

# A constrained optimization problem in quantum statistical physics

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June 28, 2021

## Abstract

In this paper, we consider the problem of minimizing quantum free energies under the constraint that the density of particles is fixed at each point of  $\mathbb{R}^d$ , for any  $d \geq 1$ . We are more particularly interested in the characterization of the minimizer, which is a self-adjoint nonnegative trace class operator, and will show that it is solution to a nonlinear self-consistent problem. This question of deriving quantum statistical equilibria is at the heart of the quantum hydrodynamical models introduced by Degond and Ringhofer in [4]. An original feature of the problem is the local nature of constraint, i.e. it depends on position, while more classical models consider the total number of particles in the system to be fixed. This raises difficulties in the derivation of the Euler-Lagrange equations and in the characterization of the minimizer, which are tackled in part by a careful parameterization of the feasible set.

## 1 Introduction

This work is concerned with the minimization of quantum free energies of the form

$$F(\varrho) = \text{Tr}(H\varrho) + T \text{Tr}(\beta(\varrho)), \quad (1)$$

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where  $\varrho$  is a density operator, i.e. a self-adjoint, trace class, and nonnegative operator on some Hilbert space,  $H$  is a given Hamiltonian,  $T$  the temperature,  $\text{Tr}(\cdot)$  denotes the operator trace, and  $\beta$  is an entropy function, for instance the Boltzmann or the Fermi-Dirac entropy. The free energy  $F(\varrho)$  is minimized under a constraint of local density, namely the density of particles is prescribed at each point of space: if  $\rho(x, y)$  is the integral kernel associated with the operator  $\varrho$ , then the local density, defined as  $\rho(x, x)$ , is fixed and equal to a given function.

The problem considered here is the building block of the quantum hydrodynamical models introduced by Degond et al in [4]. Their strategy consists in adapting to the quantum setting the moments closure method by entropy minimization that was developed by Levermore in the context of kinetic equations [10]. This requires the construction of quantum statistical equilibria, which are obtained by minimizing  $F(\varrho)$  under appropriate constraints. We focus in this work on the local density constraint (i.e. the zero order moment of  $\varrho$ ) explicitated above, which leads to the so-called quantum drift-diffusion model, see [2]. Different models can be obtained by considering additional constraints, in particular the local current and energy constraints (first and second order moments), which lead to the quantum Euler or quantum Navier-Stokes equations. We refer to [3, 1] for more details. See also e.g. [7, 9, 8] for additional references on quantum hydrodynamics.

At the mathematical level, it is proved in [12], for  $H = -\Delta + V$  defined on  $L^2(\mathbb{R}^d)$ , with  $d \geq 1$  and  $V$  a given potential, that  $F(\varrho)$ , with  $\beta$  the Boltzmann or the Fermi-Dirac entropy, admits a unique minimizer under the constraint  $\rho(x, x) = n(x)$ , where  $n$  is nonnegative and verifies

$$\sqrt{n} \in H^1(\mathbb{R}^d), \quad \int_{\mathbb{R}^d} n(x)dx = 1, \quad n \log n \in L^1(\mathbb{R}^d). \quad (2)$$

The first condition above is necessary for the energy to be finite (i.e. the first term in the definition of  $F(\varrho)$ ). The second condition is not crucial and can be modified. The proof is based on compactness and convexity methods. An important ingredient is a logarithmic Sobolev inequality for systems that yields a bound from below for the free energy. This requires the third condition in (2), which prevents leakage of particles at the infinity. Without this condition, the free energy is not bounded below and the minimization problem does not admit a solution. The reference [12] addresses in addition a local current constraint, while (local) density, current and energy constraints are considered in [6] in a one-dimensional setting in a bounded (periodic) domain. The energy constraint is difficult to handle in that there is no sufficient compactness on the minimizing sequences to directly pass to the limit in the constraint, and one has to resort to subtle monotonicity arguments inspired by thermodynamics to conclude.

Knowing from [12] that a minimizer exists and is unique, our main motivation in this work is its characterization. This is actually a quite more difficult problem than just establishing well-posedness. Formal calculations, performed e.g. in [3] in the case of the Boltzmann entropy and when  $V = 0$ , yield that the minimizer  $\varrho_*$  satisfies the following self-consistent relation

$$\varrho_* = \exp(-H[\varrho_*]/T), \quad (3)$$

where  $H[\varrho_\star]$  is an Hamiltonian of the form

$$H[\varrho_\star] = -\Delta + A[\varrho_\star], \quad A[\varrho_\star] = \frac{\Delta n}{2n} - \frac{Tn[\varrho_\star \log(\varrho_\star)] + k[\varrho_\star]}{n}.$$

Above,  $n[\varrho_\star \log \varrho_\star]$  and  $k[\varrho_\star]$  are respectively the local entropy and local kinetic energy, defined by

$$n[\varrho_\star \log(\varrho_\star)](x) = \sum_{p \in \mathbb{N}} \rho_p \log(\rho_p) |\phi_p(x)|^2, \quad k[\varrho_\star](x) = \sum_{p \in \mathbb{N}} \rho_p |\nabla \phi_p(x)|^2, \quad (4)$$

where  $\{\rho_p\}_{p \in \mathbb{N}}$  and  $\{\phi_p\}_{p \in \mathbb{N}}$  are the eigenvalues and the eigenvectors of  $\varrho_\star$ . Throughout the paper, the eigenvalues are counted with multiplicity and form a nonincreasing nonnegative sequence that accumulates at zero. At this stage, the kernel of  $\varrho_\star$  could be zero, finite, or infinite, but we will prove that it is actually zero when the constraint verifies  $n(x) > 0$  almost everywhere on  $\mathbb{R}^d$ . The solution  $\varrho_\star$  obtained in (3) is referred to in [3] as the “quantum Maxwellian”, and  $A[\varrho_\star]$  is the chemical potential, the Lagrange parameter associated with the density constraint. In [11], in a periodic one-dimensional domain  $\Omega$ , it is proved under the assumptions that  $n$  is uniformly bounded from below, i.e.  $n(x) \geq \underline{n} > 0$  a.e., and that  $n \in H^1(\Omega)$ , that the Hamiltonian  $H[\varrho_\star]$  is self-adjoint in the sense of quadratic forms. This is possible since the hypotheses (2) on  $n$  eventually lead to  $A[\varrho_\star] \in H^{-1}(\Omega)$ , which, in one dimension only in general, allows one to define  $H[\varrho_\star]$  in the sense of quadratic forms. In the case where the spatial domain is  $\mathbb{R}^d$ , the condition  $n(x) \geq \underline{n} > 0$  is not compatible with  $n \in L^1(\mathbb{R}^d)$ , and even if we had  $A[\varrho_\star] \in H^{-1}(\mathbb{R}^d)$ , this is in general too low a regularity to construct a self-adjoint operator using classical results such as the KLMN theorem [14] for instance. One of the main difficulties is therefore to give a proper meaning for (3) for the low regularity self-consistent potential  $A[\varrho_\star]$ . One could consider adding regularity conditions on  $\Delta n$  for instance, but on the one hand it is unclear how this improves the regularity of the self-consistent terms  $n[\varrho_\star \log \varrho_\star]$  and  $k[\varrho_\star]$ , and on the other any additional assumptions to (2) are not natural since they are not necessary for the existence theory.

The main result of this work is to rigorously define (3) under the minimal assumptions (2) when the constraint verifies  $n(x) > 0$  almost everywhere on  $\mathbb{R}^d$ . We will characterize  $\{\rho_p\}_{p \in \mathbb{N}}$  and  $\{\phi_p\}_{p \in \mathbb{N}}$  and show they are obtained by minimizing an appropriate quadratic form whose closure is  $-\log(\varrho_\star)$ . The method of proof is based on a proper rewriting of the chemical potential  $A[\varrho_\star]$  and on exploiting the obtained particular form. While a potential with a regularity as low as that of  $A[\varrho_\star]$  would not in general lead to a self-adjoint operator, it is the distinct structure of  $A[\varrho_\star]$  inherited from the minimization problem that allows us to justify (3). We will also briefly address the case where  $n(x)$  vanishes on a set of positive measure, which can be treated in a very similar fashion as the case when  $n$  has a full support.

There are several steps in our approach. Since we expect that  $\log \varrho_\star = -H[\varrho_\star]/T$ , the first one is to establish that  $\log \varrho_\star$  is well-defined, which amounts to prove that the kernel of  $\varrho_\star$  is zero; we then associate  $H[\varrho_\star]$  with an adequate quadratic form  $\mathcal{Q}_\star$ , and finally relate  $\mathcal{Q}_\star$  with  $\log \varrho_\star$ . All of this is done by deriving the Euler-Lagrange equations associated with the minimization problem, and a key difficulty is to appropriately parametrize the feasible set in order to define variations around  $\varrho_\star$ . The self-consistent nature of the problem and the singularity of the derivative of the entropy at zero make

the proofs somewhat involved and technical. We will in particular need to regularize the entropy in order to derive many results.

The article is structured as follows: we present our main result in Section 2; the proof is broken down into several parts in Section 3, and the proofs of some technical lemmas are given in Section 4.

**Acknowledgments.** OP's work is supported by NSF CAREER Grant DMS-1452349 and NSF grant DMS-2006416. The authors would like to thank the referees whose suggestions helped improve this manuscript.

## 2 Main result

We start by introducing some notation.

**Notation.** We write  $(\cdot, \cdot)$  for the inner product on  $L^2(\mathbb{R}^d)$ , with the convention  $(f, g) = \int_{\mathbb{R}^d} \bar{f}g dx$ , and  $\|\cdot\|$  for the corresponding norm. The free Hamiltonian  $-\Delta$  is denoted by  $H_0$ , equipped with the domain  $H^2(\mathbb{R}^d)$ .  $\mathcal{L}(L^2(\mathbb{R}^d))$  is the space of bounded operators on  $L^2(\mathbb{R}^d)$ ,  $\mathcal{J}_1 \equiv \mathcal{J}_1(L^2(\mathbb{R}^d))$  is the space of trace class operators and  $\mathcal{J}_2$  the space of Hilbert-Schmidt operators, both on  $L^2(\mathbb{R}^d)$ . In the sequel, we will refer to a density operator as a self-adjoint, trace class, nonnegative operator on  $L^2(\mathbb{R}^d)$ . For  $|\varrho| = \sqrt{\varrho^* \varrho}$ , we introduce the following space:

$$\mathcal{E} = \left\{ \varrho \in \mathcal{J}_1 : \overline{\sqrt{H_0}|\varrho|\sqrt{H_0}} \in \mathcal{J}_1 \right\},$$

where  $\overline{\sqrt{H_0}|\varrho|\sqrt{H_0}}$  denotes the extension of the operator  $\sqrt{H_0}|\varrho|\sqrt{H_0}$  to  $L^2(\mathbb{R}^d)$ . We will drop the extension sign in the sequel to ease notation. The space  $\mathcal{E}$  is a Banach space when endowed with the norm

$$\|\varrho\|_{\mathcal{E}} = \text{Tr}(|\varrho|) + \text{Tr}(\sqrt{H_0}|\varrho|\sqrt{H_0}),$$

where  $\text{Tr}(\cdot)$  denotes the operator trace. Finally, the energy space is the following closed convex subspace of  $\mathcal{E}$ :

$$\mathcal{E}_+ = \left\{ \varrho \in \mathcal{E} : \varrho \geq 0 \right\}.$$

Operators in  $\mathcal{E}_+$  are automatically self-adjoint since they are nonnegative. The local kinetic energy of  $\varrho \in \mathcal{E}_+$  is defined by

$$k[\varrho](x) = \sum_{p \in \mathbb{N}} \lambda_p |\nabla \psi_p(x)|^2, \quad \text{with} \quad \|k[\varrho]\|_{L^1} = \text{Tr}(\sqrt{H_0} \varrho \sqrt{H_0}),$$

where the series converges in  $L^1(\mathbb{R}^d)$  and  $\{\lambda_p\}_{p \in \mathbb{N}}$  and  $\{\psi_p\}_{p \in \mathbb{N}}$  are the eigenvalues and eigenvectors of  $\varrho$ .

**Setting of the problem.** The local density constraint is defined in a different, more convenient form than the one given in the introduction as follows: let  $\varrho$  be a density operator; for any function  $\varphi \in L^\infty(\mathbb{R}^d)$ , and identifying a function with its associated multiplication operator, the density  $n[\varrho]$  is uniquely defined by duality by

$$\int_{\mathbb{R}^d} n[\varrho] \varphi dx = \text{Tr}(\varrho \varphi). \quad (5)$$

A familiar equivalent expression is

$$n[\varrho] = \sum_{p \in \mathbb{N}} \lambda_p |\psi_p|^2, \quad (6)$$

where the series converges in  $L^1(\mathbb{R}^d)$ . Given a nonnegative function  $n$  satisfying (2), the admissible set is then

$$\mathcal{A} = \{\varrho \in \mathcal{E}_+ : n[\varrho] = n\}.$$

The kinetic energy and the entropy of  $\varrho \in \mathcal{E}_+$  are denoted by

$$E(\varrho) = \text{Tr}(\sqrt{H_0} \varrho \sqrt{H_0}), \quad S(\varrho) = \text{Tr}(\beta(\varrho)),$$

where  $\beta$  is the Boltzmann entropy  $\beta(x) = x \log(x) - x$ . We will state and prove our main result for such a  $\beta$ , and explain why it directly extends to the Fermi-Dirac entropy for instance. Setting  $T = 1$  to simplify notation, we write  $F(\varrho) = E(\varrho) + S(\varrho)$  and consider the minimization problem

$$\min_{\varrho \in \mathcal{A}} F(\varrho). \quad (7)$$

It is proven in [12] that there exists a unique solution  $\varrho_*$  to (7), that we characterize in our main result further. Before stating it, we need to introduce a few more notations. For  $n(x) > 0$  a.e., consider the nonnegative potential

$$V_* = \frac{|\nabla \sqrt{n}|^2 - n[\varrho_* \log(\varrho_*)]}{n},$$

where a series expression of  $n[\varrho_* \log(\varrho_*)]$  is given in (4). Note that  $-n[\varrho_* \log(\varrho_*)]$  is nonnegative since the eigenvalues of  $\varrho_*$  are less than one since  $\text{Tr}(\varrho_*) = \|n\|_{L^1} = 1$ . Since  $\sqrt{n} \in H^1(\mathbb{R}^d)$ , and we will see later that  $n[\varrho_* \log(\varrho_*)] \in L^1(\mathbb{R}^d)$ , the potential  $V_*$  is only in  $L^1(\mathbb{R}^d; ndx)$ . The introduction of  $V_*$  is motivated by the following observation: the first term in the definition of  $A[\varrho_*]$  can actually be written as

$$\frac{\Delta n}{2n} = \frac{\Delta \sqrt{n}}{\sqrt{n}} + \frac{|\nabla \sqrt{n}|^2}{n},$$

so that

$$A[\varrho_*] = \frac{\Delta \sqrt{n}}{\sqrt{n}} + \frac{|\nabla \sqrt{n}|^2 - n[\varrho_* \log(\varrho_*)] - k[\varrho_*]}{n}.$$

The first term on the right-hand-side above is called the Bohm potential, and can be absorbed into the Laplacian leading to

$$H[\varrho_\star] = -\frac{1}{\sqrt{n}} \nabla \cdot \left( n \nabla \left( \frac{\cdot}{\sqrt{n}} \right) \right) + V_\star - \frac{k[\varrho_\star]}{n}. \quad (8)$$

We then define the following weighted Sobolev space

$$H_\star^1(\mathbb{R}^d) = \{u \in L^2(\mathbb{R}^d; (1 + V_\star)dx) : \nabla u \in (L^2(\mathbb{R}^d))^d\},$$

which is complete as a closed subspace of  $H^1(\mathbb{R}^d)$ . Furthermore, based on (8), let  $\mathcal{Q}_\star$  be the quadratic form

$$\mathcal{Q}_\star(u, v) = \int_{\mathbb{R}^d} n \nabla \left( \frac{u^*}{\sqrt{n}} \right) \cdot \nabla \left( \frac{v}{\sqrt{n}} \right) dx + \int_{\mathbb{R}^d} \left( V_\star - \frac{k[\varrho_\star]}{n} \right) u^* v dx, \quad u, v \in H_\star^1(\mathbb{R}^d),$$

where  $k[\varrho_\star]$  is the local kinetic energy defined in (4). It is not clear at this point that  $\mathcal{Q}_\star$  is indeed well defined on  $H_\star^1(\mathbb{R}^d)$ . For this, we will see on the one hand that, and this is a consequence of the fact that  $\varrho_\star$  is the minimizer of  $F$ ,

$$\int_{\mathbb{R}^d} \frac{k[\varrho_\star]}{n} |u|^2 dx \leq \int_{\mathbb{R}^d} n \left| \nabla \left( \frac{u}{\sqrt{n}} \right) \right|^2 dx + \int_{\mathbb{R}^d} V_\star |u|^2 dx,$$

and on the other, after a short calculation, that

$$\int_{\mathbb{R}^d} n \left| \nabla \left( \frac{u}{\sqrt{n}} \right) \right|^2 dx = \int_{\mathbb{R}^d} |\nabla u|^2 dx - \int_{\mathbb{R}^d} \frac{\nabla \sqrt{n} \cdot \nabla |u|^2}{\sqrt{n}} dx + \int_{\mathbb{R}^d} \frac{|\nabla \sqrt{n}|^2}{n} |u|^2 dx,$$

which explains why  $\mathcal{Q}_\star$  is well-defined on  $H_\star^1(\mathbb{R}^d)$  using the Cauchy-Schwarz inequality. We will write  $\mathcal{Q}_\star(u)$  for  $\mathcal{Q}_\star(u, u)$ . Let finally  $\mathfrak{H}$  be defined by

$$\mathfrak{H} = \left\{ \varphi \in L^2(\mathbb{R}^d) : - \sum_{p \in \mathbb{N}} \log(\rho_p) |(\phi_p, \varphi)|^2 < \infty \right\},$$

where we recall that  $\{\rho_p\}_{p \in \mathbb{N}}$  is the nonnegative and nonincreasing sequence of eigenvalues of  $\varrho_\star$  and  $\{\phi_p\}_{p \in \mathbb{N}}$  its eigenvectors, which form an orthonormal basis of  $L^2(\mathbb{R}^d)$ . The space  $\mathfrak{H}$  is a Hilbert space when equipped with the inner product

$$(u, v)_{\mathfrak{H}} = - \sum_{p \in \mathbb{N}} \log(\rho_p) (\phi_p, u)^* (\phi_p, v).$$

Note that  $\mathfrak{H}$  is well-defined since we will see that  $\rho_p > 0$  for all  $p \in \mathbb{N}$ , and that  $\mathfrak{H}$  is the domain of self-adjointness of  $\sqrt{-\log(\varrho_\star)}$ .

We state now our main result.

**Theorem 2.1** *Let  $\varrho_\star$  be the unique solution to the minimization problem (7) with the constraint  $n$  satisfying (2) and  $n > 0$  a.e. in  $\mathbb{R}^d$ , and denote by  $\{\rho_p\}_{p \in \mathbb{N}}$  and  $\{\phi_p\}_{p \in \mathbb{N}}$*

the eigenvalues and eigenfunctions of  $\varrho_*$ . Then  $\varrho_*$  is full rank, i.e.  $\rho_p > 0$  for all  $p \in \mathbb{N}$ , and

$$-\log(\rho_p) = \min_{\varphi \in \mathcal{K}_p} \mathcal{Q}_*(\varphi) = \mathcal{Q}_*(\phi_p), \quad p \in \mathbb{N}, \quad (9)$$

where

$$\mathcal{K}_p = \{\varphi \in H_*^1(\mathbb{R}^d) : \|\varphi\| = 1, (\phi_q, \varphi) = 0, q = 0, \dots, p-1\},$$

with the convention that  $\mathcal{K}_0 = \{\varphi \in H_*^1(\mathbb{R}^d) : \|\varphi\| = 1\}$ . Moreover, denoting by  $\mathcal{Q}_{*,S}$  the restriction of  $\mathcal{Q}_*$  to  $S = \text{span}\{\phi_p, p \in \mathbb{N}\}$ , we have that  $\mathcal{Q}_{*,S}$  is densely defined and closable, and that  $-\log(\varrho_*)$  is the unique self-adjoint operator associated with the closure  $\overline{\mathcal{Q}_{*,S}}$ . Finally,  $H_*^1(\mathbb{R}^d) \subset \mathfrak{H}$ .

Let us make a few remarks. The self-consistent eigenvalue problem (9) is the rigorous formulation of (3). Also, while the form  $\mathcal{Q}_0$  obtained by setting  $k[\varrho_*] = 0$  in  $\mathcal{Q}_*$  can be shown to be closed in  $H_*^1(\mathbb{R}^d)$ , and is therefore associated to a self-adjoint operator, we do not know if  $\mathcal{Q}_*$  is closed in  $H_*^1(\mathbb{R}^d)$ . This is because  $-k[\varrho_*]$  is negative and is only in  $L^1(\mathbb{R}^d)$ , and there does not seem to be a way to consider the term involving  $k[\varrho_*]$  as a perturbation of  $\mathcal{Q}_0$  with such a low regularity. We obtain though that  $\mathcal{Q}_*$  is positive, and that it is closable when defined on a dense, smaller set than  $H_*^1(\mathbb{R}^d)$ . Note that since  $\{\phi_p\}_{p \in \mathbb{N}} \subset H_*^1(\mathbb{R}^d)$ , and that  $\{\phi_p\}_{p \in \mathbb{N}}$  is an orthonormal basis of  $L^2(\mathbb{R}^d)$ , the set  $H_*^1(\mathbb{R}^d)$  is dense in  $L^2(\mathbb{R}^d)$ .

Theorem 2.1 can be directly generalized to the Fermi-Dirac entropy  $x \log(x) + (1-x) \log(1-x)$ ,  $x \in [0, 1]$ . The Boltzmann and Fermi-Dirac entropies share indeed the same technical difficulties, in particular the fact that the eigenvalues of  $\varrho_*$  accumulate at zero. The Fermi-Dirac entropy has another singularity at  $x = 1$ , which is not an issue since there is only a finite number of eigenvalues arbitrarily close to one.

**Remark on the condition  $n > 0$  almost everywhere.** When  $n(x)$  vanishes on a set of positive measure, the statement of Theorem 2.1 has to be modified as follows. We only address the case where the support of  $n$  is not too “wild”, which is what we expect in the applications we have in mind: one can imagine nanostructures where particles are free to move in all of  $\mathbb{R}^d$  except in some open disjoint bounded domains  $\Omega_i$ ,  $i = 1, \dots, N$  (with smooth boundaries  $\partial\Omega_i$ ) where the particle density is then zero. Let  $\Omega = \mathbb{R}^d \setminus \bigcup_{i=1}^N \overline{\Omega_i}$ . We could treat as well the case where  $n$  vanishes outside of a bounded domain  $\Omega_0$ , and define instead  $\Omega = \Omega_0 \setminus \bigcup_{i=1}^N \overline{\Omega_i}$ .

Suppose that  $n > 0$  a.e. on  $\Omega$  and that  $n = 0$  a.e. on  $\bigcup_{i=1}^N \Omega_i$ . With the assumption that  $\sqrt{n} \in H^1(\mathbb{R}^d)$ , it follows that  $\sqrt{n}$  admits a trace on  $\partial\Omega_i$ , and therefore that  $\sqrt{n}|_{\partial\Omega_i} = 0$ ,  $i = 1, \dots, N$ . The main difference with the full support case is that the minimizer  $\varrho_*$  is not full rank any longer. Indeed, the eigenfunctions associated with strictly positive eigenvalues (denoted  $\{\phi_p\}_{p \in I}$ ) have the same support as  $n$ , and it is clear that functions supported in  $\bigcup_{i=1}^N \Omega_i$  are in the kernel of  $\varrho_*$ . Now, if we restrict  $\varrho_*$  to  $L^2(\Omega)$  by defining  $\varrho_{*,\Omega} = \mathbb{1}_\Omega \varrho_* \mathbb{1}_\Omega$ , the analysis that we pursue in the case  $n(x) > 0$  a.e. on  $\mathbb{R}^d$  carries over to the operator  $\varrho_{*,\Omega}$  with the following modifications: the potential  $V_*$  has the same expression as before and is restricted to  $\Omega$ , the set  $H_*^1(\mathbb{R}^d)$  is replaced by

$$H_*^1(\Omega) = \{u \in L^2(\Omega; (1 + V_*)dx) : \nabla u \in (L^2(\Omega))^d, u|_{\Omega_i} = 0, i = 1, \dots, N\},$$

and the domain of integration of the form  $\mathcal{Q}_*$  is set to  $\Omega$ . Note that  $\varrho_{*,\Omega}$  has a finite kinetic energy since the  $\{\phi_p\}_{p \in I}$  have a zero trace on  $\partial\Omega_i$ , and therefore

$$\int_{\mathbb{R}^d} |\nabla \phi_p|^2 dx = \int_{\Omega} |\nabla \phi_p|^2 dx, \quad p \in I.$$

One can then show with almost identical proofs as those given further that the operator  $\varrho_{*,\Omega}$  is full rank and that its eigenvalues/eigenfunctions satisfy a modified version of (9). In particular, the kernel of  $\varrho_*$  consists of  $L^2(\mathbb{R}^d)$  functions that vanish a.e. on  $\Omega$ .

**Strategy of proof.** One of the main difficulties is to construct admissible directions in order to derive the Euler-Lagrange equations. For  $\varphi \in L^2(\mathbb{R}^d)$ , we will choose operators of the form (with the Dirac bra-ket notation)

$$\varrho(t) = \sqrt{\frac{n}{n(t)}} (\varrho_* + t|\varphi\rangle\langle\varphi|) \sqrt{\frac{n}{n(t)}},$$

where  $n(t) = n[\varrho_* + t|\varphi\rangle\langle\varphi|]$ . An issue here is to make sure that  $\varrho_* + t|\varphi\rangle\langle\varphi|$  is nonnegative. This is true for any  $\varphi \in L^2(\mathbb{R}^d)$  when  $t \geq 0$ , but is false if  $t < 0$ , leading only to an inequality when  $t \geq 0$  in the Euler-Lagrange equations and not to an equality. We will use this inequality to prove an important estimate in the derivation of (9) and to obtain that  $\varrho_*$  is full rank. We will then replace  $|\varphi\rangle\langle\varphi|$  by  $|\phi_p\rangle\langle\phi_q| + |\phi_q\rangle\langle\phi_p|$ , which will allow us to work with negative and sufficiently small  $t$  to obtain the Euler-Lagrange equations as an equality. Note that it is tempting to use operators of the form  $C(t)\varrho_*C^*(t)$  for appropriate  $C(t)$  since positivity is ensured, but this does not eventually bring more information.

Note that because of the particular expression of  $H[\varrho_*]$  given in (8), it is not necessary to make hypotheses on the regularity of  $\Delta\sqrt{n}$  and those in (2) are sufficient.

### 3 Proof of Theorem 2.1

The proof is divided into four parts. In the first one, we obtain important results about the differentiability (in appropriate directions) of the functional  $F(\varrho)$ . In the second part, we prove that the minimizer is full rank. In the third part, we derive the crucial relation  $\mathcal{Q}_*(\phi_p, \phi_q) = -\log(\rho_p)\delta_{pq}$ , while we conclude the proof in the fourth part.

Throughout this section, we will use the following notations. For  $\varphi \in L^2(\mathbb{R}^d)$ ,  $P_\varphi$  denotes the rank-one projector  $P_\varphi = |\varphi\rangle\langle\varphi|$ . For  $t \geq 0$ , we consider perturbations of the minimizer of the form  $\varrho_* + tP_\varphi$ , and introduce the local density

$$n(t) = n[\varrho_* + tP_\varphi], \quad a(t) = \sqrt{\frac{n}{n(t)}},$$

as well as

$$\varrho(t) = a(t) (\varrho_* + tP_\varphi) a(t).$$

The operator  $\varrho(t)$  is designed to belong to the admissible set  $\mathcal{A}$ . Consider finally the weight

$$\omega(x) = 1 + V_*(x) + \frac{k[\varrho_*]}{n},$$

and introduce the space

$$H_\omega^1(\mathbb{R}^d) = \{u \in L^2(\mathbb{R}^d, \omega dx) : \nabla u \in (L^2(\mathbb{R}^d))^d\}.$$

Note that we actually have  $H_\omega^1(\mathbb{R}^d) = H_\star^1(\mathbb{R}^d)$ , but this fact is unknown at this stage. We will need the following logarithmic Sobolev for systems proved in [5, Corollary 18], which holds for any  $\varrho \in \mathcal{E}_+$  such that  $n[\varrho] \log n[\varrho] \in L^1(\mathbb{R}^d)$ :

$$\int_{\mathbb{R}^d} n[\varrho] \log(n[\varrho]) dx \leq \sum_{p \in \mathbb{N}} \rho_p \log(\rho_p) + \frac{d}{2} \log \left( \frac{e}{2\pi d} \frac{E(\varrho)}{\text{Tr}(\varrho)} \right) \text{Tr}(\varrho). \quad (10)$$

Above,  $\{\rho_p\}_{p \in \mathbb{N}}$  denotes the set of eigenvalues of  $\varrho$  and  $E(\varrho)$  its kinetic energy. Since  $E(\varrho) < \infty$  for any admissible  $\varrho$  and  $x \log(x) \leq 0$  for  $x \in [0, 1]$ , this inequality shows that the entropy of an admissible density operator is indeed well-defined as

$$0 \leq - \sum_{p \in \mathbb{N}} \rho_p \log(\rho_p) = -\text{Tr}(\beta(\varrho)) \leq \frac{d}{2} \log \left( \frac{e}{2\pi d} E(\varrho) \right) - \int_{\mathbb{R}^d} n \log(n) dx < \infty. \quad (11)$$

Above, we used that  $\text{Tr}(\varrho) = 1 = \|n\|_{L^1}$  and  $n \log(n) \in L^1(\mathbb{R}^d)$ .

### 3.1 Preliminary results

For  $u, v \in H_\omega^1(\mathbb{R}^d)$ , consider the quadratic form

$$\begin{aligned} \mathcal{Q}_e(u, v) &= \int_{\mathbb{R}^d} \left( -\frac{\nabla \sqrt{n} \cdot \nabla(u^* v)}{\sqrt{n}} + \frac{2|\nabla \sqrt{n}|^2 u^* v}{n} \right) dx \\ &\quad + \int_{\mathbb{R}^d} \nabla u^* \cdot \nabla v dx - \int_{\mathbb{R}^d} \frac{k[\varrho_\star] u^* v}{n} dx, \end{aligned} \quad (12)$$

with the notation  $\mathcal{Q}_e(\varphi) \equiv \mathcal{Q}_e(\varphi, \varphi)$ . Note that it follows from the Cauchy-Schwarz inequality for the first term on the right above that  $\mathcal{Q}_e$  is indeed well defined on  $H_\omega^1(\mathbb{R}^d)$ . The first lemma below pertains to the kinetic energy  $E(\varrho(t))$ , and is proven in section 4.1.

**Lemma 3.1** *Suppose  $\varphi \in H_\omega^1(\mathbb{R}^d)$ . Then, for all  $t \geq 0$ ,  $\varrho(t)$  belongs to the admissible set  $\mathcal{A}$ . Moreover,  $E(\varrho(t)) \in C^1(\mathbb{R}^+)$  with*

$$\frac{dE(\varrho(t))}{dt} \Big|_{t=0^+} = \mathcal{Q}_e(\varphi). \quad (13)$$

We then consider the entropy  $S(\varrho)$  for which we will need the next lemma.

**Lemma 3.2** *Let  $\varphi \in H^1(\mathbb{R}^d)$  with  $|\varphi| \leq M\sqrt{n}$  a.e. for some  $M > 0$ . Then,  $\varrho(t) \in C^1(\mathbb{R}^+, \mathcal{J}_1)$ .*

Because of the singularity of  $\beta'(x)$  at  $x = 0$  and of the particular form of  $\varrho(t)$ , it is difficult to justify some calculations that directly involve  $S(\varrho(t))$ . We therefore need to regularize and introduce, for  $x \in [0, 1]$  and  $\eta > 0$ ,

$$\beta_\eta(x) = (x + \eta) \log(x + \eta) - x - \eta \log(\eta),$$

and define

$$S_\eta(\varrho) = \text{Tr}(\beta_\eta(\varrho)), \quad F_\eta(\varrho) = E(\varrho) + S_\eta(\varrho).$$

Note that

$$\beta_\eta(x) - \beta(x) = \int_0^\eta (\log(u+x) - \log(u)) du \geq 0, \quad (14)$$

since  $\log$  is an increasing function. We then obtain the following lemma.

**Lemma 3.3** *Let  $\varphi \in L^2(\mathbb{R}^d)$  with  $|\varphi| \leq M\sqrt{n}$  a.e. for some constant  $M > 0$ . Then  $S_\eta(\varrho(t)) \in C^1(\mathbb{R}^+)$ , and for all  $t \geq 0$ ,*

$$h(\eta) + S_\eta(\varrho(t)) - S_\eta(\varrho(0)) \geq S(\varrho(t)) - S(\varrho(0)), \quad (15)$$

where  $h(\eta)$  is a nonnegative function independent of  $t$  and  $\varphi$  that goes to zero as  $\eta \rightarrow 0$ . Moreover,

$$\frac{dS_\eta(\varrho(t))}{dt} \Big|_{t=s} = \text{Tr}(\log(\eta + \varrho(s))P_{\varphi a(s)}) - \text{Tr}\left(\varrho(s)\log(\eta + \varrho(s))\frac{|\varphi|^2}{n(s)}\right). \quad (16)$$

*Proof.* That  $S_\eta(\varrho(t)) \in C^1(\mathbb{R}^+)$  is a direct consequence of Lemma 3.2 and that, according to [11, Lemma 5.3],  $S_\eta(\varrho)$  is differentiable at any nonnegative density operator  $\varrho$  in any direction  $\delta\rho \in \mathcal{J}_1$ , with  $DS_\eta[\varrho](\delta\rho) = \text{Tr}(\log(\eta + \varrho)\delta\rho)$ . Regarding (15), we have first, thanks to (14),  $S_\eta(\varrho(t)) \geq S(\varrho(t))$ . We now show that  $S_\eta(\varrho_\star) \rightarrow S(\varrho_\star)$  as  $\eta \rightarrow 0$ . Set  $\eta \in (0, 1/2)$ , then  $\beta_\eta(x) \leq 0$  for  $x \in [0, 1]$ . Then, by Fatou's lemma for series and (14),

$$\begin{aligned} -\sum_{p \in \mathbb{N}} \beta(\rho_p) &= \sum_{p \in \mathbb{N}} \liminf_{\eta \rightarrow 0} -\beta_\eta(\rho_p) \\ &\leq \liminf_{\eta \rightarrow 0} -\sum_{p \in \mathbb{N}} \beta_\eta(\rho_p) \leq \limsup_{\eta \rightarrow 0} -\sum_{p \in \mathbb{N}} \beta_\eta(\rho_p) \leq -\sum_{p \in \mathbb{N}} \beta(\rho_p), \end{aligned}$$

which yields the desired result. Then, with  $h(\eta) = S_\eta(\varrho(0)) - S(\varrho(0))$  and  $S_\eta(\varrho(t)) \geq S(\varrho(t))$ , we have

$$h(\eta) + S_\eta(\varrho(t)) - S_\eta(\varrho(0)) = S_\eta(\varrho(0)) - S(\varrho(0)) + S_\eta(\varrho(t)) - S_\eta(\varrho(0)) \geq S(\varrho(t)) - S(\varrho(0)),$$

which proves (15). Finally,

$$\begin{aligned} \frac{dS_\eta(\varrho(t))}{dt} \Big|_{t=s} &= \text{Tr}(\log(\eta + \varrho(s))\partial_t \varrho(s)) \\ &= \text{Tr}(\log(\eta + \varrho(s))P_{\varphi a(s)}) + \text{Tr}(\log(\eta + \varrho(s))\varrho(s)b(s)), \end{aligned}$$

where  $b(s) = -|\varphi|^2/n(s)$ . Above, we used the cyclicity of the trace and  $|b(s)| \leq |\varphi|^2/n \in L^\infty(\mathbb{R}^d)$ , which proves (16).  $\square$

**Remark 3.4** Note that both terms in (16) are finite since  $\varrho(s)$  and  $P_{\varphi a(s)}$  are trace class,  $\log(\eta + \varrho(s))$  is bounded, and  $|\varphi|^2/n(s) \leq |\varphi|^2/n \in L^\infty(\mathbb{R}^d)$  by assumption.

### 3.2 The minimizer is full rank

We have the following proposition.

**Proposition 3.5** *The minimizer  $\varrho_*$  is full rank, that is  $\rho_p > 0$  for all  $p \in \mathbb{N}$ .*

*Proof.* We prove the result by contradiction, in the spirit of [11], section 5, by differentiating in a direction related to a nonzero eigenfunction in the kernel of  $\varrho_*$ . Compared to [11], there are complications though since on the one hand, there is the additional term  $h(\eta)$  in (15) that needs to be handled carefully, and on the other admissible directions do not admit as simple expressions as in [11].

**Step 1:** Assume first that the kernel of  $\varrho_*$  is not  $\{0\}$ , and consider an orthonormal basis  $\{\psi_p\}_{p \in I}$  of  $\text{Ker } \varrho_*$  ( $I$  may be empty, finite or infinite, and we write  $|I|$  for its cardinal). Then, we denote by  $(\rho_p)_{1 \leq p \leq N}$  the nonincreasing sequence of nonzero eigenvalues of  $\varrho_*$  (here  $N$  is finite or not), associated to the orthonormal family of eigenfunctions  $(\phi_p)_{1 \leq p \leq N}$ . We thus obtain a Hilbert basis  $\{(\psi_p)_{1 \leq p \leq |I|}, (\phi_p)_{1 \leq p \leq N}\}$  of  $L^2(\mathbb{R}^d)$ . Pick then for instance  $\psi_1$ , that we denote for simplicity by  $\phi$ . Having little information about its regularity (we only know it is in  $L^2(\mathbb{R}^d)$ ), we need to regularize it in order to apply Lemmas 3.1 and 3.3. Let then  $\varphi_\varepsilon = \phi_\varepsilon \left( \frac{n}{n + \varepsilon |\phi_\varepsilon|^2} \right)^{1/2}$ , where  $\phi_\varepsilon \in C_c^\infty(\mathbb{R}^d)$  and  $\phi_\varepsilon \rightarrow \phi$  in  $L^2(\mathbb{R}^d)$ . We verify that  $\varphi_\varepsilon \in H_\omega^1(\mathbb{R}^d)$ . First of all,

$$\begin{aligned} \int_{\mathbb{R}^d} |\varphi_\varepsilon(x)|^2 \omega(x) dx &= \int_{\mathbb{R}^d} |\phi_\varepsilon(x)|^2 \frac{n(x)}{n(x) + \varepsilon |\phi_\varepsilon(x)|^2} dx \\ &\quad + \int_{\mathbb{R}^d} |\phi_\varepsilon(x)|^2 \frac{|\nabla \sqrt{n(x)}|^2 - n[\varrho_* \log(\varrho_*)] + k[\varrho_*]}{n(x) + \varepsilon |\phi_\varepsilon(x)|^2} dx \\ &\leq \|\phi_\varepsilon\|^2 + \varepsilon^{-1} \left( \|\nabla \sqrt{n}\|^2 - \text{Tr}(\varrho_* \log(\varrho_*)) + \|k[\varrho_*]\|_{L^1} \right), \end{aligned}$$

which is finite thanks to (11) and the fact that  $\|k[\varrho_*]\|_{L^1} = E(\varrho_*) < \infty$ . Moreover, we have

$$\begin{aligned} \nabla \varphi_\varepsilon &= \left( \frac{n}{n + \varepsilon |\phi_\varepsilon|^2} \right)^{1/2} \nabla \phi_\varepsilon + \phi_\varepsilon \nabla \sqrt{n} \left( \frac{1}{(n + \varepsilon |\phi_\varepsilon|^2)^{1/2}} - \frac{n}{(n + \varepsilon |\phi_\varepsilon|^2)^{3/2}} \right) \\ &\quad - \varepsilon \frac{\phi_\varepsilon \sqrt{n} \Re(\phi_\varepsilon^* \nabla \phi_\varepsilon)}{(n + \varepsilon |\phi_\varepsilon|^2)^{3/2}}, \end{aligned} \tag{17}$$

leading to the estimate

$$|\nabla \varphi_\varepsilon| \leq 2(|\nabla \phi_\varepsilon| + \varepsilon^{-1/2} |\nabla \sqrt{n}|).$$

This yields  $\varphi_\varepsilon \in H_\omega^1(\mathbb{R}^d)$ . Note that we also have  $|\varphi_\varepsilon| \leq \varepsilon^{-1/2} \sqrt{n}$ . Consider now

$$\varrho_\varepsilon(t) = a_\varepsilon(t) (\varrho_* + t P_{\varphi_\varepsilon}) a_\varepsilon(t),$$

where

$$n_\varepsilon(t) = n[\varrho_* + t P_{\varphi_\varepsilon}], \quad a_\varepsilon(t) = \sqrt{\frac{n}{n_\varepsilon(t)}}.$$

According to Lemma 3.1,  $\varrho_\varepsilon$  is admissible and  $\varrho_\varepsilon \in C^1(\mathbb{R}^+, \mathcal{J}_1)$ . As a consequence,  $\varrho_\varepsilon(t) \rightarrow \varrho_\varepsilon(0) = \varrho_*$  in  $\mathcal{J}_1$  as  $t \rightarrow 0^+$ . We will use the following Lemma, taken from [11, Lemma A.2].

**Lemma 3.6** Let a sequence  $(\varrho^k)_{k \in \mathbb{N}}$  converging to  $\varrho$  in  $\mathcal{J}_1$  as  $k \rightarrow +\infty$ . Then the corresponding nonincreasing sequence of eigenvalues  $(\rho_p^k)_{p \in \mathbb{N}}$ ,  $(\rho_p)_{p \in \mathbb{N}}$  converge as follows:

$$\forall p \in \mathbb{N}, \quad \lim_{k \rightarrow +\infty} \rho_p^k \rightarrow \rho_p.$$

Moreover, there exist a sequence of orthonormal eigenbasis  $(\phi_p^k)_{p \in \mathbb{N}}$  of  $\varrho^k$  and an orthonormal eigenbasis  $(\phi_p)_{p \in \mathbb{N}}$  of  $\varrho$  such that

$$\forall p \in \mathbb{N}, \quad \lim_{k \rightarrow +\infty} \|\phi_p^k - \phi_p\|_{L^2} = 0.$$

According to Lemma 3.6, we can choose the eigenbasis of  $\varrho_\varepsilon(t)$  and that of  $\varrho_\star$  in such a way that the eigenvectors converge to one another in  $L^2(\mathbb{R}^d)$  as  $t \rightarrow 0^+$ . We then pick  $\{(\psi_p)_{1 \leq p \leq |I|}, (\phi_p)_{1 \leq p \leq N}\}$  to be this very basis for  $\varrho_\star$ , and we denote by  $\{(\psi_p(t))_{1 \leq p \leq N(t)}\}$  that of  $\varrho_\varepsilon(t)$  ( $N(t)$  can be finite or not). Let  $\{\rho_p(t)\}_{1 \leq p \leq N(t)}$  be the eigenvalues associated with  $\{\psi_p(t)\}_{1 \leq p \leq N(t)}$ . We suppose that  $\psi_1(t)$  is the eigenvector of  $\varrho_\varepsilon(t)$  converging to  $\phi$ , and we denote for simplicity  $\psi_1(t) \equiv \phi(t)$ . As a consequence, Lemma 3.6 yields  $\rho_1(t) \rightarrow 0$  as  $t \rightarrow 0^+$ , which we will use below.

**Step 2:** According to (16), we find

$$\frac{dS_\eta(\varrho_\varepsilon(t))}{dt} \Big|_{t=s} = \text{Tr} \left( \log(\eta + \varrho_\varepsilon(s)) P_{\varphi_\varepsilon a_\varepsilon(s)} \right) - \int_{\mathbb{R}^d} \frac{n[\varrho_\varepsilon(s) \log(\eta + \varrho_\varepsilon(s))]}{n(s)} |\varphi_\varepsilon|^2 dx.$$

Let  $P_0(t)$  the set of indices such that  $\rho_p(t) \geq 1 - \eta$  for  $p \in P_0(t)$ . Then, since  $\log(\eta + x) \geq 0$  for  $x \geq 1 - \eta$ , and since  $\log(\eta + x) \leq 0$  for  $0 \leq x \leq 1 - \eta$ ,

$$\begin{aligned} \text{Tr} \left( \log(\eta + \varrho_\varepsilon(s)) P_{\varphi_\varepsilon a_\varepsilon(s)} \right) &\leq |(\varphi_\varepsilon a_\varepsilon(s), \phi(s))|^2 \log(\eta + \rho_1(s)) \\ &\quad + \sum_{p \in P_0(t)} |(a_\varepsilon(s) \varphi_\varepsilon, \psi_p(s))|^2 \log(\rho_p(s) + \eta). \end{aligned}$$

Moreover, since  $|\varphi_\varepsilon|^2 \leq \varepsilon^{-1} n$ , since  $n(s) \geq n$  for all  $s \geq 0$ , and  $x \log(x) \leq 0$  on  $[0, 1]$ , and  $-\log(\eta + x)$  is decreasing on  $[0, 1]$ , we find

$$-\int_{\mathbb{R}^d} \frac{n[\varrho_\varepsilon(s) \log(\eta + \varrho_\varepsilon(s))]}{n(s)} |\varphi_\varepsilon|^2 dx \leq -\varepsilon^{-1} \text{Tr} (\varrho_\varepsilon(s) \log(\varrho_\varepsilon(s))).$$

Choosing  $\eta \in (0, 1)$ , we then obtain, since  $\rho_p(t) \leq 1$ ,

$$\begin{aligned} \frac{dS_\eta(\varrho_\varepsilon(t))}{dt} \Big|_{t=s} &\leq |(\varphi_\varepsilon a_\varepsilon(s), \phi(s))|^2 \log(\eta + \rho_1(s)) + \log(2) \sum_{p \in P_0(t)} |(a_\varepsilon(s) \varphi_\varepsilon, \psi_p(s))|^2 \\ &\quad - \varepsilon^{-1} \text{Tr} (\varrho_\varepsilon(s) \log(\varrho_\varepsilon(s))). \end{aligned}$$

The bound  $a_\varepsilon(s) \leq 1$  for  $s \geq 0$  shows that the second term on the right can be bounded by  $\varepsilon^{-1} \log(2) \|\varphi_\varepsilon\|^2$ . Regarding the third term, the logarithmic Sobolev inequality (10) yields, since  $E(\varrho_\varepsilon(t)) \in C^1(\mathbb{R}^+)$  according to Lemma 3.1,

$$\begin{aligned} 0 \leq -\text{Tr} (\varrho_\varepsilon(s) \log(\varrho_\varepsilon(s))) &\leq -\int_{\mathbb{R}^d} n \log(n) dx + \frac{d}{2} \log \left( \frac{e}{2\pi d} E(\varrho_\varepsilon(s)) \right) \\ &\leq C + \frac{d}{2} \log \left( \frac{e}{2\pi d} \max_{s \in [0,1]} E(\varrho_\varepsilon(s)) \right) = C_{1,\varepsilon}. \end{aligned}$$

For any  $t \in [0, 1]$ , we have therefore arrived at

$$S_\eta(\varrho_\varepsilon(t)) - S_\eta(\varrho_\varepsilon(0)) \leq \int_0^t |(\varphi_\varepsilon a_\varepsilon(s), \phi(s))|^2 \log(\eta + \rho_1(s)) ds + tC_{2,\varepsilon}.$$

for another constant  $C_{2,\varepsilon}$ . Furthermore, since  $E(\varrho_\varepsilon(t)) \in C^1(\mathbb{R}^+)$ , there exists a constant  $C_{3,\varepsilon}$  such that

$$E(\varrho_\varepsilon(t)) - E(\varrho_\varepsilon(0)) \leq C_{3,\varepsilon}t, \quad \forall t \in [0, 1].$$

Gathering the previous estimates, we find, for  $t \in [0, 1]$ ,

$$F_\eta(\varrho_\varepsilon(t)) - F_\eta(\varrho_\varepsilon(0)) + h(\eta) \leq \int_0^t |(\varphi_\varepsilon a_\varepsilon(s), \phi(s))|^2 \log(\eta + \rho_1(s)) ds + tC_{4,\varepsilon} + h(\eta),$$

for a new constant  $C_{4,\varepsilon}$ .

**Step 3:** We will show that we can choose  $t$  and  $\eta$  such that the right hand side is negative. First, write

$$(\varphi_\varepsilon, \phi) = (\phi_\varepsilon, \phi) + \left( \left( \left( \frac{n}{n + \varepsilon |\phi_\varepsilon|^2} \right)^{1/2} - 1 \right) \phi_\varepsilon, \phi \right).$$

Since  $\phi_\varepsilon \rightarrow \phi$  in  $L^2(\mathbb{R}^d)$  as  $\varepsilon \rightarrow 0$ , the first term on the right above converges to one and the second to zero. Indeed, we write

$$\begin{aligned} \left( \left( \left( \frac{n}{n + \varepsilon |\phi_\varepsilon|^2} \right)^{1/2} - 1 \right) \phi_\varepsilon, \phi \right) &= \left( \left( \left( \frac{n}{n + \varepsilon |\phi_\varepsilon|^2} \right)^{1/2} - 1 \right) \phi, \phi \right) \\ &\quad + \left( \left( \left( \frac{n}{n + \varepsilon |\phi_\varepsilon|^2} \right)^{1/2} - 1 \right) (\phi_\varepsilon - \phi), \phi \right), \end{aligned}$$

and realize that the second term on the right converges to zero since  $\phi_\varepsilon \rightarrow \phi$  in  $L^2(\mathbb{R}^d)$ . The first term converges to zero by dominated convergence and the fact that  $n > 0$  a.e. on  $\mathbb{R}^d$  (if  $n$  were to vanish on a set of positive measure, then taking a function  $\phi$  supported on the complementary of that set would yield that this first term is actually  $-(\phi, \phi)$  and not zero).

We then choose  $\varepsilon$  sufficiently small so that  $|(\phi_\varepsilon, \phi)| > 1/2$ . Also, since

$$|(\varphi_\varepsilon a_\varepsilon(s), \phi(s))|^2 \rightarrow |(\varphi_\varepsilon, \phi)|^2 \geq \frac{1}{4} \quad \text{as } s \rightarrow 0,$$

there is an  $s_0(\varepsilon) > 0$  such that, for all  $s \in [0, s_0(\varepsilon)]$ ,

$$|(\varphi_\varepsilon a_\varepsilon(s), \phi(s))|^2 \geq \frac{1}{8}.$$

Besides, since  $\rho_1(s) \rightarrow 0$  as  $s \rightarrow 0$ , there exists  $s_1(\varepsilon, \delta) > 0$  such that  $0 \leq \rho_1(s) \leq \delta$ , for all  $s \in [0, s_1(\varepsilon, \delta)]$ . Finally, set  $\eta_0$  and  $\delta$  sufficiently small so that

$$\frac{1}{8} \log(\eta_0 + \delta) + 1 + C_{4,\varepsilon} < 0,$$

and choose  $\eta_1$  such that  $h(\eta) \leq \min(s_0(\varepsilon), s_1(\varepsilon, \delta), 1)$  for  $\eta \leq \eta_1$  (we recall that such a  $\eta_1$  exists since  $h(\eta) \rightarrow 0$  as  $\eta \rightarrow 0$ ). Then, for  $\eta \leq \min(\eta_0, \eta_1)$ , since  $\log(x)$  is increasing,

$$\begin{aligned} \int_0^{h(\eta)} \left( |(\varphi_\varepsilon a_\varepsilon(s), \phi(s))|^2 \log(\eta + \rho_1(s)) + 1 + C_{3,\varepsilon} \right) ds \\ \leq \int_0^{h(\eta)} \left( \frac{1}{8} \log(\eta + \delta) + 1 + C_{4,\varepsilon} \right) ds < 0. \end{aligned}$$

As a consequence, using (15), for all  $t \in [0, h(\eta)]$ ,

$$0 > h(\eta) + F_\eta(\varrho_\varepsilon(t)) - F_\eta(\varrho_\varepsilon(0)) \geq F(\varrho_\varepsilon(t)) - F(\varrho_\varepsilon(0)),$$

which contradicts the fact that  $\varrho_*$  is the unique minimizer of  $F$ . Hence, the kernel of  $\varrho_*$  is  $\{0\}$ , and the proof is complete.  $\square$

### 3.3 Euler-Lagrange equations

We prove here the relation

$$\mathcal{Q}_*(\phi_p, \phi_q) = -\log(\rho_p) \delta_{pq}, \quad p, q \in \mathbb{N}.$$

In the previous section, we were able to use an arbitrary test function  $\varphi$  in the perturbation since we only considered positive values for  $t$ . This ensured the positivity of  $\varrho(t)$ , with the drawback of only yielding an inequality in Euler-Lagrange equations (see e.g. (31)). This was enough though to prove that the minimizer is full rank. In order to obtain an equality in the Euler-Lagrange equations, we need to consider negative values of  $t$  as well, which limits the choice of the test functions since  $\varrho(t)$  has to be positive. We will choose below test functions related to the eigenfunctions  $\phi_p$ , for which the positivity of the perturbation holds.

We will need once again to regularize to justify the calculations. While we got away in the previous section with only regularizing the entropy term (this was justified by (15)), we need here to regularize as well the minimizer in order to obtain properly the Euler-Lagrange equation. Consider then the problem

$$\min_{\varrho \in \mathcal{A}} F_\eta(\varrho).$$

As (7), the above problem admits a unique solution denoted by  $\varrho_\eta$ , with eigenvalues and eigenvectors  $\{\rho_{p,\eta}\}_{p \in \mathbb{N}}$  and  $\{\phi_{p,\eta}\}_{p \in \mathbb{N}}$ . The proof of this fact is omitted since it is similar to the one of the non-regularized problem.

**Step 1: Euler-Lagrange equations for the regularized problem.** For  $p$  and  $q$  given, consider the operator

$$P_\eta = |\phi_{p,\eta}\rangle\langle\phi_{q,\eta}| + |\phi_{q,\eta}\rangle\langle\phi_{p,\eta}|,$$

that will be used to define a new direction of perturbation. It is not difficult to see that  $\varrho_\eta + tP_\eta$  is positive for  $t > -\min(\rho_{p,\eta}, \rho_{q,\eta})$ . It is also clear that  $\varrho_\eta + tP_\eta$  is self-adjoint and trace class, and that  $n_\eta(t) := n[\varrho_\eta + tP_\eta] = n + 2t\Re(\phi_{p,\eta}\phi_{q,\eta}^*)$ . This last

expression is deduced from the definition of the local density given in (5) and from a direct calculation. We define then

$$\varrho_\eta(t) = a_\eta(t)(\varrho_\eta + tP_\eta)a_\eta(t), \quad a_\eta(t) = \sqrt{\frac{n}{n_\eta(t)}}.$$

The lemma below, proved in Section 4.3, shows that  $\varrho_\eta(t)$  is in fact admissible for appropriate  $t$ .

**Lemma 3.7** *Let  $t_0 = \min(\rho_{p,\eta}, \rho_{q,\eta})/2$ . Then  $\varrho_\eta(t) \in \mathcal{A}$  for any  $t \in [-t_0, t_0]$ .*

We want to apply Lemma 3.3 next to obtain the Euler-Lagrange equations. For this, we will see in Lemma 3.8 that  $\rho_{j,\eta} \rightarrow \rho_j$  as  $\eta \rightarrow 0$ , for all  $j \in \mathbb{N}$ . As a consequence, since  $\rho_j > 0$  for all  $j \in \mathbb{N}$  according to Proposition 3.5, there exists  $\eta_0 > 0$  such that  $\rho_{p,\eta} > 0$  and  $\rho_{q,\eta} > 0$  for all  $\eta \in (0, \eta_0)$ . Since  $n[\varrho_\eta] = n$ , this leads to

$$|\phi_{p,\eta}| \leq \rho_{p,\eta}^{-1/2} \sqrt{n}, \quad a.e., \quad (18)$$

with a similar estimate for  $\phi_{q,\eta}$ . An easy adaptation of Lemmas 3.2 and 3.3 shows then that  $\varrho_\eta \in C^1([-t_0, t_0], \mathcal{J}_1)$ , and that

$$\frac{dS(\varrho_\eta(t))}{dt} \Big|_{t=0} = 2\log(\eta + \rho_{p,\eta})\delta_{pq} - 2\Re \int_{\mathbb{R}^d} \frac{n[\varrho_\eta \log(\eta + \varrho_\eta)]}{n} \phi_{p,\eta} \phi_{q,\eta}^* dx.$$

We consider now the kinetic energy term. Since  $\varrho_\eta \in \mathcal{E}$ , we have the relation

$$\|\nabla \phi_{p,\eta}\|^2 \leq \rho_{p,\eta}^{-1} E(\varrho_\eta) < \infty, \quad (19)$$

with a similar estimate for  $\phi_{q,\eta}$ . With (18), this shows that  $\phi_{p,\eta}$  and  $\phi_{q,\eta}$  belong to  $H_\omega^1(\mathbb{R}^d)$ . Adapting Lemma 3.1 then yields

$$\frac{dE(\varrho_\eta(t))}{dt} \Big|_{t=0} = 2\Re \mathcal{Q}_e(\phi_{p,\eta}, \phi_{q,\eta}).$$

Finally, since  $\varrho_\eta$  is the minimizer, the derivative of  $F_\eta(\varrho_\eta(t))$  at  $t = 0$  vanishes, and we find, gathering the above results,

$$2\Re \mathcal{Q}_\eta(\phi_{p,\eta}, \phi_{q,\eta}) = -2\log(\eta + \rho_{p,\eta})\delta_{pq}, \quad (20)$$

where

$$\mathcal{Q}_\eta(\varphi) = \int_{\mathbb{R}^d} n \left| \nabla \left( \frac{\varphi}{\sqrt{n}} \right) \right|^2 dx + \int_{\mathbb{R}^d} \frac{|\nabla \sqrt{n}|^2 - k[\varrho_\eta] - n[\varrho_\eta \log(\eta + \varrho_\eta)]}{n} |\varphi|^2 dx. \quad (21)$$

Note that direct calculations show that  $\mathcal{Q}_\eta$  is actually equal to

$$\begin{aligned} \mathcal{Q}_\eta(\varphi) &= \mathcal{Q}_e(\varphi) - \int_{\mathbb{R}^d} \frac{n[\varrho_\eta \log(\eta + \varrho_\eta)]}{n} |\varphi|^2 dx \\ &= \int_{\mathbb{R}^d} |\nabla \varphi|^2 dx - \int_{\mathbb{R}^d} \frac{\nabla \sqrt{n} \cdot \nabla |\varphi|^2}{\sqrt{n}} dx \\ &\quad + \int_{\mathbb{R}^d} \frac{2|\nabla \sqrt{n}|^2 - k[\varrho_\eta] - n[\varrho_\eta \log(\eta + \varrho_\eta)]}{n} |\varphi|^2 dx. \end{aligned}$$

Replacing  $P_\eta$  in the definition of  $\varrho_\eta(t)$  by  $i|\phi_{p,\eta}\rangle\langle\phi_{q,\eta}| - i|\phi_{q,\eta}\rangle\langle\phi_{p,\eta}|$ , we find that  $n[\varrho_\eta(t)] = n - 2t\Im(\phi_{p,\eta}\phi_{q,\eta}^*)$ . Repeating the above procedure, we find

$$2\Im\mathcal{Q}_\eta(\phi_{p,\eta}, \phi_{q,\eta}) = 0,$$

which, together with (20), yields

$$\mathcal{Q}_\eta(\phi_{p,\eta}, \phi_{q,\eta}) = -\log(\eta + \rho_{p,\eta})\delta_{pq}.$$

Note that we are able to obtain this equality since  $\varrho_\eta$  is the minimizer of  $F_\eta$ , had we just regularized the entropy term we would have only obtained an inequality of the form  $\mathcal{Q}_\eta(\phi_p, \phi_q) \geq -\log(\eta + \rho_p)\delta_{pq}$ .

**Step 2: Passing to the limit.** Choose for instance for  $\eta$  the sequence  $\eta \equiv \eta_\ell = 1/\ell$  which converges to zero as  $\ell \rightarrow \infty$ . The following lemma lists the convergence properties of  $\varrho_\eta$ .

**Lemma 3.8** *Let  $\varrho_\ell := \varrho_{\eta_\ell}$ . Then, as  $\ell \rightarrow \infty$ :*

- (i)  $\varrho_\ell$  converges to  $\varrho_\star$  in  $\mathcal{J}_1$ .
- (ii)  $\sqrt{H_0}\varrho_\ell\sqrt{H_0}$  converges to  $\sqrt{H_0}\varrho_\star\sqrt{H_0}$  in  $\mathcal{J}_1$ , and  $\sqrt{H_0}\sqrt{\varrho_\ell}$  converges to  $\sqrt{H_0}\sqrt{\varrho_\star}$  in  $\mathcal{J}_2$ .
- (iii)  $\forall p \in \mathbb{N}$ ,  $\rho_{p,\ell}$  converges to  $\rho_p$ , where  $\{\rho_{p,\ell}\}_{p \in \mathbb{N}}$  are the eigenvalues of  $\varrho_\ell$  and  $\{\rho_p\}_{p \in \mathbb{N}}$  those of  $\varrho_\star$ .
- (iv) there exist a sequence of orthonormal eigenbasis  $\{\phi_{p,\ell}\}_{p \in \mathbb{N}}$  of  $\varrho_\ell$  and an orthonormal eigenbasis  $\{\phi_p\}_{p \in \mathbb{N}}$  of  $\varrho_\star$  such that,  $\forall p \in \mathbb{N}$ ,

$$\lim_{\ell \rightarrow +\infty} \|\phi_{p,\ell} - \phi_p\| = 0 \quad \text{and} \quad \lim_{\ell \rightarrow +\infty} \|\sqrt{\rho_{p,\ell}}\nabla\phi_{p,\ell} - \sqrt{\rho_p}\nabla\phi_p\| = 0.$$

- (v)  $\beta_{\eta_\ell}(\varrho_\ell)$  converges to  $\beta(\varrho_\star)$  in  $\mathcal{J}_1$ .
- (vi)  $\varrho_\ell \log(\eta_\ell + \varrho_\ell)$  converges to  $\varrho_\star \log(\varrho_\star)$  in  $\mathcal{J}_1$ .

*Proof.* The proof will use the following two ingredients: the first one is the logarithmic Sobolev (10), and the second is the following Lemma proved in [11, Lemma 3.1], providing us with compactness results for sequences of density operators bounded in  $\mathcal{E}$ .

**Lemma 3.9** *Let  $(\varrho_k)_{k \in \mathbb{N}}$  be a bounded sequence of  $\mathcal{E}_+$ . Then, up to an extraction of a subsequence, there exists  $\varrho \in \mathcal{E}_+$  such that*

$$\varrho_k \rightarrow \varrho \text{ in } \mathcal{J}_1 \quad \text{as } k \rightarrow +\infty, \tag{22}$$

and

$$\text{Tr}(\sqrt{H_0}\varrho\sqrt{H_0}) \leq \liminf_{k \rightarrow +\infty} \text{Tr}(\sqrt{H_0}\varrho_k\sqrt{H_0}). \tag{23}$$

Furthermore, if one has

$$\text{Tr}(\sqrt{H_0}\varrho\sqrt{H_0}) = \lim_{k \rightarrow +\infty} \text{Tr}(\sqrt{H_0}\varrho_k\sqrt{H_0}),$$

then one can conclude in addition that

$$\sqrt{H_0}\sqrt{\varrho_k} \rightarrow \sqrt{H_0}\sqrt{\varrho} \text{ in } \mathcal{J}_2 \quad \text{and} \quad \sqrt{H_0}\varrho_k\sqrt{H_0} \rightarrow \sqrt{H_0}\varrho\sqrt{H_0} \text{ in } \mathcal{J}_1 \quad \text{as } k \rightarrow +\infty. \tag{24}$$

We now begin the proof of Lemma 3.8.

**Step 1:** We start with (i). Let  $\sigma = |\sqrt{n}\rangle\langle\sqrt{n}|$ . Since  $\sigma \in \mathcal{A}$ , we have

$$F_\eta(\varrho_\eta) \leq F_\eta(\sigma).$$

Besides, (14) yields  $F(\varrho_\eta) \leq F_\eta(\varrho_\eta)$ . It follows from (10) and  $\text{Tr}(\varrho_\eta) = \|n\|_{L^1} = 1$  that

$$\int_{\mathbb{R}^d} n(x) \log(n(x)) dx - \frac{d}{2} \log \left( \frac{eE(\varrho_\eta)}{2\pi d} \right) - 1 \leq S(\varrho_\eta),$$

This gives the estimate

$$\int_{\mathbb{R}^d} n(x) \log(n(x)) dx - \frac{d}{2} \log \left( \frac{eE(\varrho_\eta)}{2\pi d} \right) - 1 + E(\varrho_\eta) \leq F(\varrho_\eta) \leq F_\eta(\sigma) = \|\nabla\sqrt{n}\|^2 + \beta_\eta(1),$$

which shows that

$$E(\varrho_\eta) \leq M, \quad (25)$$

for some  $M > 0$  independent of  $\eta$ . Together with  $\text{Tr}(\varrho_\eta) = 1$ , we can apply Lemma 3.9 and find a subsequence  $\varrho_k := \varrho_{\eta_{\ell_k}}$  (recall that  $\eta = \eta_\ell = 1/\ell$ ) and a  $\varrho$  satisfying the convergence results of Lemma 3.9.

**Step 2:** We identify now  $\varrho$  with  $\varrho_\star$ . For this, we remark first that  $\varrho_\star \in \mathcal{A}$ , and therefore,

$$F_\eta(\varrho_\eta) \leq F_\eta(\varrho_\star). \quad (26)$$

Furthermore, it is proven in [12, Step 6 in Section 3], that  $S(\varrho_k) \rightarrow S(\varrho)$  as  $k \rightarrow \infty$ , and the proof can be directly adapted to yield that

$$\text{Tr}(|\beta_{\eta_{\ell_k}}(\varrho_\ell)|) \xrightarrow{k \rightarrow \infty} \text{Tr}(|\beta(\varrho)|) \quad \text{and} \quad \text{Tr}(|\beta_{\eta_{\ell_k}}(\varrho_\star)|) \xrightarrow{k \rightarrow \infty} \text{Tr}(|\beta(\varrho_\star)|). \quad (27)$$

As a consequence, we obtain from (26) and (23) of Lemma 3.9 that

$$F(\varrho) \leq F(\varrho_\star),$$

which, by uniqueness of the minimizer, yields  $\varrho = \varrho_\star$ . This also implies that the entire sequence  $\{\varrho_{\eta_\ell}\}_{\ell \in \mathbb{N}^*}$ , denoted with an abuse of notation by  $\{\varrho_\ell\}_{\ell \in \mathbb{N}^*}$ , converges to  $\varrho_\star$ . Then, (i) and (ii) follow from Lemma 3.9 by replacing  $\varrho$  by  $\varrho_\star$ . Furthermore, (iii) and the first result of (iv) follow from Lemma 3.6.

**Step 3:** We address now the second result of (iv). From (25), we have

$$\rho_{p,\eta} \|\nabla \phi_{p,\eta}\|^2 \leq \text{Tr}(\sqrt{H_0} \varrho_\eta \sqrt{H_0}) \leq M,$$

which, together with (iii) and the first result of (iv), shows that  $\sqrt{\varrho_{p,\ell}} \phi_{p,\ell}$  converges weakly in  $H^1(\mathbb{R}^d)$  to  $\sqrt{\varrho_p} \phi_p$ . In order to obtain strong convergence, we remark that, according to (ii),  $\sqrt{H_0} \sqrt{\varrho_\ell}$  converges to  $\sqrt{H_0} \sqrt{\varrho_\star}$  strongly in  $\mathcal{J}_2$ , so that

$$\rho_{p,\ell} \|\nabla \phi_{p,\ell}\|^2 = \text{Tr}(\sqrt{H_0} \sqrt{\varrho_\ell} P_{\phi_{p,\ell}} \sqrt{\varrho_\ell} \sqrt{H_0}) \rightarrow \text{Tr}(\sqrt{H_0} \sqrt{\varrho_\star} P_{\phi_p} \sqrt{\varrho_\star} \sqrt{H_0}) = \rho_p \|\nabla \phi_p\|^2.$$

Above, we used the fact that  $P_{\phi_{p,\ell}} \rightarrow P_{\phi_p}$  strongly in  $\mathcal{L}(L^2(\mathbb{R}^d))$  because of the first result of (iv). Together with the weak convergence of  $\sqrt{\rho_{p,\ell}} \nabla \phi_{p,\ell}$ , this proves the second result of (iv).

**Step 4:** Regarding (v), as stated in (27), we already have the convergence of  $|\beta_{\eta_\ell}(\varrho_\ell)|$  in  $\mathcal{J}_1$ . With (iii) and (iv), it is then not difficult to obtain weak convergence of  $\beta_{\eta_\ell}(\varrho_\ell)$  to  $\beta(\varrho_\star)$  in the sense of operators, which, according to [15, Theorem 2.21 and addendum H], yields the convergence in  $\mathcal{J}_1$ .

**Step 5:** Finally, for (vi), we write

$$x \log(\eta + x) - x \log(x) = \beta_\eta(x) - \beta(x) - g_\eta(x) \quad \text{with} \quad g_\eta(x) = \eta(\log(\eta) - \log(\eta + x)).$$

Since  $|g_\eta(x)| \leq |x|$  for all  $x \geq 0$ , we have that  $g_\eta(\varrho_\eta) \in \mathcal{J}_1$ . Then

$$\|g_{\eta_\ell}(\varrho_\ell)\|_{\mathcal{J}_1} = \sum_{p \in \mathbb{N}} |g_{\eta_\ell}(\rho_{p,\ell})| \xrightarrow{\ell \rightarrow \infty} 0,$$

as an application of generalized dominated convergence for series together with (iii),  $g_{\eta_\ell}(\rho_{p,\ell}) \rightarrow 0$  and  $\rho_p > 0$  for all  $p \in \mathbb{N}$ . Hence, we have

$$\|\varrho_\ell \log(\eta_\ell + \varrho_\ell) - \varrho_\star \log \varrho_\star\|_{\mathcal{J}_1} \leq \|\beta_{\eta_\ell}(\varrho_\ell) - \beta(\varrho_\star)\|_{\mathcal{J}_1} + \|g_{\eta_\ell}(\varrho_\ell)\|_{\mathcal{J}_1},$$

which converges to zero as  $\ell \rightarrow \infty$  according to (v). This ends the proof.  $\square$

Following this last lemma, we suppose that the basis of eigenvectors  $\{\phi_p\}_{p \in \mathbb{N}}$  introduced in the previous sections is the one of item (iv). We have then the

**Proposition 3.10** *For all  $p, q \in \mathbb{N}$ ,*

$$\mathcal{Q}_\star(\phi_p, \phi_q) = -\delta_{pq} \log(\rho_q).$$

*Note that  $\log(\rho_p)$  is well defined for all  $p \in \mathbb{N}$  since  $\rho_p > 0$  according to Proposition 3.5.*

*Proof.* Set first  $\rho_{p,\ell} := \rho_{p,\eta_\ell}$  and  $\phi_{p,\ell} := \phi_{p,\eta_\ell}$ . Then, since  $\rho_p > 0$  for all  $p \in \mathbb{N}$ , Lemma 3.8 (iii) shows that  $\log(\eta_\ell + \rho_{p,\ell}) \rightarrow \log(\rho_p)$  for all  $p \in \mathbb{N}$  as  $\ell \rightarrow \infty$ . Consider now  $\sqrt{\rho_{p,\ell} \rho_{q,\ell}} \mathcal{Q}_{\eta_\ell}(\phi_{p,\ell}, \phi_{q,\ell})$ , that we split into five terms  $Q_i^\ell$  defined below,  $i = 1, \dots, 5$ . Then, by Lemma 3.8 (iii)-(iv), as  $\ell \rightarrow \infty$ ,

$$Q_1^\ell := \sqrt{\rho_{p,\ell} \rho_{q,\ell}} \int_{\mathbb{R}^d} \nabla \phi_{p,\ell}^* \cdot \nabla \phi_{q,\ell} dx \rightarrow \sqrt{\rho_p \rho_q} \int_{\mathbb{R}^d} \nabla \phi_p^* \cdot \nabla \phi_q dx.$$

Furthermore,

$$\begin{aligned} Q_2^\ell &:= -\sqrt{\rho_{p,\ell} \rho_{q,\ell}} \int_{\mathbb{R}^d} \frac{\nabla \sqrt{n} \cdot \nabla (\phi_{p,\ell}^* \phi_{q,\ell})}{\sqrt{n}} dx \\ &= -\sqrt{\rho_{p,\ell} \rho_{q,\ell}} \int_{\mathbb{R}^d} \frac{\nabla \sqrt{n} \cdot (\nabla (\phi_{p,\ell}^* \phi_{q,\ell}) + \nabla (\phi_{q,\ell} \phi_{p,\ell}^*))}{\sqrt{n}} dx \\ &:= Q_{2,1}^\ell + Q_{2,2}^\ell. \end{aligned}$$

We write

$$\begin{aligned}
Q_{2,1}^\ell &= -\sqrt{\rho_p \rho_q} \int_{\mathbb{R}^d} \frac{\nabla \sqrt{n} \cdot \nabla \phi_p^* \phi_q}{\sqrt{n}} dx \\
&\quad - \sqrt{\rho_{q,\ell}} \int_{\mathbb{R}^d} \frac{\nabla \sqrt{n} \cdot (\nabla(\sqrt{\rho_{p,\ell}} \phi_{p,\ell}^* - \sqrt{\rho_p} \phi_p^*) \phi_{q,\ell})}{\sqrt{n}} dx \\
&\quad - \sqrt{\rho_p} \int_{\mathbb{R}^d} \frac{\nabla \sqrt{n} \cdot \nabla \phi_p^* (\sqrt{\rho_{q,\ell}} \phi_{q,\ell} - \sqrt{\rho_q} \phi_q)}{\sqrt{n}} dx.
\end{aligned} \tag{28}$$

The second term on the right is controlled by

$$\|\nabla \sqrt{n}\| \|\nabla(\sqrt{\rho_{p,\ell}} \phi_{p,\ell}^* - \sqrt{\rho_p} \phi_p^*)\| \|\sqrt{\rho_{q,\ell}} \phi_{q,\ell} / \sqrt{n}\|_{L^\infty},$$

and goes to zero as  $\ell \rightarrow \infty$  because of Lemma 3.8 (iv) and the fact that

$$\frac{\sqrt{\rho_{q,\ell}} |\phi_{q,\ell}|}{\sqrt{n}} \leq 1, \quad a.e. \tag{29}$$

since  $n[\varrho_\ell] = n$ . For the third term, we deduce from Lemma 3.8 (iii)-(iv) that there is a subsequence  $\{k_\ell\}_{\ell \in \mathbb{N}}$  such that  $\sqrt{\rho_{q,k_\ell}} \phi_{q,k_\ell}$  converges to  $\sqrt{\rho_q} \phi_q$  a.e.. Since  $\nabla \sqrt{n}$  and  $\nabla \phi_p$  belong to  $L^2(\mathbb{R}^d)$ , and  $\sqrt{\rho_{q,k_\ell}} |\phi_{q,k_\ell}| / \sqrt{n} \leq 1$  a.e. as well as  $\sqrt{\rho_q} |\phi_q| / \sqrt{n} \leq 1$  a.e., we can invoke dominated convergence and obtain that the limit of the third term is zero. We have therefore obtained that  $Q_{2,1}^{k_\ell}$  converges as  $\ell \rightarrow \infty$  to the first term on the right in (28). The term  $Q_{2,2}^\ell$  is handled exactly as  $Q_{2,1}^\ell$ .

We treat now the term  $Q_3^\ell$  that reads

$$Q_3^\ell := -\sqrt{\rho_{p,\ell} \rho_{q,\ell}} \int_{\mathbb{R}^d} \frac{k[\varrho_\ell] \phi_{p,\ell}^* \phi_{q,\ell}}{n} dx$$

According to Lemma 3.8 (ii), we can conclude that  $k[\varrho_\ell]$  converges to  $k[\varrho_\star]$  strongly in  $L^1(\mathbb{R}^d)$ , and we have, using (29),

$$\lim_{\ell \rightarrow \infty} Q_3^\ell := -\lim_{\ell \rightarrow \infty} \sqrt{\rho_{p,k_\ell} \rho_{q,k_\ell}} \int_{\mathbb{R}^d} \frac{k[\varrho_\star] \phi_{p,\ell}^* \phi_{q,\ell}}{n} dx.$$

Proceeding in the same way as  $Q_{2,1}^\ell$ , with dominated convergence and (29), we find

$$\lim_{\ell \rightarrow \infty} Q_3^{k_\ell} = -\sqrt{\rho_p \rho_q} \int_{\mathbb{R}^d} \frac{k[\varrho_\star] \phi_p^* \phi_q}{n} dx.$$

The term

$$Q_4^\ell := -\sqrt{\rho_{p,\ell} \rho_{q,\ell}} \int_{\mathbb{R}^d} \frac{n[\varrho_\ell \log(\eta_\ell + \varrho_\ell)] \phi_{p,\ell}^* \phi_{q,\ell}}{n} dx$$

is treated exactly as  $Q_3^\ell$  since  $n[\varrho_\ell \log(\eta_\ell + \varrho_\ell)] \rightarrow n[\varrho_\star \log(\varrho_\star)]$  in  $L^1(\mathbb{R}^d)$  according to Lemma 3.8 (vi). Finally,

$$\begin{aligned}
\lim_{\ell \rightarrow \infty} Q_5^{k_\ell} &:= 2 \lim_{\ell \rightarrow \infty} \sqrt{\rho_{p,k_\ell} \rho_{q,k_\ell}} \int_{\mathbb{R}^d} \frac{|\nabla \sqrt{n}|^2 \phi_{p,k_\ell}^* \phi_{q,k_\ell}}{n} dx \\
&= 2\sqrt{\rho_p \rho_q} \int_{\mathbb{R}^d} \frac{|\nabla \sqrt{n}|^2 \phi_p^* \phi_q}{n} dx,
\end{aligned}$$

as an application, as earlier, of dominated convergence and (29). Gathering the different limits, we find

$$\sqrt{\rho_p} \sqrt{\rho_q} (\mathcal{Q}_\star(\phi_p, \phi_q) + \delta_{pq} \log(\rho_p)) = 0,$$

which ends the proof since  $\rho_p$  and  $\rho_q$  are strictly positive according to Proposition 3.5.

□

**An important estimate.** The next result is central in proving the eigenvalue relation (9).

**Proposition 3.11** *Let  $\varphi \in H_\omega^1(\mathbb{R}^d)$ . Then,*

$$\|\varphi\|_{\mathfrak{H}}^2 \leq \mathcal{Q}_\star(\varphi).$$

*Proof.* For  $t \geq 0$  and  $\varphi \in H_\omega^1(\mathbb{R}^d)$ , consider the operator

$$\varrho_\eta(t) = a_\eta(t) (\varrho_\eta + tP_\varphi) a_\eta(t),$$

where

$$n_\eta(t) = n[\varrho_\eta + tP_\varphi], \quad a_\eta(t) = \sqrt{\frac{n}{n_\eta(t)}}.$$

We need to regularize  $\varphi$  in order to have the estimate  $|\varphi| \leq M\sqrt{n}$  and use Lemma 3.3. Let then  $\varphi_\varepsilon = \varphi \left( \frac{n}{n+\varepsilon|\varphi|^2} \right)^{1/2}$ . We can see that  $|\varphi_\varepsilon| \leq \varepsilon^{-1/2}\sqrt{n}$  and it follows from similar computations as in (17) that

$$|\nabla \varphi_\varepsilon| \leq 2 \left( |\nabla \varphi| + \frac{|\nabla \sqrt{n}|}{\sqrt{n}} |\varphi| \right), \quad (30)$$

which gives  $\varphi_\varepsilon \in H_\omega^1(\mathbb{R}^d)$ . Denoting by  $\varrho_\varepsilon(t)$  (and dropping the dependency on  $\eta_\ell$  to ease notation) the operator  $\varrho_{\eta_\ell}(t)$  for  $\varphi \equiv \varphi_\varepsilon$ , Lemma 3.1 and (16) then yield, since  $\varrho_{\eta_\ell}$  is the minimizer,

$$\frac{dF_{\eta_\ell}(\varrho_\varepsilon(t))}{dt} \Big|_{t=0^+} = \mathcal{Q}_{\eta_\ell}(\varphi_\varepsilon) + \text{Tr}(\log(\eta_\ell + \varrho_{\eta_\ell}) P_{\varphi_\varepsilon}) \geq 0. \quad (31)$$

We will pass to the limit in the above relation. We have first

$$\text{Tr}(\log(\eta_\ell + \varrho_{\eta_\ell}) P_{\varphi_\varepsilon}) = \sum_{p \in \mathbb{N}} |(\varphi_\varepsilon, \phi_{p,\ell})|^2 \log(\rho_{p,\ell} + \eta_\ell).$$

Choose  $\eta_\ell \in (0, 1/2]$  and  $p_0$  such that  $\rho_p \leq 1/2$  for  $p \geq p_0$ . Since  $\rho_{p,\ell} \rightarrow \rho_p$  by Lemma (3.8) (iii), we can choose  $\ell$  sufficiently large that  $\rho_{p,\ell} \leq 1/2$  for  $p \geq p_0$ . Since  $\varphi_\varepsilon \rightarrow \varphi$  in  $L^2(\mathbb{R}^d)$  (note that we use here the fact that  $n > 0$  a.e.), it follows that, with Lemma 3.8 (iii)-(iv),

$$\lim_{\varepsilon \rightarrow 0} \lim_{\ell \rightarrow \infty} \sum_{p < p_0} |(\varphi_\varepsilon, \phi_{p,\ell})|^2 \log(\rho_{p,\ell} + \eta_\ell) = \sum_{p < p_0} |(\varphi, \phi_p)|^2 \log(\rho_p).$$

Note that  $\log(\rho_p)$  is well defined according to Proposition 3.5. Then, since  $-\log(\eta_\ell + \rho_{p,\ell}) \geq 0$  for  $p \geq p_0$ , it follows from Fatou's lemma for series that

$$-\sum_{p \geq p_0} |(\varphi, \phi_p)|^2 \log(\rho_p) \leq -\liminf_{\varepsilon \rightarrow 0, \ell \rightarrow \infty} \sum_{p \geq p_0} |(\varphi_\varepsilon, \phi_{p,\ell})|^2 \log(\rho_{p,\ell} + \eta_\ell).$$

It remains now to pass to the limit in  $\mathcal{Q}_{\eta_\ell}(\varphi_\varepsilon)$ . The limit in  $\eta_\ell$  is done in the exact same way as in the proof of Proposition 3.10, we simply use  $|\varphi_\varepsilon| \leq \varepsilon^{-1/2} \sqrt{n}$  instead of (29) in order to apply dominated convergence. We then replace all terms in  $\eta_\ell$  by their limit and treat now the term in  $\mathcal{Q}_\star(\varphi_\varepsilon)$  involving  $\nabla \varphi_\varepsilon$ . We have that  $\nabla \varphi_\varepsilon$  is given by (17) and converges to  $\nabla \varphi$  a.e. as  $\varepsilon \rightarrow 0$ . With the estimate (30) and the fact that the r.h.s is in  $L^2(\mathbb{R}^d)$  because  $\varphi \in H_\omega^1(\mathbb{R}^d)$ , we can invoke dominated convergence and pass to the limit and obtain

$$\lim_{\varepsilon \rightarrow 0} \int_{\mathbb{R}^d} |\nabla \varphi_\varepsilon|^2 dx = \int_{\mathbb{R}^d} |\nabla \varphi|^2 dx.$$

It remains to treat

$$\int_{\mathbb{R}^d} \left( -\frac{\nabla \sqrt{n} \cdot \nabla |\varphi_\varepsilon|^2}{\sqrt{n}} + \frac{2|\nabla \sqrt{n}|^2 - k[\varrho_\star]}{n} |\varphi_\varepsilon|^2 \right) dx.$$

Using that  $\nabla \varphi_\varepsilon \rightarrow \nabla \varphi$  and  $\varphi_\varepsilon \rightarrow \varphi$  both a.e., together with (30) and  $|\varphi_\varepsilon| \leq |\varphi|$ , we can use dominated convergence to pass to the limit above and obtain the desired result. This ends the proof.  $\square$

### 3.4 Conclusion and proof of the main theorem

We have already obtained in Proposition 3.5 that  $\varrho_\star$  is full rank. We prove now relation (9). According to Proposition 3.11, we have, since  $\rho_p < 1$  for all  $p \in \mathbb{N}$ ,

$$-\log(\rho_0) \|\varphi\|^2 \leq \|\varphi\|_{\mathfrak{H}}^2 \leq \mathcal{Q}_\star(\varphi), \quad \forall \varphi \in H_\omega^1(\mathbb{R}^d). \quad (32)$$

This shows in particular that  $\mathcal{Q}_\star$  is nonnegative and as a consequence

$$\int_{\mathbb{R}^d} \frac{k[\varrho_\star]}{n} |\varphi|^2 dx \leq \int_{\mathbb{R}^d} n \left| \nabla \left( \frac{\varphi}{\sqrt{n}} \right) \right|^2 dx + \int_{\mathbb{R}^d} V_\star |\varphi|^2 dx,$$

which yields that  $H_\omega^1(\mathbb{R}^d) = H_\star^1(\mathbb{R}^d)$ . Besides, we deduce from (32) that

$$-\log(\rho_0) \leq \inf_{\varphi \in H_\star^1, \|\varphi\|=1} \mathcal{Q}_\star(\varphi).$$

According to Proposition 3.10, we have  $\mathcal{Q}_\star(\phi_0) = -\log(\rho_0)$ , and therefore the above infimum is attained at  $\phi_0$ . At any order  $p > 1$ , we have, for any  $\varphi \in \mathcal{K}_p$ ,

$$-\log(\rho_p) \|\varphi\|^2 \leq \|\varphi\|_{\mathfrak{H}}^2 \leq \mathcal{Q}_\star(\varphi) \quad \text{so that} \quad -\log(\rho_p) \leq \inf_{\varphi \in \mathcal{K}_p} \mathcal{Q}_\star(\varphi),$$

and, according to Proposition 3.10, the infimum is attained at  $\phi_p$ . This proves (9). Consider now  $\mathcal{Q}_{\star,S}$ , which is densely defined since  $\{\phi_p\}_{p \in \mathbb{N}}$  is an orthonormal basis of  $L^2(\mathbb{R}^d)$ . Following Proposition 3.10, we have

$$\mathcal{Q}_{\star,S}(u, v) = (u, v)_{\mathfrak{H}}, \quad \forall u, v \in S.$$

Since  $\mathfrak{H}$  is complete, this shows that  $\mathcal{Q}_{\star,S}$  is closable and that

$$\overline{\mathcal{Q}}_{\star,S}(u, v) = (u, v)_{\mathfrak{H}} = (u, -\log(\varrho_{\star})v), \quad \forall u \in \mathfrak{H}, \forall v \in D(-\log(\varrho_{\star})),$$

where

$$D(-\log(\varrho_{\star})) = \left\{ \varphi \in L^2(\mathbb{R}^d) : \sum_{p \in \mathbb{N}} (\log(\rho_p))^2 |(\phi_p, \varphi)|^2 < \infty \right\}.$$

Finally, the fact that  $H_{\star}^1(\mathbb{R}^d) \subset \mathfrak{H}$  is a consequence of Proposition 3.11. This ends the proof of the theorem.

## 4 Proofs of some lemmas

### 4.1 Proof of Lemma 3.1

**Step 1:** We show first that  $\varrho(t) \in \mathcal{A}$  for all  $t \geq 0$ . It is direct to see that  $\varrho(t)$  is nonnegative since  $t \geq 0$ , and that it is trace class as products of the trace class operator  $\varrho_{\star} + tP_{\varphi}$  and the bounded multiplication operator by  $a(t) \leq 1$ . It then follows that

$$n[\varrho(t)] = a(t)^2(n + t|\varphi|^2) = n,$$

i.e.  $\varrho(t)$  satisfies the constraint  $n[\varrho(t)] = n$

**Step 2:** We want to prove that  $\varrho(t) \in \mathcal{E}$ . For this, we write, by linearity of the trace,

$$E(\varrho(t)) = E(a(t)\varrho_{\star}a(t)) + tE(a(t)P_{\varphi}a(t)),$$

and use the following result, which is just a consequence of the definition of Hilbert-Schmidt operators:

**Lemma 4.1** *Let  $\sigma$  be a bounded operator and  $A$  be a self-adjoint operator. Then  $A\sigma\sigma^*A \in \mathcal{J}_1$  if and only if  $A\sigma \in \mathcal{J}_2$ .*

According to [13, Theorem 6.22, item (g)],  $A\sigma \in \mathcal{J}_2$  holds provided there is an orthonormal basis  $\{e_p\}_{p \in \mathbb{N}}$  of  $L^2(\mathbb{R}^d)$  such that

$$\sum_{p \in \mathbb{N}} \|A\sigma e_p\|^2 < \infty.$$

We use this result with  $A = \sqrt{H_0}$  and  $\sigma = a(t)\sqrt{\varrho_{\star}}$  as follows. Noticing first that

$$\left\| \sqrt{H_0} (a(t)\varrho_{\star}^{1/2}\phi_p) \right\| = \left\| \nabla (a(t)\varrho_{\star}^{1/2}\phi_p) \right\|,$$

we have

$$\begin{aligned} E(a(t)\varrho_{\star}a(t)) &= \sum_{p \in \mathbb{N}} \left\| \sqrt{H_0} (a(t)\varrho_{\star}^{1/2}\phi_p) \right\|^2 = \sum_{p \in \mathbb{N}} \rho_p \|\nabla(a(t)\phi_p)\|^2 \\ &= \int_{\mathbb{R}^d} \sum_{p \in \mathbb{N}} \rho_p (|\nabla a(t)|^2 |\phi_p|^2 + 2a(t)\nabla a(t) \cdot \Re(\phi_p^* \nabla \phi_p) + a(t)^2 |\nabla \phi_p|^2) dx \\ &= \int_{\mathbb{R}^d} (n|\nabla a(t)|^2 + a(t)\nabla a(t) \cdot \nabla n + a(t)^2 k[\varrho_{\star}]) dx. \end{aligned} \tag{33}$$

Above, the exchange of the integral and the summation is justified since the integrand is positive. We also used the fact that

$$n = \sum_{p \in \mathbb{N}} \rho_p |\phi_p|^2, \quad \nabla n = 2 \sum_{p \in \mathbb{N}} \rho_p \Re(\phi_p^* \nabla \phi_p), \quad \text{and} \quad k[\varrho_\star] = \sum_{p \in \mathbb{N}} \rho_p |\nabla \phi_p|^2,$$

with convergence of the series in  $L^1(\mathbb{R}^d)$  and almost everywhere. Regarding  $E(a(t)P_\varphi a(t))$ , we have

$$E(a(t)P_\varphi a(t)) = \|\nabla(a(t)\varphi)\|^2 = \|\varphi \nabla a(t)\|^2 + \|a(t) \nabla \varphi\|^2 + 2\Re(\varphi \nabla a(t), a(t) \nabla \varphi),$$

which also gives

$$\begin{aligned} & \int_{\mathbb{R}^d} (n |\nabla a(t)|^2 + a(t) \nabla a(t) \cdot \nabla n) dx + t E(a(t)P_\varphi a(t)) \\ &= \int_{\mathbb{R}^d} ((n(t) \nabla a(t) + a(t) \nabla n(t)) \cdot \nabla a(t) + t a(t)^2 |\nabla \varphi|^2) dx. \end{aligned}$$

Thus, we find the expression

$$E(\varrho(t)) = \int_{\mathbb{R}^d} ((n(t) \nabla a(t) + a(t) \nabla n(t)) \cdot \nabla a(t) + a(t)^2 (k[\varrho_\star] + t |\nabla \varphi|^2)) dx.$$

Note that it is crucial to express  $E(\varrho(t))$  in terms of the moments of  $\varrho_\star$  in order to exploit the fact that  $\varphi \in H_\omega^1(\mathbb{R}^d)$ . Working directly with  $\varrho_\star$  and  $a(t)$  as operators would make it difficult to justify the calculations leading to (13). From there, with the relation

$$\nabla a(t) = \frac{\nabla \sqrt{n}}{\sqrt{n(t)}} - \frac{a(t) \nabla \sqrt{n(t)}}{\sqrt{n(t)}},$$

we find

$$\begin{aligned} & (n(t) \nabla a(t) + a(t) \nabla n(t)) \cdot \nabla a(t) \\ &= \left( \sqrt{n(t)} \nabla \sqrt{n} - \sqrt{n(t)} a(t) \nabla \sqrt{n(t)} + a(t) \nabla n(t) \right) \cdot \nabla a(t) \\ &= \left( \nabla \sqrt{n} - a(t) \nabla \sqrt{n(t)} + a(t) \frac{\nabla n(t)}{\sqrt{n(t)}} \right) \cdot (\nabla \sqrt{n} - a(t) \nabla \sqrt{n(t)}) \\ &= \left( \nabla \sqrt{n} + a(t) \nabla \sqrt{n(t)} \right) \cdot (\nabla \sqrt{n} - a(t) \nabla \sqrt{n(t)}) \\ &= |\nabla \sqrt{n}|^2 - a(t)^2 |\nabla \sqrt{n(t)}|^2, \end{aligned}$$

leading to

$$E(\varrho(t)) = \int_{\mathbb{R}^d} \left( |\nabla \sqrt{n}|^2 - a(t)^2 |\nabla \sqrt{n(t)}|^2 + a(t)^2 (k[\varrho_\star] + t |\nabla \varphi|^2) \right) dx. \quad (34)$$

We remark that

$$|\nabla \sqrt{n(t)}| \leq |\nabla \sqrt{n}| + \sqrt{t} |\nabla \varphi|,$$

so that  $\nabla \sqrt{n(t)} \in (L^2(\mathbb{R}^d))^d$  for any  $t \geq 0$ . Since  $a(t)$  bounded by one,  $\nabla \sqrt{n}$  and  $\nabla \varphi$  are in  $(L^2(\mathbb{R}^d))^d$  and  $k[\varrho_\star]$  is in  $L^1(\mathbb{R}^d)$ , it follows that  $E(\varrho(t))$  is finite and, as a consequence, that  $\varrho(t) \in \mathcal{E}$ .

**Step 3:** We show that  $t \rightarrow E(\varrho(t))$  is differentiable. First of all, it is clear that  $a(t)$  and  $\sqrt{n(t)}$  are continuously differentiable as functions of  $t$ , for almost all  $x$ . Denote by  $a_1(t, x)$  the integrand in  $E(\varrho(t))$ , which is then continuously differentiable as a function of  $t$ . With the following relations

$$\partial_t a(t) = -\frac{a(t)|\varphi|^2}{2n(t)} \quad \text{and} \quad \partial_t \nabla \sqrt{n(t)} = \frac{\Re(\varphi^* \nabla \varphi)}{\sqrt{n(t)}} - \frac{|\varphi|^2 \nabla \sqrt{n(t)}}{2n(t)},$$

tedious but straightforward calculations show that

$$|\partial_t a_1(t)| \leq C \left( \frac{|\nabla \sqrt{n}|^2}{n} |\varphi|^2 + |\nabla \varphi|^2 + \frac{k[\varrho_\star]}{n} |\varphi|^2 \right).$$

Since  $\varphi \in H_\omega^1(\mathbb{R}^d)$ , the function of the r.h.s above is integrable, and standard results about Lebesgue integration imply then that  $E(\varrho(t)) \in C^1(\mathbb{R}^+)$ .

**Step 4:** We consider now (13). Differentiating  $E(\varrho(t))$  leads to

$$\begin{aligned} \partial_t E(\varrho(t)) &= -2 \int_{\mathbb{R}^d} a(t) \left( |\nabla \sqrt{n(t)}|^2 \partial_t a(t) + a(t) \nabla \sqrt{n(t)} \cdot \partial_t \nabla \sqrt{n(t)} \right) dx \\ &\quad + \int_{\mathbb{R}^d} (2a(t) \partial_t a(t) (k[\varrho_\star] + t|\nabla \varphi|^2) + a(t)^2 |\nabla \varphi|^2) dx \\ &= \int_{\mathbb{R}^d} a(t)^2 \left( 2 \frac{|\nabla \sqrt{n(t)}|^2}{n(t)} |\varphi|^2 - \frac{\nabla \sqrt{n(t)}}{\sqrt{n(t)}} \cdot \nabla |\varphi|^2 \right) dx \\ &\quad + \int_{\mathbb{R}^d} a(t)^2 \left( |\nabla \varphi|^2 - \frac{|\varphi|^2}{n(t)} (k[\varrho_\star] + t|\nabla \varphi|^2) \right) dx. \end{aligned}$$

Since

$$a(0) = 1 \quad \text{and} \quad n(0) = n,$$

we directly deduce that

$$\frac{dE(\varrho(t))}{dt} \Big|_{t=0} = \int_{\mathbb{R}^d} \left( |\nabla \varphi|^2 + 2 \frac{|\nabla \sqrt{n}|^2}{n} |\varphi|^2 - \frac{\nabla \sqrt{n}}{\sqrt{n}} \cdot \nabla |\varphi|^2 - \frac{|\varphi|^2}{n} k[\varrho_\star] \right) dx,$$

which is the desired result.

## 4.2 Proof of Lemma 3.2.

First of all, it is clear that for any  $t \geq 0$  and  $x \in \mathbb{R}^d$ ,

$$a(t, x) = \frac{\sqrt{n(x)}}{\sqrt{n(x) + t|\varphi(x)|^2}}$$

is bounded by one. Furthermore, we have

$$\partial_t a(t) = -\frac{a(t)|\varphi|^2}{2n(t)}$$

which is bounded by  $M^2/2$  according to the assumption on  $\varphi$ . With

$$\partial_t \varrho(t) = a(t)P_\varphi a(t) + \partial_t a(t)(\varrho_\star + tP_\varphi)a(t) + a(t)(\varrho_\star + tP_\varphi)\partial_t a(t),$$

it follows by inspection that  $\varrho(t) \in C^1(\mathbb{R}^+, \mathcal{J}_1)$  since  $\varrho_\star$  and  $P_\varphi$  are trace class and  $a$  and  $\partial_t a$  are bounded and continuous w.r.t  $t$ .

### 4.3 Proof of Lemma 3.7

We can see that  $a_\eta$  is bounded a.e. since, for any  $t \in [-t_0, t_0]$ ,

$$a_\eta^2(t) \leq \frac{\sum_{j \neq p, q} \rho_{j,\eta} |\phi_{j,\eta}|^2 + \rho_{p,\eta} |\phi_{p,\eta}|^2 + \rho_{q,\eta} |\phi_{q,\eta}|^2}{\sum_{j \neq p, q} \rho_{j,\eta} |\phi_{j,\eta}|^2 + (\rho_{p,\eta} - |t|) |\phi_{p,\eta}|^2 + (\rho_{q,\eta} - |t|) |\phi_{q,\eta}|^2} \leq 2. \quad (35)$$

This shows in particular that  $\varrho_\eta(t)$  is trace class for  $t \in [-t_0, t_0]$ , and that  $n[\varrho_\eta(t)] = n$ . Furthermore, it is positive so that  $\varrho_\eta(t)$  is a density operator for  $t \in [-t_0, t_0]$ . It remains to show that  $\varrho_\eta(t) \in \mathcal{E}$ . We now follow the arguments of Step 2 of the proof of Lemma 3.1. We obtain first that

$$E(a_\eta(t)\varrho_\eta a_\eta(t)) = \int_{\mathbb{R}^d} (n|\nabla a_\eta(t)|^2 + a_\eta(t)\nabla a_\eta(t) \cdot \nabla n + a_\eta(t)^2 k[\varrho_\eta]) dx.$$

Furthermore, we have

$$\begin{aligned} E(a_\eta(t)P_\eta a_\eta(t)) &= \int_{\mathbb{R}^d} 2\Re(\nabla(a_\eta(t)\phi_{p,\eta}) \cdot \nabla(a_\eta(t)\phi_{q,\eta}^*)) dx \\ &= \int_{\mathbb{R}^d} (2\Re(\phi_{p,\eta}\phi_{q,\eta}^*) |\nabla a_\eta(t)|^2 + 2a_\eta(t)^2 \Re(\nabla\phi_{p,\eta} \cdot \nabla\phi_{q,\eta}^*)) dx \\ &\quad + \int_{\mathbb{R}^d} 2a_\eta(t)\nabla a_\eta(t) \cdot \Re(\phi_{p,\eta}\nabla\phi_{q,\eta}^* + \phi_{q,\eta}^*\nabla\phi_{p,\eta}) dx, \end{aligned}$$

leading to

$$\begin{aligned} E(\varrho_\eta(t)) &= \int_{\mathbb{R}^d} (n_\eta(t)\nabla a_\eta(t) + a_\eta(t)\nabla n_\eta(t)) \cdot \nabla a_\eta(t) dx \\ &\quad + \int_{\mathbb{R}^d} (a_\eta(t)^2(k[\varrho_\eta] + 2t\Re(\nabla\phi_{p,\eta} \cdot \nabla\phi_{q,\eta}^*))) dx. \end{aligned}$$

By using the fact that

$$\nabla a_\eta(t) = \frac{\nabla \sqrt{n}}{\sqrt{n_\eta(t)}} - \frac{a_\eta(t)\nabla \sqrt{n_\eta(t)}}{\sqrt{n_\eta(t)}},$$

we deduce the expression

$$E(\varrho_\eta(t)) = \int_{\mathbb{R}^d} \left( |\nabla \sqrt{n}|^2 - a_\eta(t)^2 \left| \nabla \sqrt{n_\eta(t)} \right|^2 + a_\eta(t)^2 (k[\varrho_\eta] + 2t\Re(\nabla\phi_{p,\eta} \cdot \nabla\phi_{q,\eta}^*)) \right) dx. \quad (36)$$

Finally, since the following estimate holds for any  $t \in [-t_0, t_0]$

$$|n_\eta(t)| = |n + 2t\Re(\phi_{p,\eta}\phi_{q,\eta}^*)| \geq n/2,$$

we deduce that

$$\begin{aligned} \left| \nabla \sqrt{n_\eta(t)} \right| &\leq \frac{|\nabla n| + \rho_{p,\eta} |\phi_{p,\eta} \nabla \phi_{q,\eta}| + \rho_{q,\eta} |\phi_{q,\eta} \nabla \phi_{p,\eta}|}{n} \\ &\leq \frac{1}{2} |\nabla \sqrt{n}| + |\nabla \phi_{p,\eta}| + |\nabla \phi_{q,\eta}|, \end{aligned}$$

which enables us to bound each term of (36) since  $\phi_{p,\eta}$  and  $\phi_{q,\eta}$  belong to  $H^1(\mathbb{R}^d)$  according to (19). This shows that  $\varrho_\eta(t) \in \mathcal{E}$  for  $t \in [-t_0, t_0]$  and concludes the proof.

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