(\beta_s^1(\widetilde{\varrho}_k))| = 0 \quad \text{and} \quad \lim_{\eta\to 0} |\mathrm{Tr}(\beta_s^1(\widetilde{\varrho}))| = 0. \tag{3.25}$$

Assuming this claim, from (3.21) and (3.24), one deduces that, for all R,

$$\lim_{k\to+\infty} \mathrm{Tr}(\beta_s(\chi_R\,\varrho_k\,\chi_R)) = \mathrm{Tr}(\beta_s(\chi_R\,\varrho\,\chi_R)). \tag{3.26}$$

Let us now prove the claim (3.25). We first remark that

$$\mathrm{Tr}(\sqrt{-\Delta}\widetilde{\varrho}_k\sqrt{-\Delta}) = \sum_{i\in\mathbb{N}^*} \lambda_{k,i}\|\nabla(\chi_R\psi_{k,i})\|_{L^2}^2 \leq C\left(\mathrm{Tr}(\varrho_k) + E(\varrho_k)\right) \leq C', \tag{3.27}$$

where C' is independent of k and R. Similarly, denoting by $(\lambda_i, \psi_i)_{i\in\mathbb{N}^*}$ the eigenvalues and eigenfunctions of ϱ, we have

$$\operatorname{Tr}(\sqrt{-\Delta}\widetilde{\varrho}\sqrt{-\Delta}) = \sum_{i\in\mathbb{N}^*} \lambda_i \|\nabla(\chi_R\psi_i)\|^2_{L^2} \leq C\left(\operatorname{Tr}(\varrho) + E(\varrho)\right) < +\infty. \tag{3.28}$$

Moreover, we remark that

$$n_{\widetilde{\varrho}_k} = (\chi_R)^2 n, \quad n_{\widetilde{\varrho}} = (\chi_R)^2 n. \tag{3.29}$$

Indeed, for all $\phi \in L^\infty(\mathbb{R}^d)$, we have

$$\begin{aligned} \int_{\mathbb{R}^d} n_{\widetilde{\varrho}_k}(x)\phi(x)dx &= \operatorname{Tr}\left(\chi_R\,\varrho_k\,\chi_R\,\phi\right) = \operatorname{Tr}\left(\varrho_k\,\chi_R\,\phi\,\chi_R\right) \\ &= \int_{\mathbb{R}^d} n_{\varrho_k}(x)\phi(x)(\chi_R(x))^2dx = \int_{\mathbb{R}^d} n(x)\phi(x)(\chi_R(x))^2dx, \end{aligned}$$

and similarly for $\widetilde{\varrho}$, which yields (3.29).

From (3.28) and (3.29), one deduces that $\widetilde{\varrho} \in \mathcal{E}_+$ and that $n_{\widetilde{\varrho}} \log n_{\widetilde{\varrho}}$ belongs to L^1. By the logarithmic Sobolev inequality (2.6), this implies that $|\operatorname{Tr}\beta_s(\widetilde{\varrho}))| < \infty$: the second part of the claim (3.25) is proved.

Let us now prove the first part of this claim, by comparing the spectrum of the operator $\widetilde{\varrho}_k$ with the one of the harmonic oscillator $H_{ho} = -\Delta + |x|^2$. Recall that the i-th eigenvalue μ_i of H_{ho} (counted with multiplicities) satisfies $\mu_i \sim Ci^{1/d}$. We will use the following classical lemma proved e.g. in [17]:

Lemma 3.3. *Let $\varrho \in \mathcal{E}_+$ and denote by $(\lambda_i)_{i\geq 1}$ the nonincreasing sequence of nonzero eigenvalues of ϱ. Let $(\mu_i)_{i\geq 1}$ be the nondecreasing sequence of eigenvalues of the quantum harmonic oscillator H_{ho}. Then we have*

$$\operatorname{Tr}(\sqrt{-\Delta}\rho\sqrt{-\Delta}) + \int_{\mathbb{R}^3} |x|^2 n_\varrho(x)dx \geq \sum_{i\geq 1} \lambda_i\,\mu_i. \tag{3.30}$$

By (3.29), we have

$$\int_{\mathbb{R}^3} |x|^2 n_{\widetilde{\varrho}_k}(x)dx \leq \int_{|x|\leq 2R} |x|^2 n(x)dx \leq (2R)^2, \tag{3.31}$$

since $\int n(x)dx = 1$. Therefore, one deduces from (3.30), (3.27) and (3.31) the estimate

$$\sum_{i\geq 1} \widetilde{\lambda_{k,i}}\,\mu_i \leq C(R), \tag{3.32}$$

where $(\widetilde{\lambda_{k,i}})_{i\in\mathbb{N}^*}$ denote the eigenvalues of $\widetilde{\varrho}_k$ and $C(R)$ is a constant depending on R but not on k. Let us now introduce the constant

$$C_d := \sup_{\lambda\in(0,1]} \left(|\beta_s(\lambda)|\lambda^{-\frac{1+4d}{2+4d}} \right) < +\infty,$$

where we used that $\beta_s(\lambda) \sim \lambda\log\lambda$ near 0. We estimate:

$$\begin{aligned} \left|\operatorname{Tr}(\beta_s^1(\widetilde{\varrho}_k))\right| &= \sum_{\widetilde{\lambda_{k,i}}\leq\eta} |\beta_s(\widetilde{\lambda_{k,i}})| \leq C_d \sum_{\widetilde{\lambda_{k,i}}\leq\eta} \widetilde{\lambda_{k,i}}^{\frac{1+4d}{2+4d}} \leq C_d\,\eta^{\frac{1}{2+4d}} \sum_{i\in\mathbb{N}^*} \widetilde{\lambda_{k,i}}^{\frac{2d}{1+2d}} \\ &\leq C_d\,\eta^{\frac{1}{2+4d}} \left(\sum_{i\in\mathbb{N}^*} \widetilde{\lambda_{k,i}}\,\mu_i \right)^{\frac{2d}{1+2d}} \left(\sum_{i\in\mathbb{N}^*} \mu_i^{-2d} \right)^{\frac{1}{1+2d}} \end{aligned}$$

where we used a Hölder inequality. Since $\mu_i \sim C i^{1/d}$, the series $\sum_i \mu_i^{-2d}$ converges. By (3.32), this gives

$$\sup_{k\in\mathbb{N}^*} \left|\mathrm{Tr}(\beta_s^1(\widetilde{\varrho}_k))\right| \leq C'(R)\, \eta^{\frac{1}{2+4d}}$$

and the claim (3.25) is proved.

Step 7: convergence of the entropy, part 2. We now consider the second term $\mathrm{Tr}(\beta_s(\xi_R\, \varrho_k\, \xi_R))$ in (3.20). Let $\widehat{\varrho}_k = \xi_R\, \varrho_k\, \xi_R$ and $\widehat{\varrho} = \xi_R\, \varrho\, \xi_R$. Similarly as (3.27) and (3.28), we have

$$\mathrm{Tr}(\sqrt{-\Delta}\widehat{\varrho}_k\sqrt{-\Delta}) = \sum_{i\in\mathbb{N}^*} \lambda_{k,i}\|\nabla(\xi_R\psi_{k,i})\|_{L^2}^2 \leq C\left(\mathrm{Tr}(\varrho_k) + E(\varrho_k)\right) \leq C \tag{3.33}$$

$$\mathrm{Tr}(\sqrt{-\Delta}\widehat{\varrho}\sqrt{-\Delta}) = \sum_{i\in\mathbb{N}^*} \lambda_i\|\nabla(\xi_R\psi_i)\|_{L^2}^2 \leq C\left(\mathrm{Tr}(\varrho) + E(\varrho)\right) < +\infty, \tag{3.34}$$

and, similarly as (3.29), one has

$$n_{\widehat{\varrho}_k} = (\xi_R)^2 n \quad \text{and} \quad n_{\widehat{\varrho}} = (\xi_R)^2 n. \tag{3.35}$$

Therefore, from (3.33), (3.34), (3.35) and the optimized logarithmic Sobolev inequality (3.1), one gets

$$2\int_{\mathbb{R}^d} (\xi_R)^2 n \log\left((\xi_R)^2 n\right) dx - C\int_{\mathbb{R}^d} (\xi_R)^2 n dx \leq \mathrm{Tr}(\beta_s(\widehat{\varrho}_k)) + \mathrm{Tr}(\beta_s(\widehat{\varrho})) \leq 0$$

(for the right inequality, recall simply that the eigenvalues of $\widehat{\varrho}_k$ and $\widehat{\varrho}$ belong to $[0,1]$). Thus, since the left-hand side is independent of k, one deduces from $n \in L^1$, $n\log n \in L^1$, from the definition of ξ_R and from dominated convergence that

$$\lim_{R\to+\infty} \sup_{k\in\mathbb{N}^*} \mathrm{Tr}(\beta_s(\xi_R\, \varrho_k\, \xi_R)) = 0 \quad \text{and} \quad \lim_{R\to+\infty} \mathrm{Tr}(\beta_s(\xi_R\, \varrho\, \xi_R)) = 0. \tag{3.36}$$

The last ingredient of the proof of (3.19) is the following result taken from [2]:

Lemma 3.4 ([2], Lemmas 3 and 4)**.** *Let f be a continuous and decreasing function on $[0,1]$ with $f(0) = 0$. Let $\varrho \in \mathcal{E}_+$ and let X be a self-adjoint operator on $L^2(\mathbb{R}^d)$ such that $X^2 \leq 1$. Then we have*

$$\mathrm{Tr}(f(\varrho)) \leq \mathrm{Tr}(Xf(\varrho)X).$$

We use this lemma with the functions $f(\lambda) := \beta_s(\lambda) = \lambda\log\lambda - \lambda$, with the density matrices $\varrho_k \in \mathcal{E}_+$ or $\varrho \in \mathcal{E}_+$ and with $X = \chi_R$. Recalling (3.20) (and the similar inequality for ϱ), one gets

$$\mathrm{Tr}(\beta_s(\varrho_k)) \leq \mathrm{Tr}(\beta_s(\chi_R\, \varrho_k\, \chi_R)) \leq \mathrm{Tr}(\beta_s(\varrho_k)) - \mathrm{Tr}(\beta_s(\xi_R\, \varrho_k\, \xi_R)), \tag{3.37}$$

and

$$\mathrm{Tr}(\beta_s(\varrho)) \leq \mathrm{Tr}(\beta_s(\chi_R\, \varrho\, \chi_R)) \leq \mathrm{Tr}(\beta_s(\varrho)) - \mathrm{Tr}(\beta_s(\xi_R\, \varrho\, \xi_R)). \tag{3.38}$$

We have the tools to conclude: from (3.37), (3.38), (3.26) and (3.36), one deduces (3.19). Finally, (3.14) and (3.19) yield (3.13).

Step 8: conclusion. From (3.5), (3.7), (3.13) and $\mathrm{Tr}(\varrho_k) \to \mathrm{Tr}(\varrho)$, one deduces that $F(\varrho) \leq \inf_{\sigma\in\mathcal{A}} F(\sigma)$. Since we have proved in Step 4 that $\varrho \in \mathcal{A}$, this shows that the infimum is realized:

$$F(\varrho) = \min_{\sigma\in\mathcal{A}} F(\sigma).$$

To conclude the proof of the theorem, it remains to remark that the strict convexity of the function β implies that $\varrho \mapsto \mathrm{Tr}(\beta(\varrho))$ is strictly convex (see e.g. [17], Lemma 3.3). Hence the function F is also strictly convex and the minimizer ϱ is unique. The proof of Theorem 2.1 is complete. □

4. **Extensions**

In this section, we give various extensions to our Theorem 2.1.

4.1. **Other entropies.** We have chosen to work with the more interesting physical cases, the Boltzmann entropy or the Fermi-Dirac entropy, but one can deal with other entropies. If, instead of (2.5), we choose β as a strictly convex function, of class C^1 on $[0,1]$ and satisfying $\beta(0) = 0$, then one can prove that the minimization problem (2.8), with F, E and S defined by (2.9), (2.3) and (2.4), admits a unique minimizer under the following assumption on n:

$$\int_{\mathbb{R}^d} n(x)dx = 1, \qquad \sqrt{n} \in H^1(\mathbb{R}^d).$$

Note that we do not need here to assume that $n \log n \in L^1$. This case is in fact more regular than the one treated in Theorem 2.1. Indeed, the entropy is now continuous on the energy space, which was not true for β given by (2.5). In Step 5 of Section 3, we have in fact proved the following result:

Lemma 4.1. *If β is continuous on $[0,1]$ and if $|\beta(x)| \leq C|x|$, then the functional $\varrho \mapsto S(\varrho) = \mathrm{Tr}(\beta(\varrho))$ is continuous on $\mathcal{J}_1$.*

Thanks to this lemma, the proof of the result is significantly shorter than the one of Theorem 2.1, since one can skip Steps 6 and 7 and conclude directly after Step 5.

4.2. **Bounded domains.** Instead of the whole space $\mathbb{R}^d$, one can be interested in considering the problem on a smooth bounded domain Ω, with Dirichlet or Neumann boundary conditions. Let $H = -\Delta$ on $L^2(\Omega)$ equipped with the domain $D(H) = H^2(\Omega) \cap H^1_0(\Omega)$ if we choose Dirichlet boundary conditions, or $D(H) = H^2(\Omega)$ for the case of Neumann boundary conditions. The energy space is then defined as the following set of operators on $L^2(\Omega)$:

$$\mathcal{E}_+(\Omega) = \left\{ \varrho \in \mathcal{J}_1,\ \varrho = \varrho^*,\ 0 \leq \varrho \leq 1 \text{ and } \sqrt{H}\varrho\sqrt{H} \in \mathcal{J}_1 \right\}.$$

Then we consider the problem of minimization (2.8), with

$$E(\varrho) = \mathrm{Tr}\left(\sqrt{H}\varrho\sqrt{H}\right),$$

and $S(\varrho)$ still defined by (2.4), (2.5) (more regular entropies can of course be considered). It can be proved that this problem admits a unique minimizer under the assumption

$$\int_\Omega n(x)dx = 1, \qquad \sqrt{n} \in H^1_0(\Omega),$$

in the case of Dirichlet boundary conditions, or

$$\int_\Omega n(x)dx = 1, \qquad \sqrt{n} \in H^1(\Omega),$$

in the case of Neumann boundary conditions. Again, no assumption is required on the function $n \log n$. The reason for it is that one has the following lemma:

Lemma 4.2. *Let β be given by (2.5), then the functional $\varrho \mapsto S(\varrho) = \mathrm{Tr}(\beta(\varrho))$ is continuous on $\mathcal{E}_+(\Omega)$.*

This lemma is proved in the case of the dimension $d = 1$ in [17], but this proof can easily be extended, by an argument similar as the one that we used here in Step 6. The crucial point is that, for a density matrix in the energy space, one has (see Lemma 3.3):

$$\sum_{i\in\mathbb{N}^*} \lambda_i \, \mu_i < +\infty,$$

where $(\lambda_i)_{i\in\mathbb{N}^*}$ is the nonincreasing sequence of eigenvalues of ϱ and $(\mu_i)_{i\in\mathbb{N}^*}$ is the nondecreasing sequence of eigenvalues of H, which satisfies the Weyl asymptotics $\mu_i \leq C i^{2/d}$.

4.3. **Other interaction terms and non linear energies.** Instead of using the simple kinetic energy (2.3), one can take into account some additional terms in the energy of the density matrices, modeling interactions. In dimension $d = 3$ (for simplicity), consider the following energy for a density matrix, composed of four terms:

$$\widetilde{E}(\varrho) = \mathrm{Tr}(\sqrt{-\Delta}\varrho\sqrt{-\Delta}) + \int_{\mathbb{R}^3} V(x) n_\varrho(x)dx + W_H(\varrho) + W_{HF}. \tag{4.1}$$

The first term in (4.1) is $E(\varrho)$, the kinetic energy of the particles. The second term is the potential energy in a given external potential $V(x)$. We assume that $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, for instance $V(x) = \sum_{j=1}^m q_j |x - \overline{x_j}|^{-1}$ models the interaction with m fixed ions. The third and the fourth terms model some non linear interactions between particles. In order to take into account the most physical cases, we consider the Hartree energy

$$W_H(\varrho) = \alpha \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{n_\varrho(x)n_\varrho(y)}{|x-y|} dxdy,$$

and the Hartree-Fock exchange energy

$$W_{HF}(\varrho) = \beta \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{(\varrho(x,y))^2}{|x-y|} dxdy,$$

where α and $\beta < 0$ are real-valued parameters and where $\varrho(x, y)$ denotes the integral kernel of the operator ϱ.

Let us first make a simple remark. The linear term $\int V n_\varrho dx$ and the Hartree term W_H depend on ϱ only through its density n_ϱ: since this density is prescribed in our problem (2.8), these terms will be constant ! Hence, we only have to check that they are well-defined under our assumptions. It is immediate for the case of Hartree interaction only, namely when $\beta = 0$. Indeed, the fact that $\sqrt{n_\varrho} \in H^1(\mathbb{R}^3)$ implies by standard Sobolev embeddings that $n_\varrho \in L^1(\mathbb{R}^3) \cap L^3(\mathbb{R}^3) \subset L^{\frac{6}{5}}(\mathbb{R}^3)$ and the Hardy-Littlewood-Sobolev inequality [18] yields

$$|W_H| \leq C \|n_\varrho\|^2_{L^{\frac{6}{5}}}.$$

When $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, it is also clear that $\int V n_\varrho dx$ is finite from the previous regularity of n_ϱ.

When the Hartree-Fock exchange term is included, we set $\alpha = -\beta = 1$, without loss of generality. The result of Theorem 2.1 can be extended to such a case provided two facts are satisfied: W_{HF} must be well-defined and the non-linear term $W_H + W_{HF}$ must be lower semi-continuous. The first item follows from the Cauchy-Schwarz inequality and the simple observation that, almost everywhere on $\mathbb{R}^3 \times \mathbb{R}^3$,

$$(\varrho(x, y))^2 \leq n_\varrho(x) n_\varrho(y).$$

Recall indeed that $\varrho(x, y) = \sum_{i \in \mathbb{N}^*} \lambda_i \psi_i(x) \overline{\psi}_i(y)$, where $(\lambda_i, \psi_i)_{i \in \mathbb{N}^*}$ are the spectral elements of ϱ. This implies that $|W_{HF}|$ is controlled by W_H which is finite. The second item is proved in [11] and uses the Fatou lemma with the fact that $W_H + W_{HF}$ is non-negative.

4.4. **Constraint on the current density.** As already mentioned in the introduction, the theory of Degond and Ringhofer involves constraints on higher order moments of the density operator in addition to the density. These moments of interest are the current density and the energy density. We explain below how Theorem 2.1 can be extended to both the charge density and the current density constraints. Because of a lack of compactness, we do not tackle the energy constraint yet.

Denoting by $(\lambda_i, \psi_i)_{i \in \mathbb{N}^*}$ the spectral elements of ϱ, the current density associated to ϱ is defined by

$$j_\varrho(x) = \sum_{i \in \mathbb{N}^*} \lambda_i \, \mathcal{I}m \; \psi_i^* \nabla \psi_i. \tag{4.2}$$

This can be recast in a weak formulation as

$$\int_{\mathbb{R}^d} j_\varrho \cdot \psi \, dx = -i \, \mathrm{Tr} \left(\varrho \left(\psi \cdot \nabla + \frac{1}{2} \nabla \cdot \psi \right) \right), \qquad \forall \psi \in (W^{1,\infty}(\Omega))^d.$$

We make the following assumption:

Assumption A. *The functions $n(x)$ and $j(x)$ are given such that there exists a density operator $\varrho_0 \in \mathcal{E}_+$ satisfying $\mathrm{Tr}(\varrho_0) = 1$, $n_{\varrho_0} = n$ and $j_{\varrho_0} = j$.*

We already know (see Section 2) that Assumption A implies that $\sqrt{n} \in H^1(\mathbb{R}^d)$. Moreover, as consequences of Lieb-Thirring inequalities, see [1], Assumption A implies that the current density j belongs to $(L^q(\mathbb{R}^d))^d$, with

$$\begin{cases} 1 \leq q \leq 2 & \text{if} \quad d = 1, \\ 1 \leq q < 2 & \text{if} \quad d = 2, \\ 1 \leq q \leq \frac{d}{d-1} & \text{if} \quad d \geq 3. \end{cases} \tag{4.3}$$

Assumption A is verified for instance if there exists u (regular enough) whose curl vanishes and such that $j = nu$. Indeed, since $\nabla \times u = 0$, there exists S such that $u = \nabla S$. Defining then $\Psi = \sqrt{n} e^{iS}$, a possible choice for $\varrho_0[n, j]$ is given by

$$\varrho_0[n, j] = |\Psi\rangle \langle \Psi| \, .$$

In such a context, Theorem 2.1 becomes:

Theorem 4.3. *Consider a charge density $n(x)$ and a current density $j(x)$ that verify Assumption A and such that $n \log n \in L^1(\mathbb{R}^d)$. Then the following minimization problem with constraint:*

$$\min F(\varrho) \; \textit{for} \; \varrho \in \mathcal{E}_+ \; \textit{such that} \; n_\varrho = n, \quad \textit{and} \quad j_\varrho = j,$$

where F, E and S are defined by (2.9)*,* (2.3)*,* (2.4)*,* (2.5)*, is attained for a unique density operator.*

The proof of Theorem 2.1 can easily be modified so as to include the current constraint, one only needs to verify two facts: first, that the space of admissible density operators

$$\mathcal{A} = \{\varrho \in \mathcal{E}_+ \text{ such that } n_\varrho = n, \quad j_\varrho = j\}$$

is not empty. This is a direct consequence of Assumption A. Second, that the limit of the minimizing sequence verifies the current constraint. To see this, consider a minimizing sequence $(\varrho_k)_k$ as in Step 3 of the proof. We know from Steps 3 and 4 that ϱ_k converges strongly to ϱ in $\mathcal{J}_1$, that $(1-\Delta)^{1/2}\varrho_k(1-\Delta)^{1/2}$ converges in the $\mathcal{J}_1$ weak-$*$ topology to $(1-\Delta)^{1/2}\varrho(1-\Delta)^{1/2}$ as $k \to +\infty$ and that $n_\varrho = n$. We have to show that $j_\varrho = j$. For this, for all $\psi \in (W^{1,\infty}(\Omega))^d$, denoting also by ψ the (component by component) multiplication operator by ψ, the weak formulation of the constraint reads

$$\int_{\mathbb{R}^d} j \cdot \psi \, dx = -i \operatorname{Tr}\left(\varrho_k \left(\psi \cdot \nabla + \frac{1}{2}\nabla \cdot \psi\right)\right).$$

Since $\nabla \cdot \psi \in L^\infty(\mathbb{R}^d)$ and $\varrho_k \to \varrho$ strongly in $\mathcal{J}_1$, we find directly

$$\operatorname{Tr}\left(\varrho_k \nabla \cdot \psi\right) \to \operatorname{Tr}\left(\varrho \nabla \cdot \psi\right). \tag{4.4}$$

Regarding the second term in the definition of the current, we have

$$\operatorname{Tr}\left(\varrho_k\left(\psi \cdot \nabla\right)\right) = \operatorname{Tr}\left(\varrho_k\left(\psi \cdot \nabla\right)(1-\chi_R)\right) + \operatorname{Tr}\left((1-\Delta)^{1/2}\varrho_k(1-\Delta)^{1/2}K_R\right), \tag{4.5}$$

where χ_R is the same function as in Step 4 and

$$K_R = (1-\Delta)^{-1/2}\left(\psi \cdot \nabla\right)\chi_R(1-\Delta)^{-1/2}.$$

Since $(1-\Delta)^{-1/2}\left(\psi \cdot \nabla\right)$ is a bounded operator and $\chi_R(1-\Delta)^{-1/2}$ is compact, we deduce that K_R is compact and therefore, for all $R > 0$, as $k \to \infty$:

$$\operatorname{Tr}\left((1-\Delta)^{1/2}\varrho_k(1-\Delta)^{1/2}K_R\right) \to \operatorname{Tr}\left((1-\Delta)^{1/2}\varrho(1-\Delta)^{1/2}K_R\right). \tag{4.6}$$

For the first term of r.h.s of (4.5), we write

$$\operatorname{Tr}\left(\varrho_k\left(\psi \cdot \nabla\right)(1-\chi_R)\right) = \operatorname{Tr}\left((1-\chi_R)\sqrt{\varrho_k}\sqrt{\varrho_k}(1-\Delta)^{1/2}(1-\Delta)^{-1/2}\left(\psi \cdot \nabla\right)\right).$$

Denoting by $\mathcal{J}_2$ the space of Hilbert-Schmidt operators on $L^2(\mathbb{R}^d)$, we find

$$\begin{aligned}&\left|\operatorname{Tr}\left(\varrho_k\left(\psi \cdot \nabla\right)(1-\chi_R)\right)\right| \\ &\qquad \le \|(1-\chi_R)\sqrt{\varrho_k}\|_{\mathcal{J}_2}\|\sqrt{\varrho_k}(1-\Delta)^{1/2}\|_{\mathcal{J}_2}\|(1-\Delta)^{-1/2}\left(\psi \cdot \nabla\right)\|_{\mathcal{L}(L^2(\mathbb{R}^d))}.\end{aligned}$$

As already mentioned, $(1-\Delta)^{-1/2}\left(\psi \cdot \nabla\right)$ is a bounded operator and moreover $\sqrt{\varrho_k}(1-\Delta)^{1/2}$ is bounded in $\mathcal{J}_2$ independently of k as

$$\|\sqrt{\varrho_k}(1-\Delta)^{1/2}\|_{\mathcal{J}_2}^2 = \operatorname{Tr}\left((1-\Delta)^{1/2}\varrho_k(1-\Delta)^{1/2}\right) \le C.$$

This implies that

$$\left|\operatorname{Tr}\left(\varrho_k\left(\psi \cdot \nabla\right)(1-\chi_R)\right)\right| \le C\|(1-\chi_R)\sqrt{\varrho_k}\|_{\mathcal{J}_2}.$$

Let us now denote by $(\lambda_{k,i},\psi_{k,i})_{i\in\mathbb{N}^*}$ the spectral elements of ϱ_k. Then

$$\begin{aligned}\|(1-\chi_R)\sqrt{\varrho_k}\|^2_{\mathcal{J}_2} &= \sum_{i\in\mathbb{N}^*}\|(1-\chi_R)\sqrt{\varrho_k}\psi_{k,i}\|^2_{L^2(\mathbb{R}^d)},\\ &= \sum_{i\in\mathbb{N}^*}\lambda_{k,i}\int_{\mathbb{R}^d}(1-\chi_R)^2|\psi_{k,i}|^2dx,\\ &= \int_{\mathbb{R}^d}(1-\chi_R)^2 n dx,\end{aligned}$$

since $\varrho_k\in\mathcal{A}$ so that $n_{\varrho_k}=n$. The Lebesgue dominated convergence theorem then implies that

$$\lim_{R\to\infty}\sup_{k\in\mathbb{N}^*}\left|\mathrm{Tr}\left(\varrho_k\left(\psi\cdot\nabla\right)(1-\chi_R)\right)\right|=0. \tag{4.7}$$

Gathering (4.4), (4.5), (4.6) and (4.7) finally yields, when $k\to\infty$,

$$\begin{aligned}-i\,\mathrm{Tr}\left(\varrho_k\left(\psi\cdot\nabla+\frac{1}{2}\nabla\cdot\psi\right)\right) &\to -i\,\mathrm{Tr}\left(\varrho\left(\psi\cdot\nabla+\frac{1}{2}\nabla\cdot\psi\right)\right),\\ &= \int_{\mathbb{R}^d} j\cdot\psi\,dx.\end{aligned}$$

This means that $j_\varrho=j$ and therefore that $\varrho\in\mathcal{A}$. The rest of the proof of Theorem 4.3 is identical to that of Theorem 2.1.

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