Spectral theory and applications. An elementary introductory course.

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Abstract

We intend to present in this course the basic tools in spectral analysis and to illustrate the theory by presenting examples coming from the Schrödinger operator theory and from various branches of physics : statistical mechanics, superconductivity, fluid mechanics.

Contents

1 Introduction

Our starting point could be the theory of hermitian matrices, that is satisfying : $A^\star = A$. If we look for eigenvalues and corresponding eigenvectors of A, that is for pairs (u, λ) with $u \in \mathbb{C}^k$, $u \neq 0$ and $\lambda \in \mathbb{C}$ such that $Au = \lambda u$, we know that the eigenvalues are real and that one can find an orthonormal basis of eigenvectors associated with real eigenvalues.

In order to extend this theory to the case of spaces with infinite dimension (that is replacing the space $\mathbb{C}^m$ by a general Hilbert space $\mathcal{H}$), the first attempt consists in developing the theory of compact selfadjoint operators. But it is far to cover all the interesting cases that are present in Quantum Mechanics. So our aim is to present a general theory but it is perhaps good to start by looking at specific operators and to ask naive questions about the existence of pairs (u, λ) with u in some suitable domain, $u \neq 0$ and $\lambda \in \mathbb{C}$ such that $Au = \lambda u$. We shall discover in particular that the answer at these questions may depend strongly on the choice of the domain and on the precise definition of the operator.

1.1 The free Laplacian

The Laplacian $-\Delta$ has no eigenvectors in L^2, but it has for any $\lambda \in \mathbb{R}^+$ an eigenvector in $\mathcal{S}'(\mathbb{R}^m)$ and for any $\lambda \in \mathbb{C}$ an eigenvector in $\mathcal{D}'(\mathbb{R}^m)$. So what is the right way to extend the theory of Hermitian matrices on $\mathbb{C}^k$?
On the other hand, it is easy to produce (take for simplicity $m = 1$) approximate eigenvectors in the form $u_n(x) = \frac{1}{\sqrt{n}} \exp ix \cdot \xi \; \chi(\frac{x-n^2}{n})$, where χ is a compactly supported function of L^2-norm equal to 1.

1.2 The harmonic oscillator

As we shall see the harmonic oscillator

$$H = -d^2/dx^2 + x^2$$

plays a central role in the theory of quantum mechanics. When looking for eigenvectors in $\mathcal{S}(\mathbb{R})$, we obtain that there is a sequence of eigenvalues λ_n $(n \in \mathbb{N})$

$$\lambda_n = (2n - 1)\ .$$

In particular the fundamental level (in other words the lowest eigenvalue) is

$$\lambda_1 = 1$$

and the splitting between the two first eigenvalues is 2.
The first eigenfunction is given by

$$\phi_1(x) = c_1 \exp -\frac{x^2}{2} \tag{1.2.1}$$

and the other eigenvectors are obtained by applying the creation operator

$$L^+ = -d/dx + x \ . \tag{1.2.2}$$

We observe indeed that

$$H = L^+ \cdot L^- \ + \ 1 \ , \tag{1.2.3}$$

where

$$L^- = d/dx + x \ , \tag{1.2.4}$$

and has the property

$$L^- \phi_1 = 0. \tag{1.2.5}$$

Note that if $u \in L^2$ is a distributional solution of $L^+ u = 0$, then $u = 0$. Note also that if $u \in L^2$ is a distributional solution of $L^- u = 0$, then $u = \mu\phi_1$ for some $\mu \in I\!R$.
The n^{th}-eigenfunction is then given by

$$\phi_n = c_n (L^+)^{n-1} \phi_1 \ .$$

This can be shown by recursion using the identity

$$L^+(H+2) = HL^+ \ . \tag{1.2.6}$$

It is easy to see that $\phi_n(x) = P_n(x) \exp -\frac{x^2}{2}$ where $P_n(x)$ is a polynomial of order $n-1$. One can also show that the ϕ_n are mutually orthogonal. The proof of this point is identical to the finite dimensional case, if we observe the following identity (expressing that H is symmetric) :

$$< Hu, v >_{L^2} = < u, Hv >_{L^2} \ , \ \forall u \in \mathcal{S}(I\!R), \forall v \in \mathcal{S}(I\!R) \ , \tag{1.2.7}$$

which is obtained through an integration by parts.
Then it is a standard exercise to show that the family $(\phi_n)_{n \in I\!N}$ is total and that we have obtained an orthonormal hilbertian basis of L^2, which in some sense permits to diagonalize the operator H.
Another way to understand the completeness is to show that starting of an eigenvector u in $\mathcal{S}'(I\!R)$ associated with $\lambda \in I\!R$ solution (in the sense of distribution) of

$$Hu = \lambda u \ ,$$

then there exists $k \in I\!N$ and $c_k \neq 0$ such that $(L^-)^k u = c_k \phi_1$ and that the corresponding λ is equal to $(2k+1)$.
For this proof, we admit that any eigenvector can be shown to be in $\mathcal{S}(I\!R)$ and use the identity

$$L^-(H-2) = HL^- \ , \tag{1.2.8}$$

and the inequality

$$< Hu, u >\geq 0 \ , \ \forall u \in \mathcal{S}(I\!\!R) \ . \tag{1.2.9}$$

This property is called "positivity" of the operator.
Actually one can show by various ways that

$$< Hu, u >\geq ||u||^2 \ , \ \forall u \in \mathcal{S}(I\!\!R) \ . \tag{1.2.10}$$

One way is to first establish the Heisenberg Principle[1] :

$$||u||^2_{L^2(I\!\!R)} \leq 2||xu||_{L^2}||u'||_{L^2} \ , \ \forall u \in \mathcal{S}(I\!\!R) \ . \tag{1.2.11}$$

The trick is to observe the identity

$$1 = \frac{d}{dx} \cdot x - x \cdot \frac{d}{dx} \ . \tag{1.2.12}$$

The inequality (1.2.10) is simply the consequence of the identity

$$< Hu, u >= ||u'||^2 + ||xu||^2 \ , \tag{1.2.13}$$

which is proved through an integration by parts, and of the application in (1.2.11) of Cauchy-Schwarz inequality.

Another way is to directly observe the identity

$$< Hu, u >= ||L^- u||^2 + ||u||^2 \ , \ \forall u \in \mathcal{S} \ . \tag{1.2.14}$$

1.3 The problem of the boundary

We consider the operator $-\frac{d^2}{dx^2}$ and look at various problems that can be asked naively about the existence of eigenvectors for the problem in $L^2(]0, 1[)$.

1.3.1 Ill-posed problems

Look at pairs $(u, \lambda) \in H^2(]0, 1[) \times \mathbb{C}$ $(u \neq 0)$ such that

$$-d^2u/dx^2 = \lambda u \ .$$

We can find for any λ two linearly independent solutions.

[1]Here is a more "physical" version. If u is normalized by $||u||_{L^2(I\!\!R)} = 1$, $|u|^2 \ dx$ defines a probability measure. One can define $\langle x \rangle = \int x|u|^2 dx$, mean value of the position and the variance $\sigma_x = \langle (x - \langle x \rangle)^2 \rangle$. Similarly, we can consider: $\langle D_x \rangle := \int (D_x u) \cdot \bar{u}(x) dx$ and $\sigma_{D_x} := ||(D_x - \langle D_x \rangle)u||^2$. Then (1.2.11) can be extended in the form :

$$\sigma_x \cdot \sigma_{D_x} \geq \frac{1}{4} \ .$$

1.3.2 The periodic problem

Here we consider pairs $(u,\lambda) \in H^{2,per}(]0,1[) \times \mathbb{C}$ $(u \neq 0)$ such that

$$-d^2u/dx^2 = \lambda u \; .$$

Here

$$H^{2,per}(]0,1[) = \{u \in H^2(]0,1[) \; , \; u(0) = u(1) \text{ and } u'(0) = u'(1)\} \; .$$

Here we recall that $H^2(]0,1[)$ is included in $C^1([0,1])$ by the injection theorem of Sobolev. It is an easy exercise to show that the pairs are described by two families

- $$\lambda = 4\pi^2 n^2 \; , \; u_n = \mu \cos 2\pi n x \; , \quad \text{for } n \in \mathbb{N} \; , \; \mu \in \mathbb{R} \setminus 0 \; ,$$

- $$\lambda = 4\pi^2 n^2 \; , \; v_n = \mu \sin 2\pi n x \; , \quad \text{for } n \in \mathbb{N}^* , \; \mu \in \mathbb{R} \setminus 0 \; .$$

One observes that $\lambda = 0$ is the lowest eigenvalue and that its multiplicity is one. This means that the corresponding eigenspace is of dimension one (the other eigenspaces are of dimension 2). Moreover an eigenvector in this subspace neither vanishes in $]0,1[$. This is quite evident because $u_0 = \mu \neq 0$.
One observes also that one can find an orthonormal basis in $L^2(]0,1[)$ of eigenvectors by normalizing the family $(\cos 2\pi n x \; (n \in \mathbb{N}), \sin 2\pi n x \; (n \in \mathbb{N}^*))$ or the family $\exp 2\pi i n x$ $(n \in \mathbb{Z})$.
We are just recovering the L^2-theory of the Fourier series.

1.3.3 The Dirichlet problem

Here we consider pairs $(u,\lambda) \in H^{2,D}(]0,1[) \times \mathbb{C}$ $(u \neq 0)$ such that $-d^2u/dx^2 = \lambda u$.
Here

$$H^{2,D}(]0,1[) = \{u \in H^2(]0,1[) \; , \; u(0) = u(1) = 0\} \; .$$

It is again an easy exercise to show that the pairs are described by

$$\lambda = \pi^2 n^2 \; , \; v_n = \mu \sin \pi n x \; , \quad \text{for } n \in \mathbb{N}^* , \; \mu \in \mathbb{R} \setminus 0 \; .$$

One observes that $\lambda = \pi^2$ is the lowest eigenvalue, that its multiplicity is one (Here all the eigenspaces are one-dimensional) and that an eigenvector in this subspace neither vanishes in $]0,1[$.

1.3.4 The Neumann problem

Here we consider pairs
$(u,\lambda) \in H^{2,N}(]0,1[) \times \mathbb{C}$ $(u \neq 0)$ such that

$$-d^2u/dx^2 = \lambda u \; .$$

Here

$$H^{2,N}(]0,1[) = \{u \in H^2(]0,1[)\ ,\ u'(0) = u'(1) = 0\}\ .$$

It is again an easy exercise to show that the pairs are described by

$$\lambda = \pi^2 n^2\ ,\ v_n = \mu \cos \pi n x\ ,\quad \text{for } n \in \mathbb{N},\ \mu \in \mathbb{R} \setminus 0\ .$$

One observes that $\lambda = 0$ is the lowest eigenvalue, that its multiplicity is one (Here all the eigenspaces are one-dimensional) and that the corresponding eigenspace is of dimension one and that an eigenvector in this subspace neither vanishes in $]0,1[$.

1.3.5 Conclusion

All these examples enter in the so called Sturm-Liouville theory. We emphasize on one property which was always verified in each case: the eigenspace corresponding to the lowest eigenvalue is one dimensional and one can find a strictly positive (in $]0,1[$ or in $]-\infty,+\infty[$ in the case of the harmonic oscillator) corresponding eigenvector. This will be explained later. **We suggest to the reader to come back at this introduction after have read the course. He will surely realize that the theory has permitted to clarify many badly posed problems.**

2 Unbounded operators, adjoints, Selfadjoint operators

2.1 Unbounded operators

We consider an Hilbert space $\mathcal{H}$. The scalar product will be denoted by : $< u\ ,\ v >_{\mathcal{H}}$ or more simply by : $< u\ ,\ v >$ when no confusion is possible. We take the convention that the scalar product is antilinear with respect to the second argument.
A linear operator (or more simply an operator) T in $\mathcal{H}$ is a linear map $u \mapsto Tu$ defined on a subspace $\mathcal{H}_0$ of $\mathcal{H}$, denoted by $D(T)$ and which is called the domain of T. We shall also denote by $R(T)$ (or Im T or $Range(T)$) the range of $\mathcal{H}_0$ by T. We shall say that T is bounded if it is continuous from $D(T)$ into $\mathcal{H}$. When $D(T) = \mathcal{H}$, we recover the notion of linear continuous operators on $\mathcal{H}$. We recall that with

$$||T||_{\mathcal{L}(\mathcal{H})} = \sup_{u \neq 0} \frac{||Tu||_{\mathcal{H}}}{||u||_{\mathcal{H}}}\ , \tag{2.1.1}$$

$\mathcal{L}(\mathcal{H})$ is a Banach space. When $D(T)$ is not equal to $\mathcal{H}$, we shall always assume that

$$D(T) \text{ is dense in } \mathcal{H}. \tag{2.1.2}$$

Note that, if T is bounded, then it admits a unique continuous extension to $\mathcal{H}$. In this case the generalized notion is not interesting.
We are mainly interested in extensions of this theory and would like to consider unbounded operators.
– When using this word, we mean more precisely "non necessarily bounded operators". –
The point is to find a natural notion replacing this boundedness. This is the object of the next definition.

The operator is called **closed** if the graph $G(T)$ of T is closed in $\mathcal{H} \times \mathcal{H}$. We recall that

$$G(T) := \{(x, y) \in \mathcal{H} \times \mathcal{H} \ , \ x \in D(T) \ , \ y = Tx\} \ . \tag{2.1.3}$$

Equivalently, we can say

Definition 2.1.1. *(Closed operators).*
Let T be an operator in $\mathcal{H}$ with (dense) domain $D(T)$. We say that T is closed if the conditions

- $u_n \in D(T)$,
- $u_n \to u$ *in* $\mathcal{H}$,
- $Tu_n \to v$ *in* $\mathcal{H}$

imply

- $u \in D(T)$,
- $v = Tu$.

Example 2.1.2. .
$T_0 = -\Delta$ *with* $D(T_0) = C_0^\infty(\mathbb{R}^m)$ *is not closed.*
For this, it is enough to consider[2] some u in $H^2(\mathbb{R}^m)$ and not in $C_0^\infty(\mathbb{R}^n)$ and to consider a sequence $u_n \in C_0^\infty$ such that $u_n \to u$ in H^2. The sequence $(u_n, -\Delta u_n)$ is contained in $G(T_0)$ and converges in $L^2 \times L^2$ to $(u, -\Delta u)$ which does not belong to $G(T_0)$.

[2] We recall that the Sobolev space $H^s(\mathbb{R}^m)$ is defined as the space

$$H^s(\mathbb{R}^m) := \{u \in \mathcal{S}'(\mathbb{R}^m) \mid (1 + |\xi|^2)^{\frac{s}{2}} \hat{u} \in L^2(\mathbb{R}^m)\} \ .$$

Here $\mathcal{S}'$ is the set of tempered distributions. $H^s(\mathbb{R}^m)$ is equipped with the natural Hilbertian norm :

$$||u||^2_{H^s} := \int_{\mathbb{R}^m} (1 + |\xi|^2)^s |\hat{u}(\xi)|^2 d\xi \ .$$

By Hilbertian norm, we mean that the norm is associated to a scalar product.
When $s \in \mathbb{N}$, we can also describe H^s by

$$H^s(\mathbb{R}^m) := \{u \in L^2(\mathbb{R}^m) \mid D_x^\alpha u \in L^2 \ , \forall \alpha \text{ s. t. } |\alpha| \leq s\} \ .$$

The natural norm associated with the second definition is equivalent to the first one.

$T_1 = -\Delta$ with $D(T_1) = H^2(I\!\!R^m)$ is closed.
We observe indeed that if $u_n \to u$ in L^2 and $(-\Delta u_n) \to v$ in L^2 then $-\Delta u = v \in L^2$. The last step is to observe that this implies that $u \in H^2(I\!\!R^m)$ (take the Fourier transform) and $(u, -\Delta u) \in G(T_1)$.

This example suggests another definition.

Definition 2.1.3. .
The operator T is called **closable** *if the closure of the graph of T is a graph.*

We can then define the closure $\overline{T}$ of the operator by a limit procedure via its graph. We observe indeed that we can consider

$$D(\overline{T}) := \{x \in \mathcal{H} \mid \exists y \text{ s. t. } (x, y) \in \overline{G(T)}\}.$$

For any $x \in D(\overline{T}$, the assumption that $\overline{G(T)}$ is a graph says that y is unique. One can consequently define $\overline{T}$ by

$$\overline{T}x = y\ .$$

In a more explicit way, the domain of $\overline{T}$ is the set of the $x \in \mathcal{H}$ such that $x_n \to x \in \mathcal{H}$ and Tx_n is a Cauchy sequence and for such x's we define $\overline{T}$ by

$$\overline{T}x = \lim_{n \to +\infty} Tx_n\ .$$

Example 2.1.4. .
$T_0 = -\Delta$ with $D(T_0) = C_0^\infty$ is closable and is closure is T_1.

Let us prove it, as an exercise. Let $\overline{T_0}$ the closure of T_0. Let $u \in L^2$ such that there exists $u_n \in C_0^\infty$ such that $u_n \to u$ in L^2 and $-\Delta u_n \to v$ in L^2. We get by distribution theory that $u \in L^2$ satisfies $-\Delta u = v \in L^2$. By the ellipticity of the Laplacian (use the Fourier transform), we get that $u \in H^2$. We have consequently shown that $D(\overline{T_0}) \subset H^2$. But C_0^∞ is dense in H^2 and this gives the inverse inclusion : $H^2 \subset D(\overline{T_0})$. We have consequently,

$$H^2 = D(T_1) = D(\overline{T_0})\ ,$$

and it is then easy to verify that $T_1 = \overline{T_0}$.

These examples lead to a more general question.

Realization of differential operators as unbounded operators. Let $\Omega \subset I\!\!R^n$ and let $P(x, D_x)$ be a partial differential operator with C^∞ coefficients in Ω. Then the operator P^Ω defined by

$$D(P^\Omega) = C_0^\infty(\Omega)\ ,\ P^\Omega u = P(x, D_x)u, \forall u \in C_0^\infty(\Omega)\ ,$$

is closable. Here $\mathcal{H} = L^2(\Omega)$. We have indeed

$$\overline{G(P^\Omega)} \subset \tilde{G}_\Omega := \{(u,f) \in \mathcal{H} \times \mathcal{H} \mid P(x,D_x)u = f \text{ in } \mathcal{D}'(\Omega)\} \ .$$

The proof is then actually a simple exercise in distribution theory. This inclusion shows that $\overline{G(P^\Omega)}$ is a graph. Note that the corresponding operator is defined as P^Ω_{min} with domain

$$D(P^\Omega_{min}) = \\ \{u \in L^2(\Omega) \mid \exists \text{ a sequence } u_n \in C_0^\infty(\Omega) \text{ s.t } \left\{ \begin{array}{l} u_n \to u \text{ in } L^2(\Omega) \\ P(x,D_x)u_n \text{ converges in } L^2(\Omega) \end{array} \right. \} .$$

The operator P^Ω_{min} is then defined for such u by

$$P^\Omega_{min} u = \lim_{n\to+\infty} P(x,D_x)u_n \ .$$

Using the theory of distributions, this gives :

$$P^\Omega_{min} u = P(x,D_x)u \ .$$

Note that there exists also a natural closed operator whose graph is $\tilde{G}_\Omega$ and extending P^Ω : this is the operator $\tilde{P}^\Omega$, with domain

$$\tilde{D}^\Omega := \{u \in L^2(\Omega) \ , \ P(x,D_x)u \in L^2(\Omega)\} \ ,$$

and such that

$$\tilde{P}^\Omega u = P(x,D_x)u \ , \forall u \in \tilde{D}^\Omega \ ,$$

where the last equality is in the distributional sense. Note that $\tilde{P}^\Omega$ is an extension of P^Ω_{min} in the sense that :

$$\tilde{P}^\Omega u = P^\Omega_{min} u \ , \ \forall u \in D(P^\Omega_{min}) \ .$$

Conclusion.

We have associated with a differential operator $P(x,D_x)$ in an open set Ω three natural operators. It would be important to know better the connection between these three operators.

Remark 2.1.5. *(Link between continuity and closeness).*
If $\mathcal{H}_0 = \mathcal{H}$, the closed graph Theorem says that a closed operator T is continuous.

2.2 Adjoints.

When we have an operator T in $\mathcal{L}(\mathcal{H})$, it is easy to define the Hilbertian adjoint $T^\star$ by the identity :

$$\langle T^\star u, v\rangle_{\mathcal{H}} = \langle u, Tv\rangle_{\mathcal{H}} \ , \forall u \in \mathcal{H}, \forall v \in \mathcal{H} \ . \tag{2.2.1}$$

The map $v \mapsto \langle u, Tv\rangle_{\mathcal{H}}$ defines a continuous antilinear map on $\mathcal{H}$ and can be expressed, using Riesz's Theorem, by the scalar product by an element which is called $T^* u$. The linearity and the continuity of T^* is then easily proved using (2.2.1).

Let us now give the definition of the adjoint of an unbounded operator.

Definition 2.2.1. *(Adjoint).*
If T is an unbounded operator whose domain $D(T)$ is dense in $\mathcal{H}$, we first define the domain of T^* by

$$\begin{aligned} D(T^*) \quad &= \{u \in \mathcal{H}, D(T) \ni v \mapsto \langle u, Tv\rangle, \\ &\text{can be extended as an antilinear continuous form on } \mathcal{H}\} \ . \end{aligned}$$

Using the Riesz's Theorem, there exists $f \in \mathcal{H}$ such that

$$(f, v) = (u, Tv) \ , \ \forall u \in D(T^*), \forall v \in D(T) \ .$$

The uniqueness of f is a consequence of the density of $D(T)$ in $\mathcal{H}$ and we can then define T^* by

$$T^* u = f \ .$$

Remark 2.2.2. *.*
When $D(T) = \mathcal{H}$ and if T is bounded , then we recover as T^* the Hilbertian adjoint.

Example 2.2.3. *.*

$$T_0^* = T_1 \ .$$

Let us treat in detail this example. We get

$$\begin{aligned} D(T_0^*) \quad &= \{u \in L^2 \mid \text{ the map } C_0^\infty \ni v \mapsto \langle u, -\Delta v\rangle, \\ &\text{can be extended as an antilinear continuous form on } L^2\} \ . \end{aligned}$$

We observe that

$$\langle u, -\Delta v\rangle_{L^2} = \int_{I\!R^m} u(\overline{-\Delta v}) dx = (-\Delta u)(\bar{v}) \ .$$

The last equality just means that we are considering the distribution $(-\Delta u)$ on the test function $\bar{v}$. The condition appearing in the definition is just that this distribution is in $L^2(I\!R^m)$. Coming back to the definition of $D(T_0^*)$, we get

$$D(T_0^*) = \{u \in L^2 \mid -\Delta u \in L^2\} \ .$$

But as already seen, this gives

$$D(T_0^*) = H^2 \ , \ T_0^* u = -\Delta u \ , \ \forall u \in H^2 \ .$$

Proposition 2.2.4. *.*
T^* is a closed operator.

Proof.
Let (v_n) be a sequence in $D(T^*)$ such that $v_n \to v$ in $\mathcal{H}$ and $T^* v_n \to w^*$ in $\mathcal{H}$ for some pair (v, w^*). We would like toshow that (v, w^*) belongs to the graph of T^*.
For all $u \in D(T)$, we have :

$$< Tu, v > = \lim_{n \to +\infty} < Tu, v_n > = \lim_{n \to +\infty} < u, T^* v_n > = < u, w^* > \ . \qquad (2.2.2)$$

Coming back to the definition of $D(T^*)$, we get from (2.2.2) that $v \in D(T^*)$ and $T^*v = w^*$. This means that (v, w^*) belongs to the graph of T^*.

Proposition 2.2.5. .
Let T be an operator in $\mathcal{H}$ with domain $D(T)$. Then the graph $G(T^*)$ of T^* can be characterized by

$$G(T^*) = \{V(\,\overline{G(T)}\,)\}^\perp \,, \tag{2.2.3}$$

where V is the unitary operator defined on $\mathcal{H} \times \mathcal{H}$ by

$$V\{u, v\} = \{v, -u\} \,. \tag{2.2.4}$$

Proof.
We just observe that for any $u \in D(T)$ and $(v, w^*) \in \mathcal{H} \times \mathcal{H}$ we have the identity

$$< V(u, Tu)\,,\,(v, w^*) >_{\mathcal{H}\times\mathcal{H}} = < Tu, v >_{\mathcal{H}} - < u, w^* >_{\mathcal{H}} \quad .$$

The right hand side vanishes for all $u \in D(T)$ iff $v \in D(T^*)$ and $w^* = T^*v$, that is if (v, w^*) belongs to $G(T^*)$. The left hand side vanishes for all $u \in D(T)$ iff (v, w^*) belongs to $V(G(T))^\perp$.
Standard Hilbertian analysis, using the continuity of V and $V^{-1} = -V$, then shows that

$$V(G(T))^\perp = \overline{V(G(T))}^\perp = V(\overline{G(T)})^\perp \,.$$

End of proof We have not analyzed till now under which condition the domain of the adjoint is dense in $\mathcal{H}$. This is one of the objects of the next theorem.

Theorem 2.2.6. .
Let T be a closable operator. Then we have

1. *$D(T^*)$ is dense in $\mathcal{H}$,*
2. *$T^{**} := (T^*)^* = \overline{T}$, where we have denoted by $\overline{T}$ the operator whose graph is $\overline{G(T)}$.*

Proof.
For the first point, let us assume that $D(T^*)$ is not dense in $\mathcal{H}$. Then there exists $w \neq 0$ such that w is orthogonal to $\overline{D(T^*)}$.
We consequently get that for any $v \in D(T^*)$, we have

$$< (0, w)\,,\,(T^*v, -v) >_{\mathcal{H}\times\mathcal{H}} = 0 \,.$$

This shows that $(0, w)$ is orthogonal to $V(G(T^*))$.
But the previous proposition gives :

$$V(\overline{G(T)}) = G(T^*)^\perp \,.$$

We now apply V to this identity and get, using $V^2 = -I$,

$$V\left(G(T^*)^\perp\right) = \overline{G(T)} \; .$$

But, for any closed subspace $\mathcal{M} \subset \mathcal{H}$, we have

$$V(\mathcal{M}^\perp) = [V(\mathcal{M})]^\perp \; ,$$

as a consequence of the identity

$$< V(u,v) \; , \; (x,y) >_{\mathcal{H}\times\mathcal{H}} = < (u,v) \; , \; V(x,y) >_{\mathcal{H}\times\mathcal{H}} \; .$$

We finally obtain that $(0,w)$ belongs to the closure of the graph of T, that is the graph of $\overline{T}$ because T is closable, and consequently that $w = 0$. This gives the contradiction.
For the second point, we first observe that, $D(T^*)$ being dense in $\mathcal{H}$, we can of course define $(T^*)^*$. Using again the proposition and the closeness of T^*, we obtain $G(T^{**}) = \overline{G(T)}$ and $T^{**} = \overline{T}$.
This means more explicitly that

$$D(T^{**}) = D(\overline{T}) \; , \; T^{**}u = \overline{T}u \; , \; \forall u \in D(\overline{T}) \; .$$

End of the proof.

2.3 Symmetric and selfadjoint operators.

Definition 2.3.1. *(symmetric operators).*
We shall say that $T : \mathcal{H}_0 \mapsto \mathcal{H}$ is **symmetric** *if it satisfies*

$$\langle Tu, v\rangle_{\mathcal{H}} = \langle u, Tv\rangle_{\mathcal{H}} \; , \forall u, v \; \in \mathcal{H}_0 \; .$$

Example 2.3.2. .
$T = -\Delta$ *with* $D(T) = C_0^\infty(I\!R^m)$.

If T is symmetric it is easy to see that

$$D(T) \subset D(T^*) \tag{2.3.1}$$

and that

$$Tu = T^*u \; , \; \forall u \in D(T) \; . \tag{2.3.2}$$

The two conditions (2.3.1) and (2.3.2) express the property that $(T^*, D(T^*))$ is an extension of $(T, D(T))$.

Exercise 2.3.3. .
Show that a symmetric operator is closable.

Hint :
Show that, if u_n is a sequence in $D(T)$ such that, for some $\ell \in \mathcal{H}$, we have $u_n \to 0$ and $Tu_n \to \ell$, then $\ell = 0$.

For a symmetric operator, we have consequently two natural closed extensions:

- The **minimal** one denoted by T_{min} (or previously $\overline{T}$), which is obtained by taking the operator whose graph is the closure of the graph of T,
- The **maximal** one denoted by T_{max} the adjoint of T.

If T^{sa} is a selfadjoint extension of T, then T^{sa} is automatically an extension of T_{min} and admits[3] as an extension T_{max}.

Definition 2.3.4. .
We shall say that T is **selfadjoint** *if $T^* = T$, i. e.*

$$D(T) = D(T^*) \ , \quad \textit{and} \ \ Tu = T^* u \ , \quad \forall u \in D(T) \ .$$

Starting of a symmetric operator, it is a natural question to ask for the existence and the uniqueness of a selfadjoint extension. We shall see later that a natural way is to prove the equality between T_{min} and T_{max}.

Exercise 2.3.5. Analysis of differential operators.
Give simple criteria in the case of operators with constant coefficients for obtaining symmetric operators on $C_0^\infty(\mathbb{R}^m)$. In particular, verify that the operator $D_{x_j} = \frac{1}{i}\partial_{x_j}$ is symmetric.

Proposition 2.3.6. .
A selfadjoint operator is closed.

This is immediate because T^* is closed.

Proposition 2.3.7. .
Let T be a selfadjoint operator which is invertible. Then T^{-1} is also selfadjoint.

By invertible, we mean here that T admits an inverse T^{-1} from $R(T)$ into $D(T)$. Let us first show that $R(T)$ is dense in $\mathcal{H}$. Let $w \in \mathcal{H}$ such that $< Tu, w >_{\mathcal{H}} = 0$, $\forall u \in D(T)$.
Coming back to the definition of T^*, this implies in particular that $w \in D(T^*)$ and $T^* w = 0$. But T is selfadjoint and injective and this implies that $w = 0$.
We consequently know that $D(T^{-1})$ is dense in $\mathcal{H}$.
Coming back to the analysis of the corresponding graphs it is now easy to show the second assertion by coming back to the corresponding graphs and by using Proposition 2.2.5.

Remark 2.3.8. .
If T is selfadjoint $T + \lambda I$ is selfadjoint for any real λ.

[3] Use Proposition 2.2.5.

3 Representation theorems

We assume that the reader knows about this material but recall it for completeness[4].

3.1 Riesz's Theorem.

Theorem 3.1.1. *(Riesz's Theorem).*
Let $u \mapsto F(u)$ a linear continuous form on $\mathcal{H}$. Then there exists a unique $w \in \mathcal{H}$ such that

$$F(u) = < u, w >_{\mathcal{H}} \, , \; \forall u \in \mathcal{H} \, . \tag{3.1.1}$$

There is a similar version with antilinear maps :

Theorem 3.1.2. *.*
Let $u \mapsto F(u)$ a antilinear continuous form on $\mathcal{H}$. Then there exists a unique $w \in \mathcal{H}$ such that

$$F(u) = < w, u >_{\mathcal{H}} \, , \; \forall u \in \mathcal{H} \, . \tag{3.1.2}$$

3.2 Lax-Milgram's situation.

Let us now consider a continuous sesquilinear form a defined on $V \times V$:

$$(u, v) \mapsto a(u, v) \, .$$

We recall that the continuity can be expressed by the existence of C such that

$$|a(u, v)| \leq C||u||_V \cdot ||v||_V \, , \; \forall u, v \in V \, . \tag{3.2.1}$$

It is immediate to associate, using the Riesz Theorem, a linear map $A \in \mathcal{L}(V)$ such that

$$a(u, v) = < Au, v >_V \, . \tag{3.2.2}$$

Definition 3.2.1. *(V-ellipticity) .*
We shall say that a is V-elliptic, if there exists $\alpha > 0$, such that

$$|a(u, u)| \geq \alpha ||u||_V^2 \, , \; \forall u \in V \, . \tag{3.2.3}$$

Theorem 3.2.2. *(Lax-Milgram's Theorem) .*
Let a be a continuous sesquilinear form on $V \times V$. If a is V-elliptic, then A is an isomorphism from V onto V.

[4]Here we follow, almost verbatim, the book of D. Huet [Hu].

The proof is in three steps.

Step 1.
A is injective. We get indeed from (3.2.3)

$$| < Au, u >_V | \geq \alpha ||u||_V^2 \ , \ \forall u \in V \ . \tag{3.2.4}$$

Using Cauchy-Schwarz in the left hand side, we first get

$$||Au||_V \cdot ||u||_V \geq \alpha ||u||_V^2 \ , \ \forall u \in V \ ,$$

and consequently

$$||Au||_V \geq \alpha ||u||_V \ , \ \forall u \in V \ . \tag{3.2.5}$$

This gives clearly the injectivity but actually more.

Step 2.
$A(V)$ is dense in V.
Let us consider $u \in V$ such that $< Av, u >_V = O$, $\forall v \in V$. In particular, we can take $v = u$. This gives $a(u, u) = 0$ and $u = 0$ using (3.2.3).

Step 3.
$R(A) := A(V)$ is closed in V.
Let v_n a Cauchy sequence in $A(V)$ and u_n the sequence such that $Au_n = v_n$. But using (3.2.5), we get that u_n is a Cauchy sequence which is consequently convergent to some $u \in V$. But the sequence Au_n tends to Au by continuity and this shows that $v_n \to v = Au$ and $v \in R(A)$.

Step 4.
The three previous steps show that A is bijective. The continuity of A^{-1} is a consequence of (3.2.5) or of the Banach Theorem.

Remark 3.2.3. .
Let us suppose for simplicity that V is a real Hilbert space. Using the isomorphism $\mathcal{I}$ between V and V' given by the Riesz Theorem, one gets also a natural operator $\mathcal{A}$ from V onto V' such that

$$a(u, v) = (\mathcal{A}u)(v) \ , \ \forall v \in V \ . \tag{3.2.6}$$

We have

$$\mathcal{A} = \mathcal{I} \circ A \ .$$

3.3 An alternative point of view: $V, \mathcal{H}, V'$.

We now consider two Hilbert spaces V and $\mathcal{H}$ such that

$$V \subset \mathcal{H} \ . \tag{3.3.1}$$

By this notation of inclusion, we mean also that the injection of V into $\mathcal{H}$ is continuous or equivalently that there exists a constant $C > 0$ such that, for any $u \in V$, we have

$$||u||_{\mathcal{H}} \leq C||u||_V \, .$$

We also assume that

$$V \text{ is dense in } \mathcal{H}. \tag{3.3.2}$$

In this case, there exists a natural injection from $\mathcal{H}$ into the space V' which is defined as the space of continuous linear forms on V. We observe indeed that if $h \in \mathcal{H}$ then $V \ni u \mapsto < u, h >_{\mathcal{H}}$ is continuous on V. So there exists $\ell_h \in V'$ such that

$$\ell_h(u) = < u, h >_{\mathcal{H}} \, , \forall u \in V \, .$$

The injectivity is a consequence of the density of V in $\mathcal{H}$.
We can also associate to the sesquilinear form a an unbounded operator S on $\mathcal{H}$.
We first define $D(S)$ by

$$D(S) = \{u \in V \mid v \mapsto a(u, v) \text{ is continuous on } V \text{ for the topology induced by } \mathcal{H}\}. \tag{3.3.3}$$

Using again the Riesz Theorem and assumption (3.3.2), this defines Su in $\mathcal{H}$ by

$$a(u, v) = < Su, v >_{\mathcal{H}} \, , \; \forall v \in V \, . \tag{3.3.4}$$

Theorem 3.2.2 is completed by

Theorem 3.3.1. .
Under the same assumptions, S is bijective from $D(S)$ onto $\mathcal{H}$ and $S^{-1} \in \mathcal{L}(\mathcal{H})$. Moreover $D(S)$ is dense in $\mathcal{H}$.

Proof.
We first show that S is injective. This is a consequence of

$$\alpha||u||^2_{\mathcal{H}} \leq C\,\alpha||u||^2_V \leq Ca(u, u) = C \, < Su, u >_{\mathcal{H}} \leq C\,||Su||_{\mathcal{H}} \cdot ||u||_{\mathcal{H}} \, , \; \forall u \in D(S) \, ,$$

which leads to

$$\alpha||u||_{\mathcal{H}} \leq C\,||Su||_{\mathcal{H}} \, , \; \forall u \in D(S) \, . \tag{3.3.5}$$

We get directly the surjectivity in the following way. If $h \in \mathcal{H}$ and if $w \in V$ is chosen such that

$$< h, v >_{\mathcal{H}} = < w, v >_V \, , \forall v \in V \, ,$$

(which follows from Riesz's Theorem), we can take $u = A^{-1}w$ in V, which is a solution of

$$a(u, v) = < w, v >_V \quad .$$

We then show that $u \in D(S)$, using the identity

$$a(u,v) =< h, v >_{\mathcal{H}} \ , \ \forall v \in V \ ,$$

and get simultaneously

$$Su = h \ .$$

The continuity of S^{-1} is a consequence of (3.3.5).
Let us show the last statement of density.
Let $h \in \mathcal{H}$ s. t.

$$< u, h >_{\mathcal{H}} = 0 \ , \ \forall u \in D(S) \ .$$

By the surjectivity of S, there exists v s. t. :

$$Sv = h \ .$$

We get

$$< Sv, u >_{\mathcal{H}} = 0 \ , \ \forall u \in D(S)$$

Taking $u = v$ and using the $V - ellipticity$, we get that $v = 0$ and consequently $h = 0$.

We now consider an hermitian sesquilinear form, that is satisfying

$$a(u,v) = \overline{a(v,u)} \ , \ \forall u, v \in V \ . \tag{3.3.6}$$

This property is transmitted to S in the following way

Theorem 3.3.2. .
If a is hermitian and V-elliptic, we have

1. *S is closed;*
2. *$S = S^*$;*
3. *$D(S)$ is dense in V.*

Proof of 2.
We first observe that the assumption of Hermiticity gives

$$< Su, v >_{\mathcal{H}} =< u, Sv >_{\mathcal{H}} \ , \ \forall u \in D(S) \ , \ \forall v \in D(S) \ . \tag{3.3.7}$$

In other words S is symmetric. This means in particular that

$$D(S) \subset D(S^*) \ . \tag{3.3.8}$$

Let $v \in D(S^*)$. Using the surjectivity of S, there exists $v_0 \in D(S)$ such that

$$Sv_0 = S^* v \ .$$

For all $u \in D(S)$, we get that

$$< Su, v_0 >_{\mathcal{H}} =< u, Sv_0 >_{\mathcal{H}} =< u, S^* v >_{\mathcal{H}} =< Su, v >_{\mathcal{H}} \ .$$

Using again the surjectivity of S, we get $v = v_0 \in D(S)$. This shows that $D(S) = D(S^*)$ and $Sv = S^*v$, $\forall v \in D(S)$.

Proof of 1.
S is closed because S^* is closed and $S = S^*$.

Proof of 3.
Let $h \in V$ such that

$$< u, h >_V = 0 \ , \ \forall u \in D(S) \ .$$

Let $f \in V$ such that $Af = h$ (A is an isomorphism from V onto V).
We then have

$$0 =< u, h >_V =< u, Af >_V = \overline{< Af, u >_V} = \overline{a(f, u)} = a(u, f) =< Su, f >_{\mathcal{H}} \ .$$

Using the surjectivity, we get $f = 0$ and consequently $h = 0$.

3.4 Neumann problem.

The reader should have some minimal knowledge of Sobolev Spaces and traces of distributions for reading this subsection (See for example Brézis [Br]). Let Ω be a bounded domain with regular boundary in $I\!R^m$. Take $\mathcal{H} = L^2(\Omega)$ and $V = H^1(\Omega)$. Let us consider the sesquilinear form :

$$a(u, v) = \int_\Omega \langle \nabla u \ , \ \nabla v \rangle_{\mathbb{C}^m} \, dx + \int_\Omega u \bar{v} dx \ .$$

According to the definition of the domain of S, we observe that, for $u \in D(S)$, then it should exist some $f \in L^2(\Omega)$ such that, for all $v \in H^1(\Omega)$:

$$a(u, v) = \int_\Omega f(x) \overline{v(x)} dx \ . \tag{3.4.1}$$

Then, one can find first show (by taking in (3.4.1) $v \in C_0^\infty(\Omega)$) that, in the sense of distribution,

$$-\Delta u + u = f \ , \tag{3.4.2}$$

and consequently that :

$$D(S) \subset W(\Omega) := \{ u \in H^1(\Omega) \ | \ -\Delta u \in L^2(\Omega) \} \ . \tag{3.4.3}$$

But this is not enough for characterizing the domain.
We refer to [Lio1], [Lio2], [LiMa] or better [DaLi], Vol. 4 (p. 1222-1225)) for a detailed explanation. We first recall the Green-Riemann Formula :

$$\int_\Omega \langle \nabla u \mid \nabla v \rangle = \int_\Omega (-\Delta u) \cdot \bar{v} dx + \int_{\partial\Omega} (\partial u / \partial \nu) \bar{v} \ d\mu_{\partial\Omega} \ , \tag{3.4.4}$$

where $d\mu_{\partial\Omega}$ is the induced measure on the boundary, which is clearly true for $u \in H^2(\Omega)$ (or for $u \in C^1(\overline{\Omega})$) and $v \in H^1(\Omega)$. We unfortunately do not know that $W(\Omega) \subset H^2(\Omega)$ and the inclusion in $H^1(\Omega)$ is not sufficient for defining the normal trace. But this formula can be extended in the following way.

We first observe that, for $v \in H^1_0(\Omega)$ and $u \in W$, we have :

$$\int_\Omega \langle \nabla u \mid \nabla v \rangle = \int_\Omega (-\Delta u) \cdot \bar{v} dx \ . \tag{3.4.5}$$

This shows that the expression

$$\Phi_u(v) := \int_\Omega \langle \nabla u \mid \nabla v \rangle - \int_\Omega (-\Delta u) \cdot \bar{v} dx \ ,$$

which is well defined for $u \in W$ and $v \in H^1(\Omega)$ depends only of the restriction of v to $\partial\Omega$.

If $v_0 \in C^\infty(\partial\Omega)$, we can then extend v_0 inside Ω as a function $v = Rv_0$ in $C^\infty(\overline{\Omega})$ and the distribution [5] is defined as the map $v_0 \mapsto \Phi_u(Rv_0)$.

One observes also that, when $u \in C^1(\overline{\Omega})$ or $u \in H^2(\Omega)$, the Green-Riemann formula shows that :

$$\Phi_u(v_0) = \int_{\partial\Omega} (\partial u / \partial \nu) \bar{v}_0 \ d\mu_{\partial\Omega} \ .$$

So we have found a natural way to extend the notion of trace of the normal derivative for $u \in W$ and we write :

$$\gamma_1 u = \Phi_u \ .$$

We then conclude (using (3.4.2) and again (3.4.1) this time in full generality) that :

$$D(S) = \{ u \in W(\Omega) \mid \gamma_1 u = 0 \} \ ,$$

and that

$$S = -\Delta + 1 \ .$$

The operator S is called the Neumann realization of the Laplacian in $L^2(\Omega)$.

Remark 3.4.1. .
Another "standard" regularity theorem shows that

$$D(S) = \{ u \in H^2(\Omega) \mid \gamma_1 u = 0 \} \ ,$$

and the notion of normal trace $u \mapsto \gamma_1 u$ for $u \in H^2(\Omega)$ is more standard[6].

[5] By chosing a more specific R continuous from $H^{\frac{1}{2}}(\partial\Omega)$ into $H^1(\Omega)$, we get that Φ_u can be extended as a linear form on $H^{\frac{1}{2}}(\partial\Omega)$.

[6] The trace is in $H^{\frac{1}{2}}(\partial\Omega)$.

4 Semi-bounded operators and Friedrichs extension.

4.1 Definition

Definition 4.1.1. .
Let T_0 be a symmetric unbounded operator of domain $D(T_0)$. We say that T_0 is semibounded (from below) if there exists a constant C such that

$$< T_0 u, u >_{\mathcal{H}} \geq -C ||u||^2_{\mathcal{H}} \ , \ \forall u \in D(T_0) \ . \tag{4.1.1}$$

Example 4.1.2. *(The Schrödinger operator).*
We consider on $\mathbb{R}^m$ the operator

$$P_V(x, D_x) := -\Delta + V(x) \ , \tag{4.1.2}$$

where $V(x)$ is a continuous function on $\mathbb{R}^m$ (called the potential) such that there exists C s.t. :

$$V(x) \geq -C \ , \ \forall x \in \mathbb{R}^m \ . \tag{4.1.3}$$

Then the operator T_0 defined by $D(T_0) = C_0^\infty(\mathbb{R}^m)$ and

$$T_0 u = P_V(x, D_x) u \ , \ \forall u \in D(T_0) \ ,$$

is a symmetric, semibounded operator.
We have indeed, with $\mathcal{H} = L^2(\mathbb{R}^m)$,

$$\begin{array}{ll} < P(x, D_x) u, u >_{\mathcal{H}} & = \int_{\mathbb{R}^m} (-\Delta u + V u) \cdot \bar{u} \ dx \\ & = \int_{\mathbb{R}^m} |\nabla u(x)|^2 dx + \int_{\mathbb{R}^m} V(x) |u(x)|^2 \ dx \\ & \geq -C ||u||^2_{\mathcal{H}} \ . \end{array} \tag{4.1.4}$$

Exercise 4.1.3. .
Let us consider on $L^2(\mathbb{R}^2; \mathbb{C}^2)$ the operator $\sum_{j=1}^2 \alpha_j D_{x_j}$ with domain $\mathcal{S}(\mathbb{R}^2; \mathbb{C}^2)$. Here the α_j are 2×2 Hermitian matrices such that :

$$\alpha_j \cdot \alpha_k + \alpha_k \cdot \alpha_j = 2 \delta_{jk} \ .$$

Show that this operator symmetric but not semi-bounded.

4.2 Analysis of the Coulomb case.

There are two important inequalities which are useful when considering the Coulomb case which plays an important role in atomic Physics. By Coulomb case, we mean the analysis on $\mathbb{R}^3$ of the operator

$$S_Z := -\Delta - \frac{Z}{r} \ ,$$

or of the Klein-Gordon operator

$$K_Z := \sqrt{-\Delta+1} - \frac{Z}{r} \; .$$

The operator $\sqrt{-\Delta+1}$ can easily defined on $\mathcal{S}(I\!\!R^3)$, using the Fourier transform $\mathcal{F}$, by

$$\mathcal{F}(\sqrt{-\Delta+1}u)(p) = \sqrt{p^2+1}(\mathcal{F}u)(p) \; .$$

The first one is the Hardy Inequality (which can be found for example in the book of Kato ([Ka], p. 305-307)) :

$$\int_{I\!\!R^3} |x|^{-2}|u(x)|^2 dx \leq 4\int_{I\!\!R^3} |p|^2|\hat{u}(p)|^2 dp \tag{4.2.1}$$

and the second one is due to Kato and says that

$$\int_{I\!\!R^3} |x|^{-1}|u(x)|^2 dx \leq \frac{\pi}{2}\int_{I\!\!R^3} |p|\;|\hat{u}(p)|^2 dp \tag{4.2.2}$$

One proof of the Hardy inequality consists in writing that, for any $\gamma \in I\!\!R$ and any $u \in C_0^\infty(I\!\!R^3)$, we have :

$$\int_{I\!\!R^3} |\nabla u - \gamma\frac{x}{|x|^2}u|^2 \; dx \geq 0 \; . \tag{4.2.3}$$

This leads to :

$$\int_{I\!\!R^3} |\nabla u|^2 + \gamma^2\frac{1}{|x|^2}u|^2 \; , dx \geq 2\gamma\int_{I\!\!R^3} \nabla u \cdot \frac{x}{|x|^2}u \; dx \; .$$

But an integration by part gives :

$$\begin{aligned} 2\int_{I\!\!R^3} \nabla u \cdot \tfrac{x}{|x|^2}u \; dx &= \int_{I\!\!R^3} |u|^2(\mathrm{div}\,(\tfrac{x}{|x|^2}))\; dx \\ &= \int_{I\!\!R^3} |u|^2(\mathrm{div}\,(\tfrac{x}{|x|^2}))\; dx \\ &= \int_{I\!\!R^3} |u|^2(\tfrac{1}{|x|^2})\; dx \; . \end{aligned}$$

Optimizing over γ leads to $\gamma = \frac{1}{2}$ and gives then the result.

Remark 4.2.1. .
The same idea works for $N \geq 3$ but fails for $N = 2$. So a good exercise[7] is to look for substitutes in this case by starting from the inequality :

$$\int_{I\!\!R^3} |\nabla u - \gamma(x)\frac{x}{|x|^2}u|^2 \; dx \geq 0 \; . \tag{4.2.4}$$

The function $\gamma(x)$ can be assumed radial : $\gamma(x) = g(|x|)$ and the question is to find a differential inequality on g leading at a weaker Hardy's type inequality. One can for example try $g(r) = \ln(r)$.

[7] We thank M.J. Esteban for explaining to us the trick.

For the proof of Kato's inequality, there is a another tricky nice estimate which, as far as we know, goes back to Hardy and Littlewood. In the case of the Coulomb potential, we can write:

$$\begin{aligned}\int_{I\!R^3}\int_{I\!R^3}\hat{u}(p)\tfrac{1}{|p-p'|^2}\overline{\hat{u}}(p')dp\cdot dp' &= \int_{I\!R^3\times I\!R^3}\hat{u}(p)\tfrac{h(p)}{h(p')}\cdot\tfrac{h(p')}{h(p)}\tfrac{1}{|p-p'|^2}\overline{\hat{u}}(p')dp\cdot dp' \\ &= \int_{I\!R^3\times I\!R^3}\tfrac{1}{|p-p'|}\hat{u}(p)\tfrac{h(p)}{h(p')}\cdot\tfrac{h(p')}{h(p)}\tfrac{1}{|p-p'|}\overline{\hat{u}}(p')dp\cdot dp'\ ,\end{aligned}$$

and we then Cauchy-Schwarz this equality in order to get

$$\begin{aligned} &|\int\int\hat{u}(p)\tfrac{1}{|p-p'|^2}\overline{\hat{u}}(p')dp\cdot dp'| \\ &\leq\left(\int|\hat{u}(p)|^2|\tfrac{h(p)}{h(p')}|^2\tfrac{1}{|p-p'|^2}dp'\ dp\right)^{\frac{1}{2}}\times\left(\int|\hat{u}(p')|^2|\tfrac{h(p')}{h(p)}|^2\tfrac{1}{|p-p'|^2}dp'\ dp\right)^{\frac{1}{2}} \\ &=\int|\hat{u}(p)|^2(\int|\tfrac{h(p)}{h(p')}|^2\tfrac{1}{|p-p'|^2}dp')\ dp \\ &=\int h(p)^2|\hat{u}(p)|^2(\int|\tfrac{1}{h(p')}|^2\tfrac{1}{|p-p'|^2}dp')\ dp\ .\end{aligned}$$

We now write $|p'|=\omega'|p|$ in the integral $\int|\frac{1}{h(p')}|^2\frac{1}{|p-p'|^2}dp'$. We then take $h(p)=|p|$. The integral becomes

$$\int|\frac{1}{h(p')}|^2\frac{1}{|p-p'|^2}dp'=|p|^{-1}\int\frac{1}{|\omega'|^2|\omega-\omega'|^2}d\omega'\ ,$$

with $p=\omega|p|$.
This is clearly seen as a convergent integral and, using the invariance by rotation, independent of ω so we can compute it with $\omega=(1,0,0)$.
We finally obtain

$$|\int\int\hat{u}(p)\frac{1}{|p-p'|^2}\overline{\hat{u}}(p')\ dp.dp'|\leq\ \text{const.}\ \cdot\int_{I\!R^3}|p|||\hat{u}(p)|^2\ dp\ ,$$

for a very explicit constant. So we have proved Kato's inequality for some constant C. The optimization of the trick leads to $\frac{\pi}{2}$.

Let us now show how one can use these inequalities.
If we use (4.2.1), we get the semi-boundedness for any $Z>0$ for the Schrödinger Coulomb operator (using Cauchy-Schwarz Inequality).

$$\int_{I\!R^3}\frac{1}{r}|u|^2\ dx\leq(\int\frac{1}{r^2}|u|^2dx)^{\frac{1}{2}}\cdot||u||\ .$$

But we can rewrite the Hardy Inequality in the form

$$\int_{I\!R^3}\frac{1}{r^2}|u|^2\ dx\leq 4<-\Delta u,u>_{L^2(I\!R^3)}\ .$$

So we get, for any $\epsilon>0$,

$$\int_{I\!R^3}\frac{1}{r}|u|^2\ dx\leq\epsilon<-\Delta u,u>_{L^2}+\frac{1}{\epsilon}||u||^2\ .$$

This leads to :

$$< S_Z u, u >_{L^2} \geq (1 - \epsilon Z) < -\Delta u, u > -\frac{Z}{\epsilon} ||u||^2 \ .$$

Taking $\epsilon = \frac{1}{Z}$, we have finally shown that

$$< S_Z u, u >_{L^2} \geq -Z^2 ||u||^2 \ . \tag{4.2.5}$$

Here we are probably not optimal[8] but there is another way to see that the behavior with respect to Z is correct. We just observe some invariance of the model. Let us suppose that we have proved the inequality for $Z = 1$. In order to treat the general case, we make a change of variable $x = \rho y$. The operator S_Z becomes in the new coordinates :

$$\tilde{S}_Z = \rho^{-2}(-\Delta_y) - \frac{Z}{\rho y} \ .$$

Taking $\rho = Z^{-1}$, we obtain

$$\tilde{S}_Z = Z^2 \left(-\Delta_y - \frac{1}{y} \right) \ .$$

The other inequality (4.2.2) is with this respect much better and quite important for the analysis of the relativistic case. Let us see what we obtain in the case of Klein-Gordon using Kato's Inequality.
We have

$$< K_Z \, u \ , \ u >_{L^2} \geq (1 - Z\frac{\pi}{2}) < \sqrt{-\Delta + 1} \, u \ , \ u >_{L^2} \ .$$

Here the nature of the result is different. The proof gives only that K_Z is semibounded if $Z \leq \frac{2}{\pi}$. This is actually more than a technical problem !

4.3 Friedrichs's extension

Theorem 4.3.1. .
A symmetric semibounded operator T_0 on $\mathcal{H}$ (with $D(T_0)$ dense in $\mathcal{H}$) admits a selfadjoint extension.

The standard extension appearing in the proof is the so-called Friedrichs extension. This is a variant of Lax-Milgram's Lemma. We can assume indeed by possibly replacing T_0 by $T_0 + \lambda_0 Id$ that T_0 is strictly positive and more precisely that

$$< T_0 u, u >_{\mathcal{H}} \geq ||u||^2_{\mathcal{H}} \ , \ \forall u \in D(T_0) \ . \tag{4.3.1}$$

[8]It can be proven (see any standard book in quantum mechanics) that the negative spectrum of this operator is discrete and is described by a sequence of eigenvalues tending to 0 : $-\frac{Z}{4n^2}$ with $n \in \mathbb{N}^*$. An eigenvector related to the lowest eigenvalue $-\frac{1}{4}$ ($Z = 1$) is given by $x \mapsto \exp -\frac{1}{2}|x|$.

Let us consider the associated form a priori defined on $D(T_0) \times D(T_0)$:

$$(u,v) \mapsto a_0(u,v) := \langle T_0 u \, , \, v \rangle_{\mathcal{H}} \; . \tag{4.3.2}$$

The inequality (4.3.1) says that

$$a_0(u,u) \geq ||u||^2_{\mathcal{H}} \; , \; \forall u \in D(T_0) \; . \tag{4.3.3}$$

We introduce V as the completion in $\mathcal{H}$ of $D(T_0)$ for the norm

$$u \mapsto p_0(u) = \sqrt{a_0(u,u)} \; .$$

More concretely $u \in \mathcal{H}$ belongs to V, if there exists $u_n \in D(T_0)$ such that $u_n \to u$ in $\mathcal{H}$ and u_n is a Cauchy sequence for the norm p_0.
As a natural norm for V, we get as a candidate :

$$||u||_V = \lim_{n \to +\infty} p_0(u_n) \; , \tag{4.3.4}$$

where u_n is a Cauchy sequence for p_0 tending to u in $\mathcal{H}$.
Let us show that the definition does not depend on the Cauchy sequence. This is the object of the

Lemma 4.3.2. .
Let x_n a Cauchy sequence in $D(T_0)$ for p_0 such that $x_n \to 0$ in $\mathcal{H}$. Then $p_0(x_n) \to 0$.

Proof of the lemma.
First observe that $p_0(x_n)$ is a Cauchy sequence in $I\!R^+$ and consequently convergent in $\overline{I\!R^+}$.
Let us suppose by contradiction that

$$p_0(x_n) \to \alpha > 0 \; . \tag{4.3.5}$$

We first observe that

$$a_0(x_n, x_m) = a_0(x_n, x_n) + a_0(x_n, x_m - x_n) \; ,$$

and that a Cauchy-Schwarz inequality is satisfied :

$$|a_0(x_n, x_m - x_n)| \leq \sqrt{a_0(x_n, x_n)} \cdot \sqrt{a_0(x_m - x_n, x_m - x_n)} \; .$$

Using also that x_n is a Cauchy sequence for p_0, we obtain that

$$\forall \epsilon > 0, \exists N \text{ s. t. } \forall n \geq N, \, \forall m \geq N, |a_0(x_n, x_m) - \alpha^2| \leq \epsilon \; . \tag{4.3.6}$$

We take $\epsilon = \frac{\alpha^2}{2}$ and consider the corresponding N given by (4.3.6). Coming back to the definition of a_0 we obtain,

$$| < T_0 x_n, x_m > | \geq \frac{1}{2}\alpha^2 \; , \; \forall n \geq N, \forall m \geq N \; . \tag{4.3.7}$$

But as $m \to +\infty$, the left hand side in (4.3.7) tends to 0 because $x_m \to 0$ and this gives a contradiction.
##.
We now observe that

$$||u||_V \geq ||u||_{\mathcal{H}} , \tag{4.3.8}$$

as a consequence of (4.3.3) and (4.3.4).
This means that the injection of V in $\mathcal{H}$ is continuous. Note also that V, which contains $D(T_0)$, is dense in $\mathcal{H}$, by density of $D(T_0)$ in $\mathcal{H}$. Moreover, we get a natural scalar product on V by extension of a_0 :

$$< u, v >_V := \lim_{n \to +\infty} a_0(u_n, v_n) , \tag{4.3.9}$$

where u_n and v_n are Cauchy sequences for p_0 tending respectively to u and v in $\mathcal{H}$.
By the second version of the Lax-Milgram Theorem (in the context $V, \mathcal{H}, V'$) applied with

$$a(u, v) := \quad < u, v >_V ,$$

we get an unbounded selfadjoint operator S on $\mathcal{H}$ extending T_0 whose domain $D(S)$ satisfies $D(S) \subset V$.

4.4 Applications

Application 1: The Dirichlet realization. Let Ω be an open set in $\mathbb{R}^m$ such that $\overline{\Omega}$ is compact and let T_0 be the unbounded operator defined by

$$D(T_0) = C_0^\infty(\Omega) , \; T_0 = -\Delta .$$

The involved Hilbert space is $\mathcal{H} = L^2(\Omega)$. It is clear that T_0 is symmetric and positive[9] (hence semi-bounded). Following the previous general construction, we prefer to consider : $\tilde{T}_0 := T_0 + Id$.
It is easy to see[10] that V is the closure in $H^1(\Omega)$ of $C_0^\infty(\Omega)$. This means, at least if Ω is regular, the space $H_0^1(\Omega)$. The domain of S is then described as

$$D(S) := \{u \in H_0^1(\Omega) \mid -\Delta u \in L^2(\Omega)\}.$$

S is then the operator $(-\Delta + 1)$ acting in the sense of distributions.
When Ω is regular, a standard regularity theorem (see [Lio2], [LiMa]) permits

[9] We shall in fact see later that it is strictly positive.

[10] We recall that there are two ways for describing $H_0^1(\Omega)$. In the first definition we just take the closure of $C_0^\infty(\Omega)$ in $H^1(\Omega)$.
In the second definition, we describe $\mathcal{H}_0^1(\Omega)$ as the subspace in $H^1(\Omega)$ of the distributions whose trace is zero at the boundary. This supposes that the boundary $\Gamma = \partial\Omega$ is regular. In this case, there exists a unique application γ_0 continuous from $H^1(\Omega)$ onto $H^{\frac{1}{2}}(\Gamma)$ extending the map $C^\infty(\bar{\Omega}) \ni u \mapsto u_\Gamma$. It is a standard result (cf Brézis [Br] or Lions-Magenes [LiMa]) that $\mathcal{H}_0^1(\Omega) = H_0^1(\Omega)$, when the boundary is regular.

to show that

$$D(S) = H^2(\Omega) \cap H^1_0(\Omega) \ . \tag{4.4.1}$$

So we have shown the following theorem

Theorem 4.4.1. .
The operator T_1 defined by

$$D(T_1) = H^2(\Omega) \cap H^1_0(\Omega) \ , \ T_1 = -\Delta \ ,$$

is selfadjoint and called the Dirichlet realization of $-\Delta$ in Ω.

We have just to observe that $T_1 = S - 1$ and to use Remark 2.3.8.
Note that T_1 is a selfadjoint extension of T_0.
Note that by the technique developed in Subsection 3.4, we have also constructed another selfadjoint extension of T_0. So we have constructed, when Ω is relatively compact, two different selfadjoint realizations of T_0. We say in this case that T_0 is not essentially selfadjoint.

Application 2: The harmonic oscillator. We can start from

$$H_0 = -\Delta + |x|^2 + 1 \ ,$$

with domain

$$D(H_0) = C_0^\infty(I\!R^m) \ .$$

Following the scheme of the construction of the Friedrichs extension, we first get that

$$V = B^1(I\!R^m) := \{u \in H^1(I\!R^m) \mid x_j u \in L^2(I\!R^m) \ , \ \forall j \in [1, \cdots, m]\} \ .$$

One can indeed first show that $V \subset B^1(I\!R^m)$ and then get the equality by proving the property that $C_0^\infty(I\!R^m)$ is dense in $B^1(I\!R^m)$. One can then determine the domain of S as

$$D(S) = \{u \in B^1(I\!R^m) \mid (-\Delta + |x|^2 + 1)u \in L^2(I\!R^m)\} \ .$$

By a regularity theorem (differential quotients method [LiMa]), one can show that

$$D(S) = B^2(I\!R^m) := \{u \in H^2(I\!R^m) \mid x^\alpha u \in L^2(I\!R^m) \ , \ \forall \alpha \text{ s. t. } |\alpha| \leq 2\}.$$

5 Compact operators : general properties and examples.

5.1 Definition and properties.

We just recall here very briefly the basic properties of compact operators and their spectral theory. We will emphasize on examples. We refer to the book by H. Brézis [Br] (Chap. VI).
Let us recall that an operator T from a Banach E into a Banach F is compact if the range of the unit ball in E by T is relatively compact in F. We denote by $\mathcal{K}(E,F)$ the space of compact operators which is a closed subspace in $\mathcal{L}(E,F)$. There is an alternative equivalent definition in the case when E and F are Hilbert spaces by using sequences. The operator is compact if and only if, for any sequence x_n which converges weakly in E, Tx_n is a strongly convergent sequence in F. Here we recall that a sequence is said to be weakly convergent in $\mathcal{H}$, if, for any $y \in \mathcal{H}$, the sequence $< x_n, y >_{\mathcal{H}}$ is convergent. Such a sequence is bounded (Banach-Steinhaus's Theorem) and we recall that, in this case, there exists a unique $x \in \mathcal{H}$, such that $< x_n, y >_{\mathcal{H}} \to < x, y >_{\mathcal{H}}$ for all $y \in \mathcal{H}$. In this case, we write : $x_n \rightharpoonup y$.

Let us recall that when one composes a continuous operator and a compact operator (in any order) one gets a compact operator. This could be one way to prove the compactness.
Another efficient way for proving compactness of an operator T is to show that it is the limit (for the norm convergence) of a sequence of continuous operators with finite rank (that is whose range is a finite dimensional space). We observe indeed that a continuous operator with finite rank is clearly a compact operator (in a finite dimensional space the closed bounded sets are compact).

5.2 Examples

Continuous kernels .
The first example of this type is the operator T_K associated to the continuous kernel K on $[0,1] \times [0,1]$.
By this we mean that the operator T_K is defined by

$$E \ni u \mapsto (T_K u)(x) = \int_0^1 K(x,y) u(y) dy \, . \tag{5.2.1}$$

Here E could be the Banach space $C^0([0,1])$ (with the Sup norm) or $L^2(]0,1[)$.

Proposition 5.2.1. .
If the kernel K is continuous, then the operator T_K is compact from E into E.

There are two standard proofs for this proposition. The first one is based on Ascoli's Theorem giving a criterion relating equicontinuity of a subset of continuous functions on a compact and relatively compact sets in $C^0([0,1])$.

The other one is based on the Stone-Weierstrass Theorem permitting to recover the operator as the limit of a sequence of finite rank operators T_{K_n} associated to kernels K_n of the form $K_n(x,y) = \sum_{j=1}^{j_n} f_{j,n}(x) g_{j,n}(y)$.

Let us study three other examples.
The first example comes from statistical mechanics, the second one from the spectral theory for the Dirichlet realization of the Laplacian and the third one from Quantum Mechanics.

The transfer operator. The transfer operator is the operator associated with the kernel

$$K_t(x,y) = \exp -\frac{V(x)}{2} \exp -t|x-y|^2 \exp -\frac{V(y)}{2} \, , \tag{5.2.2}$$

where $t > 0$, and V is a $C^\infty(\mathbb{R})$ function such that

$$\int_{\mathbb{R}} \exp -V(x) dx < +\infty \, .$$

The L^2- boundedness of operators with integral kernel is proven very often through the

Lemma 5.2.2. *Schur's Lemma.*
Let $\mathbf{K}$ *an operator associated with an integral kernel* K*, that is a function* $(x,y) \mapsto K(x,y)$ *on* $\mathbb{R}^m \times \mathbb{R}^m$*, satisfying*

$$\begin{array}{l} M_1 := \sup_{x \in \mathbb{R}^m} \int_{\mathbb{R}^m} |K(x,y)| \, dy < +\infty \, , \\ M_2 := \sup_{y \in \mathbb{R}^m} \int_{\mathbb{R}^m} |K(x,y)| \, dx < +\infty \, . \end{array} \tag{5.2.3}$$

Then $\mathbf{K}$*, initially defined for* $u \in C_0^\infty(\mathbb{R}^m)$ *by*

$$(Ku)(x) = \int_{\mathbb{R}^m} K(x,y) u(y) dy \, ,$$

can be extended as a continuous linear operator in $\mathcal{L}(L^2(\mathbb{R}^m))$ *(still denoted by* $\mathbf{K}$ *or* T_K*), whose norm satisfies*

$$||\mathbf{K}|| \leq \sqrt{M_1 M_2} \, . \tag{5.2.4}$$

Proof:
By the Cauchy-Schwarz inequality, we have

$$|Ku(x)|^2 \leq \int |K(x,y)||u(y)|^2 dy \int |K(x,y)| dy \leq M_1 \int |K(x,y)||u(y)|^2 dy \, .$$

Integrating with respect to x and using Fubini's Theorem, we then obtain the result.

In our case, the operator T_K is actually an Hilbert-Schmidt operator, i.e. an operator whose integral kernel is in $L^2(\mathbb{R}^m \times \mathbb{R}^m)$ (with $m = 1$). One can indeed prove, using Cauchy-Schwarz's inequality, show that :

$$|Ku(x)|^2 \leq \int |u(y)|^2 dy \int |K(x,y)|^2 dy \,,$$

and one obtains :

$$||T_K|| \leq ||K||_{L^2(\mathbb{R}^m \times \mathbb{R}^m)} \,. \tag{5.2.5}$$

It is then easy to show that T_K is a compact operator. Its kernel K is indeed the limit in L^2 of a sequence K_n such that T_{K_n} is of finite rank. If ϕ_j is an orthonormal basis in $L^2(\mathbb{R}^m)$, one first shows that the basis $\phi_k \otimes \overline{\phi_\ell}$ is an orthonormal basis in $L^2(\mathbb{R}^m \times \mathbb{R}^m)$. Here we have by definition :

$$(\phi_k \otimes \overline{\phi_\ell})(x,y) := \phi_k(x)\overline{\phi_\ell}(y) \,.$$

We then obtain

$$K(x,y) = \sum_{k,\ell} c_{k,\ell}\phi_k(x)\overline{\phi_\ell}(y) \,.$$

We now introduce

$$K_n(x,y) := \sum_{k+\ell \leq n} c_{k,\ell}\phi_k(x)\overline{\phi_\ell}(y) \,.$$

It is then easy to see that T_{K_n} is of finite rank because its range is included in the linear space generated by the ϕ_k's ($k = 1, \cdots, n$). Moreover, we have

$$\lim_{n \to +\infty} ||K - K_n||_{L^2(\mathbb{R}^m \times \mathbb{R}^m)} = 0 \,.$$

Coming back to the corresponding operators, we get

$$\lim_{n \to +\infty} ||T_K - T_{K_n}||_{\mathcal{L}(L^2(\mathbb{R}^m))} = 0 \,.$$

The inverse of the Dirichlet operator .

We come back to the operator S, which was introduced in the study of the Dirichlet realization. One can show the following

Proposition 5.2.3. .
The operator S^{-1} is compact.

Proof.
The operator S^{-1} can indeed be considered as the composition of a continuous operator from L^2 into $V = H_0^1(\Omega)$ and of the continuous injection of V into $L^2(\Omega)$. If Ω is relatively compact, we know (cf [Br]) that we have compact

injection from $H^1(\Omega)$ into $L^2(\Omega)$. For the continuity result, we observe that, for all $u \in D(S)$:

$$||Su||_{\mathcal{H}}||u||_{\mathcal{H}} \geq \langle Su \mid u\rangle = a(u,u) \geq \alpha ||u||_V^2 \geq \alpha ||u||_V ||u||_{\mathcal{H}} \ .$$

This gives, for all $u \in D(S)$, the inequality :

$$||Su||_{\mathcal{H}} \geq \alpha ||u||_V \ . \tag{5.2.6}$$

Using the surjectivity of S, we get :

$$||S^{-1}||_{\mathcal{L}(\mathcal{H},V)} \leq \frac{1}{\alpha} \ . \tag{5.2.7}$$

Note that in our example $\alpha = 1$ but that this part of the proof is completely general.

The inverse of the harmonic oscillator. The analysis is analogous. We have seen that the Sobolev space $H^1_0(I\!R)$ has to be replaced by the space

$$B^1(I\!R) := \{u \in L^2(I\!R)\ ,\ xu \in L^2 \text{ and } du/dx \in L^2\} \ .$$

We can then prove, using a standard precompactness criterion, that $B^1(I\!R)$ has compact injection in $L^2(I\!R)$. One has in particular to use the inequality :

$$\int_{|x|\geq R} |u(x)|^2 dx \leq \frac{1}{R^2} ||u||^2_{B^1(I\!R)} \ . \tag{5.2.8}$$

It is very important to realize that the space $H^1(I\!R)$ is not compactly injected in L^2. To understand this point, it is enough to consider the sequence $u_n = \chi(x-n)$ where χ is a function in $C_0^\infty(I\!R)$ with norm in L^2 equal to 1. It is a bounded sequence in H^1, which converges weakly in H^1 to 0 and is not convergent in $L^2(I\!R)$.

5.3 Adjoints and compact operators

We recall[11] that the adjoint of a bounded operator in the Hilbertian case is bounded. When E and F are different Hilbert spaces , the Hilbertian adjoint is defined through the identity :

$$< Tx, y >_F = < x, T^* y >_E \ ,\ \forall x \in E\ ,\ \forall y \in F\ . \tag{5.3.1}$$

Example 5.3.1. .
Let Ω be an open set in $I\!R^m$ and Π_Ω the operator of restriction to Ω: $L^2(I\!R^m) \ni u \mapsto u_{/\Omega}$. Then Π_Ω^* is the operator of extension by 0.

[11] We are mainly following Brézis's exposition [Br].

Exercise 5.3.2. .
Let γ_0 be the trace operator on $x_m = 0$ defined from $H^1(I\!R^m_+)$ onto $H^{\frac{1}{2}}(I\!R^{m-1})$. Determine the adjoint.

In an Hilbert space, we have

$$M^\perp = \overline{M}^\perp .$$

In particular, if M is a closed subspace, we have already used the property

$$(M^\perp)^\perp = M . \tag{5.3.2}$$

In the case of bounded operators ($T \in \mathcal{L}(E, F)$), one gets easily the properties

$$N(T^*) = R(T)^\perp , \tag{5.3.3}$$

and

$$\overline{R(T)} = (N(T^*))^\perp . \tag{5.3.4}$$

Let us also recall the proposition

Proposition 5.3.3. .
The adjoint of a compact operator is compact.

5.4 Precompactness

We assume that the reader is aware of the basic results concerning compact sets in metric spaces. We in particular recall that in a complete metric space E, an efficient way to show that a subset M is relatively compact is to show, that for any $\epsilon > 0$, one can recover M by a finite family of balls of radius ϵ in E.

The second standard point is to remember Ascoli's Theorem, giving a criterion for a bounded subset in $C^0(K)$ (K compact in $I\!R^m$) to be relatively compact in term of uniform equicontinuity. Ascoli's Theorem gives in particular :

- the compact injection of $C^1(K)$ into $C^0(K)$
- the compact injection of $H^m(\Omega)$ into $C^0(K)$, for $m > \frac{n}{2}$ and with $K = \overline{\Omega}$.

Let us recall finally a general proposition permitting to show that a subset in L^2 is relatively compact.

Proposition 5.4.1. *Let $A \subset L^2(I\!R^m)$. Let us assume that :*

1. *A is bounded in $L^2(I\!R^m)$, that is there exists $M > 0$ such that :*

$$||u||_{L^2} \leq M \ , \ \forall u \in A .$$

2. *The expression $\epsilon(u, R) := \int_{|x|\geq R} |u(x)|^2 dx$ tends to zero as $R \to +\infty$ uniformly with respect to $u \in A$.*

3. *For $h \in I\!R^m$, let τ_h defined on L^2 by : $(\tau_h u)(x) = u(x-h)$. Then the expression $\delta(u,h) := ||\tau_h u - u||_{L^2}$ tends to zero as $h \to 0$, uniformly with respect to A.*

Then A is relatively compact in L^2.

This proposition can be applied for showing :

- the compact injection of $H_0^1(\Omega)$ in $L^2(\Omega)$ when Ω is regular and bounded,
- the compact injection of $H^1(\Omega)$ in $L^2(\Omega)$ when Ω is regular and bounded,
- the compact injection of $B^1(I\!R^m)$ in $L^2(I\!R^m)$.

6 Spectral theory for bounded operators.

6.1 Fredholm's alternative

Let us first recall Riesz's Theorem.

Theorem 6.1.1. .
Let E be a normed linear space such that $\overline{B_E}$ is compact then E is finite dimensional.

Let us now describe Fredholm's alternative.

Theorem 6.1.2. .
Let $T \in \mathcal{K}(E)$. Then
(i) $N(I-T)$ is finite dimensional.
(ii) $R(I-T)$ is closed (of finite codimension).
(iii) $R(I-T) = E$ if and only if $N(I-T) = \{0\}$.

We shall only use this theorem in the Hilbertian framework, so $E = \mathcal{H}$, and we shall prove it for simplicity under the additional assumption that $T = T^*$.
Proof.
We divide the proof in successive steps.
Step 1.
(i) is a consequence of Riesz's Theorem.
Step 2.
Let us show that $R(I-T)$ is closed.
Let y_n a sequence in $R(I-T)$ such that $y_n \to y$ in $\mathcal{H}$. We would like to show that $y \in R(I-T)$.
Let x_n in $N(I-T)^\perp$ such that $y_n = x_n - Tx_n$.

Step 2a. Let us first show the weaker property that the sequence x_n is bounded.
Let us indeed suppose that there exists a subsequence x_{n_j} such that $||x_{n_j}|| \to +\infty$. Considering $u_{n_j} = x_{n_j}/||x_{n_j}||$, we observe that

$$(*) \quad u_{n_j} - Tu_{n_j} \to 0 \; .$$

The sequence being bounded, we observe that (after possibly extracting a subsequence) one can consider that the sequence u_{n_j} is weakly convergent. This implies that Tu_{n_j} is convergent (T is compact). Using now $(*)$, we get the convergence of u_{n_j} to u :

$$u_{n_j} \to u \; , \; Tu = u \; , \; ||u|| = 1 \; .$$

But $u \in N(I-T)^\perp$, hence we get $u = 0$ and a contradiction.

Step 2b. We have consequently obtained that the sequence x_n is bounded. One can consequently extract a subsequence x_{n_j} that weakly converges to x_∞ in $\mathcal{H}$. Using the compactness of T, we get Tx_{n_j} converges strongly to Tx_∞.

Hence the sequence x_{n_j} tends strongly to $y + Tx_\infty$.
We have finally

$$y + Tx_\infty = x_\infty \ ,$$

and consequently proved that $y = x_\infty - Tx_\infty$.

Step 3.
If $N(I-T) = \{0\}$, then $N(I - T^*) = 0$ (here we use for simplification our additional assumption) and $R(I-T)$ being closed, we get

$$R(I-T) = N(I-T^*)^\perp = \mathcal{H} \ .$$

The converse is also immediate as $T = T^*$.

Step 4.
We have

$$R(I-T)^\perp = N(I-T^*) = N(I-T) \ .$$

This shows, according to (i) that $R(I-T)$ is of finite codimension (second statement of (ii)).

This ends the proof of Fredholm's alternative in the particular case that T is selfadjoint.

Remark 6.1.3. .
Under the same asumptions, it is possible to show that

$$dim \ N(I-T) = \ dim \ N(I-T^*) \ .$$

6.2 Resolvent set for bounded operators

In this subsection, E could be a Banach on $\mathbb{R}$ or $\mathbb{C}$, but we will essentially need the Hilbertian case in the applications treated here.

Definition 6.2.1. *(Resolvent set).*
For $T \in \mathcal{L}(E)$, the resolvent set is defined by

$$\varrho(T) = \{\lambda \in \mathbb{C} \ ; \ (T - \lambda I) \textit{ is bijective from } E \textit{ on } E\}. \tag{6.2.1}$$

Note that in this case $(T-\lambda I)^{-1}$ is continuous (Banach's Theorem). It is easy to see that $\varrho(T)$ is an open set in $\mathbb{C}$. If $\lambda_0 \in \varrho(T)$, we oberve that

$$(T-\lambda) = (T-\lambda_0)\left(Id + (\lambda-\lambda_0)(T-\lambda_0)^{-1}\right)$$

Hence $(T-\lambda)$ is invertible if $|\lambda - \lambda_0| < ||(T-\lambda_0)^{-1}||^{-1}$. We also get the following identity for all $\lambda,\ \lambda_0 \in \varrho(T)$:

$$(T-\lambda)^{-1} - (T-\lambda_0)^{-1} = (\lambda-\lambda_0)(T-\lambda)^{-1}(T-\lambda_0)^{-1} \ . \tag{6.2.2}$$

Definition 6.2.2. *(Spectrum).*
The spectrum of T, $\sigma(T)$, is the complementary set of $\varrho(T)$ in $\mathbb{C}$.

Note that $\sigma(T)$ is a closed set in $\mathbb{C}$. This is typically the case when T is a compact injective operator in a Banach space of infinite dimension.

We say that λ is an eigenvalue if $N(T-\lambda I) \neq 0$. $N(T-\lambda I)$ is called the eigenspace associated with λ.

Definition 6.2.3. *(Point spectrum).*
The point spectrum $\sigma_p(T)$ of T is defined as the set of the eigenvalues of T.

Example 6.2.4. *(Basic example) .*
Let $\mathcal{H} = L^2(]0,1[)$ and $f \in C^0([0,1])$. Let T_f be the operator of multiplication by f. Then one has :

$$\sigma(T_f) = \ Im\ f =: \{\lambda \in \mathbb{C} \mid \exists x \in [0,1] \text{ with } f(x) = \lambda\}\ .$$

$$\sigma_p(T_f) = Sta(f) =: \{\lambda \in \mathbb{C} \mid meas(f^{-1}(\lambda)) > 0\}\ .$$

For the first assertion, it is first immediate to see that if $\lambda \notin\ Im\ f$, then $T_{(f-\lambda)^{-1}}$ is a continuous inverse of $T_f - \lambda$. On the other side, if $\lambda = f(x_0)$ for some $x_0 \in]0,1[$ then we have $(T_f - \lambda)u_n \to 0$ and $||u_n|| = 1$ for $u_n = \frac{1}{\sqrt{n}}\chi(\frac{x-x_0}{n})$, where χ is a C_0^∞ function such that $||\chi|| = 1$. This shows that $f(]0,1[) \subset \sigma(T_f)$ and we can conclude by considering the closure.

Note that the point spectrum is not necessarily closed. Note also that one can have a strict inclusion of the point spectrum in the spectrum as can be observed in the following example :

Example 6.2.5. .
Let us consider $E = \ell^2(\mathbb{N})$ and let T be the shift operator defined by :

$$(Tu)_0 = 0\ ,\ (Tu)_n = u_{n-1}\ ,\ n > 0\ ,$$

where $u = (u_0, \cdots, u_n, \cdots) \in \ell^2(\mathbb{N})$. Then it is easy to see that T est injective (so 0 is not an eigenvalue) and is not surjective (so 0 is in the spectrum of T).

As another interesting example, one can consider :

Example 6.2.6. .
Let $E = \ell^2(\mathbb{Z}, \mathbb{C})$ and let T be the operator defined by :

$$(Tu)_n = \frac{1}{2}(u_{n-1} + u_{n+1})\ ,\ n \in \mathbb{Z}\ ,$$

for $u \in \ell^2(\mathbb{Z})$. Then it is easy to see (by using expansion in Fourier series [12]) that T has no eigenvalues and its spectrum is $[-1,+1]$.

[12] Using the isomorphism between $\ell^2(\mathbb{Z};\mathbb{C})$ and $L^2(S^1\ ;\ \mathbb{C})$, which associates to the sequence $(u_n)_{n\in\mathbb{Z}}$ the fonction $\sum_{n\in\mathbb{Z}} u_n \exp in\theta$, one has to analyze the operator of multiplication by $\cos\theta$:

$$f \mapsto \mathcal{T}f = \cos\theta f\ .$$

It is then analyzed as in example 6.2.4. One concludes that the spectrum of $\mathcal{T}$ is $[-1,+1]$.

Exercise 6.2.7. .
Let $\alpha \in [0,1]$. Let p and q integers which are mutually prime. Analyze the spectrum Σ_α of the operator H_α defined on $\ell^2(\mathbb{Z})$ by

$$(H_\alpha u)_n = \frac{1}{2}(u_{n-1}+u_{n+1}) + \cos 2\pi(\frac{p}{q}n+\alpha)\, u_n\ ,\ n \in \mathbb{Z}\ .$$

In order to make the analysis easier, one can admit (particular case of the so-called Floquet theory), that one has $\Sigma = \cap_{\theta\in[0,1]}\Sigma_\theta$, where Σ_θ is the spectrum of H_α reduced to the space of the u's in ℓ^∞ such that $u_{n+q} = \exp 2i\pi\theta\ u_n$, for $n \in \mathbb{Z}$.
This operator plays an important role in Solid State Physics and is called the Harper's operator.
We now replace the rational $\frac{p}{q}$ by an irrational number β. So we consider the operator $H_{\beta,\alpha} := \frac{1}{2}(\tau_{+1}+\tau_{-1}) + \cos 2\pi(\beta\cdot + \alpha)$ on $\ell^2(\mathbb{Z},\mathbb{C})$, where τ_k ($k \in \mathbb{Z}$) is the operator defined on $\ell^2(\mathbb{Z},\mathbb{C})$ by $(\tau_k u)_n = u_{n-k}$.
Show that, if $\beta \notin \mathbb{Q}$, then the spectrum of $H_{\beta,\alpha}$ is independent of α. For this, one can first prove that $H_{\beta,\alpha}$ is unitary equivalent with $H_{\beta,\alpha+k\beta}$ for any $k \in \mathbb{Z}$. Secondly, one can use the density of the set $\{\alpha + \beta\mathbb{Q}\}$ in $\mathbb{R}$. Finally, one can use the inequality

$$||H_{\beta,\alpha} - H_{\beta,\alpha'}|| \leq |\alpha - \alpha'|\ .$$

Proposition 6.2.8. .
The spectrum $\sigma(T)$ is a compact set included in the ball $\overline{B}(0, ||T||)$.

This proposition is immediate if we observe that $(I - \frac{T}{\lambda})$ is invertible if $|\lambda| > ||T||$.

6.3 Spectral theory for compact operators

In the case of a compact operator, one has a more precise description of the spectrum.

Theorem 6.3.1. .
Let $T \in \mathcal{K}(E)$ where E is an infinite dimensional Banach space. Then

1. $$0 \in \sigma(T)\ .$$
2. $$\sigma(T)\setminus\{0\} = \sigma_p(T)\setminus\{0\}\ .$$
3. *We are in one (and only one) of the following cases*
   - *either $\sigma(T) = \{0\}$,*
   - *either $\sigma(T)\setminus\{0\}$ is finite,*
   - *or $\sigma(T)\setminus\{0\}$ can be described as a sequence of distincts points tending to 0.*

Proof.

a) If $0 \notin \sigma(T)$, then T admits a continuous inverse T^{-1} and the identity, which can be considered as :

$$I = T \circ T^{-1} ,$$

is a compact operator, as the composition of the compact operator T and the continuous operator T^{-1}. Using Riesz's Theorem we get a contradiction in the case E is supposed of infinite dimension.

b) The fact that, if $\lambda \neq 0$ and $\lambda \in \sigma(T)$, then λ is an eigenvalue, comes directly from the Fredholm's alternative applied to $(I - \frac{T}{\lambda})$.

c) The last step comes essentially from the following lemma :

Lemma 6.3.2. .
Let $(\lambda_n)_{n\geq 1}$ a sequence of distincts points $\lambda_n \to \lambda$ and $\lambda_n \in \sigma(T) \setminus \{0\}$, for all $n > 0$.
Then $\lambda = 0$.

Proof.

We just give the proof in the Hilbertian case. For all $n > 0$, let e_n be a normalized eigenvector such that $(T - \lambda_n)e_n = 0$ and let E_n be the vectorial space spanned by $\{e_1, e_2, \cdots, e_n\}$. Let us show that we have a strict inclusion of E_n in E_{n+1}.

We prove this point by recursion. Let us assume the result up to order $n-1$ and let us show it at order n. If $E_{n+1} = E_n$, then $e_{n+1} \in E_n$ and we can write

$$e_{n+1} = \sum_{j=1}^{n} \alpha_j e_j .$$

Let us apply T to this relation. Using the property that e_{n+1} is an eigenvector, we obtain

$$\lambda_{n+1} \left(\sum_{j=1}^{n} \alpha_j e_j \right) = \sum_{j=1}^{n} \alpha_j \lambda_j e_j .$$

Using the recursion assumption, $\{e_1, \cdots, e_n\}$ is a basis of E_n and the λ_j being distincts, we obtain $\alpha_j = 0$ for all $j = 1, \cdots, n$ and a contradiction with $||e_{n+1}|| = 1$.

So we can find a sequence u_n such that $u_n \in E_n \cap E_{n-1}^{\perp}$ and $||u_n|| = 1$. T being compact, one would extract a convergent subsequence (still denoted by Tu_n) from the sequence (Tu_n) and, if $\lambda_n \to \lambda \neq 0$, one would also have the convergence of this subsequence $(\frac{1}{\lambda_n} T u_n)$ and consequently the Cauchy property.

Let us show that this leads to a contradiction. We remark that

$$(T - \lambda_n)E_n \subset E_{n-1} .$$

Let $n > m \geq 2$. We have

$$\begin{aligned}
||\frac{Tu_n}{\lambda_n} - \frac{Tu_m}{\lambda_m}||^2 &= ||\frac{(T-\lambda_n)u_n}{\lambda_n} - \frac{(T-\lambda_m)u_m}{\lambda_m} + u_n - u_m||^2 \\
&= ||\frac{(T-\lambda_n)u_n}{\lambda_n} - \frac{(T-\lambda_m)u_m}{\lambda_m} - u_m||^2 + ||u_n||^2 \\
&\geq ||u_n||^2 = 1 .
\end{aligned}$$

We can consequently not extract a Cauchy subsequence from the sequence $\frac{1}{\lambda_n} T u_n$. This is in contradiction with the assumption $\lambda \neq 0$.
This ends the proof of the lemma and of the theorem.

We shall now consider the Hilbertian case and see which new properties can be obtained by using the additional assumption that T is selfadjoint.

6.4 Spectrum of selfadjoint operators.

As $T = T^*$, the spectrum is real. If $\text{Im}\,\lambda \neq 0$, one immediately verifies that :

$$|\text{ Im }\lambda|\ ||u||^2 \leq |\text{ Im }\langle (T-\lambda)u, u\rangle \leq ||(T-\lambda)u|| \cdot ||u||\ .$$

This shows immediately that the map $(T-\lambda)$ is injective and with close range. But the orthogonal of the range of $(T-\lambda)$ is the kernel of $(T-\bar{\lambda})$ which is reduced to 0. So $(T-\lambda)$ is bijective.
This was actually, a consequence of the Lax-Milgram theorem (in the simple case when $V = H$), once we have observed the inequality

$$|\langle (T-\lambda)u, u\rangle| \geq |\text{ Im }\lambda| ||u||^2\ .$$

Using again Lax-Milgram's theorem, we can show

Theorem 6.4.1. .
Let $T \in \mathcal{L}(\mathcal{H})$ be a selfadjoint operator. Then the spectrum of T is contained in $[m, M]$ with $m = \inf \langle Tu, u\rangle / ||u||^2$ and $M = \sup \langle Tu, u\rangle / ||u||^2$. Moreover m and M belong to the spectrum of T.

Proof:
We have already mentioned that the spectrum is real. Now if $\lambda > M$, we can apply the Lax-Milgram to the sequilinear-form $(u, v) \mapsto \lambda\langle u, v\rangle - \langle Tu, v\rangle$.
Let us now show that $M \in \sigma(T)$.

We observe that, by Cauchy-Schwarz applied to the scalar product $(u, v) \mapsto M\langle u, v\rangle - \langle Tu, v\rangle$, we have :

$$|\langle Mu - Tu, v\rangle| \leq \langle Mu - Tu, u\rangle^{\frac{1}{2}}\ \langle Mv - Tv, v\rangle^{\frac{1}{2}}\ .$$

In particular, we get :

$$||Mu - Tu||_{\mathcal{H}} \leq ||M - T||^{\frac{1}{2}}_{\mathcal{L}(\mathcal{H})} \langle Mu - Tu, u\rangle^{\frac{1}{2}}\ . \tag{6.4.1}$$

Let $(u_n)_{n\in\mathbb{Z}}$ be a sequence such that $||u_n|| = 1$ and $\langle Tu_n, u_n\rangle \to M$ as $n \to +\infty$. By (6.4.1), we get that $(T - M)u_n$ tends to 0 as $n \to +\infty$. This implies that $M \in \sigma(T)$. If not, we would get that $u_n = (M-T)^{-1}((M-T)u_n)$ tends to 0 in contradiction with $||u_n|| = 1$.
This theorem admits the following important corollary

Corollary 6.4.2. .
Let $T \in \mathcal{L}(\mathcal{H})$ be a selfadjoint operator such that $\sigma(T) = \{0\}$. Then $T = 0$.

We first indeed show that $m = M = 0$ and consequently that $< Tu, u >_{\mathcal{H}} = 0$ for all $u \in \mathcal{H}$. But $< Tu, v >$ can be written as a linear combination of terms of the type $< Tw, w >_{\mathcal{H}}$ and this gives the result by taking $v = Tu$.

Another connected property which is useful is the

Proposition 6.4.3. .
If T is positive and selfadjoint then $||T|| = M$.

The proof is quite similar. We observe that :

$$|\langle Tu, v\rangle| \leq \langle Tu, u\rangle^{\frac{1}{2}} \langle Tv, v\rangle^{\frac{1}{2}} .$$

This implies, using Riesz's Theorem :

$$||Tu|| \leq ||T||^{\frac{1}{2}} (\langle Tu, u\rangle)^{\frac{1}{2}} .$$

Coming back to the definition of $||T||$, we obtain :

$$||T|| \leq ||T||^{\frac{1}{2}} M^{\frac{1}{2}} ,$$

and the inequality :

$$||T|| \leq M .$$

But it is immediate that :

$$\langle Tu, u\rangle \leq ||T|| \, ||u||^2 .$$

This gives the converse inequality and the proposition.

6.5 Spectral theory for compact selfadjoint operators

We have a very precise description of the selfadjoint compact operators.

Theorem 6.5.1. .
Let $\mathcal{H}$ be a separable Hilbert[13] space and T a compact selfadjoint operator. Then $\mathcal{H}$ admits an Hilbertian basis consisting of eigenvectors of T.

Proof.
Let $(\lambda_n)_{n\geq 1}$ be the sequence of disjoint eigenvalues of T, except 0. Their existence comes from Theorem 6.3.1 and we also observe that the eigenvalues are real.
Let us define $\lambda_0 = 0$.

[13] that is having a countable dense set.

We define $E_0 = N(T)$ and $E_n = N(T - \lambda_n I)$; We know (from Riesz's Theorem) that

$$0 < \dim \ E_n < +\infty \ .$$

Let us show that $\mathcal{H}$ is the Hilbertian sum of the $(E_n)_{n \geq 0}$.

(i) The spaces (E_n) are mutually orthogonal. If $u \in E_m$ and $v \in E_n$ with $m \neq n$, we have

$$< Tu, v >_{\mathcal{H}} = \lambda_m < u, v >_{\mathcal{H}} = < u, Tv >_{\mathcal{H}} = \lambda_n < u, v >_{\mathcal{H}} \ ,$$

and consequently

$$< u, v >_{\mathcal{H}} = 0 \ .$$

(ii) Let F be the linear space spanned by the $(E_n)_{n \geq 0}$. Let us verify that F is dense in $\mathcal{H}$. It is clear that $TF \subset F$ and, using the selfadjoint character of T, we have also $TF^\perp \subset F^\perp$. The operator $\tilde{T}$, obtained by restriction of T to $F^\perp$, is a compact selfadjoint operator. But one shows easily that $\sigma(\tilde{T}) = \{0\}$ and consequently $\tilde{T} = 0$. But $F^\perp \subset N(T) \subset F$ and hence $F^\perp = \{0\}$. F is consequently dense in $\mathcal{H}$.

(iii) To end the proof, one chooses in each E_n an Hilbertian basis. Taking the union of these bases, one obtains an Hilbertian basis of $\mathcal{H}$ effectively formed with eigenvectors of T.

Remark 6.5.2. .
If T is a compact selfadjoint operator, we can write any u in the form

$$u = \sum_{n=0}^{+\infty} u_n \ , \quad \text{with } u_n \in E_n \ .$$

This permits to write

$$Tu = \sum_{n=1}^{+\infty} \lambda_n u_n \ .$$

If, for $k \in \mathbb{N}^*$, we define T_k by

$$T_k u = \sum_{n=1}^{k} \lambda_n u_n \ ,$$

we easily see that T_k is of finite rank and that

$$||T - T_k|| \leq \sup_{n \geq k+1} |\lambda_n| \ .$$

Hence the operator T appears as the limit in $\mathcal{L}(\mathcal{H})$ of the sequence T_k as $k \to +\infty$.

7 Examples.

We go back to our previous examples and analyze their properties.

7.1 The transfer operator.

7.1.1 Compactness

The transfer operator is compact and admits consequently a sequence of eigenvalues λ_n tending to 0 as $n \to +\infty$. Let us show the

Lemma 7.1.1. .
The transfer operator is positive and injective.

Proof of the lemma.
Let $u \in L^2(\mathbb{R})$. We can write[14], with $\phi(x) = \exp -\frac{V(x)}{2} u(x)$

$$< T_K u, u >_{\mathcal{H}} = \int_{\mathbb{R}^2} \exp -t|x-y|^2 \phi(x)\overline{\phi(y)} dx dy \, .$$

Using the properties of the Fourier transform and of the convolution, we deduce

$$< T_K u, u >_{\mathcal{H}} = c_t \int_{\mathbb{R}} \exp -\frac{|\xi|^2}{4t} |\hat{\phi}(\xi)|^2 d\xi \, ,$$

where $c_t > 0$ is a normalization constant.

The spectrum is consequently the union of a sequence of positive eigenvalues and of its limit 0. T_K can be diagonalized in an orthonormal basis of eigenvectors associated with strictly positive eigenvalues. We emphasize that 0 is in the spectrum but not an eigenvalue.
Theorem 6.4.1 says also that $||T_K||$ is the largest eigenvalue and is isolated. A natural question is then to discuss the multiplicity of each eigenvalue, i. e. the dimension of each associated eigenspace. We shall see later (Krein-Rutman's Theorem) that the largest eigenvalue is of multiplicity 1.

7.1.2 About the physical origin of the problem.

Our initial problem was to find a rather general approach for the estimate of the decay of correlations attached to "gaussian like" measures of the type

$$\exp -\Phi(X) \; dX \tag{7.1.1}$$

on $\mathbb{R}^n$ with Φ. One proof of this estimate (in the case when Φ has a particular structure) is based on the analysis of the transfer matrix method, originally

[14] If we make only the weak assumption that $\exp -V \in L^1(\mathbb{R})$, it is better to start for the proof of the positivity by considering u's in $C_0^\infty(\mathbb{R})$ and then to treat the general case by using the density of C_0^∞ in L^2.

due to Kramers-Wannier, that we have already seen for the study of the Ising model. We present here briefly the technique for our toy model. We shall only consider the case when $d = 1$ and treat the periodic case, that is the case when $\{1, \cdots, n\}$ is a representation of $\Lambda^{per} = \mathbb{Z}/n\mathbb{Z}$.

We consider the particular potential Φ

$$\Phi^{(n)}(X) \equiv \Phi(X) \equiv \frac{1}{h}\left(\sum_{j=1}^{n} V(x_j) + \frac{|x_j - x_{j+1}|^2}{4}\right) \tag{7.1.2}$$

where we take the convention that $x_{n+1} = x_1$ and where h is possibly a semiclassical parameter which is sometimes chosen equal to one if we are not interested in the "semiclassical" aspects. More generally, we could more generally consider examples of the form:

$$\Phi_h(X) = \frac{1}{h}\left(\sum_{j=1}^{n} (V(x_j) + I(x_j, x_{j+1}))\right) \tag{7.1.3}$$

where I is a symmetric "interaction" potential on $\mathbb{R} \times \mathbb{R}$. Let us mention however that the example (7.1.2) appears naturally in quantum field theory when the so called "lattice approximation" is introduced. For this special class of potentials, we shall demonstrate that the informations given by the transfer operator method are complementary to the other approachs we have explained before. We shall present the "dictionary" between the properties of the measure $h^{-\frac{n}{2}} \cdot \exp -\Phi_h(X)\, dX$ on $\mathbb{R}^n$ and the spectral properties of the transfer operator K_V (which is also called Kac operator for some particular models introduced by M. Kac) whose integral kernel is real and given on $\mathbb{R} \times \mathbb{R}$ by

$$K_V(x, y) = h^{-\frac{1}{2}} \exp -\frac{V(x)}{2h} \cdot \exp -\frac{|x-y|^2}{4h} \cdot \exp -\frac{V(y)}{2h}\,. \tag{7.1.4}$$

By integral kernel (or distribution kernel), we mean[15] a distribution in $\mathcal{D}'(\mathbb{R}^2)$ such that the operator is defined from $C_0^\infty(\mathbb{R})$ into $\mathcal{D}'(\mathbb{R})$ by the formula

$$\int_{\mathbb{R}} (K_V u)(x) v(x)\, dx = \int_{\mathbb{R}\times\mathbb{R}} K_V(x, y)\, u(x)\, v(y)\, dx\, dy\ ,\ \forall u\ ,\ v \in C_0^\infty(\mathbb{R})\,. \tag{7.1.5}$$

This dictionary permits to obtain interesting connections between estimates for the quotient μ_2/μ_1 of the two first largest eigenvalues of the transfer operator and corresponding estimates controlling the speed of convergence of thermodynamic quantities. In particular this speed of convergence is exponentially rapid as $n \to +\infty$.

[15] Here we shall always consider much more regular kernels which are in particular continuous. So the notation $\int$ can be interpreted in the usual sense. In general, this means that the distribution kernel K_V is applied to the test function $(x, y) \mapsto u(x)\, v(y)$.

We know that when the operator $\mathbf{K}$ is compact, symmetric and injective, then there exists a decreasing (in modulus) sequence μ_j of eigenvalues tending to 0 and a corresponding sequence of eigenfunctions u_j which can be normalized in order to get an orthonormal basis of $L^2(\mathbb{R})$. Moreover, the operator becomes the limit in norm of the family of operators $\mathbf{K}^{(N)}$ whose corresponding kernel are defined by

$$K^{(N)}(x,y) = \sum_{j=1}^{N} \mu_j u_j(x)\, u_j(y) \ . \tag{7.1.6}$$

We recall indeed that

$$||\mathbf{K} - \mathbf{K}^{(N)}|| \leq \sup_{j>N} |\mu_j| \ . \tag{7.1.7}$$

The symmetric operators[16] are called trace class if we have in addition the property that

$$||\mathbf{K}||_{tr} := \sum_j |\mu_j| < +\infty \tag{7.1.8}$$

In this case, we get that

$$||\mathbf{K} - \mathbf{K}^{(N)}||_{tr} \leq \sum_{j>N} |\mu_j| \ . \tag{7.1.9}$$

For a trace class symmetric operator, we can in particular define the trace as

$$\text{Tr }\ \mathbf{K} = \sum_j \mu_j \ , \tag{7.1.10}$$

and this operation is continuous on the space of the trace class operators

$$|\ \text{Tr }\ \mathbf{K}\ | \leq ||\mathbf{K}||_{tr} \ . \tag{7.1.11}$$

This of course extends the usual notion of trace for matrices. We can actually compute directly the trace of a trace-class operator in the following way. We first observe that

$$\text{Tr }\ \mathbf{K} = \lim_{N\to+\infty}\ \text{Tr }\ \mathbf{K}^{(N)} \ . \tag{7.1.12}$$

Then we observe that

$$\text{Tr }\ \mathbf{K}^{(N)} = \sum_{j=1}^{N} \mu_j = \int_{\mathbb{R}} K^{(N)}(x,x)dx \ . \tag{7.1.13}$$

[16] When $\mathbf{K}$ is not symmetric, trace class operators can still be defined by considering $\sqrt{\mathbf{K}^*\mathbf{K}}$. Note that when K is trace class, one can compute the trace by considering any orthonormal basis e_i : $\text{Tr }\ \mathbf{K} = \sum_i \langle \mathbf{K}e_i, e_i\rangle$.

We consequently obtain that

$$\text{Tr } \mathbf{K} = \lim_{N\to+\infty} \int_{\mathbb{R}} K^{(N)}(x,x)dx \; . \tag{7.1.14}$$

If we observe that $x \mapsto \sum_j |\mu_j||u_j(x)|^2$ is in $L^1(\mathbb{R})$, then it is natural[17] to hope (but this is not trivial!) that $x \mapsto K(x,x)$ is in L^1 and that

$$\text{Tr } \mathbf{K} = \int_{\mathbb{R}} K(x,x)\, dx \; . \tag{7.1.15}$$

Note that it is only when $\mathbf{K}$ is positive that the finiteness of the right hand side in (7.1.15) will imply the trace class property.
In the case the operator is Hilbert-Schmidt, that is with a kernel K in L^2, then the operator is also compact and we have the identity

$$\sum_j \mu_j^2 = \int_{\mathbb{R}\times\mathbb{R}} |K(x,y)|^2\; dx\, dy \; . \tag{7.1.16}$$

This gives an easy criterion for verifying the compactness of the operator. Let us first look at the thermodynamic limit. This means that we are interested in the limit $\lim_{n\to+\infty} \frac{1}{n} \ln \left(\int_{\mathbb{R}^n} \exp -\Phi(X)\; dX \right)$. We start from the decomposition:

$$\exp -\Phi(X) = K_V(x_1,x_2)\cdot K_V(x_2,x_3)\cdots K_V(x_{n-1},x_n)\cdot K_V(x_n,x_1) \tag{7.1.17}$$

and we observe that

$$\int_{\mathbb{R}^n} \exp -\Phi(X)\; dX = \int_{\mathbb{R}} K_V^{(n)}(y,y)\; dy \tag{7.1.18}$$

where $K_V^{(n)}(x,y)$ is the distribution kernel of $(K_V)^n$. Our assumption on V permits to see that $(K_V)^n$ is trace class[18] and we rewrite (7.1.18) in the form:

$$\int_{\mathbb{R}^n} \exp -\Phi(X)\; dX = \text{ Tr } [(K_V)^n] = \sum_j \mu_j^n \; , \tag{7.1.19}$$

---

[17] Let us sketch a proof of (7.1.15) in our particular case. $\mathbf{K}$ being positive and with an explicit kernel : $\exp -\frac{V(x)}{2}\; \exp -\mathcal{J}|x-y|^2\; \exp -\frac{V(y)}{2}$, one can find an Hilbert-Schmidt operator L satisfying $L^\star L = K$. The kernel of L is given, for a suitable θ, by $L(x,y) = c_\theta\, \exp -\theta|x-y|^2 \exp -\frac{V(y)}{2}$. We note indeed that $c_\theta \exp -\theta|x-y|^2$ is the distribution kernel of $\exp t_\theta \Delta$ for a suitable $t_\theta > 0$.
Then we observe that L is Hilbert-Schmidt and that $||L||_{H.S}^2 = \sum_j \mu_j = \text{ Tr } K$. Using the previously mentioned formula for the Hilbert-Schmidt norm and the property that

$$K(x,x) = \int L^\star(x,z)\, L(z,x)\, dz = \int L^\star(z,x)\, L(z,x)\, dz \; ,$$

one obtains (7.1.15).

[18] See for example [Ro].

where the μ_j are introduced in (7.1.24).
We note also for future use that

$$K_V^{(n)}(x,y) = \sum_j \mu_j^n \, u_j(x)\, u_j(y) \ . \tag{7.1.20}$$

In particular we get for the thermodynamic limit:

$$\lim_{n\to\infty} \frac{\ln \int_{\mathbb{R}^n} \exp -\Phi(X)\, dX}{n} = \ln \mu_1 \ . \tag{7.1.21}$$

Moreover the speed of the convergence is easily estimated by:

$$-\ln \left|\frac{\ln \int_{\mathbb{R}^n} \exp -\Phi(X)\, dX}{n} - \ln \mu_1\right| = -n \ln(\frac{\mu_2}{\mu_1}) - \ln k_2 + \ln n + \mathcal{O}(\exp -\delta_2 n) \ , \tag{7.1.22}$$

where k_2 is the multiplicity of μ_2.

7.1.3 Krein-Rutman's Theorem.

We observe now that the kernel $(x,y) \mapsto K_V(x,y)$ satisfies the condition

$$K_V(x,y) > 0 \ , \ \forall x, y \in \mathbb{R} \ . \tag{7.1.23}$$

In particular it satisfies the assumptions of the extended Perron-Frobenius Theorem also called Krein-Rutman's Theorem and our positive operator K_V admits consequently a largest eigenvalue μ_1 equal to $||K_V||$ which is simple and corresponds to a unique strictly positive normalized eigenfunction which we denote by u_1. Let μ_j the sequence of eigenvalues that we order as a decreasing sequence tending to 0:

$$0 \leq \mu_{j+1} \leq \mu_j \leq .... \leq \mu_2 < \mu_1 . \tag{7.1.24}$$

We shall denote by u_j a corresponding orthonormal basis of eigenvectors with

$$K_V u_j = \mu_j u_j \ , \ ||u_j|| = 1 \ . \tag{7.1.25}$$

Let us present the statements:

Definition 7.1.2. .
Let A be a bounded positive operator on a Hilbert space $\mathcal{H} = L^2(X, d\nu)$ where (X,ν) is a measured space. Then we say that A has a strictly positive kernel if, for each choice of a non negative function $\theta \in \mathcal{H}$ ($||\theta|| \neq 0$), we have

$$0 < A\theta$$

almost everywhere.

It is immediate to see that the transfer operator satisfies this condition. The theorem generalizing the Perron-Frobenius Theorem is then the following:

Theorem 7.1.3. .
Let A be a bounded positive compact symmetric operator on $\mathcal{H}$ having a strictly positive kernel and let[19] $||A|| = \lambda$ *be the largest eigenvalue of A. Then λ has multiplicity* 1 *and the corresponding eigenvector Ω can be chosen to be a strictly positive function.*

Proof:
Since A maps real functions into real functions, we may assume that Ω is real. We now prove that

$$\langle A\Omega, \Omega\rangle \leq \langle A|\Omega|, |\Omega|\rangle.$$

This is an immediate consequence of the strict positivity of the kernel. We just write:

$$\Omega = \Omega_+ - \Omega_-$$

and

$$|\Omega| = \Omega_+ + \Omega_-$$

and the above inequality is then a consequence of

$$\langle A\Omega_+, \Omega_-\rangle \geq 0 \ ,$$

and

$$\langle \Omega_+, A\Omega_-\rangle \geq 0 \ .$$

We then obtain

$$\lambda||\Omega||^2 = \langle A\Omega, \Omega\rangle \leq \langle A|\Omega|, |\Omega|\rangle \leq ||A|| \ ||\Omega||^2 = \lambda||\Omega||^2 \ .$$

This implies

$$\langle A\Omega, \Omega\rangle = \langle A|\Omega|, |\Omega|\rangle \ .$$

This equality means

$$\langle \Omega_+, A\Omega_-\rangle + \langle \Omega_-, A\Omega_+\rangle = 0 \ .$$

We then get a contradiction unless $\Omega_+ = 0$ or $\Omega_- = 0$. We can then assume $\Omega \geq 0$ and the assumption gives again

$$0 < \langle \theta, A\Omega\rangle = \lambda\langle \theta, \Omega\rangle \ ,$$

for any positive θ. This gives

$$\Omega \geq 0 \quad a.e \ .$$

But

$$\Omega = \lambda^{-1}A\Omega$$

[19] See Proposition 6.4.3

and this gives

$$\Omega > 0 \quad a.e \ .$$

Finally if there was two linearly independent eigenvectors Ψ and Ω corresponding to λ, we would obtain the same property for Ψ by considering as new Hilbert space the orthogonal of Ω in $\mathcal{H}$. But it is impossible to have two orthogonal vectors which are strictly positive.
q.e.d.

Remark 7.1.4. .
In the case $t = 0$, we keep the positivity but lose the injectivity ! The spectrum is easy to determine. We are indeed dealing with the orthonormal projector associated to the function $x \mapsto \exp -\frac{V(x)}{2}$. The real 1 is a simple eigenvalue and 0 is an eigenvalue whose corresponding eigenspace is infinite dimensional.

7.2 The Dirichlet realization, a model of operator with compact resolvent.

We can apply Theorem 6.5.1 to the operator $(-\Delta_D + Id)^{-1}$. We have seen that this operator is compact and it is clearly injective (by construction). It was also seen as a selfadjoint and positive. Moreover, the norm of this operator is less or equal to 1.
There exists consequently a sequence of distinct eigenvalues μ_n tending to 0 (with $0 < \mu_n \leq 1$) and a corresponding orthonormal basis of eigenvectors such that $(\Delta_D + I)^{-1}$ is diagonalized. If $\phi_{n,j}$ is a corresponding eigenvector associated with μ_n, that is, if

$$(-\Delta_D + I)^{-1}\phi_{n,j} = \mu_n \phi_{n,j} \ ,$$

we first observe that $\phi_{n,j} \in D(-\Delta_D + I)$; hence $\phi_{n,j} \in H_0^1(\Omega) \cap H^2(\Omega)$ (if Ω is relatively compact with regular boundary) and

$$-\Delta_D \phi_{n,j} = (\frac{1}{\mu_n} - 1)\phi_{n,j} \ .$$

The function $\phi_{n,j}$ is consequently an eigenvector of $-\Delta_D$ associated with the eigenvalue $\lambda_n = (\frac{1}{\mu_n} - 1)$.
Let us show, as easily imagined, that this basis $\phi_{n,j}$ permits effectively the diagonalization of $-\Delta_D$.
Let us indeed consider $u = \sum_{n,j} u_{n,j}\phi_{n,j}$ in the domain of $-\Delta_D$. Let us consider the scalar product $< -\Delta_D u, \phi_{m,\ell} >_{\mathcal{H}}$. Using the selfadjoint character of $-\Delta_D$, we get

$$< -\Delta_D u, \phi_{m,\ell} >_{\mathcal{H}} = < u, -\Delta_D \phi_{m,\ell} >_{\mathcal{H}} = \lambda_m u_{m,\ell} \ .$$

Observing, that $D(\Delta_D) = R(S^{-1})$, one obtains that the domain of $-\Delta_D$ is characterized by

$$D(-\Delta_D) = \{u \in L^2 \mid \sum_{n,j} \lambda_n^2 |u_{n,j}|^2 < +\infty\} \ .$$

Here we have used the property that for any N, we have the identity :

$$\sum_{n\leq N} u_{n,j}\phi_{n,j} = S(\sum_{n\leq N} \lambda_n u_{n,j}\phi_{n,j}) \ .$$

We have consequently given a meaning to the following diagonalization formula

$$-\Delta_D = \sum_n \lambda_n \Pi_{E_n} \ , \tag{7.2.1}$$

where Π_{E_n} is the orthogonal projector on the eigenspace E_n associated with the eigenvalue λ_n.
Let us remark that it results from the property that the sequence μ_n tends to 0 the property that λ_n tend to $+\infty$.
Let us also prove the

Lemma 7.2.1. .
The lowest eigenvalue of the Dirichlet realization of the Laplacian in a relatively compact domain Ω is strictly positive :

$$\lambda_1 > 0 \ . \tag{7.2.2}$$

Proof.
We know that $\lambda_1 \geq 0$; the Dirichlet realization of the Laplacian is indeed positive. If $\lambda_1 = 0$, a corresponding normalized eigenvector ϕ_1 would satisfy

$$< -\Delta\phi_1, \phi_1 >= 0 \ ,$$

and consequently

$$\nabla\phi_1 = 0 \ , \ \text{ dans } \Omega \ .$$

This leads first $\phi_1 =$ Cste in each connected component of Ω but because the trace of ϕ_1 on $\partial\Omega$ vanishes ($\phi_1 \in H_0^1(\Omega)$) implies that $\phi_1 = 0$. So we get a contradiction.

Finally it results from standard regularity theorems (See [Br], [LiMa]) that the eigenvectors belong (if Ω is regular) to $C^\infty(\overline{\Omega})$.

7.3 Extension to operators with compact resolvent

What we have done for the analysis of the Dirichlet realization is indeed quite general. It can be applied to selfadjoint operators, which are bounded from below and with compact resolvent.
We show that in this case, there exists an infinite sequence (if the Hilbert space is infinite dimensional) of real eigenvalues λ_n tending to $+\infty$ such that the corresponding eigenspaces are mutually orthogonal, of finite dimension and such that their corresponding Hilbertian sum is equal to $\mathcal{H}$.
Typically, one can apply the method to the Neumann realization of the Laplacian in a relatively compact domain Ω or to the harmonic oscillator in $I\!R^m$.

7.4 Operators with compact resolvent : the Schrödinger operator in an unbounded domain.

We just recall some criteria of compactness for the resolvent of the Schrödinger operator $P = -\Delta + V$ in $\mathbb{R}^m$ in connection with the precompactness criterion. In the case of the Schrödinger equation on $\mathbb{R}^m$ and if V is C^∞ and bounded from below, the domain of the selfadjoint extension is always contained in

$$Q(P) := H^1_V(\mathbb{R}^m) = \{u \in H^1(\mathbb{R}^m) | (V + C)^{\frac{1}{2}} u \in L^2(\mathbb{R}^m)\} .$$

$Q(P)$ is usually called the form domain of the form

$$u \mapsto \int_{\mathbb{R}^m} |\nabla u|^2 dx + \int_{\mathbb{R}^m} V(x) |u(x)|^2 \, dx .$$

It is then easy to see that, if V tends to ∞, then the injection of H^1_V in L^2 is compact (using a criterion of precompactness). We then obtain, observing that $(P+1)^{-1}$ is continuous from L^2 into H^1_V, that the resolvent $(P+\lambda)^{-1}$ is compact for $\lambda \notin \sigma(P)$.
In the case of a compact manifold M and if we consider the Laplace-Beltrami operator on M, then the compactness of the resolvent is obtain without additional assumption on V. The domain of the operator is $H^2(M)$ and we have compact injection from $H^2(M)$ into $L^2(M)$.
The condition that $V \to \infty$ as $|x| \to \infty$ is not a necessary condition. We can indeed replace it by the weaker sufficient condition

Proposition 7.4.1. .
Let us assume that the injection of $H^1_V(\mathbb{R}^m)$ into $L^2(\mathbb{R}^m)$ is compact then P is with compact resolvent.

More concretely, the way to verify this criterion is to show the existence of a continuous function $x \mapsto \rho(x)$ tending to ∞ as $|x| \to +\infty$ such that

$$H^1_V(\mathbb{R}^m) \subset L^2_\rho(\mathbb{R}^m) . \tag{7.4.1}$$

Of course, the preceding case corresponds to $\rho = V$, but, as typical example of this strategy, we shall show in exercise 7.4.3 that the Schrödinger operator on $\mathbb{R}^2$, $-\Delta + x^2 \cdot y^2 + 1$, is with compact inverse.
On the other hand, the criterion that $V \to +\infty$ as $|x| \to +\infty$ is not not too far from optimality.
We can indeed prove

Lemma 7.4.2. .
Suppose that $V \geq 0$ and that there exists $r > 0$ and a sequence σ_n such that $|\sigma_n| \to +\infty$ and such that

$$\sup_{n \in \mathbb{N}} \sup_{x \in B(\sigma_n, r)} V(x) < +\infty . \tag{7.4.2}$$

Then $-\Delta + V + 1$ is not with compact inverse.

Proof.
Let us consider the sequence

$$\phi_n(x) = \psi(x - \sigma_n) \ . \tag{7.4.3}$$

Here ψ is a compactly supported function of L^2 norm 1 and with support in $B(0, r)$.
We observe that the ϕ_n are an orthogonal sequence (after possibly extracting a subsequence for obtaining that the supports of ϕ_n and $\phi_{n'}$ are disjoint for $n \neq n'$) which satisfies for some constant C

$$||\phi_n||^2_{H^2} + ||V\phi_n||^2_{L^2} \leq C \ . \tag{7.4.4}$$

In particular, there exists C such that :

$$||(-\Delta + V + 1)\phi_n||_{L^2} \leq C \ , \ \forall n \in I\!N \ .$$

But we can not extract from this sequence a strongly convergent sequence in L^2, because ϕ_n is weakly convergent to 0 and $||\phi_n|| = 1$. So the operator $(-\Delta + V + I)^{-1}$ can not be a compact operator.

Exercise 7.4.3. .
Show that the unbounded operator on $L^2(I\!R^2)$

$$P := -\frac{d^2}{dx^2} - \frac{d^2}{dy^2} + x^2y^2 \ ,$$

is with compact resolvent.

Hint.
One can introduce

$$X_1 = \frac{1}{i}\partial_x \ , \ X_2 = \frac{1}{i}\partial_y \ , \ X_3 = xy \ ,$$

and show, for $j = 1, 2$ and for a suitable constant C, the following inequality :

$$||(x^2 + y^2 + 1)^{-\frac{1}{4}}[X_j, X_3]u||^2 \leq C \left(< Pu, u >_{L^2(I\!R^2)} + ||u||^2\right) \ ,$$

for all $u \in C_0^\infty(I\!R^2)$.
One can also observe that

$$i[X_1, X_3] = y \ , \ i[X_2, X_3] = x \ ,$$

and then

$$\begin{aligned} &||(x^2 + y^2 + 1)^{-\frac{1}{4}}[X_1, X_3]u||^2 + ||(x^2 + y^2 + 1)^{-\frac{1}{4}}[X_2, X_3]u||^2 + ||u||^2 \\ &\quad \geq ||(x^2 + y^2 + 1)^{\frac{1}{4}}u||^2 \ . \end{aligned}$$

For the control of $||(x^2 + y^2 + 1)^{-\frac{1}{4}}[X_1, X_3]u||^2$, one can remark that

$$||(x^2 + y^2 + 1)^{-\frac{1}{4}}[X_1, X_3]u||^2 = \langle \frac{y}{(x^2 + y^2 + 1)^{\frac{1}{4}}} u \mid (X_1\, X_3 - X_3\, X_1)u \rangle \ ,$$

and perform an integration by parts.

7.5 The Schrödinger operator with magnetic field

We can consider on $\mathbb{R}^m$ the so-called Schrödinger operator with magnetic field :

$$P_{A,V} := -\Delta_A + V \ , \tag{7.5.1}$$

where

$$-\Delta_A := \sum_{j=1}^{m} (\frac{1}{i}\partial_{x_j} - A_j(x))^2 \ . \tag{7.5.2}$$

Here $x \mapsto \vec{A} = (A_1(x), \cdots, A_n(x))$ is a vector field on $\mathbb{R}^m$ called the "magnetic potential" and V is called the electric potential. It is easy to see that, when V is semi-bounded, the operator is symmetric and semi-bounded on $C_0^\infty(\mathbb{R}^m)$. We can therefore consider the Friedrichs extension and analyze the property of this selfadjoint extension.
A general question arises if one can get operator of the type $P_{A,V}$ which are with compact resolvent if $V = 0$. This is the problem which is called the problem of the magnetic bottle.
The "heuristical" idea is that the module of the magnetic field can play in some sense the role of the electric potential if it does not oscillate too rapidly ($m \geq 2$).
For defining the magnetic field it is probably easier to consider the magnetic potential as a one-form

$$\sigma_A = \sum_{j=1}^{n} A_j(x) dx_j \ .$$

The magnetic field is then defined as the two form

$$\omega_B = d\sigma_A = \sum_{j<k} (\partial_{x_j} A_k - \partial_{x_k} A_j) dx_j \wedge dx_k \ .$$

The case when $m = 2$ is particularly simple. In this case,

$$\omega_B = B dx_1 \wedge dx_2 \ ,$$

and we can identify ω_B with the function[20] $x \mapsto B(x) = \text{curl } (\vec{A})(x)$.
The proof is particularly simple in the case when $B(x)$ has a constant sign (say $B(x) \geq 0$). In this case, we immediately have the inequality

$$\int_{\mathbb{R}^2} B(x)|u(x)|^2 dx \leq < -\Delta_A u, u >_{L^2} \ . \tag{7.5.3}$$

We observe indeed the following identities between operators

$$B(x) = \frac{1}{i}[X_1, X_2] \ , \ -\Delta_A = X_1^2 + X_2^2 \ . \tag{7.5.4}$$

[20] Here, for french readers, curl denotes the rotational (in french "rotationnel") rot .

Here

$$X_1 = \frac{1}{i}\partial_{x_1} - A_1(x)\ ,\ X_2 = \frac{1}{i}\partial_{x_2} - A_2(x)\ .$$

Note also that :

$$\langle -\Delta_A u\ ,\ u\rangle = ||X_1 u||^2 + ||X_2 u||^2\ ,$$

for all $u \in C_0^\infty(I\!R^2)$.
To obtain (7.5.3) is then easy through an integration by parts. One can also use, introducing $Z = X_1 + iX_2$, the positivity of $Z^* Z$ or ZZ^*.
We then easily obtain as in the previous example that the operator is with compact resolvent if $B(x) \to +\infty$.
As a simple example, one can think of

$$\vec{A} = (-x_1^2 x_2, +x_1 x_2^2)\ ,$$

which gives

$$B(x) = x_1^2 + x_2^2\ .$$

Note that the case $m = 2$ is rather particular and it is more difficult to treat $m > 2$. We have indeed to introduce partition of unity.

7.6 Laplace Beltrami operators on a Riemannian compact manifold

If M is a compact riemannian manifold, it is well known that in this case one can canonically define a measure $d\mu_M$ on M and consequently the Hilbertian space $L^2(M)$. We have also a canonical definition of the gradient. At each point x of M, we have indeed a scalar product on $T_x M$ giving an isomorphism between $T_x M$ and $T_x^* M$. Using this family of isomorphisms we have a natural identification between the C^∞-vector fields on M and the 1-forms on M. In this identification, the vector field $\mathrm{grad}\, u$ associated to a C^∞ function on M corresponds to the 1-form du.
Considering on $C^\infty(M) \times C^\infty(M)$ the sesquilinear form

$$(u, v) \mapsto a_0(u, v) := \int_M < \mathrm{grad}\, u(x)\ ,\ \mathrm{grad}\, v(x) >_{T_x M}\ d\mu_M\ .$$

There is a natural differential operator $-\Delta_M$ called the Laplace-Beltrami operator on M such that

$$a_0(u, v) =< -\Delta_M u\ ,\ v >_{L^2(M)}\ .$$

In this context, it is not diffficult to define the Friedrichs extension and to get a selfadjoint extension of $-\Delta_M$ as a selfadjoint operator on $L^2(M)$. The domain is easily characterized as being $H^2(M)$, the Sobolev space naturally associated to $L^2(M)$ and one can show that the injection of $H^2(M)$ into $L^2(M)$ is compact because M is compact. The selfadjoint extension of $-\Delta_M$ is with compact resolvent and the general theory can be applied to this example.

The simplest model is the operator $-d^2/d\theta^2$ on the circle of radius one whose spectrum is $\{n^2\ ,\ n \in I\!N\}$. For $n > 0$ the multiplicity is 2. An orthonormal basis is given by the functions $\theta \mapsto (2\pi)^{-\frac{1}{2}} \exp in\theta$ for $n \in Z\!\!\!Z$. Here the form domain of the operator is $H^{1,per}(S^1)$ and the domain of the operator is $H^{2,per}(S^1)$. These spaces have two descriptions. One is to describe these operators as $H^{1,per} := \{u \in H^1(]0, 2\pi[\ \mid\ u(0) = u(2\pi)\}$ and $H^{2,per} := \{u \in H^2(]0, 2\pi[\ \mid u(0) = u(2\pi)\ ,\ u'(0) = u'(2\pi)\}$.
The other way is to consider the Fourier coefficients of u.
The Fourier coefficients of $u \in H^{k,per}$ are in $\mathbf{h}^k$. Here

$$\mathbf{h}^k := \{u_n \in \ell^2(Z\!\!\!Z) \mid n^k u_n \in \ell^2(Z\!\!\!Z)\}.$$

It is then easy to prove the compact injection from $H^{1,per}$ in $L^2(S^1)$ or equivalently from $\mathbf{h}^1$ into ℓ^2.
More generally, elliptic symmetric positive operators of order $m > 0$ admit a selfadjoint extension with compact resolvent. We refer to the book by Berger-Gauduchon-Mazet [BGM] for this central subject in Riemannian geometry.

8 Selfadjoint unbounded operators and spectral theory.

8.1 Introduction

Once we have a selfadjoint operator we can apply the basic spectral decomposition, which we shall now describe without to give complete proofs. Before to explain the general case, let us come back to the spectral theorem for compact operators T or operators with compact resolvent. This will permit us to introduce a new vocabulary.
We have seen that one can obtain a decomposition of $\mathcal{H}$ in the form

$$\mathcal{H} = \oplus_{k\in \mathbb{N}} V_k \;, \tag{8.1.1}$$

such that

$$T u_k = \lambda_k u_k \;, \;\text{ if } u_k \in V_k \;. \tag{8.1.2}$$

Hence we have decomposed $\mathcal{H}$ into a direct sum of subspaces V_k in which the selfadjoint operator T is reduced to multiplication by λ_k.
If P_k denotes the orthogonal projection operator onto V_k, we can write

$$I = \sum_k P_k \;, \tag{8.1.3}$$

and

$$T u = \sum_k \lambda_k P_k u \;,\; \forall u \in D(T) \;. \tag{8.1.4}$$

Here we recall the definition

Definition 8.1.1. .
An operator $P \in \mathcal{L}(\mathcal{H})$ is called an orthogonal projection if $P = P^*$ and $P^2 = P$.

If we assume that T is semibounded (with compact resolvent), we can introduce for any $\lambda \in \mathbb{R}$

$$G_\lambda = \oplus_{\lambda_k \leq \lambda} V_k \;, \tag{8.1.5}$$

and E_λ is the orthogonal projection onto G_λ :

$$E_\lambda = \sum_{\lambda_k \leq \lambda} P_k \;. \tag{8.1.6}$$

It is easy to see that the function $\lambda \mapsto E_\lambda$ has values in $\mathcal{L}(\mathcal{H})$ and satisfy the following properties :

- $E_\lambda \cdot E_\mu = E_{\inf(\lambda,\mu)}$;

- for all λ, $E_{\lambda+0} = E_\lambda$;
- $\lim_{\lambda\to-\infty} E_\lambda = 0$, $\lim_{\lambda\to+\infty} E_\lambda = Id$.

We also observe that

$$E_{\lambda_k} - E_{\lambda_k - 0} = P_k \ .$$

Then in the sense of vectorvalued distributions, we have

$$dE_\lambda = \sum_k \delta_{\lambda_k} \otimes P_k \ , \tag{8.1.7}$$

where δ_{λ_k} is the Dirac measure at the point λ_k. Hence, in the sense of Stieltjes integrals, one can write

$$x = \int_{-\infty}^{+\infty} dE_\lambda(x) \ ,$$

and

$$T = \int_{-\infty}^{+\infty} \lambda dE_\lambda \ .$$

This is in this form that we shall generalize the previous formulas to the case of any selfadjoint operator T.

Functional calculus for operators with compact resolvent :
If f is a continuous (or piecewise continuous function) one can also define $f(T)$ as

$$f(T) = \sum_k f(\lambda_k) \cdot P_k \ ,$$

as an unbounded operator whose domain is

$$D(f(T)) = \{x \in \mathcal{H} \mid \sum_k |f(\lambda_k)|^2 ||x_k||^2 < +\infty\} \ ,$$

where $x_k = P_k x$.

We can also write $f(T)$ in the form :

$$< f(T)x, y >_{\mathcal{H}} = \int_{\mathbb{R}} f(\lambda) \ d < E_\lambda x, y > \ ,$$

where the domain of $f(T)$ is described as

$$D(f(T)) = \{x \in \mathcal{H} \mid \int_{\mathbb{R}} |f(\lambda)|^2 \ d < E_\lambda x, x >_{\mathcal{H}} < +\infty\} \ .$$

Remark 8.1.2. .
There are two conventions for the notation of the eigenvalues. The first one is to classify them into an increasing sequence

$$\mu_j \leq \mu_{j+1}$$

counting each eigenvalue according to its multiplicity. The second one is to describe them as a strictly increasing sequence λ_k with λ_k eigenvalue of multiplicity m_k.

We now present a list of properties which are easy to verify in this particular case and which will be still true in the general case.

Remarks 8.1.3. .

1. *If f and g coincide on $\sigma(T)$, then $f(T) = g(T)$. For any $(x, y) \in \mathcal{H} \times \mathcal{H}$, the support of the measure $d\langle E_\lambda x, y\rangle$ is contained in $\sigma(T)$.*

2. *If f and g are functions on $\mathbb{R}$,*
$$f(T)g(T) = (f \cdot g)(T)\ .$$
In particular, if $(T - z)$ is invertible, the inverse is given by $f(T)$ where f is a continuous function such that $f(\lambda) = (\lambda - z)^{-1}$, $\forall \lambda \in \sigma(T)$.

3. *If f is bounded, then $f(T)$ is bounded and we have*
$$||f(T)|| \leq \sup_{\lambda \in \sigma(T)} |f(\lambda)|\ . \tag{8.1.8}$$

4. *The function f may be complex. Note that, in this case, we get*
$$f(T)^\star = \overline{f}(T)\ . \tag{8.1.9}$$
An interesting case is, for $z \in \mathbb{C} \setminus \mathbb{R}$, the function $\lambda \mapsto (\lambda - z)^{-1}$. Then we get from (8.1.8)
$$||(T - z)^{-1}||_{\mathcal{L}(\mathcal{H})} \leq |\ Im\ z|^{-1}\ . \tag{8.1.10}$$

5. *More generally, this works also for $z \in \mathbb{R} \setminus \sigma(T)$. We then obtain in this case the spectral theorem*
$$||(T - z)^{-1}||_{\mathcal{L}(\mathcal{H})} \leq d(z, \sigma(T))^{-1}\ . \tag{8.1.11}$$

6. *If $f \in C_0^\infty(\mathbb{R})$, we have :*
$$f(T) = \frac{1}{\pi} \lim_{\epsilon \to 0+} \int_{|Imz|>\epsilon} (\frac{\partial \tilde{f}}{\partial \bar{z}})(T - z)^{-1} dx.dy\ . \tag{8.1.12}$$

Here $\tilde{f}$ is defined by :

$$\tilde{f}(x,y) = (f(x) + iyf'(x))\chi(y) \ ,$$

where $\chi(y)$ is equal to 1 in a neighborhood of 0 and with compact support. This formula can be proven using the Green-Formula (first prove it with T replaced by the scalar λ) or using that :

$$\partial_{\bar{z}} \frac{1}{z-\lambda} = \pi \delta_0 \ ,$$

where δ_0 is the Dirac measure at $(0,0) \in \mathbb{R}^2$, $\partial_{\bar{z}} = \frac{1}{2}(\partial_x + i\partial_y)$. One should observe that $\tilde{f}$ is not holomorphic but "almost" holomorphic in the sense that :

$$\partial \tilde{f} / \partial \bar{z} = \mathcal{O}(y) \ ,$$

as $y \to 0$.

8.2 Spectrum.

We now come back to the notion of spectrum that we have only met for bounded operators.

Definition 8.2.1. .
The resolvent set of a closed operator T is the set of the λ in $\mathbb{C}$ such that the range of $(T-\lambda)$ is equal to $\mathcal{H}$ and such that $(T-\lambda)$ admits a continuous operator denoted by $R(\lambda)$ whose range is included in $D(T)$ such that :

$$R(\lambda)(T-\lambda) = I_{D(T)} \ ,$$

and

$$(T-\lambda)R(\lambda) = I_{\mathcal{H}} \ .$$

As in the bounded case, we observe that the resolvent set is open. Note also that the continuity of $R(\lambda)$ is actually a consequence of the property that the graph of $R(\lambda)$ is closed (using that T is closed).

Definition 8.2.2. .
The spectrum of a closed operator T is defined as the complementary set in $\mathbb{C}$ of the resolvent set.

The spectrum $\sigma(T)$ is closed in $\mathbb{C}$ and real if T is selfadjoint.

8.3 Spectral family and resolution of the identity.

Definition 8.3.1. .
A family of orthogonal projectors $E(\lambda)$ (or E_λ), $-\infty < \lambda < \infty$ in an Hilbert space $\mathcal{H}$ is called a resolution of the identity (or spectral family) if it satisfies the following conditions :

- $$E(\lambda)E(\mu) = E(\min(\lambda,\mu)) \ , \tag{8.3.1}$$

- $$E(-\infty) = 0, E(+\infty) = I, \tag{8.3.2}$$

  where $E(\pm\infty)$ *is defined* [21] *by*

  $$E(\pm\infty)x = \lim_{\lambda\to\pm\infty} E(\lambda)x$$

  for all x *in* $\mathcal{H}$,

- $$E(\lambda+0) = E(\lambda) \ , \tag{8.3.3}$$

  where $E(\lambda+0)$ *is defined by*

  $$E(\lambda+0)x = \lim_{\mu\to\lambda\ ,\ \mu>\lambda} E(\mu)x \ .$$

Remark 8.3.2. .
We have shown an example of such a family in the previous subsection.

Proposition 8.3.3. .
Let $E(\lambda)$ *be a resolution of identity (=spectral family); then for all* $x,y\in\mathcal{H}$, *the function*

$$\lambda \mapsto < E(\lambda)x, y > \tag{8.3.4}$$

is a function of bounded variation whose total variation [22] *satisfies*

$$V(x,y) \leq ||x||\cdot||y||\ ,\ \forall x,y\in\mathcal{H}\ . \tag{8.3.5}$$

Proof.
Let $\lambda_1 < \lambda_2 < \cdots < \lambda_n$. We first get from the assumption (8.3.1) that

$$E_{]\alpha,\beta]} = E_\beta - E_\alpha$$

is an orthogonal projection. From the Cauchy-Schwarz inequality we have

$$\begin{aligned}
\sum_{j=2}^n |< E_{]\lambda_{j-1},\lambda_j]}x, y >| \ & = \sum_{j=2}^n |< E_{]\lambda_{j-1},\lambda_j]}x, E_{]\lambda_{j-1},\lambda_j]}y >| \\
& \leq \sum_{j=2}^n ||E_{]\lambda_{j-1},\lambda_j]}x||\ ||E_{]\lambda_{j-1},\lambda_j]}y|| \\
& \leq \left(\sum_{j=2}^n ||E_{]\lambda_{j-1},\lambda_j]}x||^2\right)^{\frac{1}{2}} \left(\sum_{j=2}^n ||E_{]\lambda_{j-1},\lambda_j]}y||^2\right)^{\frac{1}{2}} \\
& = \left(||E_{]\lambda_1,\lambda_n]}x||^2\right)^{\frac{1}{2}} \left(||E_{]\lambda_1,\lambda_n]}y||^2\right)^{\frac{1}{2}}\ .
\end{aligned}$$

[21] (8.3.1) gives the existence of the limit (cf also Lemma 8.3.4). Here the limit is taken in the norm of $\mathcal{H}$. We observe indeed that $\lambda\mapsto\langle E(\lambda)x,x\rangle = ||E(\lambda)x||^2$ is monotonically increasing.

[22] See the definition in (8.3.7)

But for $m > n$, we get

$$||x||^2 \geq ||E_{]\lambda_n,\lambda_m]}x||^2 = \sum_{i=n}^{m-1} ||E_{]\lambda_i,\lambda_{i+1}]}x||^2 \, . \tag{8.3.6}$$

We finally obtain that, for any finite sequence $\lambda_1 < \lambda_2 < \cdots < \lambda_n$, we have

$$\sum_{j=2}^{n} | < E_{]\lambda_{j-1},\lambda_j]}x, y > | \leq ||x|| \cdot ||y|| \, .$$

This shows the bounded variation and the estimate of the total variation defined as

$$V(x,y) := \sup_{\lambda_1,\cdots,\lambda_n} \sum_{j=2}^{n} | < E_{]\lambda_{j-1},\lambda_j]}x, y > | \, . \tag{8.3.7}$$

We now observe that, for all x and y in $\mathcal{H}$, the function $\lambda \mapsto \langle E(\lambda)x, y\rangle$ is with bounded variation and one can then show the existence of $E(\lambda+0)$ and $E(\lambda-0)$. This is the object of

Lemma 8.3.4. .
If $E(\lambda)$ is a family of projectors satisfying (8.3.1) and (8.3.2), then, for all $\lambda \in \mathbb{R}$, the operators

$$E_{\lambda+0} = \lim_{\mu\to\lambda \;\; \mu>\lambda} E(\mu) \; , \; E_{\lambda-0} = \lim_{\mu\to\lambda \;\; \mu<\lambda} E(\mu) \; , \tag{8.3.8}$$

are well defined when considering the limit for the strong convergence topology.

Proof.
From (8.3.6), we get that for any $\epsilon > 0$ there exists $\lambda_0 < \lambda$ such that, $\forall \lambda'$, $\forall \lambda'' \in [\lambda_0, \lambda[$, such that $\lambda' < \lambda''$

$$||E_{]\lambda',\lambda'']}x||^2 \leq \epsilon \, .$$

It is then easy to show that $E_{\lambda-\frac{1}{n}}x$ is a Cauchy sequence converging to a limit and that this limit does not depend on the choice of the sequence tending to λ. The proof of the existence of the limit from above is the same. This ends the proof of the lemma.

It is then classical (Stieltjes integrals) that one can define for any continuous complex valued function $\lambda \mapsto f(\lambda)$ the integrals $\int_a^b f(\lambda) d\langle E(\lambda)x, y\rangle$ as a limit[23] of Riemann sums.

[23] The best is to first consider the case when $x = y$.

Proposition 8.3.5. .
Let f be a continuous function on $I\!R$ with complex values and let $x \in \mathcal{H}$. Then it is possible to define for $\alpha < \beta$, the integral

$$\int_\alpha^\beta f(\lambda)\, dE_\lambda x$$

as the strong limit in $\mathcal{H}$ of the Riemann sum :

$$\sum_j f(\lambda'_j)(E_{\lambda_{j+1}} - E_{\lambda_j})x\ , \tag{8.3.9}$$

where

$$\alpha = \lambda_1 < \lambda_2 < \cdots < \lambda_n = \beta\ ,$$

and

$$\lambda'_j \in]\lambda_j, \lambda_{j+1}]\ ,$$

when $\max_j |\lambda_{j+1} - \lambda_j| \to 0$.

The proof is easy using the uniform continuity of f. Note also that the notation could be misleading. May be $\int_{]\alpha,\beta]} f(\lambda) dE_\lambda x$ is less ambiguous.

We now arrive like in the standard theory to the undefined integral.

Definition 8.3.6. .
For any given $x \in \mathcal{H}$ and any continuous function f on $I\!R$, the integral :

$$\int_{-\infty}^{+\infty} f(\lambda) dE_\lambda x$$

is defined as the strong limit in $\mathcal{H}$, if it exists of $\int_\alpha^\beta f(\lambda) dE_\lambda x$ when $\alpha \to -\infty$ and $\beta \to +\infty$.

Remark 8.3.7. .
The theory works more generally for any borelian function (cf Reed-Simon, Vol. 1 [RS-I]). This can be important, because we are in particular interested in the case when $f(t) = 1_{]-\infty,\lambda]}(t)$.
One possibility for the reader who wants to understand how this can be made is to take the Rudin's book [Ru1], which gives the following theorem (Theorem 8.14, p. 173)

Theorem 8.3.8. .

1. *If μ is a complex Borel measure on $I\!R$ and if*

$$(\star) \quad f(x) = \mu(]-\infty, x])\ ,\ \forall x \in I\!R\ ,$$

   then f is a normalized function with bounded variation (NBV). By NBV we mean, with bounded variation, but also continuous from the right and such that $\lim_{x\to-\infty} f(x) = 0$.

2. *Conversely, to every $f \in NBV$, there corresponds a unique complex Borel measure μ such that $(\star)$ is satisfied.*

Theorem 8.3.9. .
For x given in $\mathcal{H}$ and f a complex valued continuous on $I\!R$, the following conditions are equivalent

- $$\int_{-\infty}^{+\infty} f(\lambda) dE_\lambda x \text{ exists } ; \tag{8.3.10}$$

- $$\int_{-\infty}^{+\infty} |f(\lambda)|^2 d||E_\lambda x||^2 < +\infty; \tag{8.3.11}$$

- $$y \mapsto \int_{-\infty}^{+\infty} f(\lambda) d(< E_\lambda y, x >_{\mathcal{H}}) \tag{8.3.12}$$

  is a continuous linear form.

Hint for the proof.

a)
(8.3.10) implies (8.3.12) essentially by using repeatedly the Banach-Steinhaus's theorem (also called Uniform Boundedness Theorem) and the definition of the integral.

b)
Let us prove that (8.3.12) implies (8.3.11).

Let F be the linear form appearing in (8.3.12). If we introduce $y = \int_\alpha^\beta \overline{f(\lambda)} dE_\lambda x$, then we first observe (coming back to the Riemann integrals) that

$$y = E_{]\alpha,\beta]} y \; .$$

It is then not too difficult to show that

$$\begin{array}{ll} \overline{F(y)} & = \int_{-\infty}^{+\infty} \overline{f(\lambda)} d < E_\lambda x, y > \\ & = \int_{-\infty}^{+\infty} \overline{f(\lambda)} d < E_\lambda x, E_{]\alpha,\beta]} y > \\ & \int_{-\infty}^{+\infty} \overline{f(\lambda)} d < E_{]\alpha,\beta]} E_\lambda x, y > \\ & = \int_\alpha^\beta \overline{f(\lambda)} d < E_\lambda x, y > \\ & = ||y||^2 \; . \end{array}$$

Using (8.3.12), we get $||y||^2 \leq ||F|| \cdot ||y||$ and consequently

$$||y|| \leq ||F|| \, . \tag{8.3.13}$$

Here we observe that the r.h.s. is independent of α and β.

On the other hand, coming back to Riemann sums, we get

$$||y||^2 = \int_\alpha^\beta |f(\lambda)|^2 d||E_\lambda x||^2 \,.$$

We finally obtain

$$\int_\alpha^\beta |f(\lambda)|^2 d||E_\lambda x||^2 \leq ||F||^2 \,. \tag{8.3.14}$$

Hence, taking the limits $\alpha \to -\infty$ and $\beta \to +\infty$, we obtain (8.3.11).

c)
For the last implication, it is enough to observe that, for $\alpha' < \alpha < \beta < \beta'$, we have

$$|| \int_{\alpha'}^{\beta'} f(\lambda) dE_\lambda x - \int_\alpha^\beta f(\lambda) dE_\lambda x||^2 = \int_{\alpha'}^{\alpha} |f(\lambda)|^2 d||E_\lambda x||^2 + \int_\beta^{\beta'} |f(\lambda)|^2 d||E_\lambda x||^2 \,.$$

Theorem 8.3.10. .
Let $\lambda \mapsto f(\lambda)$ be a real-valued continuous function. Let

$$D_f := \{x \in \mathcal{H}, \int_{-\infty}^{+\infty} |f(\lambda)|^2 \; d\langle E(\lambda)x, x\rangle \; < \; \infty \; , \; \}.$$

Then D_f is dense in $\mathcal{H}$ and we can define T_f whose domain is defined by

$$D(T_f) = D_f \;,$$

and

$$\langle T_f x, y\rangle \; = \; \int_{-\infty}^{+\infty} f(\lambda) d\langle E(\lambda)x, y\rangle$$

for all x in $D(T_f)$ and y in $\mathcal{H}$.
The operator T_f is selfadjoint.
Finally, we have

$$TE_\lambda \textit{ is an extension of } E_\lambda T \,. \tag{8.3.15}$$

Proof of the theorem.
From property (8.3.2), we obtain that, for any y in $\mathcal{H}$, there exists a sequence (α_n, β_n) such that $E_{]\alpha_n,\beta_n]} y \to y$ as $n \to +\infty$.
But $E_{]\alpha,\beta]} y$ belongs to D_f, for any α, β, and this shows the density of D_f in $\mathcal{H}$.
We now observe that f being real and E_λ being symmetric the symmetry is clear.
We observe that, for $f_0 = 1$, we have $T_{f_0} = I$ and for $f_1(\lambda) = \lambda$, we obtain a

selfadjoint operator $T_{f_1} := T$.
In this case we say that

$$T = \int_{-\infty}^{+\infty} \lambda \; dE(\lambda)$$

is a spectral decomposition of T and we shall note that

$$||Tx||^2 = \int_{-\infty}^{+\infty} \lambda^2 d\left\langle E(\lambda)x, x\right\rangle \; = \; \int_{-\infty}^{+\infty} \lambda^2 d\, ||E(\lambda)x||^2 \; ,$$

for $x \in \; D(T)$.
More generally

$$||T_f x||^2 = \int_{-\infty}^{+\infty} |f(\lambda)|^2 d((E(\lambda)x, x)) = \int_{-\infty}^{+\infty} |f(\lambda)|^2 d(||E(\lambda)x||^2)$$

for $x \in D(T_f)$.

Conclusion. We have consequently seen in this subsection how one can associate to a spectral family of projectors a selfadjoint operator. We have seen in the introduction that the converse was true for a compact operator or an operator with compact resolvent. It remains to prove that this is the general case.

8.4 The spectral decomposition Theorem.

The spectral decomposition Theorem makes explicit that the preceding situation is actually the general one.

Theorem 8.4.1. .
Any selfadjoint operator T in an Hilbert space $\mathcal{H}$ admits a spectral decomposition such that

$$\begin{array}{l} < Tx, y >= \int_{\mathbb{R}} \lambda \; d < E_\lambda x, y >_{\mathcal{H}} \; , \\ Tx = \int_{\mathbb{R}} \lambda d(E_\lambda x) \; . \end{array} \tag{8.4.1}$$

"Proof".
We shall not give a detailed proof. We refer to [Hu] or [DaLi] for one possible proof or to [RS-I] for another proof which we describe now shortly. Another interesting proof is based on Formula 8.1.12 and presented in the book of Davies [Da].

Step 1.
It is rather natural to imagine that it is essentially enough to treat the case when T is a bounded selfadjoint operator (or at least a normal bounded operator, that is satisfying $T^*T = TT^*$). If A is indeed a general semibounded selfadjoint operator, one can come back to the bounded case by considering $(A + \lambda_0)^{-1}$, with

λ_0 real, which is bounded and selfadjoint. In the general case[24], one can consider $(A+i)^{-1}$.

Step 2.
We analyze first the spectrum of $P(T)$ where P is a polynomial.

Lemma 8.4.2. .
If P is a polynomial, then

$$\sigma(P(T)) = \{P(\lambda) \mid \lambda \in \sigma(T)\} \tag{8.4.2}$$

Hint.
Use the identity $P(x) - P(\lambda) = (x-\lambda)Q_\lambda(x)$ and the corresponding identity between bounded operators $P(T) - P(\lambda) = (T-\lambda)Q_\lambda(T)$. This permits to construct the inverse of $(T-\lambda)$ if one knows the inverse of $P(T) - P(\lambda)$.
More generally, we observe if $z \in \mathbb{C}$ and if $\lambda_j(z)$ are the roots of $\lambda \mapsto (P(\lambda) - z)$, we can write :

$$(P(T) - z) = c \prod_j (T - \lambda_j(z)) \,.$$

This permits to construct the inverse of $(P(T) - z)$ if one has the inverses of $(T - \lambda_j(z))$ (for all j).

Lemma 8.4.3. .
Let T be a bounded self-adjoint operator. Then

$$||P(T)|| = \sup_{\lambda \in \sigma(T)} |P(\lambda)| \,. \tag{8.4.3}$$

We first observe that

$$||P(T)||^2 = ||P(T)^* P(T)||$$

This is the consequence of the general property that :

$$||A^* A|| = ||A||^2 \,.$$

The proof is obtained by observing first that :

$$\begin{array}{ll} ||A^*A|| & = \sup_{||x||\leq 1, ||y||\leq 1} |\langle A^*Ax, y\rangle| \\ & = \sup_{x,y\ ||x||\leq 1, ||y||\leq 1} |\langle Ax, Ay\rangle \\ & \leq ||A||^2 \,, \end{array}$$

and secondly that :

$$||A||^2 = \sup_{||x||\leq 1} \langle Ax, Ax\rangle = \sup_{||x||\leq 1} \langle A^*Ax, x\rangle \leq ||A^*A|| \,.$$

[24] Here we recall that an example of operator which is not semibounded is given in Exercise 4.1.3

We then observe that :

$$\begin{array}{ll} ||P(T)||^2 & = ||(\bar{P}P)(T)|| \\ & = \sup_{\lambda \in \sigma(\bar{P}P)(T)} |\lambda| \qquad \text{(using Theorem 6.4.1)} \\ & = \sup_{\lambda \in \sigma(T)} |(\bar{P}P)(\lambda)| \qquad \text{(using Lemma 8.4.2)} \\ & = \left(\sup_{\lambda \in \sigma(T)} |P(\lambda)|^2\right) \qquad . \end{array}$$

Step 3.
We have defined a map Φ from the set of polynomials into $\mathcal{L}(\mathcal{H})$ defined by

$$P \mapsto \Phi(P) = P(T) , \tag{8.4.4}$$

which is continuous

$$||\Phi(P)||_{\mathcal{L}(\mathcal{H})} = \sup_{\lambda \in \sigma(T)} |P(\lambda)| . \tag{8.4.5}$$

The set $\sigma(T)$ is a compact in $I\!R$ and using the Stone-Weierstrass theorem (which states the density of the polynomials in $C^0(\sigma(T))$), the map Φ can be uniquely extended in a unique map Φ on $C^0(\sigma(T))$. The properties of Φ are described in the following theorem

Theorem 8.4.4. .
Let T be as selfadjoint continuous operator on $\mathcal{H}$. Then there exists a unique map Φ from $C^0(\sigma(T))$ into $\mathcal{L}(\mathcal{H})$ with the following properties :

1. $$\begin{array}{ll} \Phi(f+g) = \Phi(f) + \Phi(g) \ , & \Phi(\lambda f) = \lambda \Phi(f) \ ; \\ \Phi(1) = Id \ , & \Phi(\bar{f}) = \Phi(f)^* \ ; \\ \Phi(fg) = \Phi(f) \circ \Phi(g) \ . & \end{array}$$

2. $$||\Phi(f)|| = \sup_{t \in \sigma(T)} |f(t)| .$$

3. *If f is defined by $f(x) = x$, then $\Phi(f) = T$.*

4. $$\sigma(\Phi(f)) = \{f(\lambda) \mid \lambda \in \sigma(T)\} .$$

5. *If ψ satisfies $T\psi = \lambda\psi$, then $\Phi(f)\psi = f(\lambda)\psi$.*

6. *If $f \geq 0$, then $\Phi(f) \geq 0$.*

All these properties are obtained by showing first the properties for P and then extending the properties by continuity.
For the last item, note that :

$$\Phi(f) = \Phi(\sqrt{f}) \cdot \Phi(\sqrt{f}) = \Phi(\sqrt{f})^* \cdot \Phi(\sqrt{f}) .$$

Step 4.
We are now ready to introduce the measures. Let $\psi \in \mathcal{H}$. Then

$$f \mapsto < \psi, f(T)\psi >_{\mathcal{H}} = < \psi, \Phi(f)\psi >_{\mathcal{H}}$$

is a positive linear functional on $C^0(\sigma(T))$. By measure theory (Riesz Theorem) (cf Rudin [Ru1]), there exists a unique measure μ_ψ on $\sigma(T)$, such that

$$< \psi, f(T)\psi >_{\mathcal{H}} = \int_{\sigma(T)} f(\lambda) d\mu_\psi(\lambda) \ . \tag{8.4.6}$$

This measure is called the spectral measure associated with the vector $\psi \in \mathcal{H}$. This measure is a Borel measure. This means that we can extend the map Ψ and (8.4.6) for Borelian functions.
Using the standard Hilbert calculus (that is the link between sesquilinear form and quadratic forms) we can also construct for any x and y in $\mathcal{H}$ a complex measure $d\mu_{x,y}$ such that

$$< x, \Phi(f)y >_{\mathcal{H}} = \int_{\sigma(T)} f(\lambda) d\mu_{x,y}(\lambda) \ . \tag{8.4.7}$$

Using the Riesz representation Theorem (Theorem 3.1.1), this gives as, when f is bounded, an operator $f(T)$. If $f = 1_{]-\infty,\mu]}$, we recover the operator $E_\mu = f(T)$ which permits to recover indeed the spectral family announced in the theorem.

Remark 8.4.5. .
Modulo some care concerning the domains of the operator, the properties mentioned in Remark 8.1.3 are preserved in the case of an unbounded selfadjoint operator.

8.5 Applications of the spectral theorem:

One of the first applications of the spectral theorem (Property 2.) is the following property :

Proposition 8.5.1. .

$$d(\lambda, \sigma(T)) ||x|| \leq ||(T - \lambda)x|| \ , \tag{8.5.1}$$

for all x in $D(T)$.

This proposition is frequently used in the following context. It is usually difficult to get explicitely the values of the eigenvalues of an operator. One consequently tries to localize these eigenvalues by using approximations. Let us suppose for example that one has found λ_0 and y in $D(L)$ such that

$$||(T - \lambda_0)y|| \leq \epsilon \tag{8.5.2}$$

and $||y|| = 1$ then we deduce the existence of λ in the spectrum of L such that $|\lambda - \lambda_0| \leq \epsilon$.
Standard examples are the case of hermitian matrices or the case of the anharmonic oscillator $T := -h^2 \frac{d^2}{dx^2} + x^2 + x^4$. In the second case the first eigenfunction of the harmonic oscillator $-h^2 \frac{d^2}{dx^2} + x^2$ can be used as approximate eigenfunction y in (8.5.2) with $\lambda_0 = h$. We then find (8.5.2) with $\epsilon = \mathcal{O}(h^2)$.
Another application is, using the property that the spectrum is real, the following inequality

$$| \operatorname{Im} \lambda| \; ||x|| \leq ||(T - \lambda)x|| \tag{8.5.3}$$

and this gives an upper bound on the norm of $(T - \lambda)^{-1}$ in $\mathcal{L}(\mathcal{H})$ by $1/| \operatorname{Im} \lambda|$.
One can also consider the operator $T_\epsilon = -d^2/dx^2 + x^2 + \epsilon x^4$. One can show that near each eigenvalue of the harmonic oscillator $(2n + 1)$, then there exists, when $\epsilon > 0$ is small enough, an eigenvalue $\lambda_n(\epsilon)$ of T_ϵ.
Another good example to analyze is the construction of a sequence of approximate eigenvectors considered in Subsection 1.1. From the construction of u_n such that, with $T = -\Delta$,

$$||(T - \xi^2)u_n||_{L^2(I\!\!R^m)} = \mathcal{O}(\frac{1}{n}) \; ,$$

one obtains that

$$d(\sigma(T), \xi^2) \leq \frac{C}{n} \; , \; \forall n \in I\!\!N \; .$$

As $n \to +\infty$, we get $\xi^2 \in \sigma(T)$.
It is then easy to show that

$$\sigma(P) = [0, +\infty[.$$

It is enough to prove indeed, using the Fourier transform, that, for any $b > 0$, $(-\Delta + b)$ has an inverse $(-\Delta + b)^{-1}$ sending L^2 onto H^2.

Here we have followed in a particular case the proof of the following general theorem

Theorem 8.5.2. .
Let T be a selfadjoint operator. Then $\lambda \in \sigma(P)$ if and only if there exists a sequence $(u_n)_{n \in I\!\!N}$, $u_n \in D(T)$ such that $||u_n|| = 1$ and $||(T - \lambda)u_n|| \to 0$ as $n \to +\infty$.

Exercise 8.5.3. .
Show the only if, after reading of the proof of Proposition 8.5.4.

Note also the following characterization.

Proposition 8.5.4. .

$$\sigma(T) = \{\lambda \in I\!\!R, \; s.t. \; \forall \epsilon > 0, E(]\lambda - \epsilon, \lambda + \epsilon[) \neq 0\} \tag{8.5.4}$$

The proof uses in one direction the explicit construction of $(T - \lambda)$ through Proposition 8.5.1. If λ and $\epsilon_0 > 0$ are such $E_{]\lambda-\epsilon_0,\lambda+\epsilon_0[} = 0$. Then there exists a continous function f on $I\!R$, such that $f(t) = (t - \lambda)^{-1}$ on the support of the measure dE_λ. This permits to construct the inverse and to show that λ is in the resolvent set of T.
Let λ in the set defined by the r.h.s of (8.5.4) later denoted by $\tilde{\sigma}(T)$. For any $n \in I\!N^*$, let us take x_n such that $||x_n|| = 1$ and $E(]\lambda - \frac{1}{n}, \lambda + \frac{1}{n}[)x_n = x_n$. Using property 2., with the function $f_n(t) = (t-\lambda)1_{]\lambda-\frac{1}{n},\lambda+\frac{1}{n}[}(t)$, we get :

$$||(T-\lambda)x_n|| = ||(T-\lambda)E(]\lambda - \frac{1}{n}, \lambda + \frac{1}{n}[)x_n|| \leq \frac{1}{n}||x_n|| = \frac{1}{n} .$$

Applying Proposition 8.5.1, we obtain :

$$\tilde{\sigma}(T) \subset \sigma(T) .$$

8.6 Examples of functions of a selfadjoint operator

We shall for example meet usually in spectral theory the functions

1. f is the characteristic function of $]-\infty, \lambda]$, $Y_{]-\infty,\lambda]}$; $\Phi(f) = f(T)$ is then $\Phi(f) = E(\lambda)$.
2. f is the characteristic function of $]-\infty, \lambda[$, $Y_{]-\infty,\lambda[}$; $f(T)$ is then $\Phi(f) = E(\lambda - 0)$.
3. f is a compactly supported continuous function. $f(T)$ will be an operator whose spectrum is localized in the support of f.
4. $f_t(\lambda) = \exp(it\lambda)$ with t real.
   $f_t(T)$ is then a solution of the functional equation

$$\begin{array}{ll} (\partial_t - iT)(f(t,T)) & = 0 \\ f(0,T) & = Id \end{array}$$

   We note here that, for all real t, $f_t(T) = \exp(itT)$ is a bounded unitary operator .

5. $g_t(\lambda) = \exp(-t\lambda)$ with t real positive. $g_t(T)$ is then a solution of the functional equation

$$\begin{array}{ll} (\partial_t + T)(g(t,T)) & = 0 \text{ , for } t \geq 0 \\ g(0,T) & = Id . \end{array}$$

We have discussed in the introduction the case of an operator with compact resolvent. The other case to understand for the beginner is of course the case of the free Laplacian $-\Delta$ on $I\!R^n$. Using the Fourier transform $\mathcal{F}$, we get as unbounded operator the operator of multiplication by ξ^2. It is not difficult to develop the functional calculus which simply becomes for a borelian function ϕ :

$$\phi(-\Delta) = \mathcal{F}^{-1}\phi(\xi^2)\mathcal{F} \; . \qquad (8.6.1)$$

One possibility is to start from $(-\Delta+1)^{-1}$, for which this formula is true and to then follow what was our construction of the functional calculus. Another possibility is to use the Formula (8.1.12) and to use that (8.6.1) is satisfied for $(-\Delta+z)^{-1}$, with $z \in \mathbb{C} \setminus \mathbb{R}$.

The spectral family is then defined by

$$< E(\lambda)f, g >_{L^2(\mathbb{R}^m)} = \int_{\xi^2 \leq \lambda} \hat{f}(\xi) \cdot \overline{\hat{g}}(\xi) \; d\xi \; .$$

8.7 Spectrum and spectral measures

Another interest of the spectral theorem is to permit the study of the different properties of the spectrum according to the nature of the spectral measure and this leads to the definition of the continuous spectrum and of the pure point spectrum. Let us briefly discuss (without proof) these notions.
Starting of a selfadjoint operator T, one defines $\mathcal{H}_{pp}$ (pure point subspace) as the set defined as

$$\mathcal{H}_{pp} = \{\psi \in \mathcal{H} \mid f \mapsto < f(T)\psi, \psi >_{\mathcal{H}} \text{ is a pure point measure } \} \qquad (8.7.1)$$

We recall that a measure on X is pure point if

$$\mu(X) = \sum_{x \in X} \mu(\{x\}) \; . \qquad (8.7.2)$$

One can verify that H_{pp} is a closed subspace of $\mathcal{H}$ and that the corresponding orthogonal projection $\Pi_{\mathcal{H}_{pp}}$ satisfies

$$\Pi_{\mathcal{H}_{pp}} D(T) \subset D(T) \; .$$

In this case $T_{/\mathcal{H}_{pp}}$ is naturally defined as unbounded operator on $\mathcal{H}_{pp}$ and one defines the pure point spectrum of T by

$$\sigma_{pp}(T) = \sigma(T_{/\mathcal{H}_{pp}}) \; . \qquad (8.7.3)$$

We can similarly define $\mathcal{H}_c$ (continuous subspace) as the set defined as

$$\mathcal{H}_c = \{\psi \in \mathcal{H} \mid f \mapsto < f(T)\psi, \psi >_{\mathcal{H}} \text{ is a continuous measure } \} \qquad (8.7.4)$$

We recall that a measure on X is continuous if

$$\mu(\{x\})) = 0 \; , \; \forall x \in X \; . \qquad (8.7.5)$$

One can verify that H_c is a closed subspace of $\mathcal{H}$ and that the corresponding orthogonal projection $\Pi_{\mathcal{H}_c}$ satisfies

$$\Pi_{\mathcal{H}_c} D(T) \subset D(T) \; .$$

Moreover, it can be shown (See [RS-I]), that

$$\mathcal{H} = \mathcal{H}_{pp} \oplus \mathcal{H}_c \; . \tag{8.7.6}$$

In this case $T_{/\mathcal{H}_c}$ is naturally defined as unbounded operator on $\mathcal{H}_c$ and one defines the continuous spectrum of T by

$$\sigma_c(T) = \sigma(T_{/\mathcal{H}_c}) \; . \tag{8.7.7}$$

Example 8.7.1. .
The spectrum of $-\Delta$ is continuous.

We observe indeed that

$$\lim_{\epsilon \to 0 \; , \; \epsilon > 0} \int_{||\xi|^2 - \lambda| \leq \epsilon} |\hat{f}(\xi)|^2 d\xi = 0 \; , \; \forall f \in L^2(\mathbb{R}^m) \; .$$

One can still refine this discussion by using the natural decomposition of the measure given by the Radon-Nikodym Theorem. This leads to the notion of absolutely continuous spectrum and of singularly continuous spectrum.

9 Essentially selfadjoint operators

9.1 Introduction

In most of the examples which were presented, the abstract operators are associated with differential operators. These differential operators are naturally defined on $C_0^\infty(\Omega)$ or $\mathcal{D}'(\Omega)$. Most of the time (for suitable potentials increasing slowly at ∞) they are also defined (when $\Omega = I\!R^m$) on $\mathcal{S}(I\!R^m)$ or $\mathcal{S}'(I\!R^m)$. It is important to understand how the abstract point of view can be related to the PDE point of view. The theory of the essential selfadjointness gives a clear understanding of the problem. The question is to decide if, starting from a symmetric operator T, whose domain $D(T) = \mathcal{H}_0$ is dense in $\mathcal{H}$, there exists a unique selfadjoint extension T^{ext} of T. We recall that it means that $D(T) \subset D(T^{ext})$ and $T^{ext}u = Tu$, $\forall u \in D(T)$. This leads to

Definition 9.1.1. .
A symmetric operator T with domain $\mathcal{H}_0$ is called essentially selfadjoint if its closure is selfadjoint.

Proposition 9.1.2. .
If T is essentially selfadjoint, then its selfadjoint extension[25] is unique.

Indeed suppose that S is a selfadjoint extension of T. Then S is closed and being an extension of T, is also an extension of its smallest extension $\overline{T}$. We recall from Theorem 2.2.6 that $\overline{T} = T^{**}$. Thus, $S = S^* \subset (T^{**})^* = T^{**}$, and so $S = T^{**}$.

Example 9.1.3. .
Here we give a list of examples and counter-examples which will be analyzed later.

1. The differential operator $-\Delta$ with domain $\mathcal{H}_0 = C_0^\infty(I\!R^m)$ is essentially selfadjoint (see later).

2. The differential operators $-\Delta + |x|^2$ with domain $\mathcal{H}_0 = C_0^\infty(I\!R^m)$ or $H_1 = \mathcal{S}(I\!R^m)$ are essentially selfadjoint and admit consequently a unique selfadjoint extension. This extension is the same for the two operators. The domain can be explicitely described as

$$\begin{aligned} &B^2(I\!R^m) = \\ &\quad \{u \in L^2(I\!R^m) \mid x^\alpha D_x^\beta u \in L^2(I\!R^m) \ , \ \forall \alpha, \beta \in I\!N^m \text{ with } |\alpha| + |\beta| \leq 2\} \ . \end{aligned}$$

3. The differential operator $-\Delta$ with domain $C_0^\infty(\Omega)$ (where Ω is an open bounded set with smooth boundary) is not essentially selfadjoint. There exists a lot of selfadjoint extensions related to the choice of a boundary problem. As we have seen before, we have already met two such extensions :

[25] Although, it will not help in this course, note that the converse is true. See for example the book [Ro], in which the essential selfadjointness is defined differently.

- the Dirichlet realization whose domain is the set $H_0^1(\Omega) \cap H^2(\Omega)$,
- the Neumann realization whose domain is the set : $\{u \in H^2(\Omega) \mid (\partial u/\partial \nu)_{/\partial\Omega} = 0\}$

4. The Laplace Beltrami operator on a compact manifold M with domain $C^\infty(M)$ is essentially selfadjoint on $L^2(M)$. The domain of the selfadjoint extension can be described as $H^2(M)$ (which can be described using local charts).

9.2 Basic criteria.

We now give some criteria in order to verify that an operator is essentially selfadjoint. As already mentioned, one can prove essential selfadjointness by proving that the minimal closed extension $T_{min} := \overline{T}$ coincides with T^*. One easily verifies (see Proposition 2.2.5 in conjonction with the definition of $\overline{T}$) that $T^* = \overline{T}^*$ and we recall that $T^{**} = \overline{T}$.
We now observe the

Proposition 9.2.1. .
Any closed symmetric extension of T is a restriction of T^*.

Proof.
Let S is a closed symmetric extension of T.
We have indeed $T \subset S \subset S^*$ and, observing that $S^* \subset T^*$, we consequently get $S \subset T^*$.

In particular, if $\overline{T}$ is selfadjoint then $\overline{T}$ is the unique selfadjoint extension of T.

We can characterize the selfadjointness through the following general criterion

Theorem 9.2.2. .
Let T be a closed symmetric operator. Then the following statements are equivalent :

1. *T is selfadjoint.*
2. *Ker $(T^\star \pm i) = \{0\}$;*
3. *Range $(T \pm i) = \mathcal{H}$.*

Proof.
1. implies 2.
This property was already observed (because $T = T^*$ and $\pm i \notin \sigma(T)$).
2. implies 3. .
We first observe that the property that ker $(T^\star + i) = \{0\}$ implies that $R(T - i)$ is dense in $\mathcal{H}$. Note that the converse is also true. For getting 3., it remains

to show that $R(T-i)$ is closed. But, for all ϕ in $D(T)$, we have (using the symmetry of T)

$$||(T-i)\phi||^2 = ||T\phi||^2 + ||\phi||^2 \,. \tag{9.2.1}$$

If ϕ_n is a sequence in $D(T)$ such that $(T+i)\phi_n$ converges to some ψ_∞. The previous identity shows that ϕ_n is a Cauchy sequence, so there exists ϕ_∞ such that $\phi_n \to \phi_\infty$ in $\mathcal{H}$. But $T\phi_n = (T+i)\phi_n - i\phi_n$ is convergent and using that the graph is closed, we obtain that $\phi_\infty \in D(T)$ and $T\phi_\infty = \psi_\infty$.

3. implies 1. .

Let $\phi \in D(T^*)$. Let $\eta \in D(T)$ such that $(T-i)\eta = (T^*-i)\phi$. T being symmetric, we have also $(T^*-i)(\eta-\phi) = 0$. But, if $(T+i)$ is surjective, then (T^*-i) is injective and we get $\phi = \eta$. This proves that $\phi \in D(T)$.

Remark 9.2.3. .

Here we have used and proved during the proof of the assertion "2. implies 3." the following lemma

Lemma 9.2.4. .

If T is closed and symmetric, then $R(T \pm i)$ is closed.

This theorem gives as a corollary a criterion for essential selfadjointness in the form

Corollary 9.2.5. .

Let A with domain $D(A)$ be a symmetric operator. Then the following are equivalent

1. *A is essentially selfadjoint.*
2. *$Ker(A^* \pm i) = \{0\}$.*
3. *The two spaces $R(A \pm i)$ are dense in $\mathcal{H}$.*

We have indeed essentially to apply the previous theorem to $\overline{A}$, oberving in addition that $\overline{A}$ is symmetric and that Lemma 9.2.4 is true.

Let us here emphasize that in this case, to specify the operator A, it is not necessary to give the exact domain of A but a core for A that is a subspace D such that the closure of $A_{/D}$ is $\overline{A}$.

In the same spirit, we have in the semibounded case the following

Theorem 9.2.6. .

Let T be a positive, symmetric operator. Then the following statements are equivalent :

1. *T is essentially selfadjoint.*
2. $$ker\ (T^* + b) = \{0\} \text{ for some } b > 0 \,.$$

3. Range $(T+b)$ is dense for some $b > 0$.

The proof essentially the same as for the previous corollary, if one observes that if T is positive then the following trivial estimate is a good substitute for (9.2.1) :

$$\langle (T+b)u, u\rangle \geq b||u||^2 \,.$$

Example 9.2.7. *(The free Laplacian).*
The operator $-\Delta$ with domain C_0^∞ is essentially selfadjoint. Its selfadjoint extension is $-\Delta$ with domain H^2.

9.3 The Kato -Rellich theorem

We would like to consider the case when $P = -\Delta + V$ when V is regular and tends to 0 as $|x| \rightarrow +\infty$. Here V can be considered as a perturbation of the Laplacian. One can then apply a general theorem due to Kato-Rellich.

Theorem 9.3.1. .
Let A be a selfadjoint operator, B be a symmetric operator whose domain contains $D(A)$. Let us assume the existence of a and b such that $0 \leq a < 1$ and $b \geq 0$ such that

$$||Bu|| \leq a\,||Au|| + b\,||u|| \tag{9.3.1}$$

for all $u \in D(A)$. Then $A+B$ is selfadjoint on $D(A)$. If A is essentially selfadjoint on[26] *$D \subset D(A)$, then $A+B$ has the same property.*

Proof.

Step 1.
We start from the following identity which only uses that $(A+B)$ with domain $D(A)$ is symmetric.

$$||(A+B\pm i\lambda)u||^2 = ||(A+B)u||^2 + \lambda^2||u||^2 \,,\ \forall u \in D(A)\,. \tag{9.3.2}$$

By the triangle inequality and the symmetry of $A+B$, we get for a real $\lambda > 0$, and for any $u \in D(A)$:

$$\begin{aligned} \sqrt{2}||(A+B-i\lambda)u|| \ &\geq ||(A+B)u|| + \lambda||u|| \\ &\geq ||Au|| - ||Bu|| + \lambda||u|| \\ &\geq (1-a)||Au|| + (\lambda - b)||u||. \end{aligned} \tag{9.3.3}$$

We now choose $\lambda > b$.

Step 2.
Let us show that $(A+B)$ with domain $D(A)$ is closed. If we start indeed from a pair (u_n, f_n) with $u_n \in D(A)$ and $f_n = (A+B)u_n$ such that $(u_n, f_n) \rightarrow (u, f)$

[26] By this we mean that the closure of $A_{/D}$ is A.

in $\mathcal{H}$. From (9.3.3), we get that Au_n is a Cauchy sequence in $\mathcal{H}$. A being closed, we get $u \in D(A)$ and the existence of g such that $Au_n \to g = Au$.
Now from (9.3.2) and (9.3.1), we get also that Bu_n is a Cauchy sequence and there exists v such that $Bu_n \to v$ in $\mathcal{H}$.
We claim that $Bu = v$. We have indeed, for any $h \in D(A)$,

$$< v, h >_{\mathcal{H}} = \lim_{n \to +\infty} < Bu_n, h >_{\mathcal{H}} = \lim_{n \to +\infty} < u_n, Bh >_{\mathcal{H}} = < u, Bh >_{\mathcal{H}} = < Bu, h >_{\mathcal{H}} \; .$$

Using the density of $D(A)$, we get $v = Bu$. (We could have also used that B is closable).
We conclude by observing that $(A + B)u = f$ (with $f = g + v$) as expected.

Step 3.
In order to apply Theorem 9.2.2, we have to show that $(A+B \pm i\lambda)$ is surjective. The main element in the proof is the following

Lemma 9.3.2. .
For $\lambda > 0$ large enough, we have

$$||B(A \pm i\lambda)^{-1}|| < 1 \; . \tag{9.3.4}$$

Proof.
We observe that, for $u \in D(A)$,

$$||(A \pm i\lambda)u||^2 = ||Au||^2 + \lambda^2 ||u||^2 \; . \tag{9.3.5}$$

For $u \in D(A)$, we have, using two times (9.3.5) and then (9.3.1)

$$\begin{aligned} ||Bu|| \; & \leq a||Au|| + b||u|| \\ & \leq a||(A + i\lambda)u|| + \tfrac{b}{\lambda}||(A + i\lambda)u|| \\ & \leq (a + \tfrac{b}{\lambda})||(A + i\lambda)u|| \; . \end{aligned} \tag{9.3.6}$$

It is then enough to choose $\lambda > 0$ large enough such that

$$(a + \frac{b}{\lambda}) < 1 \; .$$

Writing

$$A + B - i\lambda = [I + B(A - i\lambda)^{-1}](A - i\lambda) \; , \tag{9.3.7}$$

it is easy to deduce the surjectivity using the lemma and the surjectivity of $(A - i\lambda)$.

Application.

As an application, let us treat the case of the Schrödinger operator with Coulomb potential.

Proposition 9.3.3. .
The operator $-\Delta - \frac{1}{|x|}$ *with domain* $C_0^\infty(I\!R^3)$ *is essentially selfadjoint.*

We recall that the operator is well defined because $\frac{1}{r}$ belongs to $L^2_{loc}(I\!R^3)$. We first observe a Sobolev type inequality.

Lemma 9.3.4. :
There exists a constant C *such that for all* $u \in H^2(I\!R^3)$, *all* $a > 0$ *and all* $x \in I\!R^3$, *we have*

$$|u(x)| \leq C(a||\Delta u||_0 + a^{-3}||u||_0) .$$

(Prove first the inequality[27] for all u with $x = 0$ and $a = 1$, then use translation and dilation.)
In the second step, we show that the potential $V = -\frac{1}{r}$ is a perturbation of the Laplacian.
There exists indeed a constant C such that for all $u \in H^2(I\!R^3)$ and all $b > 0$, we have

$$||Vu||_0 \leq C(b||\Delta u||_0 + b^{-1}||u||_0) .$$

For this proof we observe that, for any $R > 0$,

$$\int V(x)^2|u(x)|^2 dx = \int_{|x|\leq R} V(x)^2|u(x)|^2 dx + \int_{|x|\geq R} V(x)^2|u(x)|^2 dx ,$$

and treat the first term of the right hand side using the Sobolev's type inequality and the second term by the trivial estimate $|V(x)| \leq \frac{1}{R}$.

Remark 9.3.5. .
We note that the same proof shows that $-\Delta + V$ *is essentially selfadjoint starting from* $C_0^\infty(I\!R^m)$ *if* $V \in L^2 + L^\infty$, *that is if* $V = V_1 + V_2$ *with* $V_1 \in L^2$ *and* $V_2 \in L^\infty$.

9.4 Other criteria of selfadjointness for Schrödinger operators

We present in this subsection two criteria which are specific of the Schrödinger case. The first one seems due to Rellich (See [Sima]) and we present it in the easy case when the potential is regular. The second one permits to treat singular potentials and is due to Kato (cf [HiSi] or [Ro]).

The first theorem is adapted to operators which are already know to be positive on $C_0^\infty(I\!R^m)$.

Theorem 9.4.1. .
A Schrödinger operator $T = -\Delta + V$ *on* $I\!R^n$ *associated with a* C^0 *potential* V, *which is semibounded on* $C_0^\infty(I\!R^n)$, *is essentially selfadjoint. In other words, the Friedrichs extension is the unique selfadjoint extension starting from* $C_0^\infty(I\!R^m)$.

[27] In this case, this is just the Sobolev's injection theorem of $H^2(\boldsymbol{R}^3)$ into $C_b^0(\boldsymbol{R}^3)$, where $C_b^0(\boldsymbol{R}^3)$ is the space of the continuous bounded functions.

This theorem is complementary to the second theorem (Theorem 9.4.4) because we do not have to assume the positivity of the potential.

Proof.

Let T be our operator. Possibly by adding a constant, we can assume that

$$< Tu, u >_{\mathcal{H}} \geq ||u||^2 \; , \; \forall u \in C_0^\infty(I\!\!R^m) \; . \tag{9.4.1}$$

Of course this inequality can be rewritten in the form :

$$||\nabla u||^2 + \int_{I\!\!R^m} V(x)|u(x)|^2 dx \geq ||u||^2 \; , \; \forall u \in C_0^\infty(I\!\!R^m) \; .$$

In this form, the inequality can be extended to the elements of $H^1_{comp}(I\!\!R^m)$, corresponding to the distributions of $H^1(I\!\!R^m)$ with compact support :

$$||\nabla u||^2 + \int_{I\!\!R^m} V(x)|u(x)|^2 dx \geq ||u||^2 \; , \; \forall u \in H^1_{comp}(I\!\!R^m) \; . \tag{9.4.2}$$

According to the general criterion of essential selfadjointness (cf Theorem 9.2.6), it is enough to verify that $R(T)$ is dense. Let us show this property.
Let $f \in L^2(I\!\!R^m)$, such that

$$< f, Tu >_{\mathcal{H}} = 0 \; , \; \forall u \in C_0^\infty(I\!\!R^m) \; . \tag{9.4.3}$$

We have to show that $f = 0$.
Because T is real, one can assume that f is real.
We first observe that (9.4.3) implies that : $(-\Delta + V)f = 0$ in $\mathcal{D}'(I\!\!R^m)$. A standard regularity theorem for the Laplacian[28] implies that $f \in H^2_{loc}(I\!\!R^m)$.
We now introduce a family of cutoff functions ζ_k by

$$\zeta_k := \zeta(x/k) \; , \; \forall k \in I\!\!N \; , \tag{9.4.4}$$

where ζ is a C^∞ function satisfying $0 \leq \zeta \leq 1$, $\zeta = 1$ on $B(0,1)$ and $\operatorname{supp} \zeta \subset B(0,2)$.
For any $u \in C_0^\infty$, we have the identity

$$\begin{array}{l} \int \nabla(\zeta_k f) \cdot \nabla(\zeta_k u) dx + \int \zeta_k(x)^2 V(x) u(x)\, f(x)\; dx \\ \quad = \int |(\nabla \zeta_k)(x)|^2 u(x) f(x)\; dx + \sum_{i=1}^m \int \left(f(\partial_i u) - u(\partial_i f)\right)(x) \zeta_k(x) (\partial_i \zeta_k)(x)\; dx \\ \quad + \langle f(x)\; ,\; T\zeta_k^2 u\rangle \; . \end{array} \tag{9.4.5}$$

When f satisfies (9.4.3), we get :

$$\begin{array}{l} \int_{I\!\!R^m} \nabla(\zeta_k f) \cdot \nabla(\zeta_k u) dx + \int \zeta_k(x)^2 V(x) u(x)\, f(x)\; dx \\ \quad = \int |(\nabla \zeta_k)(x)|^2 u(x) f(x)\; dx + \sum_{i=1}^m \int \left(f(\partial_i u) - u(\partial_i f)\right)(x) \zeta_k(x) (\partial_i \zeta_k)(x)\; dx \; , \end{array} \tag{9.4.6}$$

[28] This is the property that $f \in L^2_{loc}(I\!\!R^m)$, $\Delta f \in L^2_{loc}(I\!\!R^m)$ implies that $f \in H^2_{loc}(I\!\!R^m)$.

for all $u \in C_\infty(I\!R^m)$.
This formula can be extended to functions $u \in H^1_{loc}$. In particular, we can take $u = f$.
We obtain

$$< \nabla(\zeta_k f) \ , \ \nabla(\zeta_k f) > + \int \zeta_k^2 V(x)|f(x)|^2 \, dx = \int |\nabla \zeta_k|^2 |f(x)|^2 dx \ . \quad (9.4.7)$$

Using (9.4.1), (9.4.7) and taking the limit $k \to +\infty$, we get

$$\begin{array}{ll} ||f||^2 & = \lim_{k\to+\infty} ||\zeta_k f||^2 \\ & \leq \limsup_{k\to+\infty} \left(< \nabla(\zeta_k f) \ , \ \nabla(\zeta_k f) > + \int \zeta_k^2 V(x)|f(x)|^2 \, dx\right) \\ & = \limsup_{k\to+\infty} \int f(x)^2 |(\nabla \zeta_k)(x)|^2 \, dx = 0 \ . \end{array} \quad (9.4.8)$$

This proves the theorem.

Remark 9.4.2. .
When V is C^∞, we get, in the previous proof, that $f \in C^\infty$ and we immediately can prove (9.4.7) without going through the previous discussion.

Example 9.4.3. .

- *If $V \geq 0$ and C^∞, then the Schrödinger operator $-\Delta + V$ with domain $C_0^\infty(I\!R^m)$ is essentially selfadjoint. The operator $-\Delta + V$ is indeed positive.*
- *If ϕ is C^∞ on $I\!R^m$, then the operators $-\Delta + |\nabla\phi|^2 \pm \Delta\phi$ are essentially selfadjoint. They are indeed positive on $C_0^\infty(I\!R^m)$. They can actually be written in the form $\sum_j Z_j^* Z_j$ with $Z_j = \partial_{x_j} \mp \partial_{x_j}\phi$. These operators appear naturally in statistical mechanics.*

Let us now mention, without proof, a quite general theorem due to Kato (See for example [Ro]).

Theorem 9.4.4. .
Let V in $L^2_{loc}(I\!R^m)$ such that $V \geq 0$ almost everywhere on $I\!R^m$. Then $-\Delta + V$ with domain $C_0^\infty(I\!R^m)$ is essentially selfadjoint.

This theorem is based on the so called Kato's inequality.

Remark 9.4.5. .
This last theorem may be extended to the case of the Schrödinger operator with magnetic regular potential A (See Subsection 7.5).

10 Discrete spectrum, essential spectrum

10.1 Discrete spectrum

We have already recalled in Proposition 8.5.4 a characterization of the spectrum. Let us now complete this characterization by introducing different spectra.

Definition 10.1.1. .
If T is a selfadjoint operator, we shall call discrete spectrum of T the set

$$\sigma_{disc}(T) = \{\lambda \in \sigma(T) \ s.\ t.\ \exists \epsilon > 0, \dim range\,(E(]\lambda - \epsilon, \lambda + \epsilon[)) < +\infty\}\ .$$

With this new definition, we get the following:
For a selfadjoint operator with compact resolvent, the spectrum is reduced to the discrete spectrum.
For a compact selfadjoint operator, the spectrum is discrete outside 0. We see in this case that the discrete spectrum is not closed.
Equivalently, let us observe now give another characterization :

Proposition 10.1.2. .
A complex λ is in the discrete spectrum if and only if :
λ is an isolated point in $\sigma(T)$ and if λ is an eigenvalue of finite multiplicity.

Proof.
If $\lambda \in \sigma_{disc}(T)$, we immediately see that there exists ϵ_0 such that, $\forall \epsilon$ such that $0 < \epsilon < \epsilon_0$, $E_{]\lambda-\epsilon,\lambda+\epsilon[}$ becomes a projector independent of ϵ with finite range. This is actually the projector $\Pi_\lambda = 1_{\{\lambda\}}(T)$ and we observe moreover $E_{]\lambda,\lambda+\epsilon[} = 0$ and $E_{]\lambda-\epsilon,\lambda[} = 0$. This shows that λ is an isolated point in $\sigma(T)$. Using the spectral representation of T, one immediately get that, if $x = \Pi_\lambda x$ $(x \neq 0)$, then x is an eigenvector of T. Moreover, one easily obtains that $(T - \lambda)$ is invertible on $R(I - \Pi_\lambda)$. One can indeed find a continuous bounded f such that $f(T)(T - \lambda)(I - \Pi_\lambda) = (I - \Pi_\lambda)$.

Conversely, let λ be isolated. The previous proof as already shown that in this case the range of Π_λ is an eigenspace. The assumption of finite multiplicity permits then to conclude.

10.2 Essential spectrum

Definition 10.2.1. .
The essential spectrum is the complementary in the spectrum of the discrete spectrum.

Intuitively, a point of the essential spectrum corresponds

- either to a point in the continuous spectrum,
- or to a limit point of a sequence of eigenvalues with finite multiplicity,
- or to an eigenvalue of infinite multiplicity.

The discrete spectrum being composed of isolated points, we get

Proposition 10.2.2. .
The essential spectrum of a selfadjoint operator T is closed in $\mathbb{R}$.

10.3 Basic examples:

1. The essential spectrum of a compact selfadjoint operator is reduced to 0.
2. The essential spectrum of an operator with compact resolvent is empty.
3. The Laplacian on $\mathbb{R}^n$ $-\Delta$ is a selfadjoint operator on $L^2(\mathbb{R}^n)$ whose domain is the Sobolev space $H^2(\mathbb{R}^n)$. The spectrum is continuous and equal to $\overline{\mathbb{R}^+}$. The essential spectrum is also $\overline{\mathbb{R}^+}$ and the operator has no discrete spectrum.
4. The Schrödinger operator with constant magnetic field ($B \neq 0$) in $\mathbb{R}^2$:
$$S_B := (D_{x_1} - \frac{Bx_2}{2})^2 + (D_{x_2} + \frac{Bx_1}{2})^2 \,, \tag{10.3.1}$$
with
$$D_{x_j} := \frac{1}{i}\partial_{x_j} = \frac{1}{i}\frac{\partial}{\partial x_j} \,.$$
The spectrum is formed with eigenvalues $(2k+1)|B|$ but the spectrum is not discrete because each eigenvalue is with infinite multiplicity. This example will be analyzed later.

10.4 Weyl's criterion:

We have already mentioned that the essential spectrum is a closed set. In order to determine the essential spectrum it is useful to have theorems proving the invariance by perturbation. The following characterization is in this spirit quite useful.

Theorem 10.4.1. .
Let T be a selfadjoint operator. Then λ belongs to the essential spectrum iff there exists a sequence u_n in $D(T)$ with $||u_n|| = 1$ such that u_n tends weakly[29] *to 0 and such that $||(T-\lambda)u_n|| \to 0$ as $n \to \infty$.*

Let us give a partial proof of the Theorem and we refer to [Ro], [HiSi] or [RS-IV] for a complete proof.
The sequence appearing in the theorem is called a Weyl sequence. A point λ such that there exists an associated Weyl sequence is said to belong to the Weyl spectrum $W(T)$. Let us show the inclusion
$$W(T) \subset \sigma_{ess}(T) \,. \tag{10.4.1}$$

[29] We recall that we say that a sequence u_n in a separable Hilbert space $\mathcal{H}$ is weakly convergent if, for any g in $\mathcal{H}$, $< u_n|g >_{\mathcal{H}}$ is convergent. In this case, there exists a unique f such that $< u_n|g >_{\mathcal{H}} \to < f|g >_{\mathcal{H}}$ and $||u_n||$ is a bounded sequence.

We have already seen that

$$W(T) \subset \sigma(T) . \tag{10.4.2}$$

Let us suppose by contradiction that $\lambda \in \sigma_{disc}(T)$. Let $\Pi_\lambda := E_{\{\lambda\}}$ be the associated spectral projector. We first observe that, Π_λ being finite range, hence compact, we have :

$$\Pi_\lambda u_n \to 0 \in \mathcal{H} . \tag{10.4.3}$$

Let us define

$$w_n = (I - \Pi_\lambda) u_n .$$

We get $||w_n|| \to +1$ and $(T - \lambda) w_n = (I - \Pi_\lambda)(T - \lambda) u_n \to 0$.
But $(T - \lambda)$ is invertible on $R(I - \Pi_\lambda)$, so we get $w_n \to 0$ and the contradiction. This shows the announced inclusion (10.4.1).

Corollary 10.4.2. .
The operator $-h^2\Delta + V$ with V a continuous function tending to 0 as $|x| \to \infty$ ($x \in I\!R^D$) has $\overline{I\!R^+}$ as essential spectrum.

For proving the inclusion of $\overline{I\!R^+}$ in the essential spectrum, we can indeed consider the sequence

$$u_n(x) = \exp(ix \cdot \xi) n^{-(D/2)} \cdot \chi((x - R_n)/n)$$

with $\chi \geq 0$ and supported in the ball $B(0,1)$ and equal to one on say $B(0, \frac{1}{2})$. The sequence R_n is chosen such that $|R_n|$ (for example $|R_n| = n^2$) tends to ∞ and such that the support of the u_n are disjoints.
This is a particular case of a Weyl sequence (called in [HiSi] a Zhislin sequence). The converse can be obtained by abstract analysis and the fact that we know that the essential spectrum of $-\Delta$ is $[0, +\infty[$. This idea is formalized through the notion of relative compactness.

Definition 10.4.3. .
If T is a closed operator with a dense domain D_L, we shall say that the operator V is relatively compact with respect to T or T-compact if $D_T \subset D_V$ and if the image by V of a closed ball in D_T (for the graph-norm $u \mapsto \sqrt{||u||^2 + ||Tu||^2}$) is relatively compact in $\mathcal{H}$.

In other words, we shall say that V is T-compact, if, from each sequence u_n in D_T bounded in $\mathcal{H}$ and such that Tu_n is bounded in $\mathcal{H}$, one can extract a subsequence u_{n_i} such that Vu_{n_i} is convergent in $\mathcal{H}$. Here we recall (exercise) that when T is closed, then $D(T)$ equipped with the graph norm is an Hilbert space.

Example 10.4.4. .
If V is the multiplication operator by a continuous function V tending to 0 then V is $(-\Delta)$-compact. This is a consequence of Proposition 5.4.1 and of the uniform continuity of V on each compact.

Weyl's Theorem says

Theorem 10.4.5. .
Let T be a selfadjoint operator, and V be symmetric and T-compact, then $T + V$ is selfadjoint and the essential spectrum of $T+V$ is equal to the essential spectrum of T.

The first part was discussed in the previous subsection (See Theorem 9.3.1). We observe indeed the following variant of Lions's Lemma :

Lemma 10.4.6. .
If V is T-compact and closable, then, for any $a > 0$, there exists $b > 0$ such that

$$||Vu|| \leq a||Tu|| + b||u|| \, , \, \forall u \in D(T) \, . \tag{10.4.4}$$

Proof of the lemma.
The proof is by contradiction. If (10.4.4) is not true, then there exists $a > 0$ such that, $\forall n \in \mathbb{N}^*$, there exists $u_n \in D(T)$ such that

$$a||Tu_n|| + n||u_n|| < ||Vu_n|| \, . \tag{10.4.5}$$

Observing that $||Vu_n|| \neq 0$ and that the inequation is homogeneous, we can in addition assume that u_n satisfies the condition :

$$||Vu_n|| = 1 \, . \tag{10.4.6}$$

From these two properties we get that the sequence Tu_n is bounded and that $u_n \to 0$.
On the other hand, by T-compactness, we can extract a subsequence u_{n_k} such that Vu_{n_k} is convergent to v with $||v|| = 1$. But $(0, v)$ is in the closure of the graph of V, hence in the graph of the closure of V and consequently $v = 0$ (contradiction).

For the second part we can use the Theorem 10.4.1. If we take a Weyl's sequence u_n such that $u_n \to 0$ (weakly) and $(T - \lambda)u_n \to 0$ strongly, let us consider $(T + V - \lambda)u_n$. We have simply to show that one can extract a subsequence u_{n_k} such that $(T + V - \lambda)u_{n_k} \to 0$.
But Tu_n is a bounded sequence. By the T-compactness, we can extract a subsequence such that Vu_{n_k} converges strongly to some v in $\mathcal{H}$. It remains to show that $v = 0$. But here we can observe that for any $f \in D(T)$, we have

$$< v, f >= \lim_{k \to +\infty} < Vu_{n_k}, f >= \lim_{k \to +\infty} < u_{n_k}, Vf >= 0 \, .$$

Here we have used the symmetry of V and the weak convergence of u_n to 0. Using the density of $D(T)$ in $\mathcal{H}$, we obtain $v = 0$.
This shows that a Weyl sequence for T is a Weyl sequence for $T + V$. For the converse, one can intertwine the roles of T and $T + V$, once we have shown that

V is $(T+V)$-compact. For this, we can use Lemma 10.4.6, and observe that the following inequality is true :

$$||Tu|| \leq \frac{1}{1-a}\left(||(T+V)u|| + b||u||\right) . \tag{10.4.7}$$

This shows that if u_n is a sequence such that $(||u_n|| + ||(T+V)u_n||)$ is bounded, then this sequence has also the property that $(||u_n|| + ||Tu_n||)$ is bounded.

11 The max-min principle

11.1 Introduction

The max-min principle is an alternative way for describing the lowest part of the spectrum when it is discrete. It gives also an efficient way to localize these eigenvalues or to follow their dependence on various parameters.

11.2 On positivity

We first recall the following definition

Definition 11.2.1. .
Let A be a symmetric operator. We say that A is positive (and we write $A \geq 0$), if

$$< Au, u > \geq 0 \ , \ \forall u \in D(A) \ . \tag{11.2.1}$$

The following proposition relates the positivity with the spectrum

Proposition 11.2.2. .
Let A be a selfadjoint operator. Then $A \geq 0$ if and only if $\sigma(A) \subset [0, +\infty[$.

Proof.
It is clear that if the spectrum is in $\mathbb{R}^+$, then the operator is positive. This can be seen for example through the spectral representation :

$$< Au, u > = \int_{\lambda \in \sigma(A)} \lambda \ d||E_\lambda u||^2 \ .$$

Now, if $A \geq 0$, then, for any $a > 0$, $A + a$ is invertible. We have indeed

$$a||u||^2 \leq < (A + a)u, u > \leq ||(A + a)u|| \ ||u|| \ ,$$

which leads to

$$a||u|| \leq ||(A + a)u|| \ , \ \forall u \in D(A) \ . \tag{11.2.2}$$

This inequality gives the closed range and the injectivity. A being selfadjoint, we get also from the injectivity, the density of the image of $(A + a)$. This shows that $-a$ is not in the spectrum of A.

Example 11.2.3. .
Let us consider the Schrödinger operator $P := -\Delta + V$, with $V \in C^\infty$ and semi-bounded, then

$$\sigma(P) \subset [\inf V, +\infty[\ . \tag{11.2.3}$$

11.3 Variational characterization of the discrete spectrum

Theorem 11.3.1. .
Let A be a selfadjoint semibounded operator. Let $\Sigma := \inf \sigma_{ess}(A)$ and let us consider $\sigma(A) \cap]-\infty, \Sigma[$, described as a sequence (finite or infinite) of eigenvalues that we write in the form

$$\lambda_1 < \lambda_2 < \cdots < \lambda_n \cdots .$$

Then we have

$$\lambda_1 = \inf_{\phi \in D(A), \phi \neq 0} ||\phi||^{-2} < A\phi, \phi > , \quad (11.3.1)$$

$$\lambda_2 = \inf_{\phi \in D(A) \cap K_1^{\perp}, \phi \neq 0} ||\phi||^{-2} < A\phi, \phi > , \quad (11.3.2)$$

and, for $n \geq 2$,

$$\lambda_n = \inf_{\phi \in D(A) \cap K_{n-1}^{\perp}, \phi \neq 0} ||\phi||^{-2} < A\phi, \phi > , \quad (11.3.3)$$

where

$$K_j = \oplus_{i \leq j} \; Ker \; (A - \lambda_i) \; .$$

Proof.

Step 1. Let us start, with the lowest eigenvalue. Let us define $\mu_1(A)$ by

$$\mu_1(A) := \inf_{\phi \in D(A), \phi \neq 0} ||\phi||^{-2} < A\phi, \phi > \; . \quad (11.3.4)$$

If ϕ_1 is an eigenvector associated to λ_1, we get immediately the inequality

$$\mu_1(A) \leq \lambda_1(A) \; . \quad (11.3.5)$$

Let us prove the converse inequality. Using the spectral theorem, one get immediately that $A \geq \inf \sigma(A)$.
So we get

$$\inf \sigma(A) \leq \mu_1(A) \; . \quad (11.3.6)$$

Now, if the spectrum below Σ is not empty, we get

$$\lambda_1(A) \leq \mu_1(A) \; .$$

We have consequently the equality. We have actually a little more.

We have indeed proved that, if $\mu_1(A) < \Sigma$, then, the spectrum below Σ is not empty, and the lowest eigenvalue is $\mu_1(A)$.

Step 2. The proof is by recursion, applying Step 1 to $A_{/D(A)\cap K_{n-1}^{\perp}}$.

This ends the proof of Theorem 11.3.1.

Example 11.3.2. *(Payne-Polya-Weinberger Inequality.)*
Let $P = -\Delta + V$ with $V \in C^\infty$ positive and $V \to +\infty$ as $|x| \to +\infty$.
Let us assume that V is even

$$V(x) = V(-x)\ . \tag{11.3.7}$$

Then λ_2 satisfies

$$\lambda_2 \leq \inf_{\phi \in Q(P), \phi \text{ odd}} < P\phi, \phi > \tag{11.3.8}$$

Let u_1 be the first normalized eigenvector. We admit that the lowest eigenvalue of the Schrödinger operator is simple (variant of the Krein-Rutman's Theorem) and that the first eigenvector can be chosen strictly positive, with exponential decay at ∞ together with ∇u_1 (this is a consequence of Agmon's inequality [Ag]). Then it is not difficult to verify that u_1 is even. Let us consider $v_j := x_j u_1$. v_j is in the form domain of P. We observe that

$$P(x_j u_1) = \lambda_1 x_j u_1 - 2\partial_j u_1\ .$$

Taking the scalar product with $x_j u_1$, we then obtain

$$\begin{aligned}(\lambda_2 - \lambda_1)||x_j u_1||^2 \quad & \leq -2 < \partial_j u_1, x_j u_1 > \\ & \leq ||u_1||^2 \\ & \leq 1\ .\end{aligned} \tag{11.3.9}$$

We now use the uncertainty principle (1.2.11) and get :

$$(\lambda_2 - \lambda_1) \leq 4||\partial_j u_1||^2\ . \tag{11.3.10}$$

On the other hand,

$$||\nabla u_1||^2 + \int_{\mathbb{R}^m} V(x)|u_1(x)|^2 dx = \lambda_1\ , \tag{11.3.11}$$

and this gives

$$||\nabla u_1||^2 \leq \lambda_1\ . \tag{11.3.12}$$

Putting the inequalities (11.3.9) and (11.3.12), we get, summing over j,

$$\lambda_2 - \lambda_1 \leq \frac{4}{m}\lambda_1\ . \tag{11.3.13}$$

This inequality is not optimal, in the sense that for $m = 1$ and $V(x) = x^2$, we have $\lambda_2 - \lambda_1 = 2\lambda_1$.

Example 11.3.3. .
Let us consider $S_h := -h^2\Delta + V$ on $\mathbb{R}^m$ where V is a C^∞ potential tending to 0 at ∞ and such that $\inf_{x\in\mathbb{R}^m} V(x) < 0$.
Then if $h > 0$ is small enough, there exists at least one eigenvalue for S_h. We note that the essential spectrum is $[0,+\infty[$. The proof of the existence of this eigenvalue is elementary. If x_{min} is one point such that $V(x_{min}) = \inf_x V(x)$, it is enough to show that, with $\phi_h(x) = \exp -\frac{\lambda}{h}|x-x_{min}|^2$, the quotient $\frac{<S_h\phi_h,\phi_h>}{||\phi_h||^2}$ tends as $h \to 0$ to $V(x_{min}) < 0$.

11.4 Max-min principle

We now give a more flexible criterion for the determination of the bottom of the spectrum and for the bottom of the essential spectrum. This flexibility comes from the fact that we do not need an explicit knowledge of the various eigenspaces.

Theorem 11.4.1. .
Let A be a selfadjoint semibounded operator of domain $D(A) \subset \mathcal{H}$. Let us introduce

$$\mu_n(A) = \sup_{\psi_1,\psi_2,\ldots,\psi_{n-1}} \inf_{\left\{\begin{array}{l}\phi\in[span(\psi_1,\ldots,\psi_{n-1})]^\perp;\\ \phi\in D(A)\ and\ ||\phi||=1\end{array}\right\}} \langle A\phi \mid \phi\rangle_{\mathcal{H}}\,. \qquad (11.4.1)$$

Then either
(a) $\mu_n(A)$ is the n-th eigenvalue when ordering the eigenvalues in increasing order (and counting the multiplicity) and A has a discrete spectrum in $]-\infty,\mu_n(A)]$
or
(b) $\mu_n(A)$ corresponds to the bottom of the essential spectrum. In this case, we have $\mu_j(A) = \mu_n(A)$ for all $j \geq n$.

Remark 11.4.2. .
In the case when the operator is with compact resolvent, case (b) does not occur and the supremum in (11.4.1) is a maximum. Similarly the infimum is a minimum. This explains the traditional terminology " Max-Min principle" for this theorem.

Proof.
If Ω is a borelian, let E_Ω be the projection-valued measure for A (see Remark 8.3.7).
We first prove that

$$\dim\ \left(Range E_{]-\infty,a[}\right) < n \text{ if } a < \mu_n(A). \qquad (11.4.2)$$

$$\dim\ \left(Range E_{]-\infty,a[}\right) \geq n \text{ if } a > \mu_n(A)\,. \qquad (11.4.3)$$

Step 1.
Let a and n be given such that $a < \mu_n(A)$. Let us prove (11.4.2) by contradiction. If it was false, then we would have $\dim \big(Range(E_{]-\infty,a[})\big) \geq n$ and we could find an n-dimensional space $V \subset Range(E_{]-\infty,a[})$. Note now, that A being bounded from below, $Range(E_{]-\infty,a[})$ is included in $D(A)$.
So we can find an n-dimensional space $V \subset D(A)$, such that

$$\forall \psi \in V\ ,\ < A\psi, \psi > \leq a||\psi||^2\ . \tag{11.4.4}$$

But then given any $\phi_1, \cdots, \phi_{n-1}$ in $\mathcal{H}$, we can find $\psi \in V \cap \{\phi_1, \cdots, \phi_{n-1}\}^\perp$ such that $||\psi|| = 1$ and $< A\psi, \psi > \leq a$. Coming back to the definition, this shows that $\mu_n(A) \leq a$ and a contradiction.

Note that we have proved in this step the following proposition

Proposition 11.4.3. .
Suppose that there exists a and an n-dimensional subspace $V \subset D(A)$ such that (11.4.4) is satisfied. Then we have the inequality :

$$\mu_n(A) \leq a\ . \tag{11.4.5}$$

Modulo the complete proof of the theorem, we obtain

Corollary 11.4.4. .
Under the same assumption as in Proposition 11.4.3, if a is below the bottom of the essential spectrum of A, then A has at least n eigenvalues (counted with multiplicity).

Exercise 11.4.5. .
In continuation of Example 11.3.3, show that for any $\epsilon > 0$ and any N, there exists $h_0 > 0$ such that for $h \in]0, h_0]$, S_h has at least N eigenvalues in $[\inf V, \inf V + \epsilon]$. One can treat first the case when V has a unique non degenerate minimum at 0.

Step 2.
Suppose that (11.4.3) is false. Then dim (Range $(E_{]-\infty,a[}) \leq n-1$, so we can find $(n-1)$ generators $\phi_1, \cdots, \phi_{n-1}$ of this space. Then any $\psi \in D(A) \cap span\{\phi_1, \cdots, \phi_{n-1}\}^\perp$ is in Range $(E_{[a,+\infty[})$, so

$$< A\psi, \psi > \geq a||\psi||^2\ .$$

Therefore, coming back to the definition of $\mu_n(A)$, we get $\mu_n(A) \geq a$ in contradiction with our initial assumption.

Before to continue the proof, let us emphasize on one point.

Remark 11.4.6. .
In the definition of $\mu_n(A)$, $\psi_1, \cdots, \psi_{n-1}$ are only assumed to belong to the Hilbert space $\mathcal{H}$.

Step 3.
We now observe that $\mu_n(A) < +\infty$.
First the semi-boundedness from below of A gives a uniform lower bound.
Secondly, if $\mu_n(A) = +\infty$, this would mean by (11.4.2) that :
$\dim(Range(E_{]-\infty,a[})) < n$ for all a,
and consequently that $\mathcal{H}$ is finite dimensional. This is a contradiction, if $\mathcal{H}$ is infinite dimensional.
But the finite case is trivial, we have indeed $\mu_n(A) \leq ||A||$, in this case.
According to the two first steps, there are two cases to consider.

Step 4.
Let us assume that

$$\dim\,(Range(E_{]-\infty,\mu_n+\epsilon[})) = +\infty\ ,\ \forall \epsilon > 0\ . \tag{11.4.6}$$

We claim that, we are in the second alternative in the theorem. Using (11.4.2) and (11.4.6), we get indeed

$$\dim\,(Range(E_{]\mu_n-\epsilon,\mu_n+\epsilon[})) = +\infty\ ,\ \forall \epsilon > 0\ . \tag{11.4.7}$$

This shows that $\mu_n(A) \in \sigma_{ess}(A)$.
On the other hand, using (11.4.2), we immediately get that $]-\infty, \mu_n(A)[$ does not contain any point in the essential spectrum. Thus $\mu_n(A) = \inf\{\lambda \mid \lambda \in \sigma_{ess}(A)\}$. Let us show now that $\mu_{n+1} = \mu_n$ in this case. From the definition, it is clear that $\mu_{n+1} \geq \mu_n$, since one can take $\phi_{n+1} = \phi_n$.
But if $\mu_{n+1} > \mu_n$, (11.4.6) would also be satisfied for μ_{n+1}, and, applying the previous argument, this would show that μ_n is an eigenvalue below the bottom of the essential spectrum.

Step 5.

Let us now assume that

$$\dim\,(Range(E_{]-\infty,\mu_n+\epsilon_0[})) < \infty\ ,\ \text{ for some } \epsilon_0 > 0\ . \tag{11.4.8}$$

Then it is clear, that the spectrum is discrete in $]-\infty, \mu_n + \epsilon_0[$. Therefore μ_n is an eigenvalue. Then, for $\epsilon_1 > 0$ small enough,

$$Range(E_{]-\infty,\mu_n]}) = Range(E_{]-\infty,\mu_n+\epsilon_1[})\ ,$$

and by (11.4.3)

$$\dim\,(Range E_{]-\infty,\mu_n]}) \geq n\ . \tag{11.4.9}$$

So there are at least n eigenvalues $E_1 \leq E_2 \leq \cdots \leq E_n \leq \mu_n$ for A. If E_n were strictly less than μ_n, $\dim(Range E_{]-\infty,E_n]})$ would equal n in contradiction with (11.4.2).

This ends the proof of Theorem 11.4.1.

A first natural extension of Theorem 11.4.1 is obtained by

Theorem 11.4.7. .
Let A be a selfadjoint semibounded operator and $Q(A)$ its form domain [30] .
Then

$$\mu_n(A) = \sup_{\psi_1,\psi_2,\dots,\psi_{n-1}} \inf_{\left\{ \begin{array}{l} \phi \in [span(\psi_1,\dots,\psi_{n-1})]^\perp ; \\ \phi \in Q(A) \ and \ ||\phi|| = 1 \end{array} \right\}} \langle A\phi \mid \phi \rangle_{\mathcal{H}} \ . \quad (11.4.10)$$

Proof.
Let $\tilde{\mu}_n$ be the right hand side of (11.4.10). By imitating the proof of the previous theorem, we get that each $\tilde{\mu}_n$ obeys one of the two conditions. These conditions determine μ_n and consequently $\mu_n = \tilde{\mu}_n$.
One can also note (see [?]) that, when constructing the Friedrichs extension, one has shown that the domain of the Friedrichs extension is dense in the form domain.
Applications

- It is very often useful to apply the max-min principle by taking the minimum over a dense set in $Q(A)$.
- The max-min principle permits to control the continuity of the eigenvalues with respect to parameters. For example the lowest eigenvalue $\lambda_1(\epsilon)$ of $-\frac{d^2}{dx^2} + x^2 + \epsilon x^4$ increases with respect to ϵ. Show that $\epsilon \mapsto \lambda_1(\epsilon)$ is right continuous on $[0,+\infty[$. (The reader can admit that the corresponding eigenfunction is in $\mathcal{S}(I\!\!R)$ for $\epsilon \geq 0$).
- The max-min principle permits to give an upperbound on the bottom of the spectrum and the comparison between the spectrum of two operators. If $A \leq B$ in the sense that, $Q(B) \subset Q(A)$ and[31]

  $$< Au, u > \leq < Bu, u > \ , \ \forall u \in Q(B) \ ,$$

  then

  $$\lambda_n(A) \leq \lambda_n(B) \ .$$

  Similar conclusions occur if we have $D(B) \subset D(A)$.

Example 11.4.8. *(Comparison between Dirichlet and Neumann).*
Let Ω be a bounded regular connected open set in $I\!\!R^m$. Then the N-th eigenvalue of the Neumann realization of $-\Delta + V$ is less or equal to the N-th eigenvalue of the Dirichlet realization. It is indeed enough to observe the inclusion of the form domains.

Example 11.4.9. *(monotonicity with respect to the domain).*
Let $\Omega_1 \subset \Omega_2 \subset I\!\!R^m$ two bounded regular open sets. Then the $n-th$ eigenvalue

[30] associated by completion with the form $u \mapsto \langle u|Au\rangle_{\mathcal{H}}$ initially defined on $D(A)$.
[31] It is enough to verify the inequality on a dense set in $Q(B)$.

of the Dirichlet realization of the Schrödinger operator in Ω_2 is less or equal to the n-th eigenvalue of the Dirichlet realization of the Schrödinger operator in Ω_1. We observe that we can indeed identify $H_0^1(\Omega_1)$ with a subspace of $H_0^1(\Omega_2)$ by just an extension by 0 in $\Omega_2 \setminus \Omega_1$.
We then have

$$\begin{aligned}
\lambda_n(\Omega_2) &= \sup_{\{\psi_1,\cdots,\psi_{n-1}\in L^2(\Omega_2)\}} \inf_{\left\{\begin{array}{l}\phi\in H_0^1(\Omega_2)\\ <\phi,\psi_j>_{L^2(\Omega_2)} \text{ and } ||\phi||=1\end{array}\right\}} ||\nabla\phi||^2_{L^2(\Omega_2)}\\
&\leq \sup_{\{\psi_1,\cdots,\psi_{n-1}\in L^2(\Omega_2)\}} \inf_{\left\{\begin{array}{l}\phi\in H_0^1(\Omega_1)\\ <\phi,\psi_j>_{L^2(\Omega_2)} \text{ and } ||\phi||=1\end{array}\right\}} ||\nabla\phi||^2_{L^2(\Omega_2)}\\
&= \sup_{\{\psi_1,\cdots,\psi_{n-1}\in L^2(\Omega_2)\}} \inf_{\left\{\begin{array}{l}\phi\in H_0^1(\Omega_1)\\ <\phi,\psi_j>_{L^2(\Omega_1)} \text{ and } ||\phi||=1\end{array}\right\}} ||\nabla\phi||^2_{L^2(\Omega_1)}\\
&= \sup_{\{\psi_1,\cdots,\psi_{n-1}\in L^2(\Omega_1)\}} \inf_{\left\{\begin{array}{l}\phi\in H_0^1(\Omega_1)\\ <\phi,\psi_j>_{L^2(\Omega_1)} \text{ and } ||\phi||=1\end{array}\right\}} ||\nabla\phi||^2_{L^2(\Omega_1)}\\
&= \lambda_n(\Omega_1)\,.
\end{aligned}$$

Note that this argument is not valid for the Neumann realization.

11.5 CLR inequality

In order to complete the picture, let us mention (confer [RS-IV], p. 101) that, if $m \geq 3$, then the following theorem due to Cwickel-Lieb-Rozenbljum is true :

Theorem 11.5.1. .
There exists a constant L_m, such that, for any V such that $V_- \in L^{\frac{m}{2}}$, and if $m \geq 3$, the number of strictly negative eigenvalues of S_1 N_- is finite and bounded by

$$N_- \leq L_m \int_{V(x)\leq 0} (-V)^{\frac{m}{2}}\, dx\,. \tag{11.5.1}$$

This shows that when $m \geq 3$, we could have examples of negative potentials V (which are not identically zero) and such that the corresponding Schrödinger operator S_1 has no eigenvalues. A sufficient condition is indeed

$$L_m \int_{V\leq 0} (-V)^{\frac{m}{2}}\, dx < 1\,.$$

In the other direction, we have[32] the following results.

Proposition 11.5.2. .
Let V be in $L^1(I\!R^m)$ ($m = 1, 2$). Then $S_1 = -\Delta + V$ has a negative eigenvalue if the following condition holds :

$$\int_{I\!R^m} V(x)\, dx < 0\,. \tag{11.5.2}$$

[32] These counterexamples come back (when $m = 1$ to Avron-Herbst-Simon [AHS] and when $m = 2$ to Blanchard-Stubbe [BS]).

Proof.

We just treat the case when $V \in C_0^\infty(I\!R^m)$.
We first observe that the the essential spectrum is $[0, +\infty[$. For the proof of the proposition, it is then enough to find $\psi \in D(S_1)$ such that

$$< S_1\psi, \psi >_{L^2(I\!R^m)} < 0 \ .$$

When $m = 1$, taking $\psi_a = \exp -a|x|$, $a > 0$, we find that

$$\int_{I\!R} |\psi'_a(x)|^2 \ dx = a \ ,$$

and

$$\lim_{a \to 0} \int_{I\!R} V(x)|\psi_a(x)|^2 \ dx = \int_{I\!R} V(x) \ dx < 0 \ ,$$

by the dominated convergence Theorem.
When $m = 2$, we can take $\psi_a(x) = \exp -\frac{1}{2}|x|^a$, $a > 0$, then

$$\int_{I\!R^2} ||\nabla \psi_a(x)||^2 \ dx = \frac{\pi}{2} a \ ,$$

and

$$\lim_{a \to 0} \int_{I\!R^2} V(x)|\psi_a(x)|^2 \ dx = \int_{I\!R^2} V(x) dx < 0 \ .$$

12 Essential spectrum and Persson's Theorem

12.1 Statement

We follow mainly in this section Agmon's presentation [Ag].

Theorem 12.1.1. .
Let V be a real-valued potential in the Kato-Rellich class[33]*, and let $H = -\Delta + V$ be the corresponding self-adjoint, semibounded Schrödinger operator with domain $H^2(\mathbb{R}^m)$. Then, the bottom of the essential spectrum is given by*

$$\inf \sigma_{ess}(H) = \Sigma(H) \ , \tag{12.1.1}$$

where

$$\Sigma(H) := \sup_{\mathcal{K} \subset \mathbb{R}^m} \left[\inf_{||\phi||=1} \{ < \phi, H\phi > \ | \ \phi \in C_0^\infty(\mathbb{R}^m \setminus \mathcal{K}) \} \right] \ , \tag{12.1.2}$$

where the supremum is over all compact subset $\mathcal{K} \subset \mathbb{R}^m$.

Essentially this is a corollary of Weyl's Theorem 10.4.5. We will indeed play with the fact that

Lemma 12.1.2.

$$\sigma_{ess}(H) = \sigma_{ess}(H + W) \ ,$$

for any regular potential W with compact support.

Let us now give the detailed proof.

12.2 Preliminary lemmas

As we have seen in the analysis of the compactness of the resolvent, it is useful to find weights ρ such that the form domain of the operator H has a continuous injection in L^2_ρ. In this spirit, we introduce

Definition 12.2.1. .
For any $y \in \mathbb{R}^m$ and $R > 0$, we define $\Lambda_R(y, H)$ by

$$\Lambda_R(y, H) = \inf \{ \frac{< H\phi, \phi >}{||\phi||^2} \mid \phi \in C_0^\infty(B(y, R)) \} \tag{12.2.1}$$

In other words, using the characterization of the bottom of the spectrum, $\Lambda_R(y, H)$ is the lowest eigenvalue of the Dirichlet realization of $-\Delta + V$ in the ball $B(y, R)$. The function $x \mapsto \Lambda_R(x, H)$ will play the role of this weight as shown by the :

[33] Cf Theorem 9.3.1.

Lemma 12.2.2. .
For all $\epsilon > 0$, there exists R_ϵ such that

$$< H\phi, \phi > \geq \int_{\mathbb{R}^n} (\Lambda_R(x,H) - \epsilon)|\phi(x)|^2 \, dx \,, \tag{12.2.2}$$

for all $\phi \in C_0^\infty(\mathbb{R}^m)$ and all $R \geq R_\epsilon$.

Proof of Lemma 12.2.2.
Let ζ be a real valued function in $C_0^\infty(\mathbb{R}^m)$ such that

$$\zeta(x) = 0 \text{ if } |x| \geq \frac{1}{2} \text{ and } \int_{\mathbb{R}^m} |\zeta(x)|^2 \, dx = 1 \,. \tag{12.2.3}$$

For $R > 0$ and $y \in \mathbb{R}^m$, let

$$\zeta_{R,y}(x) = \zeta(\frac{x-y}{R}) \,,\ \zeta_R(x) = \zeta_{R,0}(x) \,. \tag{12.2.4}$$

We get immediately, the existence of a constant C such that, for all $x \in \mathbb{R}^m$, all $y \in \mathbb{R}^m$ and all $R > 0$,

$$|\nabla_x \zeta_{R,y}(x)|^2 \leq \frac{C}{R^2} \,. \tag{12.2.5}$$

We now use the identity (already used in the proof of the selfadjointness)

$$\begin{array}{l} \int_{\mathbb{R}^m} \left(|(\nabla(\zeta_{R,y}\phi))(x)|^2 + V(x)|\zeta_{R,y}(x)\phi(x)|^2 \right) \, dx - \int_{\mathbb{R}^m} |(\nabla\zeta_{R,y})(x)|^2 |\phi(x)|^2 \, dx \\ \quad = \ \ \mathrm{Re} \int_{\mathbb{R}^m} (H\,\phi)(x)\, \zeta_{R,y}(x)^2 \bar{\phi}(x) \, dx \,. \end{array} \tag{12.2.6}$$

The first term of the left hand side is estimated from below by

$$\begin{array}{l} \int_{\mathbb{R}^m} \left(|(\nabla(\zeta_{R,y}\phi))(x)|^2 \ + \ V(x)|\zeta_{R,y}(x)\phi(x)|^2 \right) \, dx \\ \quad = < H(\zeta_{R,y}\phi), \phi > \\ \quad \geq \Lambda_{\frac{R}{2}}(y,H) \int_{\mathbb{R}^m} |\phi(x)\zeta_{R,y}(x)|^2 dx \,. \end{array} \tag{12.2.7}$$

Now we observe that, when $|x - y| \leq \frac{R}{2}$, we have $B(y, \frac{R}{2}) \subset B(x,R)$ and therefore

$$\Lambda_{\frac{R}{2}}(y,H) \geq \Lambda_R(x,H) \,. \tag{12.2.8}$$

This leads to the following lower bound

$$\begin{array}{l} \int_{\mathbb{R}^m} \left(|(\nabla(\zeta_{R,y}\phi))(x)|^2 \ + \ V(x)|\zeta_{R,y}(x)\phi(x)|^2 \right) \, dx \\ \quad \geq \int_{\mathbb{R}^m} \Lambda_R(x,H) |\phi(x)\zeta_{R,y}(x)|^2 dx \,. \end{array} \tag{12.2.9}$$

So the left hand side of (12.2.6) is estimated from below by

$$\begin{array}{l} \int_{\mathbb{R}^m} \left(|(\nabla(\zeta_{R,y}\phi))(x)|^2 \ + \ V(x)|\zeta_{R,y}(x)\phi(x)|^2 \right) \, dx - \int_{\mathbb{R}^m} |(\nabla\zeta_{R,y})(x)|^2 |\phi(x)|^2 \, dx \\ \quad \geq \int_{\mathbb{R}^m} \Lambda_R(x,H) |\phi(x)\zeta_{R,y}(x)|^2 dx \ - CR^{-2} \int_{B(y,R)} |\phi(x)|^2 \, dx \,. \end{array} \tag{12.2.10}$$

We have consequently obtained

$$\begin{aligned}\text{Re } &\int_{\mathbb{R}^m} (H\phi)(x)\ \zeta_{R,y}(x)^2 \bar{\phi}(x)\ dx \\ &\geq \int_{\mathbb{R}^m} \Lambda_R(x,H)|\phi(x)\zeta_{R,y}(x)|^2\ dx\ - CR^{-2}\cdot \int_{B(y,R)} |\phi(x)|^2\ dx\ .\end{aligned} \tag{12.2.11}$$

We now integrate this inequality with respect to y :

$$\begin{aligned}R^m \cdot\ \text{Re } &\int_{\mathbb{R}^m} (H\phi)(x)\ \bar{\phi}(x)\ dx \\ &\geq R^m \cdot \int_{\mathbb{R}^m} \Lambda_R(x,H)|\phi(x)|^2 dx\ - \tilde{C}R^{m-2}\cdot \int_{\mathbb{R}^m} |\phi(x)|^2\ dx\ .\end{aligned} \tag{12.2.12}$$

Dividing by R^m gives

$$\begin{aligned}\text{Re } &\int_{\mathbb{R}^m} (H\phi)(x)\ \bar{\phi}(x)\ dx \\ &\geq\ \int_{\mathbb{R}^m} \Lambda_R(x,H)|\phi(x)|^2 dx\ - \tilde{C}R^{-2} \int_{\mathbb{R}^m} |\phi(x)|^2\ dx\ .\end{aligned} \tag{12.2.13}$$

The lemma is obtained by taking $R_\epsilon = (\frac{\tilde{C}}{\epsilon})^{\frac{1}{2}}$.
This ends the proof of Lemma 12.2.2.

The relationship between the family of the $\Lambda_R(x,H)$ and $\Sigma(H)$ is described by the :

Lemma 12.2.3. .

$$\Sigma(H) = \lim_{R\to+\infty} \underline{\lim}_{|x|\to+\infty} \Lambda_R(x,H)\ . \tag{12.2.14}$$

Proof of Lemma 12.2.3.
Step 1.
Let K be a compact subset of $\mathbb{R}^m$ and $R>0$. Then if $|x|$ is large enough, the ball $B(x,R)$ is contained in $\mathbb{R}^m \setminus K$. Therefore, for such an x, we have

$$\inf \left\{ \frac{< H\phi, \phi >}{||\phi||^2}\ |\ \phi \in C_0^\infty(\mathbb{R}^m \setminus K)\ ,\ \phi \neq 0 \right\} \leq \Lambda_R(x,H)\ ,$$

and consequently

$$\inf \left\{ \frac{< H\phi, \phi >}{||\phi||^2}\ |\ \phi \in C_0^\infty(\mathbb{R}^m \setminus K)\ ,\ \phi \neq 0 \right\} \leq \underline{\lim}_{|x|\to+\infty} \Lambda_R(x,H)\ . \tag{12.2.15}$$

The left hand side is independent of R; so we can take the limit $R\to+\infty$ in this equation and get

$$\inf \left\{ \frac{< H\phi, \phi >}{||\phi||^2}\ |\ \phi \in C_0^\infty(\mathbb{R}^m \setminus K)\ ,\ \phi \neq 0 \right\} \leq \lim_{R\to+\infty} \underline{\lim}_{|x|\to+\infty} \Lambda_R(x,H)\ . \tag{12.2.16}$$

Here we note that the limit in the right hand side of (12.2.16) exists because the map $R \mapsto \underline{\lim}_{|x|\to+\infty}\Lambda_R(x,H)$ is a monotonically decreasing function.
Now the right hand side of this inequation is independent of K. Taking the infimum over K, we get

$$\Sigma(H) \leq \lim_{R\to+\infty} \underline{\lim}_{|x|\to+\infty}\Lambda_R(x,H)\ . \tag{12.2.17}$$

This is the first part of the statement in the lemma.

Step 2.
Let us now show the reverse inequality. Coming back, to the definition of $\underline{\lim}_{|x|\to+\infty}\Lambda_R(x,H)$, we get, that for any $\epsilon > 0$ and any R, there exists R_0 such that, for all $\phi \in C_0^\infty(I\!R^m \setminus \overline{B(0,R_0)})$, we have

$$\int_{I\!R^m} (\Lambda_R(x,H)|\phi(x)|^2\, dx \geq \left(\underline{\lim}_{|x|\to+\infty}\Lambda_R(x,H) - \epsilon\right) ||\phi||^2\ . \tag{12.2.18}$$

Therefore (12.2.2) and (12.2.18) imply, for any $R \geq R_\epsilon$, the existence of R_0, such that, for any $\phi \in C_0^\infty(I\!R^m \setminus \overline{B(0,R_0)})$ $(\phi \neq 0)$,

$$\frac{< H\phi,\phi >}{||\phi||^2} \geq \left(\underline{\lim}_{|x|\to+\infty}\Lambda_R(x,H) - 2\epsilon\right)\ . \tag{12.2.19}$$

Therefore, coming back to the definition of $\Sigma(H)$, we get that, for any $\epsilon > 0$, there exists $R_\epsilon > 0$ such that, for all $R \geq R_\epsilon$,

$$\Sigma(H) \geq \left(\underline{\lim}_{|x|\to+\infty}\Lambda_R(x,H) - 2\epsilon\right) \tag{12.2.20}$$

So the only restriction on R is that $R \geq R_\epsilon$. Therefore, we can take the limit $R \to +\infty$:

$$\Sigma(H) \geq \lim_{R\to+\infty}\left(\underline{\lim}_{|x|\to+\infty}\Lambda_R(x,H) - 2\epsilon\right) \tag{12.2.21}$$

But we can take the limit $\epsilon \to 0$ in (12.2.21) and get

$$\Sigma(H) \geq \lim_{R\to+\infty}\left(\underline{\lim}_{|x|\to+\infty}\Lambda_R(x,H)\right) \tag{12.2.22}$$

This is the second part of the statement in the lemma.

This ends the proof of Lemma 12.2.3.

12.3 Proof of the inequality $\inf \sigma_{ess(H)} \geq \Sigma(H)$.

To prove this inequality, we first use Lemma 12.2.2, and get, for any $\epsilon > 0$, the existence of $R > 0$ such that

$$< H\phi,\phi >_{\mathcal{H}} \geq \int_{I\!R^m} (\Lambda_R(x,H) - \frac{\epsilon}{2})|\phi(x)|^2\, dx\ ,\ \forall \phi \in C_0^\infty(I\!R^m)\ . \tag{12.3.1}$$

Since, by Lemma 12.2.3,

$$\underline{\lim}_{|x|\to+\infty}\Lambda_R(x,H) \geq \Sigma(H)\ ,$$

it follows that, for any $\epsilon > 0$, there exists a_ϵ such that

$$\Lambda_R(x,H) \geq \Sigma(H) - \frac{\epsilon}{2}\ ,$$

for $|x| \geq a_\epsilon$.
On the other hand, we have

$$\Lambda_R(x,H) \geq \inf \sigma(H)\ ,$$

and there consequently exists a constant C such that

$$\Lambda_R(x,H) \geq \Sigma(H) - C\ .$$

We now choose a function W with compact support such that

$$W(x) \geq C\ ,\ \forall x \in B(0,a_\epsilon)\ .$$

We now consider $H+W$ and obtain, from (12.3.1), that, for any $\phi \in C_0^\infty(\mathbb{R}^m)$,

$$\begin{array}{ll} < (H+W)\phi,\phi > & \geq \int (W(x) + \Lambda_R(x,H) - \frac{\epsilon}{2})|\phi(x)|^2 dx \\ & \geq (\Sigma(H) - \epsilon)\int |\phi|^2 dx\ . \end{array} \tag{12.3.2}$$

This can be interpreted as

$$\inf \sigma(H+W) \geq \Sigma(H) - \epsilon\ . \tag{12.3.3}$$

We now observe that

$$\inf \sigma_{ess}(H) = \inf \sigma_{ess}(H+W)\ , \tag{12.3.4}$$

and

$$\inf \sigma_{ess}(H+W) \geq \inf \sigma(H+W)\ . \tag{12.3.5}$$

This leads to

$$\inf \sigma_{ess}(H) \geq \Sigma(H) - \epsilon\ ,\ \forall \epsilon > 0\ ,$$

and finally to

$$\inf \sigma_{ess}(H) \geq \Sigma(H)\ , \tag{12.3.6}$$

which corresponds to the first statement in Persson's theorem.

12.4 Proof of the inequality $\inf \sigma_{ess}(H) \leq \Sigma(H)$.

Let us show the reverse inequality. Let $\mu < \inf \sigma_{ess}(H)$ and let $E_{]-\infty,\mu]}$ the spectral projection which has finite rank (we are below the essential spectrum). We first observe that there exists a finite orthonormal system of eigenvectors such that

$$E_{]-\infty,\mu]} = \sum_i < \cdot, \phi_i > \phi_i \ . \tag{12.4.1}$$

From this we get, that, for any ϵ, there exists R_ϵ such that

$$\int_{|x|\geq R_\epsilon} |E_{]-\infty,\mu]}\phi|^2 \leq \epsilon ||\phi||^2 \ , \ \forall \phi \in C_0^\infty(I\!R^m) \ . \tag{12.4.2}$$

We now get

$$\begin{aligned} < H\phi, \phi > \ &= < H(I - E(\mu))\phi, (I - E(\mu))\phi > + < HE(\mu)\phi, E(\mu)\phi > \\ &\geq \mu < (I - E(\mu))\phi, (I - E(\mu))\phi > - C < E(\mu)\phi, E(\mu)\phi > \ . \end{aligned}$$

But now we can write

$$\begin{aligned} \Sigma(H) \ &\geq \inf\{ \tfrac{< H\phi, \phi >}{||\phi||^2} \mid \phi \in C_0^\infty(I\!R^m \setminus (B(0, R_\epsilon))\} \\ &\geq \mu ||\phi||^2 - \epsilon(C + \mu)||\phi||^2 \ . \end{aligned}$$

As $\epsilon \to 0$, we get

$$\Sigma(H) \geq \mu$$

and, letting μ tend to $\sigma_{ess}(H)$, we finally obtain

$$\Sigma(H) \geq \sigma_{ess}(H) \ . \tag{12.4.3}$$

This ends the proof of Persson's Theorem.

13 Simplicity of the groundstate energy

13.1 Trotter's formula

The Trotter formula is useful in many contexts going from the Quantum Mechanics to the Numerical Analysis. It is a way to analyze in a simpler way the properties of the operators $\exp it(A + B)$ or $\exp -t(A + B)$ for selfadjoint operators having a better knowledge of $\exp itA$, $\exp itB$, $\exp -tA$ or $\exp -tB$. Here we present the analysis of $\exp -t(A + B)$.

Theorem 13.1.1. .
Let A and B be selfadjoint operators on a separable Hilbert space $\mathcal{H}$ so that $A + B$ defined on $D(A) \cap D(B)$, is selfadjoint. Let us assume that A and B are semibounded. Then

$$\exp -t(A + B) = s - \lim_{n \to +\infty} \left(\exp -\frac{tB}{2n} \ \exp -\frac{tA}{n} \ \exp -\frac{tB}{2n} \right)^n \ , \tag{13.1.1}$$

and

$$\exp -t(A+B) = s - \lim_{n\to+\infty}\left(\exp -\frac{tA}{n}\ \exp -\frac{tB}{n}\right)^n , \tag{13.1.2}$$

where the limit is considered in the sense of the strong convergence.

Proof:
Let us prove (13.1.2). It is actually sufficient to prove it on a dense set and we can also assume after translation that A and B are positive. As dense set, we shall choose at the end $D(A)\cap D(B)$. Let $S_t = \exp -t(A+B)$, $V_t = \exp -tA$, $W_t = \exp -tB$ and $U_t = V_t W_t$.If $\psi\in\mathcal{H}$, we define ψ_t by $\psi_t = S_t\psi$. Then

$$\begin{aligned} \|(S_t - U_{\frac{t}{n}}^n)\psi\| &= \|\sum_{j=0}^{n-1} U_{\frac{t}{n}}^j (S_{\frac{t}{n}} - U_{\frac{t}{n}}) S_{\frac{t}{n}}^{n-j-1}\psi\| \\ &\leq n \sup_{0\leq s\leq t} \|(S_{\frac{t}{n}} - U_{\frac{t}{n}})\psi_s\| \end{aligned} \tag{13.1.3}$$

Let $\phi\in D(A)\cap D(B)$. Then

$$s^{-1}(S_s - 1)\phi \to -(A+B)\phi \tag{13.1.4}$$

as $s\to 0$ ($s>0$) and

$$\begin{aligned} s^{-1}(U_s-1)\phi &= V_s(-B\phi) + V_s[s^{-1}(W_s-1)+B]\phi + s^{-1}(V_s-1)\phi \\ &\to -B\phi + 0 - A\phi\ . \end{aligned} \tag{13.1.5}$$

So

$$\lim_{n\to\infty}[n\|(S_{\frac{t}{n}} - U_{\frac{t}{n}})\phi\|] \to 0\ , \forall\phi\in D(A)\cap D(B)\ . \tag{13.1.6}$$

Let D denote $D(A)\cap D(B)$ with the norm $\|(A+B)\phi\| + \|\phi\| \equiv |||\phi|||$. By hypothesis, D is a Banach space. By the above calculations, $\{n(S_{\frac{t}{n}} - U_{\frac{t}{n}})\}$ is a family of bounded operators from D to $\mathcal{H}$ with $\sup_n\{n(S_{\frac{t}{n}} - U_{\frac{t}{n}})\phi\} < \infty$ for each ϕ. Using the Banach-Steinhaus theorem, we get the existence of a constant C such that

$$\|n(S_{\frac{t}{n}} - U_{\frac{t}{n}})\phi\| \leq C\,|||\phi|||\ . \tag{13.1.7}$$

But (13.1.7) implies that the limit in (13.1.6) is uniform over compact subsets of D. Let $\psi\in D$. Then $s\mapsto\psi_s$ is a continuous map from $[0,t]$ into D, so that $\{\psi_s | 0\leq s\leq t\}$ is compact in D. Thus the right-hand side of (13.1.3) goes to 0 as $n\to\infty$. We have consequently proved (13.1.2) for $\psi\in D$ and conclude for the general case by density.

13.2 Strong resolvent sense convergence.

When dealing with unbounded families of selfadjoint operators it is necessary to introduce adapted notions of convergence. The following definition will be quite useful in our context.

Definition 13.2.1. .
Let A be a selfadjoint operator and A_n be a sequence of selfadjoint operators A_n ($n \in I\!N$). We shall say that $A_n \to A$ in the strong resolvent sense if we have

$$s - \lim_{n \to +\infty} (A_n - \lambda)^{-1} = (A - \lambda)^{-1} , \qquad (13.2.1)$$

for any $\lambda \in \mathbb{C}$ with $Im\, \lambda \neq 0$.

One can actually show that this is enough to have the property for one λ_0 with $\operatorname{Im} \lambda_0 > 00$ and one λ_0' with $\operatorname{Im} \lambda_0' < 0$. We observe indeed that, if

$$|\lambda - \lambda_0| < \frac{1}{|\operatorname{Im} \lambda_0|} ,$$

then

$$(A - \lambda)^{-1} - (A_n - \lambda)^{-1} = \left(I - (\lambda - \lambda_0)(A - \lambda_0)^{-1}\right)^{-1} W_n , \qquad (13.2.2)$$

with

$$W_n := \left(I + (\lambda - \lambda_0)(A_n - \lambda_0)^{-1}\right) \left((A - \lambda_0)^{-1} - (A_n - \lambda_0)^{-1}\right) . \qquad (13.2.3)$$

We now observe that, for any $\psi \in \mathcal{H}$, $W_n \psi \to 0$ as $n \to +\infty$ and the completion of the proof is then immediate.

The following criterion gives an easy way for verifying this property.

Theorem 13.2.2. .
Let A be a selfadjoint operator and A_n be a sequence of selfadjoint operators A_n ($n \in I\!N$). Let us assume that there exists a common core D for A and A_n. If

$$A_n \phi \to A\phi \ , \ \forall \phi \in D , \qquad (13.2.4)$$

then $A_n \to A$ in the strong resolvent sense.

Proof.
Let $\phi \in D$ and $\psi = (A + i)\phi$.
Then

$$\left[(A_n + i)^{-1} - (A + i)^{-1}\right] \psi = (A_n + i)^{-1}(A - A_n)\phi .$$

Since $(A - A_n)\phi \to 0$ and $(A_n + i)^{-1}$ is uniformly bounded, we get

$$\lim_{n \to +\infty} \left[(A_n + i)^{-1} - (A + i)^{-1}\right] \psi = 0 .$$

Now the image by $(A+i)$ of D is dense in $\mathcal{H}$ because D is a core[34]. Using again the uniform boundedness of $(A_n + i)^{-1}$, we immediately see that it is enough to verify the strong convergence of the resolvent on a dense set.

[34] Let indeed $f \in \mathcal{H}$. Then $(A + i)^{-1} f \in D(A)$, and there exists a sequence $\phi_j \in D$ such that $\phi_j \to (A + i)^{-1} f$ in $\mathcal{H}$ and $A\phi_j$ converges to $A(A + i)^{-1} f$ in $\mathcal{H}$. But this implies that $(A + i)\phi_j \to f$ in $\mathcal{H}$.

13.3 Positivity preserving operators

Definition 13.3.1. .
We say that an operator A *on* $\mathcal{H} = L^2$ *is positivity preserving if it has the property to send a non zero, positive element in* $\mathcal{H}$ *into a non zero positive element in* L^2.

Remark 13.3.2. .
Note that the condition "non zero" is not systematically included in the definition of positivity preserving. Here following [RS-IV], positive function means non-negative (almost everywhere) and not identically 0. *The verification of "positivity preserving" goes usually through the verification of "non-negativity preserving" and injectivity.*

Example 13.3.3. .
The operator $\exp t\Delta$ *is positivity preserving. The distribution kernel is indeed given by* $(x,y) \mapsto c(t) \exp -\frac{1}{t}|x-y|^2$.
The fact that a non zero positive functions is sent onto a non zero positive function can be seen by looking at the Fourier transform. The operator becomes a multiplication operator by $\exp -t|\xi|^2$.

Example 13.3.4. .
The operator $(-\Delta+1)^{-1}$ *is positivity preserving. The distribution kernel is indeed given, when* $m = 3$, *by* $(x,y) \mapsto \frac{1}{4\pi}\frac{1}{|x-y|}\exp -|x-y|$.
The fact that a non zero positive function is sent onto a non zero positive function can be seen by looking at the Fourier transform. The operator becomes a multiplication operator by $(|\xi|^2+1)^{-1}$.

Definition 13.3.5. .
We say that an operator A *on* $\mathcal{H} = L^2$ *is positivity improving if it has the property to send a non zero, almost everywhere positive element in* $\mathcal{H}$ *into an almost every-where strictly positive element in* L^2.

Note that a positivity improving operator is also called an operator with strictly positive kernel (cf Definition 7.1.2).

Example 13.3.6. .
The operators $\exp t\Delta$ *and* $(-\Delta+1)^{-1}$ *are positivity improving.*

13.4 Basic theorem

We now analyze the link between positivity preserving and simplicity of the ground state. In some sense this naturally follows our presentation of the Krein-Rutman theorem.

Theorem 13.4.1. .
Let A *be a bounded selfadjoint*[35] *positive operator on* L^2. *Suppose that* A *is*

[35] This assumption is not done in the statement in [RS-IV] (Theorem XII.43) but the given proof makes use of this property at many points in the proof.

positivity preserving and that $||A||$ is an eigenvalue. Then the following are equivalent :

1. *$||A||$ is a simple eigenvalue and the associated eigenvector is strictly positive.*
2. *A has the property that for u, v in L^2 that are both positive (with $||u||||v|| \neq 0$) there exists some $n > 0$ such that $< u, A^n v > \neq 0$.*
3. *$\{A\} \cup L^\infty$ acts irreducibly, i.e., no nontrivial closed subspace is left invariant by both A and every bounded multiplication operator.*

Proof.

1. implies 2.
We can assume that $||A|| = 1$.
Let Π_Ω the family of spectral projections for A.
Since $x^n \to 0$ if $0 \leq x < 1$ and $x^n \to 1$ if $x = 1$, the functional calculus implies that

$$s - \lim_{n \to +\infty} A^n = \Pi_{\{1\}} \ . \tag{13.4.1}$$

By assumption $\Pi_{\{1\}} =< \psi, \cdot > \psi$ where ψ is the strictly positive eigenvector attached to the eigenvalue 1.
Thus, for any non zero, positive functions u and v, we have

$$\lim_{n \to +\infty} < u, A^n v > = < u, \psi > < \psi, v > > 0 \ . \tag{13.4.2}$$

This shows 2..

2. implies 3.
Suppose that 3. does not hold. Then there exists a non trivial subspace S which is left invariant by A and every bounded multiplication operator. Let $f \in S$. Then $h = \bar{f}/|f| \in L^\infty$ and so $|f| \in S$. Similarly, if $g \in S^\perp$, then $|g| \in S^\perp$. But if we choose $f \neq 0$ and $g \neq 0$, we obtain, since A leaves S invariant, that $A^n|f| \in S$ and so

$$< |g|, A^n|f| > = 0 \ , \ \forall n \geq 1$$

in contradiction with 2.

3. implies 1.
The proof is quite near the proof of the Krein-Rutman theorem but we can not apply it directly (our operator is not assumed to be positivity improving and we shall actually use only the non-negativity preserving property)).
Let ψ an eigenvector of A with eigenvalue $||A||$.
Step 1.
Suppose first that ψ is real valued. Since $|\psi| \pm \psi \geq 0$, we know that $A(|\psi| \pm \psi) \geq 0$. So we get

$$|A\psi| \leq A|\psi| \ .$$

Thus

$$< |\psi|, A|\psi| >_{L^2} \geq < |\psi|, |A\psi| > \geq < \psi, A\psi >= ||A|| \cdot ||\psi||^2 \ .$$

As a result, we have the equality

$$< |\psi|, A|\psi| >_{L^2} = < |\psi|, |A\psi| > = < \psi, A\psi >= ||A|| \cdot ||\psi||^2 \ .$$

We get, using this equality and the property that A is selfadjoint, that $A|\psi| = ||A||\,|\psi|$. We can indeed write that

$$< A(|\psi| + \epsilon v), |\psi| + \epsilon v > \leq ||A||\, ||\psi| + \epsilon v||^2 \ ,$$

for all $v \in L^2$, and this implies

$$< (A - ||A||)|\psi|, v >= 0 \ , \ \forall v \ .$$

We have shown that $|\psi|$ is an eigenvector. We would like now to prove that $|\psi|$ is strictly positive.
Let $S := \{f \in L^2 \mid f\psi = 0 \ a.e\}$.
S is clearly invariant by multiplication by L^∞. Let us analyze the invariance by A. Let $S_\pm = \{g \in S \mid \ \pm g \geq 0\}$. We have clearly $S = S_+ - S_- + i(S_+ - S_-)$. Now, for $f \in S_+$, we have

$$< Af, |\psi| >=< f, A|\psi| >= ||A|| < f, |\psi| >= 0 \ .$$

This shows that $Af \in S_+$. A leaves consequently S invariant. Thus by assumption we have $S = \{0\}$ or $S = L^2$. But $\psi \notin S$ so $S = \{0\}$.
Step 2.
Thus we know that any real eigenvector with eigenvalue $||A||$ is non zero almost everywhere and that $|\psi|$ is also an eigenvector with the same eigenvalue $||A||$. Thus $|\psi| - \psi$ is either an eigenvector with eigenvalue $||A||$ or is identically 0, so that $|\psi| - \psi$ is either almost everywhere vanishing or almost everywhere non-vanishing. This means that every real eigenvector with eigenvalue $||A||$ is a.e strictly positive or a.e strictly negative. But we can not have two orthogonal eigenvectors which are both with constant sign. So we conclude that A has only one real eigenvector of eigenvalue $||A||$ and that this eigenvector is strictly positive.
Step 3.
We apply the previous argument separately to $\mathrm{Re}\,\psi$ and $\mathrm{Im}\,\psi$ observing that they are (if non *zero*) eigenvectors.

Theorem 13.4.2. .
Let H and H_0 be semibounded selfadjoints operators on L^2. Suppose that there exists a sequence of bounded multiplication operators V_n so that $H_0 + V_n$ converges to H in strong resolvent sense and so that $H - V_n$ to H_0 converges in strong resolvent sense. Suppose, moreover, that $H - V_n$ and $H_0 + V_n$ are uniformly bounded from below. Then

1. *The operator* $\exp -tH$ *is positivity preserving iff* $\exp -tH_0$ *is positivity preserving.*

2. $\{\exp -tH\} \cup L^\infty$ *acts irreducibly on* L^2 *iff* $\{\exp -tH_0\} \cup L^\infty$ *acts irreducibly on* L^2.

Proof.
We first observe that

$$\exp -tH = s - \lim_{n\to+\infty} \left(\exp -t(H_0 + V_n)\right) \ , \tag{13.4.3}$$

and

$$\exp -tH_0 = s - \lim_{n\to+\infty} \left(\exp -t(H - V_n)\right) \ , \tag{13.4.4}$$

This will be a consequence of the lemma

Lemma 13.4.3. .
If $A_n \geq 0$, $A \geq 0$ *are selfadjoint operators and if* $A_n \to A$ *in the strong resolvent sense convergence, then, for* $t > 0$,

$$s - \lim \exp -tA_n = \exp -tA \ .$$

Thiscan be proved by using a formula relating, for a selfadjoint, semi-bounded from below operator A, $\exp -tA$ $(t > 0)$ to the resolvent $(A - z)^{-1}$. One possibility is to first approximate $f(s) = \exp -ts$ by a sequence of compactly supported functions $\theta_k := f(s)\chi_k$ such that $\chi_k(s) := \chi(s/k)$ wth $\chi \in C_0^\infty$ satisfying :

- $0 \leq \chi \leq 1$,
- $\chi = 1$ on $[-1, 1]$,
- $\mathrm{supp}\chi \subset [-2, 2]$.

We get the following control

$$\sup_{s\in\mathbb{R}^+} |\theta_k(s) - \exp -ts| \leq \exp -tk \ .$$

One easily gets from this control, that, if $A \geq 0$, then

$$||\theta_k(A) - \exp -tA||_{\mathcal{L}(\mathcal{H})} \ \leq \ \exp -tk \ .$$

It is then enough to show that if $A_n \to A$ in the strong resolvent convergence sense, with A_n, A positive, then, for a C^∞ function with compact support θ, we have

$$s - \lim \theta(A_n) = \theta(A) \ . \tag{13.4.5}$$

We now relate $\theta(A)$ and $(A-z)^{-1}$. This can be done by some variant of the Cauchy formula. Let us introduce the function defined on $\mathbb{C}$ by

$$\tilde{\theta}(z) = \theta(x) + i\theta'(x)y\chi(y) - \frac{1}{2}\theta''(x)\chi(y)y^2 \; . \tag{13.4.6}$$

The function $\tilde{\theta}$ is called an almost analytic extension of θ. We have the property that

$$(\partial_{\bar{z}}\tilde{\theta})(z) = \mathcal{O}(|Imz|^2) \; . \tag{13.4.7}$$

Using the functional calculus, one observes the identity (introduced in this context by Helffer-Sjöstrand and consequence of the Stokes formula)

$$\theta(A) = \frac{i}{2\pi}\int_{\mathbb{C}} (\partial_{\bar{z}}\tilde{\theta})(z)(A-z)^{-1}dz\wedge d\bar{z} \; . \tag{13.4.8}$$

where the r.h.s. can be defined as

$$\frac{i}{2\pi}\int_{\mathbb{C}} (\partial_{\bar{z}}\tilde{\theta})(z)(A-z)^{-1}dz\wedge d\bar{z} \; := \; \lim_{\epsilon\to 0}\frac{1}{\pi}\int_{|y|\geq\epsilon} (\partial_{\bar{z}}\tilde{\theta})(z)(A-z)^{-1}dx\cdot dy \; .$$

Here the limit is in $\mathcal{L}(\mathcal{H})$ and the convergence is controlled in $\mathcal{O}(\epsilon)$ uniformly with respect to A selfadjoint (due to the inequality $||(A-z)^{-1}|| \leq \frac{1}{|Imz|}$).
The proof of (13.4.5) is then not too difficult, but one has to control the dependence with respect to z of the convergence, for a fixed ψ, of $(A_n - z)^{-1}\psi$ to $(A-z)^{-1}\psi$ as $\mathrm{Im}\, z \to 0$. This is done using (13.2.2)-(13.2.3).

Remark 13.4.4. .
Note that we have the formula

$$\exp -tA = s - \lim_{p\to+\infty}(1+\frac{t}{p}A)^{-p} \; . \tag{13.4.9}$$

This can be obtained through the functional calculus and (13.4.9) in the scalar case.
Note that conversely we have

$$(A-\lambda)^{-1}\phi = \int_0^\infty \exp\lambda t \; \exp -tA \; \phi \; dt \; , \; \forall\phi\in\mathcal{H} \; , \tag{13.4.10}$$

if $\lambda < \inf\sigma(A)$.

Let us come back to the proof of the theorem.
By the Trotter product formula (13.1.2), we have

$$\exp -tH = s - \lim_{n\to+\infty}\left(s - \lim_{m\to+\infty}\left[\exp -t\frac{H_0}{m}\; \exp -t\frac{V_n}{m}\right]^m\right) \; , \tag{13.4.11}$$

and

$$\exp -tH_0 = s - \lim_{n\to+\infty}\left(s - \lim_{m\to+\infty}\left[\exp -t\frac{H}{m}\; \exp +t\frac{V_n}{m}\right]^m\right) \; . \tag{13.4.12}$$

Since $\exp - \pm t\frac{V_n}{m}$ is positivity preserving, it is easy to prove that it is "non-negativity preserving". We additionally observe that $\exp -tH$ and $\exp -tH_0$ are injective. The first part of the theorem is proved.
Now, for the second part, it is enough to observe that $\exp \pm t\frac{V_n}{m}$ being in L^∞ any subspace which is left invariant by $\exp -tH_0$ and L^∞ is left invariant by $\exp -tH$. Similarly any subspace which is left invariant by $\exp -tH$ and L^∞ is left invariant by $\exp -tH_0$.

Application .

We will apply in the next subsection this theorem with $H_0 = -\Delta$. So we have to prove the

Lemma 13.4.5. .
For any $t > 0$, the set $\{\exp t\Delta\} \cup L^\infty$ acts irreducibly on $L^2(\mathbb{R}^m)$.

Proof.
We have already observed that the operator is positivity improving. This shows that Property 2. in Theorem 13.4.1 is satisfied and the proof of the implication :" 2. implies 3. " can be used, although all the assumptions of the theorem are not satisfied.

13.5 Simplicity of the ground state.

We recall that a groundstate is an eigenvector corresponding to the lowest eigenvalue when it exists.

Theorem 13.5.1. .
Let $V \in L^2_{loc}(\mathbb{R}^m)$ be positive and suppose that $\lim_{|x|\to+\infty} V(x) = +\infty$. Then $-\Delta + V$ has a nondegenerate strictly positive ground state.

We have seen that $-\Delta + V$ has a purely discrete spectrum. The operator is indeed with compact resolvent. In order to apply Theorem 13.4.2 , it is enough to introduce the sequence of truncated potential $V_n = \inf(V, n)$ for $n \in \mathbb{N}$ and to use Lemma 13.4.5. Then using Theorem 9.4.4, one immediately gets that the operators $-\Delta + V_n$, $-\Delta + V$, $-\Delta + V - V_n$ and $-\Delta$ are essentially selfadjoint. Moreover, for any $\psi \in C_0^\infty(\mathbb{R}^m)$, we have $V_n\psi \to V\psi$ in L^2. This implies by Theorem 13.2.2 that we have the necessary strong resolvent convergence.
Finally, we can apply Theorem 13.4.1 to $\exp -(-\Delta + V)$.

Remark 13.5.2. .
Let us observe that $-\Delta + V_n$ has an essential spectrum included in $[n, +\infty[$. So $-\Delta + V_n$ has a non empty discrete spectrum below n for n large enough. Apply the Max-min Principle with ψ groundstate of $-\Delta + V$ or just observe that $\inf \sigma(H_0 + V_n) \leq \inf \sigma(H_0 + V)$ by monotonicity.

13.6 Notes

In this section, we mainly followed the presentation by Reed-Simon [RS-IV].

14 On the Schrödinger Operator with constant magnetic field

The Schrödinger operator with magnetic field has been briefly introduced in Subsection 7.5. We have in particularly given examples where this operator was with compact resolvent. In this section, we analyze more in detail the properties of the Schrödinger operator with constant magnetic field in dimension 2 and 3. This appears to play an important role in Superconductivity theory.

14.1 Preliminary study: an important model

14.1.1 Main results

Let us begin with the analysis of a a family of ordinary differential operators, whose study will play an important role in the analysis of various examples. We consider the Neumann realization $H^{N,\xi}$ in $L^2(\mathbb{R}^+)$ associated to the operator $D_x^2 + (x-\xi)^2$. It is easy to see that the operator is with compact resolvent and that the lowest eigenvalue $\mu(\xi)$ of $H^{N,\xi}$ is simple . For the second point, the following simple argument can be used. Suppose by contradiction that the eigenspace is of dimension 2. Then, we can find in this eigenspace an eigenvector such that u such that $u(0) = u'(0) = 0$. But then it should be identically 0 by Cauchy uniqueness.
We denote by φ_ξ the corresponding strictly positive normal eigenvector. The minimax shows that $\mu(\xi)$ is continuous as a function of ξ. It is a little more work (admitted (see Kato [Ka]) to show that the function is C^∞ and actually analytic (see in the next Subsubsection). It is immediate to show that $\mu(\xi) \to +\infty$ as $\xi \to -\infty$. We can indeed compare by monotonicity with $D_x^2 + x^2 + \xi^2$.

The second remark is that $\mu(0) = 1$. For this, we use the fact that the lowest eigenvalue of the Neumann realization of $D_t^2 + t^2$ in $\mathbb{R}^+$ is the same as the lowest eigenvalue of $D_t^2 + t^2$ in $\mathbb{R}$, but restricted to the even functions, which is also the same as the lowest eigenvalue of $D_t^2 + t^2$ in $\mathbb{R}$.

Moreover the derivative of μ at 0 is strictly negative.
It is a little more difficult to show that

$$\lim_{\xi \to +\infty} \mu(\xi) = 1 \,.$$

The proof can be done in the following way. For the upper bound, we observe that $\mu(\xi) \leq \lambda(\xi)$ where $\lambda(\xi)$ is the eigenvalue of the Dirichlet realization. By monotonicity of $\lambda(\xi)$, it is easy to see that $\lambda(\xi)$ is larger than one and tend to 1 as $\xi \to +\infty$. Another way is to use the function $\exp -\frac{1}{2}(x-\xi)^2$ as a test function.
For the converse, we start from the eigenfunction $\phi_\xi(x)$, show some uniform decay of $\phi_\xi(x)$ near 0 as $\xi \to +\infty$ and use $x \mapsto \chi(x+\xi)\phi_\xi(x+\xi)$ as a test function for the harmonic oscillator in $\mathbb{R}$.

All these remarks lead to the observation that the infimum $\inf_{\xi\in I\!R} \inf \mathrm{Sp}\,(H^{N,\xi})$ is actually a minimum [DaHe] and stricly less than 1. Moreover one can see that $\mu(\xi) > 0$, for any ξ, so the minimum is strictly positive. To be more precise on the variation of μ, let us first establish

$$\mu'(\xi) = -[\mu(\xi) - \xi^2]\varphi_\xi(0)^2\ . \tag{14.1.1}$$

To get (14.1.1), we observe that, if $\tau > 0$, then

$$\begin{aligned} 0 &= \int_{I\!R_+} [D_t^2\varphi_\xi(t) + (t-\xi)^2\varphi_\xi(t)]\varphi_{\xi+\tau}(t+\tau)dt \\ &= -\varphi_\xi(0)\varphi'_{\xi+\tau}(\tau) + (\mu(\xi+\tau) - \mu(\xi))\int_{I\!R_+} \varphi_\xi(t)\varphi_{\xi+\tau}(t+\tau)\,dt\ . \end{aligned}$$

We then take the limit $\tau \to 0$ to get the formula.

From (14.1.1), it comes that, for any critical point ξ_c of μ in $I\!R^+$

$$\mu''(\xi_c) = 2\xi_c\varphi^2_{\xi_c}(0) > 0\ . \tag{14.1.2}$$

So the critical points are necessarily non degenerate local minima. It is then easy to deduce that there exists a unique $\xi_0 > 0$ such that $\mu(\xi)$ continues to decay monotonically till some value $\Theta_0 < 1$ and is then increasing monotonically and tending to 1 at $+\infty$. Moreover

$$\Theta_0 = \xi_0^2\ . \tag{14.1.3}$$

Finally, it is easy to see that $\varphi_\xi(x)$ decays exponentially at ∞.

Let us show additional remarks on the properties of μ and $\varphi_\xi(x)$ which are related to the Feynman-Heilmann formula. We admit again (See Kato [Ka] and the next subsection) that we can "freely" differentiate with respect to ξ.

Let us start[36] from :

$$H^N(\xi)\varphi(\cdot;\xi) = \mu(\xi)\varphi(\cdot;\xi)\ . \tag{14.1.4}$$

Differentiating with respect to ξ, we obtain :

$$(\partial_\xi H^N(\xi) - \mu'(\xi))\varphi(\cdot;\xi) + (H^N(\xi)\varphi(\cdot;\xi) - \mu(\xi))(\partial_\xi\varphi)(\cdot;\xi) = 0\ . \tag{14.1.5}$$

Taking the scalar product with φ_ξ in $L^2(I\!R^+)$, we obtain the socalled Feynman-Heilmann Formula

$$\mu'(\xi) = \langle(\partial_\xi H^N(\xi)\varphi_\xi \mid \varphi_\xi\rangle = -2\int_0^{+\infty}(t-\xi)|\varphi_\xi(t)|^2dt\ . \tag{14.1.6}$$

Taking the scalar product with $\partial_\xi\varphi)(\cdot;\xi)$, we obtain the identity :

$$\langle(\partial_\xi H^N(\xi) - \mu'(\xi))\varphi(\cdot;\xi) \mid (\partial_\xi\varphi)(\cdot;\xi)\rangle + \langle(H^N(\xi)\varphi(\cdot;\xi) - \mu(\xi))(\partial_\xi\varphi)(\cdot;\xi) \mid (\partial_\xi\varphi)(\cdot;\xi)\rangle = 0\ . \tag{14.1.7}$$

[36] We change a little the notations for $H^{N,\xi}$ (this becomes $H^N(\xi)$) and φ_ξ in order to have an easier way for the differentiation.

In particular, we obtain for $\xi = \xi_0$ that :

$$\langle(\partial_\xi H^N(\xi_0)\varphi(\cdot;\xi_0) \mid \partial_\xi\varphi)(\cdot;\xi_0)\rangle + \langle(H^N(\xi)\varphi(\cdot;\xi_0) - \mu(\xi_0))(\partial_\xi\varphi)(\cdot;\xi_0) \mid (\partial_\xi\varphi)(\cdot;\xi_0)\rangle = 0\ . \tag{14.1.8}$$

We observe that the second term is positive (and with some extra work coming back to (14.1.5) strictly positive) :

$$\langle(\partial_\xi H^N(\xi_0))\varphi(\cdot;\xi_0) \mid \partial_\xi\varphi)(\cdot;\xi_0)\rangle < 0\ . \tag{14.1.9}$$

Let us differentiate one more (14.1.5) with respect to ξ.

$$\begin{array}{l} 2(\partial_\xi H^N(\xi) - \mu'(\xi))\partial_\xi\varphi(\cdot;\xi) \\ +(H^N(\xi) - \mu(\xi))(\partial_\xi^2\varphi)(\cdot;\xi) \\ +(\partial_\xi^2 H^N(\xi) - \mu''(\xi))\varphi(\cdot;\xi) = 0\ . \end{array} \tag{14.1.10}$$

Taking the scalar product with φ_ξ and $\xi = \xi_0$, we obtain

$$\mu''(\xi_0) = 2 + \langle(\partial_\xi H^N(\xi_0)\varphi(\cdot;\xi_0) \mid \partial_\xi\varphi)(\cdot;\xi_0)\rangle < 2\ . \tag{14.1.11}$$

14.1.2 Regularity

Proposition 14.1.1. *The eigenvalue $\mu(\xi)$ and the corresponding eigenvector ϕ_ξ are of class C^∞ with respect to ξ.*

Proof :
Step 1 :
Let $\mu(\xi_0)$ the lowest eigenvalue of $H^N(\xi_0)$. We recall that it is simple. Let φ_{ξ_0} the normalized eigenvector attached to $\mu(\xi_0)$. Let us denote by $\varphi_{\xi_0}^*$ the orthogonal projection on $varphi_{\xi_0}$. The domain of the operator can be seen as

$$D(H^N(\xi)) = \{u \in B^2(\mathbb{R}^+) \mid u'(0) = 0\ ,$$

and we observe that it is independent of ξ. We will use a variant of the so called Grushin's method. Let us introduce the unbounded operator on $L^2(\mathbb{R}^+) \times \mathbb{C}$

$$M_0 : = \begin{pmatrix} H^N(\xi_0) - \mu(\xi_0) & \varphi_{\xi_0} \\ \varphi_{\xi_0}^* & 0 \end{pmatrix}$$

with domain $D(H^N(\xi_0))$. Let us show its invertibility. By elementary algebra, we get that the inverse is

$$R_0 = \begin{pmatrix} E_0 & E_0^+ \\ E_0^- & E_0^{+-} \end{pmatrix},$$

with :

$$E_0 = ((H^N(\xi_0) - \mu(\xi_0))_{|\varphi_{\xi_0}^\perp})^{-1} \tag{14.1.12}$$

$$E_0^+ = \varphi_{\xi_0} \tag{14.1.13}$$

$$E_0^- = \varphi_{\xi_0}^* \tag{14.1.14}$$

$$E_0^{+-} = 0. \tag{14.1.15}$$

Step 2 :
Let us now introduce

$$M(\xi,\mu) = \begin{pmatrix} H^N(\xi)-\mu & \varphi_{\xi_0} \\ \varphi^*_{\xi_0} & 0 \end{pmatrix}.$$

Let us show that the inversibility is stable when ξ remains near ξ_0, and μ remains near $\mu(\xi_0)$. We observe that :

$$\begin{aligned} M(\xi,\mu) &= M_0 + \begin{pmatrix} (H(\xi)-H(\xi_0))-(\mu-\mu(\xi_0)) & 0 \\ 0 & 0 \end{pmatrix} \\ &= M_0 \left(\mathrm{Id} + R_0 \begin{pmatrix} (H^N(\xi)-H^N(\xi_0))-(\mu-\mu(\xi_0)) & 0 \\ 0 & 0 \end{pmatrix}\right). \end{aligned}$$

But the map $\xi \mapsto H^N(\xi)$ is continuous from $\mathbb{C}$ into $\mathcal{L}(D(H^N(\xi_0),L^2)$. So the result is clear and the inverse can be given by the convergent Neumann series :

$$M(\xi,\mu)^{-1} = \sum_{j\in\mathbb{N}} (-1)^j \left(R_0 \begin{pmatrix} (H(\xi)-H(\xi_0))-(\mu-\mu(\xi_0)) & 0 \\ 0 & 0 \end{pmatrix}\right)^j R_0. \tag{14.1.16}$$

Let us denote by

$$R(\xi,\mu) = \begin{pmatrix} E(\xi,\mu) & E^+(\xi,\mu) \\ E^-(\xi,\mu) & E^{+-}(\xi,\mu) \end{pmatrix}$$

the inverse of $M(\xi,\mu)$. The following result is standard :

Lemma 14.1.2.
The inverse of $M(\xi,\mu)$ is a C^∞ map in a neighborhood of $(\xi_0,\mu(\xi_0))$ with value in $D(H^N(\xi_0))\times\mathbb{C}$).

Proof of Lemma 14.1.2 :
It is clear that

$$T(\xi,\mu) = \left(R_0 \begin{pmatrix} (H(\xi)-H(\xi_0))-(\mu-\mu(\xi_0)) & 0 \\ 0 & 0 \end{pmatrix}\right) \tag{14.1.17}$$

is C^∞. Let us also observe that :

$$M(\xi,\mu)^{-1} = \sum_{j\in\mathbb{N}} (-1)^j T^j(\xi,\mu) R_0. \tag{14.1.18}$$

Consider

$$r(\xi,\mu) = (H(\xi)-H(\xi_0)) - (\mu-\mu(\xi_0))\,.$$

The derivatives of $r(\xi,\mu)$ are given by :

$$\begin{aligned} \partial_\xi r(\xi,\mu) &= \partial_\xi H(\xi) = -2(t-\xi) \\ \partial_\mu r(\xi,\mu) &= -1. \end{aligned} \tag{14.1.19}$$

In view of (14.1.18), we will estimate $T(\xi,\mu)^j$:

$$\begin{aligned}\left(R_0\begin{pmatrix} r(\xi,\mu) & 0\\ 0 & 0\end{pmatrix}\right)^j &= \left(\begin{pmatrix} E_0 & \varphi_{\xi_0}\\ \varphi^*_{\xi_0} & 0\end{pmatrix}\begin{pmatrix} r(\xi,\mu) & 0\\ 0 & 0\end{pmatrix}\right)^j\\ &= \begin{pmatrix} (E_0 r(\xi,\mu))^j & 0\\ (\varphi^*_{\xi_0} r(\xi,\mu))(E_0 r(\xi,\mu))^{j-1} & 0\end{pmatrix}.\end{aligned} \tag{14.1.20}$$

So

$$M(\xi,\mu)^{-1} = \sum_{j\in\mathbb{N}}(-1)^j \begin{pmatrix} (E_0 r(\xi,\mu))^j & 0\\ (\varphi^*_{\xi_0} r(\xi,\mu))(E_0 r(\xi,\mu))^{j-1} & 0\end{pmatrix} R_0. \tag{14.1.21}$$

It is then easy to show the C^∞ property.

Lemma 14.1.3.
μ is an eigenvalue of $H^N(\xi)$ if and only if $E^{+-}(\xi,\mu)=0$.
Moreover, if μ is an eigenvalue, $E^+(\xi,\mu)$ is the associated eigenvector in a neighborhood of $(\xi_0,\mu(\xi_0))$.

Proof of 14.1.3 :
Again this is simple linear algebra. Expressing that $R(\xi,\mu)$ is the inverse of $M(\xi,\mu)$ gives :

$$\begin{aligned}
E(\xi,\mu)(H(\xi)-\mu)+E^+(\xi,\mu)\varphi^*_{\xi_0} &= \mathrm{Id} &(14.1.22)\\
E^-(\xi,\mu)\varphi_{\xi_0} &= 1 &(14.1.23)\\
E(\xi,\mu)\varphi_{\xi_0} &= 0 &(14.1.24)\\
E^-(\xi,\mu)(H(\xi)-\mu)+E^{+-}(\xi,\mu)\varphi^*_{\xi_0} &= 0 &(14.1.25)\\
(H(\xi)-\mu)E(\xi,\mu)+\varphi_{\xi_0}E^-(\xi,\mu) &= \mathrm{Id} &(14.1.26)\\
\varphi^*_{\xi_0}E^+_{\xi,\mu} &= 1 &(14.1.27)\\
(H(\xi)-\mu)E^+(\xi,\mu)+\varphi_{\xi_0}E^{+-}(\xi,\mu) &= 0 &(14.1.28)\\
\varphi^*_{\xi_0}E(\xi,\mu) &= 0. &(14.1.29)
\end{aligned}$$

Taking the composition of $E^+(\xi,\mu)$ with (14.1.25) on the left, we get

$$E^+(\xi,\mu)E^-(\xi,\mu)(H(\xi)-\mu)+E^{+-}(\xi,\mu)E^+(\xi,\mu)\varphi^*_{\xi_0}=0,$$

so

$$E^+(\xi,\mu)\varphi^*_{\xi_0} = -\frac{E^+(\xi,\mu)E^-(\xi,\mu)(H(\xi)-\mu)}{E^{+-}(\xi,\mu)}. \tag{14.1.30}$$

This quantity (14.1.30) is well defined if $E^{+-}_{\xi,\mu}\neq 0$. So using (14.1.22) et(14.1.30) we get,

$$(H(\xi)-\mu)^{-1} = E(\xi,\mu)-\frac{E^+(\xi,\mu)E^-(\xi,\mu)}{E^{+-}(\xi,\mu)}. \tag{14.1.31}$$

So we have shown that if $E^{+-}_{\xi,\mu} \neq 0$, then $H(\xi) - \mu$ is invertible.

Conversely, let us assume that $E^{+-}_{\xi,\mu} = 0$. Then using (14.1.28), $E^+(\xi,\mu)$ is an eigenvector as soon that $E^+(\xi,\mu)$ is different from 0. But $E^+_{\xi_0,\mu(\xi_0)} = E^+_0 = \varphi_{\xi_0}$ is non zero, so by continuityit is also true for $E^+(\xi,\mu)$.

Step 3 : Analysis of the equation $E^{+-}(\xi,\mu) = 0$.
We have just to compute the implicit function theorem in the neighborhood of $(\xi_0, \mu(\xi_0)$. But by elementary computations, we have

$$E^{+-}(\xi,\mu) = \sum_{j\geq 1} (-1)^j (\varphi^*_{\xi_0} r_{\xi,\mu})(E_0 r(\xi,\mu))^{j-1} \varphi_{\xi_0}. \tag{14.1.32}$$

The derivatives at $(\xi_0, \mu(\xi_0)$ are easily computed as :

$$\begin{aligned} \partial_\xi E(\xi,\mu)^{+-}(\xi_0,\mu(\xi_0)) &= -\varphi^*_{\xi_0} \partial_\xi r(\xi_0,\mu(\xi_0))\varphi_{\xi_0} && (14.1.33)\\ &= 2\int_{I\!R^+} (t-\xi_0)\varphi^2_{\xi_0}(t)\ dt && (14.1.34)\\ \partial_\mu E^{+-}_{\xi,\mu}(\xi,\mu(\xi_0)) &= -1. && (14.1.35) \end{aligned}$$

In particular $\partial_\mu E^{+-}_{\xi,\mu}(\xi_0,\mu(\xi_0)) \neq 0$ and the implicit function theorem leads to

Lemma 14.1.4.
There exists $\eta > 0$ and a C^∞ map $\tilde{\mu}$ on $]\xi_0 - \eta, \xi_0 + \eta[$ such that

$$\forall \xi \in]\xi_0 - \eta, \xi_0 + \eta[,\ \forall \mu \in]\mu(\xi_0) - \eta, \mu(\xi_0) + \eta[,\ E^{+-}_{\xi,\mu} = 0 \Longleftrightarrow \mu = \tilde{\mu}(\xi).$$

We then obtain a C^∞ function $\xi \mapsto \tilde{\mu}(\xi)$ such that $\tilde{\mu}(\xi)$ is an eigenvalue of $H^N(\xi)$ and which is equal to $\mu(\xi)$ at ξ_0. By uniqueness, we get that for $|\xi - \xi_0|$ small enough $\tilde{\mu}(\xi) = \mu(\xi)$.

14.2 Dimension 2

We would like to analyze the spectrum of :

$$S_B := (D_{x_1} - \frac{B}{2}x_2)^2 + (D_{x_2} + \frac{B}{2}x_1)^2 . \tag{14.2.1}$$

14.2.1 The case of $I\!R^2$

We first look at the selfadjoint realization in $I\!R^2$. Let us show briefly, how one can analyze its spectrum. We leave as an exercise to show that the spectrum (or the discrete spectrum) of two selfadjoints operators S and T are the same if there exists a unitary operator U such that $U(S \pm i)^{-1} U^{-1} = (T \pm i)^{-1}$. We note that this implies that U sends the domain of S onto the domain of T.
In order to determine the spectrum of the operator S_B, we perform a succession

of unitary conjugations. The first one is called a gauge transformation. We introduce U_1 on $L^2(\mathbb{R}^2)$ defined, for $f \in L^2$ by

$$U_1 f = \exp iB\frac{x_1 x_2}{2} f \ . \tag{14.2.2}$$

It satisfies

$$S_B U_1 f = U_1 S_B^1 f \ , \ \forall f \in \mathcal{S}(\mathbb{R}^2) \ , \tag{14.2.3}$$

with

$$S_B^1 := (D_{x_1})^2 + (D_{x_2} + Bx_1)^2 \ . \tag{14.2.4}$$

Remark 14.2.1. .
U_1 is a very special case of what is called a gauge transform. More generally, we can consider $U = \exp i\phi$ where ϕ is C^∞. If $\Delta_A := \sum_j (D_{x_j} - A_j)^2$ is a general Schrödinger operator associated with the magnetic potential A, then $U^{-1}\Delta_A U = \Delta_{\tilde{A}}$ where $\tilde{A} = A + \operatorname{grad}\phi$. Here we observe that $B := \operatorname{rot} A = \operatorname{rot} \tilde{A}$. The associated magnetic field is unchanged in a gauge transformation. We are discussing in our example the very special case (but important!) when the magnetic potential is constant.

We have now to analyze the spectrum of S_B^1.
Observing that the operator is with constant coefficients with respect to the x_2-variable, we perform a partial Fourier transform with respect to the x_2 variable

$$U_2 = \mathcal{F}_{x_2 \mapsto \xi_2} \ , \tag{14.2.5}$$

and get by conjugation, on $L^2(\mathbb{R}^2_{x_1,\xi_2})$,

$$S_B^2 := (D_{x_1})^2 + (\xi_2 + Bx_1)^2 \ . \tag{14.2.6}$$

We now introduce a third unitary transform U_3

$$(U_3 f)(y_1, \xi_2) = f(x_1, \xi_2) \ , \ \text{ with } y_1 = x_1 + \frac{\xi_2}{B} \ , \tag{14.2.7}$$

and we obtain the operator

$$S_B^3 := D_y^2 + B^2 y^2 \ , \tag{14.2.8}$$

operating on $L^2(\mathbb{R}^2_{y,\xi_2})$.
The operator depends only on the y variable. It is easy to find for this operator an orthonormal basis of eigenvectors. We observe indeed that if $f \in L^2(\mathbb{R}_{\xi_2})$, and if ϕ_n is the $(n+1)$-th eigenfunction of the harmonic oscillator, then

$$(x, \xi_2) \mapsto |B|^{\frac{1}{4}} f(\xi_2) \cdot \phi_n(|B|^{\frac{1}{2}} y)$$

is an eigenvector corresponding to the eigenvalue $(2n+1)|B|$. So each eigenspace has an infinite dimension. An orthonormal basis of this eigenvalue can be given by vectors $e_j(\xi_2)|B|^{\frac{1}{4}} f(\xi_2)\ \phi_n(|B|^{\frac{1}{2}} y)$ where e_j $(j \in \mathbb{N})$ is a basis of $L^2(\mathbb{R})$.
We have consequently an empty discrete spectrum. The eigenvalues are usually called Landau levels.

14.2.2 The case of $\mathbb{R}^{2,+}$

For the analysis of the spectrum of the Neumann realization of the Schrödinger operator with constant magnetic field S_B in $\mathbb{R}^{2,+}$, we start like in the case of $\mathbb{R}^2$ till (14.2.6). Then we can use the preliminary study in dimension 1. The bottom of the spectrum is effectively given by :

$$\inf \sigma(S_B^{N,\mathbb{R}^{2,+}}) = |B| \inf \mu(\xi) = \Theta_0 |B| \,. \tag{14.2.9}$$

Similarly, for the Dirichlet realization, we find (See Problem 16.3.3, for details) :

$$\inf \sigma(S_B^{D,\mathbb{R}^{2,+}}) = |B| \inf \lambda(\xi) = |B| \,. \tag{14.2.10}$$

14.3 Magnetic Schrödinger operators in dimension 3

14.3.1 The case of $\mathbb{R}^3$

We start with the Schrödinger operator with constant magnetic field in dimension 3. After some rotation in $\mathbb{R}^3$, we arrive to the model :

$$P(h,\vec{b}) = D_{x_1}^2 + (D_{x_2} - bx_1)^2 + D_{x_3}^2 \,, \tag{14.3.1}$$

with

$$b = ||B|| \,.$$

This time, we can take the Partial Fourier transform, with respect to x_2 and x_3 in order to get the operator

$$D_{x_1}^2 + (\xi_2 - bx_1)^2 + \xi_3^2 \,.$$

When $b \neq 0$, we can translate in the x_1 variable and get the operator on $L^2(\mathbb{R}^3)$

$$D_{y_1}^2 + (|b| y_1)^2 + \xi_3^2 \,.$$

It is then easy to see that the spectrum is $[|b|, +\infty[$.

14.3.2 The case of $\mathbb{R}^{3,+}$: preliminary reductions

We now look at the case of $\mathbb{R}^{3,+}$. We would proceed as in the previous case, but our rotations have to conserve $\mathbb{R}^{3,+}$ and its boundary. Let us start from :

$$P(h,\vec{b}) := h^2 D_{x_1}^2 + (hD_{x_2} - b_{12}x_1)^2 + (hD_{x_3} - b_{13}x_1 - b_{23}x_2)^2 \,,$$

in $\{x_1 > 0\}$.
After scaling, we can assume that $h = 1$ and $b_{12}^2 + b_{13}^2 + b_{23}^2 = 1$.

After some rotation in the (x_2, x_3) variables, we can assume that the new magnetic field $\tilde{B}$ satisfies $\tilde{b}_{12} = 0$, the new $\tilde{b}_{13}$ satisfying :

$$\tilde{b}_{13}^2 = b_{12}^2 + b_{13}^2 \,.$$

So we have now reduced to the problem of analyzing :

$$P(\beta_1,\beta_2) := D_{x_1}^2 + D_{x_2}^2 + (D_{x_3} - \beta_1 x_1 - \beta_2 x_2)^2 \,,$$

in $\{x_1 > 0\}$, where :

$$\beta_1^2 + \beta_2^2 = 1 \,.$$

Here we have :

$$\beta_1^2 = b_{23}^2 \,,\ \beta_2^2 = b_{12}^2 + b_{13}^2 \,.$$

Changing of variables $x_2 \mapsto -x_2$ or $x_3 \mapsto -x_3$ (which respect the boundary) lead to the following model :

$$L(\vartheta, D_t) = D_{x_1}^2 + D_{x_2}^2 + (D_t - \cos\vartheta x_1 - \sin\vartheta x_2)^2 \,.$$

By Partial Fourier transform, we arrive to :

$$L(\vartheta,\tau) = D_{x_1}^2 + D_{x_2}^2 + (\tau - \cos\vartheta x_1 - \sin\vartheta x_2)^2 \,,$$

in $x_1 > 0$ and with Neumann condition on $x_1 = 0$. It is enough to consider the variation with respect to $\vartheta \in [0, \frac{\pi}{2}]$.

The bottom the spectrum is given by :

$$\sigma(\vartheta) := \inf \mathrm{Sp}\,(L(\vartheta, D_t) = \inf_\tau (\inf \mathrm{Sp}\,(L(\vartheta,\tau))) \,.$$

We first observe the following lemma :

Lemma 14.3.1. .
If $\vartheta \in [0, \frac{\pi}{2}[$, then $\mathrm{Sp}\,(L(\vartheta,\tau))$ *is independent of τ.*

This is trivial by translation.

Lemma 14.3.2. .
The function $\vartheta \mapsto \sigma(\vartheta)$ is continuous on $]0, \frac{\pi}{2}[$.

After a change of variable $y_1 = \cos\vartheta x_1$, $y_2 = \sin\vartheta x_2$ and we arrive with a continuous family of operators with a fixed domain. Using the mini-max principle, the lemma becomes easy to prove.

Lemma 14.3.3. .

$$\sigma(0) = \Theta_0 < 1 \,.$$

Proof We first observe that :

$$L(0, D_t) = D_{x_1}^2 + D_{x_2}^2 + (D_t - x_1)^2 \,.$$

We have then to analyze the bottom of the spectrum of the family :

$$L(0,\tau,\xi_2) := D_{x_1}^2 + \xi_2^2 + (x_1 - \tau)^2 \,.$$

This infimum is obtained as the infimum over $\tau \in \mathbb{R}$ of the spectrum of the family :

$$L(0,\tau,0) = D_{x_1}^2 + (x_1 - \tau)^2 \,.$$

This is the model which was analyzed in Subsection 14.1.

Lemma 14.3.4. .

$$\sigma(\frac{\pi}{2}) = 1 \ .$$

Proof.
We start from

$$L(\frac{\pi}{2}, \tau) = D_{x_1}^2 + D_{x_2}^2 + (\tau - x_2)^2 \ .$$

The bottom of the spectrum is the same as the bottom of the Neumann realization of :

$$D_{x_1}^2 + D_{x_2}^2 + x_2^2 \ ,$$

in $x_1 > 0$.
This is easily computed as equal to 1.

14.3.3 Lower bounds

Let us now consider the case when $\vartheta \in]0, \frac{\pi}{2}[$. According to Lemma 14.3.1, we can take $\tau = 0$ and we have to analyze :

$$L(\vartheta) = D_{x_1}^2 + D_{x_2}^2 + (x_1 \cos\vartheta + x_2 \sin\vartheta)^2.$$

Let us introduce a parameter $\rho \in [0, 1]$ and we then associate the following decomposition :

$$\begin{aligned} L(\vartheta) \ \ &:= D_{x_1}^2 + \rho^2 (x_1 \cos\vartheta + x_2 \sin\vartheta)^2 \\ &+ D_{x_2}^2 + (1 - \rho^2)(x_1 \cos\vartheta + x_2 \sin\vartheta)^2 \ . \end{aligned}$$

We will find a lower bound of the spectrum of $L(\vartheta)$ by considering the sum of the lower bounds of the spectra of the two following operators :

$$P_1(\rho, \vartheta) = D_{x_1}^2 + \rho^2 (x_1 \cos\vartheta + x_2 \sin\vartheta)^2 \ ,$$

and

$$P_2(\rho, \vartheta) = D_{x_2}^2 + (1 - \rho^2)(x_1 \cos\vartheta + x_2 \sin\vartheta)^2 \ .$$

Easy computations lead to :

$$\inf \sigma(P_1(\rho, \vartheta)) = \rho\Theta_0 \cos\vartheta \ ,$$

and

$$\inf \sigma(P_2(\rho, \vartheta)) = \sqrt{1 - \rho^2} \sin\vartheta \ ,$$

Choosing $\rho = \cos\vartheta$, we obtain :

$$\sigma(\vartheta) \geq \Theta_0 (\cos\vartheta)^2 + (\sin\vartheta)^2 \ .$$

Coming back to the initial problem, we have shown that :

$$\inf \sigma(P_{h,A_0}) \geq h(\Theta_0 (b_{13}^2 + b_{12}^2) + b_{23}^2)(b_{13}^2 + b_{12}^2 + b_{23}^2)^{-\frac{1}{2}}.$$

Moreover, one verifies that we have equality when $b_{23} = 0$:

$$\inf \sigma(P_{h,A_0}) = h(\Theta_0(b_{13}^2 + b_{12}^2))^{\frac{1}{2}} \, .$$

This clearly shwows that when $|B|$ is fixed the energy is minimal when the magnetic field is parallel to the hyperplane $x_1 = 0$.

14.3.4 Analysis of the essential spectrum

Proposition 14.3.5. *If $\vartheta \in]0, \frac{\pi}{2}$, then the essential spectrum of $L(\vartheta, 0)$ is contained in $[1, +\infty[$.*

Proof:
Using Persson's criterion, we have to show that if the support of u is in $\{x_1 > R\}$ or $\{|x_2| > R\}$, then we have

$$< Lu, u >\geq (1 - \epsilon(R))||u||_2^2 \, ,$$

with $\epsilon(R) \to 0$ as $R \to +\infty$. We proceed like for the lower bound. We treat the first case by observing that one can in this case use the Dirichlet result. This is for the second case that one use the decomposition with $\rho = \cos\vartheta$. But we have:

$$< P_1(\rho, \vartheta))u, u >\geq \cos\vartheta \rho\mu(R\cot(\vartheta))||u||^2 \, ,$$

when $\operatorname{supp} u \subset \{|x_2| > R\}$ and $\mu(\tau)$ is the first eigenvalue of the Neumann realization of the operator $D_t^2 + (t-\tau)^2$ in $I\!R^+$. We have also seen that :

$$< P_2(\rho, \vartheta))u, u >\geq \sin\vartheta\sqrt{1-\rho^2}||u||^2 \, .$$

This gives the result if one observe that $\lim_{\tau\to+\infty} \mu(\tau) = 1$ and that $\lim_{\tau\to-\infty} \mu(\tau) = +\infty$.

14.3.5 The upperbound: $\sigma(\vartheta) < 1$

We take the version :

$$L = -\frac{d^2}{dx_1^2} - \frac{d^2}{dx_2^2} + (x_1\cos\vartheta + x_2\sin\vartheta)^2 \, ,$$

in $x_1 > 0$.
We use first the change of variables :

$$u_1 = x_1\cos\vartheta + x_2\sin\vartheta \, , \; u_2 = -x_1\sin\vartheta + x_2\cos\vartheta \, ,$$

whose inverse is given by :

$$x_1 = u_1\cos\vartheta - u_2\sin\vartheta \, , \; x_2 = u_1\sin\vartheta + u_2\cos\vartheta \, .$$

This gives :

$$L' = -\frac{d^2}{du_1^2} - \frac{d^2}{du_2^2} + u_1^2 ,$$

in $\{u_1 > \tan\vartheta u_2\}$.
A new change of variable :

$$y_1 = -u_1 \ , \ y_2 = -\tan\vartheta u_2 ,$$

shows that this problem is equivalent to the Neumann realization of

$$L^{new} = -\frac{d^2}{dy_1^2} - \tan^2(\vartheta)\frac{d^2}{dy_2^2} + y_1^2 ,$$

in $\{y_2 > y_1\}$.
We now introduce :

$$f(t) = \exp -\frac{t^2}{2} ,$$

and

$$F(t) = \int_{-\infty}^{t} \exp -s^2 \ ds .$$

We observe that F is strictly positive :

$$\lim_{t\to+\infty} F(t) = \sqrt{\pi} ,$$

and

$$F(t) \sim \frac{2}{t}\exp -t^2 \ , \ \text{as } t \to -\infty .$$

We shall apply the minimax principle with the test function :

$$\Psi(y_1, y_2) = f(y_1)g(y_2) ,$$

with g to be determined in $L^2(I\!R)$.
Integrating Ψ^2 in the domain, we first have :

$$||\Psi||^2 = \int_{-\infty}^{+\infty} g(y_2)^2 F(y_2) dy_2 .$$

Let us now compute the corresponding energy of Ψ. We first get :

$$\begin{aligned} E(\Psi) \ &= \int g(y_2)^2 (\int_{-\infty}^{y_2} \left((f'(y_1))^2 + y_1^2 f(y_1)^2\right) dy_1) dy_2 \\ &+ (\tan\vartheta)^2 \int g'(y_2) F(y_2) dy_2 . \end{aligned}$$

After a few computations, we first get

$$\begin{aligned} E(\Psi) \ &= ||\Psi||^2 \\ &+ \int g(y_2)^2 f(y_2) f'(y_2) \, dy_2 \\ &+ (\tan\vartheta)^2 \int g'(y_2)^2 F(y_2) dy_2 , \end{aligned}$$

and then, after one integration by parts :

$$\begin{aligned} E(\Psi) \;&= ||\Psi||^2 \\ &\quad - \int g(y_2)g'(y_2)f(y_2)^2\, dy_2 \\ &\quad + (\tan\vartheta)^2 \int g'(y_2)^2 F(y_2) dy_2 \;. \end{aligned}$$

This sum can be rewritten in the form :

$$E(\Psi) = ||\Psi||^2 + \Sigma(g) \;,$$

where

$$\Sigma(g) := \int g'(y_2)\left((\tan\vartheta)^2 g'(y_2)F(y_2) - g(y_2)F'(y_2)\right) dy_2 \;.$$

We observe that we are done if we find some $g \in L^2$ such that $\Sigma(g)$ is strictly negative.

Let us first see what is going on if we try to get that the sum is zero. A natural try is then to solve the equation :

$$(\tan\vartheta)^2 g'(y_2)F(y_2) - g(y_2)F'(y_2) = 0 \;,$$

which leads to

$$g := cg_\alpha \;,$$

where

$$\alpha = (\cot\vartheta)^2$$

and

$$g_\alpha = F^\alpha \;.$$

We can compute $\Sigma(g_\alpha)$ for more general α. We get :

$$\Sigma(g_\alpha) = \alpha(\tan\vartheta^2\alpha - 1)\int f^4 F^{2\alpha-1} dy_2 \;.$$

Let us first control that this integral is well defined. No problem at $+\infty$ because F tends to a constant and f is exponentially decreasing. Near $-\infty$, F decreases like f^2 (see above), so this is OK for $\alpha > 0$. Now the sign of the expression is negative if :

$$0 < \alpha < \cot\vartheta^2 \;.$$

But...... g_α is not in L^2 at $+\infty$.
So we are obliged to introduce a cut-off function χ_n defined by :

$$\chi_n(t) = \chi(\frac{t}{n}) \;,$$

where χ is equal to 1 for $t \leq 1$ and equal to 0 for $t \geq 2$.
We now take

$$g = g_{n,\alpha} = \chi_n(t)g_\alpha(t) \;.$$

We observe that the corresponding $||\Psi_{n,\alpha}||^2$ increases like n as $n \to +\infty$. More precisely, we have :

$$-C + n\pi^{\alpha+1} \leq ||\Psi_{n,\alpha}||^2 \leq (2n)\pi^{\alpha+1} + C \ .$$

Let us compare $\Sigma(g_{\alpha,n})$ and $\Sigma(g_\alpha)$ as $n \to +\infty$.
We have

$$g'_{\alpha,n}(t) = \frac{1}{n}\chi'(\frac{t}{n})g_\alpha(t) + \chi(\frac{t}{n})g_\alpha(t) \ .$$

The more problematic term is :

$$\frac{1}{n^2}\int \chi'(\frac{t}{n})^2 g_\alpha^2(t)F(t)\ dt \ .$$

But this term is less than $\frac{C}{n^2}||\Psi_{n,\alpha}||^2$, that is of order $n \times \mathcal{O}(\frac{1}{n^2}) = \mathcal{O}(\frac{1}{n})$. The other terms appearing in the computation of $\Sigma(g_{\alpha,n}) - \Sigma(g_\alpha)$ are $\mathcal{O}(\frac{1}{n})$. Now, observing that $\Sigma(g_\alpha) < 0$, we get, for n large enough, that

$$E(\Psi_{\alpha,n}) \leq \Sigma(g_\alpha) + \frac{C}{n} + ||\Psi_{\alpha,n}||^2 < ||\Psi_{\alpha,n}||^2 \ .$$

This shows the property. Let us observe that

$$E(\Psi_{\alpha,n})/||\Psi_{\alpha,n}||^2 = 1 - \mathcal{O}(\frac{1}{n}) \ .$$

So there is no hope for using this function $\Psi_{\alpha,n}$ as a good quasimode.

14.3.6 Monotonicity

Let $\sigma(\vartheta)$ the lowest eigenvalue. This value exists if we show show that :

$$\inf_u < Lu, u > /||u||^2 < 1 \ .$$

We shall recall the proof of Lu-Pan in another sequence.

For the monotonicity, it is better (following Lu-Pan) to first do the dilation leading to the new operator:

$$\hat{L} = (\cos\vartheta)^2 D_{y_1}^2 + (\sin\vartheta)^2 D_{y_2}^2 + (y_1 + y_2)^2 \ .$$

We then apply Feynmann-Heilman formula at a possible minimum in $(0, \pi/2)$ and get a contradiction. So $\sigma'(\vartheta)$ does not vanish in the open interval of definition.
More precisely, if u_ϑ is the strictly positive normalized groundstate, we have:

$$\sigma'(\vartheta) = -(\sin\vartheta\cos\vartheta)\left(||D_{y_1}u_\vartheta||^2 - ||D_{y_2}u_\vartheta||^2\right) \ .$$

The size of this expression is not evident but let us assume that $b'(\vartheta_0) = 0$ for some $\vartheta_0 \in (0, \pi/2)$. Then we obtain that:

$$||D_{y_1}u_{\vartheta_0}||^2 = ||D_{y_2}u_{\vartheta_0}||^2 \ .$$

We then obtain the contradiction by writing :

$$1 > b(\vartheta_0) =< Lu_{\vartheta_0}, u_{\vartheta_0} >= ||D_{y_2}u_{\vartheta_0}||^2 + ||(y_1 + y_2)u_{\vartheta_0}||^2 \geq 1 \ .$$

14.3.7 Another rough upperbound

Lemma 14.3.6. .
When $\vartheta \in]0, \frac{\pi}{2}[$,

$$\inf \mathrm{Sp}\, L(\vartheta) \ \leq \cos(\vartheta)\Theta_0 + \sin(\vartheta). \tag{14.3.2}$$

Proof:
Let us write

$$\begin{aligned} L(\vartheta) \quad &= D_{x_1}^2 + (\cos\vartheta^2 x_1 - z)^2 \\ &\quad + D_{x_2}^2 + (\sin\vartheta x_2 + z)^2 \\ &\quad + 2(x_1 \cos\vartheta - z)(x_2 \sin\vartheta + z)\ . \end{aligned}$$

Use as quasimode the product of the eigenvector attached to the lowest eigenvalue of $D_{x_1}^2 + (\cos\vartheta x_1 - z)^2$ and of the eigenvector attached to the lowest eigenvalue of $D_{x_2}^2 + (\sin\vartheta x_2 + z)^2$. This gives, by a good choice of $z = -\xi_0/\sqrt{\sin\vartheta}$) an upper bound by $\Theta_0 \cos\vartheta + \sin\vartheta$.

14.4 Notes

Old results are due to Kato [Ka] and Avron-Herbst-Simon [AHS], but we have also added more recent results of Dauge-Helffer [DaHe] (for Subsection 14.1), Bernoff-Sternberg [BeSt], and of Lu-Pan [LuPa1]-[LuPa3] and Helffer-Morame [HeMo1]-[HeMo4] for the three dimensional case.

15 On spectral questions around the Rayleigh equation

15.1 On the physical motivation of the problem

The starting point in fluid mechanics is the analysis of the following differential systems in $I\!R^4 = I\!R^3_x \times I\!R_t$.

$$\begin{aligned} &\partial_t \rho + \mathrm{div}\,(\rho \vec{u}) = 0 \\ &\partial_t (\rho \vec{u}) + \rho (\vec{u} \cdot \nabla) \vec{u} + \nabla p = \rho \vec{g} \end{aligned} \tag{15.1.1}$$

The unknowns are $\vec{u} = (u_1, u_2, u_3)$, the density ρ and the pressure p. We assume that $\vec{g} = (0, 0, 1)g$.

This system models the so-called Rayleigh-Taylor instability, which occurs when a heavy fluid is on a light fluid in a gravity field directed from the heavy to the light fluid. We intend to study the linear growth rate of this instability in a situation where there is a mixing region. This linear growth rate will corresponds to γ in (15.1.15) below.

We would like to analyze the linearized problem around the solution

$$\rho = \rho^0 \ , \ u = u^0 = 0 \ , \ p = p^0 \ , \tag{15.1.2}$$

where ρ^0 is assumed to depend only on x_3 and p^0 and ρ^0 are related by :

$$\nabla p^0 = \rho^0 \vec{g} \ . \tag{15.1.3}$$

We assume that the perturbation $(\vec{\hat{u}}, \hat{p}, \hat{\rho})$ is incompressible that is satisfying :

$$\mathrm{div}\, \vec{\hat{u}} = 0 \ . \tag{15.1.4}$$

The linearized system takes the form :

$$\partial_t \hat{\rho} + (\rho^0)' \hat{u}_3 = 0 \ . \tag{15.1.5}$$

$$\rho^0 \partial_t \hat{u}_1 + \partial_1 \hat{p} = 0 \ . \tag{15.1.6}$$

$$\rho^0 \partial_t \hat{u}_2 + \partial_2 \hat{p} = 0 \ . \tag{15.1.7}$$

$$\rho^0 \partial_t \hat{u}_3 + \partial_3 \hat{p} = g \hat{\rho} \ . \tag{15.1.8}$$

In order to analyze (at least formally this system) we exhibit now an equation for $\hat{u}_3$ (by eliminating the other unknowns).

We first differentiate with respect to t (15.1.8). This leads to :

$$\rho^0 \partial_t^2 \hat{u}_3 + \partial_t \partial_3 \hat{p} = g \frac{\partial \hat{\rho}}{\partial t} . \tag{15.1.9}$$

We now use (15.1.5) in order to eliminate $\frac{\partial \hat{\rho}}{\partial t}$. We get :

$$\rho^0 \partial_t^2 \hat{u}_3 + \partial_t \partial_3 \hat{p} + g(\rho^0)'(x_3)\hat{u}_3 = 0 . \tag{15.1.10}$$

We now differentiate (15.1.6) and (15.1.7) respectively with respect to x_1 and x_2. This gives :

$$\rho^0 \partial_t \partial_1 \hat{u}_1 + \partial_1^2 \hat{p} = 0 , \tag{15.1.11}$$

and

$$\rho^0 \partial_t \partial_2 \hat{u}_2 + \partial_2^2 \hat{p} = 0 . \tag{15.1.12}$$

Differentiating (15.1.4) with respect to t and using (15.1.11) and (15.1.12), we get :

$$\Delta_{1,2} \hat{p} = \rho^0 \partial_t \partial_3 \hat{u}_3 . \tag{15.1.13}$$

It remains to eliminate $\hat{p}$ between (15.1.10) and (15.1.13) :

$$\Delta_{12}(\rho^0 \partial_t^2 \hat{u}_3 + (\rho^0)' g \hat{u}_3) + \partial_3 \rho^0 \partial_3 \partial_t^2 \hat{u}_3 = 0 . \tag{15.1.14}$$

We now look for a solution $\hat{u}_3$ in the form :

$$\hat{u}_3 = v(x_3) \exp(\gamma t + i k_1 x_1 + i k_2 x_2) . \tag{15.1.15}$$

This leads to the ordinary differential equation :

$$-(k_1^2 + k_2^2)(\rho^0 \gamma^2 v + (\rho^0)' g v) + \gamma^2 \frac{d}{dx^3} \rho^0 \frac{d}{dx_3} v = 0 . \tag{15.1.16}$$

Replacing x_3 by x ($x \in I\!R$) and dividing by $\gamma^2 k^2$ with $k^2 = k_1^2 + k_2^2$, we get :

$$\left[-\frac{1}{k^2} \frac{d}{dx} \rho^0 \frac{d}{dx} + \rho^0 + (\rho^0)' \frac{g}{\gamma^2} \right] v = 0 . \tag{15.1.17}$$

15.2 Introduction

So the mathematical problem is to analyze as a function of $\delta \in I\!R$ the kernel of the following operator :

$$P(h, \delta) := -h^2 \frac{d}{dx} \rho(x) \frac{d}{dx} + \rho(x) + \delta \rho'(x) . \tag{15.2.1}$$

Although it is not a standard spectral theory, we will see that the same techniques apply. Here $h > 0$ and $\rho(x)$ is a C^1 function satisfying the following properties :

$$\begin{aligned} \lim_{x\to-\infty}\rho(x) &= \rho_1 > 0\ ; \\ \lim_{x\to+\infty}\rho(x) &= \rho_2 > 0\ ; \end{aligned} \tag{15.2.2}$$

and

$$\rho(x) > 0\ ,\ \forall x \in \mathbb{R}\ . \tag{15.2.3}$$

We also assume that ρ' satisfies :

$$\lim_{|x|\to+\infty}\rho'(x) = 0\ , \tag{15.2.4}$$

and that

$$\rho_1 \neq \rho_2\ . \tag{15.2.5}$$

Notice that this in particular implies that $\rho'(x)$ can not be identically 0. Note that the question we are interested in could be semi-classical (that is $h \to 0$) or corresponding to the asymptotics $h \to +\infty$. Notice also that the most physical case is the case when ρ' is negative and in particular when

$$\rho_2 < \rho_1. \tag{15.2.6}$$

15.3 General spectral theory

We first observe that there is no problem[37] to define the selfadjoint extension of $P(h,\delta)$ (we keep the same notation) with domain $H^2(\mathbb{R})$ and it is immediate to observe that $P(h,0)$ is injective (actually stricly positive).

Definition 15.3.1. .
We call "generalized spectrum " of the family $P(h,\delta)$ the set of δ's such that $P(h,\delta)$ is not injective.

Remark 15.3.2. .
The standard analysis of the solutions of ordinary differential equations at ∞ (see for example the book by Sibuya [Sib]) shows that for any δ, the dimension of $\ker P(h,\delta)$ *is zero or one.*

The first result is

Proposition 15.3.3. .
Let us take the above assumptions and let us assume that ρ' is not identically

[37] The proof is the same as for the Schrödinger operator in Subsection 9.4. The presence of ρ is not a problem.

0. *Then the set of δ's such that* $\ker P(h,\delta)$ *is not zero can be described by two sequences (possibly empty or finite)* δ_n^+ *and* δ_n^- *such that :*

$$\begin{array}{l} 0 < \delta_n^+ < \delta_{n+1}^+ \,, \\ \lim_{n\to+\infty} \delta_n^+ = +\infty \,, \end{array} \tag{15.3.1}$$

(the second condition being only introduced in the infinite case)

$$\begin{array}{l} 0 < -\delta_n^- < -\delta_{n+1}^- \,, \\ \lim_{n\to+\infty} \delta_n^- = -\infty \,. \end{array} \tag{15.3.2}$$

Proof.
Observing that :

$$\ker P(h,\delta) \neq \{0\} \text{ iff } \ker(K(h) + \frac{1}{\delta}) \neq \{0\} \,, \tag{15.3.3}$$

with

$$K(h) = P(h,0)^{-\frac{1}{2}} \rho'(x) P(h,0)^{-\frac{1}{2}} \,.$$

So the problem is immediately reduced to a standard result in spectral analysis for a selfadjoint compact operator $K(h)$.

Actually some of the sequences could be empty. Here are some remarks, which could be instructive.
1. If $\rho'(x)$ is identically 0, then the spectrum of $K(h)$ is zero and the set of δ such $P(h,\delta)$ is not injective is empty.
2. If $\rho'(x) > 0$, then we have only the negative sequence δ_n^-.
3. Note that if ρ' vanishes in an open set, then 0 is in the spectrum of $K(h)$, but we are actually only interested in the non-zero eigenvalues of $K(h)$.

We note also that a particular role is played by the quantity $\inf_{||u||=1}\langle Ku \,,\ u\rangle$ and $\sup_{||u||=1}\langle Ku \,,\ u\rangle$. We now that they belong to the spectrum of $K(h)$. We observe that if δ_1^+ exists, then it is given by :

$$1/\delta_1^+ = - \inf_{||u||=1} \langle Ku \,, u\rangle \,. \tag{15.3.4}$$

Similarly, if δ_1^- exists, then it is given by :

$$1/\delta_1^- = - \sup_{||u||=1} \langle Ku \,, u\rangle \,. \tag{15.3.5}$$

Until now, we are doing abstract analysis and $h > 0$ was considered as a fixed parameter.

The next remark in this spirit (cf Theorem 6.4.1) is that :

$$\sup_{||u||=1} |\langle Ku \,,\ u\rangle| \leq \Lambda = \frac{\sup|\rho'(x)|}{\inf \rho(x)} \,.$$

As a consequence, we see that there exists some interval $I :=]-\frac{1}{\Lambda_0}, +\frac{1}{\Lambda_0}[$ independent of h such that :

$$\ker P(h,\delta) = \{0\} \ , \ \forall \delta \in I \ . \tag{15.3.6}$$

A different estimate can be obtained rather easily. If u is a solution for some $\delta \neq 0$, we get, by taking the scalar product in L^2 with u :

$$\int_{-\infty}^{+\infty} \rho(h^2 u'(x)^2 + u(x)^2)\, dx = -\delta \int_{-\infty}^{+\infty} \rho'(x) u(x)^2\, dx = 2\delta \int_{-\infty}^{+\infty} \rho u(x) u'(x)\, dx \ . \tag{15.3.7}$$

Using Cauchy-Schwarz, we get :

$$\int_{-\infty}^{+\infty} \rho(x)(1 - \frac{|\delta|}{h})(u'(x)^2 + u(x)^2) dx \leq 0 \ . \tag{15.3.8}$$

So we have shown the

Proposition 15.3.4.

$$\ker P(h,\delta) = \{0\} \ , \ \forall \delta \in]-h, h[\ . \tag{15.3.9}$$

We observe that this estimate is not interesting in the semiclassical regime (unless $\inf \rho = 0$).

Exercise 15.3.5.
Assuming that $\rho' > 0$, show the same results by using a proof similar to the uncertainty principle. Introduce the change of function $u = \rho^{\frac{1}{2}} v$ and the differential operators $X_1 = \rho^{\frac{1}{2}} \frac{d}{dx} \rho^{\frac{1}{2}}$ and $X_2 = \rho$.

A last a priori estimate is also interesting and can be obtained by starting of

$$\langle P(h,\delta) \rho^{-\frac{1}{2}} u \mid \rho^{-\frac{1}{2}} u \rangle = 0 \ .$$

15.4 More simple examples

15.4.1 The initial toy model

In the case when $\rho(x) = \rho_1$ for $x < 0$ and $\rho(x) = \rho_2$ for $x > 0$ with $\rho_1 \neq \rho_2$, the generalized eigenvalue is unique and given by :

$$\delta^c(h) = h(\rho_1 + \rho_2)/(\rho_1 - \rho_2) \ . \tag{15.4.1}$$

This model was investigated by Rayleigh in 1893. There are at least two points of view for understanding this problem.

The first point of view is a good exercise in distribution theory and consists in using the general description of solution in $L^2(I\!R^{\pm})$ for $\pm x > 0$. For $x > 0$, the solution should be $C_+ \exp -\frac{1}{h} x$ and for $x < 0$ the solution should be $C_- \exp \frac{1}{h} x$. The possible generalized eigenfunction, for some δ, is found by imposing that the two functions can be matched as an H^1 function u satisfying (in the sense of distributions) $P(h,\delta)u = 0$. Here $\rho'(x)$ should be understood as the operator (well defined on H^1) : $u \mapsto (\rho_2 - \rho_1)u(0)\mu_0$, where μ_0 is the Dirac measure at the origin. So we take $u(x) = \exp -\frac{1}{h}|x|$ and look for δ's such that : $P(h,\delta)u = 0$. We now note that

$$(-h^2 \frac{d}{dx}\rho(x)\frac{d}{dx} + \rho(x))u = h(\rho_1 + \rho_2)\mu_0$$

This gives the computation.

The second point of view is to observe that the associated compact operator K is actually of rank one. The range of K is on one side described as the vector spaced generated by : $(-h^2 \frac{d}{dx}\rho\frac{d}{dx} + \rho)^{-\frac{1}{2}}\mu_0$. On the other hand, we know that it is also related to the kernel of $P(h,\delta)$ through the map :

$$v \mapsto Sv = P(h,0)^{-\frac{1}{2}}v \ .$$

An eigenvector u is easier to compute by the first approach, and the associate v generating the range of K is then determined by the map S^{-1}.

15.4.2 Toward a more realistic model

We now suppose that ρ is equal to ρ_1 and ρ_2 in the neighborhhod of $\pm\infty$.

We analyze some asymptotic regime, corresponding to a transition between ρ_1 and ρ_2 over an interval of size ϵ. The initial problem is to find δ such that the operator :

$$P_\epsilon(\delta) = -\frac{d}{dx}\rho_\epsilon\frac{d}{dx} + \rho_\epsilon(x) + \delta\rho_\epsilon'(x) \ , \tag{15.4.2}$$

with $\rho_\epsilon(x) = \rho(\frac{x}{\epsilon})$, has a non zero kernel.

If we assume that ρ is constant outside $[-1,+1]$ the analysis of the L^2 solutions outside this interval is easy. We prefer to look at the analysis for a scaled operator :

$$H(\epsilon,\delta) = -\frac{d}{dx}\rho\frac{d}{dx} + \epsilon^2\rho(x) + \delta\epsilon\rho'(x) \ . \tag{15.4.3}$$

We would like to analyze in the limit $\epsilon \to 0$. We are then reduced, using the explicit description of the solutions outside $[-1,+1]$ (the solution should be $A_+ \exp -\epsilon x$ in $[1,+\infty[$ and consequently satisfies $u' = -\epsilon u$ in this interval and similarly the solution should be $A_- \exp \epsilon x$ in $]-\infty,-1]$ and consequently satisfies $u' = \epsilon u$ in $]-\infty,-1]$) to an analysis in $[-1,+1]$ of the following problem :

$$\begin{array}{ll} H(\epsilon,\delta)u & = 0 \ , \\ u'(+1) & = -\epsilon u(1) \ , \\ u'(-1) & = +\epsilon u(-1) \ . \end{array}$$

We note first that we can perform, assuming that δ has a formal expansion in powers of ϵ, a formal expansion of the system in powers of ϵ that can be solved by recursion.

On the other hand, this is also a consequence of a rather standard perturbation theory. One can indeed proceed as follows. For treating this problem, it is good to eliminate the dependence on ϵ of the boundary problem. But this is easily done by writing : $u = \exp -\sqrt{2}\,\epsilon < x > v$ and by considering

$$\hat{H}(\epsilon,\delta) := \exp \sqrt{2}\epsilon < x > \; H(\epsilon,\delta) \; \exp -\sqrt{2}\epsilon < x > ,$$

and the Neumann condition at ± 1.

We have then to analyze the spectrum near 0 of the operator corresponding to the Neumann realization in $]-1,+1[$ of :

$$\tilde{H}(\epsilon,\gamma) := -(\frac{d}{dx} - \epsilon\sqrt{2}\frac{x}{< x >})\rho(\frac{d}{dx} - \epsilon\sqrt{2}\frac{x}{< x >}) + \epsilon^2\rho + \gamma\rho' ,$$

as a function of ϵ and γ, where $\gamma = \delta\epsilon$.
For $\epsilon = \gamma = 0$, $\tilde{H}(0,0)$ has 0 as isolated eigenvalue of multiplicity 1, with $u_0 = 1$ has eigenvector. So by regular perturbation, the eigenvalue (near 0) $F(\epsilon,\gamma)$ depends analytically on ϵ and γ (Kato's theory [Ka]). For this we can proceed like in Subsection 14.1.2.
We get

$$(\partial F/\partial\gamma) = \frac{1}{2}\int_{-1}^{+1} \rho'(x)\,dx = \frac{1}{2}(\rho_2 - \rho_1) \neq 0 .$$

This permits to apply the implicit function theorem, and we get $\gamma(\epsilon)$ such that $F(\gamma(\epsilon),\epsilon) = 0$ and we observe that $\gamma(0) = 0$. We then recover

$$\delta = \delta^c + \sum_{j\geq 1} c_j\epsilon^j , \tag{15.4.4}$$

by dividing by ϵ. In order to get the main term in (15.4.4), let us compute $(\partial F/\partial\epsilon)(0,0)$. We obtain :

$$(\partial F/\partial\epsilon)(0,0) = \frac{1}{2}\langle(\partial\tilde{H}/\partial\epsilon)_{\epsilon=0}\, u_0 \mid u_0\rangle = \frac{1}{2}(\rho_1 + \rho_2) .$$

This gives :

$$\delta^c = \frac{\rho_1 + \rho_2}{\rho_1 - \rho_2} . \tag{15.4.5}$$

Remark 15.4.1.
Let us emphasize a few points. The new problem is not selfadjoint but weakly non selfadjoint (the principal part -that is $-\frac{d}{dx}\rho\frac{d}{dx}$*-of the operator is selfadjoint.) We are looking to a regular holomorphic perturbation which is relatively regular. Above, we have found an holomorphic function* $\epsilon \mapsto \gamma(\epsilon)$*. The fact that* $\gamma(\epsilon)$ *is real for* ϵ *real is verified a posteriori by uniqueness.*

15.5 The general case

15.5.1 Main theorem

We would like to treat now the case when ρ is not constant at ∞. This is more difficult because the reduction to a finite interval is less evident. The main result is the following

Theorem 15.5.1. .
Let us assume that ρ is of class C^1 and that

$$M := \int_{-\infty}^{0} |\rho(x) - \rho_1|^2 \, dx + \int_{0}^{+\infty} |\rho(x) - \rho_2|^2 \, dx < +\infty \, . \tag{15.5.1}$$

Then for any $C > \delta^c$, there exists ϵ_0 and C_0 such that for $\epsilon \in]0, \epsilon_0]$, $P_\epsilon(\delta)$ admits a unique generalized eigenvalue δ_ϵ in the interval $]0, C]$. Moreover we have :

$$|\delta_\epsilon - \delta^c| \leq C\epsilon^{\frac{1}{2}} \, .$$

We will now describe different approachs for proving this result. Each approach gives a different information (localization, uniqueness, existence and asymptotics).

15.5.2 First approach

Proposition 15.5.2. .
Under the assumptions of the theorem, let $\mathcal{A}$ be some subset in $]0, \epsilon_0]$ with 0 as accumulation point.
Let us assume that, for $\epsilon \in \mathcal{A}$, $(\delta_\epsilon, U_\epsilon)$ is a solution of

$$P_\epsilon(\delta_\epsilon) \, U_\epsilon = 0 \, , \tag{15.5.2}$$

with

$$U_\epsilon > 0 \, , \tag{15.5.3}$$

$$||U_\epsilon||_{L^2(\mathbb{R})} = 1 \tag{15.5.4}$$

and

$$0 < c_1 < \delta_\epsilon < c_2 \, . \tag{15.5.5}$$

Then, if c_1 and c_2 satisfy :

$$0 < c_1 < \delta^c < c_2 \, , \tag{15.5.6}$$

we have :
i)

$$\lim_{\epsilon \to 0} \delta_\epsilon = \delta^c \, . \tag{15.5.7}$$

ii)

$$\lim_{\epsilon \to 0} U_\epsilon = \frac{1}{\sqrt{2}}\, e^{-|X|}\ , \tag{15.5.8}$$

strongly in $L^2(\mathbb{R})$.

Proof

Preliminaries.
We have the following inequality of uniform coercivity of P_ϵ:

$$\min \rho\ ||\phi||^2_{H^1} \leq \langle P_\epsilon \phi \mid \phi \rangle \leq \max \rho\ ||\phi||^2_{H^1}\ . \tag{15.5.9}$$

This implies in particular that :

Lemma 15.5.3. .
There exists a constant C *such that* $P_\epsilon^{\frac{1}{2}}$ *satisfies, for all* $\epsilon \in]0, \epsilon_0]$ *:*

$$||P_\epsilon^{\frac{1}{2}}||_{\mathcal{L}(L^2, H^{-1})} + ||P_\epsilon^{\frac{1}{2}}||_{\mathcal{L}(H^1, L^2)} \leq C\ . \tag{15.5.10}$$

Similarly, we have :

$$||P_\epsilon^{-\frac{1}{2}}||_{\mathcal{L}(L^2, H^1)} + ||P_\epsilon^{-\frac{1}{2}}||_{\mathcal{L}(H^{-1}, L^2)} \leq C\ . \tag{15.5.11}$$

Finally, we have also :

$$||P_\epsilon^{-1}||_{\mathcal{L}(H^{-1}, H^1)} \leq C\ . \tag{15.5.12}$$

Now we observe that

Lemma 15.5.4.

$$||U_\epsilon||_{H^1} \leq C\ . \tag{15.5.13}$$

Proof.
We start from :

$$\langle P_\epsilon U_\epsilon \mid U_\epsilon \rangle = -\delta_\epsilon \int \rho_\epsilon (U_\epsilon^2)'\ dx\ . \tag{15.5.14}$$

This gives :

$$(\inf \rho_\epsilon) ||U_\epsilon||^2_{H^1} \leq 2 c_2 (\sup \rho_\epsilon) \cdot ||U_\epsilon||_{L^2} ||U_\epsilon'||_{L^2}\ ,$$

so :

$$||U_\epsilon||_{H^1} \leq 2 c_2 (\frac{\sup \rho_\epsilon}{\inf \rho_\epsilon}) \cdot ||U_\epsilon||_{L^2}\ .$$

The proof is then immediate.

We now extract from $U_\epsilon, \delta_\epsilon, U_\epsilon(0)$ a sequence such that $U_\epsilon \rightharpoonup U$ in H^1, $\delta_\epsilon \to \delta$, $U_\epsilon(0) \to U(0) = A$. From the variational formulation, if we denote by $H(x)$ the distribution equal to ρ_1 in $-\infty, 0[$ and to ρ_2 on $]0, +\infty[$, we have, using assumption (15.5.1):

$$-\frac{d}{dx}(H(x)\frac{dU}{dx}) + H(x)U + \delta(\rho_2 - \rho_1)\mu_0 U = 0 \ , \tag{15.5.15}$$

which implies that

$$U(X) = A\ e^{-|X|} \ . \tag{15.5.16}$$

Now, we need to have a uniform lower bound for $U_\epsilon(0)$ in order to show that $A \neq 0$. Admitting this point and using once again the equation (15.5.15), we obtain δ^c.

Lemma 15.5.5. .
U is not identically 0.

Proof.
In the same spirit than above, we start from :

$$\langle P_\epsilon U_\epsilon \mid U_\epsilon \rangle = -\delta_\epsilon \int \rho'_\epsilon (U_\epsilon^2)\ dx \ .$$

Introducing, a free parameter $a > 0$, we cut the right hand integral, in two parts that we shall estimate separately :

$$\begin{aligned} ||\, U_\epsilon \,||^2_{H^1} \quad &\leq C \int_{-a}^{+a} |\rho'_\epsilon|(U_\epsilon^2)\ dx \\ &\quad +C \int_{|x|\geq a} \rho'_\epsilon (U_\epsilon^2)\ dx \ . \end{aligned}$$

This leads to :

$$\begin{aligned} ||U_\epsilon||^2_{H^1} \quad &\leq C_1\ ||\rho'_\epsilon||_{L^1}|\ \sup_{x\in[-a,+a]}(U_\epsilon(x)^2) \\ &\quad +\tfrac{C_2}{a}\ ||x\rho'(x)||_{L^\infty}\ \int_{|x|\geq a}(U_\epsilon^2)\ dx \ . \end{aligned} \tag{15.5.17}$$

Choosing a large enough (independently of $\epsilon \in \mathcal{A}$), we get :

$$||U_\epsilon||^2_{H^1} \leq C_2 \ . \sup_{x\in[-a,+a]} (U_\epsilon(x)^2) \ . \tag{15.5.18}$$

This implies :

$$1 \leq C_2 \ . \sup_{x\in[-a,+a]} (U_\epsilon(x)^2) \ . \tag{15.5.19}$$

Now, if U_ϵ converges weakly to U in H^1, it converges strongly to U in $C^0([-a, +a])$. This implies :

$$1 \leq C_2 \ . \sup_{x\in[-a,+a]} (U(x)^2) \ . \tag{15.5.20}$$

This gives a proof that $A \neq 0$.

Up to now, we have shown that for any family $(\delta_\epsilon, U_\epsilon)$ satisfying the above solution, there exists a subsequence such that $\delta_\epsilon \to \delta$ and such that U_ϵ tends weakly to a non zero U in H^1, for some $A > 0$. But this A may depend on this subsequence.

It remains to show the lemma :

Lemma 15.5.6. *The convergence of U_ϵ to U in L^2 is strong.*

Once we have this lemma, it is easy to determine A as a consequence of the relation

$$||U_\epsilon||_{L^2} = 1 \ ,$$

which implies

$$||\,U\,|| = 1 \ ,$$

and

$$A = 1/\sqrt{2} \ .$$

Proof of Lemma 15.5.6.
The proof is a consequence of a compactness argument that we shall get through the so-called Agmon estimates for U_ϵ.

Our starting point is, for any Lipschitzian function ϕ, the identity :

$$\langle \exp 2\phi P_\epsilon U_\epsilon \mid U_\epsilon\rangle = ||\rho_\epsilon^{\frac{1}{2}}(\exp\phi U_\epsilon)'(x)||^2 + \int \rho_\epsilon (1-\phi'(x)^2)\exp 2\phi(x)|U_\epsilon|^2(x)\,dx \tag{15.5.21}$$

Using the equation satisfied by U_ϵ, we get :

$$-\delta_\epsilon \int \rho_\epsilon' \exp 2\phi |U_\epsilon(x)^2\,dx = ||\rho_\epsilon^{\frac{1}{2}}(\exp\phi U_\epsilon)'(x)||^2 + \int \rho_\epsilon(1-\phi'(x)^2)\exp 2\phi(x)|U_\epsilon|^2(x)\,dx \tag{15.5.22}$$

Let us define :

$$V_\epsilon = \exp\phi(x) U_\epsilon \ . \tag{15.5.23}$$

We now obtain, choosing a function $\phi(x) = \alpha\sqrt{1+x^2}$ with α small enough :

$$||V_\epsilon||_{H^1}^2 \leq C\int |\rho_\epsilon'||V_\epsilon(x)|^2 dx \tag{15.5.24}$$

As in te proof of (15.5.18), there exists some $a > 0$, such that :

$$||V_\epsilon||_{H^1}^2 \leq 2C \sup_{x\in[-a,+a]} |V_\epsilon(x)|^2 \ . \tag{15.5.25}$$

But we can estimate the right hand side of the previous inequality. We get :

$$||\exp\phi\, U_\epsilon||_{H^1}^2 \leq 2C\exp 2\alpha\sqrt{1+a^2}\ ||U_\epsilon||_{H^1}^2 \leq \tilde{C} \ . \tag{15.5.26}$$

In particular U_ϵ is bounded in $E := H^1(I\!R) \cap L^2(I\!R\ , \ \exp 2\phi\, dx)$. But the injection of E in L^2 is compact. After extraction of a subsequence, we get that U_ϵ converges strongly to U. Taking into account the two conditions (15.5.3) and (15.5.4) on U_ϵ, this determines the choice of U and we can consequently (the accumulation point of $(\delta_\epsilon, U_\epsilon, U_\epsilon(0))$ being unique) get the convergence for all the sequence.

15.5.3 A second approach

One could hope a better result by using another point of view.

We introduce :

$$v_\epsilon = P_\epsilon^{\frac{1}{2}} U_\epsilon\ ,$$

and observe that v_ϵ is a solution in $L^2(I\!R)$ of

$$\frac{1}{\delta_\epsilon} v_\epsilon + P_\epsilon^{-\frac{1}{2}} \rho'_\epsilon P_\epsilon^{-\frac{1}{2}}\ v_\epsilon = 0\ .$$

This leads to the analysis of the operator :

$$K_\epsilon = P_\epsilon^{-\frac{1}{2}} \rho'_\epsilon P_\epsilon^{-\frac{1}{2}}\ . \tag{15.5.27}$$

We introduce the distribution $T_\epsilon = \rho'_\epsilon - (\rho_2 - \rho_1)\mu_0$, where μ_0 is the Dirac measure at 0. It is immediate that T_ϵ tends to 0, but we may need a stronger control. We observe that :

$$- < T_\epsilon, \phi >= \int_{-\infty}^0 (\rho(x) - \rho_1)\epsilon\phi'(\epsilon x) dx + \int_0^{+\infty} (\rho(x) - \rho_2)\epsilon\phi'(\epsilon x) dx\ ,$$

and a Cauchy-Schwarz inequality leads to

$$| < T_\epsilon, \phi > | \leq M\sqrt{\epsilon} ||\phi'||_{L^2}\ .$$

Associated to this distribution, we can introduce the operator of multiplication by T_ϵ, denoted by $\mathcal{T}_\epsilon$, which is well defined as an operator from H^1 into H^{-1}. We have actually the

Lemma 15.5.7. .

$$||\mathcal{T}_\epsilon||_{\mathcal{L}(H^1,H^{-1})} \leq C\sqrt{\epsilon}\ . \tag{15.5.28}$$

Proof.
We observe that, for $u \in H^1$, $\mathcal{T}_\epsilon u$ is the distribution defined by :

$$(\mathcal{T}_\epsilon u)(\phi) = T_\epsilon(u\phi)\ .$$

Using the estimate on T_ϵ, which gives a control of the norm of T_ϵ in H^{-1} and the property that H^1 is an algebra, we get :

$$|(\mathcal{T}_\epsilon u)(\phi)| \leq C\ \sqrt{\epsilon} ||u||_{H^1} ||\phi||_{H^1}\ .$$

The lemma is proved.

Our aim is to compare K_ϵ with a limit operator. So the natural guess would be to compare with the operator :

$$K_0 := P_0^{-\frac{1}{2}} \mu_0 P_0^{-\frac{1}{2}} ,$$

with

$$P_0 = \lim_{\epsilon \to 0} P_\epsilon = -\frac{d}{dx} H \frac{d}{dx} + H .$$

We start from the following identity :

$$K_\epsilon = -P_\epsilon^{-\frac{1}{2}} \mathcal{T}_\epsilon P_\epsilon^{-\frac{1}{2}} + (\rho_1 - \rho_2) P_\epsilon^{-\frac{1}{2}} \mu_0 P_\epsilon^{-\frac{1}{2}} := R_\epsilon + K_\epsilon^0 . \tag{15.5.29}$$

From the previous lemmas, we easily obtain that :

$$||R_\epsilon||_{\mathcal{L}(L^2)} \leq C\sqrt{\epsilon} . \tag{15.5.30}$$

This leads to the spectral analysis of K_ϵ^0 which is an ϵ-dependent rank one operator. The analysis of this operator is unfortunately incomplete.

This point of view leads however to interesting inequalities. The equality satisfied by v_ϵ is

$$\frac{1}{\delta_\epsilon} v_\epsilon = (\rho_1 - \rho_2)(P_\epsilon^{-\frac{1}{2}} v_\epsilon)(0)(P_\epsilon^{-\frac{1}{2}} \mu_0)(x) - P_\epsilon^{-\frac{1}{2}} \mathcal{T}_\epsilon P_\epsilon^{-\frac{1}{2}} v_\epsilon .$$

Hence we obtain :

$$\frac{1}{c_2} ||v_\epsilon||_{L^2} \leq C\,\sqrt{\epsilon} ||v_\epsilon||_{L^2} + |\rho_2 - \rho_1|\; |(P_\epsilon^{-\frac{1}{2}} v_\epsilon)(0)|\; ||(P_\epsilon^{-\frac{1}{2}} \mu_0)||_{L^2} .$$

We now observe that $\mu_0 \in H^{-1}(\mathbb{R})$. So using Lemma 15.5.3, we immediately obtain that $P_\epsilon^{-\frac{1}{2}} \mu_0$ is bounded in L^2.

This leads to the existence of $c_0 > 0$ such that :

$$U_\epsilon(0) = |(P_\epsilon^{-\frac{1}{2}} v_\epsilon)(0)| \geq c_0 > 0 . \tag{15.5.31}$$

Here we note (compare with (15.5.20)) that this is an alternative way to show that $A \neq 0$.

Another information is that it gives a way to show that there is at most, K_ϵ^0 having only one non zero eigenvalue of multiplicity 1, one negative eigenvalue in $]-\infty, -C\sqrt{\epsilon}]$, which is consequently the eigenvalue found before which tends to $-1/\delta$.

15.5.4 Quasimodes and generaized spectrum

Here we discuss in a simple case how one can use the construction of approximate solutions for localizing the generalized spectrum. Let us start of $U = \frac{1}{\sqrt{2}} \exp -|x|$. Let us assume that we have shown that :

$$||P_\epsilon(\delta^c)U||_{H^{-1}} \leq C\sqrt{\epsilon}\,. \tag{15.5.32}$$

Then let us show that there exists a generalized eigenvalue δ_ϵ such that :

$$|\delta_\epsilon - \delta^c| \leq C_1\sqrt{\epsilon}\,. \tag{15.5.33}$$

This is simply done by applying the spectral theorem to the compact operator K_ϵ, where

$$K_\epsilon = P_\epsilon^{-\frac{1}{2}} \rho'_\epsilon P_\epsilon^{-\frac{1}{2}}\,,$$

with the quasimode $W_\epsilon := P_\epsilon^{\frac{1}{2}} U$.
For this we observe that

$$||(K_\epsilon + \frac{1}{\delta^c})W_\epsilon||_{L^2}^2 = ||\frac{1}{\delta^c} P_\epsilon^{-\frac{1}{2}}\,(P_\epsilon(\delta^c)U)\,||_{L^2} \leq C\,||P_\epsilon(\delta^c)U||_{H^{-1}}^2 \leq \tilde{C}\sqrt{\epsilon}\,,$$

where we have used Lemma 15.5.3.
If we know observe that :

$$||W_\epsilon||_{L^2} \geq \frac{1}{C}\,||U||_{H^1}^2 \geq \frac{1}{C}\,,$$

we have completed the argument.

Let us now show (15.5.32). First we compute in the distribution sense :

$$P_\epsilon(\delta^c)U = \frac{1}{\sqrt{2}}\,(\rho'_\epsilon((\mathrm{sign}x) + \delta^c)\exp -|x|) + \sqrt{2}\rho(0)\mu_0\,.$$

So we have now to compute the different terms by testing on a function ϕ.
We have :

$$\begin{aligned}
&\int \rho'_\epsilon(\mathrm{sign}x)\exp -|x|\phi(x)dx\\
&\quad = \int_0^\infty \rho'_\epsilon \exp -x\phi(x)dx - \int_{-\infty}^0 \rho'_\epsilon \exp x\phi(x)dx\\
&\quad = -2\rho(0)\phi(0) - \int_0^\infty \rho_\epsilon(\exp -x\phi(x))'dx + \int_{-\infty}^0 \rho_\epsilon(\exp x\phi(x))'dx
\end{aligned}$$

Similarly, we have :

$$\begin{aligned}
\int \rho'_\epsilon \exp -|x|\phi(x)dx &= \int_0^\infty \rho'_\epsilon \exp -x\phi(x)\,dx + \int_{-\infty}^0 \rho'_\epsilon \exp x\phi(x)\,dx\\
&= -\int_0^\infty \rho_\epsilon(\exp -x\phi(x))'\,dx - \int_{-\infty}^0 \rho_\epsilon(\exp x\phi(x))'\,dx
\end{aligned}$$

Summing up, we get with $S_\epsilon := P_\epsilon(\delta^c)U$,

$$\begin{aligned}
S_\epsilon(\phi) &= \tfrac{1}{\sqrt{2}}\left(-\int_0^\infty \rho_\epsilon(\exp -x\phi(x))'dx + \int_{-\infty}^0 \rho_\epsilon(\exp x\phi(x))'dx\right)\\
&\quad +\delta^c \tfrac{1}{\sqrt{2}}\left(-\int_0^\infty \rho_\epsilon(\exp -x\phi(x))'\,dx - \int_{-\infty}^0 \rho_\epsilon(\exp x\phi(x))'\,dx\right)
\end{aligned} \tag{15.5.34}$$

In a similar way as in Subsubsection 15.5.3, we get :

$$\begin{aligned} S_\epsilon(\phi) \quad &= \frac{1}{\sqrt{2}}(-1+\delta^c)\int_0^\infty(\rho_\epsilon-\rho_2)(\exp -x\phi(x))'dx \\ &+\frac{1}{\sqrt{2}}(1+\delta^c)\int_{-\infty}^0(\rho_\epsilon-\rho_1)(\exp x\phi(x))'dx \end{aligned} \tag{15.5.35}$$

Using then Cauchy-Schwarz and the assumption (15.5.1), we obtain the inequality :

$$|S_\epsilon(\phi)| \leq C\sqrt{\epsilon}(||(\exp -x\phi)'||_{L^2(I\!R^+)} + ||(\exp x\phi)'||_{L^2(I\!R^-)}) \ , \tag{15.5.36}$$

and this achieves the proof of (15.5.32).

15.6 Notes

This material is extracted of a common paper with O. Lafitte [HelLaf], which was in continuation of previous papers by [ChLa], [La] and [CCLaRa].

16 Exercises and Problems

16.1 Introduction

We present some exercises or problems proposed in the last years. They sometimes strongly intersect with the course.

16.2 Exercises

Exercise 16.2.1. *(After Effros, Avron-Seiler-Simon).*
Let P and Q two selfadjoint projectors in a Hilbert space $\mathcal{H}$. i) Let us assume that $A = P - Q$ is compact. Show that if $\lambda \neq \pm 1$ is in the spectrum, then $-\lambda$ is in the spectrum with the same multiplicity. For this, one can first show that with $B = I - P - Q$,

$$A^2 + B^2 = I \ , \ AB + BA = 0 \ .$$

ii) Assume now that A is in addition trace class, that is that the series $|\mu_j|$, where μ_j are the non zero eigenvalues of A, counted with multiplicity. Compute $Tr\ A := \sum_j \mu_j$ and show that it is an integer.

Exercise 16.2.2. *(Temple's inequality).*
Let A be a selfadjoint operator on an Hilbert space and $\psi \in D(A)$. Suppose that λ is the unique eigenvalue of A in some interval $]\alpha, \beta[$¿ Suppose in addition that $\eta = \langle \psi \mid A\psi \rangle$ belongs to the interval $]\alpha, \beta[$ and assusme that $\epsilon^2 = ||(A - \eta)\psi||^2 \leq (\beta - \eta)(\eta - \alpha)$. Then show that :

$$\eta - \frac{\epsilon^2}{\beta - \eta} \leq \lambda \leq \eta + \frac{\epsilon^2}{\beta - \eta} \ .$$

As a preliminary result, show that $(A - \alpha)(A - \lambda)$ and $(A - \beta)(A - \lambda)$ are positive operators. Then apply the inequalities with ψ.

Exercise 16.2.3. .
Let $A(x_1, x_2) = (A_1(x_1, x_2)\ , \ A_2(x_1, x_2))$ be a C^∞ vector field on $\mathbb{R}^2$. Let V be a C^∞ positive function on $\mathbb{R}^2$.
Let $P := (D_{x_1} - A_1(x_1, x_2))^2 + (D_{x_2} - A_2(x_1, x_2))^2 + V(x)$ the differential operator defined on $C_0^\infty(\mathbb{R}^2)$.
a) Show that P admits a selfadjoint extension in $L^2(\mathbb{R}^2)$.
b) Show that P is essentially selfadjoint.

Exercise 16.2.4. .
We admit the results of Exercise 16.2.3. Show that the selfadjoint extension in $L^2(\mathbb{R}^2)$ of

$$T := -(\frac{d}{dx_1} - ix_2 x_1^2)^2 - \frac{d^2}{dx_2^2} + x_2^2 \ ,$$

is with compact resolvent.

Exercise 16.2.5. .
Let V be a C^∞ positive potential in $\mathbb{R}^2$. Let us consider, with $B \in \mathbb{R} \setminus \{0\}$, the operator
$$P = D_{x_1}^2 + (D_{x_2} + B\, x_1)^2 + V(x)\ .$$
a) Recall briefly the spectrum of its selfadjoint extension in the case $V = 0$.
b) We assume that V tends to 0 as $|x| \to +\infty$. Determine the essential spectrum of $\bar{P}$.

Exercise 16.2.6. .
Let K be a kernel in $\mathcal{S}(\mathbb{R}^2)$ which is strictly positive and symmetric.
a) Show that the associated operator $\mathcal{K}$ which is defined on $\mathcal{S}(\mathbb{R})$ by
$$(\mathcal{K}u)(x) = \int_{\mathbb{R}} K(x,y) u(y) dy\ ,$$
can be extended as a compact operator on $L^2(\mathbb{R})$. b) Let I be an open interval in $\mathbb{R}$ and let us denote by $\mathcal{K}_I$ the operator on $L^2(I)$ defined by
$$(\mathcal{K}_I u)(x) = \int_I K(x,y) u(y) dy\ .$$
Let λ_I^1 be the largest eigenvalue of $\mathcal{K}_I$. Show that
$$\lambda_I^1 \leq \lambda_{\mathbb{R}}^1\ .$$
Show that we have strict inequality when I is not $\mathbb{R}$.
c) Let u^1 be a normalized eigenfunction of $\mathcal{K}$ associated with $\lambda_{\mathbb{R}}^1$. Using its restriction to I, show the inequality :
$$\lambda_{\mathbb{R}}^1 \leq \lambda_I^1\, (1 - ||u^1||_{L^2(I^C)})^{-1}\ .$$
d) Let $I_n = [-n, n]$. Show that $\lambda_{I_n}^1$ converges rapidly to $\lambda_{\mathbb{R}}^1$ as $n \to +\infty$. More precisely, show that, for all $j \in \mathbb{N}$, there exists a constant C_j such that :
$$|\lambda_{\mathbb{R}}^1 - \lambda_{I_n}^1| \leq C_j\, n^{-j}\ ,\ \forall n \in \mathbb{N}^*\ .$$

Exercise 16.2.7. .
Let us consider in $\Omega =]0,1[\times \mathbb{R}$, a positive C^∞ function V and let S_0 be the Schrödinger operator $S_0 = -\Delta + V$ defined on $C_0^\infty(\Omega)$.
(a) Show that S_0 admits a selfadjoint extension on $L^2(\Omega)$. Let S this extension.
(b) Determine if S is with compact resolvent in the following cases :

1. $V(x) = 0$,
2. $V(x) = x_1^2 + x_2^2$,
3. $V(x) = x_1^2$,
4. $V(x) = x_2^2$

5. $V(x) = (x_1 - x_2)^2$.

Determiner the spectrum in the cases (1) and (4). One can first determine the spectrum of the Dirichlet realization (or of Neumann) of $-d^2/dx^2$ on $]0,1[$.

Exercise 16.2.8. .
We consider in $\mathbb{R}^2$ the operator defined on $\mathcal{S}(\mathbb{R}^2;\mathbb{C}^2)$ by

$$\mathcal{D}_0 = \alpha_1 D_{x_1} + \alpha_2 D_{x_2} + \alpha_3 \, .$$

Here the matrices α_j are hermitian 2×2 matrices such that :

$$\alpha_i\alpha_j + \alpha_j\alpha_i = 2\delta_{ij} \, ,$$

and we recall that $D_{x_j} = \frac{1}{i}\frac{\partial}{\partial_{x_j}}$ for $j = 1, 2$.

a) Is $\mathcal{D}_0$ symmetric? semi-bounded ? It is suggested to use the Fourier transform.

b) Compute $\mathcal{D}_0^2$.

c) Show that $\mathcal{D}_0$ admits a selfadjoint extension $\mathcal{D}_1$ in $L^2(\mathbb{R}^2;\mathbb{C}^2)$, and determine its domain.

d) Determine the spectrum of $\mathcal{D}_1$.

e) We suppose that, for all $x \in \mathbb{R}^2$, $V(x)$ is a 2×2 hermitian matrix, with bounded C^∞ coefficients. Show that $\mathcal{D}_V = \mathcal{D}_0 + V$ admits a selfadjoint extension and determine its domain.

Exercise 16.2.9. .
Let H_a be the Dirichlet realization of $-d^2/dx^2 + x^2$ in $]-a,+a[$. Show that the lowest eigenvalue $\lambda_1(a)$ of H_a is strictly positive, monotonically decreasing as $a \to +\infty$ and tend exponentially fast to 1 as $a \to +\infty$. Give an estimate as fine as possible of $|\lambda_1(a) - 1|$.

Exercise 16.2.10. .
We consider on $C_0^\infty(\mathbb{R}^2)$, the operator

$$P_0 := (D_{x_1} - x_2)^2 + (D_{x_2} - x_1)^2 \, .$$

We recall that $D_{x_j} = \frac{1}{i}\partial_{x_j}$.

Show that its natural selfadjoint extension P is unitary equivalent to the operator $-\Delta$ (of domain H^2). Determine its spectrum and its essential spectrum.

Exercise 16.2.11. .
Show that one can associate to the differential operator on $C_0^\infty(\mathbb{R}\times]0,1[)$:

$$T_0 := (D_{x_1} - x_2 x_1^2)^2 + (D_{x_2})^2 \, ,$$

an unbounded selfadjoint operator T on $L^2(\mathbb{R}\times]0,1[)$ whose spectrum is with compact resolvent.

Exercise 16.2.12. .
Let ϕ be a C^2- function on $I\!R^m$ such that $|\nabla\phi(x)| \to +\infty$ as $|x| \to +\infty$ and with uniformly bounded second derivatives. Let us consider the differential operator on $C_0^\infty(I\!R^2)$ $-\Delta + 2\nabla\phi \cdot \nabla$. We consider this operator as an unbounded operator on $\mathcal{H} = L^2(I\!R^m, \exp -2\phi\ dx)$. Show that it admits a selfadjoint extension and that its spectrum is discrete.
We assume in addition that : $\int_{I\!R^m} \exp -2\phi dx < +\infty$. Show that its lowest eigenvalue is simple and determine a corresponding eigenvector.

Exercise 16.2.13. .
We consider in $I\!R^3$ the differential operator $S_0 := -\Delta - \frac{1}{r}$, a priori defined on $C_0^\infty(I\!R^3)$.
a) Show that the operator admits a selfadjoint extension S.
b) Show the continuous injection of $H^2(I\!R^3)$ into the space of the Hölder functions $C^s(I\!R^3)$, with $s \in]0, \frac{1}{2}[$, and the compact injection for all compact K of $C^s(K)$ into $C^0(K)$.
c) Determine the essential spectrum of S. One possibility is to start with the analysis of $S_\chi = -\Delta - \frac{\chi}{r}$ where χ is C^∞ with compact support.
d) Show using the minimax-principle that S has at least one eigenvalue. One can try to minimize over a $u \mapsto < S_0 u\ ,\ u\rangle/||u||^2$ with $u(x) = \exp -ar$.
e) Determine this lowest eigenvalue (using the property that the groundstate should be radial).

Exercise 16.2.14. .
a) Let g be a continuous function on $I\!R$ such that $g(0) = 0$. Analyze the convergence of the sequence $(g(t)u_n(t))_{n\geq 1}$ in $L^2(I\!R)$ where $u_n(t) = \sqrt{n}\chi(nt)$ and χ is a C^∞ function with compact support.
b) let $f \in C^0([0,1]; I\!R)$. Let T_f be the multiplication operator by f defined on $L^2(]0,1[)$: $u \mapsto T_f u = fu$.
Determine the spectrum of T_f. Discuss in function of f the possible existence of eigenvalues. Determine the essential spectrum of T_f.

Exercise 16.2.15. .
Discuss in function of $\alpha \geq 0$ the possibility of associating to the differential operator define on $C_0^\infty(I\!R^3)$

$$-\Delta - r^{-\alpha}$$

a selfadjoint operator on $L^2(I\!R^3)$.

Exercise 16.2.16. .
Let Ω be a non empty open subset in $I\!R^d$ and let us consider the multiplication operator on $L^2(I\!R^d)$ defined by the multiplication by χ_Ω where χ_Ω is equal to 1 in Ω and 0 outside. Determine the spectrum, the essential spectrum, the discrete spectrum.

Exercise 16.2.17. .
Show that the spectrum in $I\!R^2$ of $P = D_x^2 + x^2 + D_y^2$ is $[1, +\infty[$.

Exercise 16.2.18. .
Let $V \in \mathcal{S}(\mathbb{R}^d)$ be positive and let us consider the operator :

$$T := (-\Delta + 1)^{-\frac{1}{2}} V (-\Delta + 1)^{-\frac{1}{2}} \,.$$

a) Explain how to define $(-\Delta+1)^{-\frac{1}{2}}$, as an operator on $L^2(\mathbb{R}^d)$.
b) Show that T is a bounded, selfadjoint, positive, compact operator on $L^2(\mathbb{R}^d)$.
c) Discuss the injectivity in function of V ?
d) Establish a link with the research of pairs (u, μ) in $H^2(\mathbb{R}^d) \times \mathbb{R}^+$ such that :

$$(-\Delta + 1 - \mu V) u = 0 \,.$$

Exercise 16.2.19. .
Let $\delta \in \mathbb{R}$.
(a) Show that the operator P_δ defined on $C_0^\infty(\mathbb{R}^2)$ by

$$P_\delta := D_x^2 + D_y^2 + x^2 y^4 + x^4 y^2 + \delta(x+y)$$

is semibounded.
One can first show the inequality :

$$\langle P_0 u \,,\ u \rangle \geq ||xu||^2 + ||yu||^2 \,.$$

(b) Show that there exists a natural selfadjoint extension of P_δ.
(c) What is the corresponding form domain ?
(d) Show that the selfadjoint extension is with compact resolvent.

Exercise 16.2.20. .
Let us consider in $\mathbb{R}^+$, the Neumann realization in $\mathbb{R}^+$ of $P_0(\xi) := D_t^2 + (t-\xi)^2$, where ξ is a parameter in $\mathbb{R}$. We would like to find an uppr bound for $\Theta_0 = \inf_\xi \mu(\xi)$ where $\mu(\xi)$ is the smallest eigenvalue of $P_0(\xi)$. Following the physicist Kittel, one can proceed by minimizing $\langle P_0(\xi)\phi(\cdot;\rho) \mid \phi(\cdot;\rho)\rangle$ over the normalized functions $\phi(t;\rho) := c_\rho \exp -\rho t^2$ ($\rho > 0$). For which value of ξ is this quantity minimal ?? Deduce the inequality :

$$\Theta_0 < \sqrt{1 - \frac{2}{\pi}} \,.$$

16.3 Problems

Problem 16.3.1. .
Let us consider in the disk of $\mathbb{R}^2$ $\Omega := D(0,R)$ the Dirichlet realization of the Schrödinger operator

$$S(h) := -\Delta + \frac{1}{h^2} V(x) \,, \tag{16.3.1}$$

where V is a C^∞ potential on $\bar{\Omega}$ satisfying :

$$V(x) \geq 0 \,. \tag{16.3.2}$$

Here $h > 0$ is a parameter.

a) Show that this operator is with compact resolvent.

b) Let $\lambda_1(h)$ be the lowest eigenvalue of $S(h)$. We would like to analyze the behavior of $\lambda_1(h)$ as $h \to 0$. Show that $h \to \lambda_1(h)$ is monotonically increasing.

c) Let us assume that $V > 0$ on $\bar{\Omega}$; show that there exists $\epsilon > 0$ such that

$$h^2 \lambda_1(h) \geq \epsilon \,. \tag{16.3.3}$$

d) We assume now that $V = 0$ in an open set ω in Ω. Show that there exists a constant $C > 0$ such that, for any $h > 0$,

$$\lambda_1(h) \leq C \,. \tag{16.3.4}$$

One can use the study of the Dirichlet realization of $-\Delta$ in ω.

e) Let us assume that :

$$V > 0 \textit{ almost everywhere in } \Omega \,. \tag{16.3.5}$$

Show that, under this assumption :

$$\lim_{h \to 0} \lambda_1(h) = +\infty \,. \tag{16.3.6}$$

One could proceed by contradiction supposing that there exists C such that

$$\lambda_1(h) \leq C \,,\ \forall h \textit{ such that } 1 \geq h > 0 \,. \tag{16.3.7}$$

and establishing the following properties.

- *For $h > 0$, let us denote by $x \mapsto u_1(h)(x)$ an L^2-normalized eigenfunction associted with $\lambda_1(h)$. Show that the family $u_1(h)$ $(0 < h \leq 1)$ is bounded in $H^1(\Omega)$.*
- *Show the existence of a sequence h_n $(n \in I\!N)$ tending to 0 as $n \to +\infty$ and $u_\infty \in L^2(\Omega)$ such that*

  $$\lim_{n \to +\infty} u_1(h_n) = u_\infty$$

  in $L^2(\Omega)$.
- *Deduce that :*

  $$\int_\Omega V(x)\, u_\infty(x)^2 \, dx = 0 \,.$$

- *Deduce that $u_\infty = 0$ and make explicite the contradiction.*

f) Let us assume that $V(0) = 0$; show that there exists a constant C, such that :

$$\lambda_1(h) \leq \frac{C}{h} \,.$$

g) Let us assume that $V(x) = \mathcal{O}(|x|^4)$ près de 0. Show that in this case :

$$\lambda_1(h) \leq \frac{C}{h^{\frac{2}{3}}} .$$

h) We assume that $V(x) \sim |x|^2$ near 0; discuss if one can hope a lower bound in the form

$$\lambda_1(h) \geq \frac{1}{C\,h} .$$

Justify the answer by illustrating the arguments by examples and counterexamples.

Problem 16.3.2. .
We consider on $\mathbb{R}$ and for $\epsilon \in I := [-\frac{1}{4}, +\infty[$ the operator $H_\epsilon = -d^2/dx^2 + x^2 + \epsilon|x|$.
a) Determine the form domain of H_ϵ and show that it is independent of ϵ.
b) What is the nature of the spectrum of the associated selfadjoint operator?
c) Let $\lambda_1(\epsilon)$ the smallest eigenvalue. Give rough estimates permitting to estimate from above or below $\lambda_1(\epsilon)$ independently of ϵ on every compact interval of I.
d) Show that, for any compact sub-interval J of I, there exists a constant C_J such that, for all $\epsilon \in J$, any L^2-normalized eigenfunction u_ϵ of H_ϵ associated with $\lambda_1(\epsilon)$ satisfies :

$$||u_\epsilon||_{B^1(\mathbb{R})} \leq C_J .$$

For this, on can play with : $\langle H_\epsilon u_\epsilon, u_\epsilon\rangle_{L^2(\mathbb{R})}$.
e) Show that the lowest eigenvalue is a monotonically increasing sequence of $\epsilon \in I$.
f) Show that the lowest eigenvalue is a locally Lipschitzian function of $\epsilon \in I$. On utilisera de nouveau le principe du max-min.
g) Show that $\lambda(\epsilon) \to +\infty$, as $\epsilon \to +\infty$ and estimate the asymptotic behavior.
h) Discuss the same questions for the case $H_\epsilon = -d^2/dx^2 + x^2 + \epsilon x^4$ (with $\epsilon \geq 0$).

Problem 16.3.3. .
The aim of this problem is to analyze the spectrum $\Sigma^D(P)$ of the Dirichlet realization of the operator $P := (D_{x_1} - \frac{1}{2}x_2)^2 + (D_{x_2} + \frac{1}{2}x_1)^2$ in $\mathbb{R}^+ \times \mathbb{R}$.

1. *Show that one can a priori compare the infimum of the spectrum of P in $\mathbb{R}^2$ and the infimum of $\Sigma^D(P)$.*
2. *Compare $\Sigma^D(P)$ with the spectrum $\Sigma^D(Q)$ of the Dirichlet realization of $Q := D_{y_1}^2 + (y_1 - y_2)^2$ in $\mathbb{R}^+ \times \mathbb{R}$.*
3. *We first consider the following family of Dirichlet problems associated with the family of differential operators : $\alpha \mapsto H(\alpha)$ defined on $]0, +\infty[$ by :*

   $$H(\alpha) = D_t^2 + (t - \alpha)^2 .$$

   Compare with the Dirichlet realization of the harmonic oscillator in $]-\alpha, +\infty[$.

4. Show that the lowest eigenvalue $\lambda(\alpha)$ of $H(\alpha)$ is a monotonic function of $\alpha \in I\!R$.
5. Show that $\alpha \mapsto \lambda(\alpha)$ is a continuous function on $I\!R$.
6. Analyze the limit of $\lambda(\alpha)$ as $\alpha \to -\infty$.
7. Analyze the limit of $\lambda(\alpha)$ as $\alpha \to +\infty$.
8. Compute $\lambda(0)$. For this, one can compare the spectrum of $H(0)$ with the spectrum of the harmonic oscillator restricted to the odd functions.
9. Let $t \mapsto u(t;\alpha)$ the positive L^2-normalized eigenfunction associated with $\lambda(\alpha)$. Let us admit that this is the restriction to $I\!R^+$ of a function in $\mathcal{S}(I\!R)$. Let, for $\alpha \in I\!R$, T_α be the distribution in $\mathcal{D}'(I\!R^+ \times I\!R)$ défined by

$$\phi \mapsto T_\alpha(\phi) = \int_0^{+\infty} \phi(y_1, \alpha) u_\alpha(y_1) dy_1 \; .$$

Compute QT_α.

10. By constructing starting from T_α a suitable sequence of L^2-functions tending to T_α, show that $\lambda(\alpha) \in \Sigma^D(Q)$.
11. Determine $\Sigma^D(P)$.

Problem 16.3.4. .
Let H_a be the Dirichlet realization of $-d^2/dx^2 + x^2$ in $]-a, +a[$.
(a) Briefly recall the results concerning the case $a = +\infty$.
(b) Show that the lowest eigenvalue $\lambda_1(a)$ of H_a is decreasing for $a \in]0, +\infty[$ and larger than 1.
(c) Show that $\lambda_1(a)$ tends exponentially fast to 1 as $a \to +\infty$. One can use a suitable construction of approximate eigenvectors.
(d) What is the behavior of $\lambda_1(a)$ as $a \to 0$. One can use the change of variable $x = ay$ and analyze the limit $\lim_{a\to 0} a^2 \lambda_1(a)$.
(e) Let $\mu_1(a)$ be the smallest eigenvalue of the Neumann realization in $]-a, +a[$. Show that $\mu_1(a) \leq \lambda_1(a)$.
(f) Show that, if u_a is a normalized eigenfunction associated with $\mu_1(a)$, then there exists a constant C such that, for all $a \geq 1$, we have :

$$||xu_a||_{L^2(]-a,+a[)} \leq C \; .$$

(g) Show that, for u in $C^2([-a, +a])$ and χ in $C_0^2(]-a, +a[)$, we have :

$$-\int_{-a}^{+a} \chi^2 u''(t) u(t) dt = \int_{-a}^{+a} |(\chi u)'(t)|^2 dt - \int_{-a}^{+a} \chi'(t)^2 u(t)^2 dt \; .$$

(h) Using this identity with $u = u_a$, a suitable χ which should be equal to 1 on $[-a+1, a-1]$, the estimate obtained in (f) and the minimax principle, show that there exists C such that, for $a \geq 1$, we have :

$$\lambda_1(a) \leq \mu_1(a) + Ca^{-2} \; .$$

Deduce the limit of $\mu_1(a)$ as $a \to +\infty$.

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