COMPACTNESS PROPERTIES FOR TRACE-CLASS OPERATORS AND APPLICATIONS TO QUANTUM MECHANICS

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Abstract. Interpolation inequalities of Gagliardo-Nirenberg type and compactness results for self-adjoint trace-class operators with finite kinetic energy are established. Applying these results to the minimization of various free energy functionals, we determine for instance stationary states of the Hartree problem with temperature corresponding to various statistics.

Key-words. Compact self-adjoint operators – Trace-class operators – mixed states – occupation numbers – Lieb-Thirring inequality – Gagliardo-Nirenberg inequality – logarithmic Sobolev inequality – optimal constants – orthonormal and sub-orthonormal systems – Schrödinger operator – asymptotic distribution of eigenvalues – free energy – embeddings – compactness results

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1. Introduction

The first eigenvalue $\lambda_{V,1}$ of a Schrödinger operator $-\Delta + V$ can be estimated using Sobolev's inequalities, [24, 22, 11]. In some recent papers, [2, 25, 5], a precise connection has been given between the optimal estimates of $\lambda_{V,1}$ in terms of a norm of V, and the optimal constants in some related *Gagliardo-Nirenberg inequalities*. Such inequalities admit optimal functions, see [26, 5]. In the case of orthonormal and sub-orthonormal systems, interpolation inequalities of Gagliardo-Nirenberg type provide information on optimal constants in inequalities, see [16, 15, 9, 8], which can be extended to *Lieb-Thirring type inequalities*, [14]. We refer to [5] for references in this direction and precise statements concerning the relation between optimal constants in these two families of inequalities, in the case of the euclidean space $\mathbb{R}^d$.

Conversely, the knowledge of Lieb-Thirring inequalities can be rephrased into interpolation inequalities for *mixed states*, which are infinite systems of orthogonal functions with occupation numbers, see [5]. It is well known that an equivalent formulation holds in terms of operators. In this paper we rewrite and extend these interpolation inequalities for *trace-class self-adjoint operators* and focus on the case of a bounded domain $\Omega \subset \mathbb{R}^d$. We also study, at the level of operators,

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the *compactness properties* of the corresponding embeddings, which somehow extend the well known properties of Sobolev's embeddings to trace-class self-adjoint operators.

An important source of motivation for us is the paper by Markowich, Rein and Wolansky, [18], which was devoted to the analysis of the stability of the Schrödinger-Poisson system. It involves in a crucial way some functionals which are a key tool of our approach, and that we will call *free energy functionals* because of their interpretation in physics. In [18], the authors refer to such functionals as *Casimir* functionals, for historical reasons in mechanics, see for example [28].

During the last few years, various results based on free energy functionals, which are sometimes also called *generalized entropy functionals,* have been achieved in the theory of partial differential equations. We can for instance quote nonlinear stability results for fluid and kinetic equations, see for instance [28, 12, 13, 21], studies of the qualitative behavior of the solutions of kinetic and diffusion equations, including large time asymptotics and diffusion limits, see for example [1, 4, 6], and applications to free boundary problems: [7], or quantum mechanics: [17, 18]. At a formal level, these various functionals are all more or less the same object, but the precise connection among them is still being studied at the moment from a mathematical point of view.

Minimizing the free energy functional for a given potential is equivalent to proving Lieb-Thirring inequalities, while the optimization on the potential provides interpolation inequalities. Such questions have been only tangentially studied in [18], since in this paper the potential is an electrostatic Poisson potential with homogeneous Dirichlet boundary conditions and therefore always positive. Here we work in a much more general setting which physically could correspond to external potentials with a singularity (for instance created by doping charged impurities in a semi-conductor) and our first task is therefore to bound from below the free energy functional, that is to establish adapted Lieb-Thirring inequalities. Our second step consists in reformulating these inequalities in terms of Gagliardo-Nirenberg type interpolation inequalities for operators, and to study the compactness properties of the corresponding embeddings. Afterwards, the minimization procedure becomes more or less trivial, thus giving for almost no work the existence of minimizers, including the case of non-linear models involving, for instance, a Poisson coupling.

This paper is organized as follows. Section 2 is devoted to definitions and preliminary results. In Subsection 2.1 we present the operator setting, that is the Sobolev-like cone $\mathcal{H}^1_+$, an appropriate set of positive trace-class operators acting on $L^2(\Omega)$. Basic properties of these cones are given in Proposition 2.1 and a regularity result concerning the density functions associated to $\mathcal{H}^1_+$ is established in Proposition 2.2. In Subsection 2.2 we define a set of trace-class operators having the form $F(-\Delta)$. To this class belong the operators generated by the Boltzmann distribution and the Fermi-Dirac statistics, see Example 2.4. In Subsection 2.2 we also introduce the *free energy functional* $\mathcal{F}_{V,\beta}(L)$, for every $L \in \mathcal{H}^1_+$.

In Section 3 we present our main results. In Subsection 3.1 we start by recovering Lieb-Thirring and Gagliardo-Nirenberg inequalities, as obtained in [5], but in the language of operators and for the case of a bounded domain, in Theorem 3.1 and 3.2 respectively. The key estimate here is a convexity inequality obtained in Lemma 3.1. In Subsection 3.2 we prove Proposition 3.2 which is crucial for dealing with non-positive potentials. Then in Subsection 3.3 we prove Theorem 3.3 which is the anounced extension of Lieb-Thirring and Gagliardo-Nirenberg inequalities, the first of our main results. Finally in Subsection 3.4 we prove our second main result, in Theorem 3.4 and Corollary 3.4, on compactness properties of the space $\mathcal{H}^1_+$.

As a simple consequence, in Section 4, we obtain the existence of minimizers in several cases of interest in quantum mechanics. Some additional references for applications in quantum mechanics are given at the end of this paper.

2. Definitions and preliminary results

Along the paper we shall assume that Ω is a bounded domain in $\mathbb{R}^d$, $d \in \mathbb{N}$. Even though all our results will be proved under this assumption on Ω, most results also hold if Ω is unbounded and appropriate assumptions are made. These assumption whould involve the eigenvalues of the Laplacian with Dirichlet boundary condition and/or the behavior of the external potential. By convention, $\mathbb{N}$ denotes the set of positive integers only.

2.1. **The operators setting.**

We denote by $\mathcal{L} = \mathcal{L}(L^2(\Omega))$ the space of bounded linear operators acting on $L^2(\Omega)$. We denote by $\mathcal{I}_\infty$ and $\mathcal{S}_\infty$ the subspaces of $\mathcal{L}$ respectively made of compact and compact self-adjoint operators.

We shall deal with elements of the space of *trace-class* operators,

$$\mathcal{I}_1 \equiv \left\{ L \in \mathcal{I}_\infty \ : \ \sum_{i \in \mathbb{N}} \left| \langle \chi_i, \, L\chi_i \rangle_{L^2(\Omega)} \right| < \infty \right\},$$

which is a subspace of the space of *Hilbert-Schmidt* operators,

$$\mathcal{I}_2 \equiv \Big\{ L \in \mathcal{I}_\infty \; : \; \sum_{i\in\mathbb{N}} \big| \big\langle \chi_i, \, |L|^2 \, \chi_i \big\rangle_{\mathrm{L}^2(\Omega)} \big| < \infty \Big\} ,$$

where $\{\chi_i\}_{i\in\mathbb{N}}$ is *any* complete orthonormal system in $\mathrm{L}^2(\Omega)$. The trace of an operator $L \in \mathcal{I}_1$ is given by

$$\mathrm{Tr}\,[L] \equiv \sum_{i\in\mathbb{N}} \big\langle \chi_i, \, L\chi_i \big\rangle_{\mathrm{L}^2(\Omega)} .$$

For the basic properties of $\mathcal{I}_1$, $\mathcal{I}_2$ and the spaces $\mathcal{S}_q$ (see definition below), we refer the reader to [19, 20]. We just recall a couple of important facts. The space $\mathcal{I}_2$ is a Hilbert space when equipped with the product $\langle L, R\rangle_2 \equiv \mathrm{Tr}\,[R^* L]$; the corresponding norm is denoted by $\|\cdot\|_2$. It is also well known that an operator $L \in \mathcal{L}$ belongs to the Hilbert-Schmidt space if and only if there is a function $K_L \in \mathrm{L}^2(\Omega\times\Omega)$, the *kernel of* L, such that

$$\begin{aligned} \|L\|_2^2 &= \iint_{\Omega\times\Omega} |K_L(x,y)|^2 \, dx\, dy \\ (L\eta)(x) &= \int_\Omega K_L(x,y)\, \eta(y)\, dy \quad \text{for } x \in \Omega \text{ a.e.} , \quad \forall\, \eta \in \mathrm{L}^2(\Omega) . \end{aligned}$$

Remark 2.1. From now on we only deal with self-adjoint operators. For $L \in \mathcal{S}_\infty$ we denote by $\{\nu_i(L)\}_{i\in\mathbb{N}}$, or simply $\{\nu_i\}_{i\in\mathbb{N}}$ if there is no ambiguity, the sequence of eigenvalues of L counted with multiplicity (which is well defined by the Hilbert-Schmidt theorem). We adopt the convention that $\{\nu_i\}_{i\in\mathbb{N}}$ is ordered in a way such that $\{|\nu_i|\}_{i\in\mathbb{N}}$ is non-increasing, and if both ν and $-\nu$ are eigenvalues, $-|\nu|$ comes first. We will denote by $\{\psi_i(L)\}_{i\in\mathbb{N}}$, or simply $\{\psi_i\}_{i\in\mathbb{N}}$ if there is no ambiguity, an associated $\mathrm{L}^2(\Omega)$-*complete orthonormal* system of eigenfunctions.

We also consider the Banach space

$$\mathcal{S}_q \equiv \Big\{ L \in \mathcal{S}_\infty \; : \; \|L\|_q \equiv \Big(\sum_{i\in\mathbb{N}} |\nu_i|^q \Big)^{1/q} < \infty \Big\} ,$$

where $q \in [1,\infty)$, which is the closure of the space of finite rank self-adjoint operators with respect to the norm $\|\cdot\|_q$. It can be proved that the two given definitions of $\|L\|_2$ coincide. If $1 \le q \le \infty$ and $q^{-1} + r^{-1} = 1$, then

$$\|A\,B\|_1 \le \|A\|_q \, \|B\|_r, \quad \forall\, A \in \mathcal{S}_q\,,\; B \in \mathcal{S}_r\,.$$

It is also well known that for $L \in \mathcal{S}_1$ the function ρ_L given by

$$\rho_L(x) \equiv \sum_{i\in\mathbb{N}} \nu_i \, |\psi_i(x)|^2, \quad x \in \Omega \text{ a.e.} , \tag{2.1}$$

is in $L^1(\Omega)$ and does not depend on the special choice of the complete orthonormal sequence $\{\psi_i\}_{i\in\mathbb{N}}$. If, additionally, L is a non-negative operator, ρ_L is also non-negative and it is called the *density function associated to* L. Such a definition is consistent with the density operator formalism in quantum mechanics.

Definition 2.1. An operator $L \in \mathcal{S}_1$ is in the *Sobolev-like cone* $\mathcal{H}^1$ if $\{\psi_i(L)\}_{i\in\mathbb{N}} \subset H^1_0(\Omega)$ and

$$\langle\!\langle L \rangle\!\rangle_2 \equiv \sum_{i\in\mathbb{N}} |\nu_i| \cdot \|\psi_i\|^2_{H^1_0(\Omega)} < \infty \,. \tag{2.2}$$

The following proposition collects some basic facts:

Proposition 2.1. *The Sobolev-like cone $\mathcal{H}^1$ of trace-class operators satisfies the following properties:*

i) *Given $L \in \mathcal{H}^1$, $\langle\!\langle L \rangle\!\rangle_2$ depends only on L and not on the particular basis of eigenfunctions of L.*

ii) *$\mathcal{H}^1$ is a cone in the sense that for every $L \in \mathcal{H}^1$ and for all $\alpha \in \mathbb{R}$, $\alpha L \in \mathcal{H}^1$.*

iii) *For every $L \in \mathcal{H}^1$ and $\alpha \in \mathbb{R}$*

$$\langle\!\langle \alpha L \rangle\!\rangle_2 = |\alpha| \langle\!\langle L \rangle\!\rangle_2 \,,$$

and $\langle\!\langle \alpha L \rangle\!\rangle_2 = 0$ if and only if $L = 0$ or $\alpha = 0$.

iv) *There exists a constant $c_2 = c_2(\Omega)$ such that*

$$\|L\|_1 \le c_2 \, \langle\!\langle L \rangle\!\rangle_2, \quad \forall\, L \in \mathcal{H}^1 \,. \tag{2.3}$$

Property (iii) justifies the denomination of *cone*. We define the *kinetic energy* functional on the *positive cone* of positive operators $\mathcal{H}^1_+ \equiv \{L \in \mathcal{H}^1 :\; L \ge 0\}$, as

$$\mathcal{K}(L) \equiv \sum_{i\in\mathbb{N}} \nu_i \int_\Omega |\nabla\psi_i(x)|^2 \, dx \,, \quad L \in \mathcal{H}^1_+ \,.$$

We shall simply say that $\mathcal{K}(L)$ is the *kinetic energy* of L.

Remark 2.2. We may extend the definitions given before to a more general situation. Given $l \in \mathbb{N}$ and $p \in [1, \infty[$, we say that an operator $L \in \mathcal{S}_1$ is in the *Sobolev-like cone* $\mathcal{W}^{l,p}$ if $\{\psi_i(L)\}_{i\in\mathbb{N}} \subset W^{1,p}_0(\Omega) \cap W^{l,p}(\Omega)$ and

$$\sum_{i\in\mathbb{N}} |\nu_i| \cdot \|\psi_i\|^p_{W^{l,p}(\Omega)} < \infty \,.$$

We observe that the above term may be basis-dependent, but we could still define a notion similar to $\langle\!\langle \cdot \rangle\!\rangle_2$ by taking the infimum on all possible bases. Many properties of usual Sobolev spaces can be adapted to $\mathcal{W}^{l,p}$

sets of operators. For instance, $\mathcal{W}^{l_2,p} \subset \mathcal{W}^{l_1,p}$ if $l_1 \le l_2$ and $\mathcal{W}^{l,q} \subset \mathcal{W}^{l,p}$ if $1 \le p < q < \infty$. Although some of our results can be extended to these cones, for simplicity we will not go further in this direction.

The following result, which is a short version of Theorem 3.4, says that the embedding $\mathcal{H}^1_+ \subset \mathcal{I}_1$ equipped with $\mathcal{K}$ is compact and plays a role similar to the embedding $H^1_0(\Omega) \hookrightarrow \mathrm{L}^2(\Omega)$.

Theorem 2.1. *Let $\{L_n\}_{n\in\mathbb{N}}$ be a sequence in $\mathcal{H}^1_+$ such that $\{\mathcal{K}(L_n)\}_{n\in\mathbb{N}}$ is bounded. Then, up to a subsequence, $\{L_n\}_{n\in\mathbb{N}}$ converges in trace norm $\|\cdot\|_1$ to some L in $\mathcal{H}^1_+$.*

Exactly as for the embedding $\mathrm{H}^1_0(\Omega) \hookrightarrow \mathrm{L}^2(\Omega)$, some interpolation inequalities are associated with this compactness result. These inequalities are presented in Theorem 3.2, thus generalizing to self-adjoint trace-class operators the usual Gagliardo-Nirenberg inequalities.

The Sobolev-like cones $\mathcal{H}^1$ and $\mathcal{H}^1_+$ are analogues of $\mathrm{H}^1_0(\Omega)$ and $\mathrm{H}^1_{0,+}(\Omega) = \{u \in \mathrm{H}^1_0(\Omega) \,:\, u \ge 0\}$ at the level of self-adjoint compact operators. This results in integrability properties for the function $\rho_L(x) = \sum_{i\in\mathbb{N}} \nu_i\,|\psi_i(x)|^2$, defined in (2.1), which are the counterpart of Sobolev's embeddings.

Proposition 2.2. *For any $L \in \mathcal{H}^1$, the function ρ_L belongs to the space $\mathrm{W}^{1,r}(\Omega) \cap \mathrm{L}^q(\Omega)$ with r and q in the following ranges:*

- ***i)*** *for all $q \in [1,\infty]$ and $r \in [1,2]$ if $d = 1$,*
- ***ii)*** *for all $q \in [1,\infty[$ and $r \in [1,2]$ if $d = 2$,*
- ***iii)*** *for all $q \in [1, d/(d-2)]$ and $r \in [1, d/(d-1)]$ if $d \ge 3$.*

Proof. Assume that $d \ge 3$ and $r \in [1, d/(d-1)]$. Using the convexity of $s \mapsto |s|^r$, Hölder's and Sobolev's inequalities, we obtain

$$\begin{aligned}
\int_\Omega |\nabla\rho_L|^r\,dx &\le 2^r \int_\Omega \Big(\sum_{i\in\mathbb{N}} |\nu_i\,\psi_i\,\nabla\psi_i|\Big)^r dx \\
&\le \Big(2\sum_{j\in\mathbb{N}}|\nu_j|\Big)^r \int_\Omega \sum_{i\in\mathbb{N}} \Big(\tfrac{|\nu_i|}{\sum_{j\in\mathbb{N}}|\nu_j|}\Big) |\psi_i|^r |\nabla\psi_i|^r\,dx \\
&\le 2^r \Big(\sum_{j\in\mathbb{N}}|\nu_j|\Big)^{r-1} \sum_{i\in\mathbb{N}} |\nu_i| \left(\int_\Omega |\nabla\psi_i|^2\right)^{\frac{r}{2}} \left(\int_\Omega |\psi_i|^{\frac{2r}{2-r}}\right)^{1-\frac{r}{2}} \\
&\le 2^r\, s_r^r\, \|L\|_1^{r-1}\, \mathcal{K}(L)
\end{aligned}$$

where s_r is the optimal constant in Sobolev's embedding $H^1_0(\Omega) \hookrightarrow L^{\frac{2r}{2-r}}(\Omega)$ found by Aubin and Talenti. Thus, from (2.3) we find

$$\|\nabla\rho_L\|_{L^r(\Omega)} \le 2\,s_r\,\|L\|_1^{1-\frac{1}{r}} \mathcal{K}^{\frac{1}{r}}(L) \le 2\,s_r\,c_2^{1-\frac{1}{r}}\,\mathcal{K}(L)$$

where $c_2 = c_2(\Omega, 2)$ is the Poincaré constant. Therefore, by the critical Sobolev embedding, we finally have

$$\|\rho_L\|_{L^{d/(d-2)}(\Omega)} \leq s_{d/(d-1)} \|\nabla \rho_L\|_{L^{d/(d-1)}(\Omega)} \leq 2\, s_{d/(d-1)}^2\, c_2^{1-\frac{1}{r}}\, \mathcal{K}(L) < \infty\,.$$

The cases $d = 1,\, 2$ follow similarly from the Sobolev inequalities, with the corresponding restrictions on q and r. □

2.2. **Operators of the form $\mathbf{F(-\Delta)}$ and Free Energy functionals.** We recall that $\Omega \subset \mathbb{R}^d$ is assumed to be bounded. For a potential $V = V(x)$ defined on Ω and a positive number $\alpha > 0$, we consider the following condition:

(V_α) The Schrödinger operator $-\alpha\,\Delta + V$, with Dirichlet boundary conditions, has a sequence of eigenelements

$$\{(\lambda^\alpha_{V,i},\, \phi^\alpha_{V,i})\}_{i\in\mathbb{N}} \subset \mathbb{R} \times \mathrm{H}^1_0(\Omega) \tag{2.4}$$

such that $\{\phi^\alpha_{V,i}\}_{i\in\mathbb{N}}$ is a complete orthonormal system in $\mathrm{L}^2(\Omega)$ and $\lambda^\alpha_{V,i} \to \infty$ as $i \to \infty$.

When V and α satisfies (V_α), we shall say that a function $F : \mathbb{R} \to \mathbb{R} \cup \{\infty\}$ is of Casimir class $\mathcal{C}^\alpha_V$ if it is convex and

$$\sum_{i\in\mathbb{N}} F(\lambda^\alpha_{V,i}) \quad \text{is finite.}$$

It is clear that $\mathcal{C}^\alpha_V$ is a convex cone, that is, it is convex and stable under addition and multiplication by a positive constant. When $\alpha = 1$ we consider condition (V_1) and we shall simply write $\lambda_{V,i}$, $\phi_{V,i}$ and $\mathcal{C}_V$ instead of $\lambda^1_{V,i}$, $\phi^1_{V,i}$ and $\mathcal{C}^1_V$, respectively.

Example 2.1. The properties of the Laplacian with homogeneous Dirichlet boundary conditions are well known (see *e.g.* [3, Theorem IX.31]). This corresponds to $V = 0$ and $\alpha = 1$ in Condition (V_α). We notice that if V is a potential which is bounded from below, say by a constant λ, the eigenvalues $\lambda_{V,i}$ satisfy $\lambda_{V,i} \geq \lambda_{0,i} + \lambda$, for all $i \in \mathbb{N}$, and therefore the sequence $\{\lambda_{V,i}\}_{i\in\mathbb{N}}$ diverges, since $\{\lambda_{0,i}\}_{i\in\mathbb{N}}$ diverges.

The Spectral Theorem, see for instance [19, Theorem VIII.5] allows us to define the trace-class operator $F(-\alpha\,\Delta + V)$ for each $F \in \mathcal{C}^\alpha_V$, whenever $\alpha \in \mathbb{R}_+$ and V verifies (V_α). In this case, it follows that the spectrum $\sigma(-\alpha\,\Delta + V) \equiv \{\lambda^\alpha_{V,i} :\ i \in \mathbb{N}\}$ is contained in $\mathrm{Dom}(F) \equiv \{s \in \mathbb{R} :\ F(s) < \infty\}$.

Example 2.2. Let $\gamma > \gamma_d \equiv d/2$. Then, as we shall see below,

$$\sum_{i\in\mathbb{N}} (\lambda_{0,i})^{-\gamma} < \infty\,, \tag{2.5}$$

so that the function

$$F(s) = \begin{cases} s^{-\gamma} & \text{if } s \geq 0 \;, \\ +\infty & \text{if } s < 0 \;, \end{cases}$$

belongs to the Casimir class $\mathcal{C}_0$ and therefore $(-\Delta)^{-\gamma}$ is a trace-class operator.

Example 2.3. More generally, let $F : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ be a non-increasing convex function which is non-negative and such that for any $s \geq 0$ large,

$$F(s) \leq \frac{C}{(1+s)^{\varepsilon + d/2}} \;,$$

for some constants C, $\varepsilon > 0$. Then heuristically we have that $F(\lambda_{0,i})$ is summable and can be estimated by $\sum_{k\in\mathbb{N}} F(k) \cdot \#A(k)$, for $d \geq 3$, where $A(k) \equiv \{i \in \mathbb{N} : \; k < \lambda_{0,i} \leq k+1\}$. Using Weyl's estimate [27], $\#A(k)$ grows like $k^{d/2-1}$ for large k, it follows that $F(k)\cdot\#A(k)$ behaves like $k^{-1-\varepsilon}$ as $k \to \infty$. Consequently $\sum_{i\in\mathbb{N}} F(\lambda_{0,i})$ is finite and then F belongs to the Casimir class $\mathcal{C}_0$.

Example 2.4. Assume $f : \mathbb{R} \to \mathbb{R}$ is a *Casimir function* (see [18]), that is a function that satisfies the following properties:

- **i)** There exists $s_1 \in [-\infty, \infty)$ such that $f(s) = \infty$ for any $s \in (-\infty, s_1)$.
- **ii)** f is continuous on (s_1, ∞).
- **iii)** There exists $s_2 \in (s_1, \infty]$ such that $f(s) > 0$ for any $s \in (s_1, s_2)$ and $f(s) = 0$ for any $s \geq s_2$.
- **iv)** f is strictly decreasing on (s_1, s_2) .
- **v)** If $s_2 = \infty$, there exists two positive constants ε and C such that for any $s \geq 0$, large,

$$f(s) \leq \frac{C}{(1+s)^{\varepsilon+1+d/2}} \;.$$

Then the function

$$F(s) = \int_s^\infty f(t)\; dt \tag{2.6}$$

falls in the class of functions of the Example 2.3. Under these conditions $f(-\Delta)$ is also a trace-class operator if one requires $\varepsilon > 1$, see [18]. The function of Example 2.2, the Fermi-Dirac statistics defined by $f(s) = \int_{\mathbb{R}^d} \frac{dv}{\alpha + e^{s+|v|^2/2}}$ and the Boltzmann distribution $f(s) = e^{-\alpha s}$, where $\alpha > 0$, are Casimir functions.

We continue by introducing the entropy functionals, which can be generated by elements in the class $\mathcal{C}_V^\alpha$.

Definition 2.2. Given $L \in \mathcal{H}^1_+$ and a convex function $\beta : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ such that $\beta(0) = 0$, we shall call the value

$$\mathcal{E}_\beta(L) \equiv \mathrm{Tr}\,[\beta(L)] = \sum_{i \in \mathbb{N}} \beta(\nu_i(L))$$

the *β-entropy* of L provided $\mathcal{E}_\beta(L) \in (-\infty, \infty]$. In this case we say that β is an *entropy seed*. Additionally, if $V \in \mathrm{L}^1_{\mathrm{loc}}(\Omega)$ and $L \in \mathcal{H}^1_+$ are such that $\rho_L V \in \mathrm{L}^1(\Omega)$, then we shall define the *(V, β)-free energy* of L by

$$\mathcal{F}_{V,\beta}(L) \equiv \mathcal{E}_\beta(L) + \mathcal{K}(L) + \mathcal{P}_V(L), \tag{2.7}$$

where

$$\mathcal{P}_V(L) \equiv \mathrm{Tr}\,[VL] = \int_\Omega V(x)\rho_L(x)dx$$

shall be referred to as the *V-potential energy of L.*

We shall say that an entropy seed β is *generated* by the convex function F if

$$\beta(s) = F^*(-s)\ , \quad s \in \mathbb{R}\ ,$$

where for a convex function $\theta : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ such that $\theta \not\equiv +\infty$, we denote by θ^* the Legendre-Fenchel transform of θ, that is the function defined by

$$\theta^*(\nu) \equiv \sup_{\lambda \in \mathbb{R}} \{\nu\lambda - \theta(\lambda)\} \quad \forall\, \nu \in \mathbb{R}\ . \tag{2.8}$$

Example 2.5. Let $\gamma > \gamma_d \equiv d/2$ and

$$\beta_m(s) = \begin{cases} \infty & \text{if} \quad s < 0\ , \\ -\,c_m\, s^m & \text{if} \quad s \geq 0\ , \end{cases}$$

where $c_m = (1-m)^{m-1} m^{-m}$ and $m = \frac{\gamma}{\gamma+1} \in \left(\frac{d}{d+2}, 1\right)$. The entropy seed β_m is generated by the function F of Example 2.2.

The V-potential energy functional is bounded from below in $\mathcal{H}^1_+$ if and only if V is non-negative. To be precise, we can make the following observation.

Proposition 2.3. *Let V be a potential and assume that $A \subseteq \mathcal{H}^1_+$ is such that $\alpha\, A \subseteq A$, for all $\alpha > 0$. Then*

$$\inf_{L \in A} \mathcal{P}_V(L) \geq C \tag{2.9}$$

for some constant $C \in \mathbb{R}$ if and only if

$$\inf_{L \in A} \mathcal{P}_V(L) = 0\ , \tag{2.10}$$

which is equivalent to $V \geq 0$ a.e.

Proof. If we assume (2.9) and there is $L \in A$ such that $0 > \mathcal{P}_V(L) > C$, then it should also be true that

$$0 > \mathcal{P}_V(\alpha L) = \alpha\, \mathcal{P}_V(L) > C \quad \forall\, \alpha > 0\;,$$

but this is impossible for $\alpha > |C|/|\mathcal{P}_V(L)|$. Then, as $\lim_{\alpha\to 0} \mathcal{P}(\alpha L) = 0$, we have (2.10). Next, assuming (2.10) we see that $V \geq 0$ a.e., since in the contrary we can find L such that $\mathcal{P}_V(L) < 0$. Finally, if $V \geq 0$ a.e., then (2.9) follows with $C = 0$. □

3. Main results

3.1. Lieb-Thirring and Gagliardo-Nirenberg inequalities (I).

In this subsection we interpret the results obtained in [5] in terms of the operator formalism and we adapt those results originally written in $\mathbb{R}^d$ to our context, a bounded domain $\Omega \subset \mathbb{R}^d$.

Following the setting defined in [5], we let g be a non-negative function on $\mathbb{R}_+$ such that

$$\int_0^\infty g(t)\,\left(1 + t^{-d/2}\right)\,\frac{dt}{t} < \infty \tag{3.1}$$

and consider F and G such that

$$F(s) = \int_0^\infty e^{-t\,s}\, g(t)\,\frac{dt}{t}\;, \quad G(s) = \int_0^\infty e^{-t\,s}\,(4\pi\, t)^{-d/2}\, g(t)\,\frac{dt}{t}\;. \tag{3.2}$$

Observe that $F, G : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ are convex non-increasing functions. By considering a bounded domain Ω instead of $\mathbb{R}^d$ we obtain the following adaptation of Theorem 3 in [5].

Theorem 3.1. *Let $V \in \mathrm{L}^1_{\mathrm{loc}}(\Omega)$ be a potential bounded from below. Assume moreover that $G(V)$ is in $\mathrm{L}^1(\Omega)$, with F and G given by (3.2) and g satisfying (3.1). Then we have*

$$\sum_{i\in\mathbb{N}} F(\lambda_{V,i}) = \mathrm{Tr}\left[F\left(-\Delta + V\right)\right] \leq \int_\Omega G(V(x))\, dx\;.$$

Recall that $\lambda^\alpha_{V,i}$ has been defined in (2.4). A proof of this theorem is easily achieved using [5, Th. 3] with an appropriate increasing sequence of potentials $\{V_n\}$, so that its limit is $+\infty$ outside Ω, and V in Ω. Notice that [5, Th. 3] can be recovered by taking larger and larger sets Ω.

Remark 3.1. Having in mind Example 2.1, under the hypotheses of Theorem 3.1, the function F given by (3.2), is convex and satisfies $\sum_{i\in\mathbb{N}} F(\lambda_{V,i}) < \infty$, so that F belongs to the Casimir class $\mathcal{C}_V$.

Theorem 3.1 is well illustrated with the following examples.

Example 3.1. If $V \in \mathrm{L}^1_{\mathrm{loc}}(\Omega)$ is a non-negative potential such that $V^{\frac{d}{2}-\gamma}$ is in $L^1(\Omega)$ and F is the function given in Example 2.2, then Theorem 3.1 takes the following special form

$$\mathrm{Tr}\left[(-\Delta+V)^{-\gamma}\right] = \sum_{i\in\mathbb{N}}(\lambda_{V,i})^{-\gamma} \le \frac{\Gamma(\gamma-\frac{d}{2})}{(4\pi)^{d/2}\,\Gamma(\gamma)}\int_\Omega V^{\frac{d}{2}-\gamma}\,dx\,.$$

See Theorem 1 in [5].

Example 3.2. If $V \in \mathrm{L}^1_{\mathrm{loc}}(\Omega)$ is bounded from below and such that $e^{-V} \in L^1(\Omega)$ and $F(s) = e^{-s}$ for any $s \in \mathbb{R}$, then $G(s) = (4\pi)^{-d/2}\,e^{-s}$ and Theorem 3.1 takes the following special form

$$\mathrm{Tr}\left[e^{-\Delta+V}\right] = \sum_{i\in\mathbb{N}} e^{-\lambda_{V,i}} \le \frac{1}{(4\pi)^{d/2}}\int_\Omega e^{-V}\,dx\,.$$

See Theorem 3 in [5].

We will now extend the above results to a potential that may be unbounded from below and obtain some Gagliardo-Nirenberg inequalities in the context of the operator formalism. We also bring Theorem 15 in [5], which is stated at the level of mixed states and for the whole space $\mathbb{R}^d$, to the level of operators and for a bounded domain $\Omega \subset \mathbb{R}^d$.

Theorem 3.2. *Let V be a potential verifying (V_1). Let β be an entropy seed generated by F in the Casimir class $\mathcal{C}_V$, and G a strictly convex function with with F and G related by (3.1) and (3.2). Then*

$$\mathrm{Tr}\left[F(-\Delta+V)\right] \le \int_\Omega G(V(x))\,dx\,. \tag{3.3}$$

If τ is such that $G(s) = \tau^*(-s)$ for any $s \in \mathbb{R}$, where τ and τ^* are related according to (2.8), *then for any $L \in \mathcal{H}^1_+$, we have*

$$\mathcal{K}(L) + \mathcal{E}_\beta(L) \ge \int_\Omega \tau(\rho_L)\,dx\,.$$

In order to prove Theorem 3.2, we first need to know that $\mathcal{F}_{V,\beta}$ is bounded from below.

Lemma 3.1. *Let V be a potential verifying (V_1) and let β be an entropy seed generated by $F \in \mathcal{C}_V$. Then,*

$$\mathcal{F}_{V,\beta}(L) \ge -\mathrm{Tr}\left[F(-\Delta+V)\right]\,,\quad \forall\, L \in \mathcal{H}^1_+\,. \tag{3.4}$$

Remark 3.2. Before proving Lemma 3.1, let us observe that a similar result was stated in Lemma 3 of [18], in the context of mixed states for the case of a non-negative Poisson coupling $V \in \mathrm{H}^1_0(\Omega)$. There the function F was obtained through (2.6) by a Casimir function as in

Example 2.4, and $d=3$. However, in the proof the authors use [18, Lemma 2] which is valid for functions $\psi \in \mathrm{H}^1_0(\Omega)\cup\mathrm{H}^2(\Omega)$. Our result is stated for functions $\psi\in\mathrm{H}^1_0(\Omega)$ and $F\in\mathcal{C}_V$, for an arbitrary $d\in\mathbb{N}$ and for any V verifying (V_1), not only for a nonnegative potential or a potential given by a Poisson coupling, hence slightly generalizing the results of [18].

Proof of Lemma 3.1. Let $\psi\in\mathrm{H}^1_0(\Omega)$ such that $\|\psi\|_{L^2(\Omega)}=1$. Then there exists a sequence $\{\alpha_i\}_{i\in\mathbb{N}}\subset\mathbb{R}$ such that $\psi=\sum_{i\in\mathbb{N}}\alpha_i\,\phi_{V,i}$ and $\sum_{i\in\mathbb{N}}\alpha_i^2=1$. By convexity of F, we obtain

$$\begin{aligned} F\Big(\int_\Omega|\nabla\psi|^2\,dx+\int_\Omega V\,|\psi|^2\,dx\Big) &= F\Big(\sum_{i\in\mathbb{N}}\alpha_i^2\,\lambda_{V,i}\Big)\\ &\le \sum_{i\in\mathbb{N}}\alpha_i^2\,F(\lambda_{V,i})=\big\langle\psi,\,F(-\Delta+V)\,\psi\big\rangle_{\mathrm{L}^2(\Omega)}\,. \end{aligned}\tag{3.5}$$

Observe that if ψ is an eigenfunction of $-\Delta+V$ then this inequality becomes an equality.

Since β is given by $\beta(s)=F^*(-s)$ for all $s\in\mathbb{R}$, we get

$$\beta(\nu)+\nu\,\lambda\ge-F(\lambda)\quad\forall\,\nu,\,\lambda\in\mathbb{R}\,.\tag{3.6}$$

Using (3.6) and (3.5) and substituting ν_i for ν, $\int_\Omega|\nabla\psi_i|^2+V|\psi_i|^2\,dx$ for λ and by adding over $i\in\mathbb{N}$, we get

$$\begin{aligned} \mathcal{E}_\beta(L)+\mathcal{K}(L)+\mathcal{P}_V(L) &= \sum_{i\in\mathbb{N}}\Big[\beta(\nu_i)+\nu_i\int_\Omega\big(\,|\nabla\psi_i|^2+V\,|\psi_i|^2\,\big)\,dx\Big]\\ &\ge-\sum_{i\in\mathbb{N}}F\Big(\int_\Omega|\nabla\psi_i|^2\,dx+\int_\Omega V\,|\psi_i|^2\,dx\Big)\\ &\ge-\sum_{i\in\mathbb{N}}\big\langle\psi_i,\,F(-\Delta+V)\,\psi_i\big\rangle_{\mathrm{L}^2(\Omega)}\\ &=-\mathrm{Tr}\,[F(-\Delta+V)]\ , \end{aligned}$$

which is the desired lower bound. Here $\{\psi_i\}$ is an orthonormal basis of $L^2(\Omega)$ of eigenfunctions of L, with eigenvalues $\{\nu_i\}$. □

Proof of Theorem 3.2. Using (3.3), (3.4) and using the fact that

$$\tau(s)\equiv-\big[\big(G\circ(G')^{-1}\big)(-s)+s\,(G')^{-1}(-s)\big]\ ,$$

we follow the steps as in the proof of Theorem 15 in [5]. We observe that, with no restriction, the potential can be taken bounded from below, and not only positive. Shifting g by the corresponding constant, the inequality follows. Since the inequality is independent of the lower bound, we can then extend the result to unbounded potentials. Of course, in many cases, one side or both sides of Inequality (3.3) might then be infinite, when the potential for instance takes negative values. □

This theorem provides interesting insights in the following two typical examples.

Example 3.3. We continue the case of Examples 2.2 and 2.5. Here we have $G(s) = \mathcal{C}(\gamma)\, s^{\frac{d}{2}-\gamma}$ for $s \geq 0$, extended as $+\infty$ to the interval $(-\infty, 0)$. Writing $q = \frac{2\gamma-d}{2(\gamma+1)-d} \in (0,1)$, Theorem 3.2 takes the following special form

$$\mathcal{K}(L) + \kappa(\gamma) \int_\Omega \rho_L^q \, dx \geq c_m \operatorname{Tr}[L^m] , \quad \forall L \in \mathcal{H}_+^1 , \tag{3.7}$$

where $\kappa(\gamma) \equiv (\mathcal{C}(\gamma))^{1-q} \, [(\frac{q}{q-1})^{1-q} + (\frac{q}{q-1})^{-q}]$.

Example 3.4. Consider the convex function β defined as

$$\beta(s) = \begin{cases} s \log s - s & \text{if } s > 0 , \\ 0 & \text{if } s = 0 , \\ +\infty & \text{if } s < 0 . \end{cases}$$

which is generated by the function $F(s) = e^{-s}$. If $G(s) = (4\pi)^{-d/2} \, e^{-s}$, for any $s \in \mathbb{R}$, then Theorem 3.2 shows that for $L \in \mathcal{H}_+^1$,

$$\mathcal{K}(L) + \operatorname{Tr}[L \, \log L] \geq \int_\Omega \rho_L \log \rho_L \, dx + \frac{d}{2} \log(4\pi) \int_\Omega \rho_L \, dx .$$

3.2. **Coercivity Estimates.** Our first result in this subsection shows that the free energy functional has coercivity properties, which are direct consequences of Lemma 3.1.

Proposition 3.1. *Let $\alpha > 0$ and V a potential verifying (V_α). Assume that β is an entropy seed generated by F in the Casimir class $\mathcal{C}_V^\alpha$. Then for any $L \in \mathcal{H}_+^1$ we have*

$$\mathcal{E}_\beta(L) + \alpha\, \mathcal{K}(L) + \mathcal{P}_V(L) \geq -\operatorname{Tr}[F(-\alpha\, \Delta + V)] \ .$$

Moreover, if $\alpha = 1 - \varepsilon$ with $\varepsilon \in (0,1]$, then for any $L \in \mathcal{H}_+^1$ we have

$$\mathcal{F}_{V,\beta}(L) \geq \varepsilon\, \mathcal{K}(L) - \operatorname{Tr}[F(-(1-\varepsilon)\, \Delta + V)] \ . \tag{3.8}$$

Definition 3.1. We say that the Schrödinger operator $-\Delta + V$ on $\mathrm{H}_0^1(\Omega)$ is *ε-coercive* for some $\varepsilon \in (0,1]$ if and only if

$$\lambda_{V,1}^{(1-\varepsilon)} = \sup\{\mu \in \mathbb{R} \ : \ -(1-\varepsilon)\, \Delta + V \geq \mu\} > -\infty . \tag{3.9}$$

For $\lambda \leq \lambda_{V,i}^{(1-\varepsilon)}$ we now define the free energy functional $\mathcal{F}_{V,\beta}^{\lambda} : \mathcal{H}_+^1 \to \mathbb{R} \cup \{\infty\}$ as

$$\mathcal{F}_{V,\beta}^{\lambda}(L) \equiv \mathcal{F}_{V,\beta}(L) - \lambda \, \|L\|_1 \tag{3.10}$$

where $\mathcal{F}_{V,\beta}(L)$ is defined by (2.7).

The ε-coercivity means that

$$-\Delta + V - \lambda_{V,1}^{(1-\varepsilon)} \geq -\varepsilon \, \Delta,$$

in the sense of operators with Dirichlet boundary conditions, that is in $\mathrm{H}_0^1(\Omega)$. We also observe that Condition (3.9) for $\varepsilon = 1$ means that V is bounded from below while $\lambda_{V,1}^1 = 0$ means that V is non-negative. We have the following

Proposition 3.2. *Let $\varepsilon \in (0,1]$ and V a potential such that $-\Delta + V$ is ε-coercive. Let β be an entropy seed generated by a function F. If F belongs to the Casimir class $\mathcal{C}_0^{\varepsilon/2}$, then for any $\lambda \leq \lambda_{V,1}^{(1-\varepsilon)}$ and any $L \in \mathcal{H}_+^1$ we have that*

$$\mathcal{F}_{V,\beta}^{\lambda}(L) \geq -\mathrm{Tr}\left[F\left(-\frac{\varepsilon}{2}\,\Delta\right)\right] + \frac{\varepsilon}{2}\,\mathcal{K}(L)\,. \tag{3.11}$$

If $F \in \mathcal{C}_{V-\lambda}^{1-\varepsilon}$, then for any $\lambda \leq \lambda_{V,1}^{(1-\varepsilon)}$ and any $L \in \mathcal{H}_+^1$ we have that

$$\mathcal{F}_{V,\beta}^{\lambda}(L) \geq -\mathrm{Tr}\left[F(-(1-\varepsilon)\Delta + V - \lambda)\right]. \tag{3.12}$$

Proof. Let $L \in \mathcal{H}_+^1$ and write

$$\mathcal{F}_{V,\beta}^{\lambda}(L) = \Big\{\mathcal{E}_\beta(L) + \frac{\varepsilon}{2}\,\mathcal{K}(L)\Big\} + \frac{\varepsilon}{2}\,\mathcal{K}(L) + \Big\{(1-\varepsilon)\,\mathcal{K}(L) + \mathcal{P}_V(L) - \lambda\,\|L\|_1\Big\}\,. \tag{3.13}$$

If $F \in \mathcal{C}_0^{\varepsilon/2}$, then from Proposition 3.1 we have that

$$\mathcal{E}_\beta(L) + \frac{\varepsilon}{2}\,\mathcal{K}(L) \geq -\mathrm{Tr}\left[F\left(-\frac{\varepsilon}{2}\,\Delta\right)\right]\,. \tag{3.14}$$

On the other hand, from (3.9) it follows that

$$\begin{aligned} &(1-\varepsilon)\,\mathcal{K}(L) + \mathcal{P}_V(L) - \lambda\,\|L\|_1 \\ &\quad = \sum_{i\in\mathbb{N}} \nu_i \int_\Omega \Big((1-\varepsilon)\,|\nabla\psi_i|^2 + (V-\lambda)\,|\psi_i|^2\Big)\,dx \geq 0\,, \end{aligned} \tag{3.15}$$

which together with (3.13) and (3.14) proves (3.11).

Inequality (3.12) also comes as a direct consequence of Proposition 3.1. □

As an easy consequence of Proposition 3.2 we have the following useful corollary.

Corollary 3.3. *Let $\varepsilon \in (0,1]$ and V be a potential such that $-\Delta + V$ is ε-coercive. Let β be an entropy seed generated by a function F in $\mathcal{C}_0^{\varepsilon/2} \cap \mathcal{C}_{V-\lambda}^{1-\varepsilon}$ and $\lambda \leq \lambda_{V,1}^{(1-\varepsilon)}$. If $\{L_\sigma\}_{\sigma\in\Sigma}$ is a family in $\mathcal{H}_+^1$ such that $\{\mathcal{F}_{V,\beta}^\lambda(L_\sigma)\}_{\sigma\in\Sigma}$ is bounded, then the families $\{\|L_\sigma\|_1\}_{\sigma\in\Sigma}$, $\{\mathcal{K}(L_\sigma)\}_{\sigma\in\Sigma}$, $\{\mathcal{E}_\beta(L_\sigma)\}_{\sigma\in\Sigma}$ and $\{\mathcal{P}_V(L_\sigma)\}_{\sigma\in\Sigma}$ are also bounded.*

Proof. As follows from (3.14) and (3.15) in the proof of Proposition 3.2, it is clear that the boundedness of $\mathcal{F}_{V,\beta}^\lambda(L_\sigma)$ implies the boundedness from above of $(1-\varepsilon)\,\mathcal{K}(L_\sigma) + \mathcal{P}_V(L_\sigma) - \lambda\,\|L_\sigma\|_1$ and of $\mathcal{E}_\beta$. Then we obtain the boundedness from above of $\mathcal{K}(L_\sigma)$ and therefore that of $\|L_\sigma\|_1$, by (2.3). Now the boundedness of $\mathcal{P}_V(L_\sigma)$ follows. □

3.3. **Lieb-Thirring and Gagliardo-Nirenberg inequalities (II).** We shall see in this subsection that for a potential V verifying (3.9) for some $\varepsilon \in (0,1]$, a Lieb-Thirring inequality holds and therefore an interpolation inequality can also be established. For the convenience of the reader, we recall that according to (3.10),

$$\mathcal{F}_{V,\beta}^\lambda(L) = \mathrm{Tr}\,[\,\beta(L) + (-\Delta + V - \lambda)\,L\,]\;.$$

The aim of this section is to prove the following result.

Theorem 3.3. *Let $\varepsilon \in (0,1]$ and V a potential such that $-\Delta + V$ is ε-coercive. Let F and G be defined by (3.2), with g satisfying (3.1). We assume that the entropy seeds β and G are generated by F and τ, respectively. Then, for any non-negative potential W and any $L \in \mathcal{H}_+^1$, we have that*

$$\mathcal{F}_{V+W,\beta}^\lambda(L) \geq -\varepsilon^{-d/2}\int_\Omega G(W)\,dx\;, \tag{3.16}$$

and, moreover

$$\mathcal{F}_{V,\beta}^\lambda(L) \geq \varepsilon^{-\frac{d}{2}}\int_\Omega \tau\left(\varepsilon^{\frac{d}{2}}\,\rho_L(x)\right)\,dx\;. \tag{3.17}$$

To start with, we use a change of scale to rewrite Theorem 3.1 with $-\Delta$ replaced by $-\varepsilon\,\Delta$.

Lemma 3.2. *Let W be a non-negative potential, $\varepsilon \in (0,1]$, and F and G be defined by (3.2), with g satisfying (3.1). We denote by β the entropy seed generated by F. Then, for any $L \in \mathcal{H}_+^1$,*

$$\mathcal{E}_\beta(L) - \varepsilon\,\mathcal{K}(L) + \mathcal{P}_W(L) \geq -\,\varepsilon^{-\frac{d}{2}}\int_\Omega G(W)\,dx\;. \tag{3.18}$$

Proof. Let us consider an operator $L \in \mathcal{H}_+^1$. Then we consider the scaling $\psi_i^\varepsilon(x) = \varepsilon^{d/4}\psi_i(\sqrt{\varepsilon}\,x)$, $W^\varepsilon(x) = W(\sqrt{\varepsilon}\,x)$ for any $x \in \varepsilon^{-1/2}\,\Omega$

and denote by L^ε the operator associated to L after the scaling, that is,

$$L^\varepsilon \eta = \sum_{i\in\mathbb{N}} \nu_i \langle \psi_i^\varepsilon |\, \eta\rangle_{\mathrm{L}^2(\varepsilon^{-1/2}\,\Omega)} \psi_i^\varepsilon \ , \quad \eta \in \mathrm{L}^2(\varepsilon^{-1/2}\,\Omega)\ .$$

Now observe that

$$\mathcal{E}_\beta(L) - \varepsilon\,\mathcal{K}(L) + \mathcal{P}_W(L) = \mathcal{E}_\beta(L^\varepsilon) - \varepsilon\,\mathcal{K}(L^\varepsilon) + \mathcal{P}_{W^\varepsilon}(L^\varepsilon)$$

since for all $i \in \mathbb{N}$ it verifies that

$$\int_\Omega \left(\varepsilon\,|\nabla\psi_i|^2 + W\,|\psi_i|^2\right)\,dx = \int_{\varepsilon^{-1/2}\,\Omega} \left(|\nabla\psi_i^\varepsilon|^2 + W^\varepsilon\,|\psi_i^\varepsilon|^2\right)\,dx\ .$$

Therefore, applying Theorem 3.1 to L^ε we find

$$\begin{aligned}\mathcal{E}_\beta(L^\varepsilon) - \varepsilon\,\mathcal{K}(L^\varepsilon) + \mathcal{P}_{W^\varepsilon}(L^\varepsilon) \ &\geq\ -\mathrm{Tr}\left[F(-\varepsilon\Delta + W^\varepsilon)\right]\\ &\geq\ -\int_{\varepsilon^{-1/2}\,\Omega} G(W^\varepsilon)\,dx\ .\end{aligned}$$

The conclusion then holds by undoing the change of variables. □

Proof of Theorem 3.3. Since $-\Delta + V$ is ε-coercive, Lemma 3.2 shows that

$$\begin{aligned}\mathcal{F}^\lambda_{V+W,\beta}(L) \ &=\ \{(1-\varepsilon)\,\mathcal{K}(L) + \mathcal{P}_{V-\lambda}(L)\} + \{\mathcal{E}(L) - \varepsilon\,\mathcal{K}(L) + \mathcal{P}_W(L)\}\\ &\geq\ -\,\varepsilon^{-\frac{d}{2}} \int_\Omega G(W)\,dx\ .\end{aligned}$$

Then we can rearrange this estimate as

$$\mathcal{F}^\lambda_{V,\beta}(L) \geq -\int_\Omega \Big(\rho_L\,W + \varepsilon^{-\frac{d}{2}}\,G(W)\Big)\,dx\ .$$

Optimizing on W as in the proof of [5, Th. 15], we get

$$-\int_\Omega \Big(\rho_L\,W + \varepsilon^{-\frac{d}{2}}\,G(W)\Big)\,dx \geq \varepsilon^{-\frac{d}{2}}\ \int_\Omega \tau\left(\varepsilon^{\frac{d}{2}}\,\rho_L(x)\right)\,dx\ ,$$

which completes the proof of Theorem 3.3. □

3.4. **Compactness results.** Theorem 3.2 is the analogous at operators level of the embedding $\mathrm{H}^1_0(\Omega) \hookrightarrow \mathrm{L}^2(\Omega)$. Similarly, a compactness result can be proved.

Theorem 3.4. *Consider $d \geq 2$, and assume that $m \in (d/(d+2), 1)$. Let $\{L_n\}_{n\in\mathbb{N}}$ be a sequence in $\mathcal{H}^1_+$ such that*

$$K_\infty \equiv \sup_{n\in\mathbb{N}} \mathcal{K}(L_n) < \infty\ ,$$

for some constant $K_\infty > 0$. Then $\{\|L_n\|_1\}_{n\in\mathbb{N}}$ is bounded and

$$\sup_{n\in\mathbb{N}} \sum_{i\in\mathbb{N}} |\nu_i^n|^m < \infty\ .$$

Moreover, up to a subsequence, $\lim_{n\to\infty} \nu_i^n = \bar{\nu}_i$*, for all* $i \in \mathbb{N}$*, and the following properties hold:*

i) *If* $\bar{\nu}_i \neq 0$ *for all* $i \in \mathbb{N}$*, then, up to a subsequence,*

$$\lim_{n\to\infty} \sum_{i\in\mathbb{N}} |\nu_i^n|^m = \sum_{i\in\mathbb{N}} |\bar{\nu}_i|^m \ .$$

ii) *For any* $m' \in (m, 1]$*, up to a subsequence,*

$$\lim_{n\to\infty} \sum_{i\in\mathbb{N}} |\nu_i^n|^{m'} = \sum_{i\in\mathbb{N}} |\bar{\nu}_i|^{m'} \ .$$

iii) *Up to a subsequence,* $\{L_n\}_{n\in\mathbb{N}}$ *converges in trace norm* $\|\cdot\|_1$ *to some operator* $\bar{L} \in \mathcal{H}^1_+$*, whose eigenvalues are* $\{\bar{\nu}_i^n\}_{i\in\mathbb{N}}$*.*

Proof. For each $n \in \mathbb{N}$, let us denote by $\{\nu_i^n\}_{i\in\mathbb{N}}$ and $\{\psi_i^n\}_{i\in\mathbb{N}}$ the sequence of eigenvalues and a sequence of orthonormalized eigenfunctions of L_n, respectively. By (2.3), $\sup_{n\in\mathbb{N}} \|L_n\|_1 < \infty$. For $i \in \mathbb{N}$, $n \in \mathbb{N}$, let

$$E_i^n \equiv \int_\Omega |\nabla \psi_i^n(x)|^2 \, dx \ .$$

The uniform bound on $\|L_n\|_1$ follows from Proposition 2.2. The uniform bound of $\sum_{i\in\mathbb{N}} |\nu_i^n|^m$ comes from (3.7) and Hölder's inequality. Up to the extraction of a subsequence, ν_i converges to some $\bar{\nu}_i$ for any $i \in \mathbb{N}$.

Proof of i) Assume first that $\bar{\nu}_i \neq 0$ for any $i \in \mathbb{N}$. Then, for each $i \in \mathbb{N}$, the sequence $\{E_i^n\}_{n\in\mathbb{N}}$ is bounded and, consequently, there is a function $\bar{\psi}_i \in H^1_0(\Omega)$ for which, up to a subsequence,

$$\lim_{n\to\infty} \psi_i^n = \bar{\psi}_i \quad \text{in } \mathrm{L}^2(\Omega) \ .$$

It is clear that $\{\bar{\psi}_i\}_{i\in\mathbb{N}}$ is orthonormal in $\mathrm{L}^2(\Omega)$. Recall that, counting multiplicity, $|\bar{\nu}_1| \geq |\bar{\nu}_2| \geq \ldots$ We denote by $P_N : L^2(\Omega) \to F_N$ the orthogonal projection operator over

$$F_N \equiv \operatorname{span}\{\bar{\psi}_i \ : \ 1 \leq i \leq N-1\}$$

and let $Q_N \equiv I_d - P_N$ be the projection operator onto $F_N^\perp$.

Next we claim that for all $\varepsilon > 0$, there exists $N \in \mathbb{N}$ such that

$$\sum_{i=N}^{\infty} |\nu_i^n|^m \leq \varepsilon \quad \forall\, n \in \mathbb{N} \ . \tag{3.19}$$

This can be proved as follows. First, using (2.5), we choose $N \in \mathbb{N}$ such that

$$\left(\sum_{\ell=N}^{\infty} (\lambda_{0,\ell})^{-\gamma}\right)^{m/\gamma} \quad \leq \quad \frac{\varepsilon}{2}$$

where $\gamma = \frac{m}{1-m}$, and $\{\lambda_{0,i}\}_{i\in\mathbb{N}}$ and $\{\phi_{0,i}\}_{i\in\mathbb{N}}$ are chosen as in (2.4). Consider for each $n \in \mathbb{N}$ the expansion

$$\psi_i^n = \sum_{k=1}^{\infty} \alpha_{i,k}^n \, \phi_{0,k} \quad n \in \mathbb{N} \, ,$$

where $\alpha_{i,k}^n \equiv \left\langle \psi_i^n ,\, \phi_{0,k} \right\rangle_{\mathrm{L}^2(\Omega)}$. According to the reverse Hölder inequality, which states that for any $p \in (0,1)$, $q \in (-\infty, 0)$ such that $\frac{1}{p}+\frac{1}{q} = 1$,

$$\sum_{i\in\mathbb{N}} a_i \, b_i \geq \left(\sum_{i\in\mathbb{N}} a_i^p \right)^{1/p} \left(\sum_{i\in\mathbb{N}} b_i^q \right)^{1/q} \quad \forall \, \{a_i\}_{i\in\mathbb{N}}, \, \{b_i\}_{i\in\mathbb{N}} \in (\mathbb{R}^+)^{\mathbb{N}},$$

applied for $p = m = \gamma/(\gamma+1)$, $q = -\gamma$, $a_i = |\nu_i^n|$ and $b_i = E_i^n$, we get, for all $N \in \mathbb{N}$, that

$$\left(\sum_{i=N}^{\infty} |\nu_i^n|^m \right)^{1/m} \leq K_\infty \left(\sum_{i=N}^{\infty} (E_i^n)^{-\gamma} \right)^{1/\gamma} .$$

Next we find $N \in \mathbb{N}$ large enough so that

$$\|P_N(\phi_{0,\ell})\|_{L^2(\Omega)} \geq 1 - \frac{1}{2} \, \varepsilon^{\gamma/m} \quad \ell = 1, 2, ...N-1 \, ,$$

or, which is equivalent,

$$\|Q_N(\phi_{0,\ell})\|_{L^2(\Omega)} \leq \frac{1}{2} \, \varepsilon^{\gamma/m}, \quad \ell = 1, 2, ...N-1 \, .$$

Then, there is $n_0 \in \mathbb{N}$ large enough so that,

$$\sum_{i=N}^{\infty} (\alpha_{i,\ell}^n)^2 \leq \varepsilon^{\gamma/m} \quad \forall \, n \geq n_0 \, , \; \ell = 1, 2, ..., N-1 \, .$$

Using $E_i^n = \sum_{\ell=1}^{\infty} \lambda_{0,\ell} \, (\alpha_{i,\ell}^n)^2$ and $\sum_{\ell=1}^{\infty} (\alpha_{i,\ell}^n)^2 = 1$, by concavity of $s \mapsto s^{-\gamma}$ we have

$$(E_i^n)^{-\gamma} \leq \sum_{\ell=1}^{\infty} (\alpha_{i,\ell}^n)^2 \, (\lambda_{0,\ell})^{-\gamma}.$$

Hence, collecting the above estimates, we obtain

$$\begin{aligned} \sum_{i=N}^{\infty} (E_i^n)^{-\gamma} \leq \sum_{i=N}^{\infty} \sum_{\ell=1}^{\infty} (\alpha_{i,\ell}^n)^2 \, (\lambda_{0,\ell})^{-\gamma} &= \sum_{\ell=1}^{M-1} \sum_{i=N}^{\infty} \cdots + \sum_{\ell=M}^{\infty} \sum_{i=N}^{\infty} \cdots \\ &\leq \frac{M-1}{\lambda_1^\gamma} \sum_{i=N}^{\infty} (\alpha_{i,\ell}^n)^2 + \sum_{l=M}^{\infty} \frac{\varepsilon^{\gamma/m}}{\lambda_{0,l}^\gamma} \\ &\leq c \, \varepsilon^{\gamma/m} \, , \end{aligned}$$

for some constant $c > 0$. This completes the proof of Claim (3.19).

Since $\{\|L_n\|_1\}_{n\in\mathbb{N}}$ is uniformly bounded with respect to $n \in \mathbb{N}$,

$$\sum_{i\in\mathbb{N}} |\bar{\nu}_i| < \infty .$$

For any $\eta \in \mathrm{L}^2(\Omega)$, by the Cauchy-Schwarz and the triangle inequality,

$$\left\| \sum_{i\in\mathbb{N}} \left\langle \eta,\, \bar{\psi}_i \right\rangle_{\mathrm{L}^2(\Omega)} \bar{\nu}_i\, \bar{\psi}_i \right\|_{L^2(\Omega)} \le \|\eta\|_{L^2(\Omega)} \sum_{i\in\mathbb{N}} |\bar{\nu}_i| < \infty .$$

Hence, the operator defined by

$$\bar{L}\eta = \sum_{i\in\mathbb{N}} \bar{\nu}_i \,\langle \bar{\psi}_i |\, \eta\rangle_{\mathrm{L}^2(\Omega)} \bar{\psi}_i \;, \quad \eta \in \mathrm{L}^2(\Omega) \;,$$

is in $\mathcal{S}_1$. Let us prove now that $\{L_n\}_{n\in\mathbb{N}}$ converges to $\bar{L}$ in $\mathcal{S}_1$. Given $N \in \mathbb{N}$, denote by $P_N^n : L^2(\Omega) \to F_N^n$ the orthogonal projection onto $F_N^n = \mathrm{span}\{\psi_i^n : 1 \le i \le N-1\}$ and by $Q_N^n = I - P_N^n$ the projection onto $(F_N^n)^\perp$:

$$\|L_n - L\|_1 \le \|(L_n - L)\, P_N\|_1 + \|L_n\, Q_N^n\|_1 + \|L Q_N\,\|_1 + \|L_n\,(Q_N^n - Q_N)\|_1 .$$

The first term converges to zero, because of the strong convergence of the first $N-1$ eigenvalues and eigenfunctions in $\mathbb{R}$ and $\mathrm{L}^2(\Omega)$ respectively. From (3.19) we have that the second and third terms are small if $N \in \mathbb{N}$ is large enough, independent of $n \in \mathbb{N}$, since

$$\Big(\sum_{i\in\mathbb{N}} |\nu_i|^n \Big)^m \le C_2 \sum_{i\in\mathbb{N}} |\nu_i^n|^m < \varepsilon .$$

The constant C_2 appears because of $\sum_{i\in\mathbb{N}} |\nu_i^n|$. Now we have that

$$\|L_n(Q_N^n - Q_N)\|_1 \le \|L_n\|_1 \cdot \|Q_N^n - Q_N\|$$

which converges to zero as $n \to \infty$, since $Q_N^n - Q_N = P_N^n - P_N$ converges to zero for the same reasons as the first term.

Proof of ii) Assume now that $\sup_{n\in\mathbb{N}} \sum_{i\in\mathbb{N}} |\nu_i^n|^m = C_1$ is finite, so that using the monotonicity of $\{|\nu_i^n|^m\}_{i\in\mathbb{N}}$, for any $m' > m$ and any $N \in \mathbb{N}$,

$$\sum_{i=N}^{\infty} |\nu_i^n|^{m'} \le (\nu_N^n)^{m'-m} \sum_{i=N}^{\infty} |\nu_i^n|^m \le |\nu_N^n|^{m'-m}\, C_1 .$$

If $\bar{\nu}_i = 0$ for all $i \in \mathbb{N}$, then

$$\lim_{n\to\infty} \sum_{i\in\mathbb{N}} |\nu_i^n|^{m'} \le \lim_{n\to\infty} |\nu_N^n|^{m'-m}\, C_1 = 0 .$$

From here on, taking $m' = 1$ and arguing as before we obtain that $\{L_n\}_{n\in\mathbb{N}}$ converges to 0 in $\mathcal{S}_1$. The general case, *i.e.*, when there is $i_0 \in \mathbb{N}$ such that $|\bar\nu_{i_0}| > 0$, follows from similar arguments.

Proof of iii) The convergence of the kernels K_{L_n} to the kernel of the limit operator L follows from ii) with $m' = 1$ and from the strong convergence of ψ_i^n to $\bar\psi_i$ in $\mathrm{L}^2(\Omega)$.

Finally let us see that the limit operator $\bar L$ actually belongs to $\mathcal{H}^1_+$. In fact, given a fixed $N \in \mathbb{N}$, we have that

$$\begin{aligned} \liminf_{n\to\infty} \sum_{i\in\mathbb{N}} \nu_i^n \int_\Omega |\nabla\psi_i^n(x)|^2\,dx \;&\geq\; \liminf_{n\to\infty} \sum_{i=1}^N \nu_i^n \int_\Omega |\nabla\psi_i^n(x)|^2\,dx \\ &\geq\; \sum_{i=1}^N \bar\nu_i \int_\Omega |\nabla\bar\psi_i(x)|^2\,dx\;, \end{aligned}$$

whence, since N is arbitrary, we get

$$\liminf_{n\to\infty} \mathcal{K}(L_n) \geq \mathcal{K}(\bar L)\;, \tag{3.20}$$

so that $\bar L \in \mathcal{H}^1_+$.

□

The following result is a direct consequence of Theorem 3.4 and Corollary 3.3.

Corollary 3.4. *Consider $d \geq 2$. Take $\varepsilon \in (0,1]$ and let V be a potential such that the Schrödinger operator $-\Delta + V$ is ε-coercive. Let β be an entropy seed generated by $F \in \mathcal{C}_0^{\varepsilon/2} \cap \mathcal{C}^{1-\varepsilon}_{V-\lambda}$ and $\lambda \leq \lambda^{(1-\varepsilon)}_{V,1}$. If $\{L_n\}_{n\in\mathbb{N}}$ is a sequence in $\mathcal{H}^1_+$ such that $\{\mathcal{F}^\lambda_{V,\beta}(L_n)\}_{n\in\mathbb{N}}$ is bounded, where $\mathcal{F}^\lambda_{V,\beta}$ is given in (3.10), then $\{L_n\}_{n\in\mathbb{N}}$, up to a subsequence, converges in trace norm $\|\cdot\|_1$ to some positive operator $L \in \mathcal{S}_1$. Moreover, ρ_{L_n} converges to ρ_L in $L^q(\Omega)$, for any $q \in [1,\infty]$ if $d = 1$, $q \in [1,\infty)$ if $d = 2$ and $q \in [1, d/(d-2)]$ if $d \geq 3$.*

4. Applications

In this section we present three applications of the results discussed in this paper. The three cases correspond to minimization problems arising in Quantum Mechanics.

4.1. **Minimization of the free energy functional.** Consider first the free energy functional $\mathcal{F}^\lambda_{V,\beta}$ defined in $\mathcal{H}^1_+$ by (3.10).

Theorem 4.1. *Let V a potential verifying (V_1) and such that $-\Delta+V$ is ε-coercive for some $\varepsilon \in (0,1]$. Take $\lambda \leq \lambda_{V,1}^{(1-\varepsilon)}$. Let β be an entropy seed generated by $F \in \mathcal{C}_0^{\varepsilon/2} \cap \mathcal{C}_{V-\lambda}^{1-\varepsilon}$. Then there exists a unique $L_\infty \in \mathcal{H}_+^1$ such that*

$$\mathcal{F}_{V,\beta}^{\lambda}(L_\infty) = \inf_{L \in \mathcal{H}_+^1} \mathcal{F}_{V,\beta}^{\lambda}(L) ,$$

provided one of the following conditions is satisfied:

i) *if $d=1$, $V \in \mathrm{L}^q(\Omega)$, for some $q \in [1,\infty]$,*
ii) *if $d=2$, $V \in \mathrm{L}^q(\Omega)$, for some $q \in]1,\infty]$,*
iii) *if $d \geq 3$, $V \in \mathrm{L}^q(\Omega)$, for some $q \in [\frac{d}{2},\infty]$.*

Proof. By Proposition 3.2, the functional $\mathcal{F}_{V,\beta}^{\lambda}$ is bounded from below. Let $\{L_n\}_{n\in\mathbb{N}} \subset \mathcal{H}_+^1$ be a minimizing sequence, that is

$$\lim_{n\longrightarrow\infty} \mathcal{F}_{V,\beta}^{\lambda}(L_n) = \inf_{L \in \mathcal{H}_+^1} \mathcal{F}_{V,\beta}^{\lambda}(L) .$$

Then the sequences

$$\{\|L_n\|_1\}_{n\in\mathbb{N}},\ \{\mathcal{K}(L_n)\}_{n\in\mathbb{N}},\ \{\mathcal{E}_\beta(L_n)\}_{n\in\mathbb{N}} \text{ and } \{\mathcal{P}_V(L_n)\}_{n\in\mathbb{N}}$$

are bounded according to Corollary 3.3. Now Theorem 3.4 provides the existence of $L_\infty \in \mathcal{H}_+^1$ such that, up to a subsequence, $\{L_n\}_{n\in\mathbb{N}}$ converges to L_∞ in trace norm $\|\cdot\|_1$ so that, in particular,

$$\lim_{n\longrightarrow\infty} \|L_n\|_1 = \|L_\infty\|_1 .$$

In order to study the entropy term we consider the space ℓ^1 with the usual norm. Consider the set

$$\mathcal{A}_+ \equiv \{\mu = \{\mu_i\}_{i\in\mathbb{N}} \in \ell^1 : \sum_{i\in\mathbb{N}} \beta(\mu_i) \geq A\} ,$$

where $A \equiv \inf_{n\in\mathbb{N}} \mathcal{E}_\beta(L_n)$. Both the function $D : \mathcal{A}_+ \to \mathbb{R}$ defined by

$$D(\mu) \equiv \sum_{i\in\mathbb{N}} \beta(\mu_i) \quad \forall\ \mu = \{\mu_i\}_{i\in\mathbb{N}} \in \mathcal{A}_+ ,$$

and the set $\mathcal{A}_+$ are convex. Thus D is weakly lower semi-continuous, so that $\liminf_{n\to\infty} D(\nu_n) \geq D(\nu_0)$, where $\nu^n = \{\nu_i^n\}_{i\in\mathbb{N}}$ and $\nu_0 = \{\bar{\nu}_i\}_{i\in\mathbb{N}}$. This amounts to say that

$$\liminf_{n\to\infty} \mathcal{E}_\beta(L_n) \geq \mathcal{E}_\beta(L_\infty) .$$

For the kinetic energy term we have (3.20). As for the potential energy, we obtain

$$\lim_{n\to\infty} \mathcal{P}_V(L_n) = \mathcal{P}_V(L_\infty)$$

using Proposition 2.2. Therefore L_∞ is a minimizer for $\mathcal{F}_{V,\beta}^{\lambda}$.

At this point we relate this minimization problem with the one studied in [5]. For this purpose we denote by S the set of non-increasing sequences $\{\nu_i\}_{i\in\mathbb{N}} \subset \mathbb{R}_+$ converging to zero, such that $\sum_{i\in\mathbb{N}} \beta(\nu_i)$ is absolutely convergent and let

$$\mathcal{X} \equiv \{(\nu, \psi) \in S \times \left(\mathrm{H}^1_0(\Omega)\right)^{\mathbb{N}} : \left\langle \psi_i,\, \psi_j \right\rangle_{\mathrm{L}^2(\Omega)} = \delta_{ij},\, \forall\, i, j \in \mathbb{N}\}$$

be the space of mixed states. Then we define an associated free energy functional acting on mixed states as

$$\mathcal{F}^\lambda_{V,\beta}[\nu, \psi] \equiv \sum_{i\in\mathbb{N}} \left[\beta(\nu_i) + \nu_i \int_\Omega \left(|\nabla\psi_i|^2 + (V-\lambda)|\psi_i|^2\right)\, dx\right] .$$

We observe that the function F is given by

$$F(s) = \beta \circ (\beta')^{-1}(-s) - s\,(\beta')^{-1}(-s) .$$

As a consequence of Theorem 4.1, the problem

$$\min_{(\nu,\psi)\in\mathcal{X}} \mathcal{F}^\lambda_{V,\beta}[\nu, \psi] . \tag{4.1}$$

has a solution $(\nu, \psi) \in \mathcal{X}$ given by $\nu_i = \nu_i(L_\infty)$ and $\psi_i = \psi_i(L_\infty)$.

The minimizer of (4.1) is unique, up to the choice of a basis for non-simple eigenvalues, as proved in [5]. As a consequence, the minimization problem at the level of operators

$$\min_{L\in\mathcal{H}^1_+} \mathcal{F}^\lambda_{V,\beta}(L)$$

has a unique minimizer $L_\infty \in \mathcal{H}^1_+$. □

Remark 4.1. In the Heisenberg formalism we see that the solution to the minimization problem given by Theorem 4.1 is a stationary solution to the Heisenberg equation

$$[-\Delta + V - \lambda,\, L_\lambda] = 0 ,$$

where the commutator operator is given by $[L, R] = L\,R - R\,L$. Moreover, since a solution of (4.1) is given by

$$(\bar\nu, \bar\psi) = \{(\bar\nu_i, \bar\psi_i)\}_{i\in\mathbb{N}} \in \mathcal{X} ,$$

where

$$\bar\nu_i = (\beta')^{-1}(\lambda - \lambda_{V,i}) ,$$

and $\bar\psi_i$ is an eigenfunction of $-\Delta+V-\lambda$ associated to $\lambda_{V,i}$, the operator L_∞ can actually be written as

$$L_\infty = (\beta')^{-1}(\Delta - V + \lambda) .$$

4.2. **Free energy involving a non-linear but local function of the density function.** Consider the free energy functional given by

$$\mathcal{F}_{V,\beta}^{\lambda,g}(L) \equiv \mathcal{F}_{V,\beta}^{\lambda} + \mathcal{G}(L) \quad \forall\, L \in \mathcal{H}_+^1 \ ,$$

where

$$\mathcal{G}(L) = \int_\Omega g(\rho_L(x))\, dx$$

and g is some real function, which is not necessarily convex. Using an argument similar to that in the proof of Theorem 4.1, we can obtain the following result.

Theorem 4.2. *Let V a potential verifying (V_1) and such that $-\Delta + V$ is ε-coercive for some $\varepsilon \in (0,1]$. Take $\lambda \leq \lambda_{V,1}^{(1-\varepsilon)}$. Let β be an entropy seed generated by $F \in \mathcal{C}_0^{\varepsilon/2}$. Let $g \in \mathrm{C}([0,\infty))$ be such that for non-negative constants c_1, c_2*

$$c_1 \leq g(s) \leq c_2 s^q \quad \forall\, s \geq 0 \ , \tag{4.2}$$

where

i) *$q \in [1,\infty)$ if $d = 1$ or $d = 2$,*
ii) *$q \in [1, d/(d-2)]$ if $d \geq 3$.*

If $F \in \mathcal{C}_{V-\lambda}^{1-\varepsilon}$, then there exists $L_\infty \in \mathcal{H}_+^1$ such that

$$\mathcal{F}_{V,\beta}^{\lambda,g}(L_\infty) = \inf_{L \in \mathcal{H}_+^1} \mathcal{F}_{V,\beta}^{\lambda,g}(L) \ .$$

Proof. It is similar to the one of Theorem 4.1. We use condition (4.2) to show via Fatou's lemma that

$$\mathcal{G}(L_\infty) \leq \liminf_{n \longrightarrow \infty} \mathcal{G}(L_n) \ ,$$

where $\{L_n\}_{n\in\mathbb{N}} \subset \mathcal{H}_+^1$ is a minimizing sequence for $\mathcal{F}_{V,\beta}^{\lambda,g}$. □

Remark 4.2. If $g \in \mathrm{C}^1([0,\infty))$, L_∞ is a fixed point of the map $Y : \mathcal{H}_+^1 \longrightarrow \mathcal{H}_+^1$ given by

$$Y(L) = (\beta')^{-1}\left(-(-\Delta + V) + \lambda - g' \circ \rho_L\right) \ .$$

4.3. **Stationary states for the Hartree problem with temperature.** Consider a Heisenberg equation with a Poisson coupling, namely

$$\begin{cases} i\,\partial_t L(t) = [-\Delta + V(t,\cdot), L(t)] & t \geq 0 \ , \\ -\Delta V(t,x) = \rho_{L(t)}(x) & x \in \Omega\,, \quad t \geq 0 \ , \\ L(0) = \tilde{L} \end{cases} \tag{4.3}$$

where $L(t)$, the *density operator of the system*, is a positive trace-class operator acting on $\mathrm{L}^2(\Omega)$. This system is known as the Hartree evolution system, or Schrödinger-Poisson system in the mixed states formulation, and a large literature has been devoted to its study, which goes far beyond the scope of this paper. We refer to [18] for further references. We restrict our study to the case of homogeneous Dirichlet boundary conditions, $V = 0$ on $\partial\Omega$. The stationary states of (4.3) are then solutions of

$$\begin{cases} [-\Delta + V, L] = 0 \;, \\ -\Delta V = \rho_L \;. \end{cases} \tag{4.4}$$

Stationary states of (4.3) can be obtained through the minimization of the free energy

$$\mathcal{F}_\beta(L) = \mathcal{E}_\beta(L) + \mathcal{K}(L) + \mathcal{P}(L) \;, \quad \forall\, L \in \mathcal{H}^1_+ \;,$$

where

$$\mathcal{P}(L) = \frac{1}{2}\int_\Omega V_L \rho_L \, dx = \frac{1}{2}\int_\Omega |\nabla V_L|^2 \, dx$$

is the *Poisson potential energy* of $L \in \mathcal{H}^1_+$. Since we minimize the free energy $\mathcal{F}_\beta$ and not only the energy $\mathcal{K} + \mathcal{P}$, the solutions we find correspond to the so-called *Hartree problem with temperature.* By virtue of Proposition 2.2 we have, for $d \leq 4$, that ρ_L is in $\mathrm{L}^2(\Omega)$, for any $L \in \mathcal{H}^1_+$, so that the *Poisson potential* $V_L \in \mathrm{H}^1_0(\Omega)$, is well defined as the solution of

$$\begin{cases} -\Delta V = \rho_L & \text{in} \quad \Omega \;, \\ \quad V = 0 & \text{on} \quad \partial\Omega \;. \end{cases}$$

Using Proposition 2.2 we get the following result, whose proof easily follows by using the regularity machinery provided for instance in [10].

Proposition 4.1. *Assume that $d \leq 4$. Let $L \in \mathcal{H}^1_+$. If $d = 1$ or $d = 2$, then $V_L \in \mathrm{C}^0(\overline{\Omega})$. Moreover, $V_L \in \mathrm{W}^{1,p}_0(\Omega) \cap \mathrm{L}^q(\Omega)$ for any $q \in [1, \infty)$ and for any $p \in [1, \infty)$ if $d = 3$, and for any $p \in [1, 4]$ if $d = 4$. If additionally $\partial\Omega$ is of class C^2, then $V_L \in \mathrm{W}^{2,r}(\Omega) \cap \mathrm{C}^{0,1/2}(\Omega)$ for any $r \in [1, 3/2]$ if $d = 3$, and $V_L \in \mathrm{W}^{2,r}(\Omega)$ for any $r \in [1, 4/3]$ if $d = 4$.*

We have the following

Theorem 4.3. *Assume that $d \leq 4$. Let β be an entropy seed generated by $F \in \mathcal{C}_0$. Then there exists $L_F \in \mathcal{H}^1_+$ such that*

$$\mathcal{F}_\beta(L_F) \leq \mathcal{F}_\beta(L) \quad \forall\, L \in \mathcal{H}^1_+ \;.$$

Moreover if β is of class C^1 in the interior of its support, then

$$L_F = (\beta')^{-1}(\Delta - V_{L_F})$$

is the unique minimizer of $\mathcal{F}_\beta$ and solves (4.4) as well.

Proof. The proof follows the same lines as the one for Theorem 4.1. The argument changes only to reach $\lim_{n\to\infty} \mathcal{P}(L_n) = \mathcal{P}(L_F)$, but this still follows from Proposition 2.2. □

Let us notice that if β is non-negative then the minimizer in Theorem 4.3 is $L_F = 0$. However, the result also applies to functions β for which $\{\beta < 0\} \neq \emptyset$ as it is the case of the one defined in Example 3.4, or if we replace β by $\beta - \lambda$ for some constant $\lambda > \beta'(0)$ (see below).

Remark 4.3. The case of an attracting Poisson coupling, that is when the potential is given by

$$+\Delta V = \rho_L \quad \text{in } \Omega \, ,$$

can be dealt with the same methods although it makes less sense from the point of view of physics. Some additional work is necessary to establish spectral properties of $\Delta + V_L$.

Finally we present a result for stationary states having a prescribed total charge, which brings to the level of operators a result obtained by Markowich, Rein and Wolansky in [18, Th. 2]. There the authors consider the case of F generated by a Casimir function, as in Example 2.4, with $d = 3$, and work at the level of mixed states requiring that the eigenstates ψ_i to belong to $\mathrm{H}^1_0(\Omega) \cap \mathrm{H}^2(\Omega)$. In our setting we need $\psi_i \in \mathrm{H}^1_0(\Omega)$, $F \in \mathcal{C}_0$, and $d \leq 4$.

Proposition 4.2. *Assume that $d \leq 4$. Let $\Lambda > 0$ and F be a non-negative non-increasing C^1-function in the Casimir class $\mathcal{C}_0$ such that $F' \in \mathcal{C}_0$ and, for every $\mu > 1$,*

$$F(s) \geq -\mu\, s + C \, , \quad s \leq 0 \, ,$$

for some $C = C(\mu) \in \mathbb{R}$. Then the functional defined by

$$\Phi(V,\lambda) = \frac{1}{2}\int_\Omega |\nabla V|^2 + \mathrm{Tr}\left[F(-\Delta + V - \lambda)\right] + \lambda\,\Lambda \, ,$$

for $\lambda \in \mathbb{R}$ and $\mathrm{H}^1_0(\Omega) \ni V \geq 0$, is continuous, strictly convex, and coercive. In particular, there exists a unique minimizer (V_F, λ_F) of Φ. Moreover, the operator

$$L_F \equiv -F'(-\Delta + V_F - \lambda_F)$$

is in $\mathcal{H}^1_+$ with $\|L\|_1 = \mathrm{Tr}\,[L] = \Lambda$ and, (L_F, V_F) is a solution of (4.4).

Mathematically, the free energy is changed only by an integral term $-\lambda \int_\Omega \rho_L \, dx$, where λ is the Lagrange multiplier associated to the mass constraint. The entropy seed β is now changed into $\nu \mapsto \beta(\nu) - \lambda\,\nu$, which results in the fact that the set $\{\nu \in \mathbb{R} \, : \, \nu \mapsto \beta(\nu) - \lambda\,\nu < 0\}$ is automatically non-empty. Because of the compactness property, the mass constraint will be verified when passing to the limit in the minimizing sequence.

Remark 4.4. With almost no work, we may add an external potential which takes negative values and eventually has singularities, of Coulomb type, for instance. This situation is highly relevant from a physics point of view, for the modelization of atomic and molecular systems, without temperature, see for instance [23] and references therein, or with temperature, see [17]. In such a case, the appropriate model is rather the Hartree-Fock system than the Hartree system.

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