Analysis tools and spectral theory for quantum mechanics

Internship supervised by Arnaud Triay
Ludwig-Maximilian University (LMU), Munich

Pierre Larivé

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Introduction : formalism of quantum mechanics

In quantum mechanics, we model a system using a set of axioms that postulate the existence of mathematical objects and tools to describe a system. Let us expose them taking the example of a particle of mass m in a given potential energy $V : \mathbb{R}^3 \to \mathbb{R}$.

The quantum description of the system assumes the existence of a Hilbert space $\mathcal{H}$, called the state space, whose each normalised vector, up to a phase, represents a state of a system and contains all information to describe it. For the case of our particle, a possible choice is $\mathcal{H} = L^2(\mathbb{R}^3)$ and a normalised vector $\psi \in L^2(\mathbb{R}^3)$, called wave fonction (complex-valued), enables to write the probability of presence of the particle at a certain point of the space using the probability density function $|\psi|^2$.

To talk about the measure of a physical quantity (such as position, momentum, energy), we associate to each quantity a self-adjoint operator, acting on $\mathcal{H}$. The values that the quantity can take for any system are given by the operator's spectrum. The physical quantity for the system is a random variable, following a law over the operator's spectrum given by ψ and the operator.

In our example, the self-adjoint operator for energy, called Hamiltonian, is the following :

$$H = \frac{-\hbar^2}{2m}\Delta + V(x)$$

The mean value of the energy for a state described by the wave function ψ would then be obtained by $\langle \psi, H\psi \rangle_{L^2}$. We can also get the probability law on the spectrum of H with more advanced tools that will arise with the spectral theorem (see the measure in theorem 2.4).

A first question arises when we see the expression of the Hamiltonian, as we are working on the space $L^2(\mathbb{R}^3)$: this operator cannot be defined on the whole space, because if $u \in L^2(\mathbb{R}^3)$, it is not guaranteed that $Hu \in L^2(\mathbb{R}^3)$. It is then necessary to consider operators that are only defined on subspaces of $\mathcal{H}$ and to have a spectral theory for them.

So far, we have only considered a system at a fixed moment, but quantum mechanics allows to describe its evolution over time. Indeed, the state $\psi(t)$ evolves in $\mathcal{H}$ satisfying the Schrödinger equation :

$$i\hbar \frac{d\psi}{dt}(t) = H\psi$$

Studying the Hamiltonian does not only provide information about the energy of the system, but also about its evolution in time.

If we now take the example of the Hydrogen atom, i.e. our particle is an electron and the potential is the Coulombian potential created by a proton fixed at the origin, we know empirically that the atom can be stable with a minimal energy, and with its electron staying bound to the nucleus. Mathematically, this stability is described by a system evolving from an eigenfunction ψ_0 of the Hamiltonian, called ground state, corresponding to a minimal eigenvalue E called groud state energy. The solution of the Schrödinger equation from this state is $\psi(t) = \psi_0 \exp\left(i\frac{E}{\hbar}t\right)$, so the only thing that change is the phase, which does not change the state of the system.

Therefore, we want to be able to study the existence of a ground state, of eigenvalues in the spectrum. A difficulty is that in infinite dimension, the spectrum can contain other elements than eigenvalues.

In this report, we begin by listing some tools of analysis (section 1) which we apply essentially in the section 3. Then, we explain the spectral theory for self-adjoint operators, with the difficulties of the domain we highlighted in this introduction (section 2). We obtain first results just after that shed light on the general structure of the spectrum of self-adjoint operators.

The section 3 is dedicated to an application of this general theory. We are interested in describing many-body systems, as for example the electrons of an atom. We first see classical reasoning to study the Hamiltonian and its domain (section 3.1), before diving into the comprehension of a fundamental result about the spectrum of many-body Hamiltonian, namely the HVZ Theorem (theorem 3.4). We introduce a formalism enabling to theorise the methods we use in the proof of this theorem, and which are used in other applications (section 3.2).

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Contents

1 Tools of analysis

In this section, we recall or write classical tools of analysis that will be useful in our journey. Some of them are useful inequalities, other are related to the theory of Sobolev spaces.

Theorem 1.1 *Young inequality with parameter*

Let $a, b \geq 0$.
Then, for all $\eta > 0$, $2ab \leq \eta a^2 + \eta^{-1} b^2$.

Young inequality is used in this report in the proof of lemma 3.2.

Theorem 1.2 *Variant of Hölder inequality*

Let $p_1, \cdots, p_n, r \geq 1$, and $\theta_1, \cdots, \theta_n > 0$ such that $\frac{\theta_1}{p_1} + \cdots + \frac{\theta_n}{p_n} = \frac{1}{r}$.
Then, for all $f_1 \in L^{p_1}, \cdots, f_n \in L^{p_n}$:

$$\|f_1 \cdots f_n\|_{L^r} \leq \|f_1\|_{L^{p_1}}^{\theta_1} \cdots \|f_n\|_{L^{p_n}}^{\theta_n} .$$

For our purpose, it will be often used with Sobolev inequalities.

Theorem 1.3 *Sobolev embeddings / Sobolev inequalities for $H^s(\mathbb{R}^d)$*

Let $s > 0$ and $d \in \mathbb{N}^*$.
We have the following continuous injections.

- If $0 < s < d/2$:
$$\forall 2 \leq p \leq \frac{2d}{d-2s}, \quad H^s(\mathbb{R}^d) \hookrightarrow L^p(\mathbb{R}^d)$$
- If $s = d/2$:
$$\forall 2 \leq p < \infty, \quad H^s(\mathbb{R}^d) \hookrightarrow L^p(\mathbb{R}^d)$$
- If $s > d/2$:
$$H^s(\mathbb{R}^d) \hookrightarrow \mathscr{C}^0_0(\mathbb{R}^d) \hookrightarrow L^\infty(\mathbb{R}^d)$$

An example of application of Hölder and Sobolev inequalities together is detailed later in this report, in the proof of theorem 3.3.

Theorem 1.4 *Rellich-Kondrachov theorem*

Let $\Omega \subset \mathbb{R}^d$ be a bounded open set.
For all $s > 0$, the injection $H^s(\Omega) \hookrightarrow L^2(\mathbb{R}^d)$ is compact.

An application of this theorem can be found in the proof of the proposition 3.4.

2 Spectral theory in infinite dimension

In the whole section, let $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ be a separable Hilbert space.

2.1 Defining self-adjonction in infinite dimension

As we need to consider operators that are only defined on subspaces of $\mathcal{H}$, the definition of self-adjonction is more difficult, because we need to take the domain of the adjoint into account. To overcome this difficulty, we will use the graph of the operator.

Definition 2.1 *Operator*

An *operator* on $\mathcal{H}$ is a couple $(A, D(A))$ where $D(A) \subset \mathcal{H}$ is a dense subspace of $\mathcal{H}$, called *domain*, and $A : D(A) \to \mathcal{H}$ is a linear map.

Definition 2.2 *Graph*

The *graph* of an operator $(A, D(A))$ is the subset $G(A) = \{(v, Av) \mid v \in D(A)\} \subset \mathcal{H} \times \mathcal{H}$.

Now, let us see how we would like to define the adjoint $(A^\dagger, D(A^\dagger))$ of an operator $(A, D(A))$. We want it to verify the following property :

$$\forall u \in D(A), \forall v \in D(A^\dagger), \langle v, Au \rangle = \left\langle A^\dagger v, u \right\rangle \Leftrightarrow \left\langle (v, A^\dagger v), (Au, -u) \right\rangle_{\mathcal{H}\times\mathcal{H}} = 0$$

We are encouraged to define $G(A^\dagger) = \{(Au, -u) \mid u \in D(A)\}^\perp$, where the orthogonal is taken in $\mathcal{H} \times \mathcal{H}$. But to be the graph of an operator, we need more hypothesis on A, motivating the following definitions.

Definition 2.3 *Extension*

Let $(A, D(A))$ be an operator. We say that $(B, D(B))$ is an *extension* of $(A, D(A))$ when $D(A) \subset D(B)$ and $B|_{D(A)} = A$. In this case, we note $A \subset B$.

Definition 2.4 *Closed operator, closable operator, closure of an operator*

An operator $(A, D(A))$ is *closed* when its graph is closed in $\mathcal{H} \times \mathcal{H}$, which means that if $(x_n)_{n\in\mathbb{N}} \in D(A)^{\mathbb{N}}$ converges to $x \in \mathcal{H}$, such that $(Ax_n)_{n\in\mathbb{N}}$ also converges to $y \in \mathcal{H}$, then $x \in D(A)$ and $Ax = y$.
An operator $(A, D(A))$ is said to be *closable* if it admits a closed extension. In this case, we note $(\bar{A}, D(\bar{A}))$ its smallest closed extension, called *closure of* A.

Let us now prove that, with this additional hypothesis on A, the adjoint is well defined.

Proposition 2.1 *Adjoint of an closable operator*

Let $(A, D(A))$ be a closable operator.
Then the operator $(A^\dagger, D(A^\dagger))$, defined by its graph $G(A^\dagger) = \{(Au, -u) \mid u \in D(A)\}^\perp \subset \mathcal{H} \times \mathcal{H}$, is well defined. It is called *adjoint* of $(A, D(A))$.

Proof.

We start by establishing a caracterisation of the graph of an operator, then we will verify the criteria on our particular graph.

Lemma 2.1 *Caracterisation of the graph*

A subspace $G \subset \mathcal{H} \times \mathcal{H}$ is the graph of an operator if and only if :

(i) $(0, y) \in G \Rightarrow y = 0$

(ii) The subspace $\{v \in \mathcal{H} \mid \exists w \in \mathcal{H}, (v, w) \in G\}$ is dense in $\mathcal{H}$.

Proof.

The direct implication is clear, noticing that the set of (ii) is the domain of the operator.

Conversely, we call $D(A)$ the set of (ii) and define $A : D(A) \to \mathcal{H}$ by $A(u) = v$ for $(u, v) \in G$. A is well defined thanks to (i) and the fact that G is a vector space. It is linear because G is a vector space. (ii) gives the density of the domain. ■

First, $G(A^\dagger)$ is a subspace of $\mathcal{H} \times \mathcal{H}$. Then, let $(0, w) \in G(A^\dagger)$. We have, for all $v \in D(A), \langle v, w\rangle = 0$ i.e. $w \in D(A)^\perp = \{0\}$ as $D(A)$ is dense. Finally, let us show that $D(A^\dagger)$ is dense. Let $v \in D(A^\dagger)^\perp$. This means that $(v, 0) \in G(A)^\perp = \overline{\{(Au, -u) \mid u \in D(A)\}}$. So $(0, v) \in \overline{G(A)}$. We use that A is closable and apply the lemma to its closure $\bar{A}$ to conclude that $v = 0$. ■

Now we are ready to correctly define symmetry and self-adjonction for our operators.

Definition 2.5 *Symmetric, self-adjoint operator*

Let $(A, D(A))$ be an operator. We say that it is *symmetric* when $A \subset A^\dagger$, i.e. $\forall u, v \in D(A), \langle u, Av\rangle = \langle Au, v\rangle$. We say that it is *self-adjoint* when $A = A^\dagger$.

In the definition, we do not assume A to be closable, whereas it is a necessary hypothesis to define the adjoint, as we saw before. This is due to the fact that if A is symmetric, then it is closeable. Indeed :

- $D(A) \subset D(A^\dagger)$, which means that $(A^\dagger, D(A^\dagger))$ is well-defined as an operator (its domain is dense) ;
- $(A^\dagger, D(A^\dagger))$ is closed thanks to the continuity of the scalar product. Thus, $A \subset A^\dagger$ is a closed extension of A, meaning that A is in fact a closable operator.

Then, our goal is to study the spectrum of a self-adjoint operator. We recall the definition of the spectrum and the associated subtilities in infinite dimensions for general operators, and we establish a caracterisation of self-adjonction which we will use in the following proofs.

Definition 2.6 *Resolvant set, spectrum*

Let $(A, D(A))$ be an operator.
We define the following subsets of $\mathbb{C}$:

- its *resolvant set* $\rho(A) = \{z \in \mathbb{C} \mid (A - z)^{-1} : \mathcal{H} \to D(A) \text{ is well defined and bounded}\}$
- its *spectrum* $\sigma(A) = \mathbb{C} \backslash \rho(A)$

We recall that in infinite dimension, the spectrum can contain $z \in \mathbb{C}$ for several reasons :

- $(A - z)$ is not injective (z is called an *eigenvalue*) ;
- $(A - z)$ is not surjective ;
- $(A - z)^{-1}$ is well-defined but unbounded.

Proposition 2.2 *Caracterisation of self-adjoint operators*

Let $(A, D(A))$ be a symmetric operator.
The following are equivalent :

(i) A is self-adjoint ;

(ii) $\sigma(A) \subset \mathbb{R}$;

(iii) There exists $\lambda \in \mathbb{C}$ such that $A - \lambda, A - \bar{\lambda} : D(A) \to \mathcal{H}$ are surjective.

Proof.

$(i) \Rightarrow (ii)$: Suppose that A is self-adjoint and let $\lambda \in \mathbb{C} \backslash \mathbb{R}$. We know that λ is not an eigenvalue : if $u \in D(A)$ satisfies $Au = \lambda u$, then :

$$\lambda \|u\|^2 = \langle u, Au \rangle = \langle Au, u \rangle = \bar{\lambda} \|u\|^2$$

so $\|u\| = 0$. The same holds for $\bar{\lambda}$.

Hence, $\{0\} = \operatorname{Ker}(A - \bar{\lambda}) = \operatorname{Ker}(A^\dagger - \bar{\lambda}) = \operatorname{Im}(A - \lambda)^\perp$, showing that the image of $A - \lambda$ is dense in $\mathcal{H}$. We now show that it is closed, using the following useful relation, that we show by developing the inner product.

Lemma 2.2

Let $(A, D(A))$ be a symmetric operator, and $a, b \in \mathbb{R}$.

$$\|(A - (a + ib))u\|^2 = \|(A - a)u\|^2 + b^2 \|u\|^2 \geq b^2 \|u\|^2$$

Let $(u_n)_{n \in \mathbb{N}} \in D(A)^{\mathbb{N}}$ such that $(A - \lambda)u_n \to w$. Then, for all $n, m \in \mathbb{N}$, $\operatorname{Im} \lambda \|u_n - u_m\|^2 \leq \|(A - \lambda)(u_n - u_m)\|^2$. This tells us that (u_n) is a Cauchy sequence in the Hilbert space $\mathcal{H}$. It converges to some limit $u \in \mathcal{H}$. Using the fact that $A = A^\dagger$ is closed, we obtain $u \in D(A)$ and $(A - \lambda)u = w$.

Finally, the inequality of the lemma justifies that $(A - \lambda)^{-1}$ is a bounded operator, whence $\lambda \in \rho(A)$.

$(ii) \Rightarrow (iii)$ is clear.

$(iii) \Rightarrow (i)$: Suppose to have $\lambda \in \mathbb{C}$ such that (iii) holds. We want to show that $D(A^\dagger) \subset D(A)$. Let $u \in D(A^\dagger)$. We use the fact that $A - \bar{\lambda}$ is surjective to get $v \in D(A)$ such that $(A - \bar{l}ambda)v = (A^\dagger - \bar{\lambda})u$. Then, we write, for $w \in D(A)$:

$$\langle u, (A-\lambda)w\rangle = \left\langle (A^\dagger - \bar{\lambda})u, w \right\rangle = \left\langle (A - \bar{\lambda})v, w \right\rangle = \langle v, (A-\lambda)w\rangle$$

where we use that A is symmetric for the last equality. As $A - \lambda$ is surjective, we established : $\forall \tilde{w} \in \mathcal{H}, \langle u, \tilde{w}\rangle = \langle v, \tilde{w}\rangle$, hence $u = v \in D(A)$. ■

N.B.

The point (ii) of the proposition is important for the fundamentals of quantum mechanics. Indeed, it guarantees that the theory described at the begining enables only real measures for physical quantities.

Example 2.1 *The Laplacian on $\mathbb{R}^d$*

We illustrate the notions of this section with the example of the operator Δ, working in $\mathcal{H} = L^2(\mathbb{R}^d)$. We are able to define the Laplacian on the subsets $\mathscr{C}_c^\infty(\mathbb{R}^d)$ or $H^2(\mathbb{R}^d)$.

We start by showing that $(\Delta, H^2(\mathbb{R}^d))$ is the closure of $(\Delta, \mathscr{C}_c^\infty(\mathbb{R}^d))$.

First, $(\Delta, H^2(\mathbb{R}^d))$ is closed. Indeed, let $(f_n, \Delta f_n)_{n\in\mathbb{N}}$ be a sequence in $G(\Delta)$ converging to (f, g) in $L^2(\mathbb{R}^d) \times L^2(\mathbb{R}^d)$. We want to obtain that $f \in H^2(\mathbb{R}^d)$ and $g = \Delta f$.

Let $\varphi \in \mathscr{C}_c^\infty(\mathbb{R}^d)$ be a test function. In the sense of distributions :

$$\begin{aligned}
\langle g, \varphi\rangle &= \lim_{n\to\infty} \langle \Delta f_n, \varphi\rangle \\
&= \lim_{n\to\infty} \langle f_n, \Delta\varphi\rangle \\
&= \langle f, \Delta\varphi\rangle \\
&= \langle \Delta f, \varphi\rangle
\end{aligned}$$

So $g = \Delta f$ in the sense of distributions, hence $f \in H^2(\mathbb{R}^d)$.

Then, it remains to justify that $H^2(\mathbb{R}^d) \subset D(\overline{\Delta})$, where the closure is the one of $(\Delta, \mathscr{C}_c^\infty(\mathbb{R}^d))$. For $f \in H^2(\mathbb{R}^d)$, we want to approach $(f, \Delta f)$ with compactly supported functions. It comes from the density of $\mathscr{C}_c^\infty(\mathbb{R}^d)$ in $H^2(\mathbb{R}^d)$ for its norm.

Finally, we show that $(\Delta, H^2(\mathbb{R}^d))$ is self-adjoint. By definition of the derivation for distributions, it is symmetric. To see that it is self-adjoint, we use the proposition 2.2 and show that $\Delta - 1$ is surjective. Let $g \in L^2(\mathbb{R}^d)$. We are looking for $f \in H^2(\mathbb{R}^d)$ such that $(\Delta - 1)f = g$. Taking the Fourier transform, we find that :

$$\hat{f}(\xi) = -\frac{\hat{g}(\xi)}{1 + |\xi|^2}$$

f is well defined in $L^2(\mathbb{R}^d)$ because $\hat{f} \in L^2(\mathbb{R}^d)$. Moreover, $f \in H^2(\mathbb{R}^d)$ because $(1 + |\xi|^2)^{2/2}\hat{f} \in L^2(\mathbb{R}^d)$. We use here the caracterisation of $H^2(\mathbb{R}^d)$ by the Fourier transform.

2.2 The spectral theorem

We then want to study more precisely the spectrum of a self-adjoint operator. Until now, we have proved that it is real-valued. Our first goal to do that is to establish the spectral theorem for all self-adjoint operators. It generalises the case of finite dimension and unlocks a lot of tools to work with self-adjoint operators.

Preliminary work is needed to achieve this aim. The sketch of the proof is to establish the spectral theorem for bounded self-adjoint operators, then generalising it for bounded normal operators, and finally using this version to get the general spectral theorem. We present here a version, called *multiplication operator form*, of the theorem that looks like the diagonalisation in finite dimension, and then deduce from it another version, called functional calculus. Actually, both formulations are equivalent, and functional calculus will partially arise in the proof of the spectral theorem we follow.

We begin with this lemma, well-known for bounded operators. Its proof remains the same. It will be useful to say that $\sigma(A)$ is compact if A is a bounded operator on $\mathcal{H}$.

Lemma 2.3 *Closure, compactness of the spectrum*

Let $(A, D(A))$ be an operator.
$\sigma(A)$ is a closed subset of $\mathbb{C}$. Moreover, if A is bounded on $\mathcal{H}$, $\sigma(A)$ is compact.

Proof.

We show that $\rho(A)$ is open. Let $z \in \rho(A)$. We write

$$A - z' = A - z + z - z' = (1 + (z - z')(A - z)^{-1})(A - z)$$

and have that $A - z : D(A) \to \mathcal{H}$ is invertible, such as $(1 + (z - z')(A - z)^{-1}) : \mathcal{H} \to \mathcal{H}$ for z' sufficiently small to have $|z - z'| \left\|(A - z)^{-1}\right\| < 1$.

If A is bounded on $\mathcal{H}$, we have $\sigma(A) \subset [-\|A\|, \|A\|]$, so $\sigma(A)$ is also bounded. ■

We will admit the following theorem, but we give some insights about its proof.

Theorem 2.1 *Riesz-Markov representation theorem*

Let $B \subset \mathbb{R}^d$ be a Borel set, and $\mathscr{L} : \mathscr{C}_c(B) \to \mathbb{C}$ a linear positive map (i.e. $f \geq 0 \Rightarrow \mathscr{L}(f) \geq 0$).
There exists a unique Borel regular measure μ on B such that :

$$\forall f \in \mathscr{C}_c(B), \mathscr{L}(f) = \int_B f(x) d\mu(x)$$

Proof. *(sketch)*

We want to define μ for the open and compact sets by :

- for $U \subset B$ open, $\mu(U) = \sup\{\mathscr{L}(f) \mid f \in \mathscr{C}_c(B), 0 \leq f \leq 1, \operatorname{supp} f \subset U\}$;
- for $K \subset B$ compact, $\mu(K) = \inf\{\mathscr{L}(f) \mid f \in \mathscr{C}_c(B), 0 \leq f \leq 1, f \equiv 1 \text{ on } K\}$.

  Then, we have to extend this definition of μ to a Borel regular measure on B. Eventually, we verify that $\mathscr{L}(f) = \int_B f d\mu$ by approximation.

■

The following operators will be the formulation of the diagonalisation in infinite dimension. The parallel is explained in the next section.

Definition 2.7 *Multiplication operator*

Let (B, μ) be a measured space, and $a : B \to \mathbb{C}$ a measurable function.
We work here in $\mathcal{H} = L^2(B, d\mu)$. We define the *multiplication operator* associated to a on the domain $D(M_a) = \{f \in L^2(B, d\mu) \mid af \in L^2(B, d\mu)\}$ by

$$\forall f \in D(M_a), M_a f = af$$

2.2.1 The spectral theorem for bounded self-adjoint operators

We want to establish the following result.

Theorem 2.2 *Spectral theorem for bounded self-adjoint operators*

Let A be a bounded self-adjoint operator on $\mathcal{H}$.
There exists :

- a measured space (B, μ) where $B \subset \mathbb{R}^d$ is a Borel set and μ is a finite measure on B ;
- a unitary operator $U : \mathcal{H} \to L^2(B, d\mu)$;
- a measurable and real-valued function $a \in L^\infty_{\text{loc}}(B, d\mu)$;

such that $UAU^\dagger = M_a$.

Let us first explain to what extent it generalises the spectral theorem in finite dimension by explicitly building such objects in the way they will make sense in the proof.

Example 2.2 *Link with finite dimension*

Let A be a self-adjoint (Hermitian) matrix of $M_d(\mathbb{C})$. There exists a orthonormal basis of eigenvectors $(u_{i,k})_{1\leq i\leq p, 1\leq j\leq N_i}$ corresponding to distinct eigenvalues $(\lambda_i)_{1\leq i\leq p}$. We have written things to take into account the multiplicity of eigenvalues.

We set :

- $B = \sigma(A) \times \mathbb{N}$, $\mu = \sum\limits_{1\leq i\leq p, 1\leq k\leq N_i} \delta_{\lambda_i,k}$;
- $U : u_{i,k} \mapsto \mathbb{1}_{(\lambda_i,k)}$;
- $a(\lambda, k) = \lambda$.

U is a unitary operator because it maps the orthonormal basis $(u_{i,k})$ of $\mathcal{H}$ to the orthonormal basis $(\mathbb{1}_{(\lambda_i,k)})$ of $L^2(B, d\mu)$. Indeed, μ has the effect to "ignore" the part of $\sigma(A) \times \mathbb{N}$ that is not used to register the eigenvectors. We have for $(i, k) \in [\![1, p]\!] \times \mathbb{N}$ for which $\mu(\{(\lambda_i, k)\}) \neq 0$:

$$(UAU^\dagger \mathbb{1}_{(\lambda_i,k)}) = UAu_{i,k} = \lambda_i U u_{i,k} = \lambda_i \mathbb{1}_{(\lambda_i,k)}$$

So $UAU^\dagger = M_a$ on $L^2(B, d\mu)$.

> **Here, things are easy to make explicitly because the spectrum is only composed with eigenvalues. But the strength of the space $L^2(B, d\mu)$ is that it can also work with a more general spectrum in infinite dimension, thanks to the use of the measure.**

Now we move on to the proof of the spectral theorem. We will decompose the whole space with the same idea as cyclic decomposition for Frobenius reduction in finite dimension. We therefore introduce a notion of cyclic vector. Then, on each cyclic subspace, we will define a functional calculus using polynoms of the operator, extending it to continuous functions thanks to the Stone-Weierstrass theorem. To conclude, we will use the cyclic vector and the Riesz-Markov theorem to access L^2.

Definition 2.8 *Cyclic vector*

Let A be a bounded self-adjoint operator on $\mathcal{H}$.
We say that a vector $u \in \mathcal{H}$ is cyclic if $\mathrm{Span}(A^k u)_{k\in\mathbb{N}}$ is dense in $\mathcal{H}$.

Lemma 2.4 *Continuous functional calculus for bounded self-adjoint operators*

Let A be a bounded self-adjoint operator on $\mathcal{H}$.
There exists a unique continuous linear map $f \in \mathscr{C}(\sigma(A)) \mapsto f(A) \in \mathcal{B}(\mathcal{H})$ such that :

(i) if $f = \sum_i a_i t^i$ is a polynom, then $f(A) = \sum_i a_i A^i$;

(ii) it is an isometry of C^*-algebra, meaning that for $f, g \in \mathscr{C}(\sigma(A))$:

- $\|f(A)\| = \|f\|_{L^\infty(\sigma(A))}$;
- $(fg)(A) = f(A)g(A)$;
- $f(A)^\dagger = \bar{f}(A)$;
- $\sigma(f(A)) = f(\sigma(A))$.

Proof.

We first define the linear map

$$\mathscr{L} : \left| \begin{array}{ccc} \mathbb{C}[t] & \to & \mathcal{B}(\mathcal{H}) \\ \sum_i a_i t^i & \mapsto & \sum_i a_i A^i \end{array} \right.$$

We prove that $\|P(A)\| = \|P\|_{L^\infty(\sigma(A))}$ for $P \in \mathbb{C}[t]$ by showing first that $\sigma(P(A)) = P(\sigma(A))$. To see this, for $\mu \in \mathbb{C}$, we write the polynom $P(t) - \mu$ in its factorised form and we apply $\mathscr{L}$. We obtain :

$$P(A) - \mu = \alpha \prod_i (A - \lambda_i)$$

Now, if $\mu = P(\lambda) \in P(\sigma(A))$, then there exists i such that $\lambda_i = \lambda$. Therefore, as $A - \lambda$ is not invertible, $P(A) - P(\lambda)$ is also not invertible, meaning that $P(\lambda) \in \sigma(P(A))$. Conversely, if $\mu \in \sigma(P(A))$, $P(A) - \mu$ is not invertible, so there exists i such that $A - \lambda_i$ is not invertible. Then $\lambda_i \in \sigma(A)$ and valuing the polynom in λ_i, we obtain $\mu = P(\lambda_i) \in P(\sigma(A))$.

The result on norms we wanted follows, using that for a bounded self-adjoint operator,

$\|A\| = \sup\{|\lambda| \mid \lambda \in \sigma(A)\}$, and $\|A\|^2 = \left\|A^\dagger A\right\|$:

$$\|P(A)\|^2 = \left\|P(A)^\dagger P(A)\right\| = \left\|\bar{P}P(A)\right\| = \sup_{\lambda\in\sigma(\bar{P}P(A))} |\lambda| = \sup_{\lambda\in\sigma(A)} |\bar{P}P(\lambda)| = \sup_{\lambda\in\sigma(A)} |P(\lambda)|^2 = \|P\|^2_{L^\infty(\sigma(A))}$$

To conclude, we use Lemma 2.3 and the Stone-Weierstrass theorem to say that $\mathbb{C}[t]$ is dense in $\mathscr{C}(\sigma(A))$ for $\|\cdot\|_{L^\infty(\sigma(A))}$. The continuous linear map $\mathscr{L}$ has therefore a unique continuous linear extension to $\mathscr{C}(\sigma(A))$, satisfying $\|f(A)\| = \|f\|_{L^\infty(\sigma(A))}$. The other properties are true for polynomials and are extended by density. ■

Lemma 2.5 *Spectral theorem on cyclic subspace*

Let A be a bounded self-adjoint operator on $\mathcal{H}$.
Assume that A has a cyclic vector $u \in \mathcal{H}$.
Then there exists a finite measure μ_u on $\sigma(A)$ and a unitary operator $U : \mathcal{H} \to L^2(\sigma(A), d\mu_u)$ such that $UAU^\dagger = M_a$, where $a(\lambda) = \lambda$.

Proof.

First, we use the continuous functional calculus and the Riesz-Markov theorem (theorem 2.1) to get a measure from u.

The linear map $f \in \mathscr{C}(\sigma(A)) \mapsto \langle u, f(A)u\rangle \in \mathbb{C}$ is positive. Indeed, if $f \geq 0$, then :

$$\langle u, f(A)u\rangle = \left\langle u, (\sqrt{f}\sqrt{f})(A)u\right\rangle = \left\langle u, \sqrt{f}(A)\sqrt{f}(A)u\right\rangle = \left\langle \sqrt{f}(A)u, \sqrt{f}(A)u\right\rangle = \left\|\sqrt{f}(A)u\right\| \geq 0$$

Here we can observe the strength of functional calculus, allowing us to use the self-adjonction very efficiently.

By the Riesz-Markov theorem, there exists a (unique) Borel regular measure μ_u on $\sigma(A)$ such that :

$$\forall f \in \mathscr{C}(\sigma(A)), \langle u, f(A)u\rangle = \int_{\sigma(A)} f(\lambda)d\mu_u(\lambda)$$

The fact that it is regular gives that it is finite because the measure of any compact set is finite.

Now, it remains to make the Hilbert space $L^2(\sigma(A), d\mu_u))$ appear, by considering the following linear map :

$$\mathscr{L} : \left| \begin{array}{ccc} \mathscr{C}(\sigma(A)) & \to & \mathcal{H} \\ f & \mapsto & f(A)u \end{array} \right.$$

Using again the strength of functional calculus, we observe that for $f \in \mathscr{C}(\sigma(A))$:

$$\|f(A)u\|^2 = \left\langle u, f(A)^\dagger f(A)u\right\rangle = \left\langle u, |f|^2(A)u\right\rangle = \int_{\sigma(A)} |f|^2 d\mu_u = \|f\|^2_{L^2(\sigma(A),d\mu_u)}$$

Since $\mathscr{C}(\sigma(A))$ is dense in $L^2(\sigma(A), d\mu_u)$, there exists a unique continuous linear extension of $\mathscr{L}$ to $L^2(\sigma(A), d\mu_u)$, and it satisfies $\|f(A)u\| = \|f\|_{L^2(\sigma(A),d\mu_u)}$ for $f \in L^2(\sigma(A), d\mu_u)$.

To conclude, we want to define the unitary operator of the statement U_u by its adjoint :

$$U_u^\dagger : \left| \begin{array}{ccc} L^2(\sigma(A), d\mu_u) & \to & \mathcal{H} \\ f & \mapsto & f(A)u \end{array} \right.$$

It is indeed legitimate as :

- $U_u^\dagger$ is an isometry ;
- $U_u^\dagger$ is surjective (because u is cyclic and $\sigma(A)$ is compact, so polynomials are in $L^2(\sigma(A), d\mu_u)$) ;
- $L^2(\sigma(A), d\mu_u)$ and $\mathcal{H}$ are two Hilbert spaces, so the well-defined operator U_u is also bounded.

  We finally verify with the functional calculus that $U_u A U_u^\dagger = M_a$ where $a(\lambda) = \lambda$. For $f \in L^2(\sigma(A), d\mu_u)$, we have, for μ_u-almost every $\lambda \in \sigma(A)$:

$$(U_u A U_u^\dagger f)(\lambda) = (U_u A f(A)u)(\lambda) = (t \mapsto t f(t))(\lambda) = \lambda f(\lambda)$$

■

The general case follows applying Zorn's lemma to get a decomposition of $\mathcal{H}$ in cyclic subspaces.

Proof. *(Theorem 2.2)*

Let $\mathcal{X} = \{(u_n)_{n\in\mathcal{N}} \subset \mathcal{H} \mid \mathcal{N} = [\![0, N]\!]$ or $\mathcal{N} = \mathbb{N}$, and $(u_n)_{n\in\mathcal{N}}$ is an orthonormal family$\}$, with the partial order :

$$(u_n)_n \preccurlyeq (v_n)_n \Leftrightarrow \begin{cases} (u_n)_n \subset (v_n)_n \\ \bigoplus_n \mathcal{H}_{u_n} \subset \bigoplus_n \mathcal{H}_{v_n} \end{cases}$$

where we define $\mathcal{H}_{u_n} = \overline{\mathrm{Span}(A^k u_n)_{k\in\mathbb{N}}}$.

We verify Zorn's lemma hypothesis. If $\mathcal{Y} \subset \mathcal{X}$ is a totally order subset, the maximal element to consider is the orthonormal family $\bigcup_{u\subset\mathcal{Y}} u$. Thus, there is a maximal element $(u_n)_{n\in\mathcal{N}}$ for $\mathcal{X}$.

Assume a moment that $\bigoplus \mathcal{H}_{u_n} \subsetneq \mathcal{H}$. Then there exists a normalised $u \in \mathcal{H}$ such that $\forall n \in \mathcal{N}, u \perp \mathcal{H}_{u_n}$. The orthonormal family $(u_n) \cup \{u\}$ contradicts the maximality of (u_n).

Let us now use this decomposition and the lemma 2.5 to get the spectral theorem for bounded operators.

For $n \in \mathcal{N}$, we have a unitary operator $U_{u_n} : \mathcal{H} \to L^2(\sigma(A), d\mu_{u_n})$ such that $U_{u_n} A_{u_n} U_{u_n}^\dagger = M_a$ with $a(\lambda) = \lambda$, where A_{u_n} is the bounded self-adjoint operator induced by A on the stable subspace $\mathcal{H}_{u_n}$.

Then, we define the unitary operator

$$U = \bigoplus_{n\in\mathcal{N}} U_{u_n} : \mathcal{H} = \bigoplus_{n\in\mathcal{N}} \mathcal{H}_{u_n} \to L^2(\sigma(A) \times \mathbb{N}, d\mu) \simeq \bigoplus_{n\in\mathcal{N}} L^2(\sigma(A), d\mu_{u_n})$$

where $\mu = \bigoplus_{n\in\mathcal{N}} 2^{-n} \mu_{u_n}$. The measure μ on $\sigma(A) \times \mathbb{N}$ is finite :

$$\mu(\sigma(A) \times \mathbb{N}) = \sum_{n\in\mathcal{N}} 2^{-n} \mu_{u_n}(\sigma(A)) = \sum_{n\in\mathcal{N}} 2^{-n} \leq 2$$

Eventually, with $a(\lambda, n) = \lambda$, we have :

$$UAU^\dagger = \bigoplus_{n\in\mathcal{N}} (U_{u_n} A_{u_n} U_{u_n}^\dagger) = \bigoplus_{n\in\mathcal{N}} M_{a(\cdot,n)} = M_a$$

2.2.2 Extension to bounded normal operators

To prove the spectral theorem for unbounded operators, we need to extend the spectral theorem to bounded normal operators. We will use it on the normal operator $(A+i)^{-1}$. The main idea of this extension is that two bounded self-adjoint operators which commute can be simultaneously diagonalised, i.e. turned into multiplication operators by the same unitary operator.

To show this, we need to use another functional calculus, defined for bounded measurable functions, because we will work with multi-valued functions, so Stone-Weierstrass theorem is no more valid.

To define it, we use the spectral theorem to write $UAU^\dagger = M_a$, and then, for $f \in L^\infty(B, d\mu)$ (see Theorem 2.2 for the notations), let $f(A) = U^\dagger M_{f(a)} U$. To do so, we have to verify that it does not depend of the unitary operator chosen when we applied the spectral theorem. We admit here this point, but the idea is to identify a dense subset of $L^\infty(B, d\mu)$ on which the definition arising from two different unitary operators would be the same, and then to use the uniqueness of the continuous linear extension to $L^\infty(B, d\mu)$.

Theorem 2.3 *Spectral theorem for bounded normal operators*

Let A be a bounded normal operator on $\mathcal{H}$, i.e. such that A and $A^\dagger$ commute.
There exists :

- a measured space (B, μ) where $B \subset \mathbb{R}^d$ is a Borel set and μ is a finite measure on B ;
- a unitary operator $U : \mathcal{H} \to L^2(B, d\mu)$;
- a measurable (no more real-valued in general) function $a \in L^\infty_{\text{loc}}(B, d\mu)$;

such that $UAU^\dagger = M_a$.

Proof.

We decompose $A = A_1 + iA_2$ where $A_1 = \frac{A+A^\dagger}{2}$ and $A_2 = \frac{A-A^\dagger}{2i}$, and notice that A_1 and A_2 are two bounded self-adjoint operator (true for every bounded operator A) that commute (because A is normal).

We now want to simultaneously diagonalise A_1 and A_2. To do so, we reproduce the proof for one single operator, but getting this time a functional calculus on $\mathscr{C}(\sigma(A_1) \times \sigma(A_2))$. We use the following map $\mathscr{L}$, defined for step functions of $\mathbb{R} \times \mathbb{R}$ by :

$$\mathscr{L}(\mathbb{1}_{B_1}\mathbb{1}_{B_2}) = \mathbb{1}_{B_1}(A_1)\mathbb{1}_{B_2}(A_2) \in \mathcal{B}(\mathcal{H})$$

As A_1 and A_2 commute, and using functional calculus, we see that $\mathbb{1}_{B_1}(A_1)\mathbb{1}_{B_2}(A_2)$ is self-adjoint and that $\mathscr{L}$ is bounded for $\|\cdot\|_{L^\infty(\sigma(A_1)\times\sigma(A_2))}$:

$$(\mathbb{1}_{B_1}(A_1)\mathbb{1}_{B_2}(A_2))^\dagger = \mathbb{1}_{B_2}(A_2)^\dagger \mathbb{1}_{B_1}(A_1)^\dagger = \overline{\mathbb{1}_{B_2}}(A_2)\overline{\mathbb{1}_{B_1}}(A_1) = \mathbb{1}_{B_1}(A_1)\mathbb{1}_{B_2}(A_2)$$

and therefore

$$
\begin{aligned}
\|\mathbb{1}_{B_1}(A_1)\mathbb{1}_{B_2}(A_2)\| &= \sup_{\lambda\in\sigma(\mathbb{1}_{B_1\times B_2}(A_1,A_2))} |\lambda| \\
&= \sup_{(\lambda_1,\lambda_2)\in\sigma(A_1)\times\sigma(A_2)} |\mathbb{1}_{B_1}(\lambda_1)\mathbb{1}_{B_2}(\lambda_2)| \\
&= \|\mathbb{1}_{B_1}(\lambda_1)\mathbb{1}_{B_2}(\lambda_2)\|_{L^\infty(\sigma(A_1)\times\sigma(A_2))}
\end{aligned}
$$

In the latter equalities, we used functional calculus on $\mathcal{H}\times\mathcal{H}$ for the self-adjoint operator (A_1, A_2).

The closure of the step functions for $\|\cdot\|_{L^\infty(\sigma(A_1)\times\sigma(A_2))}$ contains $\mathscr{C}(\sigma(A_1)\times\sigma(A_2))$ because $\sigma(A_1)\times\sigma(A_2)$ is compact. We can now use the same arguments as before to conclude. ■

2.2.3 The spectral theorem for unbounded self-adjoint operators

We prove at last the general spectral theorem.

Theorem 2.4 *Spectral theorem*

Let $(A, D(A))$ be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$.
There exists :

- a measured space (B,μ) where $B\subset\mathbb{R}^d$ is a Borel set and μ is a finite measure on B ;
- a unitary operator $U:\mathcal{H}\to L^2(B,d\mu)$;
- a measurable and real-valued function $a\in L^\infty_{\text{loc}}(B,d\mu)$;

such that $UAU^\dagger = M_a$.

N.B.

Until now, the function a was actually globally bounded because $\sigma(A)$ was compact. So, $D(M_a)$ was the whole space $L^2(B,d\mu)$. But now, it is no more the case, and the domain corresponding to $D(A)$ is $D(M_a)=\{f\in L^2(B,d\mu)\mid af\in L^2(B,d\mu)\}$.

Proof.

We show that $(A+i)^{-1}$ is normal, so that we can turn it to a multiplication operator. We then deduce what the multiplication operator corresponding to A should be.

We recall that $(A+i)$ is invertible as $\sigma(A)\subset\mathbb{R}$. We also know that $(A+i)^{-1}$ and $(A-i)^{-1}$ commute (this is a property of the resolvant). Now, we show that $((A+i)^{-1})^\dagger=(A-i)^{-1}$. This is not clear due to the fact that A is unbounded and is not defined on the whole space. We write :

$$
\begin{array}{rlrcl}
 & \forall u,v\in D(A), & \langle (A-i)u,v\rangle & = & \langle u,(A+i)v\rangle \\
\Leftrightarrow & \forall u,v\in D(A), & \langle (A-i)u,(A+i)^{-1}(A+i)v\rangle & = & \langle (A-i)^{-1}(A-i)u,(A+i)v\rangle \\
\Leftrightarrow & \forall \tilde{u},\tilde{v}\in \mathcal{H}, & \langle \tilde{u},(A+i)^{-1}\tilde{v}\rangle & = & \langle (A-i)^{-1}\tilde{u},\tilde{v}\rangle
\end{array}
$$

For the last equivalence, we used the fact that $A\pm i:D(A)\to\mathcal{H}$ are bijective. It remains to see that $\mathcal{H}=D((A+i)^{-1})\subset D([(A+i)^{-1}]^\dagger)\subset\mathcal{H}$ to get $((A+i)^{-1})^\dagger=(A-i)^{-1}$.

Let us now apply the spectral theorem for bounded normal operators to $(A+i)^{-1}$ to obtain a measured space (B, μ) with finite measure μ, a unitary operator $U : \mathcal{H} \to L^2(B, d\mu)$ and $f \in L^\infty_{\text{loc}}(B, d\mu)$ such that $U(A+i)^{-1}U^\dagger = M_f$.

We are looking for $a \in L^\infty_{\text{loc}}(B, d\mu)$ such that $UAU^\dagger = M_a$. As $F = (A+i)^{-1}$ corresponds to f, A might correspond to $a = \frac{1}{f} - i$. We verify :

- $a \in L^\infty_{\text{loc}}(B, d\mu)$: if not, we would have $C \subset B$ of positive measure where $a = +\infty$ i.e. where $f = 0$. Taking $\mathbb{1}_C \in D(M_f)$, we would obtain an eigenvector of eigenvalue 0 in $\mathcal{H}$ for the invertible operator $(A+i)^{-1}$.
- $UAU^\dagger = U(F^{-1} - i)U^\dagger = UF^{-1}U^\dagger - i = M_f^{-1} - i = M_{f^{-1}-i} = M_a$.
- a is real-valued because A is self-adjoint and $M_a^\dagger = M_{\bar{a}}$.

■

Example 2.3 *The Laplacian on $\mathbb{R}^d$*

We recall that the operator Δ is self-adjoint on $H^2(\mathbb{R}^d)$. The Fourier transform $\mathcal{F} : H^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d, (1+|\xi|^2)^{1/2}dx)$ is a unitary operator which turn Δ into the multiplication by $-|\xi|^2$. Indeed, for $f \in H^2(\mathbb{R}^d)$ and almost every $\xi \in \mathbb{R}^d$:

$$(\mathcal{F}\Delta\mathcal{F}^{-1}\hat{f})(\xi) = \mathcal{F}(\Delta f)(\xi) = -|\xi|^2\hat{f}(\xi)$$

2.2.4 Tools arising from spectral theorem

The spectral theorem is a very strong result that enables to use some tools to analyse the spectrum of self-adjoint operators. We sum up here the properties we will use. It is also possible to prove several properties of the following parts without these tools, but I chose to begin with the spectral theorem because it clarifies the proofs once we are used to use it, and it also offers some visualisation as it becomes to think of a self-adjoint operator as a multiplication operator on L^2 functions.

Results on multiplication operators

We can study the multiplication operators on $L^2(B, d\mu)$ to get results on self-adjoint operators. The proof can be found in [1].

Proposition 2.3 *Spectrum of multiplication operators*

Let (B, μ) be a measured space with B a Borel set of $\mathbb{R}^d$ and μ a finite measure on B. Let $a \in L^\infty_{\text{loc}}(B, d\mu)$.
The spectrum of M_a is $\sigma(M_a) = \operatorname{Im}\operatorname{Ess} a := \{y \in \mathbb{C} \mid \forall\varepsilon > 0, \mu(\{|a(x) - y| \leq \varepsilon\}) > 0\}$.
Besides, $\lambda \in \sigma(M_a)$ is an eigenvalue if and only if $\mu(\{a(x) = \lambda\}) > 0$.

We now give an example of application of this tool.

Proposition 2.4 *Bounds of $\sigma(A)$*

Let $(A, D(A))$ be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$. We have the following formulas :

$$\inf \sigma(A) = \inf_{\substack{v \in D(A) \\ \|v\|=1}} \langle v, Av\rangle \qquad \sup \sigma(A) = \sup_{\substack{v \in D(A) \\ \|v\|=1}} \langle v, Av\rangle$$

Proof.

Using the spectral theorem, it suffises to show this result for $A = M_a$ a multiplication operator on $L^2(B, d\mu)$, where B is a Borel set of $\mathbb{R}^d$, μ is a finite measure and $a \in L^\infty_{\text{loc}}(B, d\mu)$ is real-valued. From the previous proposition, we have $\sigma(M_a) = \operatorname{Im}\operatorname{Ess} a$.

Let $m = \inf \operatorname{Im}\operatorname{Ess} a$. We first suppose that $m > -\infty$. Then $m \in \operatorname{Im}\operatorname{Ess} a$ because it is closed (lemma 2.3).

Let $\varepsilon > 0$. We write $B_\varepsilon = \{a \in [m-\varepsilon, m+\varepsilon]\}$ and have, by definition of the essential image, $\mu(B_\varepsilon) > 0$. Therefore, $f = \frac{\mathbb{1}_{B_\varepsilon}}{\mu(B_\varepsilon)} \in L^2(B, d\mu)$ with $\|f\|_{L^2} = 1$. Since a is bounded on B_ε, we also have $f \in D(M_a)$, and we obtain

$$m - \varepsilon \leq \langle f, M_a f\rangle \leq m + \varepsilon$$

giving us the result with $\varepsilon \to 0$.

If $m = -\infty$, we do a similar construction but using, for $C \in \mathbb{R}$, the set $B_C = \{a \in]-\infty, C]\}$ of positive measure. The same constructions shows the other formula. ■

Spectral projections, functional calculus

We have observed during the proof of the spectral theorem the strength of functional calculus, which allows us to compute as if the operator was a variable in its spectrum. Spectral projections are useful tools to decompose a self-adjoint operator on various parts of its spectrum. They are just functional calculus for $\mathbb{1}_B$ where $B \subset \mathbb{R}$ is a Borel set. In the next part, they will be used in several proofs, for example see the proofs of the propositions 2.7 and 2.9.

2.3 Studying the spectrum of self-adjoint operators

In this part, we study more precisely the spectrum of self-adjoint operators and introduce Weyl sequences, which are powerful tools.

For the whole part, let $\mathcal{H}$ be a separable Hilbert space and $(A, D(A))$ be a self-adjoint operator.

2.3.1 Essential spectrum, discrete spectrum

We introduce a partition of the spectrum that will be meaningful from a physical point of view, and also adapted for the perturbation theory. We start by noticing remarkable elements of the spectrum.

Proposition 2.5 *Isolated points of the spectrum*

Let $\lambda \in \sigma(A)$ be an isolated point. Then it is an eigenvalue of A.

Proof.

We apply the spectral theorem to suppose that $A = M_a$ is a multiplication operator on $L^2(B, d\mu)$ with the notations of the theorem 2.4.

With the proposition 2.3, $\lambda \in \operatorname{Im}\operatorname{Ess} a$ is isolated. This means that there exists $\eta > 0$ such that $[\lambda-\eta, \lambda+\eta] \cap \operatorname{Im}\operatorname{Ess} a = \{\lambda\}$. Then, for $0 < \varepsilon < \eta$, $\mu(\{a(x) = \lambda\}) = \mu(\{|a(x)-\lambda| \leq \varepsilon\}) > 0$, using the definition of the essential image. Thus, λ is an eigenvalue of M_a. ∎

Definition 2.9 *Essential spectrum, discrete spectrum*

We call *discrete spectrum* of A, and write $\sigma_{\text{disc}}(A)$, the set of isolated eigenvalues of A with finite multiplicity.

We call *essential spectrum* of A, and write $\sigma_{\text{ess}}(A)$, the complementary of $\sigma_{\text{disc}}(A)$ in $\sigma(A)$.

2.3.2 Weyl sequences

Here, we caracterise elements of the spectrum with sequences of vectors.

Proposition 2.6 *Caracterisation of $\sigma(A)$ with Weyl sequences*

Let $\lambda \in \mathbb{R}$.

Then $\lambda \in \sigma(A)$ if and only if there exists a sequence $(v_n)_{n\in\mathbb{N}} \in D(A)^{\mathbb{N}}$ such that :

(*i*) $\|v_n\| = 1$;

(*ii*) $\|(A-\lambda)v_n\| \to 0$.

In this case, $(v_n)_{n\in\mathbb{N}}$ is called a *Weyl sequence* associated to λ.

Proof.

We notice that the caracterisation with Weyl's sequence is equivalent to :

$$inf_{v\in D(A), \|v\|=1} \|(A-\lambda)v\| = 0$$

Suppose that the infimum is 0. Then, if $(A-\lambda)^{-1} : \mathcal{H} \to D(A)$ exists, it is unbounded : if not, there exists $C > 0$ such that $\forall w \in \mathcal{H}, \|(A-\lambda)^{-1}w\| \leq C\,\|w\|$. We take, for $v \in D(A)$ normalised, $w = (A-\lambda)v$ to obtain : $1 = \|v\| \leq C\,\|(A-\lambda)v\|$. This contradicts that the infimum is 0.

Conversely, suppose that there exists $\varepsilon > 0$ such that $\forall v \in D(A)$, $\|(A-\lambda)v\| \geq \varepsilon\,\|v\|$. It shows that $\{0\} = \operatorname{Ker}(A-\lambda) = \operatorname{Im}(A-\lambda)^{\perp}$. So the image of $(A-\lambda)$ is dense. We show that it is closed. Let $(v_n)_{n\in\mathbb{N}} \in D(A)^{\mathbb{N}}$ such that $(A-\lambda)v_n \to w \in \mathcal{H}$. Using the assumed inequality, we have :

$$\forall n, m \in \mathbb{N}, \|v_n - v_m\| \leq \frac{1}{\varepsilon}\,\|(A-\lambda)(v_n - v_m)\|$$

Hence, $(v_n)_{n\in\mathbb{N}}$ is a Cauchy sequence of the Hilbert space $\mathcal{H}$: it is convergent to some $v \in \mathcal{H}$. As A is self-adjoint, it is closed, so $v \in D(A)$ and $(A-\lambda)v = w$. ∎

We have then a further criterion for essential spectrum. The proof is a nice application of the spectral theorem, particularly of the use of spectral projections.

Proposition 2.7 *Caracterisation of $\sigma_{ess}(A)$ with singular Weyl sequences*

Let $\lambda \in \mathbb{R}$.
Then $\lambda \in \sigma_{\text{ess}}(A)$ if and only if there exists a sequence $(v_n)_{n\in\mathbb{N}} \in D(A)^{\mathbb{N}}$ such that :

(i) $\|v_n\| = 1$;

(ii) $\|(A-\lambda)v_n\| \to 0$;

(iii) $v_n \rightharpoonup 0$ in $\mathcal{H}$.

In this case, $(v_n)_{n\in\mathbb{N}}$ is called a *singular Weyl sequence* associated to λ.

Proof.

Thanks to the spectral theorem, we have a multiplication operator M_a on $L^2(\sigma(A)\times\mathbb{N}, d\mu)$ associated to A on $\mathcal{H}$, where μ is a finite measure and $a \in L^\infty_{\text{loc}}(\sigma(A)\times\mathbb{N}, d\mu)$.

• Suppose that $\lambda \in \sigma_{\text{ess}}(A)$. We can caracterise essential spectrum by the following criteria, using the spectral theorem :

$$\lambda \in \sigma_{\text{ess}}(A) \Leftrightarrow \forall\varepsilon > 0, \dim(L^2([\lambda-\varepsilon, \lambda+\varepsilon]\times\mathbb{N}, d\mu)) = \infty$$

We construct by induction the orthonormal sequence $(v_n)_{n\geq 1} \in L^2(\sigma(A)\times\mathbb{N}, d\mu)$ by taking, for $n \geq 1$, $v_n \in L^2([\lambda - 1/n, \lambda + 1/n]\times\mathbb{N}, d\mu)$ such that $\|v_n\|_{L^2} = 1$ and $v_n \in \{v_1, \cdots, v_{n-1}\}^\perp$.

As $(v_n)_{n\geq 1}$ is orthonormal, the Bessel inequality combined with the Riesz representation theorem give us that $v_n \rightharpoonup 0$ in $L^2(\sigma(A)\times\mathbb{N}, d\mu)$. Besides :

$$\|(M_a-\lambda)v_n\|^2_{L^2} = \int_{[\lambda-1/n,\lambda+1/n]\times\mathbb{N}} |s-\lambda|^2 |v_n(s,j)|^2 d\mu(s,j) \leq \frac{1}{n^2}\|v_n\|^2_{L^2} = \frac{1}{n^2} \to 0$$

• Conversely, suppose that $\lambda \in \sigma_{\text{disc}}(A)$. Let $(v_n)_{n\in\mathbb{N}}$ be a Weyl sequence associated to λ. Assume that this sequence converges weakly to $v \in \mathcal{H}$. Let us show that the convergence is strong using spectral projections. We write $v_n = \mathbb{1}_{\{\lambda\}}(A)v_n + \mathbb{1}_{\mathbb{R}\setminus\{\lambda\}}(A)v_n$ and we verify that each term converge strongly :

- $v_n \rightharpoonup v$ and $\mathbb{1}_{\{\lambda\}}(A)$ is compact because it is finite rank (it is the projection on the finite dimension subspace Ker $A - \lambda$). Thus $\mathbb{1}_{\{\lambda\}}v_n \to \mathbb{1}_{\{\lambda\}}v$ strongly in $\mathcal{H}$.
- We have $(A-\lambda) = \mathbb{1}_{\mathbb{R}\setminus\{\lambda\}}(A)(A-\lambda)$, and therefore

  $$\|(A-\lambda)v_n\| = \left\|\mathbb{1}_{\mathbb{R}\setminus\{\lambda\}}(A)(A-\lambda)v_n\right\| \geq d(\lambda, \sigma(A)\setminus\{\lambda\})\left\|\mathbb{1}_{\mathbb{R}\setminus\{\lambda\}}(A)v_n\right\| \quad (\star)$$

  where the distance is by hypothesis positive (λ is isolated) so that $\mathbb{1}_{\mathbb{R}\setminus\{\lambda\}}(A)v_n \to 0$ strongly in $\mathcal{H}$ because $(A-\lambda)v_n \to 0$ strongly in $\mathcal{H}$.

Hence, $(v_n)_{n\in\mathbb{N}}$ converges strongly in $\mathcal{H}$ so it cannot converges weakly to 0 in $\mathcal{H}$. ■

N.B.

* The main use of functional calculus in the proof is hidden in the line $(\star)$. I want to give details (maybe too much) to really show how it works, with the following computations. We write $U : \mathcal{H} \to L^2(\sigma(A) \times \mathbb{N}, d\mu)$ the unitary operator of the spectral theorem.

$$\begin{aligned}
&\left\| \mathbb{1}_{\mathbb{R}\setminus\{\lambda\}}(A)(A-\lambda)v \right\| \\
&\quad = \left\| M_{\mathbb{1}_{\mathbb{R}\setminus\{\lambda\}}(a)} M_{a-\lambda} U^\dagger v \right\|_{L^2} && \text{using the unitary operator to go in } L^2 \\
&\quad = \left\| \mathbb{1}_{\mathbb{R}\setminus\{\lambda\}}(a)(a-\lambda) U^\dagger v \right\|_{L^2} \\
&\quad \geq d(\lambda, \operatorname{Im}\operatorname{Ess}(a)\setminus\{\lambda\}) \left\| \mathbb{1}_{\mathbb{R}\setminus\{\lambda\}}(a) U^\dagger v \right\|_{L^2} \\
&\quad = d(\lambda, \sigma(A)\setminus\{\lambda\}) \left\| \mathbb{1}_{\mathbb{R}\setminus\{\lambda\}}(A) v \right\| && \text{using proposition 2.3 and coming back in } \mathcal{H}
\end{aligned}$$

* Similar computation can be realised to show that $(A-\lambda) = \mathbb{1}_{\mathbb{R}\setminus\{\lambda\}}(A)(A-\lambda)$. The idea is to enable us to compute with operator A as if it was just one of the real number of its spectrum.

We finish this section with two results using Weyl sequences and describing more precisely the form of the essential spectrum.

Proposition 2.8 *Closure of $\sigma_{ess}(A)$*

The essential spectrum of a self-adjoint operator is closed.

Proof.

Let $(\lambda_k)_{k\in\mathbb{N}}$ be a sequence of $\sigma_{\text{ess}}(A)$ converging to $\lambda \in \mathbb{R}$. We already know that $\sigma(A)$ is closed, so $\lambda \in \sigma(A)$.

For each $k \in \mathbb{N}$, we have a singular Weyl sequence $(v_n^{(k)})_{n\in\mathbb{N}}$ of $D(A)$, i.e. $\left\| v_n^{(k)} \right\| = 1$, $v_n^{(k)} \xrightarrow[n\to\infty]{} 0$, $(A-\lambda_k)v_n^{(k)} \xrightarrow[n\to\infty]{} 0$.

Let $(e_j)_{j\in\mathbb{N}}$ be a complet orthonormal basis of $\mathcal{H}$.

We define by induction $(w_k)_{k\in\mathbb{N}} = (v_{\varphi(k)}^{(k)})_{k\in\mathbb{N}}$ by diagonaly extracting one term of each singular Weyl sequence such that :

- $\|(A-\lambda_k)w_k\| \leq \frac{1}{k+1}$
- $\displaystyle\sum_{j=0}^{k} |\langle w_k, e_j\rangle|^2 \leq \frac{1}{(k+1)^2}$

The second point is a valid demand because for each k, $v_n^{(k)}$ converges weakly to 0, so $\forall j \in [\![0,k]\!], \left\langle v_n^{(k)}, e_j \right\rangle \xrightarrow[n\to\infty]{} 0$.

Then, we show that $(w_k)_{k\in\mathbb{N}}$ is a singular Weyl sequence associated to λ, which caracterise $\lambda \in \sigma_{\text{ess}}(A)$. First, we have :

$$\|(A-\lambda)w_k\| \leq \|(A-\lambda_k)w_k\| + |\lambda-\lambda_k| \, \|w_k\| \leq \frac{1}{k+1} + |\lambda-\lambda_k| \xrightarrow[k\to\infty]{} 0$$

For the weak convergence, let $u \in \mathcal{H}$. For $k \in \mathbb{N}$, we use our complete orthonormal basis to write

$$\langle w_k, u\rangle = \sum_{j=0}^{k} \langle w_k, e_j\rangle \langle e_j, u\rangle + \sum_{j\geq k+1} \langle w_k, e_j\rangle \langle e_j, u\rangle$$

and we then apply Cauchy Schwartz inequality in $l^2(\mathbb{N})$ and Bessel inequality to get

$$|\langle w_k, u\rangle \leq \|u\| \left(\sum_{j=0}^{k} |\langle w_k, e_j\rangle|^2\right)^{\frac{1}{2}} + \|w_n\| \left(\sum_{j\geq k+1} |\langle u, e_j\rangle|^2\right)^{\frac{1}{2}} \leq \frac{\|u\|}{k+1} + \left(\sum_{j\geq k+1} |\langle u, e_j\rangle|^2\right)^{\frac{1}{2}} \to 0$$

recognising the rest of a convergent series. ∎

Proposition 2.9 *Minimum of $\sigma_{ess}(A)$*

We suppose that there exists $C \in \mathbb{R}$ such that $\forall v \in D(A), \langle v, Av\rangle \geq C\|v\|^2$. Then, if $\sigma_{\text{ess}}(A) \neq \varnothing$, the minimum of $\sigma_{\text{ess}}(A)$ is given by :

$$\min \sigma_{\text{ess}}(A) = \min \{\liminf_{n\to\infty} \langle v_n, Av_n\rangle \mid (v_n)_{n\in\mathbb{N}} \in D(A)^{\mathbb{N}}, \|v_n\| = 1, v_n \rightharpoonup 0\}$$

Proof.

With proposition 2.4, our hypothesis gives that $-\infty < \inf \sigma(A) \leq \inf \sigma_{\text{ess}}(A)$. Since $\sigma_{\text{ess}}(A)$ is closed, we then have that the infimum of $sigmaess(A)$ is a minimum. We write $m = \min \sigma_{\text{ess}}(A)$.

First, let $(v_n)_{n\in\mathbb{N}} \in D(A)^{\mathbb{N}}$ be a singular Weyl sequence associated to m. Then we have $\langle v_n, (A-m)v_n\rangle \to 0$ i.e. $\langle v_n, Av_n\rangle \to m$. This shows that the minimum is greater than the right-hand term.

Conversely, let $(v_n)_{n\in\mathbb{N}}$ be a sequence of $D(A)$ such that $\|v_n\| = 1$ and $v_n \rightharpoonup 0$, and let $\varepsilon > 0$. We show that $\liminf \langle v_n, Av_n\rangle \geq m - \varepsilon$ by decomposing the operator in two parts with spectral projections : $A = \mathbb{1}_{-\infty, m-\varepsilon]}(A)A + \mathbb{1}_{]m-\varepsilon,+\infty[}(A)A$.

On the one hand, $\mathbb{1}_{]-\infty,m-\varepsilon]}(A)A$ is compact because it is finite-rank. Indeed, it is the spectral projection on the discrete spectrum below $m-\varepsilon$. As $\inf \sigma(A) > -\infty$, there can only be a finite number of isolated finite-rank eigenvalues below $m-\varepsilon$, therefore the corresponding subspace is finite dimension. Since $v_n \rightharpoonup 0$, we find that $\mathbb{1}_{]-\infty,m-\varepsilon]}(A)Av_n \to 0$ strongly in $\mathcal{H}$.

On the other hand, using functional calculus,

$$\left\langle v_n, A\mathbb{1}_{]m-\varepsilon,+\infty[}(A)v_n\right\rangle \geq (m-\varepsilon)\left\langle v_n, \mathbb{1}_{]m-\varepsilon,+\infty[}(A)v_n\right\rangle,$$

and

$$\left\langle v_n, \mathbb{1}_{]m-\varepsilon,+\infty[}(A)v_n\right\rangle = \underbrace{\|v_n\|^2}_{=1} - \underbrace{\left\langle v_n, \mathbb{1}_{]-\infty,m-\varepsilon]}(A)v_n\right\rangle}_{\to 0} \to 1.$$

Finally, we obtain $\liminf \langle v_n, Av_n\rangle \geq m - \varepsilon$, giving us that the minimum is lower than the right-hand term with $\varepsilon \to 0$. ∎

2.3.3 Courant-Fischer formula

We now explain how we can access the discrete spectrum located below the essential spectrum.

Theorem 2.5 *Courant-Fischer formula*

We suppose that there exists $C \in \mathbb{R}$ such that $\forall v \in D(A), \langle v, Av\rangle \geq C\|v\|^2$. We define

$$\forall k \geq 1,\ \mu_k = \inf_{\substack{W \subset D(A)\\ \dim W = k}} \max_{\substack{v \in W\\ \|v\|=1}} \langle v, Av\rangle\,, \text{ and } m = \begin{cases} \min \sigma_{\text{ess}}(A) & \text{if } \sigma_{\text{ess}}(A) \neq \varnothing, \\ +\infty & \text{else.} \end{cases}$$

and we write $\lambda_1 \leq \cdots \leq \lambda_k \leq \cdots$ the ordered eigenvalues of A situated below $\sigma_{\text{ess}}(A)$, taken with multiplicity.
Then :

- if there is a finite number N of eigenvalues below $\sigma_{\text{ess}}(A)$, we have $\mu_k = \lambda_k$ for $1 \leq k \leq N$ and $\mu_k = m$ for $k > N$;
- else, $\mu_k = \lambda_k$ for $k \geq 1$.

N.B.

* The first hypothesis gives us this existence of a smallest eigenvalue of A.

* As we will see in the proof, the infimum is actually a minimum, reached for subspaces of dimension k included in the sum of the eigenspaces associated to eigenvalues smaller than λ_k.

* We can translate the condition of the number of eigenvalue into the language of spectral projections, which is more concise for the proof. Saying that there are N eigenvalues below $\sigma_{\text{ess}}(A)$ means that the spectral projection $\mathbb{1}_{]-\infty,m[}(A)$ has an image of dimension N. Saying that there are infinite eigenvalues below $\sigma_{\text{ess}}(A)$ means that it has an image of infinite dimension.

Proof.

Let $k \geq 1$.

• Suppose that λ_k exists. It means that $\dim(\operatorname{Im} \mathbb{1}_{]-\infty,\lambda_k]}) \geq k$. Therefore, there exists an orthonormal family $(v_1, \cdots, v_k)$ of eigenvectors associated to eigenvalues $\lambda(v_1), \lambda(v_k) \leq \lambda_k$. Defining the $k-$dimensional subspace $W = \operatorname{Span}(v_1, \cdots, v_k) \subset D(A)$, and taking $v \in W$ such that $\|v\| = 1$, we have

$$\langle v, Av\rangle = \sum_{j=1}^{k} \lambda(v_j) |\langle v, v_j\rangle|^2 \leq \lambda_k \|v\|^2 = \lambda_k.$$

This shows $\mu_k \leq \lambda_k$.

Conversely, let W be a $k-$dimensional subspace of $D(A)$. We know that $\dim(\operatorname{Im} \mathbb{1}_{]-\infty,\lambda_k[}(A)) < k$, so $W \cap (\operatorname{Im} \mathbb{1}_{]-\infty,\lambda_k[}(A))^\perp \neq \{0\}$. But noticing that $(\operatorname{Im} \mathbb{1}_{]-\infty,\lambda_k[}(A))^\perp = \operatorname{Im} \mathbb{1}_{[\lambda_k,+\infty[}(A)$, we can take $v \in W \cap \operatorname{Im} \mathbb{1}_{[\lambda_k,+\infty[}(A)$ such that $\|v\| = 1$, and then write

$$\langle v, Av\rangle = \left\langle v, A\mathbb{1}_{[\lambda_k,+\infty[}(A)v\right\rangle \geq \lambda_k \left\langle v, \mathbb{1}_{[\lambda_k,+\infty[}(A)v\right\rangle = \lambda_k \langle v, v\rangle = \lambda_k.$$

This shows that $\max\limits_{\substack{v \in W\\ \|w\|=1}} \langle v, Av\rangle \geq \lambda_k$. Since this is true for every $k-$dimensional subspace of $D(A)$, we can take the infimum to obtain $\mu_k \geq \lambda_k$.

• Suppose that there is less than k eigenvalues below $\sigma_{\text{ess}}(A)$. For $\varepsilon > 0$, $\dim(\operatorname{Im} \mathbb{1}_{]-\infty,m+\varepsilon]}(A)) =$

∞, so we can take a $k-$dimensional subspace W inside, and obtain

$$\forall v \in W, \langle v, Av \rangle = \left\langle v, A\mathbb{1}_{]-\infty,m+\varepsilon]}(A)v \right\rangle \leq (m+\varepsilon)\|v\| = m+\varepsilon.$$

Taking $\varepsilon \to 0$, we get $\mu_k \leq m$.

Conversely, let $\lambda_{\max}$ be the highest eigenvalue below $\sigma_{\text{ess}}(A)$. Since it is an isolated point of $\sigma(A)$, for $\varepsilon > 0$ sufficiently small to have $[\lambda_{\max} - \varepsilon, \lambda_{\max} + \varepsilon] \cap \sigma(A) = \{\lambda_{\max}\}$, we can use the same trick as in the reciprocal above, providing that $\dim(\text{Im}(\mathbb{1}_{]-\infty,\lambda_{m-\varepsilon}]}) < k$. We get $\mu_k \geq m - \varepsilon$, and taking $\varepsilon \to 0$, we get $\mu_k \geq m$. ■

Let us now use the tools we have developed so far to study the spectrum of the Laplacian.

Example 2.4 *Spectrum of the Laplacian on $\mathbb{R}^d$*

We recall that the Laplacian $-\Delta$ is self-adjoint on $H^2(\mathbb{R}^d)$. We show that $\sigma(-\Delta) = \sigma_{\text{ess}}(-\Delta) = [0, +\infty[$.

First, by integration by parts, we see that for all f in $H^2(\mathbb{R}^d)$:

$$\langle f, -\Delta f \rangle_{L^2(\mathbb{R}^d)} = \|\nabla f\|_{L^2(\mathbb{R}^d)} \geq 0$$

Thus, the Courant-Fischer formula for μ_1 gives the inclusion $\sigma(-\Delta) \subset [0, +\infty[$.

Conversely, let $\lambda \geq 0$. We build a singular Weyl sequence for $-\Delta$ associated to λ to show that $[0, +\infty[\subset \sigma_{\text{ess}}(-\Delta)$. We first notice that, for $k \in \mathbb{R}^d$ such that $|k|^2 = \lambda$ the function $f(x) = e^{ik\cdot x}$ verify $-\Delta f = \lambda f$. However, $f \notin H^2(\mathbb{R}^d)$. So a good candidate for a Weyl sequence would be the sequence $f_n(x) = n^{-\frac{d}{2}}\chi(\frac{x}{n})e^{ik\cdot x}$, where $\chi \in \mathscr{C}_c^\infty(\mathbb{R}^d)$ is a cut-off function :

- $\operatorname{supp} \chi \subset [-1, 1]$,
- $\chi \equiv 1$ on $[-\frac{1}{4}, \frac{1}{4}]$,
- $0 \leq \chi \leq 1$,
- $\|\chi\|_{L^2} = 1$.

Let us show that it is a singular Weyl sequence. First, it is normalised. Then, using the Fourier transform to simplify computations with the Laplacian :

$$\begin{aligned}
\left\|(-\Delta - |k|^2)f_n\right\|^2_{L^2(\mathbb{R}^d)} &= \int (|\xi|^2 - |k|^2)^2 |\hat{f}_n(\xi)|^2 d\xi && \text{(Plancherel)} \\
&= \int (|\xi|^2 - |k|^2)^2 n^{-\frac{d}{2}} |\hat{\chi}(n(\xi - k))|^2 dk \\
&= \int \left(\left| \frac{p}{n} + k \right|^2 - |k|^2 \right)^2 |\hat{f}(p)|^2 dp && \text{with } p = n(\xi - k) \\
&= \frac{1}{n^2} \int \left(\frac{|p|^2}{n} + 2k \cdot p \right)^2 |\hat{f}(p)|^2 dp \\
&\xrightarrow[n\to\infty]{} 0
\end{aligned}$$

Finally, $f_n \rightharpoonup 0$ in $L^2(\mathbb{R}^d)$ because $\forall \varphi \in \mathscr{C}_c^\infty(\mathbb{R}^d), \langle \varphi, f_n \rangle \to 0$ when $n \to \infty$, and $\mathscr{C}_c^\infty(\mathbb{R}^d)$ is dense in $L^2(\mathbb{R}^d)$.

3 Many-body quantum mechanics

In this section, we want to consider situations of N identical particles evolving in $\mathbb{R}^d$, interacting with each other and with an exterior potential. For example, it includes the case of N electrons around a nucleus.

The form of the Hamiltonian we will study is the following :

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \sum_{j=1}^{N} V(x_j) + \sum_{1\leq k<l\leq N} W(x_k - x_l)$$

The first part is the kinetic energy of the N particles. The second part is the potential energy due to the exterior potential. The third part is the potential energy due to the interactions of each particle with all the others. This interpretation makes sense if we make the following assumptions on V and W. We will do further assumptions later :

- $W : \mathbb{R}^d \to \mathbb{R}$ is even and real-valued ;
- $V : \mathbb{R}^d \to \mathbb{R}$ is real-valued.

Depending on which particles we want to study, it will be needed to work with different statistics corresponding to bosons and fermions. This is taken into account when we choose the Hilbert space. We will consider the following cases :

- $L^2(\mathbb{R}^d)^{\otimes N} \simeq L^2((\mathbb{R}^d)^N)$ when we do not choose any statistics ;
- $L^2(\mathbb{R}^d)^{\otimes_s N} \simeq L^2_s((\mathbb{R}^d)^N)$ when we work with bosons. They are represented by N-variable $x_j \in \mathbb{R}^d$ wave functions that are symmetric.
- $L^2(\mathbb{R}^d)^{\otimes_a N} \simeq L^2_a((\mathbb{R}^d)^N)$ when we work with fermions. They are represented by N-variable $x_j \in \mathbb{R}^d$ wave functions that are antisymmetric.

They are all Hilbert spaces for the same inner product $\langle \cdot, \cdot \rangle_{L^2((\mathbb{R}^d)^N)}$, so several proofs can treat all cases at once, but sometimes we will need to see each case.

3.1 On which domain is H_N self-adjoint ?

The first step to study H_N is to identify on which domain it is self-adjoint. An efficient method is to use the fact that we know on which domain the Laplacian is self-adjoint, and to see the added potentials as a symmetric perturbation of the self-adjoint operator. Under assumptions on the potentials, the self-adjointness and the domain won't be lost for the new operator.

We present two theories that exist to follow this idea. The first one works directly on the operators and really preserve the same domain. The second one introduces quadratic forms associated to the symmetric operators, and preserve the domain of the quadratic forms. It enables weaker assumptions on the perturbation but the domain of the final operator may be harder to identify.

3.1.1 Rellich-Kato's theory

Theorem 3.1 *Rellich-Kato*

Let $(A, D(A))$ be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$, and let $(B, D(A))$ be a symmetric operator.
Assume that there exists $0 \leq \alpha < 1$ and $C > 0$ such that :

$$\forall v \in D(A), \|Bv\| \leq \alpha \|Av\| + C \|v\|$$

Then $A + B$ is self-adjoint on the domain $D(A)$.

Proof. *(sketch)*

To show self-adjointness, using proposition 2.2, we want to find $\mu > 0$ for which we can prove that the following operators are surjective :

$$A + B \pm i\mu = (1 + B(A \pm i\mu)^{-1})(A \pm i\mu).$$

The perturbation of identity is inversible for large μ thanks to the control assumption of B relatively to A. ∎

3.1.2 Friedrichs' theory

The principle of Friedrichs' theory is the following : instead of studying the symmetric operator to find a self-adjoint extension, one can introduce an associated quadratic form. From it, with further assumptions, we can obtain an inner product space, and then complete it. The Hilbert space we get corresponds to a self-adjoint operator.

Here, we only give the theorem that enables to prove the existence of a self-adjoint extension of a symmetric operator.

Definition 3.1 *Quadratic form of a symmetric operator*

Let $(A, D(A))$ be a symmetric operator on a separable Hilbert space $\mathcal{H}$.
We define the following quadratic form associated to A :

$$q_A : v \in D(A) \mapsto \langle v, Av \rangle$$

Definition 3.2 *Vocabulary of quadratic form*

Let q be a quadratic form on $Q \subset \mathcal{H}$.
We say that :

- q is *bounded from below* if there exists $\alpha \in \mathbb{R}$ such that $\forall v \in Q, q(v) \geq \alpha \|v\|$.
- q is *coercive* when it is bounded from below with $\alpha > 0$.
- q is *closed* if it is coercive and (Q, q) is a Hilbert space.

N.B.

- A coercive quadratic form defines an inner product on its domain.
- If q is bounded from below by $\alpha \in \mathbb{R}$, $q + a\,\|\cdot\|^2$ is coercive for $a > -\alpha$. It is the trick hidden behind the fact that we can find self-adjoint extension for lower bounded symmetric operators, whereas their quadratic forms are not always inner products.

Lemma 3.1 *Closed extension of a quadratic form*

Let $(A, D(A))$ be a symmetric operator that is coercive.
Then q_A has a closed extension.

Proof. *(Sketch)*

We build by hand the extension $Q(A)$ of $D(A)$ on which q_A is closed by studying the Cauchy sequences of $D(A)$ for q_A. The coersion enables to get a limit for such sequences, which we add to the domain. We obtain the following set and extension of q_A :

$$Q(A) = \{v \in \mathcal{H} \mid \exists (v_n)_{n\in\mathbb{N}} \in D(A)^{\mathbb{N}}, v_n \to v \text{ et } \lim_{m,n\to\infty} q_A(v_n - v_m) = 0\}$$

$$\overline{q_A}(v) = \lim_{n\to\infty} q_A(v_n)$$

where $(v_n)_{n\in\mathbb{N}}$ is a sequence as in the definition of $Q(A)$ for v.
We then verify that $\overline{q_A}$ is well-defined and that $(Q(A), \overline{q_A})$ is a Hilbert space. ■

Theorem 3.2 *Friedrichs' extension*

Let $(A, D(A))$ be a symmetric operator that is lower bounded, and (Q, q) be the closure of its quadratic form q_A.
Then there exists a unique self-adjoint extension B of A, with quadratic form q defined on Q, and with domain $D(A) \subset D(B) \subset Q$.

Proof. *(Sketch)*

We define the self-adjoint operator by its graph and verify that it has all the wished properties. If φ denotes the polar form of q, then the graph is given by :

$$G(B) = \{(v, z) \in \mathcal{H} \mid \forall h \in Q, \varphi(v, h) = \langle z, h\rangle_{\mathcal{H}}\}$$

If we consider the definition of the quadratic form associated to B, this graph means that $\forall h \in Q, \varphi(v, h) = \langle Bv, h\rangle_{\mathcal{H}} = \langle z, h\rangle_{\mathcal{H}}$ i.e. $Bv = z$. ■

3.1.3 Application to H_N

We now apply the two theories to get self-adjoint extensions of H_N, initially defined on $\mathscr{C}_c^\infty(\mathbb{R}^d)$. As explained in the motivation of these theories, the first method uses stronger assumptions on the potentials but also gives an explicit domain for the self-adjoint extension.

Theorem 3.3 *Kato, self-adjoint extensions of H_N*

Assume $V, W : \mathbb{R}^d \to \mathbb{R}$, W even, and :

- **Assumption 1 (stronger) :** $V, W \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ with $p > \max(\frac{d}{2}, 2)$.

Then H_N has a self-adjoint extension with domain $D(H_N) = H^2((\mathbb{R}^d)^N)$.

- **Assumption 2 (weaker) :** $V, W \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ with $p > \max(\frac{d}{2}, 1)$.

Then H_N has a self-adjoint extension with quadratic form domain $Q(H_N) = H^1((\mathbb{R}^d)^N)$.

N.B.

* These assumptions on the potentials are including some applications. For example, if we consider the Coulomb potential $V(x) = \frac{1}{|x|}$ in $\mathbb{R}^3$, it can be written :

$$V(x) = \frac{1}{|x|}\mathbb{1}_{\{|x|\leq 1\}} + \frac{1}{|x|}\mathbb{1}_{\{|x|\geq 1\}} \in L^p(\mathbb{R}^3) + L^\infty(\mathbb{R}^3) \quad \forall 2 < p < 3$$

Proof.

For both methods, the process will be the same :

1. Writing the potential $V = V_p + V_\infty$ with $\|V_p\|_{L^p} < \varepsilon$, and same for W.
2. Controlling the term in V_p with Hölder and Sobolev inequalities (this is where the assumptions on p will be used).
3. Choose ε sufficiently small to have a positive constant in front of the kinetic term.

For the first point, we explain why it is possible to choose $\|V_p\|_{L^p}$ as small as wished. Indeed, if $V = V_p + V_\infty \in L^p(\mathbb{R}^d) + L\infty(\mathbb{R}^d)$ is a given decomposition, we can write, for $R > 0$, $V_p = V_p\mathbb{1}_{\{|x|\leq R\}} + V_p\mathbb{1}_{\{|x|>R\}}$. The first term is in $L^\infty(\mathbb{R}^d)$ and can be added to V_∞, whereas the second term is going to 0 in $L^p(\mathbb{R}^d)$ as $R \to +\infty$.

- **Assumption 1 :** We apply Rellich-Kato's theory and show that V and W are relatively bounded by $\sum_{j=1}^N -\Delta_{x_j}$. By the triangular inequality, we bound each potential and then sum everything.

Let $\varepsilon > 0$ and $V = V_p + V_\infty$ with $V_p \in L^p(\mathbb{R}^d), V_\infty \in L^\infty(\mathbb{R}^d)$ and $\|V_p\|_{L^p(\mathbb{R}^d)} \leq \varepsilon$. Let also $\psi_N \in H^2((\mathbb{R}^d)^N)$ be a wave function in the domain of the self-adjoint kinetic operator. We bound $\|V_p(x_1)\psi_N\|_{L^2((\mathbb{R}^d)^N)}$ using Hölder and Sobolev inequalities :

$$\begin{aligned}
&\|V_p(x_1)\psi_N\|^2_{L^2((\mathbb{R}^d)^N)} \\
&= \int_{(\mathbb{R}^d)^{N-1}} \left(\int_{\mathbb{R}^d} \underbrace{|V_p(x_1)|^2}_{\in L^{p/2}(\mathbb{R}^d)} \underbrace{|\psi(x_1,\cdots,x_N)|^2}_{\in L^{q/2}(\mathbb{R}^d)} dx_1 \right) dx_2\cdots dx_N \quad \text{by Fubini} \\
&\leq \int_{(\mathbb{R}^d)^{N-1}} \|V_p\|^2_{L^p(\mathbb{R}^d)} \|\varphi\|^2_{L^q(\mathbb{R}^d)} dx_2\cdots dx_N \quad \text{by Hölder inequality for } \frac{2}{p}+\frac{2}{q}=1
\end{aligned}$$

We have here defined $\varphi(x_1) = \varphi_{x_2,\cdots,x_N}(x_1) = \psi(x_1,\cdots,x_N)$ to have lighter notations. On the one hand, $\|V_p\|^2_{L^p(\mathbb{R}^d)} \leq \varepsilon^2$. On the other, $\|\varphi\|_{L^q(\mathbb{R}^d)}$ is controled by $\|\varphi\|_{H^2(\mathbb{R}^d)}$ thanks to Sobolev inequalities for $H^2(\mathbb{R}^d)$. Let us detail here precisely how they work. The assumption on p gives $q > 2$ and $q < \begin{cases} \frac{2d}{d-4} & \text{if } d > 4 \\ \infty & \text{else} \end{cases}$.

We have different inequalities depending on $\frac{d}{2}$ compared with $s = 2$:

1. if $d \leq 3$, we have $H^2(\mathbb{R}^d) \hookrightarrow \mathscr{C}^0_0(\mathbb{R}^d)$, and $q < \infty$, so $\|\varphi\|_{L^q} \leq \|\varphi\|_{L^\infty} \leq C \|\varphi\|_{H^2}$.
2. if $d = 4$, we have $H^2(\mathbb{R}^d) \hookrightarrow L^r(\mathbb{R}^d)$ $\forall 2 \leq r < \infty$, and $2 \leq q < \infty$. Hence, $\|\varphi\|_{L^q} \leq C \|\varphi\|_{H^2}$.
3. if $d > 4$, we have $H^2(\mathbb{R}^d) \hookrightarrow L^r(\mathbb{R}^d)$ $\forall 2 \leq r \leq \frac{2d}{d-4}$ and q satisfies this. Hence, $\|\varphi\|_{L^q} \leq C \|\varphi\|_{H^2}$.

We can choose the norm $\|(1-\Delta)f\|_{L^2(\mathbb{R}^d)}$ for $H^2(\mathbb{R}^d)$. Writing this estimate in our first inequality leads to :

$$\|V_p(x_1)\psi_N\|^2_{L^2((\mathbb{R}^d)^N)} \leq C\varepsilon^2 \|(1-\Delta_{x_1})\psi_N\|^2_{L^2((\mathbb{R}^d)^N)}$$

On the other hand, the term $\|V_\infty(x_1)\psi_N\|_{L^2((\mathbb{R}^d)^N)}$ can be bounded by $\|V_\infty\|_{L^\infty(\mathbb{R}^d)} \|\psi_N\|_{L^2((\mathbb{R}^d)^N)}$.

By suming for every potential $V(x_j)$, we obtain :

$$\begin{aligned}
\left\| \sum_{j=1}^N V(x_j)\psi_N \right\|_{L^2((\mathbb{R}^d)^N)} &\leq C\varepsilon \sum_{j=1}^N \left\| (1-\Delta_{x_j})\psi_N \right\|_{L^2((\mathbb{R}^d)^N)} + N \|V_\infty\|_{L^\infty(\mathbb{R}^d)} \|\psi_N\|_{L^2((\mathbb{R}^d)^N)} \\
&\leq C\varepsilon \sum_{j=1}^N \left\| -\Delta_{x_j}\psi_N \right\|_{L^2((\mathbb{R}^d)^N)} + C_{N,\varepsilon} \|\psi_N\|_{L^2((\mathbb{R}^d)^N)} \\
&\leq CN\varepsilon \left\| \sum_{j=1}^N -\Delta_{x_j}\psi_N \right\|_{L^2((\mathbb{R}^d)^N)} + C_{N,\varepsilon} \|\psi_N\|_{L^2((\mathbb{R}^d)^N)}
\end{aligned}$$

We justify the last inequality for $N = 2$, and deduce the general case by induction. It is true thanks to the fact that $\Delta_{x_j} \geq 0$ and commute. Let us show that $\|-\Delta_{x_1}\psi_N\|_{L^2((\mathbb{R}^d)^N)} \leq \|(-\Delta_{x_1} - \Delta_{x_2})\psi_N\|_{L^2((\mathbb{R}^d)^N)}$. We write :

$$\begin{aligned}
\|(-\Delta_{x_1} - \Delta_{x_2})\psi_N\|^2 &= \|-\Delta_{x_1}\psi_N\|^2 + \|-\Delta_{x_2}\psi_N\|^2 + 2\Re(\langle -\Delta_{x_1}\psi_N, -\Delta_{x_2}\psi_N\rangle) \\
&\geq \|-\Delta_{x_1}\psi_N\|^2 + 2\Re(\langle -\Delta_{x_1}\psi_N, -\Delta_{x_2}\psi_N\rangle)
\end{aligned}$$

The last term is positive. First, it is real because $-\Delta_{x_1}\psi_N \in D(-\Delta_{x_2})$, so we can move $-\Delta_{x_2}$ on the other side and make the operators commute. We obtain $\langle -\Delta_{x_1}\psi_N, -\Delta_{x_2}\psi_N\rangle = \overline{\langle -\Delta_{x_1}\psi_N, -\Delta_{x_2}\psi_N\rangle}$. And then, using functional calculus :

$$\begin{aligned}
\langle -\Delta_{x_1}\psi_N, -\Delta_{x_2}\psi_N\rangle &= \left\langle \sqrt{-\Delta_{x_1}}\psi_N, -\Delta_{x_2}\psi_N \right\rangle \\
&= \left\langle \sqrt{-\Delta_{x_1}}\psi_N, \sqrt{-\Delta_{x_1}}(-\Delta_{x_2})\psi_N \right\rangle \\
&= \left\langle \sqrt{-\Delta_{x_1}}\psi_N, -\Delta_{x_2}(\sqrt{-\Delta_{x_1}}\psi_N) \right\rangle \geq 0
\end{aligned}$$

because the Laplacian is positive.

We do the same estimates for $W(x_k - x_l)$, adding that $\|W(\cdot - x_l)\|_{L^p(\mathbb{R}^d)} = \|W\|_{L^p(\mathbb{R}^d)}$. This leads to the complete bound :

$$\left\| \left(\sum_{j=1}^{N} V(x_j) + \sum_{1\leq k<l\leq N} W(x_k - x_l) \right) \psi_N \right\|_{L^2} \leq C\varepsilon(N+N^2) \left\| \sum_{j=1}^{N} -\Delta_{x_j}\psi_N \right\|_{L^2} + C_{N,\varepsilon} \|\psi_N\|_{L^2}$$

We can now choose ε sufficiently small such as the constant in front of the Laplacian norm is lower than 1. The Rellich-Kato theory applies and gives that H_N is self-adjoint on the domain of $\sum_{j=1}^{N} -\Delta_{x_j} = -\Delta_{(\mathbb{R}^d)^N}$, i.e. $H^2((\mathbb{R}^d)^N)$.

• **Assumption 2 :** We apply Friedrichs' theory and show that the quadratic form associated to H_N is bounded from below.

The estimates are very similar to the ones in assumption 1, except that this time the potential V_p is no longer squared, since we control $\langle \psi_N, V_p(x_j)\psi_N \rangle$ instead of $\|V_p(x_j)\psi_N\|_{L^2}$ so Hölder inequality is applied with $\frac{1}{p} + \frac{2}{q} = 1$ this time. We do not write the details, they can be found in [6].

■

3.2 Geometric localisation

3.2.1 The HVZ theorem

To illustrate how the geometric localisation works, we will prove an interesting result about the spectrum of H_N.

Theorem 3.4 *HVZ theorem*

For $N \geq 1$, denote the bottom of the spectrum of the N-body Hamiltonian by $E_N = \inf \sigma(H_N)$ and the bottom of its essential spectrum by $\Sigma_N = \inf \sigma_{\text{ess}}(H_N)$.

Assumptions on the potentials :

1. $V, W : \mathbb{R}^d \to \mathbb{R}$ and W is even (the model means something) ;
2. $V, W \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ with $\max(\frac{d}{2}, 2) < p < +\infty$ and $V(x), W(x) \to 0$ when $|x| \to \infty$ (regularity) ;
3. $W \geq 0$ (repulsive interaction).

Under these assumptions, for all $N \geq 1$, $\sigma_{\text{ess}}(H_N) = [E_{N-1}, +\infty[$.

Let us now detail the physical interpretation of the result. We talk about the case of N electrons around a fixed nucleus.

For a first interpretation, we assume that $E_N \in \sigma_{\text{disc}}(H_N)$ and $E_{N-1} \in \sigma_{\text{disc}}(H_{N-1})$, i.e. $E_N < \Sigma_N$ and $E_{N-1} < \Sigma_{N-1}$. The spectrum of H_N looks like on Figure 1, and we add the spectrum of H_{N-1} and of the free-particle Hamiltonian $-\Delta_{\mathbb{R}^d}$ below for understanding of the following discussion.

The states described by eigenfunctions of eigenvalues in $\sigma_{\text{disc}}(H_N)$ correspond to situations where the N electrons are bound to the nucleus. The states of energy in $\sigma_{\text{ess}}(H_N)$ correspond to situations where at least one electron escaped from the nucleus potential. Under our assumptions, consider for example a wave function $\psi_N = \psi_{N-1} \otimes u$ where ψ_{N-1} is an eigenfunction of H_{N-1} for the eigenvalue E_{N-1}, and u is describing a particle escaping to infinity (see the proof below for an example of such a function).

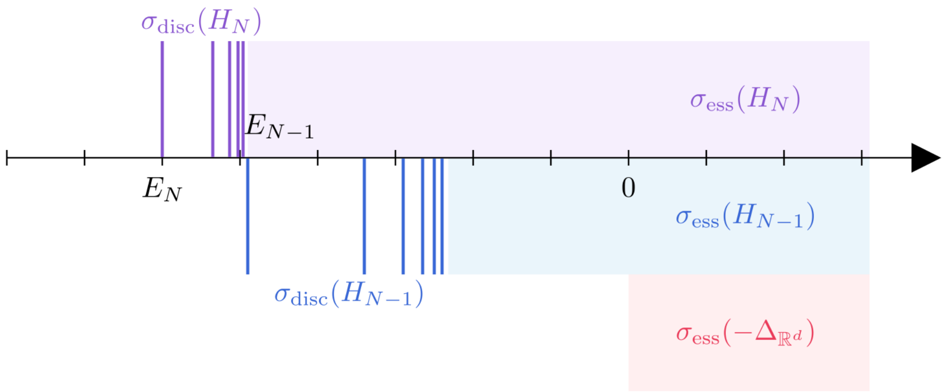

Figure 1: Spectra of H_N, H_{N-1} and of $-\Delta_{\mathbb{R}^d}$ for $N \geq 2$ when $E_N < \Sigma_N$ and $E_{N-1} < \Sigma_{N-1}$.

The gap between E_N and $\inf \sigma_{\text{ess}}(H_N)$ is called binding energy. It is the amount of energy we have to provide to the system of electrons in its ground state such that one of them escapes from the nucleus potential. It is possible for this gap to be 0, meaning that $E_{N-1} \notin \sigma_{\text{disc}}(H_N)$. In that case, the state where N electrons are bounded to the nucleus is unstable because electrons can escape without energy supply.

Geometric localisation is used in the proof for one of the two inclusions of the equality in the HVZ theorem. Let us begin by explaining the inclusion which does not use these technics. We will need the technical following lemma.

Lemma 3.2 *Weyl sequences of H_N are bounded in $H^2((\mathbb{R}^d)^N)$*

Let $N \geq 1$ and $(\psi_N^{(n)})_{n\in\mathbb{N}}$ be a Weyl sequence of H_N for E_N.
Then $(\psi_N^{(n)})_{n\in\mathbb{N}}$ is bounded in $H^2((\mathbb{R}^d)^N)$.

Proof.

The fact that $(\psi_N^{(n)})_{n\in\mathbb{N}}$ is a Weyl sequence provides that $(\psi_N^{(n)})_{n\in\mathbb{N}}$ and $(H_N\psi_N^{(n)})_{n\in\mathbb{N}}$ are both bounded sequences in $L^2((\mathbb{R}^d)^N)$.

The key fact that we use in this proof is that $(H_N\psi_N^{(n)})_{n\in\mathbb{N}}$ bounded in $L^2((\mathbb{R}^d)^N)$ can be rewritten $(\left\langle \psi_N^{(n)}, H_N^2\psi_N^{(n)} \right\rangle)_{n\in\mathbb{N}}$ is bounded. It is better to use because we manipulate a quadratic form.

We want to show that $(H_0\psi_N^{(n)})_{n\in\mathbb{N}}$ is bounded in $L^2((\mathbb{R}^d)^N)$ where $H_0 = -\Delta_{(\mathbb{R}^d)^N}$. With the same trick, let us show that $(\left\langle \psi_N^{(n)}, H_0^2\psi_N^{(n)} \right\rangle)_{n\in\mathbb{N}}$ is bounded.

We write $H_N = H_0 + \mathbb{V}(x)$ where $\mathbb{V}(x) = \sum_{i=1}^N V(x_j) + \sum_{1\leq i<j\leq N} W(x_i - x_j)$. Then :

$$H_N^2 = H_0^2 + H_0\mathbb{V}(x) + \mathbb{V}(x)H_0 + \mathbb{V}(x)^2$$

We want to bound the three quadratic forms on the right from below relatively to H_0^2, with a small constant in front of H_0^2.

For the term $\left\langle \psi_N^{(n)}, \mathbb{V}(x)\psi_N^{(n)} \right\rangle$, we use the regularity assumptions on the potentials together with Hölder and Sobolev inequalities to obtain, for all $\varepsilon > 0$:

$$\left\langle \psi_N^{(n)}, \mathbb{V}(x)\psi_N^{(n)} \right\rangle \geq -C_N\varepsilon^2 \left\langle \psi_N^{(n)}, H_0^2\psi_N^{(n)} \right\rangle - C_{N,\varepsilon}$$

where $C_N > 0$ does not depend on ε. We do not detail here the computations, as a detailed example of the use of these inequalities can be found in the proof of theorem 3.3 above. When we develop $\mathbb{V}(x)^2$, we obtain a sum of two-term products of potentials V or W. Depending on the case, we apply one time the inequalities for squared terms $V(x_i)^2$ or two times for any cross term. This is why a ε^2 comes.

For the term $\left\langle \psi_N^{(n)}, (H_0\mathbb{V}(x) + \mathbb{V}(x)H_0)\psi_N^{(n)} \right\rangle$, we use the so-called Cauchy-Schwarz inequality for operators, enabling to separe $\mathbb{V}$ from H_0.

Lemma 3.3 *Cauchy-Schwarz inequality for operators*

Let A, B be two operators on a Hilbert space $\mathcal{H}$. Then, for all $\eta > 0$:

$$\pm A^\dagger B + AB^\dagger \leq \eta AA^\dagger + \eta^{-1}B^\dagger B$$

Proof.

For $\eta = 1$, we write :

$$AA^\dagger + B^\dagger B \mp A^\dagger B + AB^\dagger = (A \mp B^\dagger)(A^\dagger \mp B) = |A \mp B^\dagger|^2 \geq 0$$

Then, we replace A by $\sqrt{\eta}A$ and B by $\sqrt{\eta}^{-1}B$ to get the $\eta-$version. ∎

This result gives here, since H_0 and $\mathbb{V}(x)$ are both self-adjoint :

$$\begin{aligned}\left\langle \psi_N^{(n)}, (H_0\mathbb{V}(x) + \mathbb{V}(x)H_0)\psi_N^{(n)} \right\rangle &\geq -\eta \left\langle \psi_N^n, H_0^2\psi_N^n \right\rangle - \frac{1}{\eta}\left\langle \psi_N^{(n)}, \mathbb{V}(x)^2\psi_N^{(n)} \right\rangle \\ &\geq \left(-\eta - \frac{C_N\varepsilon}{\eta}\right)\left\langle \psi_N^n, H_0^2\psi_N^n \right\rangle - C_{\eta,N,\varepsilon}\end{aligned}$$

using our previous estimate for $\mathbb{V}(x)^2$.

Summing our estimates, and choosing η and ε sufficiently small, we eventually obtain :

$$\left\langle \psi_N^{(n)}, H_N^2\psi_N^{(n)} \right\rangle \geq \frac{1}{2}\left\langle \psi_N^{(n)}, H_0^2\psi_N^{(n)} \right\rangle - C_N$$

i.e.

$$\left\| -\Delta\psi_N^{(n)} \right\|_{L^2}^2 = \left\| H_0\psi_N^{(n)} \right\|_{L^2}^2 \leq \left\| H_N\psi_N^{(n)} \right\|_{L^2}^2 + C_N \leq C.$$

∎

N.B.

* In the latter proof, we did not use the hypothesis that $W \geq 0$. We could use it to bound terms containing W by 0, but we prefere to emphasise that this hypothesis is not necessary to get the result. There exists a more general version of HVZ theorem without this hypothesis, so we avoid to use it as much as possible to keep a similar proof for the generalisation.

* It is possible to weaken the hypothesis of the HVZ theorem and to show that Weyl sequences are bounded in H^1 under the assumption $\max(d/2, 1) < p < +\infty$, by controlling $\left\| \nabla \psi_N^{(n)}) \right\| = \left\langle \psi_N^{(n)}, -\Delta \psi_N^{(n)} \right\rangle$. It is a sufficient result for several proofs below. In this report, we worked with the stronger assumptions $\max(d/2, 2) < p < +\infty$.

Then, we prove the first implication of the HVZ theorem, namely that $[E_{N-1}, +\infty[\subset \sigma_{\text{ess}}(H_{N-1})$. To do so, we build a singular Weyl sequence of H_N for $E_{N-1} + \lambda$, where $\lambda \geq 0$, by using a Weyl sequence $(\psi_{N-1}^{(n)})$ of H_{N-1} for the spectrum element E_{N-1} and a wave function representing a particle sent to infinity. We need to give sense to "infinity" by localising more precisely the Weyl sequence $(\psi_{N-1}^{(n)})$: this is the purpose of the construction of $(\tilde{\psi}_{N-1}^{(n)})$.

Proof. *First inclusion of the HVZ theorem : $[E_{N-1}, +\infty[\subset \sigma_{ess}(H_{N-1})$*

Let $\lambda \geq 0$. We build a singular Weyl sequence of H_N for $E_{N-1} + \lambda$.

Let $(\psi_{N-1}^{(n)})_{n\geq 1}$ be a Weyl sequence of H_{N-1} for the spectrum element E_{N-1}. We localise this sequence by creating another Weyl sequence $(\tilde{\psi}_{N-1}^{(n)})_{n\geq 1}$ as follows.

Let $\chi \in \mathscr{C}_c^\infty(\mathbb{R})$ be a cut-off function, meaning that $0 \leq \chi \leq 1$, $\operatorname{supp} \chi \subset [-1, 1]$, $\chi \equiv 1$ on $[-\frac{1}{4}, \frac{1}{4}]$ and $\|\chi\|_{L^2(\mathbb{R})} = 1$. We use this cut-off function to localise $\psi_{N-1}^{(n)}$ in the set $\{\sum_{j=1}^{N-1} |x_j| < R\}$ by multiplying it by

$$\chi_R : (x_1, \cdots, x_{N-1}) \in (\mathbb{R}^d)^{N-1} \mapsto \chi\left(\frac{\sum_{j=1}^{N-1} |x_j|^2}{R^2}\right).$$

For $n \geq 1$, as $\left\|\psi_{N-1}^{(n)} \chi_R\right\|_{L^2} \to \left\|\psi_{N-1}^{(n)}\right\|_{L^2} = 1$ when $R \to +\infty$, we let $R(n)$ be such that $R(n) \geq 2R(n-1)$ and $\left\|\psi_{N-1}^{(n)} \chi_{R(n)}\right\|_{L^2} > 1 - \frac{1}{n}$. In this way, we guaranty the following propositions : $R(n) \to \infty$ when $n \to \infty$, $\left\|\psi_{N-1}^{(n)} \chi_{R(n)}\right\|_{L^2} > 0$ for all $n \geq 1$. We now define :

$$\forall n \geq 1, \tilde{\psi}_{N-1}^{(n)} = \frac{\psi_{N-1}^{(n)} \chi_{R(n)}}{\left\|\psi_{N-1}^{(n)} \chi_{R(n)}\right\|_{L^2}}$$

Lemma 3.4

$(\tilde{\psi}_{N-1}^{(n)})_{n\geq 1}$ is still a Weyl sequence of H_{N-1} for the spectrum element E_{N-1}.

Proof.

For simplicity, we write $N-1$ as N in all the proof.

First, for $n \geq 1$, $\tilde{\psi}_N^{(n)} \in \mathscr{C}_c^\infty((\mathbb{R}^d)^N) \subset D(H_N)$, and $\left\|\tilde{\psi}_N^{(n)}\right\|_{L^2} = 1$.

Then, to control the norm of $H_N\tilde{\psi}_N^{(n)}$, we compute the Laplacian of the product of functions and regroup terms to obtain, by compactly denoting χ' the function $\chi'\left(\frac{\sum |x_j|^2}{R(n)^2}\right)$ when we want the value in x :

$$H_N\tilde{\psi}_N^{(n)} = \underbrace{\chi_{R(n)}H_N\psi_N^{(n)}}_{(1)} - \underbrace{\frac{2}{R(n)^2}\chi'\sum_{j=1}^N \nabla_{x_j}\psi_N^{(n)} \cdot x_j}_{(2)} - \underbrace{\frac{2N}{R(n)^2}\chi''\psi_N^{(n)}}_{(3)} - \underbrace{\frac{4}{R(n)^4}\chi'\psi_N^{(n)}\sum_{j=1}^N |x_j|^2}_{(4)}$$

To control each term, we use the following facts : χ, χ', χ'' are bounded, $(\psi_N^{(n)})$ is a bounded sequence in $H^2((\mathbb{R}^d)^N)$ thanks to the latter lemma 3.2, $R(n) \to \infty$ with n. ■

Then, we build a function corresponding to a particle escaping to infinity. When we studied the spectrum of the Laplacian of Rd, we built a singular Weyl sequence, which we denote here $(u_0^{(n)})_{n\in\mathbb{N}}$, of $-\Delta_{\mathbb{R}^d}$ for λ. We will now send this function far from the $N-1$ particles described by $\tilde{\psi}_{N-1}^{(n)}$ by translating it. Namely, we define

$$u^{(n)}(x) = u_0^{(n)}(x + (R(n)+n)e_1) \text{ for } x \in \mathbb{R}^d$$

where e_1 is the first vector of the canonical basis of $\mathbb{R}^d$. The sequence $(u^{(n)})_{n\in\mathbb{N}}$ we get is still a singular Weyl sequence because the weak convergence to 0 is preserved and $\left\|\Delta u^{(n)}\right\|_{L^2} = \left\|\Delta u_0^{(n)}\right\|_{L^2}$.

Finally, our N-body sequence is $(\psi_N^{(n)})_{n\in\mathbb{N}} = (\tilde{\psi}_{N-1}^{(n)} \otimes u^{(n)})_{n\in\mathbb{N}}$. We now show that it is a singular Weyl sequence. First, $\left\|\psi_N^{(n)}\right\|_{L^2} = \left\|\tilde{\psi}_{N-1}^{(n)}\right\|_{L^2}\left\|u^{(n)}\right\|_{L^2} = 1$. Then, $\psi_N^{(n)} \rightharpoonup 0$ because for all $f_1, \cdots, f_N \in L^2(\mathbb{R}^d)$, we have :

$$\begin{aligned}
\left|\left\langle f_1 \otimes \cdots \otimes f_N, \psi_N^{(n)}\right\rangle\right| &= \left|\left\langle f_1 \otimes \cdots \otimes f_{N-1}, \tilde{\psi}_{N-1}^{(n)}\right\rangle\right| \cdot \left|\left\langle f_N, u^{(n)}\right\rangle\right| \\
&\leq \|f_1 \otimes \cdots \otimes f_{N-1}\|_{L^2}\left\|\tilde{\psi}_{N-1}^{(n)}\right\|_{L_2}\left|\left\langle f_N, u^{(n)}\right\rangle\right| \\
&\xrightarrow[n\to\infty]{} 0
\end{aligned}$$

Finally, we write $H_N = H_{N-1} + -\Delta_{x_N} + V(x_N) + \sum_{k=1}^{N-1} W(x_k - x_N)$ to get three terms to control in L^2 norm :

$$(H_N - E_{N-1} - \lambda)\psi_N^{(n)} = (H_{N-1} - E_{N-1})\psi_N^{(n)} + (-\Delta_{x_N} - \lambda)\psi_N^{(n)} + \left(V(x_N) + \sum_{k=1}^{N-1} W(x_k - x_N)\right)\psi_N^{(n)}$$

The first two terms are controlled by separating the norm between the $N-1$ first particles and the last one, and using the Weyl sequences. The last two terms are controlled by Hölder and Sobolev inequalities combined with the assumed regularities of V, W and the fact that $(\psi_N^{(n)})_{n\in\mathbb{N}}$ is bounded in $H^2((\mathbb{R}^d)^N)$ thanks to the lemma 3.2 applied to $(\tilde{\psi}_{N-1}^{(n)})$. $(u^{(n)})$ is also clearly bounded in H^2. We already detailed the computations once, so we don't write everything this time. We just emphasise how we use the positions of the particles. It is used to write :

$$V(x_N)u^{(n)} = V(x_N)\mathbb{1}_{\{|x_N|\geq R(n)+n\}}u^{(n)}$$

$$W(x_k - x_N)\psi_N^{(n)} = W(x_k - x_N)\mathbb{1}_{\{|x_k - x_N|\geq n\}}\psi_N^{(n)}$$

Then, if $V \in L^p$ with $2 < p < +\infty$, $\left\|V(x_N)\mathbb{1}_{\{|x_N|\geq R(n)+n\}}\right\|_{L^p} \to 0$. And if $V \in L^\infty$ and $V(x) \to 0$ when $|x| \to \infty$, we also have $\left\|V(x_N)\mathbb{1}_{\{|x_N|\geq R(n)+n\}}\right\|_{L^\infty} \to 0$. ■

The other implication of the HVZ theorem is more difficult to prove. To motivate the following tools, we first try to explain informally the idea behind it. We take a Weyl sequence $(\Psi_N^{(n)})$ of H_N for the bottom of the essential spectrum Σ_N and examinate it in order to show that $\Sigma_N \geq E_{N-1}$. The key feature behind this fact is that at least one particle necessarely escaped to infinity. To observe this phenomenon on our sequence, we want to use a tool called geometric localisation. Instead of looking our wave functions globally on $\mathbb{R}^d$, we are interested on their description of the system only in a local domain, for example $B(0,R)$. This will give a sense to the fact that one particle escaped from the potential : whatever R we choose, at the limit the state inside the ball will contain at most $N-1$ particles only.

Geometric localisation raises modelling difficulties : so far, to describe our system of N particles, we worked with wave functions on $(\mathbb{R}^d)^N$. But here, if we only look the system inside a part of $\mathbb{R}^d$, the number of particles is no more fixed, so we will have several wave functions, one for each possibility. This is what motivates the introduction of the Fock space. It gives a formalism in which the number of particles can change.

First, we will introduce the Fock space formalism and some useful tools to work with it. With Fock space, it is possible to talk of a state *on* $\mathbb{R}^d$ whose number of particles is not fixed. Then, we will see how to localise a state on the Fock space, and define a convergence on states of the Fock space that enables to investigate the limit of our Weyl sequence together with localisation. Finally, we apply these results to prove the HVZ theorem. The goal is to get the physical sense of these tools to understand why they have been introduced and why they are working.

3.2.2 The Fock space formalism

Let $\mathcal{H}$ be a separable Hilbert space. In our case, we will always choose $\mathcal{H} = L^2(\mathbb{R}^d)$. As in our introduction for many-body quantum mechanics, there are in fact several Fock spaces, depending on the statistics of our particles.

Definition 3.3 *Fock space*

We define the *Fock space without statistics* $\mathcal{F}(\mathcal{H}) = \bigoplus_{N\geq 0} \mathcal{H}^{\otimes N} = \mathbb{C} \oplus \mathcal{H} \oplus (\mathcal{H} \otimes \mathcal{H}) \oplus \cdots$.

We also define the *bosonic* and *fermionic Fock spaces*

$$\mathcal{F}_s(\mathcal{H}) = \bigoplus_{N\geq 0} \mathcal{H}^{\otimes_s N} \qquad \mathcal{F}_a(\mathcal{H}) = \bigoplus_{N\geq 0} \mathcal{H}^{\otimes_a N}$$

where $\otimes_s$ and $\otimes_a$ are the symmetric and antisymmetric tensor products :

$$u_1 \otimes_s \cdots \otimes_s u_N = \frac{1}{\sqrt{N!}} \sum_{\sigma \in \mathfrak{S}_n} u_{\sigma_1} \otimes \cdots \otimes u_{\sigma_N}$$

$$u_1 \otimes_a \cdots \otimes_a u_N = \frac{1}{\sqrt{N!}} \sum_{\sigma \in \mathfrak{S}_n} \varepsilon(\sigma) u_{\sigma_1} \otimes \cdots \otimes u_{\sigma_N}$$

N.B.

* We defined the bosonic and fermionic Fock spaces using symmetric and antisymmetric tensor products, but for $\mathcal{H} = L^2(\mathbb{R}^d)$, this just means that we take the direct sum of symmetric or antisymmetric subspaces of wave functions.
* We will write $\mathcal{H}^N_{a/s} = \mathcal{H}^{\otimes_{a/s} N}$, and $\mathcal{H}^N = \mathcal{H}^{\otimes N}$.
* Below, the statistics will not play an important role, so we will often write statements for $\mathcal{F}(\mathcal{H})$ and use the notation $\otimes$, but they are also valid for Fock spaces with statistics.

We can extend the structure of Hilbert space of $\mathcal{H}$ to the Fock space.

Theorem 3.5 *Fock space is a Hilbert space*

The Fock space $\mathcal{F}(\mathcal{H})$ is a Hilbert space for the inner product

$$\left\langle \bigoplus_{N\geq 0} \varphi_N, \bigoplus_{N\geq 0} \psi_N \right\rangle_{\mathcal{F}} = \sum_{N\geq 0} \langle \varphi_N, \psi_N \rangle_{\mathcal{H}^N}$$

In our case, we will localise a state which contains initially N particles. So, we will work in the truncated Fock space $\mathcal{F}^{\leq N}(\mathcal{H}) = \bigoplus_{n=0}^{N} \mathcal{H}^n$.

The trace of an operator on a Hilbert space will be an important notion for what happens next.

Trace in infinite dimension

In finite dimension, we define the trace of a matrix as the sum of its diagonal coefficients. We want to generalise this notion on separable Hilbert spaces, using a complete orthonormal basis, but the sum may not converge, and only a certain class of bounded operators will have a trace.

The method to define a trace for bounded operators is similar to the one we use to define the Lebesgue integral on measurable functions. We will not detail this point in this report, we only give the steps :

- We define the trace of a positive bounded operator A on $\mathcal{H}$ (positive means $\forall u \in \mathcal{H}, \langle u, Au \rangle \geq 0$) in $\overline{\mathbb{R}}_+$ by the following formula, which does not depend of the chosen orthonormal basis $(e_i)_{i \in \mathbb{N}}$:

$$\operatorname{Tr} A = \sum_{i \in \mathbb{N}} \langle e_i, Ae_i \rangle$$

- We say that an operator is trace-class if $\operatorname{Tr} |A| < \infty$, where $|A| = \sqrt{A^\dagger A}$ is defined thanks to functional calculus for the self-adjoint operator $A^\dagger A$.

- If an operator A is trace-class, we let $\operatorname{Tr} A = \sum_{i \in \mathbb{N}} \langle e_i, Ae_i \rangle$ be its trace.

We will admit what is needed to obtain the following definition of the trace.

Definition 3.4 *Trace of an operator*

Let $\mathcal{H}$ be a separable Hilbert space and A be a positive bounded operator on $\mathcal{H}$.
The trace of A is the quantity $\operatorname{Tr}(A) = \sum_{i \in \mathbb{N}} \langle e_i, Ae_i \rangle \in \overline{\mathbb{R}}_+$, where $(e_i)_{i \in \mathbb{N}}$ is any orthonormal basis.

Let A be a bounded operator on $\mathcal{H}$.
We say that A is trace-class if $\operatorname{Tr} |A| < \infty$. In this case, we define its trace $\operatorname{Tr}(A) = \sum_{i \in \mathbb{N}} \langle e_i, Ae_i \rangle$ where $(e_i)_{i \in \mathbb{N}}$ is any orthonormal basis of $\mathcal{H}$.

We denote $\mathfrak{S}_1(\mathcal{H})$ the subspace of trace-class operators on $\mathcal{H}$. We admit the following result.

Theorem 3.6 *Properties of $\mathfrak{S}_1(\mathcal{H})$*

- $\mathfrak{S}_1(\mathcal{H})$ is a Banach space for the trace norm $\|A\|_{\operatorname{Tr}} = \operatorname{Tr} |A|$.

- $\mathfrak{S}_1(\mathcal{H})$ is a subspace of the compact operators $\mathcal{K}(\mathcal{H})$.

States on Fock space

So far, we described our states with normalised vectors ψ, but for Fock space it will be more adapted to use another definition, allowing us to work with operators.

Definition 3.5 *State on Fock space*

- A (mixed) state Γ on $\mathcal{F}(\mathcal{H})$ is a self-adjoint trace-class operator such that $\Gamma \geq 0$ and $\operatorname{Tr} \Gamma = 1$.

- A pure state on $\mathcal{F}(\mathcal{H})$ is a rank-one orthogonal projection $|\Psi\rangle \langle\Psi|$ where $\Psi \in \mathcal{F}(\mathcal{H})$ is normalised.

The set of states on Fock space is denoted $S(\mathcal{F}(\mathcal{H}))$. If we work with the truncated Fock space, it is denoted $S(\mathcal{F}^{\leq N}(\mathcal{H}))$.

N.B.

* The Dirac notation with bra and ket is just a convenient notation, where we identify ψ to $|\psi\rangle$ and the linear form $\langle\psi, \cdot\rangle$ with $\langle\psi|$. The projection $|\psi\rangle\langle\psi|$ is computed as follow :

$$\forall\varphi \in \mathcal{H}, |\psi\rangle\langle\psi|\,\varphi = |\psi\rangle\langle\psi|\,|\varphi\rangle = \langle\psi, \varphi\rangle\,\psi$$

* By the spectral theorem, a mixed state can be written as a convex combination of pure states :

$$\Gamma = \sum_j n_j |\psi_j\rangle\langle\psi_j|$$

where (ψ_j) is an orthonormal family of $\mathcal{F}(\mathcal{H})$, $n_j \geq 0$ and $\sum_j n_j = 1$.

In our case, since we work with the truncated Fock space $\mathcal{F}^{\leq N}(\mathcal{H})$, a state Γ can be thought as a matrix of operator $[G_{m,n}]_{0\leq m,n\leq N}$ where $G_{m,n} : \mathcal{H}^n \to \mathcal{H}^m$. The trace of Γ in the Fock space can be written

$$\mathrm{Tr}_{\mathcal{F}}(\Gamma) = \sum_{n=0}^{N} \mathrm{Tr}_{\mathcal{H}^n}(G_{n,n}) \tag{1}$$

However, the most adapted way to describe a state is not to write it as a matrix, but rather to use density matrices.

Definition 3.6 *Density matrices of a state*

Let Γ be a state on $\mathcal{F}(\mathcal{H})$.
For $0 \leq p, q \leq N$, the $(p, q)-$density matrix of Γ is the operator $\Gamma^{(p,q)} : \mathcal{H}^q \to \mathcal{H}^p$ such that for all $(\psi_p, \psi_q) \in \mathcal{H}^p \times \mathcal{H}^q$:

$$\mathrm{Tr}_{\mathcal{F}}(|\psi_q\rangle\langle\psi_p|\,\Gamma) = \mathrm{Tr}_{\mathcal{H}^p}(|\psi_q\rangle\langle\psi_p|\,\Gamma^{(p,q)})$$
$$\Leftrightarrow \langle\psi_p, \Gamma\psi_q\rangle_{\mathcal{F}} = \left\langle\psi_p, \Gamma^{(p,q)}\psi_q\right\rangle_{\mathcal{H}^p}$$

Informally, the $(p, q)-$density matrix is the simplification of the state when we look at it only for a small operator. It is similar to the notion of marginal in probabilities. See example 3.1 to see a concrete example of a state and of a corresponding density matrix.

Operators on Fock space

How to define the Hamiltonian on Fock space ? When we worked in $\mathcal{H}^N_{a/s}$, the Hamiltonian was given by :

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \sum_{j=1}^{N} V(x_j) + \sum_{1\leq k<l\leq N} W(x_k - x_l)$$

On the Fock space, N can take any value, so the corresponding operator will be $\bigoplus_{N\geq 0} H_N$.

There is a more systematic process to come to this result, called *second quantization*.

Definition 3.7 *Second quantization of an operator*

Let A be a self-adjoint one-body operator on $\mathcal{H}$.
The second quantization of A is the operator $d\Gamma(A)$ on $\mathcal{F}(\mathcal{H})$ defined by

$$d\Gamma(A) = \bigoplus_{N\geq 1} \sum_{i=1}^{N} A_i$$

where A_i is the operator applying A to the $i-$th particle and the identity to the others : $A_1 = A \otimes 1 \otimes \cdots \otimes 1$ and so on.

Let B be a self-adjoint two-body operator on $\mathcal{H}$.
The second quantization of B is the operator $d\Gamma(B)$ on $\mathcal{F}(\mathcal{H})$ defined by

$$d\Gamma(B) = \bigoplus_{N\geq 2} \sum_{1\leq i<j\leq N} B_{i,j}$$

where $B_{i,j}$ is the operator applying B to the two particles i, j and the identity to other.

N.B.

We do not precise the domains of these new operators but this is a question to consider when we talk about self-adjoint operators. In this report, we will admit that it works well.

With these definitions, the Hamiltonian is the sum of two second quantizations :

$$d\Gamma(H) = d\Gamma(-\Delta + V(x)) + d\Gamma(W(x-y)) \tag{2}$$

This formula means that we are looking to the energy of each single particle, which is given by the operator $-\Delta + V(x)$, plus the interaction energy between each pair of two particles, given by the operator $W(x-y)$. This formula for the Hamiltonian is important because it shows that the energy of the whole system, even if it is composed of many particles, just comes from operators acting only on one or two particles. This is where density matrices for states will be used. If Γ is a state on $\mathcal{F}(\mathcal{H})$, we will show that we have :

$$\mathrm{Tr}_{\mathcal{F}}(d\Gamma(H)\Gamma) = \mathrm{Tr}_{\mathcal{H}}((-\Delta + V(x))\Gamma^{(1,1)}) + \mathrm{Tr}_{\mathcal{H}^2}(W(x-y)\Gamma^{(2,2)}) \tag{3}$$

Before going further, let us give a concrete example in low dimension to understand these notions better.

Example 3.1 *Understanding the notions of Fock space*

Let $\psi_1, \psi_2 \in \mathcal{H} = L^2(\mathbb{R}^d)$ be two normalised wave functions.

We consider the state $\Gamma = 0 \oplus 0 \oplus |\psi_1 \otimes_s \psi_2\rangle \langle \psi_1 \otimes_s \psi_2|$ on $\mathcal{F}_s^{\leq 2}(\mathcal{H})$. Γ describes two bosons, where one of them is described by ψ_1 and the other by ψ_2. Due to the fact that the particles are undistinguishable, we cannot say that the first is described by ψ_1 and the second is described by ψ_2. This is why we symmetrise the wave function : $\psi_1 \otimes_s \psi_2 = \frac{1}{\sqrt{2}}(\psi_1 \otimes \psi_2 + \psi_2 \otimes \psi_1)$.

Now, suppose that we want to talk about the kinetic energy of the system. It is the sum of the kinetic energy of each particle. Since we work on the truncated Fock space $\mathcal{F}_s^{\leq 2}(\mathcal{H})$, the system can contain $0, 1$ or 2 particles :

$$d\Gamma(-\Delta) = 0 \oplus (-\Delta) \oplus (-\Delta_1 \otimes 1 + 1 \otimes (-\Delta_2))$$

When we read the expression of this operator, we see that we only consider one particle alone in each term. In some sense, the state Γ contains too much information for what we want to know with this operator, because it describes the two particles whereas we want to know the behaviour of the first alone or of the second alone. This simplified piece of information is the one contained in the $(1,1)-$density matrix $\Gamma^{(1,1)} : \mathcal{H} \to \mathcal{H}$. This is the sense of the formula

$$\mathrm{Tr}_{\mathcal{F}}(d\Gamma(-\Delta)\Gamma) = \mathrm{Tr}_{\mathcal{H}}(-\Delta\Gamma^{(1,1)}).$$

But why are we interested in this trace ? What is its physical meaning ? If we use the formula (1), we get :

$$\begin{aligned}\mathrm{Tr}_{\mathcal{F}}(d\Gamma(-\Delta)\Gamma) &= \mathrm{Tr}_{\mathcal{H}^2}((-\Delta_1 - \Delta_2) \left|\psi_1 \otimes_s \psi_2\right\rangle \left\langle\psi_1 \otimes_s \psi_2\right|) \\ &= \langle \psi_1 \otimes_s \psi_2, (-\Delta_1 - \Delta_2)\psi_1 \otimes_s \psi_2\rangle_{\mathcal{H}^2}\end{aligned}$$

So, the trace correspond to the mean value of the kinetic energy in the state Γ.
We can show the expression of the $(1,1)-$density matrix $\Gamma^{(1,1)} = \left|\psi_1\right\rangle\left\langle\psi_1\right| + \left|\psi_2\right\rangle\left\langle\psi_2\right|$.

Practical computations in Fock space

So far, we have written formulas such as (3), but we have not explained how to establish them by computation. In Hilbert spaces, we often use a complete orthonormal basis to compute. Here, to work on states and operators, we have elementary operators to decompose our formulas. For simplicity, we write the definition for $\mathcal{H} = L^2(\mathbb{R}^d)$, but it can be generalised for any Hilbert space.

Definition 3.8 *Creation and annihilation operators*

Let $\mathcal{H} = L^2(\mathbb{R}^d)$.
For $f \in \mathcal{H}$, the *creation operator* associated to f is the operator $a^\dagger(f)$ on $\mathcal{F}(\mathcal{H})$ defined by :

$$\forall N \geq 0, \forall \psi_N \in \mathcal{H}^N_{a/s}, a^\dagger(f)\psi_N = f \otimes_{a/s} \psi_N \in \mathcal{H}^{N+1}_{a/s}$$

For $f \in \mathcal{H}$, the *annihilation operator* associated to f is the operator $a(f)$ on $\mathcal{F}(\mathcal{H})$ defined by $a(f)|_{\mathbb{C}} = 0$ and :

$$\forall N \geq 1, \forall \psi_N \in \mathcal{H}^N_{a/s}, a(f)\psi_N = \sqrt{N}\int \overline{f(y)}\psi(y,\cdot)dy \in \mathcal{H}^{N-1}_{a/s}$$

N.B.

* In this definition, we precised $\mathcal{H}^N_{a/s}$ instead of our general notation $\mathcal{H}^N$ because if we work without statistics, the definition of these operators is different to have the same combinatorial coefficients.

* In the definition of the creation operator, one may notice that we use the (anti)symmetric tensor product with a function in $\mathcal{H}^N$ on one side. This is a generalisation of the tensor product we defined above. If $N_1, N_2 \geq 1$, and $\psi_{N_1} \in \mathcal{H}_s^{N_1}, \psi_{N_2} \in \mathcal{H}_s^{N_2}$, it is defined as follows (the antisymmetric definition is the same, adding the signature of the permutation) :

$$\psi_{N_1} \otimes_s \psi_{N_2}(x_1, \cdots, x_{N_1+N_2}) = \frac{1}{\sqrt{N_1! N_2! (N_1+N_2)!}} \sum_{\sigma \in \mathfrak{S}_{N_1+N_2}} \psi_{N_1}(x_{\sigma_{1:\sigma_{N_1}}}) \psi_{N_2}(x_{\sigma_{N_1+1:\sigma_{N_1+N_2}}})$$

* These definitions give operators on all truncated Fock spaces, but not necessarely on the whole Fock space.

These operators verify algebric relations which depend on the statistics we chose. These relations are called Canonical Commutation Relations (CCR) in the bosonic case and Canonical Anticommutation Relations (CAR) in the fermionic one. We will not use them here. As the notation underlines, $a^\dagger(f)$ is the adjoint of $a(f)$.

Intuitively, creation and annihilation operators can be thought as follows : $a^\dagger(f)$ adds to the system a particle described by the wave function f, and $a(f)$ removes a particle described by f. This gives sense to the following formula, which follows from the definition :

$$\left|\psi_1 \otimes_{a/s} \cdots \otimes_{a/s} \psi_N\right\rangle = a^\dagger(\psi_1) \cdots a^\dagger(\psi_N) |\Omega\rangle \tag{4}$$

where $|\Omega\rangle = 1 \oplus 0 \oplus \cdots$ is the *vacuum* of $\mathcal{F}(\mathcal{H})$, representing an empty system of zero particle.

We write the proof of this lemma to illustrate how computations with these operators may look like. It often uses combinatorial analysis since we work with permutations. It is always needed to treat fermionic and bosonic cases separately because the formulas are slightly different for the operators, but the combinatorial reasoning is the same.

Lemma 3.5 *Second quantization in terms of creation and annihilation operators*

Let A be a one-body operator on $\mathcal{H}$, $(u_n)_{n\in\mathbb{N}}$ be a complete orthonormal basis of $\mathcal{H}$ and $N \geq 1$.

Then, on $\mathcal{H}^N$, $\sum_{i=1}^N A_i = \sum_{n\in\mathbb{N}} a^\dagger(Au_n)a(u_n) = \sum_{m,n\in\mathbb{N}} \langle u_m, Au_n\rangle\, a^\dagger(u_m)a(u_n)$.

Proof.

We treat the bosonic case. Let $\psi \in \mathcal{H}_s^N$. For $m, n \geq 0$, we compute $a^\dagger(u_m)a(u_n)\psi$:

$$a^\dagger(u_m)a(u_n)\psi = a^\dagger(u_m)\sqrt{N}\int \overline{u_n(y)}\psi(y,\cdot)dy = \sqrt{N}\int \overline{u_n(y)} u_m \otimes_s \psi(y,\cdot)dy$$

For $x_1, \cdots, x_N \in \mathbb{R}^d$, we write :

$$
\begin{aligned}
(u_m \otimes_s \psi(y,\cdot))(x_1,\cdots,x_N) &= \frac{1}{\sqrt{N!(N-1)!}} \sum_{\sigma\in\mathfrak{S}_n} u_m(x_{\sigma_1})\psi(y, x_{\sigma_2}, \cdots, x_{\sigma_N}) \\
&= \frac{1}{\sqrt{N!}} \sum_{i=1}^{N} u_m(x_i) \cdot \frac{1}{\sqrt{(N-1)!}} \sum_{\substack{\sigma\in\mathfrak{S}_n \\ \sigma_1 = i}} \psi(y, x_{\sigma_2}, \cdots, x_{\sigma_N}) \\
&= \frac{1}{\sqrt{N}} \sum_{i=1}^{N} u_m(x_i)\psi(y, x_1, \cdots, x_{i-1}, x_{i+1}, \cdots, x_N)
\end{aligned}
$$

where we used that ψ is symmetric so the permutation sum contains $(N-1)!$ times the same term. Using the Fubini theorem and the fact that (u_n) is an orthonormal basis, we then conclude :

$$
\begin{aligned}
&\left(\sum_{m,n} \langle u_m, Au_n\rangle\, a^\dagger(u_m)a(u_n)\psi\right)(x_1,\cdots,x_N) \\
&\quad= \sum_{m,n} \langle u_m, Au_n\rangle \sum_{i=1}^{N} u_m(x_i) \int \overline{u_n(y)}\psi(y, x_1, \cdots, x_{i-1}, x_{i+1}, \cdots, x_N)dy \\
&\quad= \sum_{i=1}^{N}\sum_{n} \underbrace{\left(\sum_{m} \langle u_m, Au_n\rangle\, u_m(x_i)\right)}_{=hu_n(x_i)} \int \overline{u_n(y)}\psi(y, x_1, \cdots, x_{i-1}, x_{i+1}, \cdots, x_N)dy \\
&\quad= \sum_{i=1}^{N}\sum_{n} (|hu_n\rangle\langle u_n|)_i \psi(x_1,\cdots,x_n) \\
&\quad= \sum_{i=1}^{N} h_i\psi(x_1,\cdots,x_N)
\end{aligned}
$$

The intermediate formula is obtained through this computation, seeing that $|hu_n\rangle\langle u_n| = a^\dagger(hu_n)a(u_n)$ on $\mathcal{H}$. ∎

This lemma leads to the formula (3), at least for one body operators.

Proposition 3.1

Let A be a self-adjoint one-body operator on $\mathcal{H}$, and Γ be a state on $\mathcal{F}(\mathcal{H})$. Then $\mathrm{Tr}_{\mathcal{F}}(d\Gamma(A)\Gamma) = \mathrm{Tr}_{\mathcal{H}}(A\Gamma^{(1,1)})$.

Proof.

We can choose a basis of $\mathcal{F}(\mathcal{H})$ with each vector in one $\mathcal{H}^N$. Thus, the operator $d\Gamma(A)$ will be applied only on the spaces $\mathcal{H}^N$ for $N \geq 1$. On these spaces, the formula established in the previous lemma holds, and gives, for any orthonormal basis $(e_n)_{n\in\mathbb{N}}$ of $\mathcal{H}$:

$$\begin{aligned}
\mathrm{Tr}_{\mathcal{F}}(d\Gamma(A)\Gamma) &= \mathrm{Tr}_{\mathcal{F}}(\Gamma d\Gamma(A)) \\
&= \sum_n \mathrm{Tr}_{\mathcal{F}}(\Gamma a^\dagger(Au_n)a(u_n)) \\
&= \sum_n \left\langle u_n, \Gamma^{(1,1)} Au_n \right\rangle && \text{by definition of } \Gamma^{(1,1)} \\
&= \mathrm{Tr}_{\mathcal{H}}(\Gamma^{(1,1)} A)
\end{aligned}$$

■

We can do similar computations, but for a two-body operator, and prove in this way the formula 3.

Now that we have introduced Fock space, let us explain how to localise a state.

3.2.3 Geometric localisation

Definition 3.9 *Localised state*

Let $B \in B(\mathcal{H})$ be a bounded operator on $\mathcal{H}$ such that $0 \leq B^\dagger B \leq 1$, and Γ a state of $\mathcal{F}^{\leq N}(\mathcal{H})$.
The $B-$localisation of Γ is the unique state Γ_B on $\mathcal{F}^{\leq N}(\mathcal{H})$ such that :

$$\forall 0 \leq p, q \leq N, \Gamma_B^{(p,q)} = \underbrace{B \otimes \cdots \otimes B}_{\times p} \Gamma^{(p,q)} \underbrace{B^\dagger \otimes \cdots \otimes B^\dagger}_{\times q}.$$

N.B.

* We admit the existence and uniqueness of such a state.
* As in the example just below, B may be thought as a self-adjoint orthogonal projection on some domain. In practice, we will use $B \in \mathscr{C}_c^\infty(\mathbb{R}^d)$ to respect the domain of the operators we consider.
* In practice, to find what the localised state is from its density matrices, there exists formulas.

Example 3.2

Let $\psi \in L^2(\mathbb{R})$ be a normalised function, $D = [-1, 1] \subset \mathbb{R}$ and $\chi = \mathbb{1}_D$. We consider the state $\Gamma = |\psi\rangle\langle\psi|$ describing one particle and want to localise it on D. The definition above gives the following localised state :

$$\Gamma_\chi = \left(1 - \int_{\mathbb{R}} |\chi\psi|^2\right) \oplus |\chi\psi\rangle\langle\chi\psi|$$

We explain the meaning of this formula.

- The particle described by the wave function ψ is outside D with probability $1 - \int_D |\psi|^2 = 1 - \int_{\mathbb{R}} |\chi\psi|^2$. In this case, the state inside D is described by the vacuum $|\Omega\rangle\langle\Omega|$. This is the first term of the formula. Where precisely the particle is outside does not interest us.
- The particle is inside D with probability $\int_{\mathbb{R}} |\chi\psi|^2 = \|\chi\psi\|^2$. In this case, the particle in

> D is described by the wave function $\frac{\chi\varphi}{\|\chi\varphi\|}$: the corresponding state is $\|\chi\psi\|^2 \frac{|\chi\psi\rangle\langle\chi\psi|}{\|\chi\psi\|^2} = |\chi\psi\rangle\langle\chi\psi|$. This is the second term of the formula.

Localised states will appear in geometric localisation as follows. First, we will decompose $\mathbb{R}^d$ on domains that are adapted for what we want to see. Then, we decompose our operators between its action on these domains. Finally, we write that it is the same thing to localise the operators acting on the full state, or to apply the full operator on the localised state. Localised state sequences will have good properties with the following notion of convergence.

3.2.4 Geometric convergence

The last notion we need to apply geometric localisation to the HVZ theorem is geometric convergence. Indeed, we work with a Weyl sequence $(\psi^{(n)})_{n\in\mathbb{N}}$ and we want to see what happens when $n \to \infty$. When we worked in $\mathcal{H}^N$ only, the convergence was quite easy : we just had $\psi_N \rightharpoonup 0$. But now, we need to see the limit of subsystems with less particles. For example, if $\Gamma_n = |\varphi_1 \otimes_s \varphi_n\rangle\langle\varphi_1 \otimes_s \varphi_n|$, where $\varphi_n \rightharpoonup 0$ weakly in $\mathcal{H}$, we still have $|\varphi_1 \otimes_s \varphi_n\rangle\langle\varphi_1 \otimes_s \varphi_n| \rightharpoonup^* 0$ (we will precise just below the rigorous meaning of this weak-* convergence), but if we look at the one-body density matrix $\Gamma_n^{(1,1)} = |\varphi_1\rangle\langle\varphi_1| + |\varphi_n\rangle\langle\varphi_n|$, we have $\Gamma_n^{(1,1)} \rightharpoonup^* |\varphi_1\rangle\langle\varphi_1|$. Physically, this means that the particle described by φ_n has disappeared of the system in the limit state, while the other described by φ_1 is still here. The system of both particles had the limit 0, but it was only due to one single particle. Looking at the limit of density matrices enables to study more precisely the limit state.

First, we need to precise what we mean by looking to the convergence of density matrices sequences, which are trace-class operators. Then, we define the convergence for states that corresponds to the convergence of the density matrices. Finally, we see some properties of this convergence on localised states.

Weak-* convergence of trace-class operators

If Γ is a state, all its density matrices are trace-class. To define a convergence on density matrices, it is sufficient to get a notion of convergence on trace-class operators. As motivated in our introduction just above, this convergence should correspond to the weak convergence of wave functions : if $\psi \rightharpoonup 0$, we want that $|\psi\rangle\langle\psi| \rightharpoonup^* 0$.

N.B.

> To be very precise, in section 3.2.2, we have defined trace and trace-class operators only for operators on a single Hilbert space, whereas we are saying that $\Gamma^{(p,q)} : \mathcal{H}^q \to \mathcal{H}^p$ is trace-class even for $p \neq q$. This is because $|\Gamma^{(p,q)}| = \sqrt{(\Gamma^{(p,q)})^\dagger \Gamma^{(p,q)}} : \mathcal{H}^q \to \mathcal{H}^q$ is well-defined as an operator on $\mathcal{H}^q$, thus we can compute $\mathrm{Tr}_{\mathcal{H}^q} |\Gamma^{(p,q)}|$ and see that it is finite.

The convergence on $\mathfrak{S}_1(\mathcal{H}^q, \mathcal{H}^p)$ we will use is the weak-* convergence when $\mathfrak{S}_1(\mathcal{H}^q, \mathcal{H}^p)$ is seen as the dual of compact operators $\mathcal{K}(\mathcal{H}^p, \mathcal{H}^q)$. This is the aim of the theorem below.

Theorem 3.7 $\mathfrak{S}_1(\mathcal{H}^q, \mathcal{H}^p) \simeq \mathcal{K}(\mathcal{H}^p, \mathcal{H}^q)'$

> The following map is an isometry :
>
> $$\Phi : \left| \begin{array}{ccc} \mathfrak{S}_1(\mathcal{H}^q, \mathcal{H}^p) & \to & \mathcal{K}(\mathcal{H}^p, \mathcal{H}^q)' \\ A & \mapsto & \mathrm{Tr}_{\mathcal{H}}(A\cdot) \end{array} \right.$$

Proof.

The map is well-defined thanks to the formula

$$\forall A \in \mathfrak{S}_1(\mathcal{H}), \forall K \in \mathcal{K}(\mathcal{H}), |\operatorname{Tr}(AK)| \leq \|K\|_{\text{op}} \operatorname{Tr}|A|$$

and it gives $\|\Phi(A)\|_{\text{op}} \leq \|A\|_{\text{Tr}}$.

For the converse inequality, we approach the compact operator $|A|$ by finite rank operators using spectral projections, and we write $A = U|A|$ with U a partial unitary operator (polar decomposition, see [2] pages **PAGE**).

The surjectivity is obtained by defining A from $f \in \mathcal{K}(\mathcal{H}^p, \mathcal{H}^q)'$ on a complete orthonormal basis (φ_i) of $\mathcal{H}$, and by continuously extending it to a bounded operator on $\mathcal{H}$. Eventually, we use the isometry shown in the first part to see that A is trace-class. ■

Geometric convergence

Definition 3.10 *Geometric convergence of states*

Let $(\Gamma_n)_{n\in\mathbb{N}}$ be a sequence of states on $\mathcal{F}^{\leq N}(\mathcal{H})$, and Γ be another state on $\mathcal{F}^{\leq N}(\mathcal{H})$. We say that $(\Gamma_n)_{n\in\mathbb{N}}$ converges geometrically to Γ when $\forall 0 \leq p, q \leq N, \Gamma_n^{(p,q)} \rightharpoonup^* \Gamma^{(p,q)}$.

We write $\Gamma_n \rightharpoonup^g \Gamma$.

Proposition 3.2 *Equivalent formulations*

With the above isometry, $\Gamma_n \rightharpoonup^g \Gamma$ means by definition

$$\forall 0 \leq p, q \leq N, \forall K \in \mathcal{K}(\mathcal{H}^p, \mathcal{H}^q), \operatorname{Tr}_{\mathcal{H}^p}(\Gamma_n^{(p,q)} K) \xrightarrow[n\to\infty]{} \operatorname{Tr}_{\mathcal{H}^p}(\Gamma^{(p,q)} K).$$

By density of finite-rank operators in $\mathcal{K}(\mathcal{H})$ and by linearity, it is equivalent to

$$\forall 0 \leq p, q \leq N, \forall (\psi_p, \psi_q) \in \mathcal{H}^p \times \mathcal{H}^q, \left\langle \psi_p, \Gamma_n^{(p,q)} \psi_q \right\rangle_{\mathcal{H}^p} \xrightarrow[n\to\infty]{} \left\langle \psi_p, \Gamma^{(p,q)} \psi_q \right\rangle_{\mathcal{H}^p}.$$

For practical computation, using (4) and the definition of density matrix, it can finally be written : $\forall 0 \leq p, q \leq N, \forall f_1, \cdots, f_q, g_1, \cdots, g_p \in \mathcal{H}$,

$$\left\langle g_1 \otimes \cdots \otimes g_p, \Gamma^{(p,q)} f_1 \otimes \cdots \otimes f_q \right\rangle_{\mathcal{H}^p} = \operatorname{Tr}_{\mathcal{F}}(\Gamma a^\dagger(f_1) \cdots a^\dagger(f_q) a(g_p) \cdots a(g_1)).$$

We study an example of geometric convergence that will be used in the proof of HVZ-theorem and that enables to understand more the definition.

Example 3.3 *Sequence of states commuting with the number operator*

We introduce the number operator $\mathcal{N} = \bigoplus_{N\geq 0} N \mathbb{1}_{\mathcal{H}^N}$. It counts how many particles a state describes, and is the second quantization of the identity $\mathbb{1}_{\mathcal{H}}$, using the notions introduced previously.

In this example, we are interested in states Γ of $\mathcal{F}^{\leq N}(\mathcal{H})$ that commutes with $\mathcal{N}$. Using the spectral projections $\mathbb{1}_{\{k\}}(\mathcal{N})$, we can see that commuting with $\mathcal{N}$ is equivalent to being a "diagonal" state $\Gamma = G_{0,0} \oplus \cdots \oplus G_{N,N}$. Indeed :

$$\forall 0 \leq p, q \leq N, \forall \psi_q \in \mathcal{H}^q, \delta_{p,q} = \Gamma \mathbb{1}_p(\mathcal{N})\psi_q = \mathbb{1}_p(\mathcal{N})\Gamma\psi_q$$

Now, let $(\Gamma_n)_{n\in\mathbb{N}}$ be a sequence of states of $\mathcal{F}^{\leq N}(\mathcal{H})$ that all commute with the number operator $\mathcal{N}$. Assume that it converges geometrically to a state Γ on $\mathcal{F}^{\leq N}(\mathcal{H})$. We show that the limit state Γ also commutes with $\mathcal{N}$.

Then, for all $n \in \mathbb{N}$, and for all $0 \leq p \neq q \leq N$, we have $\Gamma_n^{(p,q)} = 0$, because if $(\psi_p, \psi_q) \in \mathcal{H}^p \times \mathcal{H}^q$, we write :

$$\begin{aligned}
\left\langle \psi_p, \Gamma_n^{(p,q)}\psi_q \right\rangle_{\mathcal{H}^p} &= \left\langle \psi_p, \Gamma_n \mathbb{1}_{\{q\}}(\mathcal{N})\psi_q \right\rangle_{\mathcal{F}} && \text{(definition of } \Gamma_n^{(p,q)} \text{ to go into Fock space)} \\
&= \left\langle \mathbb{1}_{\{q\}}(\mathcal{N})\psi_p, \Gamma_n\psi_q \right\rangle_{\mathcal{F}} && \text{(commutation assumption and self-adjointness)} \\
&= \delta_{p,q}
\end{aligned}$$

Thus, we know that for the geometric limit Γ, $\Gamma^{(p,q)} = 0$ for all $p \neq q$. This means that Γ commutes with $\mathcal{N}$. Indeed, let $(\psi_p, \psi_q) \in \mathcal{H}^p \times \mathcal{H}^q$:

$$\begin{aligned}
\langle \psi_p, \Gamma\mathcal{N}\psi_q \rangle_{\mathcal{F}} &= q \left\langle \psi_p, \Gamma^{(p,q)}\psi_q \right\rangle_{\mathcal{H}^p} && \text{(definition of } \Gamma^{(p,q)} \text{ and of } \mathcal{N}) \\
&= \delta_{p,q} \\
&= \langle \mathcal{N}\psi_p, \Gamma\psi_q \rangle_{\mathcal{F}} && \text{(by doing the same reverse)} \\
&= \langle \psi_p, \mathcal{N}\Gamma\psi_q \rangle_{\mathcal{F}} && \text{(self-adjointness of } \mathcal{N})
\end{aligned}$$

Since this convergence is close to weak-* convergence, we obtain some properties that are well-known for weak-* convergence. By definition, a state has trace 1 so every sequence of states is bounded.

Theorem 3.8 *Banach-Alaoglu theorem for geometric convergence*

Let $(\Gamma_n)_{n\in\mathbb{N}}$ be a sequence of states of $\mathcal{F}^{\leq N}(\mathcal{H})$.
There exists a subsequence $(\Gamma_{\varphi(n)})_{n\in\mathbb{N}}$ which converges geometrically.

We admit the proof of this theorem. Using Banach-Alaoglu theorem for each $0 \leq p, q \leq N$, we can extract a subsequence such that every sequence of $(p, q)-$density matrices. But then we need to see that the limit Γ we build from density matrices corresponds to a state, i.e. $\Gamma = \Gamma^\dagger \geq 0$. This can be obtained through the theory of C^*-algebra.

Eventually, we have the useful proposition saying that if we localise a sequence of states on a compact set, then geometric convergence turns into strong convergence in trace norm. For our application, we can limit ourself to obtain convergence of traces, which is weaker.

This first proposition will not be used in what follows but motivates what we want to do. We do a strong assumption on the operator. In practice, our operators will only be compactly supported, not compact. We will handle it in the next proposition, where we reinforce assumptions on the sequence of states to weaken the assumption on the operator used to localise.

Proposition 3.3 *Compact localisation and geometric convergence*

Let $(\Gamma_n)_{n\in\mathbb{N}}$ be a sequence of states on $\mathcal{F}^{\leq N}(\mathcal{H})$ which converges geometrically to Γ on $\mathcal{F}^{\leq N}(\mathcal{H})$, and K be a compact operator on $\mathcal{H}$ such that $0 \leq K^\dagger K \leq 1$.
Then $\mathrm{Tr}_{\mathcal{F}}((\Gamma_n)_K) \xrightarrow[n\to\infty]{} \mathrm{Tr}_{\mathcal{F}}((\Gamma_K))$, and more precisely :

$$\forall 0 \leq k \leq N, \mathrm{Tr}_{\mathcal{H}^k}((G_k)_{K,n}) \xrightarrow[n\to\infty]{} \mathrm{Tr}_{\mathcal{H}^k}((G_k)_K)$$

where $(G_k)_{K,n}$ is the coefficient (k,k) of Γ_n when written like a matrix of operator (see just above formula (1)).

Proof.

If $\Gamma = [G_{m,n}]_{0\leq m,n\leq N}$ is a state, we can express the diagonal operators $G_{m,m}$ in terms of density matrices $\Gamma^{(p,p)}$ with $0 \leq p \leq N$. The formula is the following (see [3]) :

$$G_{m,m} = \Gamma^{(m,m)} + \sum_{j=1}^{N-m} (-1)^j \binom{m+j}{m} \mathrm{Tr}_{m+1\to m+j}(\Gamma^{(m+j,m+j)})$$

Taking the trace on this expression, we find :

$$\mathrm{Tr}_{\mathcal{H}^m}(G_{m,m}) = \mathrm{Tr}_{\mathcal{H}^m}(\Gamma^{(m,m)}) + \sum_{j=1}^{N-m} (-1)^j \binom{m+j}{m} \mathrm{Tr}_{\mathcal{H}^{m+j}}(\Gamma^{(m+j,m+j)})$$

Using (1) and the previous formula, we can therefore express $\mathrm{Tr}_{\mathcal{F}}((\Gamma_n)_K)$ as a linear combination of $\mathrm{Tr}_{\mathcal{H}^k}((\Gamma_n)_K^{(k,k)})$ with $0 \leq k \leq N$. For each term, we use the definition of geometric convergence and of localised states to write :

$$\mathrm{Tr}_{\mathcal{H}^k}((\Gamma_n)_K^{(k,k)}) = \mathrm{Tr}_{\mathcal{H}^k}(\underbrace{K^{\otimes k}}_{\in\mathcal{K}(\mathcal{H}^k)} \Gamma_n^{(k,k)} \underbrace{(K^\dagger)^{\otimes k}}_{\in\mathcal{K}(\mathcal{H}^k)}) \xrightarrow[n\to\infty]{} \mathrm{Tr}_{\mathcal{H}^k}(K^{\otimes k}\Gamma^{(k,k)}(K^\dagger)^{\otimes k}) = \mathrm{Tr}_{\mathcal{H}^k}((\Gamma)_K^{(k,k)})$$

We use again the same formulas to come back to $\mathrm{Tr}_{\mathcal{F}}((\Gamma)_K)$ from the expression of the trace with density matrices. ∎

Proposition 3.4 *Compact support localisation and geometric convergence*

Let $(\Gamma_n)_{n\in\mathbb{N}}$ be a sequence of states on $\mathcal{F}^{\leq N}(\mathcal{H})$ which converges geometrically to Γ on $\mathcal{F}^{\leq N}(\mathcal{H})$. We assume that $(\Gamma_n)_{n\in\mathbb{N}}$ has bounded kinetic energy, i.e. the sequence $(\mathrm{Tr}_{\mathcal{F}}(d\Gamma(1-\Delta)\Gamma_n))_{n\in\mathbb{N}}$ is bounded.
Let $\chi \in \mathscr{C}_c^\infty(\mathbb{R}^d)$.
Then $\mathrm{Tr}_{\mathcal{F}}((\Gamma_n)_\chi) \xrightarrow[n\to\infty]{} \mathrm{Tr}_{\mathcal{F}}((\Gamma)_\chi)$, and more precisely :

$$\forall 0 \leq k \leq N, \mathrm{Tr}_{\mathcal{H}^k}((G_k)_{\chi,n}) \xrightarrow[n\to\infty]{} \mathrm{Tr}_{\mathcal{H}^k}((G_k)_\chi)$$

where $(G_k)_{K,n}$ is the coefficient (k,k) of Γ_n when written like a matrix of operator (see just above formula (1)).

Proof.

As in the previous proof, it is sufficient to show that for all $0 \leq k \leq N$, we have $\mathrm{Tr}_{\mathcal{H}^k}((\Gamma_n)_\chi^{(k,k)}) \xrightarrow[n\to\infty]{} \mathrm{Tr}_{\mathcal{H}^k}((\Gamma)_\chi^{(k,k)})$.

We consider $\psi_n^{(k)}(x_1, \cdots, x_k) = \sqrt{\Gamma_n^{(k,k)}(x_1, \cdots, x_k; x_1, \cdots, x_k)}$. The fact that $(\Gamma_n)_{n\in\mathbb{N}}$ has bounded kinetic energy means that $(\psi_n^{(k)})_{n\in\mathbb{N}}$ is a bounded sequence in $H^1((\mathbb{R}^d)^k)$. To show this, we want to bound $(\nabla_j \psi_n^{(k)})$ for $0 \leq j \leq k$. First, we apply the spectral theorem to the positive self-adjoint operator $\Gamma_n^{(k,k)}$ to have :

$$\psi_n^{(k)} = \sqrt{\sum_{i\in\mathbb{N}} \lambda_{n,i} |\varphi_{n,i}|^2}$$

where $\lambda_{n,i} \geq 0$ and $\sum \lambda_{n,i} = \binom{N}{k}$ because $\mathrm{Tr}_{\mathcal{F}}(\Gamma_n) = 1$ and using the formula between $\Gamma_n^{(k,k)}$ and $\Gamma^{(k,k)}$.

Then, we use the convexity inequality for gradient (see [4] page **PAGE**).

Lemma 3.6 *Convexity inequality for gradient*

Let f, g be real-valued functions in $H^1(\mathbb{R}^d)$. It holds :

$$\int_{\mathbb{R}^d} \left| \sqrt{f^2 + g^2} \right|^2 \leq \int_{\mathbb{R}^d} |\nabla f|^2 + \int_{\mathbb{R}^d} |\nabla g|^2$$

In our case, $\psi_n^{(k)}$ is positive, so $\psi_n^{(k)} = |\psi_n^{(k)}|$, which allows us to use this inequality :

$$\begin{aligned}
\int |\nabla_j \psi_n^{(k)}|^2 &= \int \left| \nabla_j \sqrt{\sum_{i\in\mathbb{N}} \lambda_{n,i} \varphi_{n,i}} \right|^2 \\
&\leq \sum_{i\in\mathbb{N}} \lambda_{n,i} \int |\nabla_j |\varphi_{n,i}||^2 \\
&\leq \sum_{i\in\mathbb{N}} \lambda_{n,i} \int |\nabla_j \varphi_{n,i}|^2 \qquad \text{applying the same inequality for } |\varphi|^2 = \sqrt{f^2 + g^2} \\
&= \mathrm{Tr}_{\mathcal{H}^k}(-\Delta_j \Gamma_n^{(k)})
\end{aligned}$$

The latter quantity is bounded because (Γ_n) has bounded kinetic energy.

Now, we use the compact Sobolev embedding to deduce that $\psi_n^{(k)} \to \psi^{(k)}$ in $L^2_{\mathrm{loc}}((\mathbb{R}^d)^k)$, which means that it converges in $L^2(\Omega)$ for every bounded open set $\Omega \subset (\mathbb{R}^d)^k$. Therefore :

$$\begin{aligned}
|\,\mathrm{Tr}_{\mathcal{H}^k}(\chi^{\otimes k}(\Gamma_n^{(k,k)} - \Gamma^{(k,k)})\chi^{\otimes k})| &= \int_{\mathrm{supp}\,\chi^k} \chi(x_1)^2 \cdots \chi(x_k)^2 (|\psi_n^{(k)}|^2 - |\psi^{(k)}|^2) dx_1 \cdots dx_k \\
&\leq \|\chi\|_{L^\infty}^{2k} \left(\left\|\psi_n^{(k)}\right\|_{L^2(\mathrm{supp}(\chi)^k)} - \left\|\psi^{(k)}\right\|_{L^2(\mathrm{supp}(\chi)^k)} \right) \\
&\xrightarrow[n\to\infty]{} 0
\end{aligned}$$

■

Proposition 3.5 *Geometric localisation and approximation of states*

Let Γ be a state on $\mathcal{F}^{\leq N}(\mathcal{H})$, and $(B_n)_{n\in\mathbb{N}}$ a sequence of bounded operators such that $0 \leq B^\dagger B \leq 1$. Assume that $B_n \to 1$ strongly in operator norm.
Then $\mathrm{Tr}_{\mathcal{F}}((\Gamma)_{B_n}) \to \mathrm{Tr}_{\mathcal{F}}(\Gamma)$, and more precisely :

$$\forall 0 \leq k \leq N, \mathrm{Tr}_{\mathcal{H}^k}((G_k)_{B_n}) \xrightarrow[n\to\infty]{} \mathrm{Tr}_{\mathcal{H}^k}(G_k)$$

where G_k is the coefficient (k,k) of Γ when written like a matrix of operator (see just above formula (1)).

Proof.

Using the same formulas as in the proof just above, it is sufficient to show that for $0 \leq k \leq N$, $\mathrm{Tr}_{\mathcal{H}^k}(B_n^{\otimes k}\Gamma^{(k,k)}(B_n^\dagger)^{\otimes k}) \to \mathrm{Tr}_{\mathcal{H}^k}(\Gamma^{(k,k)})$. We write

$$B_n^{\otimes k}\Gamma^{(k,k)}(B_n^\dagger)^{\otimes k} - \Gamma^{(k,k)} = \frac{1}{2}((B_n-1)^{\otimes k}\Gamma^{(k,k)}(B_n^\dagger+1)^{\otimes k}) + (B_n+1)^{\otimes k}\Gamma^{(k,k)}(B_n^\dagger-1)^{\otimes k})$$

in order to use the fact that $\|B_n - 1\|_{\mathrm{op}} \to 0$ as follows (we use the formula $|\mathrm{Tr}(AB)| \leq \|B\|_{op} \mathrm{Tr}\,|A|$:

$$\begin{aligned}
&\mathrm{Tr}_{\mathcal{H}^k}|B_n^{\otimes k}\Gamma^{(k,k)}(B_n^\dagger)^{\otimes k} - \Gamma^{(k,k)}| \\
&\quad\leq \frac{1}{2}(\mathrm{Tr}_{\mathcal{H}^k}|(B_n-1)^{\otimes k}\Gamma^{(k,k)}(B_n^\dagger+1)^{\otimes k}| + \mathrm{Tr}_{\mathcal{H}^k}|(B_n+1)^{\otimes k}\Gamma^{(k,k)}(B_n^\dagger-1)^{\otimes k})|) \\
&\quad\leq \|B_n+1\|_{\mathrm{op}}^k \|B_n-1\|_{\mathrm{op}}^k \mathrm{Tr}_{\mathcal{H}^k}|\Gamma^{(k,k)}| \\
&\quad\leq C\|B_n-1\|_{\mathrm{op}}^k \mathrm{Tr}_{\mathcal{H}^k}|\Gamma^{(k,k)}| \xrightarrow[n\to\infty]{} 0
\end{aligned}$$

■

3.2.5 Back to the HVZ theorem : application of geometric localisation

We finally illustrate geometric localisation method by finishing the proof of the HVZ theorem (see theorem 3.4). We recall what remains to prove. We showed that the essential spectrum of the $N-$body Hamiltonian $\sigma_{\mathrm{ess}}(H_N)$ contains $[E_{N-1}, +\infty[$ where E_{N-1} is the bottom of the spectrum of the $(N-1)-$body Hamiltonian. We now want to prove that $\sigma_{\mathrm{ess}}(H_N) \subset [E_{N-1}, +\infty[$, i.e. that $\Sigma_N \geq E_{N-1}$ where $\Sigma_N = \inf \sigma_{\mathrm{ess}}(H_N)$. We explained informally the strategy at the end of section 3.2.1.

Proof. *Second inclusion of the HVZ theorem : $\sigma_{ess}(H_N) \subset [E_{N-1}, +\infty[$*

Let $(\psi_N^{(n)})_{n\in\mathbb{N}}$ be a singular Weyl sequence for Σ_N (recall definition 2.7). It corresponds to the pure state sequence on Fock space $\mathcal{F}^{\leq N}(\mathcal{H})$

$$\Gamma_n = 0 \oplus \cdots \oplus \left|\psi_N^{(n)}\right\rangle\left\langle\psi_N^{(n)}\right|.$$

We want to show that $\Sigma_N \geq E_{N-1}$ by looking at the mean energy. We explained in example 3.1 that it is given by $\mathrm{Tr}_{\mathcal{F}}(d\Gamma(H)\Gamma_n)$. We use the formula 3 :

$$\mathrm{Tr}_{\mathcal{F}}(d\Gamma(H)\Gamma_n) = \mathrm{Tr}_{\mathcal{H}}((-\Delta + V(x))\Gamma_n^{(1,1)}) + \mathrm{Tr}_{\mathcal{H}^2}(W(x-y)\Gamma_n^{(2,2)})$$

As $(\psi_N^{(n)})_{n\in\mathbb{N}}$ is a Weyl sequence for Σ_N, the left-hand term goes to Σ_N as N goes to ∞.

To analyse the right-hand term, we want to localise in balls $B(0,R)$ with $R\to\infty$. As the domain of H_N demands a bit of regularity to states, we cannot just localise with $\mathbb{1}_{B(0,R)}$. Instead, we use a smooth partition of unity. Let $\chi\in\mathscr{C}_c^\infty(\mathbb{R}^d)$ be such that $\chi\equiv 1$ on $B(0,1)$, $0\le\chi\le 1$, and $\chi\equiv 0$ outside of $B(0,2)$. We also let $\eta=\sqrt{1-\chi^2}$. We localise in $B(0,R)$ using the rescaled functions $\chi_R(x)=\chi(x/R)$ and $\eta_R(x)=\eta(x/R)$.

Now, let us decompose the Hamiltonian according to the partition of unity $\chi_R^2+\eta_R^2=1$. The one-particle potential part is easy to decompose because it commutes with the partition functions :

$$V=V(\chi_R^2+\eta_R^2)=\chi_R V\chi_R+\eta_R V\eta_R$$

The interaction potential also commutes with the partition functions, but we need to localise both variables, so there are several terms. We use the fact that W is assumed to be even to regroup the cross terms :

$$W(x-y)=(\chi_R\otimes\chi_R)W(x-y)(\chi_R\otimes\chi_R)+(\eta_R\otimes\eta_R)W(x-y)(\eta_R\otimes\eta_R)+2(\chi_R\otimes\eta_R)W(x-y)(\chi_R\otimes\eta_R)$$

For the kinetic part, there are error terms that appear due to the derivation of the side of χ_R and η_R. The decomposition is given by the following formula, which can be proven by developing each side and see they are the same.

Lemma 3.7 *IMS formula*

Let $\varphi\in\mathscr{C}_c^\infty(\mathbb{R}^d)$. Then, in the sense of quadratic forms :

$$\frac{\varphi^2(-\Delta)+(-\Delta)\varphi^2}{2}=\varphi(-\Delta)\varphi-|\nabla\varphi|^2$$

This leads to the following formula on $\mathbb{R}^d$:

$$\begin{aligned}-\Delta&=\chi_R(-\Delta)\chi_R+\eta_R(-\Delta)\eta_R-|\nabla\chi_R|^2-|\nabla\eta_R|^2\\&\ge\chi_R(-\Delta)\chi_R+\eta_R(-\Delta)\eta_R-\frac{C}{R^2}\qquad\text{where } C=\max(\|\chi\|_{H^1},\|\eta\|_{H^1})\end{aligned}$$

Putting all decompositions together and transfering the localisation on states thanks to the cyclicity of the trace, we get the following decomposition of the right (recall definition 3.9 of localised states) :

$$\begin{aligned}\mathrm{Tr}_{\mathcal{F}}(d\Gamma(H)\Gamma_n)&\ge\mathrm{Tr}_{\mathcal{F}}(d\Gamma(H)(\Gamma_n)_{\chi_R})+\mathrm{Tr}_{\mathcal{F}}(d\Gamma(H^0)(\Gamma_n)_{\eta_R})\\&\qquad+\mathrm{Tr}_{\mathcal{H}}(V(\Gamma_n)^{(1,1)}_{\eta_R})+2\,\mathrm{Tr}_{\mathcal{H}^2}(W(x-y)(\Gamma_n)^{(2,2)}_{\chi_R\otimes\eta_R})-\frac{CN}{R^2}\end{aligned}$$

We defined H^0 to be the $N-$body Hamiltonian without potential V. Let us investigate each term.

First term. It is the energy of the particles that are still bound to the potential. We expect to relate this term to the energy $(N-1)$ after having proved that, at the limit, there are only at most $N-1$ particles still bound to the potential. To prepare this limit, we use the trace formula

(1) and the second quantization of the Hamiltonian (2). $(G_k)_{\chi_R,n}$ is the part of the state $(\Gamma_n)_{\chi_R}$ going from $\mathcal{H}^n$ to $\mathcal{H}^n$ (see above the trace formula (1)) :

$$\begin{aligned}\mathrm{Tr}_{\mathcal{F}}(d\Gamma(H)(\Gamma_n)_{\chi_R}) &= \sum_{k=0}^{N-1} \mathrm{Tr}_{\mathcal{H}^k}(H_k(G_k)_{\chi_R,n}) + \mathrm{Tr}_{\mathcal{H}^N}(H_N(G_N)_{\chi_R,n}) \\ &\geq \sum_{k=0}^{N-1} E_k \,\mathrm{Tr}_{\mathcal{H}^k}((G_k)_{\chi_R,n}) + E_N \,\mathrm{Tr}_{\mathcal{H}^N}((G_N)_{\chi_R,n}) \\ &\geq E_{N-1} \sum_{k=0}^{N-1} \mathrm{Tr}_{\mathcal{H}^k}((G_k)_{\chi_R,n}) + E_N \,\mathrm{Tr}_{\mathcal{H}^N}((G_N)_{\chi_R,n})\end{aligned}$$

We used that $H_k \geq E_k$ because $E_k = \inf \sigma(H_k)$ and $E_k \geq E_{N-1}$ thanks to the first inclusion of the HVZ theorem we already proved : $E_k \geq \Sigma_{k+1} \geq E_{k+1} \geq \cdots \geq E_{N-1}$.

Second term. It corresponds to the energy of the electrons that have escaped to infinity. This interpretation is the reason why we removed the potential of this term. Since $W \geq 0$ and $-\Delta \geq 0$, using the same formulas as for first term, $\mathrm{Tr}_{\mathcal{F}}(d\Gamma(H^0)(\Gamma_n)_{\eta_R}) \geq 0$.

Third term. It is representing the fact that V is still existing, even far from the origin. However, it is small because of the assumptions on the potential. To control it, we use Hölder and Sobolev inequalities for H^1, given that $(\psi_N^{(n)})$ is bounded in $H^1((\mathbb{R}^d)^N)$ thanks to the lemma 3.2. We will not detail this time as the method is the same as in the proof of theorem 3.3, but we indicate that we work with kernels of operators to write :

$$\mathrm{Tr}_{\mathcal{H}}(V(\Gamma_n)_{\eta_R}^{(1,1)}) = \int_{\mathbb{R}^d} V(x)\eta_R(x)^2\Gamma_n^{(1,1)}(x,x)dx$$

and we do the link with $\psi_N^{(n)}$ with a formula giving the kernel of $\Gamma_n^{(1,1)}$ from the kernel of $\left|\psi_N^{(n)}\right\rangle\left\langle\psi_N^{(n)}\right|$, which is given by $\overline{\psi_N^{(n)}}(y_1,\cdots,y_n)\psi_N^{(n)}(x_1,\cdots,x_N)$. This leads to $\left|\mathrm{Tr}_{\mathcal{H}}(V(\Gamma_n)_{\eta_R}^{(1,1)})\right| \leq C\left\|V\eta_R^2\right\|_{L^p} = o(1)$ when R goes to ∞.

Fourth term. It is describing the interaction of localised particles with escaped particles. It is positive because $W \geq 0$. Below this proof, we will see that the treatment of this term is technical if we do not have this assumption. Here, we eliminate it as the second term.

So far, we have :

$$\mathrm{Tr}_{\mathcal{F}}(d\Gamma(H)\Gamma_n) \geq E_{N-1} \sum_{k=0}^{N-1} \mathrm{Tr}_{\mathcal{H}^k}((G_k)_{\chi_R,n}) + E_N \,\mathrm{Tr}_{\mathcal{H}^N}((G_N)_{\chi_R,n}) + \varepsilon_R$$

where $\varepsilon_R \to 0$ when $R \to \infty$ and does not depend of n.

Now, we want to make $n \to \infty$ to use the fact that our Weyl sequence is singular. By the equivalent of Banach-Alaoglu theorem for geometric convergence (see theorem 3.8), up to a subsequence, we can assume that $\Gamma_n \rightharpoonup^g \Gamma$. Since (Γ_n) is a sequence of states commuting with the particle number operator $\mathcal{N}$, $\Gamma = G_0 \oplus \cdots \oplus G_N$ is a diagonal state (see example 3.3). Furthermore, $G_N = \Gamma^{(N)} = 0$ because it is the weak-* limit of $\left|\psi_N^{(n)}\right\rangle\left\langle\psi_N^{(n)}\right|$ and $\psi_N^{(n)} \rightharpoonup 0$.

This is where we prove that at least one particle escaped along the singular Weyl sequence.

Since χ_R is compactly supported, by the proposition 3.4, we have $\mathrm{Tr}_{\mathcal{H}^k}((G_k)_{\chi_R,n}) = \mathrm{Tr}_{\mathcal{H}^k}((G_k)_{\chi_R})$. With these observations, taking the limit $n \to \infty$ leads to

$$\Sigma_N \geq E_{N-1} \sum_{k=0}^{N-1} \mathrm{Tr}_{\mathcal{H}^k}((G_k)_{\chi_R}) + \varepsilon_R$$

Then, we take the limit $R \to \infty$:

- by proposition 3.5, $\sum_{k=1}^{N-1} \mathrm{Tr}_{\mathcal{H}^k}((G_k)_{\chi_R}) \to \sum_{k=1}^{N-1} \mathrm{Tr}_{\mathcal{H}^k}(G_k) = 1$, the latter equality coming from the fact that Γ is a state and $G_N = 0$.
- The trace term goes to 0 by dominated convergence (we write it as an integral using the kernel of $\Gamma^{(2,2)}$).

So we finally obtain that $\Sigma_N \geq E_{N-1}$.

$\blacksquare$

To conclude, we explain a step to generalise the result when we do not assume that $W \geq 0$. It means that the particles which escape to infinity can stay together and reduce the total energy if they have a negative energy. So the bottom of the essential spectrum can be something else that E_{N-1} (see [3]). When we do not assume $W \geq 0$, the treatment of the second and the fourth term change. We explain here how to treat the fourth term. It is describing the interaction of localised particles with escaped particles. It should be small because those particles are very far from each other. However, it is a bit technical to treat it rigorously, since the domain of χ_R and the one of η_R are not separated. To control it, we split this term into two terms : a first term for which the distance of the particles which are interacting is indeed going to ∞ with R, and an error term describing interaction on a compact annulus which will be sent to infinity with R. We do this by adding the partition of unity $\chi_{3R}^2 + \eta_{3R}^2 = 1$ on the second variable :

$$\mathrm{Tr}_{\mathcal{H}^2}(W(x-y)(\Gamma_n)^{(2,2)}_{\chi_R \otimes \eta_R}) = \mathrm{Tr}_{\mathcal{H}^2}(W(x-y)(\Gamma_n)^{(2,2)}_{\chi_R \otimes \eta_R \eta_{3R}}) + \mathrm{Tr}_{\mathcal{H}^2}(W(x-y)(\Gamma_n)^{(2,2)}_{\chi_R \otimes \eta_R \chi_{3R}})$$

With Hölder and Sobolev inequalities, again, one can control the first term by another which goes to 0 when $R \to +\infty$, and which does not depend on n. The second term also goes to 0 when $R \to +\infty$, with dominated convergence, but we need to justify before what happens when we do $n \to \infty$. It looks like in the proposition 3.4 since $\chi_R \otimes \eta_R \chi_{3R}$ is compactly supported, but there is the term in W to control before. Writing it $W = W_p + W_\infty$ with $\|W_p\|_{L^p} \leq \varepsilon$ and $W_\infty \in L^\infty(\mathbb{R}^d)$, we can show that

$$\mathrm{Tr}_{\mathcal{H}^2}(W(x-y)(\Gamma_n)^{(2,2)}_{\chi_R \otimes \eta_R \chi_{3R}}) \xrightarrow[n \to \infty]{} \mathrm{Tr}_{\mathcal{H}^2}(W(x-y)(\Gamma)^{(2,2)}_{\chi_R \otimes \eta_R \chi_{3R}})$$

up to a subsequence which converges geometrically to a state Γ.

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I used [1] to understand the tools of spectral theory in infinite dimension and the definition of Weyl sequences. References [2] and [5] were useful to see the proof of the spectral theorem, and I also used [2] for the definition of the trace and of trace-class operators in infinite dimension. [3] and [6] contain the proof of the HVZ theorem and the tools of Fock space. Many "classical" theorems of analysis can be found in [4] and at the end of [1].