Higher-order Sobolev-like cones

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Abstract

We define and study $\mathscr{H}_V^n$, $n \in \mathbb{N}$, a cone of nuclear operators working on the Sobolev space $\mathbf{H}_0^n(\Omega)$, where $\Omega \subseteq \mathbb{R}^N$ is a smooth bounded domain. We prove that $\mathscr{H}_V^{n+1}$ is compactly embedded in $\mathscr{N}_{n,1}$, the space of nuclear operators, in several ways related to monotone convergence, weak convergence, etc. In the path, we prove regularity properties for the density functions of $T \in \mathscr{H}_V^n$ as well as Lieb-Thirring type and Gagliardo-Nirenberg type inequalities. We introduce the concept of ε-quasi-self-adjoint operator, $\varepsilon > 0$ being a measure of how far from being self-adjoint an operator is, show some of their properties, and prove that given $T \in \mathscr{H}_V^n$ and $\varepsilon > 0$, there is S, a finite-rank ε-quasi-self-adjoint operator operator, such that $\|T - S\| \leq \varepsilon$. Finally, we minimize several free-energy functionals defined on $\mathscr{H}_V^n$.

Keywords: Sobolev-like cone, quasi-self-adjoint operator, nuclear operator, Gagliardo-Nirenberg type inequality, Lieb-Thirring type inequality, free-energy functional.

MSC Classification: 47L07 , 47B10 , 47B28 , 47B93 , 81Q10 , 26D15 , 47A60

1 Introduction

Nuclear (self-adjoint trace-class) operators on $\mathrm{L}^2(\Omega)$, $\Omega \subseteq \mathbb{R}^N$, are basic mathematical blocks to build quantum mechanics in the Heisenberg picture where they represent quantum systems; its space shall be denoted by $\mathscr{N}_{0,1}$. To build this axiomatic, dynamical variables, usually called *observables*, are represented by closed densely-defined non-continuous linear operators, [2, 11]; e.g., the Schrödinger operator $-\Delta+V$ is related to the total energy (kinetic plus potential energy).

By the Riesz-Schauder and Hilbert-Schmidt theorems, an element $T \in \mathscr{N}_{0,1}$ operates on $u \in \mathrm{L}^2(\Omega)$ according to

$$Tu = \sum_{i\in\mathbb{N}} (u, \psi_{i,T})_0 \, \nu_{i,T} \, \psi_{i,T}, \tag{1}$$

where $(\cdot,\cdot)_0$ denotes the inner-product of $\mathrm{L}^2(\Omega)$. Here, $(\nu_{i,T})_{i\in\mathbb{N}} \subseteq \mathbb{R}$ and $(\psi_{i,T})_{i\in\mathbb{N}} \subseteq \mathrm{L}^2(\Omega)$ are, respectively, the sequence of eigenvalues or *occupation numbers* of T and the sequence of eigenfunctions or *wavefunctions* of T, $T\psi_{i,T} = \nu_{i,T}\psi_{i,T}$, $i \in \mathbb{N}$, $B_T = \{\psi_{i,T} \,/\, i \in \mathbb{N}\}$ is a Hilbert basis of $\mathrm{L}^2(\Omega)$ and the trace of T is given by

$$\mathrm{Tr}_0(T) = \sum_{i\in\mathbb{N}} \nu_{i,T} = \sum_{i\in\mathbb{N}} (\phi_i, T\phi_i)_0,$$

where $\{\phi_i \,/\, i \in \mathbb{N}\}$ is any Hilbert basis of $\mathrm{L}^2(\Omega)$, [14, 15]. Each pair $(\nu_{i,T}, \psi_{i,T})$ is referred to as a *mixed state*. Thanks to the expansion (1), the mathematical study of a quantum system can be performed by using either a nuclear operator (see e.g. [9, 18, 19]) T or its sequence of mixed states $(\nu_{i,T}, \psi_{i,T})_{i\in\mathbb{N}}$ (see e.g. [10, 17]), each scheme having pros and cons.

For the kinetic energy T to make sense, B_T needs to be contained in a Sobolev space H. For example, in [10] and [17] the kinetic energy is computed by

$$\mathscr{K}_1(T) = \sum_{i\in\mathbb{N}} |\nu_{i,T}| \int_\Omega |\nabla\psi_{i,T}|^2 dx, \tag{2}$$

by considering, $H = \mathrm{H}_0^1(\Omega)$ and $H = \mathrm{H}_0^1(\Omega) \cap \mathrm{H}^2(\Omega)$, respectively. Observe that, formally, the right side of this formula corresponds to $\mathrm{Tr}_0(-\Delta T)$. Then, a first motivation for this paper yields in dealing with higher-order kinetic energy functionals:

$$\mathscr{K}_n(T) = \sum_{i\in\mathbb{N}} |\nu_{i,T}| \int_\Omega |\Delta^m\psi_{i,T}|^2 dx, \qquad \text{if } n = 2m,$$
$$\mathscr{K}_n(T) = \sum_{i\in\mathbb{N}} |\nu_{i,T}| \int_\Omega |\nabla\Delta^m\psi_{i,T}|^2 dx, \qquad \text{if } n = 2m+1.$$

To this purpose, the elements of B_T should have more regularity.

Another source of motivation comes from the use of free-energy functionals (entropy plus kinetic plus potential) to study the stability of quantum systems; see e.g. [5, 16, 17]. This has to do with the well-posedness of the problem of minimizing an adequate free-energy functional $\mathscr{F}_{V,\beta}$, say formally

$$\mathscr{F}_{V,\beta}(T) = \mathcal{S}_\beta(T) + \mathscr{K}_1(T) + \mathscr{P}_V(T) = \mathrm{Tr}_0(\beta(T)) + \mathrm{Tr}_0(-\Delta T) + \mathrm{Tr}_0(VT), \tag{3}$$

where, for some adequate convex function β, the nuclear operator $\beta(T)$ makes sense via the spectral theorem; see e.g. Theorem 3. Therefore, achieving the following three goals is of interest: **a)** boundedness from below of $\mathscr{F}_{V,\beta}$, **b)** existence of a minimizer of $\mathscr{F}_{V,\beta}$, and **c)** uniqueness of the minimizer of $\mathscr{F}_{V,\beta}$.

Given a potential $V:\Omega\longrightarrow\mathbb{R}$, proving point a) corresponds to obtaining inequalities of Lieb-Thirring type. On the other hand, with Lieb-Thirring type inequalities one can produce Gagliardo-Nirenberg type interpolation inequalities; see e.g. [9, 10, 18, 19]. With these tools at hand, compactness properties of the corresponding embeddings are usually established and, with them, point b) is derived by a direct method. To achieve point c), convexity arguments are commonly used.

In [9] and [19] the path just mentioned was followed. Cones of nuclear operators, referred to as Sobolev-like cones, were defined as a good environment to find minimizers of free-energy functionals where the kinetic term is given by (2) and the convex function β is generated by a Casimir-class function (see Remark 15) related to the eigenvalue problem of the Schrödinger operator with Dirichlet condition, considering that $\Omega\subseteq\mathbb{R}^N$ is either a bounded or unbounded domain, respectively. For this cone of operators, $\mathscr{H}_V^1$ (see Definition 1), the total energy behaves like the square of a norm and it's proved that $\mathscr{H}_V^1$ is compactly embedded in $\mathscr{N}_{0,1}$, a property which is an analogue of the usual Sobolev embedding but at operators level.

In [18] the results of [9] were extended. There were introduced cones $\mathscr{W}^{1,p}$ which are analogues of the space $\mathrm{W}^{1,p}(\Omega)$, $p>1$, at the level of operators. In addition, it was shown, except for $p=2$, that there is an imbalance of energies: the p-total energy of an operator $\mathscr{W}^{1,p}$ is bigger or equal than the sum of its p-kinetic energy and its p-potential energy. The case of energy balance, $p=2$, occurs because the definitions of kinetic energy and potential energy appearing at the right side of (3) are actually basis-independent.

Grossly speaking, in this paper we define and study higher-order Sobolev-like cones $\mathscr{H}_V^n$, $n\in\mathbb{N}$. Let's give more detail and context.

1. We replace $\mathrm{L}^2(\Omega)$ by other pivote space, $\mathrm{H}_n=\mathrm{H}_0^n(\Omega)$, which is also a separable Hilbert space with an adequate inner-product, $(\cdot,\cdot)_n$; see (4) and (5). This and the general framework is the matter of Section 2.1. There are introduced spaces of operators acting on H_n: $\mathscr{C}_{n,s}$ the space of compact self-adjoint operators, $\mathscr{N}_{n,1}$ the space of nuclear operators, and $\mathscr{N}_{n,2}$ the space of self-adjoint Hilbert-Schmidt operators, together with the standard norms.
2. In Section 2.2 we show that the elements of $\mathscr{C}_{n,s}$ have an integral representation, $(T\varphi)(x)=(K_T(x,\cdot),\varphi)_n$, $\varphi\in\mathrm{H}_n$, where its kernel, given by $K_T(x,y)=\sum_{i\in\mathbb{N}}|\nu_{i,T}|\psi_{i,T}(x)\psi_{i,T}(y)$, $x,y\in\Omega$, belongs to $\mathrm{L}^2(\Omega\times\Omega)$ and verifies $K_T(x,\cdot)\in\mathrm{H}_n$, for a.e. $x\in\Omega$.
3. In Section 2.3 we show that the density functions of $T\in\mathscr{N}_{n,1}$ are elements of $\mathrm{L}^1(\Omega)$. While an operator of $\mathscr{N}_{0,1}$ has a unique density function, $\rho_{0,T}$, an operator of $\mathscr{N}_{n,1}$ has $n+1$ density functions $\rho_{m,T}$, $m=0,\ldots,n$, given by (18) and (19) for m odd and even, respectively.
4. Section 3.1 introduces the Sobolev-like cone $\mathscr{H}_V^n$ and the notion of total energy, together with some preliminary properties. It's stated that $\mathscr{H}_V^n$ is in fact an algebraic cone and that the total energy behaves like the square of a norm, Proposition

2. Theorem 3 is an important tool; it states that $\beta(\mathscr{H}_V^n) \subseteq \mathscr{H}_V^n$ for any Borel function $\beta : \mathbb{R} \longrightarrow \mathbb{R}$ with $\beta(0) = 0$ which verifies a simple growing condition.

5. In Section 3.2 it's proved that a nice finite-rank operator can be used to approximate an element of $\mathscr{H}_V^n$, Theorem 5. This operator is not necessarily self-adjoint but can be chosen as close as we want to be self-adjoint, i.e., it's an *ε-quasi-self-adjoint operator*; see Definition 2. In Theorem 5 and Definition 2, ε is a measure of how far from being self-adjoint an operator is. This result seems to be important as in the last years attention has been put to problems related to *non-Hermitian quantum mechanics*. For example, physical symmetries are represented by unitary and antiunitary operators, [12, 13]. There is also interest in non-standard representations of observables by operators which could not be self-adjoint but which share some of their properties, [1, 8].
6. In Section 4 are introduced the functionals of entropy, potential energy and kinetic energy working on $\mathscr{H}_V^n$. Here it's also proved a kind of Poincaré inequality for operators in $\mathscr{H}_V^n$, Theorem 7. This could also be interpreted as an uncertainty principle in the sense that the total energy of a nuclear operator is bounded from below by the basic 'spread' of the operator, its trace norm.
7. In Section 5 are stated regularity properties of the density functions given in (18) and (19) below. Here are also introduced other energetic values of the operators in $\mathscr{H}_V^n$.
8. In Section 6 are presented lower estimates for energy functionals, some of them being Lieb-Thiring inequalities, Theorem 11, which unfortunately are not necessarily equivalent to the boundedness from below except for the nice case of $\mathscr{H}_V^1$ where the estimatives are uniform and stronger, Corollary 12. As a consequence, Gagliardo-Nirenberg type inequalities are obtained, Theorem 19.
9. In Section 7.1 we consider a sequence $(T_m)_{m\in\mathbb{N}} \subseteq \mathscr{H}_V^{n+1}$ such that $(\langle\!\langle T_m \rangle\!\rangle_{V,n})_{m\in\mathbb{N}} \subseteq \mathbb{R}$ is bounded and verifies a technical uniform condition, (B2). Then, several compactness results are obtained: there exists an operator $\overline{T} \in \mathscr{H}_V^{n+1}$ such that, up to a subsequence and as $m \longrightarrow +\infty$, it holds i) convergence of mixed states, Lemmas 20 and 22; ii) convergence in trace norm provided downward monotony, Theorem 23, or upward monotony, Corollary 27; iii) convergence of the density functions, Proposition 24; iv) a kind of $\mathrm{L}^2(\Omega)$-convergence of the kernels, Proposition 25; v) weak convergence in $\mathscr{N}_{n,1}$, Theorem 26; vi) pointwise convergence, Corollary 28. In the context of $\mathscr{H}_{V,+}^1$, condition (B2) is unnecessary, [9, Th.3.4]. In [19, Lemmas 4.1&4.2] it was dealt the case of Ω unbounded and [18, Lemma 4.2] considers $p \geq 2$.
10. In Section 7.2 the compactness properties stated in Section 7.1 are used to minimize some free-energy functionals. Here we comment on some situations were uniqueness of the minimizer is achieved.

2 Nuclear operators and density functions

In this section we give a general framework for nuclear operators, preparing the path to introduce Sobolev-like cones in Section 3.

2.1 Pivote space and general framework

Let $\Omega \subseteq \mathbb{R}^N$ be a bounded domain with smooth boundary. Let's consider the separable Hilbert spaces $\mathrm{H}_0 = \mathrm{L}^2(\Omega)$ and $\mathrm{H}_n = \mathrm{H}_0^n(\Omega)$, $n \in \mathbb{N}$. The inner-product of H_0 is that of $\mathrm{L}^2(\Omega)$ and, given $n \in \mathbb{N}$, the inner-product of H_n is given by

$$(u,v)_n = (\Delta^k u, \Delta^k v)_0 + (u,v)_0 = \int_\Omega \left[\Delta^k u \Delta^k v + uv\right] dx, \tag{4}$$

$$(u,v)_n = (\nabla\Delta^{k-1} u, \nabla\Delta^{k-1} v)_0 + (u,v)_0 = \int_\Omega \left[\nabla\Delta^{k-1} u \cdot \nabla\Delta^{k-1} v + uv\right] dx, \tag{5}$$

if $n = 2k$ or $n = 2k-1$, respectively. The corresponding norm is

$$\|u\|_n = \left(\int_\Omega \left[|\Delta^k u|^2 + |u|^2\right] dx\right)^{1/2}, \qquad \text{if } n = 2k, \tag{6}$$

$$\|u\|_n = \left(\left[|\nabla\Delta^{k-1} u|^2 + |u|^2\right] dx\right)^{1/2}, \qquad \text{if } n = 2k-1. \tag{7}$$

Let's write $\mathbb{N}_* = \mathbb{N} \cup \{0\}$. Given $n \in \mathbb{N}_*$, let's denote $\mathscr{L}_n = \mathcal{L}(\mathrm{H}_n) = \{T : \mathrm{H}_n \longrightarrow \mathrm{H}_n \,/\, T \text{ is linear and bounded}\}$, $\mathscr{L}_{n,s} = \{T \in \mathscr{L}_n \,/\, T \text{ is self-adjoint}\}$, $\mathscr{C}_n = \{T \in \mathscr{L}_n \,/\, T \text{ is compact}\}$ and $\mathscr{C}_{n,s} = \{T \in \mathscr{C}_n \,/\, T \text{ is self-adjoint}\}$. As it's well known, $\mathscr{L}_n$ is a Banach space whenever it's equipped with the usual norm, $\|T\| = \sup\{\|Tu\|_n \,/\, u \in \mathrm{H}_n \wedge \|u\|_n = 1\}$.

Let's recall that a linear operator $S : D \subseteq \mathrm{H}_n \longrightarrow \mathrm{H}_n$ is positive iff $(Su,u)_n \geq 0$, for every $u \in D$. Let's also recall, [20, Th.VI.10], that an operator $T \in \mathscr{L}_n$ has a unique polar decomposition, $T = U|T|$, where $|T| = \sqrt{T^*T}$ is positive and U is an isometry sharing the null-space with T.

Let's denote by $\mathscr{L}_n^+$ the set of positive bounded operators. In the same way we consider the sets of positive operators: $\mathscr{C}_n^+, \mathscr{C}_{n,s}^+, \mathscr{N}_{n,1}^+$, $\mathscr{L}_{n,s}^+$, etc.

Given $T \in \mathscr{L}_n^+$ and $\{\chi_i \,/\, i \in \mathbb{N}\}$, a Hilbert basis of H_n, let's write

$$\mathrm{Tr}_n(T) = \sum_{i \in \mathbb{N}} (\chi_i, T\chi_i)_n. \tag{8}$$

The last computation is actually basis-independent, [14, 15]. The space of trace-class operators is $\mathscr{I}_n^1 = \{T \in \mathscr{L}_n \,/\, \|T\|_n = \mathrm{Tr}_n(|T|) < +\infty\}$. We have, [20, 22], that $(\mathscr{I}_n^1, \|\cdot\|_n)$ is a Banach space. The trace mapping $\mathrm{Tr}_n : \mathscr{I}_n^1 \longrightarrow \mathbb{R}$, given by (8), is linear and verifies $|\mathrm{Tr}_n(T)| \leq \|T\|_n$, for every $T \in \mathscr{I}_n^1$, so that it belongs to $\mathscr{I}_n^{1,*}$, the dual of $\mathscr{I}_n^1$.

The mapping $\mathscr{L}_n \ni L \longmapsto \mathrm{Tr}_n(L\,\cdot) \in \mathscr{I}_n^{1,*}$ is, [20, Th.VI.26], an isometric isomorphism so that $\mathscr{I}_n^{1,*} \cong \mathscr{L}_n$. Therefore, a sequence $(T_m)_{m\in\mathbb{N}} \subseteq \mathscr{I}_n^1$ weakly converges (in the topology $\sigma(\mathscr{I}_n^1, \mathscr{L}_n)$) to some $\overline{T} \in \mathscr{I}_n^1$, denoted

$$T_m \rightharpoonup \overline{T}, \quad \text{as } m \longrightarrow +\infty, \text{ weakly},$$

iff $\mathrm{Tr}_n(R(T_m - \overline{T})) \longrightarrow 0$, as $m \longrightarrow +\infty$, for every $R \in \mathscr{L}_n$.

The space of Hilbert-Schmidt operators is $\mathscr{I}_n^2 = \{T \in \mathscr{L}_n \,/\, \|T\|_{\text{HS}} = \sqrt{\text{Tr}_n(T^*T)} < +\infty\}$. We have, [20, Th.VI.22], that $(\mathscr{I}_n^2, \|\cdot\|_{\text{HS}})$ is a Hilbert space with the inner-product given by $(A,B)_{\text{HS}} = \text{Tr}_n(A^*B)$. It holds $\|T\| \leq \|T\|_{\text{HS}} \leq \|T\|_n$, for every $T \in \mathscr{I}_n^1$, so that $\mathscr{I}_n^1 \subseteq \mathscr{I}_n^2 \subseteq \mathscr{C}_n$.

Remark 1. *It's well known (see e.g. [20, Th.VI.23]) that an operator $T \in \mathscr{L}_0$ belongs to $\mathscr{I}_0^2$ iff there exists a unique $K_T \in \text{L}^2(\Omega \times \Omega)$ such that, for every $u \in \text{H}_0 = \text{L}^2(\Omega)$,*

$$Tu(x) = \int_\Omega K_T(x,y)\, u(y)\, dy = (K_T(x,\cdot), u)_0, \qquad \text{for a.e. } x \in \Omega. \tag{9}$$

It also holds

$$\|K_T\|_{\text{L}^2(\Omega\times\Omega)} = \left(\int_{\Omega\times\Omega} |K_T(x,y)|^2 dx\, dy\right)^{1/2} = \|T\|_{\text{HS}}\,. \tag{10}$$

Remark 2. *Let's recall that if $S \neq \varnothing$ is a subset of a linear space W, the span of S, denoted by $\langle S\rangle$, is formed by the linear combinations of elements of S.*

By the Hilbert-Schmidt and Riesz-Schauder theorems, for $T \in \mathscr{C}_{n,s}$, there exist sequences $(\nu_{i,T})_{i\in\mathbb{N}} \subseteq \mathbb{R}$ and $(\psi_{i,T})_{i\in\mathbb{N}} \subseteq \text{H}_n$ such that

i) $B_T = \{\psi_{i,T} \,/\, i \in \mathbb{N}\}$ is a Hilbert basis of H_n;
ii) $T\psi_{i,T} = \nu_{i,T}\psi_{i,T}$, for every $i \in \mathbb{N}$.

We always assume that the sequence of eigenvalues of T, $(\nu_{i,T}) \subseteq \mathbb{R}$, is ordered: $|\nu_{i,T}| \geq |\nu_{j,T}|$, if $i \leq j$, and if both ν and $-\nu$ are eigenvalues, $-|\nu|$ comes first.

Point i) means that B_T is orthonormal and $\overline{\langle B_T\rangle} = \text{H}_n$. Point ii) says that $\psi_{i,T}$ is an eigenfunction associated to the eigenvalue $\nu_{i,T}$. Observe that point i) together with (6) and (7) imply that, for every $i \in \mathbb{N}$,

$$\|\psi_{i,T}\|_0 \leq 1. \tag{11}$$

The space of nuclear operators is $\mathscr{N}_{n,1} = \mathscr{C}_{n,s} \cap \mathscr{I}_n^1$. Observe that for $T \in \mathscr{N}_{n,1}$,

$$\|T\|_n = \sum_{i\in\mathbb{N}} |\nu_{i,T}| \quad \text{and} \quad \text{Tr}_n(T) = \sum_{i\in\mathbb{N}} \nu_{i,T}. \tag{12}$$

Even though the norms on $\mathscr{N}_{n,1}$ and H_n are both denoted by $\|\cdot\|_n$, this will not provoke confussion as operators are represented with capital letters while functions are written with small letters.

Remark 3. *It's important to note that an operator $T \in \mathscr{C}_{n,s}$ has an explicit and useful way to compute:*

$$Tu = \sum_{i\in\mathbb{N}} (u, \psi_{i,T})_n\, \nu_{i,T}\, \psi_{i,T}, \qquad u \in \text{H}_n. \tag{13}$$

In applications to quantum mechanics is important to deal with elements of $\mathscr{C}_{n,s}^+$. We have that $\mathscr{C}_{n,s} = \mathscr{C}_{n,s}^+ - \mathscr{C}_{n,s}^+$. In fact, thanks to (13), any $T \in \mathscr{C}_{n,s}$ can be written as $T = P - N$, where $P, N \in \mathscr{C}_{n,s}^+$ are given by

$$Pu = \sum_{\nu_{i,T}\geq 0} (u, \psi_{i,T})_n\, \nu_{i,T}\, \psi_{i,T}, \quad Nu = -\sum_{\nu_{i,T}<0} (u, \psi_{i,T})_n\, \nu_{i,T}\, \psi_{i,T}. \tag{14}$$

Let's denote the space of self-adjoint Hilbert-Schmidt operators by $\mathscr{N}_{n,2} = \mathscr{C}_{n,s} \cap \mathscr{I}_n^2$. Observe that, for $T \in \mathscr{N}_{n,2}$, $\|T\|_{\mathrm{HS}}^2 = \sum_{i\in\mathbb{N}} \nu_{i,T}^2$. In the context of Remark 1, the kernel K_T of an operator $T \in \mathscr{N}_{0,2}$ is explicitly given by $K_T(x,y) = \sum_{i\in\mathbb{N}} \nu_{i,T}\psi_{i,T}(x)\psi_{i,T}(y)$, $x, y \in \Omega$.

2.2 Kernel of a nuclear operator

Let's denote by $\mathrm{H}_{n,s}$ the subspace of $\mathrm{L}^2(\Omega\times\Omega)$ formed by the functions $w : \Omega\times\Omega \longrightarrow \mathbb{R}$ such that a) $w(x,y) = w(y,x)$, for a.e. $x, y \in \Omega$; b) $w(x,\cdot) \in \mathrm{H}_n$, for a.e. $x \in \Omega$.

As we shall see, we have points analogous to (9) and (10). Let's assume that $n = 2k$, $k \in \mathbb{N}$ (the case of n odd is similar). Given an operator $T \in \mathscr{N}_{n,1} \subseteq \mathscr{N}_{n,2}$, let's consider $K_T : \Omega \times \Omega \longrightarrow \mathbb{R}$, given by

$$K_T(x,y) = \sum_{i\in\mathbb{N}} \nu_{i,T}\psi_{i,T}(x)\psi_{i,T}(y), \quad x, y \in \Omega. \tag{15}$$

It's clear that

$$\|K_T\|_{\mathrm{L}^2(\Omega\times\Omega)} \le \sum_{i\in\mathbb{N}} |\nu_{i,T}| \left(\int_{\Omega\times\Omega} |\psi_{i,T}(x)|^2 |\psi_{i,T}(y)|^2 \right)^{1/2} \le \sum_{i\in\mathbb{N}} |\nu_{i,T}| \|\psi_{i,T}\|_n^2 = \|T\|_n,$$

which is similar to (10) and shows that $K_T \in \mathrm{L}^2(\Omega)$. By (15), we have that $\|K(x,\cdot)\|_n \le \sum_{i\in\mathbb{N}} |\nu_i| |\psi_i(x)|$ is finite for a.e. $x \in \Omega$, because, denoting $\tilde{K}_T = \|K(x,\cdot)\|_n$, we have $\|\tilde{K}_T\|_0 \le \sum_{i\in\mathbb{N}} |\nu_{i,T}| \|\psi_{i,T}\|_0 \le \sum_{i\in\mathbb{N}} |\nu_{i,T}| \|\psi_{i,T}\|_n = \|T\|_n$, which shows that $K_T \in \mathrm{H}_{n,s}$. Given $\varphi \in \mathrm{H}_n$ and $x \in \Omega$, we have, by (13), that

$$(T\varphi)(x) = \sum_{i\in\mathbb{N}} \nu_i(\varphi,\psi_i)_n\psi_i(x) = \sum_{i\in\mathbb{N}} \nu_i\psi_i(x) \int_\Omega \left[\Delta^k\psi_i\Delta^k\varphi + \psi_i\varphi\right] dy = (K(x,\cdot), \varphi)_n,$$

which is quite similar to (9).

2.3 Density functions

To a nuclear operator $T \in \mathscr{N}_{0,1}$ is usual to associate a density function $\rho_{0,T} \in \mathrm{L}^1(\Omega)$, given by

$$\rho_{0,T}(x) = K_{|T|}(x,x) = \sum_{i\in\mathbb{N}} |\nu_{i,T}| \, |\psi_{i,T}(x)|^2, \quad x \in \Omega, \tag{16}$$

which verifies

$$\|\rho_{0,T}\|_{\mathrm{L}^1(\Omega)} = \sum_{i\in\mathbb{N}} |\nu_{i,T}| = \mathrm{Tr}_0(|T|) = \|T\|_0. \tag{17}$$

On the other hand, it's quite natural to define several density functions for an operator $T \in \mathscr{N}_{n,1}$, $n \ge 1$. Even more, one of those density functions is expected to verify an equality like (17). We deal with this now.

Let $n \in \mathbb{N}_*$, $T \in \mathscr{N}_{n,1}$ and $m \in \mathbb{N}_*$ with $m \le n$. For $\rho_{0,T}$ we keep its definition as in (16). If m is odd, say $m = 2k+1$ with $k \in \mathbb{N}_*$, we put

$$\rho_{m,T}(x) = \sum_{i\in\mathbb{N}} |\nu_{i,T}| \left[|\nabla\Delta^k\psi_{i,T}(x)|^2 + |\psi_{i,T}(x)|^2 \right], \quad x \in \Omega. \tag{18}$$

If m is even, say $m = 2k$ with $k \in \mathbb{N}$, we put

$$\rho_{m,T}(x) = \sum_{i\in\mathbb{N}} |\nu_{i,T}| \left[|\Delta^k \psi_{i,T}(x)|^2 + |\psi_{i,T}(x)|^2 \right], \quad x \in \Omega. \tag{19}$$

By (18), (19), (4) and (5), it's quite clear that

$$\|\rho_{0,T}\|_{\mathrm{L}^1(\Omega)} \le \sum_{i\in\mathbb{N}} |\nu_{i,T}| = \|T\|_n = \|\rho_{n,T}\|_{\mathrm{L}^1(\Omega)}, \tag{20}$$

so that $\rho_{0.T}, \rho_{n,T} \in \mathrm{L}^1(\Omega)$.

Remark 4. *Let $n \in \mathbb{N}_*$, $T \in \mathscr{N}_{n,1}$ and $m \in \mathbb{N}_*$ with $m \le n$. By (18), (19) and Remark 3, we have that $\rho_{n,T} = \rho_{n,P} + \rho_{n,N}$, where $T = P - N$ with $P, N \in \mathscr{N}^+_{n,1}$ given in (14).*

Remark 5. *Let's assume that $\alpha \in [2, 2^*]$. Let's recall that there exists a constant $\check{c}_\alpha = \check{c}_\alpha(\Omega) > 0$ such that*

$$\forall u \in \mathrm{H}_1 = \mathrm{H}^1_0(\Omega): \quad \|u\|_{\mathrm{L}^\alpha(\Omega)} \le \check{c}_\alpha \|\nabla u\|_{\mathrm{L}^2(\Omega)}. \tag{21}$$

Observe that, for $\alpha = 2$, (21) becomes Poincaré's inequality; see e.g. [7, Cor.9.19]. For future use, we shall denote, for $l \in \mathbb{N}_*$, $\gamma_l = \max\{1, \check{c}_2^{2l}\}$. It's clear that, given $n \in \mathbb{N}$ and $l = 0, 1, ..., n$, it holds

$$\forall u \in \mathrm{H}_n: \quad \|u\|^2_{n-l} \le \gamma_l \|u\|^2_n. \tag{22}$$

Proposition 1. *Let $n \in \mathbb{N}$, $l = 0, ..., n$ and $T \in \mathscr{N}_{n,1}$. Then,*

$$\|\rho_{n-l,T}\|_{\mathrm{L}^1(\Omega)} \le \gamma_l \|T\|_n. \tag{23}$$

Proof. The cases of $l = 0$ and $l = n$ come from (20), having an equality for $l = 0$, even when Ω is unbounded. Now let's assume that $n - l$ is even, say $n - l = 2k$ for some $k \in \mathbb{N}$; the case of $n - l$ odd is treated in a similar way. By using (20), (22) and (21) with $\alpha = 2$, we get

$$\|\rho_{n-l,T}\|_{\mathrm{L}^1(\Omega)} \le \sum_{i\in\mathbb{N}} |\nu_i| \int_\Omega \left[\check{c}_2^2 |\nabla \Delta^k \psi_i|^2 + |\psi_i|^2 \right] \le \max\{1, \check{c}_2^{2l}\} \|\rho_{n,T}\|_{\mathrm{L}^1(\Omega)} = \gamma_l \|T\|_n.$$

□

Remark 6. *Let $n \in \mathbb{N}$, $R \in \mathscr{N}_{n,1}$ and $T \in \mathscr{N}_{n+1}$ such that $R|_{\mathrm{H}_{n+1}} = T$. Then, $R\psi_{i,T} = \nu_{i,T}\psi_{i,T}$, $i \in \mathbb{N}$, but $B_T = \{\psi_{i,T} \,/\, i \in \mathbb{N}\}$ is not necessarily orthogonal nor total in H_n. In any case, $\nu_{i,T} \ne \nu_{j,T}$ implies that $(\psi_{i,T}, \psi_{j,T})_n = 0$. Therefore, in the context of nuclear spaces, it doesn't make sense an inclusion like $\mathscr{N}_{n,1}|_{\mathrm{H}_{n+1}} \subseteq \mathscr{N}_{n+1}$. In any case, points (23) and (20) show that the norms of the density functions associated to an operator $T \in \mathscr{N}_{n,1}$ are ordered in a natural way:*

$$\begin{aligned} \|\rho_{0,T}\|_{\mathrm{L}^1(\Omega)} &\le \max\{1, \check{c}_2^2\} \|\rho_{1,T}\|_{\mathrm{L}^1(\Omega)} \le ... \le \max\{1, \check{c}_2^2\}^l \|\rho_{l,T}\|_{\mathrm{L}^1(\Omega)} \\ &\le ... \le \max\{1, \check{c}_2^2\}^n \|\rho_{n,T}\|_{\mathrm{L}^1(\Omega)}, \qquad l = 1, ..., n-1. \end{aligned} \tag{24}$$

3 Sobolev-like cones

In [9, 19] were defined cones of nuclear operators $\mathscr{H}_V^1$ which present properties analogues to those of the Sobolev space $\mathrm{H}^1(\Omega)$. On the other hand, in [18] were introduced cones $\mathscr{W}^{1,p}$ analogues to the space $\mathrm{W}^{1,p}(\Omega)$, $p > 1$. In this section we introduce cones of nuclear operators which, as we shall see, are analogues to the Sobolev space $\mathrm{H}^n(\Omega)$, $n \in \mathbb{N}$.

3.1 Definition and preliminary properties of the cone $\mathscr{H}_V^n$

From now on we assume that

(V_b) $V \in \mathrm{C}(\Omega) \cap \mathrm{L}^\infty(\Omega)$ with $V_0 = \inf_{x \in \mathbb{R}^N} V(x) > 0$.

On $\mathrm{C}_0^\infty(\Omega)$ let's consider the inner-products given by $(u,w)_{V,0} = \int_\Omega V(x)\, uw\, dx$, and, for $n \in \mathbb{N}$,

$$(u,w)_{V,n} = (\Delta^k u, \Delta^k w)_0 + (u,w)_{V,0}\,, \qquad \text{if } n = 2k, \tag{25}$$

$$(u,w)_{V,n} = (\nabla \Delta^{k-1} u, \nabla \Delta^{k-1} w)_0 + (u,w)_{V,0} \qquad \text{if } n = 2k-1. \tag{26}$$

For $n \in \mathbb{N}$, let H_V^n be the Hilbert space that results from completing $\mathrm{C}_0^\infty(\Omega)$ in the inner-product $(\cdot,\cdot)_{V,n}$. The corresponding norm is denoted by $\|\cdot\|_{V,n}$.

Remark 7. *Let $n \in \mathbb{N}$. Let's observe that, as linear spaces, $\mathrm{H}_V^n = \mathrm{H}_n$ and that, on it, the norms $\|\cdot\|_{V,n}$ and $\|\cdot\|_n$ are equivalent. This does not happen when Ω is unbounded and, in this case, most of the results of this paper can be recovered by considering a coercivity condition: (V_u) there exists a constant $d_0 > 0$ such that, for every $M > 0$, $\mathrm{meas}\{x \in \Omega \,/\, |x-y| \le d_0 \wedge V(x) \le M\} \longrightarrow 0$, as $|y| \longrightarrow +\infty$, where $\mathrm{meas}(\omega) = |\omega|$ denotes the Lebesgue measure of $\omega \subseteq \mathbb{R}^N$. Condition (V_u) is typical (see e.g. [4] and condition (V8) in [3]) to prove the compactness of the embedding $\mathrm{H}_V^1 \subseteq \mathrm{L}^q(\Omega)$, for every $q \in [2, 2^*[$, where $2^* = 2N/(N-2)$ and $N > 2$. Condition (V_u) is weaker than $V(x) \longrightarrow +\infty$, as $|x| \longrightarrow +\infty$, and the alternative condition (V3) in [3].*

Remark 8. *Let's assume that $N > 2n$ and denote $2_n^* = 2N/(N-2n)$. By [7, Th.9.16], for every $q \in [2, 2_n^*[$, the immersion $\mathrm{H}_V^n \subseteq \mathrm{L}^q(\Omega)$, is compact. The injection $\mathrm{H}_V^n \subseteq \mathrm{L}^{2_n^*}(\Omega)$ is continuous. Therefore, for every $q \in [2, 2_n^*]$, there exists $c_{q,n} > 0$ such that*

$$\forall u \in \mathrm{H}_V^n : \quad \|u\|_{\mathrm{L}^q(\Omega)} \le c_{q,n}\, \|u\|_{V,n}\,.$$

Given $n, l \in \mathbb{N}$, it's easy to prove that, $\|u\|_{V,n} \le \gamma_l\, \|u\|_{V,n+l}$, for every $u \in \mathrm{H}_{n+l}$, so that the embedding $\mathrm{H}_{n+l} \subseteq \mathrm{H}_n$ is continuous.

Let's define the set of operators we shall deal with.

Definition 1. *Let $n \in \mathbb{N}$. The* Sobolev-like cone *$\mathscr{H}_V^n$ is formed by the zero operator and the operators $T \in \mathscr{N}_{n-1} \setminus \{0\}$ such that $\psi_{i,T} \in \mathrm{H}_V^n$, $i \in \mathbb{N}$, and*

$$\langle\!\langle T \rangle\!\rangle_{V,n} = \sum_{i \in \mathbb{N}} |\nu_{i,T}|\; \|\psi_{i,T}\|_{V,n}^2 < +\infty. \tag{27}$$

We put $\langle\!\langle 0\rangle\!\rangle_{V,n} = 0$*. The value* $\langle\!\langle T\rangle\!\rangle_{V,n}$ *shall be referred to as the* total energy of the operator T.

The term "cone" is justified by the following easy result.

Proposition 2. *Let* $n \in \mathbb{N}$*. The following points hold.*

i) $\mathscr{H}_V^n$ *is an algebraic cone, i.e., for every* $\alpha \in \mathbb{R}$, $\alpha\mathscr{H}_V^n \subseteq \mathscr{H}_V^n$*.*

ii) $\langle\!\langle \alpha T\rangle\!\rangle_{V,n} = 0$ *iff* $T = 0$ *or* $\alpha = 0$*.*

iii) $\langle\!\langle T\rangle\!\rangle_{V,n} = 0$ *iff* $T = 0$*.*

Since $\langle\!\langle T\rangle\!\rangle_{V,n} \geq 0$, for every $T \in \mathscr{H}_V^n$, Proposition 2 shows that $\langle\!\langle \cdot\rangle\!\rangle_{V,n}$ behaves like the square of a norm. As in Remark 3, $\mathscr{H}_V^n = \mathscr{H}_{V,+}^n - \mathscr{H}_{V,+}^n$, $n \in \mathbb{N}$.

The following result will be helpful.

Theorem 3. *Let* $\beta : \mathbb{R} \longrightarrow \mathbb{R}$ *be a bounded Borel function with* $\beta(0) = 0$ *for which there exist* $c_1, t_0 > 0$ *and* $\alpha \geq 1$ *such that*

$$|\beta(t)| \leq c_1 |t|^\alpha, \quad \textit{for a.e. } t \in [-t_0, t_0]. \tag{28}$$

Then, $\beta(\mathscr{H}_V^n) \subseteq \mathscr{H}_V^n$ *and, for* $T \in \mathscr{H}_V^n$*, there is some* $d^* = d^*(T) > 0$ *such that*

$$\langle\!\langle \beta(T)\rangle\!\rangle_{V,n} \leq d^* \langle\!\langle T\rangle\!\rangle_{V,n}. \tag{29}$$

Proof. Let $T \in \mathscr{H}_V^n$. Since T is a compact self-adjoint operator, $\#\{i \in \mathbb{N} \,/\, |\nu_{i,T}| > t_1\} < +\infty$, where $t_1 = \min\{1, t_0\}$. Then, we pick $d > 0$ such that $|\beta(\nu_{j,T})| \leq d|\nu_{j,T}|$, for each $j \in \{i \in \mathbb{N} \,/\, |\nu_{i,T}| > t_1\}$. By the spectral theorem, [20, Th.VII.2], and (28), we get

$$\begin{aligned}\langle\!\langle \beta(T)\rangle\!\rangle_{V,n} &= \sum_{i\in\mathbb{N}} |\beta(\nu_{i,T})| \, \|\psi_{i,T}\|_{V,n}^2 = \sum_{|\nu_{i,T}|\leq t_1} \cdots + \sum_{|\nu_{i,T}|>t_1} \cdots \\ &\leq c_1 \sum_{|\nu_{i,T}|\leq t_1} |\nu_{i,T}|^\alpha \, \|\psi_{i,T}\|_{V,n}^2 + d \sum_{|\nu_{i,T}|>t_1} |\nu_{i,T}| \, \|\psi_{i,T}\|_{V,n}^2 \leq d^* \sum_{i\in\mathbb{N}} |\nu_{i,T}| \, \|\psi_{i,T}\|_{V,n}^2 = d^* \langle\!\langle T\rangle\!\rangle_{V,n},\end{aligned}$$

where $d^* = \max\{c_1, d\}$. We conclude by the arbitrariness of T. □

Remark 9. *It's clear that Theorem 3 remains true if the function* β *is assumed to belong to* $\mathrm{C}(\sigma(T))$ *with* $\beta(0) = 0$*, where* $\sigma(T)$ *denotes the spectrum of* T*.*

3.2 Density of finite-rank ϵ-QSA operators in $\mathscr{H}_V^n$

In this section it's shown that nice finite-rank operators (not necessarily self-adjoint) can be used to approximate elements of $\mathscr{H}_V^n$, and that such finite-rank operators are not far from being self-adjoint. We believe that this kind of result is important because in the last years attention has been put to mathematical problems related to non-Hermitian quantum mechanics since, for example, physical symmetries are represented by unitary and antiunitary operators, [12, 13]. There is also interest in non-standard representations of observables by operators which could not be self-adjoint but which share some of their properties, [1, 8].

The key definition is the following.

Definition 2. *Let H be a Hilbert space, $S : D \subseteq H \longrightarrow H$ linear and $\varepsilon > 0$. We say that S is an ε-quasi-self-adjoint operator (ϵ-QSA operator for short) iff*

$$\forall u, v \in D : \quad |(Su, v) - (u, Sv)| \leq \varepsilon \|u\| \, \|v\|. \tag{30}$$

It's clear that any self-adjoint operator is an ε-QSA operator, for every $\varepsilon > 0$. Therefore, in Definition 2, ε is a measure of how far from being self-adjoint an operator is. In the context of Definition 2, the following points are immediate:

i) if $\alpha \in \mathbb{R} \setminus \{0\}$, then αS is an $\varepsilon|\alpha|$-QSA operator;
ii) if $0 < \varepsilon < \tilde{\varepsilon}$, then S is an $\tilde{\varepsilon}$-QSA operator;
iii) if $|\alpha| \leq 1$, then αS is an ε-QSA operator;
iv) if $T : D \subseteq H \longrightarrow H$ is an $\tilde{\varepsilon}$-QSA operator, then $S + T$ is an $(\varepsilon + \tilde{\varepsilon})$-QSA operator.

Proposition 4. *Let H be a Hilbert space, $\varepsilon > 0$ and $S : D \subseteq H \longrightarrow H$ a bounded ε-QSA operator, $S \neq 0$. Assume that $(u_n)_{n \in \mathbb{N}} \subseteq D$ and $(v_m)_{m \in \mathbb{N}} \subseteq D$ are maximizer sequences of $\|S\| = \sup \left\{ \|Su\| \cdot \|u\|^{-1} \,/\, u \in D \right\}$. Then,*

$$\limsup_{n,m \longrightarrow +\infty} |\hat{c}_{n,m} - \check{c}_{n,m}| \leq \min \left\{ 2, \frac{\varepsilon}{\|S\|} \right\}, \tag{31}$$

where $\hat{c}_{n,m} = \cos(\hat{\theta}_{n,m})$ and $\check{c}_{n,m} = \cos(\check{\theta}_{n,m})$ with $\hat{\theta}_{n,m}$ the angle between Su_n and v_m and $\check{\theta}_{n,m}$ the angle between Sv_m and u_n, respectively.

Proof. By using (30) with $u = u_n$ and $v = v_m$ we get, for every $n, m \in \mathbb{N}$, that $\left| \|Su_n\| \cdot \|u_n\|^{-1} \hat{c}_{n,m} - \|Sv_m\| \cdot \|v_m\|^{-1} \check{c}_{n,m} \right| \leq \varepsilon$, whence it follows (31). □

Observe that if S is self-adjoint, then, by Proposition 4, for n and m big, $\hat{\theta}_{n,m} \approx \check{\theta}_{n,m}$ or $\hat{\theta}_{n,m} \approx -\check{\theta}_{n,m}$, i.e., there are only two possible limit angles for any pair of maximizer sequences of $\sup \left\{ \|Su\| \cdot \|u\|^{-1} \,/\, u \in D \right\}$.

To state the promised density result, let's denote by $\mathscr{M}_n$ the space of finite-rank linear operators $T : H \longrightarrow H$, $\check{\mathscr{M}}_n = \{ T \in \mathscr{M}_n \,/\, T(\mathrm{H}_n) \subseteq \mathrm{C}_0^\infty(\Omega) \}$ and

$$\mathscr{M}_{n,s} = \{ T \in \mathscr{M}_n \,/\, T \text{ is self-adjoint} \}. \tag{32}$$

Theorem 5. *Let $n \in \mathbb{N}$. Given $T \in \mathscr{H}_V^{n+1}$ and $\varepsilon > 0$, there exists an operator $S \in \check{\mathscr{M}}_n$ which is ϵ-QSA and verifies $\|T - S\| \leq \epsilon$. Therefore, the space $\check{\mathscr{M}}_n$ is dense in $\mathscr{H}_V^{n+1}$ in the norm $\|\cdot\|$.*

Proof. a) Let $T \in \mathscr{H}_V^{n+1}$ and $\varepsilon > 0$. Since $\mathscr{M}_n$ is dense in $\mathscr{N}_{n,1}$, we can pick $m \in \mathbb{N}$ such that the finite-rank operator $T_m : \mathrm{H}_n \longrightarrow \mathrm{H}_n$, given by $T_m u = \sum_{i=1}^m (u, \psi_{i,T})_n \, \nu_{i,T} \, \psi_{i,T}$, is self-adjoint and verifies $\|T - T_m\| < \varepsilon/2$. Now we choose functions $\phi_i \in \mathrm{C}_0^\infty(\Omega)$, $i = 1, \ldots, m$, such that $\|\psi_{i,T} - \phi_i\|_n < \varepsilon (m \cdot \max_{j \in \mathbb{N}} |\nu_{j,T}| \cdot 2^{i+1})^{-1}$ and define $S : \mathrm{H}_n \longrightarrow \mathrm{H}_n$ by $Su = \sum_{i=1}^m (u, \psi_{i,T})_n \, \nu_{i,T} \, \phi_i$, so that $S \in \check{\mathscr{M}}_n$. We have, by Cauchy-Schwartz inequality, for $u \in \mathrm{H}_n$, that

$$\|(T - S)u\|_n \leq \|T - T_m\| \, \|u\|_n + \|T_m u - Su\|_n$$

$$\leq \frac{\varepsilon}{2}\|u\|_n + \sum_{i=1}^{m} |\nu_{i,T}\,(u,\psi_{i,T})_n|\,\|\psi_{i,T}-\phi_i\|_n$$
$$\leq \frac{\varepsilon}{2}\|u\|_n + \sum_{i=1}^{m} |\nu_{i,T}|\,\|u\|_n \frac{\varepsilon}{m\cdot \max_{j\in\mathbb{N}}|\nu_{j,T}|\cdot 2^{i+1}} \leq \varepsilon\|u\|_n.$$

By the arbitrariness of u we get $\|T-S\|\leq \epsilon$.

b) Let's prove that S is an ε-QSA operator. Let $u,w\in \mathrm{H}_n$. We have that

$$(Su,w)_n - (u,Sw)_n = \sum_{i=1}^{m}\nu_{i,T}\left[(u,\psi_{i,T})_n(w,\phi)_n - (w,\psi_{i,T})_n(u,\phi)_n\right]$$
$$= \sum_{i=1}^{m}\nu_{i,T}\left[(u,\psi_{i,T}-\phi_i)_n(w,\phi_i)_n + (w,\phi_i-\psi_{i,T})_n(u,\phi_i)_n\right].$$

Then, by Cauchy-Schwartz inequality,

$$|(Su,w)_n-(u,Sw)_n| \leq 2\|u\|_n\|w\|_n\sum_{i=1}^{m}|\nu_{i,T}|\,\|\psi_{i,T}-\phi_i\|_n$$
$$\leq 2\|u\|_n\|w\|_n\sum_{i=1}^{m}|\nu_{i,T}|\frac{\varepsilon}{m\cdot\max_{j\in\mathbb{N}}|\nu_{j,T}|\cdot 2^{i+1}} \leq \varepsilon\|u\|_n\|w\|_n.$$

□

4 Energy functionals and Poincaré's-like inequality

From (27), it's immediate that $\langle\!\langle T\rangle\!\rangle_{V,n} = \mathscr{K}_n(T)+\mathscr{P}_V(T)$, $T\in\mathscr{H}_V^n$, where the *potential energy of the operator* T is given by

$$\mathscr{P}_V(T) = \int_\Omega \rho_{0,T}(x)V(x)dx = \sum_{i\in\mathbb{N}}|\nu_{i,T}|\int_\Omega|\psi_{i,T}|^2V(x)dx, \tag{33}$$

and the *kinetic energy of the operator* T is given by

$$\mathscr{K}_n(T) = \sum_{i\in\mathbb{N}}|\nu_{i,T}|\int_\Omega|\Delta^m\psi_{i,T}|^2dx, \qquad \text{if } n=2m, \tag{34}$$
$$\mathscr{K}_n(T) = \sum_{i\in\mathbb{N}}|\nu_{i,T}|\int_\Omega|\nabla\Delta^m\psi_{i,T}|^2dx, \qquad \text{if } n=2m+1. \tag{35}$$

Remark 10. *In [18] were introduced cones $\mathscr{W}^{1,p}$, analogues to the space $\mathrm{W}^{1,p}(\Omega)$, $p>1$, at the level of operators. It was shown, except for $p=2$, that there is an imbalance of energies: the p-total energy of an operator $\mathscr{W}^{1,p}$ is bigger or equal than the sum of its p-kinetic energy and its p-potential energy. The case of perfect balance, $p=2$, occurs because the definitions (33) and (34)-(35) are actually basis-independent. This kind of imbalance of energies should happen for cones $\mathscr{W}^{n,p}$ with Ω bounded or unbounded.*

Remark 11. *Let $T \in \mathscr{H}^n_V$ and V be such that the multiplication operator $\langle\{\psi_{i,T} \,/\, i \in \mathbb{N}\}\rangle \ni u \longmapsto Vu \in \mathrm{H}_{n-1}$ is well defined. This happens, for example, when $V \in \mathrm{C}^{n-1}(\overline{\Omega})$ and $\psi_{i,T} \in \mathrm{H}^n_V \cap \mathrm{L}^\infty(\Omega)$, $i \in \mathbb{N}$; see [7, Prop.9.4]. In this case, we identify V with the multiplication operator. Then, for $T \in \mathscr{H}^n_V$ we formally have, using (8), that $\mathrm{Tr}_{n-1}(V|T|) = \sum_{i\in\mathbb{N}}(\psi_{i,T}, V|T|\psi_{i,T})_{n-1} = \mathscr{P}_V(T)$.*

Remark 12. *Considering the Laplace operator, $-\Delta : \mathrm{H}^1_0(\Omega) \cap \mathrm{H}^2(\Omega) \subseteq \mathrm{L}^2(\Omega) \longrightarrow \mathrm{L}^2(\Omega)$, then it formally holds, for $T \in \mathscr{H}^n_V$, that $\mathscr{K}_n(T) = \mathrm{Tr}_{n-1}((-\Delta)^n T)$. For the last, it should happen that $\psi_{i,T} \in \mathrm{H}^{2n}_V$, $i \in \mathbb{N}$.*

Definition 3. *A function $\beta : \mathbb{R} \longrightarrow \mathbb{R}$ is referred to as an* entropy seed *iff it's convex and $\beta(0) = 0$. We say that the value $\mathcal{S}_\beta(T) = \sum_{i\in\mathbb{N}} \beta(\nu_{i,T})$ is the β-*entropy of the operator *$T \in \mathscr{N}_{n-1}$ if $\mathcal{S}_\beta(T) \in \mathbb{R} \cup \{+\infty\}$.*

As a consequence of Theorem 3, we have that the entropy functional is well-defined on $\mathscr{H}^n_V$:

Corollary 6. *Let β an entropy seed. Then, $\beta(\mathscr{H}^n_V) \subseteq \mathscr{H}^n_V$ and, for every $T \in \mathscr{H}^n_V$, (29) holds as well as*

$$\mathcal{S}_\beta(T) = \mathrm{Tr}_{n-1}(\beta(T)). \tag{36}$$

Proof. Since β is convex, it's continuous and, therefore, $\beta(\sigma(T)) \subseteq \mathbb{R}$ is compact because $\sigma(T)$ is compact. Consequently, the conditions of Theorem 3 hold and, by the spectral theorem, [20, Th.VII.2], equality (36) is also true. □

Thanks to Corollary 6, the entropy functional $\mathcal{S}_\beta : \mathscr{H}^n_V \longrightarrow \mathbb{R}$ is well defined as it is the *free-energy functional*, $\mathscr{F}_{V,\beta} : \mathscr{H}^n_V \longrightarrow \mathbb{R}$, given by

$$\mathscr{F}_{V,\beta}(T) = \mathcal{S}_\beta(T) + \langle\!\langle T \rangle\!\rangle_{V,n}. \tag{37}$$

See [5] for a discussion on the entropy concept in the context of quantum mechanics.

The proof of the following result uses the classical Poincaré's inequality, (21) with $\alpha = 2$. As we mentioned, Proposition 2 shows that $\langle\!\langle\cdot\rangle\!\rangle_{V,n}$ behaves like the square of a norm; this allows us to interpret point (38) below as a Poincaré's-like inequality but at the level of nuclear operators. It can also be interpreted as an uncertainty principle in the sense that the energy of a nuclear operator is bounded from below by the basic spread of the operator, its trace norm.

Theorem 7. *Let $n \in \mathbb{N}_*$. Then there exists $\hat{c} = \hat{c}(\Omega, V_0) > 0$ such that*

$$\forall T \in \mathscr{H}^{n+1}_V : \quad \|T\|_n \le \hat{c}\langle\!\langle T \rangle\!\rangle_{V,n+1}. \tag{38}$$

Proof. Let's assume that n is even, say $n = 2k$ with $k \in \mathbb{N}$, as the case of n odd is treated in a similar way. Let $T \in \mathscr{H}^{n+1}_V$. Since $B_T = \{\psi_{i,T} \,/\, i \in \mathbb{N}\}$ is a Hilbert basis of H_n, we have, by (21) and putting $\hat{c} = \max\{\check{c}_2^2, V_0^{-1}\} > 0$, that

$$\begin{aligned} \|T\|_n &= \sum_{i\in\mathbb{N}} |\nu_{i,T}| = \sum_{i\in\mathbb{N}} |\nu_{i,T}| \int_\Omega \left[|\Delta^k \psi_{i,T}|^2 + |\psi_{i,T}|^2\right] dx \\ &\le \sum_{i\in\mathbb{N}} |\nu_{i,T}| \int_\Omega \left[\check{c}_2^2 |\nabla\Delta^k \psi_{i,T}|^2 + \frac{V(x)}{V_0}|\psi_{i,T}|^2\right] dx \le \hat{c} \sum_{i\in\mathbb{N}} |\nu_{i,T}| \; \|\psi_{i,T}\|^2_{V,2k+1} = \hat{c}\langle\!\langle T \rangle\!\rangle_{V,n+1}. \end{aligned}$$

□

5 Regularity of density functions and k-energetic values of an operator

Let $n \in \mathbb{N}$ and $k \in \{0, 1, ..., n\}$. The *k-energetic value of an operator* $T \in \mathscr{N}_{n,1}$ is given by $\mathrm{E}_{V,k}(T) = \sum_{i \in \mathbb{N}} |\nu_{i,T}| \, \|\psi_{i,T}\|_{V,k}^2$. Observe that, for $T \in \mathscr{H}_V^{n+1}$,

$$\mathrm{E}_{V,n+1}(T) = \langle\!\langle T \rangle\!\rangle_{V,n+1}. \tag{39}$$

Proposition 8. *Let $n \in \mathbb{N}$ and $k \in \{1, ..., n\}$. There exists $\tilde{c}_k = \tilde{c}_k(\Omega) > 0$ such that*

$$\forall T \in \mathscr{H}_V^{n+1} : \quad \mathrm{E}_{V,n+1-k}(T) \le \tilde{c}_k \langle\!\langle T \rangle\!\rangle_{V,n+1}. \tag{40}$$

Proof. We work as in the proof of Theorem 7, applying (21) with $\alpha = 2$ and taking $\tilde{c}_k = \max\{1, \check{c}_2^{2k}\}$. □

Remark 13. *Let $n \in \mathbb{N}$. As it was mentioned in Remark 6, it doesn't make sense the inclusion $\mathscr{N}_{n,1}|_{\mathrm{H}_{n+1}} \subseteq \mathscr{N}_{n+1}$, but the density functions associated to an operator $T \in \mathscr{N}_{n,1}$ are ordered as in (24). In the same way, we don't have $\mathscr{H}_V^n|_{\mathrm{H}_{n+1}} \subseteq \mathscr{H}_V^{n+1}$, but, thanks to (40) and (39), the energetic values of an operator $T \in \mathscr{H}_V^{n+1}$ are also ordered in a natural way:*

$$\begin{aligned} \mathrm{E}_{V,1}(T) \le \max\{1, \check{c}_2^2\} \mathrm{E}_{V,2}(T) \le ... \le \max\{1, \check{c}_2^2\}^k \mathrm{E}_{V,n+1-k}(T) \\ \le ... \le \max\{1, \check{c}_2^2\}^n \mathrm{E}_{V,n+1}(T) = \max\{1, \check{c}_2^2\}^n \langle\!\langle T \rangle\!\rangle_{V,n+1}. \end{aligned}$$

Let's recall from Section 2.3, that given $n \in \mathbb{N}_*$, $T \in \mathscr{N}_{n,1}$ and $m \in \mathbb{N}_*$ with $m \le n$, we defined a density function by (18) and (19) for m odd and even, respectively.

Since the functions $\psi_{i,T}$, $i \in \mathbb{N}$, which appear in (18)-(19), have regularity properties, it's natural to ask for regularity properties for the density functions $\rho_{0,T}$,...,$\rho_{n-1,T}$ when the operator T belongs to $\mathscr{H}_V^n \subseteq \mathscr{N}_{n-1}$. In the coming result we deal with the main density function, which will be simply denoted by

$$\rho_W = \rho_{n-1,W}, \quad W \in \mathscr{H}_V^n,$$

but it's clear that similar results hold for the other density functions associated to W and that the regularity of ρ_W is improved when $N = 1, 2$.

Theorem 9. *Let $N \ge 3$, $n \in \mathbb{N}$, $T \in \mathscr{H}_V^n$, $R =]1, N/(N-1)]$ and $S =]1, N/(N-2)]$.*

i) For every $r \in R$, there exists $\tilde{z}_1 = \tilde{z}_1(N, r) > 0$ such that, for $L = |T|^r$,

$$\|\nabla \rho_L\|_{\mathrm{L}^r(\Omega)}^r \le \tilde{z}_1 \langle\!\langle T \rangle\!\rangle_{V,n}^r.$$

ii) For every $r \in R$ and every $s \in S$, we have that $\rho_L \in \mathrm{W}^{1,r}(\Omega) \cap \mathrm{L}^s(\Omega)$.

iii) For every $s \in S$, $\rho_T \in \mathrm{W}^{1,1}(\Omega) \cap \mathrm{L}^s(\Omega)$ *and*

$$\|\nabla \rho_T\|_{\mathrm{L}^1(\Omega)} \leq 2\check{c}_2 \langle\!\langle T \rangle\!\rangle_{V,n}.$$

Before proving Theorem 9, let's observe that if $r \in R$, then $2 \leq 2r < 2N/(N-1)$ and $1 \leq 1/(2-r) < (N-1)/(N-2)$, so that $2 \leq 2r/(2-r) < 2N/(N-2) = 2^*$. In the context of inequality (21), we shall denote $s_r = \check{c}_\alpha$, for $\alpha = 2r/(2-r)$.

Proof of Theorem 9. Thanks to Remark 4, it's enough to suppose that $T \in \mathscr{H}^n_{V,+}$ and so $L = T^r$. Since $r > 1$ and $A = \sup_{i \in \mathbb{N}} \nu_{i,T} \|\psi_i\|^2_{V,n} < +\infty$,

$$\left[A^{-1}\nu_{i,T} \|\psi_i\|^2_{V,n}\right]^r \leq A^{-1}\nu_{i,T} \|\psi_i\|^2_{V,n}, \quad \text{for every } i \in \mathbb{N}. \tag{41}$$

Let's assume that n is odd, say $n = 2k+1$ with $k \in \mathbb{N}$; the case of n even is treated in a similar way. We have, for $x \in \Omega$, that $\rho_L(x) = \Upsilon(x) + \Theta(x)$, where $\Upsilon(x) = \sum_{i\in\mathbb{N}} \nu_{i,L} |\Delta^k \psi_i(x)|^2$ and $\Theta(x) = \sum_{i \in \mathbb{N}} \nu_{i,L} |\psi_i(x)|^2$. Then,

$$\nabla \Upsilon(x) = 2\|L\|_{n-1} \sum_{i \in \mathbb{N}} \frac{\nu_{i,L}}{\sum_{j\in\mathbb{N}} \nu_{j,L}} \Delta^k \psi_i(x)\, \nabla \Delta^k \psi_i(x).$$

By the convexity of $[0,+\infty[\ni t \longmapsto \beta(t) = t^r \in \mathbb{R}$, Hölder inequality with $P = 2/r$ and $P' = 2/(2-r)$, Theorems 7 and 3, Remark 9 and (41), we get, by taking $\tilde{z}_1 = (2s_r)^r (\hat{c} d_* A)^{r-1}$, that

$$\begin{aligned}
\int_\Omega |\nabla \Upsilon|^r dx &\leq 2^r \|L\|^r_{n-1} \int_\Omega \sum_{i\in\mathbb{N}} \frac{\nu_{i,L}}{\sum_{j\in\mathbb{N}} \nu_{j,L}} |\Delta^k \psi_i|^r |\nabla \Delta^k \psi_i|^r dx \\
&= 2^r \|L\|^{r-1}_{n-1} \sum_{i\in\mathbb{N}} \nu_{i,L} \int_\Omega |\Delta^k \psi_i|^r |\nabla \Delta^k \psi_i|^r dx \\
&\leq 2^r \hat{c}^{r-1} \langle\!\langle L \rangle\!\rangle^{r-1}_{V,n} \sum_{i\in\mathbb{N}} \nu_{i,L} \left(\int_\Omega |\nabla \Delta^k \psi_i|^2\right)^{r/2} \left(\int_\Omega |\Delta^k \psi_i|^{2r/(2-r)}\right)^{(2-r)/2} \\
&\leq (2s_r)^r \left(\hat{c} \langle\!\langle T \rangle\!\rangle_{V,n} d_*\right)^{r-1} \sum_{i\in\mathbb{N}} \nu_{i,L} \left\|\Delta^k \psi_i\right\|^{2r}_{\mathrm{H}^1_0(\Omega)} \\
&\leq (2s_r)^r \left(\hat{c} \langle\!\langle T \rangle\!\rangle_{V,n} d_*\right)^{r-1} \sum_{i\in\mathbb{N}} \left(\nu_{i,T} \left\|\Delta^k \psi_i\right\|^2_{V,n}\right)^r \\
&\leq (2s_r)^r \left(A\hat{c} \langle\!\langle T \rangle\!\rangle_{V,n} d_*\right)^{r-1} \sum_{i\in\mathbb{N}} \nu_{i,T} \left\|\Delta^k \psi_i\right\|^2_{V,n} = \tilde{z}_1 \langle\!\langle T \rangle\!\rangle^r_{V,n}.
\end{aligned} \tag{42}$$

Working as it was to get (42) is obtained an estimate for $\int_\Omega |\nabla \Theta(x)|^r dx$. This, together with (42) and possibly adjusting the value of $\tilde{z}_1$, provides point i). Point ii) follows by interpolation in Lebesgue spaces; see e.g. [7, pp.93]. Point iii) is obtained by letting $r \longrightarrow 1$ in points i) and ii). □

Corollary 10. *Let* $N \geq 3$, $n \in \mathbb{N}$ *and* $T \in \mathscr{H}^n_V$. *Let's denote,* $S_l =]1, N/(N-2l)]$, $l \in \{1, ..., n\}$. *For every* $r \in R$ *and* $s \in S_l$, *we have that* $\rho_{L,n-l} \in \mathrm{W}^{l,r}(\Omega) \cap \mathrm{L}^s(\Omega)$ *and*

$\rho_{T,n-l} \in \mathrm{W}^{l,1}(\Omega) \cap \mathrm{L}^s(\Omega)$. *For each* $l \in \{1, ..., n\}$, *there exists* $\tilde{z}_l = \tilde{z}_l(r, \Omega) > 0$ *such that*

$$\|\Delta\rho_{L,n-l}\|^r_{\mathrm{L}^r(\Omega)} \le \tilde{z}_l \langle\!\langle T \rangle\!\rangle^r_{V,n}, \quad \text{if } n-l \text{ is even;} \tag{43}$$

$$\|\nabla\rho_{L,n-l}\|^r_{\mathrm{L}^r(\Omega)} \le \tilde{z}_l \langle\!\langle T \rangle\!\rangle^r_{V,n}. \quad \text{if } n-l \text{ is odd.} \tag{44}$$

Proof. We can assume that T is positive. Let's deal with (43) as the situation of (44) is treated in a similar way. Let's denote $\rho_L = \rho_{L,n-l}$ and assume that $n-l = 2j$, for some $j \in \mathbb{N}_*$. We have that $\Delta\rho_L = 2\sum_{i\in\mathbb{N}} \nu_{i,L}\left[\Delta^j\psi_i\Delta^{j+1}\psi_i + |\nabla\Delta^j\psi_i|^2\right]$. Working as in the proof of Theorem 9, we get

$$\int_\Omega |\Delta\rho_L|^r dx \le 2^r \|L\|^{r-1}_{n-1} \sum_{i\in\mathbb{N}} \nu_{i,L}[I_1^{1/r} + I_2^{1/r}]^r, \tag{45}$$

where, by using Hölder inequality,

$$I_1 = \int_\Omega |\nabla\Delta^j\psi_i|^{2r} \le |\Omega|^{r-1} \left\|\nabla\Delta^j\psi_i\right\|^{2r}_{\mathrm{L}^{2r/(2-r)}(\Omega)} \le |\Omega|^{r-1} s_r^{2r} \left\|\Delta^{j+1}\psi_i\right\|^{2r}_{\mathrm{L}^2(\Omega)}, \tag{46}$$

$$\begin{aligned} I_2 &= \int_\Omega |\Delta^{j+1}\psi_i|^r |\Delta^j\psi_i|^r \le \left\|\Delta^{j+1}\psi_i\right\|^r_{\mathrm{L}^2(\Omega)} \left\|\Delta^j\psi_i\right\|^r_{\mathrm{L}^{2r/(2-r)}(\Omega)} \\ &\le \check{c}_2^r s_r^r \left\|\Delta^{j+1}\psi_i\right\|^{2r}_{\mathrm{L}^2(\Omega)}, \end{aligned} \tag{47}$$

By (45), (46), (47) and (40), it follows that

$$\begin{aligned} \int_\Omega |\Delta\rho_L|^r dx &\le 2^r \|L\|^{r-1}_{n-1} \left(|\Omega|^{(r-1)/r} s_r^2 + \check{c}_2 s_r\right)^r \sum_{i\in\mathbb{N}} \nu_{i,L} \left\|\Delta^{j+1}\psi_i\right\|^{2r}_{\mathrm{L}^2(\Omega)} \\ &\le 2^r \hat{c}^{r-1} \langle\!\langle L \rangle\!\rangle^{r-1}_{V,n} \left(|\Omega|^{(r-1)/r} s_r^2 + \check{c}_2 s_r\right)^r \sum_{i\in\mathbb{N}} \left(\nu_{i,T} \left\|\Delta^{j+1}\psi_i\right\|^2_{\mathrm{L}^2(\Omega)}\right)^r \\ &\le 2^r \left(\hat{c} d_* D\right)^{r-1} \langle\!\langle T \rangle\!\rangle^{r-1}_{V,n} \left(|\Omega|^{(r-1)/r} s_r^2 + \check{c}_2 s_r\right)^r \sum_{i\in\mathbb{N}} \nu_{i,T} \left\|\Delta^{j+1}\psi_i\right\|^2_{\mathrm{L}^2(\Omega)} \\ &= 2^r \left(\hat{c} d_* D\right)^{r-1} \left(|\Omega|^{(r-1)/r} s_r^2 + \check{c}_2 s_r\right)^r \langle\!\langle T \rangle\!\rangle^{r-1}_{V,n} \mathrm{E}_{V,j+1}(T) \le \tilde{z}_l \langle\!\langle T \rangle\!\rangle^r_{V,n}, \end{aligned}$$

where $\tilde{z}_l = 2^r \left(\hat{c} d_* D\right)^{r-1} \left(|\Omega|^{(r-1)/r} s_r^2 + \check{c}_2 s_r\right)^r \tilde{c}_{n-1-j}$ and $D = \sup_{i\in\mathbb{N}} \nu_{i,T} \left\|\Delta^{j+1}\psi_i\right\|^2_{\mathrm{L}^2(\Omega)}$. □

6 Lower estimates for energy functionals and Gagliardo-Nirenberg type inequalities

Considering the stability of a quantum system, the following three steps are relevant (see e.g. [10, 17]):

1. $\mathscr{F}_{V,\beta}$ is bounded from below on $\mathscr{H}^n_{V,+}$
2. There exists $T_0 \in \mathscr{H}^n_{V,+}$ such that $\mathscr{F}_{V,\beta}(T_0) = \inf_{T\in\mathscr{H}^n_{V,+}} \mathscr{F}_{V,\beta}(T)$.
3. There is a unique solution of the mentioned minimization problem.

In this section we deal with point 1. In Section 7.1 we produce compactness properties which are needed to deal, in Section 7.2, with point 2. In Section 7.2 we also discuss some situations where it's possible to achieve point 3.

Let's recall that the Legendre-Fenchel transform of a function $\varphi : \mathbb{R} \longrightarrow \mathbb{R} \cup \{+\infty\}$, $\varphi \neq +\infty$, is given by $\varphi^*(y) = \sup_{\theta\in\mathbb{R}} [y\theta - \varphi(\theta)]$, $y \in \mathbb{R}$. Then,

$$\forall y, \theta \in \mathbb{R} : \quad \varphi^*(y) \geq y\theta - \varphi(\theta). \tag{48}$$

Definition 4. *We say that an entropy seed β is* generated by a function F *if*

$$\beta(y) = F^*(-y), \quad y \in \mathbb{R}. \tag{49}$$

Observe that, by (49) and (48), we have, for every $y, \theta \in \mathbb{R}$,

$$\beta(y) + y\theta \geq -F(\theta). \tag{50}$$

Example 1. *Let's consider $\gamma > N/2$, so that $N/(N+2) < r = \gamma/(\gamma+1) < 1$. The function given by $\beta_r(s) = -(1-r)^{r-1} r^{-r} s$ if $s \geq 0$ and $\beta_r(s) = +\infty$ if $s < 0$, is an entropy seed, [10], generated by $F_\gamma(s) = s^{-\gamma}$ if $s \geq 0$ and $F_\gamma(s) = +\infty$ if $s < 0$.*

The following condition will be necessary. It's related to condition (H) in [10, pp.202], condition (V_α) in [9, 19] and condition $(\mathrm{G}_{V,\alpha})$ in [18].

$(\mathrm{G}^m_{V,\alpha})$ Let $m \in \mathbb{N}$ and $\alpha > 0$. Associated to the operator $\alpha(-\Delta)^m + V$ there are sequences $\big(\lambda^{(m)}_{\alpha,i}\big)_{i\in\mathbb{N}} \subseteq \mathbb{R}$ and $\big(\phi^{(m)}_{\alpha,i}\big)_{i\in\mathbb{N}} \subseteq \mathrm{H}_m$ such that $\lambda^{(m)}_{\alpha,i} \longrightarrow +\infty$, as $i \longrightarrow +\infty$; $0 < \lambda^{(m)}_{\alpha,1} < \lambda^{(m)}_{\alpha,2} \leq \lambda^{(m)}_{\alpha,3} \leq \ldots$;

$$[\alpha(-\Delta)^m + V]\phi^{(m)}_{\alpha,i} = \lambda^{(m)}_{\alpha,i}\phi^{(m)}_{\alpha,i}, \quad \text{weakly, for every } i \in \mathbb{N}; \text{ and} \tag{51}$$

$$\{\phi^{(m)}_{\alpha,i} \,/\, i \in \mathbb{N}\} \quad \text{is a Hilbert basis of } \mathrm{L}^2(\Omega). \tag{52}$$

Remark 14. *If there is no confussion, in the context of condition $(\mathrm{G}^m_{V,\alpha})$ we shall simply denote, for $i \in \mathbb{N}$, $\lambda_i = \lambda^{(m)}_{\alpha,i}$ and $\phi_i = \phi^{(m)}_{\alpha,i}$, as well as $\hat{\lambda}_i = \lambda^{(m)}_{\alpha,i}$, and $\hat{\phi}_i = \phi^{(m)}_{\alpha,i}$ if $V \equiv 0$ and $\alpha = 1$.*

Point (51) means that, for $i \in \mathbb{N}$,

$$\forall \Psi \in \mathrm{C}^\infty_0(\Omega) : \quad \alpha(\phi_i, \Psi)_{\alpha^{-1}V,m} = \lambda_i(\phi_i, \Psi)_0, \tag{53}$$

where we are using the natural extensions of notations (25) and (26). The last implies that $\lambda_i = \alpha\|\phi_i\|^2_{\alpha^{-1}V,m}/\|\phi_i\|^2_0$.

Definition 5. *Let $n \in \mathbb{N}_*$ and assume $(\mathrm{G}^{n+1}_{V,\alpha})$. Let $T \in \mathscr{H}^{n+1}_{V,+}$ and $F : \mathbb{R} \longrightarrow \mathbb{R} \cup \{+\infty\}$ convex and non-increasing on $[0, +\infty[$. We say that T is compatible with F iff*

$$D(T, F; \alpha) = \sum_{i\in\mathbb{N}} \Big(\hat{\psi}_{i,T},\ F\left(\mathcal{E}_T\alpha^{-1}[(-\Delta)^{n+1} + V]\hat{\psi}_{i,T}\right)\Big)_0 \in \mathbb{R},$$

where $\mathcal{E}_T = \inf_{i\in\mathbb{N}} \|\psi_{i,T}\|_0$ *and* $\hat{\psi}_{i,T} = \dfrac{1}{\|\psi_{i,T}\|_0}\psi_{i,T}$*,* $i \in \mathbb{N}$*. We write* $\mathcal{F}^{n+1}_{V,+} = \{T \in \mathscr{H}^{n+1}_{V,+} \,/\, T$ *is compatible with* $F\}$*.*

Remark 15. *Under* $(\mathrm{G}^{n+1}_{V,\alpha})$*, a function* $F : \mathbb{R} \longrightarrow \mathbb{R} \cup \{+\infty\}$ *belongs to the* Casimir class $\mathcal{C}^{n+1}_{V,\alpha}$ *if it's convex, non-increasing on* $[0,+\infty[$ *and* $\sum_{i\in\mathbb{N}} F(\lambda^{(m)}_{\alpha,i}) < +\infty$*. It was shown in [9], [19] and [18], that every operator* $T \in \mathscr{H}^1_{V,+}$ *is compatible with a function* $F \in \mathcal{C}^1_\alpha$*. Actually a uniform bound for the free-energy functional was proved; see Corollary 12 below.*

Example 2. *Let's consider a non-negative non-increasing function* $F : \mathbb{R} \longrightarrow \mathbb{R}\cup\{+\infty\}$ *for which there exist some* $C, \mu > 0$ *and* $d \geq 0$ *such that* $F(t) \leq C(1+t)^{-\mu+N/2}$*, for* $t \geq d$*. Then, using Weyl's estimate, [24], it's can be shown that* F *belong to the class* $\mathcal{C}^1_{0,1}$*. For example, this is the case when* F *is a primitive of a* Casimir function *[17], i.e.,* $F(t) = \int_t^{+\infty} f(s)ds$ *where* ***a)*** *there exists* $t_1 \in [-\infty,+\infty[$ *such that* $f(t) = +\infty$ *for any* $t \in]-\infty, t_1[$*,* ***b)*** f *is continuous on* $]t_1,+\infty[$*,* ***c)*** *there exists* $t_2 \in]t_1,+\infty]$ *such that* $f(t) > 0$ *for any* $t \in]t_1,t_2[$ *and* $f(t) = 0$ *for any* $t \geq t_2$*,* ***d)*** f *is strictly decreasing on* $]t_1,t_2[$*,* ***e)*** *if* $t_2 = +\infty$*, there exist* $\mu, C > 0$ *such that for* $s \geq 0$ *large,* $f(t) \leq C(1+t)^{-\mu+1+N/2}$*. As it's shown in [17], for* $\mu > 1$*,* $f(-\Delta) \in \mathcal{N}_{0,1}$*.*

Example 3. *The function* F_γ *of Example 1 belongs to* $\mathcal{C}^1_{0,1}$*. This also happens with* F *produced by the Fermi-Dirac statistics,* $f(t) = \int_{\mathbb{R}^N}(\mu + \exp(t+|x|^2/2))^{-1}dx$*, or the Boltzmann distribution* $f(t) = e^{-\mu t}$*,* $\mu > 0$*.*

Theorem 11. *Let* $\alpha > 0$*,* $n \in \mathbb{N}_*$ *and* β *an entropy seed generated by* $F : \mathbb{R} \longrightarrow \mathbb{R} \cup \{+\infty\}$ *which is convex and non-increasing on* $[0,+\infty[$*. Assume* $(\mathrm{G}^{n+1}_{V,\alpha})$*. Then, for every* $T \in \mathcal{F}^{n+1}_{V,+}$*,*

$$\mathscr{F}_{V,\beta}(T) \geq \begin{cases} -D(T,F;\alpha) & \text{if } \alpha > 1, \\ -D(T,F;1) & \text{if } 0 < \alpha \leq 1. \end{cases} \tag{54}$$

Proof. Let's assume that n is odd, say $n = 2k+1$ with $k \in \mathbb{N}$. The case of n even is treated in a similar way.

1. Let $i \in \mathbb{N}$. Since $\psi_i \in \mathrm{H}_{n+1} \subseteq \mathrm{L}^2(\Omega)$, by (52) there exists $(\mu_{i,j})_{j\in\mathbb{N}} \subseteq \mathbb{R}$ such that

$$\psi_i = \sum_{j\in\mathbb{N}} \mu_{i,j}\phi_j, \quad \text{in } \mathrm{L}^2(\Omega), \tag{55}$$

$$\|\psi_i\|_0^2 = \sum_{j\in\mathbb{N}} \mu_{i,j}^2, \qquad \mu_{i,j} = (\psi_i, \phi_j)_0. \tag{56}$$

   By using (55), (53) and (52), we get

$$\begin{aligned} \|\psi_i\|^2_{\alpha^{-1}V,n+1} &= \left(\sum_{j\in\mathbb{N}} \mu_{i,j}\phi_j, \sum_{l\in\mathbb{N}} \mu_{i,l}\phi_l\right)_{\alpha^{-1}V,n+1} = \sum_{j\in\mathbb{N}}\sum_{l\in\mathbb{N}} \mu_{i,j}\mu_{i,l}\,(\phi_j,\,\phi_l)_{\alpha^{-1}V,n+1} \\ &= \alpha^{-1}\sum_{j\in\mathbb{N}}\sum_{l\in\mathbb{N}} \mu_{i,j}\mu_{i,l}\lambda_j\,(\phi_j,\,\phi_l)_0 = \alpha^{-1}\sum_{j\in\mathbb{N}} \mu_{i,j}^2\lambda_j. \end{aligned} \tag{57}$$

2. Let's assume that $\alpha > 1$.

(a) Let $i \in \mathbb{N}$. We have that

$$\begin{aligned}\alpha \left\|\psi_i\right\|^2_{\alpha^{-1}V,n+1} &= \int_\Omega \left[\alpha|\Delta^{k+1}\psi_i|^2 + V(x)|\psi_i|^2\right] dx \\ &= \alpha \left\|\psi_i\right\|^2_{V,n+1} - (\alpha - 1)\int_\Omega V(x)|\psi_i|^2 dx \leq \alpha \left\|\psi_i\right\|^2_{V,n+1},\end{aligned}$$

whence $-F\left(\left\|\psi_i\right\|^2_{V,n+1}\right) \geq -F\left(\left\|\psi_i\right\|^2_{\alpha^{-1}V,n+1}\right)$. Then, by choosing $y = \nu_i$ and $\theta = \left\|\psi_i\right\|^2_{V,n+1}$ in (50), we get

$$\beta(\nu_i) + \nu_i \left\|\psi_i\right\|^2_{V,n+1} \geq -F\left(\left\|\psi_i\right\|^2_{V,n+1}\right) \geq -F\left(\left\|\psi_i\right\|^2_{\alpha^{-1}V,n+1}\right),$$

so that, by (37), (36) and (27),

$$\mathscr{F}_{V,\beta}(T) \geq -\sum_{i\in\mathbb{N}} F\left(\left\|\psi_i\right\|^2_{\alpha^{-1}V,n+1}\right). \tag{58}$$

(b) Since F is convex, we get, by (57), (56) and the spectral theorem, that

$$\begin{aligned}F(\left\|\psi_i\right\|^2_{\alpha^{-1}V,n+1}) &= F\left(\alpha^{-1}\sum_{j\in\mathbb{N}} \mu^2_{i,j}\lambda_j\right) = F\left(\sum_{j\in\mathbb{N}} \frac{\mu^2_{i,j}}{\|\psi_i\|^2_0}\cdot \lambda_j\alpha^{-1}\|\psi_i\|^2_0\right) \\ &\leq \frac{\sum_{j\in\mathbb{N}} \mu^2_{i,j} F\left(\lambda_j\alpha^{-1}\|\psi_i\|^2_0\right)}{\|\psi_i\|^2_0} = \frac{\left(\psi_i, F\left(\alpha^{-1}\|\psi_i\|^2_0\left[(-\Delta)^{n+1} + V\right]\right)\psi_i\right)_0}{\|\psi_i\|^2_0}.\end{aligned} \tag{59}$$

(c) Since F is non-increasing, we get, by (58) and (59), that

$$\mathscr{F}_{V,\beta}(T) \geq -\sum_{i\in\mathbb{N}} \frac{1}{\|\psi_i\|^2_0}\left(\psi_i, F\left(\alpha^{-1}\|\psi_i\|^2_0\left[(-\Delta)^{n+1} + V\right]\right)\psi_i\right)_0 \geq -D(T, F; \alpha) > -\infty.$$

3. Let's assume that $0 < \alpha < 1$. We work as in point 1. Let's just mention that, for $i \in \mathbb{N}$, we have that $\alpha \left\|\psi_i\right\|^2_{\alpha^{-1}V,n+1} \leq \left\|\psi_i\right\|^2_{V,n+1}$ as well as

$$\begin{aligned}-F\left(\left\|\psi_i\right\|^2_{V,n+1}\right) \geq -F\left(\alpha\left\|\psi_i\right\|^2_{\alpha^{-1}V,n+1}\right), \quad \alpha\left\|\psi_i\right\|^2_{\alpha^{-1}V,n+1} = \sum_{j\in\mathbb{N}}\mu^2_{i,j}\lambda_j, \\ \mathscr{F}_{V,\beta}(T) \geq -\sum_{i\in\mathbb{N}} F\left(\left\|\psi_i\right\|^2_{V,n+1}\right) \geq -\sum_{i\in\mathbb{N}} F\left(\alpha\left\|\psi_i\right\|^2_{\alpha^{-1}V,n+1}\right).\end{aligned}$$

□

Observe that the right side of (54) does not correspond to the trace of an operator because $\{\hat{\psi}_{i,T} \,/\, i \in \mathbb{N}\}$ is neither orthogonal nor complete in $\mathrm{L}^2(\Omega)$; we just have (11). However, for the context of $\mathscr{H}^1_{V,+}$, things are much better when F belongs to a Casimir class (see Remark 15) because, for $T \in \mathscr{H}^1_{V,+}$, $B_T = \{\psi_{i,T} \,/\, i \in \mathbb{N}\}$ is also a Hilbert basis of $\mathrm{L}^2(\Omega)$. Then, we get the following slight extension of [9, Lemma 3.1] which states that the free-energy functional is actually bounded from below on $\mathscr{H}^1_{V,+}$. The case of $\alpha = 1$ is considered in [19, Prop.3.1] for $\mathscr{H}^1_{V,+}$ with Ω unbounded, and in [18, Th.3.7] for the cone $\mathscr{W}^p_V$ with $p > 1$.

Corollary 12. *Let $\alpha > 0$ and β entropy seed generated by $F \in \mathcal{C}^1_\alpha$. Then, for every $T \in \mathscr{H}^1_{V,+}$,*

$$\mathscr{F}_{V,\beta}(T) \geq \begin{cases} -\mathrm{Tr}_0\left(F(\alpha^{-1}[-\Delta + V])\right) & \text{if } \alpha > 1, \\ -\mathrm{Tr}_0\left(F(-\Delta + V)\right) & \text{if } 0 < \alpha \leq 1. \end{cases}$$

By working as in the proof of Theorem 11, we get the following result.

Theorem 13. *Let $n \in \mathbb{N}_*$ and β be entropy generated by $F : \mathbb{R} \longrightarrow \mathbb{R} \cup \{+\infty\}$ which is convex and non-increasing on $[0, +\infty[$. Assume $(\mathrm{G}^{n+1}_{V,\alpha})$. Then, for every $T \in \mathcal{F}^{n+1}_{V,+}$,*

$$\mathcal{S}_\beta(T) + \alpha\mathscr{K}_{n+1}(T) + \mathscr{P}_V(T) \geq -D(T, F; 1). \tag{60}$$

If $\alpha = 1 - \epsilon$ with $0 < \epsilon < 1$, then

$$\mathscr{F}_{V,\beta}(T) \geq \epsilon\mathscr{K}_{n+1}(T) - D(T, F; 1).$$

In the context of $\mathscr{H}^1_{V,+}$, Theorem 13 implies a coercivity property of the free-energy functional when $0 < \alpha < 1$:

Corollary 14. *[9, Prop.3.1] Let $\alpha > 0$ and β an entropy seed generated by $F \in \mathcal{C}^1_\alpha$. Then, for every $T \in \mathscr{H}^1_{V,+}$,*

$$\mathcal{S}_\beta(T) + \alpha\mathscr{K}_1(T) + \mathscr{P}_V(T) \geq -\mathrm{Tr}_0(F(-\alpha\Delta + V)).$$

If $\alpha = 1 - \epsilon$ with $0 < \epsilon < 1$, then

$$\mathscr{F}_{V,\beta}(T) \geq \epsilon\mathscr{K}_1(T) - \mathrm{Tr}_0(F(-\alpha\Delta + V)).$$

The following definition extends [9, Def.3.1] (see also [19, Def.3.4]).

Definition 6. *Let $\epsilon \in]0, 1[$ and $n \in \mathbb{N}_*$. We say that the operator $(-\Delta)^{n+1} + V$ is* ϵ-coercive *on $\mathrm{H}_{n+1} \subseteq \mathrm{L}^2(\Omega)$ iff*

$$\lambda^{(1-\epsilon)}_V = \sup\left\{\mu \in \mathbb{R} \,/\, (1 - \epsilon)(-\Delta)^{n+1} + V \geq \mu\right\} > -\infty.$$

In the context of Definition 6, given $\lambda \in]-\infty, \lambda^{(1-\epsilon)}_V]$, the operator $(1-\epsilon)(-\Delta)^{n+1} + V - \lambda$ is positive: for every $\psi \in \mathrm{H}_{n+1} \subseteq \mathrm{L}^2(\Omega)$,

$$(1 - \epsilon) \int_\Omega \left[|\Delta^k\psi|^2 + (V(x) - \lambda)|\psi|^2\right] dx \geq 0, \tag{61}$$

where we are considering the case $n + 1 = 2k$. Then, a modified free-energy functional can be defined on $\mathscr{H}^{n+1}_{V,+}$ by

$$\mathscr{F}^\lambda_{V,\beta}(T) = \mathscr{F}_{V,\beta}(T) - \lambda \left\|\rho_{0,T}\right\|_{\mathrm{L}^1(\Omega)}. \tag{62}$$

Proposition 15. *Let $n \in \mathbb{N}_*$ and β an entropy generated by $F : \mathbb{R} \longrightarrow \mathbb{R} \cup \{+\infty\}$ which is convex and non-increasing on $[0, +\infty[$. Assume that $(-\Delta)^{n+1} + V$ is ϵ-coercive, $\epsilon \in]0, 1[$, and $\lambda \leq \lambda_V^{(1-\epsilon)}$.*

i) If $(\mathrm{G}^{n+1}_{0,\epsilon/2})$ holds, then, for every $T \in \mathcal{F}^{n+1}_{V,+}$,

$$\mathscr{F}^{\lambda}_{V,\beta}(T) \geq \frac{\epsilon}{2}\mathscr{K}_{n+1}(T) - D(T, F; 1). \tag{63}$$

ii) If $(\mathrm{G}^{n+1}_{V-\lambda,1-\epsilon})$ holds, then, for every $T \in \mathcal{F}^{n+1}_{V,+}$,

$$\mathscr{F}^{\lambda}_{V,\beta}(T) \geq -\sum_{i\in\mathbb{N}} \left(\hat{\psi}_{i,T}, F(\mathcal{E}_T[(1-\epsilon)(-\Delta)^{n+1} + V - \lambda]\hat{\psi}_{i,T})\right)_0. \tag{64}$$

Proof. Let $T \in \mathcal{F}^{n+1}_{V,+}$.

i) Assume $(\mathrm{G}^{n+1}_{0,\epsilon/2})$. Then, by (62), (60) and (61),

$$\mathscr{F}^{\lambda}_{V,\beta}(T) = \left[\mathcal{S}_\beta(T) + \frac{\epsilon}{2}\mathscr{K}_{n+1}(T)\right] + \frac{\epsilon}{2}\mathscr{K}_{n+1}(T) + \left[(1-\epsilon)\mathscr{K}_{n+1}(T) + \mathscr{P}_V(T) - \lambda\,\|\rho_{0,T}\|_{\mathrm{L}^1(\Omega)}\right] \geq \frac{\epsilon}{2}\mathscr{K}_{n+1}(T) - D(T, F; 1).$$

ii) Assume $(\mathrm{G}^{n+1}_{V-\lambda,1-\epsilon})$. Point (64) is obtained by adapting the proofs of Theorems 11 and of point i).

□

In the context of $\mathscr{H}^1_{V,+}$, Proposition 15 implies a coercivity property and a lower bound of the modified free-energy functional:

Corollary 16. *[9, Prop.3.2] Let β an entropy seed generated by a function F. Assume that $-\Delta + V$ is ϵ-coercive, $\epsilon \in]0, 1[$, and $\lambda \leq \lambda_V^{(1-\epsilon)}$.*

i) If $F \in \mathcal{C}^1_{0,\epsilon/2}$,

$$\mathscr{F}^{\lambda}_{V,\beta}(T) \geq -\mathrm{Tr}_0\left(F\left(-\frac{\epsilon}{2}\Delta\right)\right) + \frac{\epsilon}{2}\mathscr{K}_1(T), \qquad T \in \mathscr{H}^1_{V,+}.$$

ii) If $F \in \mathcal{C}^1_{V-\lambda,1-\epsilon}$,

$$\mathscr{F}^{\lambda}_{V,\beta}(T) \geq -\mathrm{Tr}_0\left(F\left(-(1-\epsilon)\Delta + V - \lambda\right)\right), \qquad T \in \mathscr{H}^1_{V,+}.$$

Another consequence of Proposition 15 is the following result.

Corollary 17. *Let $n \in \mathbb{N}_*$ and β an entropy generated by $F : \mathbb{R} \longrightarrow \mathbb{R} \cup \{+\infty\}$ which is convex and non-increasing on $[0, +\infty[$. Assume that $(-\Delta)^{n+1} + V$ is ϵ-coercive, $\epsilon \in]0, 1[$, $\lambda \leq \lambda_V^{(1-\epsilon)}$ and that conditions $(\mathrm{G}^{n+1}_{0,\epsilon/2})$ and $(\mathrm{G}^{n+1}_{V-\lambda,1-\epsilon})$ hold. If $(T_\omega)_{\omega\in\Lambda}$ is a family of operators in $\mathcal{F}^{n+1}_{V,+}$ for which $(\mathscr{F}^{\lambda}_{V,\beta}(T_\omega))_{\omega\in\Lambda}$ and $(D(T_\omega, F; 1))_{\omega\in\Lambda}$ are bounded, then the families $(\rho_{0,T_\omega})_{\omega\in\Lambda}$, $(\mathscr{K}_{n+1}(T_\omega))_{\omega\in\Lambda}$, $(\mathcal{S}_\beta(T_\omega))_{\omega\in\Lambda}$ and $(\mathscr{P}_V(T_\omega))_{\omega\in\Lambda}$ are also bounded.*

Proof. The proof is obtained by using (63), (23) and (38). □

In the context of $\mathscr{H}^1_{V,+}$, the statement of Corollary 17 is simpler and gives more:

Corollary 18. *[9, Cor.3.3] Assume that* $-\Delta + V$ *is* ϵ*-coercive,* $\epsilon \in]0,1[$*,* $\lambda \le \lambda_V^{(1-\epsilon)}$*, and that* β *is an entropy seed generated by* $F \in \mathcal{C}^1_{0,\epsilon/2} \cap \mathcal{C}^1_{V-\lambda,1-\epsilon}$*. If* $(T_\omega)_{\omega\in\Lambda}$ *is a family of operators in* $\mathscr{H}^1_{V,+}$ *for which* $(\mathscr{F}^\lambda_{V,\beta}(T_\omega))_{\omega\in\Lambda}$ *is bounded, then the families* $(\|T_\omega\|_0)_{\omega\in\Lambda}$*,* $(\mathscr{K}_1(T_\omega))_{\omega\in\Lambda}$*,* $(\mathcal{S}_\beta(T_\omega))_{\omega\in\Lambda}$ *and* $(\mathscr{P}_V(T_\omega))_{\omega\in\Lambda}$ *are also bounded.*

Now that we have obtained lower estimates for energy functionals, we shall prove that Lieb-Thirring type inequalities, like (65) below, imply some Gagliardo-Nirenberg type inequalites, like (66) below; see [10] for these kind of inequalities in terms of mixed states instead of working with nuclear operators. The following result extends to higher-order Sobolev-like cones [10, Th.15] and [9, Th.3.2]; these results were extended for the cones $\mathscr{W}^{1,p}$, $p > 1$ (see Remark 10), in [18, Th.3.13]).

Theorem 19. *Let* $n \in \mathbb{N}_*$*,* β *an entropy seed generated by* $F : \mathbb{R} \longrightarrow \mathbb{R} \cup \{+\infty\}$ *which is convex and non-increasing on* $[0,+\infty[$*, and* $T \in \mathcal{F}^{n+1}_{V,+}$*. Assume* $(\mathrm{G}^{n+1}_{V,1})$ *and that the functions* τ *and* Υ *are such that*

$$\tau(s) = -(-\Upsilon)^*(s), \quad \text{and} \quad D(T,F;1) \le \int_\Omega \Upsilon(V(x))dx, \tag{65}$$

$s \in \mathbb{R}$*. Then,*

$$\mathcal{S}_\beta(T) + \mathscr{K}_{n+1}(T) \ge \int_\Omega \tau(\rho_{0,T}(x))dx. \tag{66}$$

Proof. By (65) we have that $\tau(s) \le -s\theta - \Upsilon(\theta)$, $s,\theta \in \mathbb{R}$. Therefore, taking $\theta = V(x)$ and $s = \rho_{0,T}(x)$, we get

$$\int_\Omega \tau(\rho_{0,T}(x))dx \le -\int_\Omega V(x)\rho_{0,T}(x)dx - \int_\Omega \Upsilon(V(x))dx. \tag{67}$$

By Theorem 11 and points (67) and (65), we get

$$\mathcal{S}_\beta(T) + \mathscr{K}_{n+1}(T) \ge -\mathscr{P}_V(T) - \int_\Omega \Upsilon(V(x))dx \ge \int_\Omega \tau(\rho_{0,T}(x))dx.$$

□

Example 4. *Given a continuous function* $g :]0,+\infty[\longrightarrow [0,+\infty[$ *such that*

$$\int_0^{+\infty} \frac{(1+t^{-N/2})}{t} g(t)dt < +\infty,$$

let's consider the functions $F_g, \Upsilon_g : \mathbb{R} \longrightarrow \mathbb{R} \cup \{+\infty\}$ *given as the Laplace transforms of* $t \longmapsto t^{-1}g(t)$ *and* $t \longmapsto (4\pi t)^{-N/2}t^{-1}g(t)$*, respectively, i.e.,*

$$F_g(s) = \int_0^{+\infty} \frac{g(t)}{t} e^{-ts}dt, \quad \Upsilon_g(s) = \int_0^{+\infty} \frac{(4\pi t)^{-N/2}g(t)}{t} e^{-ts}dt.$$

In [10] it was shown that F_g belongs to the Casimir class $\mathcal{C}^1_{V,1}$ and that Υ_g verifies (65), so that, Theorem 19 applies. Actually, by Corollary 12, inequality (66) holds for every $T \in \mathscr{H}^1_{V,+}$. Here, $\mathrm{Tr}_0(-\Delta + V) \leq \int_\Omega G(V(x))dx$.

Example 5. *Let $\gamma > N/2$ and $r = \gamma/(\gamma+1)$. The functions β_r and F_γ that were introduced in Example 1 verify conditions of Theorem 19* and, *by Corollary 12 (see [10, Th.1,Ex.2]), there exists $\mu = \mu(\gamma, N, \Omega) > 0$ such that, for any $T \in \mathscr{H}^1_{V,+}$,* $\mathrm{Tr}_0((-\Delta + V)^{-\gamma}) \leq (4\pi)^{-N/2}\Gamma^{-1}(\gamma)\Gamma(\gamma - N/2)\int_\Omega V^{-\gamma+N/2}dx$ *and*

$$\mathscr{K}_1(T) + \mathcal{S}_{\beta_r}(T) \geq -\mu \int_\Omega \rho^q_{0,T}(x)dx,$$

where $0 < q = (2\gamma - N)/(2\gamma - N + 2) < 1$.

Example 6. *In [21], the entropy of a density function ρ is given by $\mathcal{H}(\rho) = -\int_\Omega \rho(x)\ln(\rho(x))dx$. Now let's consider the entropy seed $\beta(t) = t\ln(t) - t$ if $t > 0$, $\beta(0) = 0$ and $\beta(t) = +\infty$ if $t < 0$, which is generated by $F(t) = e^{-t}$. By Theorem 19, with $G(t) = (4\pi)^{-N/2}e^{-t}$, it holds, for every $T \in \mathscr{H}^1_{V,+}$,*

$$\mathscr{K}_1(T) + \mathcal{S}_\beta(T) \geq -\mathcal{H}(\rho_{0,T}) + \left(\frac{N}{2}\ln(4\pi) - 1\right)\|\rho_{0,T}\|_{\mathrm{L}^1(\Omega)}.$$

7 Compactness results and applications

The results of this section state that the cone of operators is compactly embedded in the space of nuclear operators in several senses.

7.1 Compactness properties

Along this section we consider $\gamma > N/2$, $r = \gamma/(\gamma+1)$ and the functions β_r and F_γ that appear in Examples 1 and 5.

Let $n \in \mathbb{N}_*$ and $(T_m)_{m\in\mathbb{N}}$ be a sequence in the cone $\mathscr{H}^{n+1}_{V,+}$. The following conditions shall be useful.

(B1) $(\langle\!\langle T_m \rangle\!\rangle_{V,n+1})_{m\in\mathbb{N}} \subseteq \mathbb{R}$ is bounded, i.e., there exists $K_\infty > 0$ such that $\langle\!\langle T_m \rangle\!\rangle_{V,n+1} < K_\infty$, for every $m \in \mathbb{N}$;

(B2) $(D(T_m, F_\gamma; 1))_{m\in\mathbb{N}} \subseteq \mathbb{R}$ is bounded from above.

We shall denote, for every $m, i \in \mathbb{N}$, $\nu_{i,T_m} = \nu_i^{(m)}$ and $\psi_{i,T_m} = \psi_i^{(m)}$. We start with a couple of preliminary results.

Lemma 20. *Let $(T_m)_{m\in\mathbb{N}} \subseteq \mathscr{H}^{n+1}_{V,+}$ be such that (B1) and (B2) hold, and $r' \in [r, 1]$. Then,*

i) $(\|T_m\|_n)_{m\in\mathbb{N}} = \left(\sum_{i\in\mathbb{N}} \nu_i^{(m)}\right)_{m\in\mathbb{N}}$ *is bounded.*

ii) $C_{1,r'} = \sup_{m\in\mathbb{N}} \sum_{i\in\mathbb{N}} (\nu_i^{(m)})^{r'} < +\infty$.

iii) For each $i \in \mathbb{N}$, there exists $\overline{\nu}_i \in [0, +\infty[$ such that, up to a subsequence,

$$\nu_i^{(m)} \longrightarrow \overline{\nu}_i, \quad \text{as } m \longrightarrow +\infty. \tag{68}$$

Proof. By Poincaré's-like inequality, (38), and (B1), we have that $(\|T_m\|_n)_{m\in\mathbb{N}}$ is bounded. Then, (12) implies that for each $i \in \mathbb{N}$, there exists $\overline{\nu}_i \in [0,+\infty[$ such that, up to a subsequence, $\nu_i^{(m)} \longrightarrow \overline{\nu}_i$, as $m \longrightarrow +\infty$. By Theorem 11 and Example 1, we have, for every $m \in \mathbb{N}$,

$$\mathcal{S}_{\beta_r}(T_m) + \mathscr{K}_{n+1}(T_m) + \mathscr{P}_V(T_m) \geq -D(T_m, F_\gamma; 1),$$
$$(1-r)^{r-1} r^{-r} \sum_{i\in\mathbb{N}} (\nu_i^{(m)})^r \leq \langle\!\langle T_m \rangle\!\rangle_{V,n+1} + D(T_m, F_\gamma; 1),$$

and, by (B1) and (B2), we get ii) for $r' = r$. From this, we get ii) for $r' \in]r,1]$. □

Remark 16. *In the context of $\mathscr{H}^1_{V,+}$, condition (B2) is unnecessary, see [9, Th.3.4]. See [19, Lemmas 4.1&4.2] for the case of Ω unbounded and [18, Lemma 4.2] for the case of $p \geq 2$.*

Lemma 21. *Let $(T_m)_{m\in\mathbb{N}} \subseteq \mathscr{H}^{n+1}_{V,+}$ be such that (B1) and (B2) hold, and $r' \in [r,1]$. Then, up to a subsequence of $(T_m)_{m\in\mathbb{N}}$, for every $M \in \mathbb{N}$,*

$$\sum_{i=M}^{+\infty} (\nu_i^{(m)})^{r'} \leq C_{1,r} (\nu_M^{(m)})^{r'-r},$$

where $C_{1,r}$ is given in Lemma 20. In particular, it holds

$$\sum_{i\in\mathbb{N}} \nu_i^{(m)} \leq C_{1,r} (\nu_1^{(m)})^{1-r}, \tag{69}$$
$$\sum_{i\in\mathbb{N}} \overline{\nu}_i \leq C_{1,r} \overline{\nu}_1^{1-r}. \tag{70}$$

Proof. Let $M \in \mathbb{N}$. We have that

$$\sum_{i=M}^{+\infty} (\nu_i^{(m)})^{r'} = \sum_{i=M}^{+\infty} (\nu_i^{(m)})^{r'-r} (\nu_i^{(m)})^r \leq (\nu_M^{(m)})^{r'-r} \sum_{i=M}^{+\infty} (\nu_i^{(m)})^r \leq C_{1,r} (\nu_M^{(m)})^{r'-r}.$$

Therefore, for $r' = 1$ and $M = 1$, we get (69), whence, letting $m \longrightarrow +\infty$, it follows (70). □

Remark 17. *From now on, to ease a number of computations we can assume, in the context of Lemma 20, that $\overline{\nu}_i \neq 0$, for every $i \in \mathbb{N}$.*

Lemma 22. *Let $(T_m)_{m\in\mathbb{N}} \subseteq \mathscr{H}^{n+1}_{V,+}$ be such that (B1) holds. Then, there exist $\overline{B} = \{\overline{\psi}_i \,/\, i \in \mathbb{N}\} \subseteq \mathrm{H}_{n+1}$, a Hilbert basis of H_n, such that, for every $i \in \mathbb{N}$, there exists $\overline{\psi}_i \in \mathrm{H}_n$ such that, up to a subsequence,*

$$\|\psi_i^{(m)} - \overline{\psi}_i\|_n \longrightarrow 0, \quad \text{as } m \longrightarrow +\infty, \tag{71}$$
$$\left\|D^h \psi_i^{(m)} - D^h \overline{\psi}_i\right\|_{\mathrm{L}^z(\Omega)} \longrightarrow 0, \quad \text{as } m \longrightarrow +\infty, \tag{72}$$

for any $z \in [1,2]$ and any multi-index $h = (h_1, \ldots, h_N) \in \mathbb{N}^N_*$ with $|h| = h_1 + \ldots + h_N \leq n$.

Proof. a) Let $i \in \mathbb{N}$. We have that

$$\|\psi_i^{(m)}\|_{V,n+1}^2 \leq \frac{1}{\nu_i^{(m)}} \sum_{j\in\mathbb{N}} \nu_j^{(m)} \left\|\psi_j^{(m)}\right\|_{V,n+1}^2 = \frac{1}{\nu_i^{(m)}} \langle\!\langle T_m \rangle\!\rangle_{V,n+1},$$

so that, by (B1), $(\psi_i^{(m)})_{m\in\mathbb{N}}$ is bounded in H_{n+1}. Therefore, up to a subsequence, (71) holds. Then, for every multi-index h with $|h| \leq n$, $\left\|D^h\psi_i^{(m)} - D^h\overline{\psi}_i\right\|_{\mathrm{L}^2(\Omega)} \longrightarrow 0$, as $m \longrightarrow +\infty$, whence (72) follows.

b) Since, for every $m \in \mathbb{N}$, $B_m = \{\psi_j^{(m)} \,/\, j \in \mathbb{N}\}$ is a Hilbert basis of H_n, the same happens with $\overline{B} = \{\overline{\psi}_j \,/\, j \in \mathbb{N}\}$.

c) By [7, Prop.9.18], for each $m \in \mathbb{N}$ and each multi-index h with $|h| \leq n$, there exists $C_{i,m} > 0$ such that, for every $\varphi \in \mathrm{C}_0^1(\mathbb{R}^N)$ and every $j \in \{1, 2, ..., N\}$,

$$\left|\int_\Omega D^h\psi_i^{(m)}(x)\frac{\partial\varphi}{\partial x_j}(x)dx\right| \leq C_{i,m}\,\|\varphi\|_{\mathrm{L}^2(\Omega)}\,. \tag{73}$$

By using (72) and perhaps up to a subsequence, it's shown that (73) holds when we replace $(\psi_i^{(m)}, C_{i,m})$ by $(\overline{\psi}_i, C_i)$ for some $C_i > 0$. Therefore, by [7, Prop.9.18] and the arbitrariness of i, it follows that $\overline{B} \subseteq \mathrm{H}_{n+1}$.

□

The following result states that downward monotony (see (75) below) helps to prove convergence in the trace norm. A result dealing with upward monotony is presented in Corollary 27.

Theorem 23. *Let $(T_m)_{m\in\mathbb{N}} \subseteq \mathscr{H}_{V,+}^{n+1}$ be such that (B1) and (B2) hold. Then, there exists an operator $\overline{T} \in \mathscr{H}_{V,+}^{n+1}$ such that, up to a subsequence, $\|T_m - \overline{T}\|_n \longrightarrow 0$, as $m \longrightarrow +\infty$, provided $\overline{T} = 0$, or*

$$\lim_{m\longrightarrow+\infty} \|T_m\|_n \leq \|\overline{T}\|_n \tag{74}$$

and the existence of $m_0 \in \mathbb{N}$ such that

$$\forall m \geq m_0 : \qquad T_m \geq \overline{T}. \tag{75}$$

Proof. Without changing notation, let's extract a subsequence of $(T_m)_{m\in\mathbb{N}} \subseteq \mathscr{H}_{V,+}^{n+1}$ that is produced by Lemmas 20 and 22 at the same time.

1. By Lemma 21 we have that $\sum_{i\in\mathbb{N}} \overline{\nu}_i < +\infty$. For $\eta \in \mathrm{H}_n$, let's write

$$\overline{T}\eta = \sum_{i\in\mathbb{N}} \overline{\nu}_i(\eta, \overline{\psi}_i)_n\overline{\psi}_i. \tag{76}$$

By Cauchy-Schwartz's inequality,

$$\|\overline{T}\eta\|_n \leq \sum_{i\in\mathbb{N}} |(\eta, \overline{\psi}_i)|\,\overline{\nu}_i\|\overline{\psi}_i\|_n \leq \|\eta\|_n \sum_{i\in\mathbb{N}} \overline{\nu}_i < +\infty,$$

so that $\overline{T} : \mathrm{H}_n \longrightarrow \mathrm{H}_n$ is well-defined, belongs to $\mathscr{L}_n$ and $\|\overline{T}\| \leq \sum_{i\in\mathbb{N}} \overline{\nu}_i$.

2. The self-adjointness and positiveness of the operators T_m is inherited by $\overline{T}$. From (76) we immediately have that $\overline{T}\overline{\psi}_i = \overline{\nu}_i\overline{\psi}_i$, $i \in \mathbb{N}$. Therefore, we have that $\overline{T} \in \mathscr{N}^+_{n,1}$, $\|\overline{T}\|_n = \sum_{i\in\mathbb{N}} \overline{\nu}_i$ and, by Lemma 22, $\overline{B} \subseteq \mathrm{H}_{n+1}$.
3. Let's prove that $\overline{T} \in \mathscr{H}^{n+1}_{V,+}$, Let's assume that n is odd, say $n = 2k+1$ with $k \in \mathbb{N}_*$. The case of n even is treated in a similar way. Let $M \in \mathbb{N}$. For $m \in \mathbb{N}$, let's consider the non-negative function given by

$$f_m(x) = \sum_{i=1}^{M} \nu_i^{(m)} \left(|\Delta^{k+1}\psi_i^{(m)}(x)|^2 + V(x)|\psi_i^{(m)}(x)|^2 \right), \quad x \in \Omega.$$

By (B1), Fatou's lemma (see e.g. [23]) and Lemmas 20 and 22, we have that

$$\begin{aligned}
\int_\Omega \liminf_{m\longrightarrow+\infty} f_m(x)\,dx &\leq \liminf_{m\longrightarrow+\infty} \int_\Omega f_m(x)\,dx \\
\sum_{i=1}^{M} \overline{\nu}_i \left\|\overline{\psi}_i\right\|^2_{V,n} &\leq \liminf_{m\longrightarrow+\infty} \sum_{i=1}^{M} \nu_i^{(m)} \left\|\psi_i^{(m)}\right\|^2_{V,n} \\
&\leq \liminf_{m\longrightarrow+\infty} \sum_{i\in\mathbb{N}} \nu_i^{(m)} \left\|\psi_i^{(m)}\right\|^2_{V,n} = \liminf_{m\longrightarrow+\infty} \langle\!\langle T_m \rangle\!\rangle_{V,n} \leq K_\infty,
\end{aligned} \tag{77}$$

which, by letting $M \longrightarrow +\infty$, shows that $\langle\!\langle \overline{T} \rangle\!\rangle_{V,n} \leq K_\infty$.
4. If $\overline{T} = 0$, then, by (70), it follows that $\|T_m\|_m \longrightarrow 0$, as $m \longrightarrow +\infty$. Assume now that $\overline{T} \neq 0$. Let's pick $(T_{m_k})_{k\in\mathbb{N}}$, a subsequence of $(T_m)_{m\in\mathbb{N}}$, such that

$$\lim_{k\longrightarrow+\infty} \|T_{m_k}\|_n = \limsup_{m\longrightarrow+\infty} \|T_m\|_n. \tag{78}$$

Since $\overline{T}$, T_m and $T_m - \overline{T}$ are positive operators, we have by (8), for $m_k \geq m_0$ and $\{\chi_i \,/\, i \in \mathbb{N}\}$ Hilbert basis of H_n, that

$$\begin{aligned}
\|T_{m_k} - \overline{T}\|_n &= \mathrm{Tr}_n(|T_{m_k} - \overline{T}|) = \mathrm{Tr}_n(T_{m_k} - \overline{T}) \\
&= \sum_{i\in\mathbb{N}} \big((T_m - \overline{T})\chi_i, \chi_i\big)_n = \sum_{i\in\mathbb{N}} (T_m\chi_i, \chi_i)_n - \sum_{i\in\mathbb{N}} \big(\overline{T}\chi_i, \chi_i\big)_n \\
&= \mathrm{Tr}_n(T_{m_k}) - \mathrm{Tr}_n(\overline{T}) = \|T_{m_k}\|_n - \|\overline{T}\|_n.
\end{aligned}$$

Therefore, by (78) and (74), it follows, as $k \longrightarrow +\infty$, that

$$\|T_{m_k} - \overline{T}\|_n \leq \|T_{m_k}\|_n - \limsup_{m\longrightarrow+\infty} \|T_m\|_n \longrightarrow 0.$$

□

Remark 18. *Observe that under conditions (B1) and (B2), points 1-3 in the proof of Theorem 23 are valid. Therefore, for the following results, we shall consider the operator $\overline{T} \in \mathscr{H}^{n+1}_{V,+}$ given by (76).*

Proposition 24. *Let* $(T_m)_{m\in\mathbb{N}} \subseteq \mathscr{H}^{n+1}_{V,+}$ *be such that (B1) and (B2) hold, and* $l \in \{0,1,...,n\}$. *Then, there exists an operator* $\overline{T} \in \mathscr{H}^{n+1}_{V,+}$ *such that, up to a subsequence,*

i) for every $w \in \mathrm{C}(\overline{\Omega})$,

$$\int_\Omega \rho_m w\, dx \longrightarrow \int_\Omega \overline{\rho} w\, dx, \qquad \text{as } m \longrightarrow +\infty, \tag{79}$$

where $\rho_m = \rho_{n-l,T_m}$ *and* $\overline{\rho} = \rho_{n-l,\overline{T}}$;

ii) $\rho_m \longrightarrow \overline{\rho}$, *as* $m \longrightarrow +\infty$, *in* $\mathrm{L}^1(\Omega)$.

Proof. We use Remark 18. Even though point ii) implies point i), we get point ii) in two ways (either using (79) or not) as we consider that both schemes are important and useful.

1. First way.
   a) By (B1), (23) and (38), it follows, for every $m \in \mathbb{N}$, that

   $$\|\rho_m\|_{\mathrm{L}^1(\Omega)} \le \gamma_l \|T_m\|_n \le \gamma_l \hat{c} \langle\!\langle T_m \rangle\!\rangle_{V,n+1} \le \gamma_l \hat{c} K_\infty.$$

   By definition of weak convergence of Radon meaures on $\mathbb{R}^N$ (see e.g. [6]) and Banach-Alouglu-Bourbaki's theorem (see e.g. [7, Th.3.16]), there exists a subsequence - still denoted (T_m) - and a Radon measure μ_l on $\mathbb{R}^N$ such that for every $w \in \mathrm{C}(\overline{\Omega})$, $\int_\Omega \rho_m w\, dx \longrightarrow \int_\Omega w d\mu_l$, as $m \longrightarrow +\infty$. Now, by using Lemmas 20, 21 and 22, it's shown that $d\mu_l = \overline{\rho} dx$ so that (79) holds.

   b) By putting $w \equiv 1$ in (79) we get

   $$\|\rho_m\|_{\mathrm{L}^1(\Omega)} \longrightarrow \|\overline{\rho}\|_{\mathrm{L}^1(\Omega)}, \quad \text{as } m \longrightarrow +\infty. \tag{80}$$

   On the other hand, by Lemma 22 and point (79) (with w replaced by mollifiers), up to a subsequence we have that

   $$\rho_m(x) \longrightarrow \overline{\rho}(x), \quad \text{as } m \longrightarrow +\infty, \text{ for a.e. } x \in \Omega. \tag{81}$$

   From (80) and (81), it follows point ii), see e.g. [7, Ex.4.13].

2. Second way.
   a) Let's assume that $n - l = 2k$, $k \in \mathbb{N}$, as the case of $n - l$ odd is similar. Given $m, q \in \mathbb{N}$, we consider the finite-rank operators $T_{m,q}, \overline{T}_q \in \mathscr{M}_{n,s} \cap \mathscr{H}^{n+1}_{V,+}$ given by $T_{m,q}\phi = \sum_{i=1}^{q} \nu_i^{(m)} (\phi, \psi_i^{(m)})_n \psi_i^{(m)}$ and $\overline{T}_q \phi = \sum_{i=1}^{q} \overline{\nu}_i (\phi, \overline{\psi}_i)_n \overline{\psi}_i$, where $\phi \in \mathrm{H}_n$ and $\mathscr{M}_{n,s}$ is given in (32). The corresponding density functions are given by

   $$\rho_{m,q}(x) = \sum_{i=1}^{q} \nu_i^{(m)} \left[|\Delta^k \psi_i^{(m)}(x)|^2 + |\psi_i^{(m)}(x)|^2 \right],$$

   $$\overline{\rho}_q(x) = \sum_{i=1}^{q} \overline{\nu}_i \left[|\Delta^k \overline{\psi}_i(x)|^2 + |\overline{\psi}_i(x)|^2 \right].$$

We have that

$$\|\rho_m - \overline{\rho}\|_{L^1(\Omega)} \leq \|\rho_m - \rho_{m,q}\|_{L^1(\Omega)} + \left\|\rho_{m,q} - \overline{\rho}_q\right\|_{L^1(\Omega)} + \left\|\overline{\rho}_q - \overline{\rho}\right\|_{L^1(\Omega)}. \tag{82}$$

By using (22), we get

$$\|\rho_m - \rho_{m,q}\|_{L^1(\Omega)} = \int_\Omega \sum_{i=q+1}^{+\infty} \nu_i^{(m)} \left[|\Delta^k \psi_i^{(m)}(x)|^2 + |\psi_i^{(m)}(x)|^2\right] dx$$

$$= \sum_{i=q+1}^{+\infty} \nu_i^{(m)} \|\psi_i^{(m)}\|_{n-l}^2 \leq \gamma_l \sum_{i=q+1}^{+\infty} \nu_i^{(m)} \|\psi_i^{(m)}\|_n^2 \leq \gamma_l \left\{ \sum_{i=q+1}^{+\infty} \left[\overline{\nu}_i + (\nu_i^{(m)} - \overline{\nu}_i)\right] \right\}, \tag{83}$$

as well as

$$\left\|\overline{\rho}_q - \overline{\rho}\right\|_{L^1(\Omega)} \leq \gamma_l \sum_{i=q+1}^{+\infty} \overline{\nu}_i. \tag{84}$$

On the other hand, by adding and substracting $\overline{\nu}_i \left[|\Delta^k \psi_i^{(m)}|^2 + |\psi_i^{(m)}|^2\right]$, using Caucht-Schwartz and triangle inequalities and (22), we get

$$\left\|\rho_{m,q} - \overline{\rho}_q\right\|_{L^1(\Omega)} = \int_\Omega \left| \sum_{i=1}^{q} \nu_i^{(m)} \left[|\Delta^k \psi_i^{(m)}|^2 + |\psi_i^{(m)}|^2\right] - \sum_{i=1}^{q} \overline{\nu}_i \left[|\Delta^k \overline{\psi}_i|^2 + |\overline{\psi}_i|^2\right] \right| dx$$

$$\leq \sum_{i=1}^{q} |\nu_i^{(m)} - \overline{\nu}_i| \|\psi_i^{(m)}\|_{n-l}^2 + \sum_{i=1}^{q} \overline{\nu}_i \int_\Omega \left| |\Delta^k \psi_i^{(m)}|^2 + |\psi_i^{(m)}|^2 - |\Delta^k \overline{\psi}_i|^2 - |\overline{\psi}_i|^2 \right| dx$$

$$\leq \gamma_l \sum_{i=1}^{q} |\nu_i^{(m)} - \overline{\nu}_i| + \sum_{i=1}^{q} \overline{\nu}_i \int_\Omega \left[\left| |\Delta^k \psi_i^{(m)}|^2 - |\Delta^k \overline{\psi}_i|^2 \right| + \left| |\psi_i^{(m)}|^2 - |\overline{\psi}_i|^2 \right| \right] dx$$

$$\leq \sum_{i=1}^{q} \overline{\nu}_i \left[\|\Delta^k \psi_i^{(m)} + \Delta^k \overline{\psi}_i\|_0 \|\Delta^k \psi_i^{(m)} - \Delta^k \overline{\psi}_i\|_0 + \|\psi_i^{(m)} + \overline{\psi}_i\|_0 \|\psi_i^{(m)} - \overline{\psi}_i\|_0 \right]$$

$$+ \gamma_l \sum_{i=1}^{q} |\nu_i^{(m)} - \overline{\nu}_i|. \tag{85}$$

b) By using Lemmas 20, 21 and 22, we can show that, up to a subsequence, the right sides of (83), (84) and (85) become as small as we want and so the same happens to (82). To exemplify how this is done, let's prove that $\sum_{i\in\mathbb{N}} |\nu_i^{(m)} - \overline{\nu}_i| \longrightarrow 0$, as $m \longrightarrow +\infty$, i.e.,

$$\forall \epsilon > 0, \exists M \in \mathbb{N}: \quad m > M \Rightarrow \sum_{i\in\mathbb{N}} |\nu_i^{(m)} - \overline{\nu}_i| < \epsilon. \tag{86}$$

Let $\epsilon > 0$. Given $q \in \mathbb{N}$, let's denote

$$\nu_{i,q}^{(m)} = \begin{cases} \nu_i^{(m)}, & i = 1, \dots, q \\ 0, & i = q+1, q+2, \dots \end{cases} \qquad \overline{\nu}_{i,q} = \begin{cases} \overline{\nu}_i, & i = 1, \dots, q \\ 0, & i = q+1, q+2, \dots \end{cases}$$

Then, we have that

$$\sum_{i\in\mathbb{N}} |\nu_i^{(m)} - \overline{\nu}_i| \le \sum_{i\in\mathbb{N}} \left(|\nu_i^{(m)} - \nu_{i,q}^{(m)}| + |\nu_{i,q}^{(m)} - \overline{\nu}_{i,q}| + |\overline{\nu}_{i,q} - \overline{\nu}_i| \right)$$
$$= \sum_{i=q+1}^{+\infty} \nu_i^{(m)} + \sum_{i=1}^{q} |\nu_i^{(m)} - \overline{\nu}_i| + \sum_{i=q+1}^{+\infty} \overline{\nu}_i. \quad (87)$$

By (68) and (70), we can choose $q_\epsilon \in \mathbb{N}$ such that

$$\sum_{i=q+1}^{+\infty} \nu_i^{(m)} < \frac{\epsilon}{3}, \quad \sum_{i=q+1}^{+\infty} \overline{\nu}_i < \frac{\epsilon}{3}. \quad (88)$$

Now we choose $M = M(q_\epsilon) \in \mathbb{N}$ such that. for $m > M$, $|\nu_i^{(m)} - \overline{\nu}_i| < \epsilon/(3 \cdot 2^i)$, $i = 1, ..., q$. Then,

$$\sum_{i=1}^{q} |\nu_i^{(m)} - \overline{\nu}_i| < \sum_{i=1}^{q} \frac{\epsilon}{3 \cdot 2^i} \le \frac{\epsilon}{3} \sum_{i\in\mathbb{N}} \frac{1}{2^i} = \frac{\epsilon}{3}. \quad (89)$$

By (87), (88), (89) and the arbitrariness of ϵ we have proved (86).

□

The following result complements what was done in Section 2.2 on the kernel of nuclear operators.

Proposition 25. *Let $(T_m)_{m\in\mathbb{N}} \subseteq \mathscr{H}_{V,+}^{n+1}$ be such that (B1) and (B2) hold. Then, there exists an operator $\overline{T} \in \mathscr{H}_{V,+}^{n+1}$ such that, up to a subsequence, $\|\tilde{K}_{m,*}\|_0 \longrightarrow 0$, as $m \longrightarrow +\infty$, where $\tilde{K}_{m,*}(x) = \|K_m(x,\cdot) - \overline{K}(x,\cdot)\|_n$, $K_m = K_{T_m}$ and $\overline{K} = K_{\overline{T}}$.*

Proof. Given $x \in \Omega$, we have that $0 \le \tilde{K}_{m,*}(x) \le f(x) + g(x)$, where $f(x) = \sum_{i\in\mathbb{N}} \left|\nu_i^{(m)}\psi_i^{(m)}(x) - \overline{\nu}_i\overline{\psi}_i(x)\right|$ and $g(x) = \sum_{i\in\mathbb{N}} \overline{\nu}_i \|\psi_i^{(m)} - \overline{\psi}_i\|_n |\overline{\psi}_i(x)|$, so that

$$\|\tilde{K}_{m,*}\|_0^2 \le \|f\|_0^2 + \|g\|_0^2 + \|f\|_0\|g\|_0. \quad (90)$$

We have, adding and substracting $\overline{\nu}_i\psi_i^{(m)}$, that

$$\|f\|_0 \le \sum_{i\in\mathbb{N}} \|\nu_i^{(m)}\psi_i^{(m)} - \overline{\nu}_i\overline{\psi}_i\|_0 \le \sum_{i\in\mathbb{N}} |\nu_i^{(m)} - \overline{\nu}_i| + \sum_{i\in\mathbb{N}} \overline{\nu}_i \|\psi_i^{(m)} - \overline{\psi}_i\|_0, \quad (91)$$
$$\|g\|_0 \le \sum_{i\in\mathbb{N}} \overline{\nu}_i \|\psi_i^{(m)} - \overline{\psi}_i\|_n \|\overline{\psi}_i\|_0 \le \sum_{i\in\mathbb{N}} \overline{\nu}_i \|\psi_i^{(m)} - \overline{\psi}_i\|_n. \quad (92)$$

By working as in point 2.b in the proof of Proposition 24 with help of Lemma 22, we can show that, up to a subsequence, the right sides of (91) and (92) become as small as we want and, therefore, the same happens to (90). □

Theorem 26. *Let $(T_m)_{m\in\mathbb{N}} \subseteq \mathscr{H}_{V,+}^{n+1}$ be such that (B1) and (B2) hold. Then, there exists an operator $\overline{T} \in \mathscr{H}_{V,+}^{n+1}$ such that, up to a subsequence, $T_m \rightharpoonup \overline{T}$, as $m \longrightarrow +\infty$, weakly.*

Proof. Let's recall Remark 18. Let's deal with the case of $\overline{T} \neq 0$; the case of $\overline{T} = 0$ follows from Theorem 23. Let $R \in \mathscr{L}_n \setminus \{0\}$ (the case of $R = 0$ is immediate) and $\{\chi_i \,/\, i \in \mathbb{N}\}$ a Hilbert basis of H_n.

a) By (8), we have that

$$|\mathrm{Tr}_n(R(T_m - \overline{T}))| = \left|\sum_{i\in\mathbb{N}} \big(R(T_m - \overline{T})\chi_i,\, \chi_i\big)_n\right|$$

By adding and subtracting the terms $(R\overline{T}\,\overline{\psi}_i, \psi_i^{(m)})_n = \overline{\nu}_i(R\overline{\psi}_i, \psi_i^{(m)})_n$ and $\overline{\nu}_i(R\psi_i^{(m)}, \psi_i^{(m)})_n$, using Cauchy-Schwartz inequality and choosing $\chi_i = \psi_i^{(m)}$, $i \in \mathbb{N}$, we get

$$\begin{aligned}
&|\mathrm{Tr}_n(R(T_m - \overline{T}))| \leq \sum_{i\in\mathbb{N}} \left|\nu_i^{(m)}(R\psi_i^{(m)}, \psi_i^{(m)})_n - (R\overline{T}\psi_i^{(m)}, \psi_i^{(m)})_n\right| \\
&= \sum_{i\in\mathbb{N}} \left|\nu_i^{(m)}(R\psi_i^{(m)}, \psi_i^{(m)})_n - \overline{\nu}_i(R\overline{\psi}_i, \psi_i^{(m)})_n + (R\overline{T}(\overline{\psi}_i - \psi_i^{(m)}), \psi_i^{(m)})_n\right| \\
&= \sum_{i\in\mathbb{N}} \left|[\nu_i^{(m)} - \overline{\nu}_i](R\psi_i^{(m)}, \overline{\psi}_i)_n + \overline{\nu}_i(R(\psi_i^{(m)} - \overline{\psi}_i), \psi_i^{(m)})_n + (R\overline{T}(\overline{\psi}_i - \psi_i^{(m)}), \psi_i^{(m)})_n\right| \\
&\leq \sum_{i\in\mathbb{N}} |\nu_i^{(m)} - \overline{\nu}_i|\|R\| + \sum_{i\in\mathbb{N}} \overline{\nu}_i\|R\|\|\psi_i^{(m)} - \overline{\psi}_i\|_n + \sum_{i\in\mathbb{N}} \|R\overline{T}\|\|\overline{\psi}_i - \psi_i^{(m)}\|_n \\
&\leq \|R\|\left[\sum_{i\in\mathbb{N}} |\nu_i^{(m)} - \overline{\nu}_i| + \sum_{i\in\mathbb{N}} \overline{\nu}_i\|\psi_i^{(m)} - \overline{\psi}_i\|_n + \|\overline{T}\|\sum_{i\in\mathbb{N}} \|\psi_i^{(m)} - \overline{\psi}_i\|_n\right]. \qquad (93)
\end{aligned}$$

b) Again, by working as in point 2.b in the proof of Proposition 24 with help of Lemma 22, we can show that, up to a subsequence, the right side of (93) become as small as we want.

□

The following result states that upward monotony helps to prove convergence in trace norm. This complements Theorem 23 where downward monotony was considered.

Corollary 27. *Let $(T_m)_{m\in\mathbb{N}} \subseteq \mathscr{H}_{V,+}^{n+1}$ be such that (B1) and (B2) hold. Assume that for some $m_0 \in \mathbb{N}$,*

$$\forall m \geq m_0 : \qquad T_m \leq \overline{T}, \qquad (94)$$

in the sense of operators. Then, up to a subsequence, $\|T_m - \overline{T}\|_n \longrightarrow 0$, as $m \longrightarrow +\infty$.

Proof. Let's pick $(T_{m_k})_{k\in\mathbb{N}}$, a subsequence of $(T_m)_{m\in\mathbb{N}}$, such that

$$\lim_{k\longrightarrow+\infty} \|T_{m_k}\|_n = \liminf_{m\longrightarrow+\infty} \|T_m\|_n.$$

Since $\overline{T}$, T_m and $\overline{T} - T_m$ are positive operators, we have by (8), for $m_k \geq m_0$, that

$$\|\overline{T} - T_{m_k}\|_n = \mathrm{Tr}_n(\overline{T} - T_{m_k}) = \mathrm{Tr}_n(\overline{T}) - \mathrm{Tr}_n(T_{m_k}) = \|\overline{T}\|_n - \|T_{m_k}\|_n.$$

Therefore, by Theorem 26, [7, Prop.3.5] and (94), it follows, as $k \longrightarrow +\infty$, that

$$\|\overline{T} - T_{m_k}\|_n \leq \liminf_{m \longrightarrow +\infty} \|T_m\|_n - \|T_{m_k}\|_n \longrightarrow 0.$$

□

The following result states that pointwise convergence holds in the context of Theorem 26. The proof is not difficult and uses the scheme shown in previous proofs.

Corollary 28. *Let $(T_m)_{m\in\mathbb{N}} \subseteq \mathscr{H}^{n+1}_{V,+}$ be such that (B1) and (B2) hold. Then, up to a subsequence, $(T_m)_{m\in\mathbb{N}}$ pointwise converges to $\overline{T}$, i.e., for every $\varphi \in \mathrm{H}_n$, $T_m\varphi \longrightarrow \overline{T}\varphi$, as $m \longrightarrow +\infty$, in H_n.*

7.2 Applications

In this section we use the compactness properties stated in Section 7.1 to minimize some free-energy functionals.

Theorem 29. *Let $n \in \mathbb{N}_*$, β an entropy seed generated by $F : \mathbb{R} \longrightarrow \mathbb{R} \cup \{+\infty\}$ which is convex and non-increasing on $[0, +\infty[$. Assume that $(-\Delta)^{n+1} + V$ is ϵ-coercive, $\epsilon \in]0,1[$, $\lambda \leq \lambda_V^{(1-\epsilon)}$ and that conditions $(\mathrm{G}^{n+1}_{0,\epsilon/2})$ and $(\mathrm{G}^{n+1}_{V-\lambda,1-\epsilon})$ hold. Suppose that $\mathscr{D}$ is a non-empty subset of $\mathcal{F}^{n+1}_{V,+}$, weakly closed in $\mathscr{N}_{n,1}$ and such that, for some $d_1 > 0$ and $d_2 \in \mathbb{R}$,*

$$\forall T \in \mathscr{D} : \quad |D(T, F; 1)| \leq d_1; \tag{95}$$

$$\forall T \in \mathscr{D} : \quad D(T, F_\gamma; 1) \leq d_2, \tag{96}$$

where $\gamma > N/2$ and F_γ is as in Examples 1 and 5. Then, there exists $\overline{T} \in \mathscr{D}$ such that

$$\mathscr{F}^\lambda_{V,\beta}(\overline{T}) = \inf_{T \in \mathscr{D}} \mathscr{F}^\lambda_{V,\beta}(T).$$

Proof. 1. By Proposition 15 and (95), $\mathscr{F}^\lambda_{V,\beta}$ is bounded from below on $\mathscr{D}$. Let's pick $(T_m)_{m\in\mathbb{N}} \subseteq \mathscr{D}$ such that

$$\lim_{m \longrightarrow +\infty} \mathscr{F}^\lambda_{V,\beta}(T_m) = \inf_{T \in \mathscr{D}} \mathscr{F}^\lambda_{V,\beta}(T). \tag{97}$$

By (96), condition (B2) holds. Thanks to Corollary 17, the sequences $(\rho_{0,T_m})_{m\in\mathbb{N}}$, $(\mathscr{K}_{n+1}(T_m))_{m\in\mathbb{N}}$, $(\mathcal{S}_\beta(T_m))_{m\in\mathbb{N}}$ and $(\mathscr{P}_V(T_m))_{m\in\mathbb{N}}$ are bounded. Therefore, condition (B1) holds: for some $K_\infty > 0$, $\langle\!\langle T_m \rangle\!\rangle_{V,n+1} < K_\infty$, for every $m \in \mathbb{N}$.

2. By Proposition (24), there exists $\overline{T} \in \mathscr{H}^{n+1}_{V,+}$ such that, up to a subsequence, $\rho_m \longrightarrow \overline{\rho}$, as $m \longrightarrow +\infty$, in $\mathrm{L}^1(\Omega)$, where $\rho_m = \rho_{0,T_m}$ and $\overline{\rho} = \rho_{0,\overline{T}}$. Consequently,

$$\|\rho_m\|_{\mathrm{L}^1(\Omega)} \longrightarrow \|\overline{\rho}\|_{\mathrm{L}^1(\Omega)}, \quad \text{as } m \longrightarrow +\infty. \tag{98}$$

By (77) and Remark 18, we have, up to a subsequence, that

$$\langle\!\langle \overline{T} \rangle\!\rangle_{V,n} \leq \liminf_{m \longrightarrow +\infty} \langle\!\langle T_m \rangle\!\rangle_{V,n}.$$

3. Let's write $\theta = \inf_{m\in\mathbb{N}} \mathcal{S}_\beta(T_m)$ and

$$\mathscr{A}_+ = \left\{ \mu = (\mu_i)_{i\in\mathbb{N}} \in l^1(\mathbb{R}) \,/\, \sum_{i\in\mathbb{N}} \beta(\mu_i) \geq \theta \,\wedge\, \mu_i \geq 0,\, i \in \mathbb{N} \right\}.$$

The convexity of β implies the convexity of the set $\mathscr{A}_+$ and of the mapping $\mathcal{S}_{\beta,*} : \mathscr{A}_+ \longrightarrow \mathbb{R} \cup \{+\infty\}$, given by $\mathcal{S}_{\beta,*}(\mu) = \sum_{i\in\mathbb{N}} \beta(\mu_i)$. Thus, $\mathcal{S}_{\beta,*}$ is weakly lower semi-continuous and, consequently,

$$\liminf_{m\longrightarrow+\infty} \mathcal{S}_{\beta,*}(\nu_{(m)}) \geq \mathcal{S}_{\beta,*}(\overline{\nu}), \tag{99}$$

where $\overline{\nu} = (\nu_{i,\overline{T}})_{i\in\mathbb{N}}$ and $\nu_{(m)} = (\nu_{i,T_m})_{i\in\mathbb{N}}$, $m \in \mathbb{N}$.

4. By (97)-(99) and the superadditivity of lim inf, we get

$$\begin{aligned}\mathscr{F}^\lambda_{V,\beta}(\overline{T}) &= \mathcal{S}_\beta(\overline{T}) + \langle\!\langle \overline{T} \rangle\!\rangle_{V,n} - \lambda \,\|\overline{\rho}\|_{\mathrm{L}^1(\Omega)} \\ &\leq \liminf_{m\longrightarrow+\infty} \mathcal{S}_\beta(T_m) + \liminf_{m\longrightarrow+\infty} \langle\!\langle T_m \rangle\!\rangle_{V,n} - \lambda \lim_{m\longrightarrow+\infty} \|\rho_m\|_{\mathrm{L}^1(\Omega)} \\ &\leq \liminf_{m\longrightarrow+\infty} \mathscr{F}^\lambda_{V,\beta}(T_m) - \lambda \lim_{m\longrightarrow+\infty} \|\rho_m\|_{\mathrm{L}^1(\Omega)} = \inf_{T\in\mathscr{D}} \mathscr{F}^\lambda_{V,\beta}(T),\end{aligned}$$

so that $\overline{T}$ is a minimizer of $\mathscr{F}^\lambda_{V,\beta}$ on $\mathscr{D}$.

□

Let's recall that for the functional $\mathscr{F}^\lambda_{V,\beta}$ to make sense (see Definition 6) we require the value λ to belong to $]-\infty, \lambda^{(1-\epsilon)}_V]$, because this imples that the operator $(1-\epsilon)(-\Delta)^{n+1}+V-\lambda$ is positive. Observe that the functional given by $\mathscr{F}^{\lambda;*}_{V,\beta}(T) = \mathscr{F}_{V,\beta}(T) - \lambda\|T\|_n$, coincides with $\mathscr{F}^{\lambda,*}_{V,\beta}$ only if $n = 0$. For this case, the operator $\overline{T}$ provided by Theorem 29 is the unique minimizer (see [9, Th.4.3] and [19, Th.5.1]) on the whole cone $\mathscr{H}^1_{V,+}$. Even more, if β is of class C^1 in the interior of its support, we have explicitly that

$$\overline{T} = \beta'^{-1}\left(\lambda - [(-\Delta)^n + V]\right), \tag{100}$$

which is compatible with the formula for occupation numbers given in [10, Prop. 4]. In [18, Th.5.1] the minimization is produced over the p-cone $\mathscr{W}^{1,p}$ (see Remark 10), $p \geq 2$; uniqueness still holds but there is not a formula like (100).

Following the scheme of the last proof, it's possible to deal with a free energy functional involving a non-linear but local function of the principal density:

$$\mathscr{F}^{\lambda;g}_{V,\beta}(T) = \mathscr{F}^\lambda_{V,\beta}(T) + \mathscr{G}(T), \qquad T \in \mathscr{H}^{n+1}_{V,+},$$

where $\mathscr{G}(T) = \int_\Omega g(\rho_{n,T}(x))\,dx$, and $g \in \mathrm{C}([0,+\infty[)$ is such that, for some $s \in S =]1, N/(N-2)[$ and $\theta_1, \theta_2 \geq 0$,

$$\forall t \in [0,+\infty[: \quad \theta_1 \leq g(t) \leq \theta_2 t^s. \tag{101}$$

Proposition 30. *Assume the conditions of Theorem 29 and (101). Then, there exists* $T_g \in \mathscr{D}$ *such that*

$$\mathscr{F}^{\lambda,g}_{V,\beta}(T_g) = \inf_{T\in\mathscr{D}} \mathscr{F}^{\lambda,g}_{V,\beta}(T).$$

Proof. We follow the scheme used to prove Theorem 29. Let's just observe that, for $T \in \mathscr{D}$,

$$\mathscr{G}(T) \le \theta_2 \int_\Omega \rho^s_{n,T}(x)\,dx \le C\theta_2 \left\|\nabla\rho_{n,T}\right\|_{\mathrm{L}^1(\Omega)} \le 2C\theta_2\check{c}_2 \langle\!\langle T\rangle\!\rangle_{V,n+1},$$

where $C > 0$ and we have used Theorem 9 with $l = 0$. From the last estimate and Fatou's lemma, we get $\mathscr{G}(T_g) \le \liminf_{m\longrightarrow+\infty} \mathscr{G}(T_m)$, where $(T_m)_{m\in\mathbb{N}}$ is an adequate subsequence of a minimizing sequence of $\mathscr{F}^{\lambda,g}_{V,\beta}$ over $\mathscr{D}$. □

To finish this section, let's consider the following Heisenberg-type equation with Poisson coupling:

$$\begin{cases} i\partial_t L(t) = \left[(-\Delta)^n + V(t,\cdot),\, L(t)\right], & t \ge 0, \\ -\Delta V(t,x) = \rho_{0,L(t)}(x), & x\in\Omega,\ t\ge 0, \\ L(0) = \tilde{L}, \end{cases} \tag{H_t}$$

where $L(t)$, the *density operator of the system*, is a positive trace-class operator acting on $\mathrm{L}^2(\Omega)$. When $n = 1$, (H_t) is known as the Hartree evolution system or Schrödinger-Poisson system in the mixed-states formulation (see e.g. [17] and the references therein). The stationary counterpart of (H_t) for the case of homogeneous Dirichlet boundary condition is then

$$\begin{cases} \left[(-\Delta)^n + V,\, L\right] = 0, & \\ -\Delta V = \rho_{0,L}(x), & x\in\Omega, \\ V(x) = 0, & x\in\partial\Omega. \end{cases} \tag{H}$$

As it's mentioned in [9], for $n = 1$, solutions of (H) can be obtained as critical points of the free energy functional $\mathscr{F}_\beta : \mathscr{H}^n_{0,+} \longrightarrow \mathbb{R}$, given by $\mathscr{F}_\beta(L) = \mathcal{S}_\beta(L) + \mathscr{K}_{n+1}(L) + \mathscr{P}(L)$, where

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

is referred to as the *Poisson potential energy of the operator* L. Observe that if we concentrate only on ground-states of $\mathscr{F}_\beta$, we shall be dealing with a kind of *Hartree problem with temperature*.

For $N \le 4$, we have, by Theorem 9, that $\rho_{n,T} \in \mathrm{L}^2(\Omega)$, so that $V_L \in \mathrm{H}^1_0(\Omega)$ is well defined as the solution of the Poisson equation in (H). If $n = 1$, β is of class C^1 in the interior of its support and F belongs to the Casimir class $\mathcal{C}^1_{0,1}$, then ([9, Th.4.3]) there exists a unique $T_F \in \mathscr{H}^1_{0,+}$ such that $\mathscr{F}_\beta(T_F) = \inf_{T\in\mathscr{H}^1_{0,+}} \mathscr{F}_\beta(T)$, which verifies $T_F = \beta'^{-1}(\Delta - V_{T_F})$.

Statements and Declarations

Acknowledgments. The authors thank YT community for their support during the project.
Funding. This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.
Conflicts of interest/Competing interests. The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.
Code availability. Not applicable.
Data availability. Not applicable.

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