Introduction to semi-classical methods for the Schrödinger operator with magnetic field

Bernard Helffer

Cours du CIMPA: Introduction to semi-classical methods for the Schrödinger operator with magnetic field

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May 12, 2004

Contents

1 Introduction

NOTES PROVISOIRES !! (les notes sront complétées et améliorées)
PROVISORY NOTES !! (some parts have to be improved and completed)

1.1 Projet du cours- main goals of the course

Décrire en 6-8 heures quelques aspects de la théorie semi-classique. On se concentre donc sur l'équation de Schrödinger de l'opérateur de Schrödinger avec champ magnétique et l'étude du bas de son spectre.
Our aim is to describe in 6-8 hours some aspects of the semi-classical theory. We focus on the Schrödinger operator with magnetic fields and the study of the bottom of its spectrum.

1.2 Prerequisites- Background

Le cours suppose connue la théorie spectrale élémentaire et l'auditeur est supposé avoir une bonne maîtrise de l'analyse hilbertienne, de la théorie des distributions (espaces de Sobolev) et une certaine connaissance des éléments de base de la géométrie différentielle (niveau maîtrise).
Pour la théorie spectrale, l'étudiant peut par exemple consulter le livre: Introduction à la théorie spectrale, par P. Lévy-Bruhl [LB], aux éditions Dunod. Il trouvera aussi de l'aide dans les notes de cours du DEA de B. Helffer (Année 2001-2002) accessible sur le web http://webmail.math.u-psud.fr/ helffer.
The student is supposed to have a good knowledge of the elementary spectral analysis, of the Hilbertian analysis and of the theory of distributions (Sobolev spaces). For the spectral theory, Reed-Simon is more than enough and the reader can also look at [LB] (in french) or to the notes of an unpublished course which is available on the web http://webmail.math.u-psud.fr/ helffer.

1.3 Bibliographie préliminaire-preliminary bibliography

Sur le sujet du cours lui-même, je donnerai en règle générale les détails mais les références et certains compléments peuvent être utilement retrouvés dans des chapitres de mon livre [Hel1] ou dans celui plus récent de Dimassi-Sjöstrand [DiSj]. D'autres références sont aussi les livres de :

Cycon-Froese-Kirsch-Simon [CFKS] orientés vers la théorie de Morse et Hislop-Sigal [HiSi]. Des résultats sur les opérateurs de Schrödinger avec champ magnétique apparaissent aussi dans les surveys de [Hel2, Hel3] et Mohamed-Raikov [MoRa], [Hel4] pour les relations avec la supraconductivité et dans le livre de B. Thaller [Tha]. Pour des développements semi-classiques plus récents, on peut aussi regarder [Hel1] et [Hel5]. D'autres aspects de l'analyse semi-classique sont présentés dans les livres de D. Robert [Ro], Kolokoltsov [Ko] (en liaison avec les travaux de Maslov) and A. Martinez (dans l'esprit de l'analyse microlocale) [Ma]. *Details will be given in general but more substantial references and complements can be found in the books [Hel1] and [DiSj]. Other referenes are the book [CFKS](Chapter 11, which is oriented towards Morse theory) and [HiSi]. When Schrödinger operators with magnetic fields are concerned, we should also mention the surveys by [Hel2, Hel3], Mohamed-Raikov [MoRa], [Hel4] for the relations with superconductivity and the book by B. Thaller [Tha]. Other aspects in Semi-classical analysis are presented in the books by D. Robert [Ro], Kolokoltsov [Ko] (in connection with results of the Maslov's school) and A. Martinez (in the spirit of the microlocal analysis) [Ma].*

1.4 Plan du cours-Organization of the course

Le plan est le suivant. Après quelques rappels généraux de théorie spectrale concernant les liens entre la construction de vecteurs propres approchés et la construction de vrais vecteurs propres (donnés en appendice), nous rappellerons les principales propriétés de notre principal sujet d'investigation: l'opérateur de Schrödinger avec champ magnétique (en régime semi-classique). Puis nous passerons en revue quelques apsects de l'analyse semi-classique: approximation harmonique, décroissance des fonctions propres dans différents contextes dont celui provenant de la supraconductivité. Comme application, nous finirons par la détermination du bas du spectre pour la réalisation de Neumann de l'opérateur de Schrödinger avec champ magnétique.
The course is organized as follows. After recalling some elements of perturbation theory concerning the links between approximate eigenvectors or eigenvalues and exact eigenvectors or eigenvalues, we will present the main properties of the Schrödinger operators with magnetic fields. We then give some elements in semi-classical analysis : harmonic approximation, WKB constructions and analysis of the decay of eigenfunctions. We will conclude by two applications to the splitting for the double well problem and to the

analysis of the bottom of the spectrum of the Neumann realization of the Schrödinger operator with magnetic fields in connection with the superconductivity.

2 On the Schrödinger with magnetic fields

2.1 Preliminaries

Let Ω be an open set in $\mathbb{R}^n$, $\vec{A} = (A_1, A_2, \dots, A_n)$ a $C^\infty(\overline{\Omega})$ vector field on $\overline{\Omega}$, corresponding to the so called magnetic potential, and V (which can depend on h) a $C^\infty(\overline{\Omega})$ real valued function, corresponding to the so called electric potential, and let $h > 0$ is a small parameter (playing the role of the Planck constant, or in other context of the inverse of the intensity of the magnetic field). The vector $\vec{A}$ corresponds more intrinsically to a 1-form

$$\omega_A = \sum_j A_j dx_j \ . \tag{2.1}$$

One can then associate to ω_A a 2-form called the magnetic field σ_B :

$$\sigma_B := d\omega_A = \sum_{j<k} B_{jk} dx_j \wedge dx_k \ . \tag{2.2}$$

When $n = 2$, the unique B_{12} defines a function, more simply denoted by $x \mapsto B(x)$, also called the magnetic field.
When $n = 3$, the magnetic field is identified to a magnetic vector $\vec{B}$, by the Hodge map :

$$\vec{B} = (B^1, B^2, B^3) = (B_{23}, B_{31}, B_{12}) \ . \tag{2.3}$$

All these objects can be defined more generally on a Riemannian manifold (with notions like Connections, Curvature, ...) but it is outside the aim of this short course.

We would like to discuss the spectrum of selfadjoint realizations of the Schrödinger operator in an open set Ω in $\mathbb{R}^n$:

$$P_{h,A,V,\Omega} = \sum_{j=1}^{n} (h\, D_{x_j} - A_j)^2 + V(x) \ .$$

2.2 Selfadjointness

Our main interest is the analysis of the bottom of the spectrum of $P_{h,A,V,\Omega}$ in an open set Ω. This open set can be bounded or the whole space $\mathbb{R}^n$. Many physically interesting situations correspond to $n = 2, 3$. In the case of an open set Ω, we can consider the Dirichlet realization or the Neumann condition (other conditions appear also in the applications).

The Dirichlet realization

The Dirichlet realization corresponds to take the so called Friedrichs extension attached to the quadratic form :

$$
\begin{aligned}
& C_0^\infty(\Omega;\mathbb{C}) \ni u \\
& \quad \mapsto Q^D_{h,A,V,\Omega}(u) := \int_\Omega \left(|\nabla_{h,A} u|^2 + V(x)|u(x)|^2\right)\, dx\ ,
\end{aligned}
\tag{2.4}
$$

whose existence follows immediately from the proof of the existence of a constant C such that :

$$
\int_\Omega \left(|\nabla_{h,A} u|^2 + V(x)|u(x)|^2\right)\, dx \geq -C||u||^2\ ,\ \forall u \in C_0^\infty(\Omega)\ , \tag{2.5}
$$

with

$$
\nabla_{h,A} = h\nabla - i\vec{A}\ .
$$

In this case, we say that the quadratic form is semibounded (from below). When Ω is regular (bounded), the form domain of the operator is

$$
\mathcal{V}^D(\Omega) = H^1_0(\Omega)\ ,
$$

and the domain of the operator, which is denoted by $P^D_{h,A,V}$, is

$$
D(P^D_{h,A,V}) = H^1_0(\Omega) \cap H^2(\Omega)\ .
$$

The Neumann realization

The Neumann realization corresponds to take the so called Friedrichs extension attached to the quadratic form :

$$
C^\infty(\overline{\Omega};\mathbb{C}) \ni u \mapsto Q^N_{h,A,V,\Omega}(u) := \int_\Omega \left(|\nabla_{h,A} u|^2 + V(x)|u(x)|^2\right)\, dx \text{(2.6)Span}
$$

whose existence follows immediately from the proof of the existence of a constant C such that :

$$
\int_\Omega \left(|\nabla_{h,A} u|^2 + V(x)|u(x)|^2\right)\, dx \geq -C||u||^2\ ,\ \forall u \in C^\infty(\overline{\Omega})\ . \tag{2.7}
$$

When Ω is regular (bounded), the form domain of the operator is

$$
\mathcal{V}^N(\Omega) = H^1(\Omega)\ , \tag{2.8}
$$

and the domain of the operator, which is denoted by $P^N_{h,A,V}$, is

$$D(P^N_{h,A,V}) = \{u \in H^2(\Omega) \mid \vec{n} \cdot (h\nabla - iA)u = 0 \;\text{ on } \partial\Omega\ \}. \tag{2.9}$$

Here $\vec{n}$ is the normal derivative to $\partial\Omega$, this condition :

$$\vec{n} \cdot (h\nabla - iA)u = 0 \;\text{ on } \partial\Omega\ , \tag{2.10}$$

is called the magnetic-Neumann boundary condition.

The case of $\mathbb{R}^n$

In the case of $\mathbb{R}^n$, it is more difficult to characterize the domain of the operator. When $V \geq -C$, it is easy to characterize the form domain which is

$$\mathcal{V}(\mathbb{R}^n) = \{u \in L^2(\mathbb{R}^n) \mid \nabla_{h,A} u \in L^2\ ,\ (V+C)^{\frac{1}{2}} u \in L^2\ \}\ . \tag{2.11}$$

In the general case, if the operator is semi-bounded on $C_0^\infty(\mathbb{R}^n)$ in the sense of (2.5), one can show (Simader) that the operator is essentially selfadjoint. This means that the Friedrichs extension is the unique selfadjoint extension in $L^2(\mathbb{R}^n)$ starting of $C_0^\infty(\mathbb{R}^n)$ and the domain $D(P_{h,A,V})$ satisfies in this case :

$$D(P_{h,A,V}) = \{u \in L^2\ ,\ P_{h,A,V} u \in L^2\}\ . \tag{2.12}$$

2.3 Spectral theory

All the operators introduced above are selfadjoint. In particular one can analyze their spectrum, defined as the complementary in $\mathbb{C}$ of the resolvent set $\rho(P)$ corresponding to the points $z \in \mathbb{C}$ such that $(P-z)^{-1}$ exists. The spectrum $\sigma(P)$ is a closed set contained in $\mathbb{R}$. The spectrum contains in particular the set of the eigenvalues of P. We recall that λ is an eigenvalue, if there exists a non zero vector $u \in D(P)$ such that $Pu = \lambda u$. The multiplicity of λ is the dimension of $\text{Ker}\ (P-\lambda)$. We call discrete spectrum $\sigma_d(P)$ the subset of the $\lambda \in \sigma(P)$ such that λ is an eigenvalue of finite multiplicity. Finally we call essential spectrum of P (denoted by $\sigma_{ess}(P)$ the closed set :

$$\sigma_{ess}(P) = \sigma(P) \setminus \sigma_d(P)\ . \tag{2.13}$$

In this course, we will be mainly interested in the analysis of the bottom of the spectrum of P as a function of the various parameters (mainly h). Depending on the assumptions, this bottom could corresponds to an eigenvalue of to the

botttom of the essential spectrum.
This bottom being determined by

$$\inf(\sigma(P_{h,A,V})) = \inf_{u\in\mathcal{V}} Q_{h,A,V}(u)\ , \tag{2.14}$$

it is enough, in order to determine if the bottom corresponds to an eigenvalue, to find a non trivial u in the form domain such that

$$Q_{h,A,V}(u) < \inf(\sigma_{ess}(P_{h,A,V})))||u||^2\ . \tag{2.15}$$

An easy case when this is satisfied is when $\sigma_{ess}(P_{h,A,V})) = \emptyset$, corresponding to the case when P is with compact resolvent. For verifying this last property, it is enough to show that the injection of $\mathcal{V}$ in L^2 is compact. This is in particular the case (for Dirichlet and Neumann) when Ω is regular and bounded. In the case, when Ω is unbounded, it is possible to determine the bottom of the essential spectrum using Persson's Lemma (see Appendix C).

2.4 Lieb-Thirring inequalities

In order to complete the picture, let us mention (confer [ReSi], p. 101) the following theorem due to Cwickel-Lieb-Rozenbljum :

Theorem 2.1 .
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

$$N_- \leq L_m \int_{V(x)\leq 0} (-V)^{\frac{m}{2}}\, dx\ . \tag{2.16}$$

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

$$L_m \int_{V\leq 0} (-V)^{\frac{m}{2}}\, dx < 1\ .$$

If $\lambda \leq \inf \sigma_{ess}(P)$, it is natural to count the number of eigenvalues strictly below λ :

$$N(\lambda) = \#\{\lambda_j < \lambda \mid \lambda_j \in \sigma(P)\}\ , \tag{2.17}$$

each eigenvalue being counted with multiplicity.
In this situation, it is useful to have either universal estimates (Cwickel-Lieb-Rozenblum) or semiclassical asymptotics (see Robert [Ro] or Ivrii [Iv]).

More generally, we are interested in controlling the more general moments (also called Riesz means) defined for $s \geq 0$ by

$$N^s(\lambda) = \sum_{\lambda_j < \lambda} (\lambda - \lambda_j)^s \, . \tag{2.18}$$

Theorem 2.2 *(see [LieTh])*
There exists a universal constant C, such that, if V satisfies $V_- \in L^{\frac{n}{2}+s}(\mathbb{R}^n)$ and $\frac{n}{2} + s > 1$, then the eigenvalues of $P = -h^2\Delta + V$ satisfy

$$\sum_{\lambda_j < 0} (-\lambda_j)^s \leq C \int_{V<0} (-V)^{\frac{n}{2}+s} dx \, . \tag{2.19}$$

The same is true with magnetic field.

This inequality (for $s = 1$) has played an important role in the analysis of the stability of the matter in physics.

2.5 Diamagnetism

By Kato's inequality (cf for example [CFKS]), which says that, for all $u \in H^1_{loc}$, for all j,

$$|\partial_j |u|| \leq |(\partial_j - iA_j)u| \, , \; a.e. \, , \tag{2.20}$$

it can be shown that the effect of the magnetic field is to increase the bottom of the spectrum (in the case when $\inf \sigma(P_{A=0}) < \inf \sigma_{ess}(P_{A=0})$). We recall that this inequality gives, for any real potential V, the comparison :

$$\inf \text{ Sp } \left(P^D_{h,A,\Omega} + V\right) \geq \inf \text{ Sp } \left(-h^2 \Delta^D_\Omega + V\right) \, , \tag{2.21}$$

and that a similar result is true in the case of Neumann :

$$\inf \text{ Sp } \left(P^N_{h,A,\Omega} + V\right) \geq \inf \text{ Sp } \left(-h^2 \Delta^N_\Omega + V\right) \, , \tag{2.22}$$

This inequality admits a kind of converse, showing its optimality (Lavine-O'Caroll-Helffer) (see [Hel1])

Proposition 2.3
Let λ_A be the ground state of $P_A(h)$, then $\lambda_A = \lambda_{A=0}$ if and only if $B = 0$ (when Ω is simply connected).

When Ω is not simply connected, the condition $B = 0$ is NOT sufficient and one should add a quantization condition[1] on the circulation of $\vec{A}$ along any closed path.

2.6 Very rough estimates for the Dirichlet realization

When $n = 2$, it is immediate to show the inequality

$$\langle P_{h,A,\Omega} u \mid u \rangle \geq h \int_\Omega B(x)|u(x)|^2 dx \ , \ \forall u \in C_0^\infty(\Omega) \ . \tag{2.23}$$

This leads for the Dirichlet realization and when $B(x) \geq 0$, to the trivial estimate :

$$\inf \sigma(P^D_{h,A}) \geq h \inf_{x \in \overline{\Omega}} B(x) := hb \ . \tag{2.24}$$

Note that the converse is asymptotically true. In a system of coordinates, where $x = 0$ denotes a minimum of B which is assumed to be inside Ω, and in a gauge where $\vec{A}(x_1, x_2) = \frac{1}{2} b(x_2, -x_1) + \mathcal{O}(|x|^2)$, we consider the quasimode

$$u(x; h) := ch^{-\frac{1}{2}} \exp -\rho\sqrt{b}\frac{|x|^2}{h}\chi(x) \ ,$$

where χ is a cutoff function equal to 1 in a neighborhood of 0. The optimal ρ is computed by minimizing over ρ the energy corresponding to the constant magnetic field b :

$$\left(\int (|(\partial_{y_1} + i\frac{b}{2} y_2) u(y; 1)|^2 + |(\partial_{y_2} - i\frac{b}{2} y_1) u(y; 1)|^2 \ dy \right) / ||u(y, 1)||^2 \ .$$

One easily gets that this quantity is minimized for $\rho = \frac{1}{2}$ and that the corresponding energy is b.
The control of the remainders is easy, and we get :

$$\inf \sigma(P^D_{h,A}) \leq hb + \mathcal{O}(h^{\frac{3}{2}}) \ . \tag{2.25}$$

So we have proved[2] (in the 2-dimensional case) :

[1] This circulation divided by 2π should be an integer.
[2] We leave to the reader the proof for when the minimum of $|B(x)|$ is attained at the boundary. This affects only the remainder term.

Theorem 2.4 .
Under assumption (8.1), the smallest eigenvalue $\lambda^{(1)}(h)$ of the Dirichlet realization $P^D_{h,A,\Omega}$ of $P_{h,A,\Omega}$ satisfies :

$$\frac{\lambda^{(1)}(h)}{h} = b + o(1)\ . \tag{2.26}$$

Let us define the theorem in the more general case. Let us extend at each point B_{jk} as an antisymmetric matrix (more intrinsically, this is the matrix of the two-form σ_B). The the eigenvalues of iB are real and one can see that if λ is a matrix of iB, with corresponding eigenvector u, then $\bar{u}$ is an eigenvector relative to the eigenvalue $-\lambda$. If the λ_j denote the eigenvalues of iB counted with multiplicity, then one can then define

$$\mathrm{Tr}^{\,+} B(x) = \sum_{\lambda_j>0} \lambda_j(x)\ . \tag{2.27}$$

The extension of the previous result is then

Theorem 2.5 .
Under assumption (8.1), the smallest eigenvalue $\lambda^{(1)}(h)$ of the Dirichlet realization $P^D_{h,A,\Omega}$ of $P_{h,A,\Omega}$ satisfies :

$$\frac{\lambda^{(1)}(h)}{h} = \inf_{x\in\Omega}\ \mathrm{Tr}_{\,+}(B(x)) + o(1)\ . \tag{2.28}$$

The idea is to first treat the constant case, and then to make a partition of unity. For the constant case, after a change variable, we will get, for $n = 2d$, the model

$$\sum_{j=1}^{d} [-(\partial_j)^2 - (\partial_{j+d} + ib_j)^2]\ ,$$

and for $n = 2d + 1$, the model

$$-\partial^2_{2d+1} + \sum_{j=1}^{d} [-(\partial_j)^2 - (\partial_{j+d} + ib_j)^2]\ ,$$

with

$$\sum_j |b_j| = \ \mathrm{Tr}^{\,+} B\ .$$

2.7 Magnetic bottles

This problematic was introduced by Avron-Herbst-Simon [AHS] and then discussed by Colin de Verdière and Helffer-Mohamed (see later Kondratiev-Mazya-Shubin and references therein). The question was to analyze the question of compact resolvent when there is no magnetic electric field. In the case of dimension 2 the previous trivial inequality (2.23) shows that in the case of $\Omega = \mathbb{R}^2$ and if $B(x) \to +\infty$ as $|x| \to +\infty$, then the Schrödinger magnetic operator is with compact resolvent. This is indeed an easy exercise to show that its form domain has compact injection in L^2. The 2-dimensional case is too particular for guessing the right result in the general case. We just mention the following result of [HelMo1]. Let us introduce

$$m_k(x) = \sum_{|\alpha|=k,j,\ell} |D_x^\alpha B_{j\ell}|$$

Theorem 2.6
Suppose $\Omega = \mathbb{R}^n$ that there exists $r \geq 0$ such that :

$$\sum_{k\leq r} m_k(x) \to +\infty \ , \ m_{r+1} \leq C m_r \ .$$

Then $-\Delta_A$ is with compact resolvent.

This theorem is based on an iterated Bracket argument inspired by Kohn's proof of the hypoellipticity of the Hörmander's operators (see [HelNi] for discussions on recent evolutions of the subject).

2.8 Other rough lower bounds.

Let us start the analysis of the question with very rough estimates. In the case of Dirichlet, $n = 2$, and if $B(x) \neq 0$ (say for example $B(x) > 0$), we can use (2.23) which gives a comparison between selfadjoint operators in the form (for any $\rho \in [0, 1]$)

$$P_{h,A}^D \geq \rho(P_{h,A}^D) + (1-\rho)hB(x) \ . \tag{2.29}$$

The lower bound is now a new Schrödinger operator, which has this time an "effective" electric potential $(1-\rho)hB$. In order to find a lower bound for the smallest eigenvalue of the Dirichlet realization, it is enough to apply for a suitable ρ a rough lower bound for the operator :

$$\rho(P^D_{h,A}) + (1-\rho)hB(x)\ .$$

We shall show as quite preliminary result the following proposition, which improves Theorem 2.4 :

Proposition 2.7 .
Under the condition that $x \mapsto B(x)$ is ≥ 0, non constant and analytic, then there exists $\theta \in]0, \frac{1}{2}]$ and $C > 0$ such that :

$$\lambda^{(1)}(h) - bh \geq \frac{1}{C} h^{\frac{1}{\theta}}\ , \tag{2.30}$$

where $b = \inf |B(x)|$.

Proof :
Using the Lieb-Thirring bounds for the Schrödinger operator $-\epsilon\Delta + V$ (see above and [BeHeVe]) with $\epsilon = \rho h$ and $V(x) = \frac{1}{2}(B(x) - b)$, we start from the property, that there exists $\theta \in]0, \frac{1}{2}]$ and C such that, $\forall \rho \in]0, \frac{1}{2}]$,

$$\lambda^{(1)}(h) - (1-\rho)hb \geq \frac{1}{C}(\rho h^2)(\rho h)^{-\theta}\ .$$

This can be rewritten in the form :

$$\lambda^{(1)}(h) - hb \geq \frac{1}{C}\rho^{1-\theta}h^{2-\theta} - b\rho h\ ,$$

or

$$\lambda^{(1)}(h) - hb \geq \rho^{1-\theta} h \left(\frac{1}{C} h^{1-\theta} - b\rho^{\theta}\right)\ .$$

If we take $\rho = \gamma h^{\frac{1-\theta}{\theta}}$ and γb small enough, we get (2.30) for h small enough.

Remark 2.8 .
The optimality of this inequality will be discussed later in particular cases. In particular, we will discuss the case when $B(x) = b$ and the case when $B(x) - b$ has a non degenerate minimum.

Remark 2.9 .
When $b = 0$, we can take $\rho = \frac{1}{2}$, and get, for some $\theta > 0$:

$$\lambda^{(1)}(h) \geq \frac{1}{C} h^{2-\theta}\ .$$

Results in [HelMo3], [Mon], [Ue2] or [LuPa1] show that it is optimal.

3 Models with constant magnetic field in dimension 2

Before to analyze the general situation and the possible differences between the Dirichlet problem and the Neumann problem, it is useful– and it is actually a part of the proof for the general case– to analyze what is going on with models.

3.1 Preliminaries.

Let us consider in a regular domain Ω in $\mathbb{R}^2$ the Neumann realization (or the Dirichlet realization) of the operator $P_{h,bA_0,\Omega}$ with

$$A_0(x_1, x_2) = (\frac{1}{2}x_2, -\frac{1}{2}x_1) \ . \tag{3.1}$$

Note that the Neumann realization is the natural condition considered in superconductivity. We will assume $b > 0$ and we observe that the problem has a strong scaling invariance :

$$P_{h,bA_0} = h^2 P_{1,bA_0/h} \ . \tag{3.2}$$

As a consequence, the semi-classical analysis (b fixed) is equivalent to the analysis strong magnetic field (h being fixed). If the domain is invariant by dilation, one can reduce the analysis to $h = b = 1$. Let us denote by $\mu^{(1)}(h, b, \Omega)$ and by $\lambda^{(1)}(h, b, \Omega)$ the bottom of the spectrum of the Neumann and Dirichlet realizations of P_{h,bA_0} in Ω. Depending on Ω, this can correspond to an eigenvalue (if Ω is bounded) or to a point in the essential spectrum (for example if $\Omega = \mathbb{R}^2$ or if $\Omega = \mathbb{R}^2_+$). The analysis of basic examples will be crucial for the general study of the problem.

3.2 An important model

Let us begin with the analysis of 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 simpl. 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 $\xi \mapsto \mu(\xi)$ is a continuous function. It is a little more work (admitted (see Kato [Ka]) to show that the function is C^∞. 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 $\inf_{\xi \in \mathbb{R}} \inf \mathrm{Sp}\ (H^{N,\xi})$ 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 (Bolley-Dauge-Helffer)

$$\mu'(\xi) = -[\mu(\xi) - \xi^2]\varphi_\xi(0)^2 \ . \tag{3.3}$$

To get (3.3), we observe that, if $\tau > 0$, then

$$\begin{aligned} 0 &= \int_{\mathbb{R}_+} [D_t^2 \varphi_\xi(t) + (t-\xi)^2 \varphi_\xi(t) - \mu(\xi)\varphi_\xi(t)] \varphi_{\xi+\tau}(t+\tau) dt \\ &= -\varphi_\xi(0)\varphi'_{\xi+\tau}(\tau) + (\mu(\xi+\tau) - \mu(\xi)) \int_{\mathbb{R}_+} \varphi_\xi(t)\varphi_{\xi+\tau}(t+\tau)\, dt \ . \end{aligned}$$

We then take the limit $\tau \to 0$ to get the formula.

From (3.3), it comes that, for any critical point ξ_c of μ in $\mathbb{R}^+$

$$\mu''(\xi_c) = 2\xi_c \varphi_{\xi_c}^2(0) > 0 \; . \tag{3.4}$$

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 $\Theta_0 < 1$

$$\Theta_0 = \inf_\xi \mu(\xi) = \mu(\xi_0) \; , \tag{3.5}$$

and is then increasing monotonically and tending to 1 at $+\infty$. Moreover

$$\Theta_0 = \xi_0^2 \; . \tag{3.6}$$

Finally, it is easy to see that $\varphi_\xi(x)$ decays exponentially at ∞.

Let us give 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]) that we can "freely" differentiate with respect to ξ.

Let us start[3] from :

$$H^N(\xi)\varphi(\cdot;\xi) = \mu(\xi)\varphi(\cdot;\xi) \; . \tag{3.7}$$

Differentiating with respect to ξ, we obtain :

$$(\partial_\xi H^N(\xi) - \mu'(\xi))\varphi(\cdot;\xi) + (H^N(\xi) - \mu(\xi))(\partial_\xi \varphi)(\cdot;\xi) = 0 \; . \tag{3.8}$$

Taking the scalar product with φ_ξ in $L^2(\mathbb{R}^+)$, we obtain the socalled Feynman-Heilmann Formula

$$\mu'(\xi) = \langle(\partial_\xi H^N(\xi)\varphi_\xi \mid \varphi_\xi\rangle = -2\int_0^{+\infty} (t-\xi)|\varphi_\xi(t)|^2 dt \; . \tag{3.9}$$

Taking the scalar product with $\partial_\xi\varphi)(\cdot;\xi)$, we obtain the identity :

$$\begin{aligned} &\langle(\partial_\xi H^N(\xi) - \mu'(\xi))\varphi(\cdot;\xi) \mid (\partial_\xi\varphi)(\cdot;\xi)\rangle \\ &\quad + \langle(H^N(\xi)\varphi(\cdot;\xi) - \mu(\xi))(\partial_\xi\varphi)(\cdot;\xi) \mid (\partial_\xi\varphi)(\cdot;\xi)\rangle = 0 \; . \end{aligned} \tag{3.10}$$

[3] We change a little the notations for $H^{N,\xi}$ (this becomes $H^N(\xi)$) and φ_ξ (this becomes $\varphi(\cdot;\xi)$) in order to have an easier way for the differentiation.

In particular, we obtain for $\xi = \xi_0$ that :

$$\begin{aligned} &\langle (\partial_\xi H^N(\xi_0)\varphi(\cdot;\xi_0) \mid \partial_\xi \varphi)(\cdot;\xi_0)\rangle \\ &\quad + \langle (H^N(\xi)\varphi(\cdot;\xi_0) - \mu(\xi_0))(\partial_\xi\varphi)(\cdot;\xi_0) \mid (\partial_\xi\varphi)(\cdot;\xi_0)\rangle = 0\ . \end{aligned} \tag{3.11}$$

We observe that the second term is positive (and with some extra work coming back to (3.8) strictly positive) :

$$\langle (\partial_\xi H^N(\xi_0))\varphi(\cdot;\xi_0) \mid \partial_\xi\varphi)(\cdot;\xi_0)\rangle < 0\ . \tag{3.12}$$

Let us differentiate one more (3.8) with respect to ξ.

$$\begin{aligned} &2(\partial_\xi H^N(\xi) - \mu'(\xi))\partial_\xi\varphi(\cdot;\xi) \\ &+(H^N(\xi) - \mu(\xi))(\partial_\xi^2\varphi)(\cdot;\xi) \\ &+(\partial_\xi^2 H^N(\xi) - \mu''(\xi))\varphi(\cdot;\xi) = 0\ . \end{aligned} \tag{3.13}$$

Taking the scalar product with φ_ξ and $\xi = \xi_0$, we obtain

$$\mu''(\xi_0) = 2 + \langle (\partial_\xi H^N(\xi_0)\varphi(\cdot;\xi_0) \mid \partial_\xi\varphi)(\cdot;\xi_0)\rangle < 2\ . \tag{3.14}$$

Proposition 3.1 *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 φ_{ξ_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 :

$$
\begin{aligned}
E_0 &= ((H^N(\xi_0)-\mu(\xi_0))_{|\varphi_{\xi_0}^{\perp}})^{-1} && (3.15)\\
E_0^+ &= \varphi_{\xi_0} && (3.16)\\
E_0^- &= \varphi_{\xi_0}^* && (3.17)\\
E_0^{+-} &= 0. && (3.18)
\end{aligned}
$$

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 :

$$
M(\xi,\mu)^{-1}=\sum_{j\in\mathbb{N}}(-1)^j\left(R_0\begin{pmatrix} (H(\xi)-H(\xi_0))-(\mu-\mu(\xi_0)) & 0 \\ 0 & 0 \end{pmatrix}\right)^j R_0. \tag{3.19}
$$

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 3.2
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 3.2 :
It is clear that

$$T(\xi,\mu) = \left(R_0 \begin{pmatrix} (H(\xi) - H(\xi_0)) - (\mu - \mu(\xi_0)) & 0 \\ 0 & 0 \end{pmatrix} \right) \tag{3.20}$$

is C^∞. Let us also observe that :

$$M(\xi,\mu)^{-1} = \sum_{j\in\mathbb{N}} (-1)^j T^j(\xi,\mu) R_0. \tag{3.21}$$

Consider

$$r(\xi,\mu) = (H(\xi) - H(\xi_0)) - (\mu - \mu(\xi_0)) \,.$$

The derivatives of $r(\xi,\mu)$ are given by :

$$\begin{array}{rcl} \partial_\xi r(\xi,\mu) & = & \partial_\xi H(\xi) = -2(t-\xi) \\ \partial_\mu r(\xi,\mu) & = & -1. \end{array} \tag{3.22}$$

In view of (3.21), we will estimate $T(\xi,\mu)^j$:

$$\begin{array}{rl} \left(R_0 \begin{pmatrix} r(\xi,\mu) & 0 \\ 0 & 0 \end{pmatrix} \right)^j & = \left(\begin{pmatrix} E_0 & \varphi_{\xi_0} \\ \varphi^*_{\xi_0} & 0 \end{pmatrix} \begin{pmatrix} r(\xi,\mu) & 0 \\ 0 & 0 \end{pmatrix} \right)^j \\ & = \begin{pmatrix} (E_0 r(\xi,\mu))^j & 0 \\ (\varphi^*_{\xi_0} r(\xi,\mu))(E_0 r(\xi,\mu))^{j-1} & 0 \end{pmatrix}. \end{array} \tag{3.23}$$

So

$$M(\xi,\mu)^{-1} = \textstyle\sum_{j\in\mathbb{N}} (-1)^j \begin{pmatrix} (E_0 r(\xi,\mu))^j & 0 \\ (\varphi^*_{\xi_0} r(\xi,\mu))(E_0 r(\xi,\mu))^{j-1} & 0 \end{pmatrix} R_0. \tag{3.24}$$

It is then easy to show the C^∞ property.

Lemma 3.3
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 Lemma 3.3 :
Again this is simple linear algebra. Expressing that $R(\xi,\mu)$ is the inverse of

$M(\xi,\mu)$ gives :

$$\begin{aligned}
E(\xi,\mu)(H(\xi)-\mu)+E^{+}(\xi,\mu)\varphi_{\xi_0}^{*} &= \mathrm{Id} && (3.25)\\
E^{-}(\xi,\mu)\varphi_{\xi_0} &= 1 && (3.26)\\
E(\xi,\mu)\varphi_{\xi_0} &= 0 && (3.27)\\
E^{-}(\xi,\mu)(H(\xi)-\mu)+E^{+-}(\xi,\mu)\varphi_{\xi_0}^{*} &= 0 && (3.28)\\
(H(\xi)-\mu)E(\xi,\mu)+\varphi_{\xi_0}E^{-}(\xi,\mu) &= \mathrm{Id} && (3.29)\\
\varphi_{\xi_0}^{*}E^{+}_{\xi,\mu} &= 1 && (3.30)\\
(H(\xi)-\mu)E^{+}(\xi,\mu)+\varphi_{\xi_0}E^{+-}(\xi,\mu) &= 0 && (3.31)\\
\varphi_{\xi_0}^{*}E(\xi,\mu) &= 0. && (3.32)
\end{aligned}$$

Taking the composition of $E^{+}(\xi,\mu)$ with (3.28) 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

$$E^{+}(\xi,\mu)\varphi_{\xi_0}^{*}=-\frac{E^{+}(\xi,\mu)E^{-}(\xi,\mu)(H(\xi)-\mu)}{E^{+-}(\xi,\mu)}. \tag{3.33}$$

This quantity (3.33) is well defined if $E^{+-}_{\xi,\mu}\neq 0$. So using (3.25) et(3.33) we get,

$$(H(\xi)-\mu)^{-1}=E(\xi,\mu)-\frac{E^{+}(\xi,\mu)E^{-}(\xi,\mu)}{E^{+-}(\xi,\mu)}. \tag{3.34}$$

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 (3.31), $E^{+}(\xi,\mu)$ 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 continuity it is also true for $E^{+}(\xi,\mu)$.

Step 3 : Analysis of the equation $E^{+-}(\xi,\mu)=0$.
We have just to apply the implicit function theorem in the neighborhood of $(\xi_0,\mu(\xi_0)$. But by elementary computations, we have

$$E^{+-}(\xi,\mu)=\sum_{j\geq 1}(-1)^{j}(\varphi_{\xi_0}^{*}r_{\xi,\mu})(E_0 r(\xi,\mu))^{j-1}\varphi_{\xi_0}. \tag{3.35}$$

The derivatives at $(\xi_0, \mu(\xi_0))$ are easily computed as :

$$\begin{aligned} \partial_\xi E(\xi,\mu)^{+-}(\xi_0,\mu(\xi_0)) &= -\varphi_{\xi_0}^* \partial_\xi r(\xi_0,\mu(\xi_0))\varphi_{\xi_0} & (3.36)\\ &= 2\int_{\mathbb{R}^+} (t-\xi_0)\varphi_{\xi_0}^2(t)\; dt & (3.37)\\ (\partial_\mu E)(\xi,\mu)^{+-}(\xi,\mu(\xi_0)) &= -1. & (3.38)\end{aligned}$$

In particular $(\partial_\mu E)(\xi,\mu)^{+-}(\xi_0,\mu(\xi_0)) \neq 0$ and the implicit function theorem leads to

Lemma 3.4
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 $\tilde\mu(\xi) = \mu(\xi)$.

3.3 The case of $\mathbb{R}^2$

We would like to analyze the spectrum of :

$$S_B := (D_{x_1} - \frac{B}{2}x_2)^2 + (D_{x_2} + \frac{B}{2}x_1)^2 \; . \tag{3.39}$$

We first look at the selfadjoint realization in $\mathbb{R}^2$. 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

$$U_1 f = \exp iB\frac{x_1x_2}{2} f \; . \tag{3.40}$$

It satisfies

$$S_B U_1 f = U_1 S_B^1 f \; , \; \forall f \in \mathcal{S}(\mathbb{R}^2) \; , \tag{3.41}$$

with

$$S_B^1 := (D_{x_1})^2 + (D_{x_2} + Bx_1)^2 \; . \tag{3.42}$$

Remark 3.5 .
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

$$U_2 = \mathcal{F}_{x_2 \mapsto \xi_2} \,, \tag{3.43}$$

and get by conjugation, on $L^2(\mathbb{R}^2_{x_1,\xi_2})$,

$$S_B^2 := (D_{x_1})^2 + (\xi_2 + Bx_1)^2 \,. \tag{3.44}$$

We now introduce a third unitary transform U_3

$$(U_3 f)(y_1, \xi_2) = f(x_1, \xi_2) \,, \ \text{ with } y_1 = x_1 + \frac{\xi_2}{B} \,, \tag{3.45}$$

and we obtain the operator

$$S_B^3 := D_y^2 + B^2 y^2 \,, \tag{3.46}$$

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.

3.4 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 (3.44). Then we can use the preliminary study in dimension 1. The bottom of the spectrum is effectively given by :

$$\inf \sigma(S_B^{N,\mathbb{R}^{2,+}}) = |B| \inf \mu(\xi) = \Theta_0 |B| \, . \tag{3.47}$$

Similarly, for the Dirichlet realization, we find (See Problem E.14, for details) :

$$\inf \sigma(S_B^{D,\mathbb{R}^{2,+}}) = |B| \inf \lambda(\xi) = |B| \, . \tag{3.48}$$

3.5 The case of the corner

After preliminary results devoted to the case $\Omega = \mathbb{R}_+ \times \mathbb{R}_+$ and obtained by [Ja] and [Pan1], a more systematic analysis have been performed by V. Bonnaillie in [Bon]. Let us mention her main results. We consider the Neumann realization of the Schrödinger operator with $h = 1$, $b = 1$ in a sector $\Omega_\alpha : \{(x_1, x_2) \in \mathbb{R}^2 \mid |x_2| \leq \operatorname{tg} \frac{\alpha}{2} x_1\}$. One can first show, using Persson's Theorem (see for example [Ag]) that the bottom of the essential spectrum is equal to Θ_0. So the question is to know if there exists an eigenvalue below the essential spectrum. One result obtained in [Bon] is that :

$$\lim_{\alpha \to 0} \frac{\mu^{corn}(\alpha)}{\alpha} = \frac{1}{\sqrt{3}} \, . \tag{3.49}$$

Computing the energy of the quasimode u_α (following an idea of Bonnaillie-Fournais [Bon])

$$\Omega_\alpha \ni (x, y) = (\rho \cos \phi, \rho \sin \phi) \mapsto u_\alpha(x, y) := c \exp i \frac{\rho^2 \beta^2 \phi}{2} \exp - \frac{\beta \rho^2}{4} \, ,$$

with $\beta = \frac{\alpha}{\sqrt{3+\alpha^2}}$ and c such that the L^2-norm in the sector is 1, one has the universal estimate

$$\mu^{corn}(\alpha) \leq \frac{\alpha}{\sqrt{3 + \alpha^2}} \, , \tag{3.50}$$

which gives (3.49) above (the lower bound is more difficult). This also answers to the question about the existence of an eigenvalue below Θ_0 under the condition that

$$\frac{\alpha}{\sqrt{3 + \alpha^2}} < \Theta_0 \, .$$

3.6 The case of the disk.

The case of Dirichlet was considered by L. Erdös in connexion with an isoperimetric inequality [Er]. By using the techniques of [BoHe], one can then show [HelMo3] the following proposition which is a small improvment of his result

Proposition 3.6 .
As $R\sqrt{b}$ large, the following asymptotics holds :

$$\lambda^{(1)}(b, D(0,R)) - b \sim 2^{\frac{3}{2}}\pi^{-\frac{1}{2}}b^{\frac{3}{2}}R\exp(-\frac{bR^2}{2}) . \tag{3.51}$$

The Neumann case is treated in the paper by Baumann-Phillips-Tang [BaPhTa] (Theorem 6.1, p. 24) (see also [PiFeSt]) who prove the

Proposition 3.7

$$\mu^{(1)}(b, D(0,R)) = \Theta_0 b - 2M_3\,\frac{1}{R}\,b^{\frac{1}{2}} + \mathcal{O}(1) . \tag{3.52}$$

Here we recall that Θ_0 was introduced in 3.5, and that $M_3 > 0$ is a universal constant.

Remark 3.8
Another interesting case is the exterior of the disk. One first observes that the bottom of the essential spectrum is b and one can show that as b is large, there exists at least one eigenvalue below b. One shows also in [HelMo3] that the above formula for the smallest eigenvalue is still valid by replacing $\frac{1}{R}$ par $-\frac{1}{R}$. This permits to verify that it is indeed the algebraic value of the curvature which appears for all the models.

4 Harmonic approximation

In this section we discuss one of the basic technics for analyzing the ground-state energy (also called lowest eigenvalue or principal eigenvalue) of a Schrödinger operator in the case the electric potential V has non degenerate minima.

4.1 Upper bounds

4.1.1 The case of the one dimensional Schrödinger operator

We start with the simplest one-well problem:

$$S_v^h := -h^2 d^2/dx^2 + v(x) \ , \tag{4.1}$$

where v is a C^∞- function tending to ∞ and admitting a unique minimum at 0 with $v(0) = 0$.
Let us assume that

$$v''(0) > 0 \ . \tag{4.2}$$

In this very simple case, the harmonic approximation is an elementary exercise. We first consider the harmonic oscillator attached to 0 :

$$-h^2 d^2/dx^2 + \frac{1}{2} v''(0) x^2 \ . \tag{4.3}$$

This means that we replace the potential v by its quadratic approximation at 0 $\frac{1}{2}v''(0)x^2$ and consider the associated Schrödinger operator.
Using the dilation $x = h^{\frac{1}{2}} y$, we observe that this operator is unitarily equivalent to

$$h \left[-d^2/dy^2 + \frac{1}{2} v''(0) y^2 \right] \ . \tag{4.4}$$

Consequently, the eigenvalues are given by

$$\lambda_n(h) = h \cdot \lambda_n(1) = (2n+1) h \cdot \sqrt{\frac{v''(0)}{2}} \ , \tag{4.5}$$

and the corresponding eigenfunctions are

$$u_n^h(x) = h^{-\frac{1}{4}} u_n^1 (\frac{x}{h^{\frac{1}{2}}}) \tag{4.6}$$

with [4]

$$u_n^1(y) = P_n(y) \exp -\sqrt{\frac{v''(0)}{2}} \frac{y^2}{2} \ . \tag{4.7}$$

We are just looking for simplicity at the first eigenvalue. We consider the function $u_1^{h,app.}$

$$x \mapsto \chi(x) u_1^h(x) = c \cdot \chi(x) h^{-\frac{1}{4}} \exp -\sqrt{\frac{v''(0)}{2}} \frac{x^2}{2h} \ ,$$

where χ is compactly supported in a small neighborhood of 0 and equal to 1 in a smaller neighborhood of 0. We now get

$$(S_v^h - h \cdot \sqrt{\frac{v''(0)}{2}}) u_1^{h,app.} = \mathcal{O}(h^{\frac{3}{2}}) \ .$$

The coefficients corresponding to the commutation of S_v^h and χ give exponentially small terms and the main contribution is

$$||(v(x) - \frac{1}{2} v''(0) x^2) \chi(x) u_1^h(x)||_{L^2}$$

which is easily seen as $\mathcal{O}(h^{\frac{3}{2}})$. Then the spectral theorem gives the existence for S_v^h of an eigenvalue $\lambda(h)$ such that

$$|\lambda(h) - h \cdot \sqrt{\frac{v''(0)}{2}}| \leq C \cdot h^{\frac{3}{2}}$$

In particular, we get the inequality

$$\lambda_1(h) \leq h \cdot \sqrt{\frac{v''(0)}{2}} + C\, h^{\frac{3}{2}} \ . \tag{4.8}$$

Combining with other techniques, one can actually prove that

$$|\lambda_1(h) - h \cdot \sqrt{\frac{v''(0)}{2}}| \leq C \cdot h^{\frac{3}{2}} \tag{4.9}$$

[4] We normalize by assuming that the L^2-norm of u_n^h is one. For the first eigenvalue, we have seen that, by assuming in addition that the function is strictly positive, we determine completely $u_1^h(x)$.

4.1.2 Harmonic approximation in general: upper bounds

In the multidimensional case, we can proceed essentially in the same way. The analysis of the quadratic case

$$H(hD_x, x) := -h^2\Delta + \frac{1}{2}\langle Ax \mid x\rangle$$

can be done explicitly by diagonalyzing A via an orthogonal matrix U. There is a corresponding unitary transformation on $L^2(\mathbb{R}^n)$ defined by

$$(\mathcal{U}f)(x) = f(U^{-1}x)\ ,$$

such that

$$\mathcal{U}^{-1}H\mathcal{U} = \sum_j \left(-(h\partial_{y_j})^2 + \frac{1}{2}\lambda_j y_j^2\right)\ .$$

Using the Hermite functions as quasimodes we get the upper bounds.

4.1.3 Case with multiple minima

When there are more than one minimum, one can apply the above construction near each of the minima. The upper bound for the ground state is obtained by taking the infimum over all the minima of the upper bound attached to each minimum.

4.2 Harmonic approximation in general: lower bounds

Here we follow Simon's approach (See also [CFKS]) (another approach is described in [Hel1] and another variant in [DiSj]). The reader is sent to Chapter 11 of CFKS.

Given a covering by balls of radius R and a corresponding partition of unity, such that :

$$\begin{array}{l} \sum_j (\phi_j^R)^2 = 1\ , \\ \sum_j |D_x^\alpha \phi_j^R|^2 \leq \frac{C}{R^2}\ , \end{array} \tag{4.10}$$

we can write that, $\forall u \in C_0^\infty$,

$$\begin{array}{ll} \langle P_V(h)u\ ,\ u\rangle & = \sum_j \langle P_V(h)\phi_j^R u\ ,\ \phi_j^R u\rangle - h^2 \sum_{j,\ell} |||D_{x_\ell}\phi_j^R|u||^2 \\ & \geq \sum_j \langle P_V(h)\phi_j^R u\ ,\ \phi_j^R u\rangle - C\frac{h^2}{R^2}||u||^2\ . \end{array} \tag{4.11}$$

We can in addition assume that either the balls are centered at the minima of V, or that the ball are at a distance of $\frac{C}{R}$ of these minima.

In the first case, we observe that :

$$|\langle P_V(h)\phi_j^R u \ , \ \phi_j^R u\rangle - \langle P_V^0(h)\phi_j^R u \ , \ \phi_j^R u\rangle \leq CR^3||\phi_j^R u||^2$$

In the second case, using the fact that the minimas of V are non degenerate, we get :

$$|\langle P_V(h)\phi_j^R u \ , \ \phi_j^R u\rangle \geq \frac{R^2}{C}||\phi_j^R u||^2$$

The optimization between the two errors leads to the choice of

$$\frac{h^2}{R^2} = R^3 \ ,$$

that is $R = h^{\frac{2}{5}}$, and we then observe that $\frac{R^2}{C} = \frac{h^{\frac{4}{5}}}{C} >> h$. We then get the lower bound

$$\lambda_1(h) \geq \inf V + h(\inf \mu_1(h, x_\ell)) - Ch^{\frac{6}{5}} \ , \tag{4.12}$$

where the infimum is over the various minima x_ℓ (assumed to be non degenerate) and $\mu_1(h, x_\ell)$ denotes the lowest eigenvalue of the harmonic approximation at x_ℓ.
Note that in the case of a Manifold there is another term which leads to a small change in the argument (see Simon [Si]). The Laplacian has indeed the form $\sum_{ij} g^{-\frac{1}{2}}\partial_{x_i} g g^{ij}\partial_{x_j} g^{-\frac{1}{2}}$ after a change of function in order to come back to the selfadjoint case.

4.3 The case with magnetic field

Let us consider two situations.

4.3.1 V has a non degenerate minimum.

The first case is the case when V has a non degenerate minimum at 0. In this case the model which gives the approximation is

$$\sum_j (hD_{x_j} - A_j^0)^2 + \frac{1}{2}\langle V''(0)x \mid x\rangle \ ,$$

where A^0_j is a linear magnetic potential attached to the constant magnetic field $B_{jk} = B_{jk}(0)$ so that in a suitable gauge is such that $A(x) - A^0(x) = \mathcal{O}(|x|^2)$.

After the dilation $x = h^{\frac{1}{2}} y$, we get

$$h \left(\sum_j (D_{y_j} - A^0_j)^2 + \frac{1}{2} \langle V''(0) y \mid y \rangle \right) ,$$

whose spectrum can be determined explicitely (see [Mat]). One then get easily the upper bound.

The lower bound is obtained similarly once we have observed that

$$\mathrm{Re}\, \langle P_{A,V}(h) u \ , \ u \rangle = \sum_j \langle P_{A,V(}h) \phi^R_j u \ , \ \phi^R_j u \rangle - h^2 \sum_{j,\ell} |||D_{x_\ell} \phi^R_j |u||^2 \ . \quad (4.13)$$

4.3.2 Magnetic wells

We will be interested in the special case when $B(z) \in C^{3+M}(\overline{\Omega})$ satisfies, for some $z_0 \in \Omega$:

$$B(z) > b := B(z_0) > 0, \ \forall \ z \in \overline{\Omega} \setminus \{z_0\}, \quad (4.14)$$

and we assume that the minimum is non degenerate :

$$\mathrm{Hess}\, B(z_0) > 0 \ . \quad (4.15)$$

We introduce in this case the notation :

$$a = \mathrm{Tr} \left(\frac{1}{2} \mathrm{Hess}\, B(z_0) \right)^{1/2} \ . \quad (4.16)$$

Theorem 4.1 .
If $A \in C^{4+M}(\overline{\Omega}; \mathbb{R}^2)$, with $M \geq 0$, and if the hypotheses (4.14) and (4.15) are satisfied, then there exists a constant $C > 0$ such that

$$\mu(h) \sim [b + \frac{a^2}{2b} h] h + o(h^2) \ . \quad (4.17)$$

The proof can be found in [HelMo4]. It is based on the analysis of the simpler model where near 0

$$B(z) = b + \alpha x^2 + \beta y^2. \tag{4.18}$$

In this case, we can also choose a gauge $A(z)$ such that

$$A_1(z) = 0 \text{ and } A_2(z) = bx + \frac{\alpha}{3} x^3 + \beta x y^2 \,. \tag{4.19}$$

When the assumptions are not satisfied, and that B vanishes. Other models should be consider. An interesting case is the case when B vanishes along a line. This model was proposed by Montgomery. We will discuss a toy model of this type when presenting the Grushin's method.

4.4 Higher order expansion

After a dilation $x = \sqrt{h}$, we can look at

$$-\Delta_y + \frac{1}{h} V_0(\sqrt{h} y) + V_1(\sqrt{h} y) \,,$$

that we can rewrite by formal expansions :

$$\sum_j h^{\frac{j}{2}} H_j(y, D_y) \,.$$

We can then find a complete expansion by recursion.

Another idea will be to introduce a Grushin problem. This will be explained in the next section.

5 Grushin's problem- alias Feschbach method

This method (as initiated by Grushin and Sjöstrand in this context) is also called the Feschbach's projection method (and is analogous in bifurcation theory)(see also Combes-Duclos-Seiler and Martinez in the context of the Born-Oppenheimer approximation...). We have already seen how to use it in the analysis of the model on $\mathbb{R}^+$. We will present various possible applications.

5.1 High order harmonic approximations

Starting from our operator $-h^2\Delta + V(x)$ with V a C^∞ positive potential admitting a minimum at 0 such that $V(0) = V'(0) = 0$, we use the dilation

$$x = h^{\frac{1}{2}} y \,, \tag{5.1}$$

and get by Taylor expanding V at 0, the operator $hH(h)$, with

$$H(h) = -\Delta_y + \frac{1}{2}\langle V''(0)y \mid y\rangle + \sum_{j\geq 3} h^{\frac{j}{2}} T_j(y) \,, \tag{5.2}$$

where $T_j(y)$ is an homogeneous polynomial of order j. We note also that T_j is odd (resp. even) with respect to the map $y \mapsto -y$ if j is odd (resp. even). We denote by μ_0 the lowest eigenvalue of

$$H_0 := -\Delta_y + \frac{1}{2}\langle V''(0)y \mid y\rangle \,, \tag{5.3}$$

and by ψ_0 the (unique) corresponding eigenvector such that $\psi_0 > 0$, $||\psi_0|| = 1$.

The starting point is to consider the (unbounded) operator on $L^2(\mathbb{R}^n)\times\mathbb{R}$ denoted by :

$$\mathcal{P}_0 = \begin{pmatrix} P_0 & R_0^+ \\ R_0^- & 0 \end{pmatrix} \,, \tag{5.4}$$

where

$$\begin{array}{l} P_0 := H_0 - \mu_0 \,, \\ (R_0^+ z)(y) = z\psi_0(y) \,, \\ (R_0^- f) = \int f(y)\psi_0(y)dy \,. \end{array} \tag{5.5}$$

We observe that $\mathcal{P}_0 = \mathcal{P}_0^*$ (formally) and in particular we have

$$R_0^- = (R_0^+)^* \,.$$

We also verify that :

$$R_0^- R_0^+ = I \ , \ R_0^+ R_0^- = \Pi_0 \ , \tag{5.6}$$

where Π_0 is the projector on the space $\{\mathbb{R}\psi_0\}$:

$$(\Pi_0 f)(y) = (\int f(y)\psi_0(y)dy)\psi_0(y) \ . \tag{5.7}$$

The first point to observe at this stage is that this operator $\mathcal{P}_0$ is inversible with explicit inverse given by

$$\mathcal{E}_0 = \begin{pmatrix} E_0 & R_0^+ \\ R_0^- & 0 \end{pmatrix} \ , \tag{5.8}$$

where

$$E_0 := (I - \Pi_0)(P_0)^{-1}(I - \Pi_0) \ . \tag{5.9}$$

Our idea is to now consider the more general operator $\mathcal{P}(z)$:

$$\mathcal{P}(z) = \begin{pmatrix} (P - z) & R_0^+ \\ R_0^- & 0 \end{pmatrix} \ , \tag{5.10}$$

P being considered in a weak sense as a perturbation of P_0 :

$$P = P_0 + \sum_{j \geq \frac{1}{2}} T_j = P_0 + \delta P \ , \tag{5.11}$$

and z being small enough. Note that $\delta P(h)$ will gain at least $h^{\frac{1}{2}}$ in formal expansions.

So the first simple idea is that at least formally $\mathcal{P}(z)$ would be right invertible (like $\mathcal{P}_0$) and that $\mathcal{E}_0$ is an approximate inverse.

Before to verify in which sense this can be true, let us recall (formally) why it is interesting to have the inverse of $\mathcal{P}(z)$ for any small z in $\mathbb{C}$. Writing $\mathcal{E}(z)$

$$\mathcal{E}(z) = \begin{pmatrix} E(z) & E^+(z) \\ E^-(z) & E^\pm(z) \end{pmatrix} \ , \tag{5.12}$$

The main "standard result" is that $(P - z)$ is invertible (resp. left or right invertible) if $E^\pm(z)$ is invertible (resp. left or right invertible). This is immediately seen by starting of :

$$\mathcal{P}(z) \circ \mathcal{E}(z) = I \ ,$$

which in particular reads

$$
\begin{array}{l}
(P-z)E(z)+R_0^+E^-(z)=I\ ,\\
(P-z)E^+(z)+R_0^+E^\pm(z)=0\ ,\\
R_0^-E(z)=0\ ,\\
R_0^-E^+=I\ .
\end{array}
\tag{5.13}
$$

We shall use this in the following form :
If $(z(h),\phi(x;h))$ is a pair such that $E^\pm(z)\phi(x,h)=0$ (or is very small in L^2) then the pair $(z,\psi(t,x;h)$, where $\psi(t,x;h):=E_+(z)\phi(x,h))$, gives an (approximate) eigenvector of P associated to the (approximate) eigenvalue z.
Very formally, if $E^\pm$ has a right inverse, then $(P-z)$ has a left inversse given by :

$$
(P-z)^{-1}=E(z)-E^+(z)(E^\pm(z))^{-1}E^-(z)\ . \tag{5.14}
$$

So it is important to determine perturbatively $E^\pm(z)$.

We first observe that

$$
\begin{pmatrix} (P-z) & R_0^+\\ R_0^- & 0\end{pmatrix}\begin{pmatrix} E_0 & R_0^+\\ R_0^- & 0\end{pmatrix}=I+\begin{pmatrix} (\delta P-z)E_0 & (\delta P-z)R_0^+\\ 0 & 0\end{pmatrix}=I+\mathcal{K}\ .
$$

For the right inverse, we have consequently :

$$
\mathcal{E}(z)=\mathcal{E}_0(z)\left(\sum_j(-1)^j\mathcal{K}^j\right)\ .
$$

Observing that

$$
\mathcal{K}^j=\begin{pmatrix} [(\delta P-z)E_0]^j & [(\delta P-z)E_0]^{j-1}[(\delta P-z)R_0^+]\\ 0 & 0\end{pmatrix}\ .
$$

In particular we get

$$
E^\pm(z)\sim\sum_{j=1}^{+\infty}(-1)^jR_0^-[(\delta P-z)E_0]^{j-1}[(\delta P-z)R_0^+]\ . \tag{5.15}
$$

At the level of the research of quasimodes, we will look for $z(h)$ in the form

$$
z(h)\sim\sum_{\ell\geq 1}z_\ell h^{\frac{\ell}{2}}\ , \tag{5.16}
$$

and the quasimode in the form

$$\phi(y,h) \sim \sum_\ell \phi_\ell(y) h^{\frac{\ell}{2}} \ , \tag{5.17}$$

in order to solve

$$E^\pm(z(h)) \sim 0 \ . \tag{5.18}$$

It remains to expand in powers of $h^{\frac{j}{2}}$.

Coefficient of $h^{\frac{1}{2}}$.
It is given by

$$E^\pm_{\frac{1}{2}}(z) = R_0^-(T_3 - z_1)R_0^+ \ .$$

Observing that $T_3\psi_0$ is orthogonal (by parity) to ψ_0, we get

$$E^\pm_{\frac{1}{2}}(z) = -z_1 \ . \tag{5.19}$$

So we get $z_1 = 0$.

Coefficient of h.
We have to visit the terms inside the terms corresponding to $j = 1$ and 2 in the expansion. This gives :

$$\begin{aligned} E_1^\pm(z) &= R_0^-(T_4 - z_2)R_0^+ + R_0^- T_3 E_0 T_3 R_0^+ \\ &= R_0^- T_4 R_0^+ + R_0^- T_3 E_0 T_3 R_0^+ - z_2 \ , \end{aligned} \tag{5.20}$$

and leads to the determination of z_2.

The recursion argument
We can continue by recursion. Using the parity of T_j, we observe that the odd powers of $z^{\frac{1}{2}}$ should vanish in order to get (5.18).

Let us by recursion verify the statement. We first start with the case $k = 2p$ even. For the coefficient, of $h^{\frac{k}{2}}$, we get

$$R_0^-[T_{k+2} - z_k]R_0^+ - P_k(z_2, \dots, z_{k-2}) = 0 \ .$$

This gives :

$$z_k = R_0^- T_{k+2} R_0^+ + P_k(z_2, \dots, z_{k-2}) \ .$$

When $k = 2p+1$, we obtain the same equation but using the imparity of the T_j, the fact that E_0 respects the parity, and the property of k, the equation reduced to

$$z_{2p+1} = 0 \ .$$

Note that this vanishing of the odd terms for the eigenvalues did not in general occur for the expnasion of the corresponding eigenvector (except if the potential is assumed to be even).

5.2 Grushin's approach for the construction of quasi-modes of the Montgomery's approach

We now look at another example called the Montgomery's example. This model corresponds to the case when the magnetic field vanishes on uniformly along a line (here $x_1 = 0$). The initial operator is

$$-h^2 D_{x_1}^2 + (hD_{x_2} - x_1^2(1+\gamma_1 x_2^2))^2 \ ,$$

with $\gamma_1 > 0$.
For this example the magnetic field $B(x_1,x_2) = 2x_1(1+\gamma_1 x_2^2)$ vanishes along the line $x_1 = 0$. But as observed in [KwPa] the variation of ∇B along the line creeates a localization at $x_1 = x_2 = 0$. This has some similarity with the example treated in [HelSj5] of a degenerate well :

$$h^2\Delta + (1+x_1^2)(1-(x_1^2+x_2^2))^2 \ .$$

For the analysis of the Montgomery's model, we introduce the dilation $x_1 = h^{\frac{1}{3}} t$, $x_2 = h^{\frac{1}{6}} x$ which after division by $h^{\frac{4}{3}}$ leads to the model :

$$H(h) := D_t^2 + (h^{\frac{1}{6}} D_s - t^2(1+\gamma_1 h^{\frac{1}{3}} x^2))^2 \ . \tag{5.21}$$

The starting point is to consider the (unbounded) operator on $L^2(\mathbb{R}^2)\times L^2(\mathbb{R})$ denoted by :

$$\mathcal{P}_0 = \begin{pmatrix} P_0 & R_0^+ \\ R_0^- & 0 \end{pmatrix} \ , \tag{5.22}$$

where

$$\begin{array}{l} P_0 := D_t^2 + (t^2-\xi_0)^2 - \mu_0 \ , \\ P_0\psi_0 = 0, \psi_0 > 0 \ , \ ||\psi_0||_{L^2(\mathbb{R})} = 1 \ , \\ (R_0^+\varphi)(t,x) = \psi_0(t)\varphi(x) \ , \\ (R_0^- f)(x) = \int f(t,x)\psi_0(t)dt \ . \end{array} \tag{5.23}$$

We observe that $\mathcal{P}_0 = \mathcal{P}_0^*$ (formally) and in particular we have

$$R_0^- = (R_0^+)^* \ .$$

We also verify that :

$$R_0^- R_0^+ = I_{L^2(\mathbb{R})} \ , \ R_0^+ R_0^- = \Pi_0 \ , \tag{5.24}$$

where Π_0 is the projector on the space $\{\mathbb{R}\psi_0\} \otimes L^2(\mathbb{R}_x)$:

$$(\Pi_0 f)(x,t) = (\int f(t,x)\psi_0(t)dt)\psi_0(t) \ . \tag{5.25}$$

The first point to observe at this stage is that this operator $\mathcal{P}_0$ is inversible with explicit inverse given by

$$\mathcal{E}_0 = \begin{pmatrix} E_0 & R_0^+ \\ R_0^- & 0 \end{pmatrix} \ , \tag{5.26}$$

where

$$E_0 := (I - \Pi_0)(D_t^2 + (t^2 - \xi_0)^2 - \mu_0)^{-1}(I - \Pi_0) \ . \tag{5.27}$$

Our idea is to now consider the more general operator $\mathcal{P}(z)$:

$$\mathcal{P}(z) = \begin{pmatrix} (P - z) & R_0^+ \\ R_0^- & 0 \end{pmatrix} \ , \tag{5.28}$$

with

$$P = P_0 + h^{\frac{1}{6}} P_1 + h^{\frac{1}{3}} P_2 + h^{\frac{1}{2}} P_3 + h^{\frac{2}{3}} P_4 = P_0 + \delta P \ , \tag{5.29}$$

and z being small enough. Note that $\delta P(h)$ will gain at least $h^{\frac{1}{6}}$ in formal expansions. Here

$$\begin{array}{ll} P_1 & = 2(\xi_0 - t^2) D_x \ , \\ P_2 & = D_x^2 - 2\gamma_1(\xi_0 - t^2) t^2 x^2 \ , \\ P_3 & = -\gamma_1 t^2 (D_x \cdot x^2 + x^2 \cdot D_x) \ , \\ P_4 & = t^4 x^4 \ . \end{array} \tag{5.30}$$

So the first simple idea is that at least formally $\mathcal{P}(z)$ would be right invertible (like $\mathcal{P}_0$) and that $\mathcal{E}_0$ is an approximate inverse.
Using formula (5.15), we proceed as before looking for an expansion in $z(h) \sim \sum_{j \geq 1} z_j h^{\frac{j}{6}}$. In this case, it remains to expand $\mathcal{E}(z)$ in powers of $h^{\frac{j}{6}}$.

Coefficient of $h^{\frac{1}{6}}$.
It is given by the operator

$$f \mapsto R_0^-(\xi_0 - t^2)\psi_0(t)D_x f(x) + z_1 f \ .$$

Observing that $(\xi_0 - t^2)\psi_0(t)$ is orthogonal to ψ_0 we get

$$E^{\pm}_{\frac{1}{6}}(z) = z_1 \ . \tag{5.31}$$

Coefficient of $h^{\frac{1}{3}}$.
We have to visit the terms inside the terms corresponding to $j = 1$ and 2 in the expansion.

This gives :

$$\begin{aligned} E^{\pm}_{\frac{1}{3}}(z) &= z_2 - R_0^- P_2 R_0^+ + R_0^- P_1 E_0 P_1 R_0^+ \\ &= z_2 - R_0^- D_x^2 R_0^+ + 2R_0^-(\xi_0 - t^2)\gamma_1 x^2 t^2 R_0^+ \\ &\quad +4R_0^-(\xi_0 - t^2)E_0(\xi_0 - t^2)R_0^+ D_x^2 \\ &= z_2 - \tfrac{1}{2}\hat{\nu}''(\rho_0)D_x^2 - 2\gamma_1 x^2 \ . \end{aligned} \tag{5.32}$$

This leads to the choice of z_2 as lowest eigenvalue of the harmonic oscillator $\frac{1}{2}\hat{\nu}''(\rho_0)D_x^2 + 2\gamma_1||(\xi_0 - t^2)\psi_0||^2 x^2$.

We leave the reader to verify that one can find the terms of the sequence z_j at any order.

6 WKB construction for the Schrödinger operator: formal approach

6.1 WKB construction

Let $V(x) = V_0(x) + hV_1(x)$ a potential. We are looking for a WKB solution of the form

$$u^{wkb}(x;h) = h^{-\frac{p}{4}} a(x,h) \exp -\phi_0(x)/h \ ,$$

for the Schrödinger equation

$$S_V = -h^2 \Delta + V(x;h) \ ,$$

in the neighborhood of a non degenerate minimum of the potential V_0 defined on $\mathbb{R}^p$. The potentials V_0 and V_1 are C^∞, defined in a neighborhood around the minimum of V_0 which is assumed to be at 0. We emphasize that we are looking for a real positive phase ϕ_0 and for an amplitude admitting an expansion

$$a(x,h) \sim \sum_{j=0}^{\infty} h^j \ a_j(x)$$

The research of a formal WKB solution corresponds to the simultaneous research of $a(x;h)$ and of $E(h) \sim \sum_{j=0}^{\infty} E_j \ h^j$ such that

$$\left(-h^2 \Delta + V(x;h) - E(h)\right) \left(a(\cdot,h) \exp -\phi_0(\cdot)/h\right) \sim 0$$

that is

$$(V_0 - |\nabla \phi_0|^2) a + 2h \, \nabla \phi_0 \cdot \nabla a - h \, \Delta a + h \, \Delta \phi_0 \, a + hV_1 a - E(h) a \sim 0 \ . \quad (6.1)$$

This leads first to

$$V_0(x) - |\nabla \phi_0(x)|^2 - E_0 = 0 \ . \quad (6.2)$$

This equation is called the eiconal equation. Assuming that a solution of this equation has been found, we then obtain a system of equations which we shall call transport equations

$$\begin{array}{lll}
(\mathrm{T}_1) & 2\nabla\phi_0(x)\cdot\nabla a_0 + (V_1 + \Delta\phi_0 - E_1)a_0 & = 0 \ , \\
(\mathrm{T}_2) & 2\nabla\phi_0(x)\cdot\nabla a_1 + (V_1 + \Delta\phi_0 - E_1)a_1 & = \Delta a_0 + E_2 a_0, \\
\cdot & & \\
\cdot & & \\
(\mathrm{T}_{k+1}) & 2\nabla\phi_0(x)\cdot\nabla a_k + (V_1 + \Delta\phi_0 - E_1)a_k & = \sum_{j=2}^{k} E_j \, a_{k+1-j} \\
 & \qquad + \Delta a_{k-1} \ + \ E_{k+1}\, a_0 \ . &
\end{array} \quad (6.3)$$

These equations have all the same structure. There is a real vector field X defined as

$$X = 2\nabla\phi_0 \cdot \nabla$$

which will vanish at 0 (and this determine $E_0 = 0 = \min V_0$), a function $g = (V_1 + \Delta\phi_0 - E_1)$ which has to vanish at 0 (and this will determine E_1, assuming that $a_0(0) = 1$) and a function f which will be either identically 0 (in the case of (T_1)) or which will be given by

$$f = \sum_{j=2}^{k} E_j a_{k+1-j} + \Delta a_{k-1} + E_{k+1} a_0 \ ,$$

and will vanish at 0 and this will determine E_{k+1}.
We have then to solve

$$Xu + gu = f$$

with $u(0) = 1$ in the case of (T_1) and with $u(0) = 0$ in the other cases.
We shall sketch later how to solve these equations in the general case. In order to meet the difficulties in successive steps, let us first consider the one dimensional case.

6.2 The case of dimension $p = 1$

Let us first rewrite the eiconal equation. We get in dimension 1

$$\phi_0'(t)^2 = V(t) \ .$$

We write $V(t)$ in the form

$$V(t) = t^2 b(t) \ ,$$

with $b(t) \neq 0$ in a sufficiently small neighborhood of 0.
This leads to the choice

$$\phi_0'(t) = t\sqrt{b(t)} \ , \ \phi_0(0) = 0 \ ,$$

which is the only one compatible with the constraints on ϕ_0. This gives explicitely

$$\phi_0(t) = \int_0^t s\sqrt{b(s)} ds \ ,$$

which is clearly well defined and C^∞ in a neighborhood of 0. We recall that we take $E_0 = \min V = 0$. Let us now look at the transport equation

$$2\phi_0'(t)a_0'(t) + (E_1 - \phi_0''(t))a_0(t) = 0\ ,$$

with the initial condition

$$a_0(0) = 1\ .$$

E_1 is determined by

$$E_1 = \phi_0''(0)\ .$$

We can solve explicitely this ordinary differential equation by observing that

$$(\ln a_0)' = -\frac{1}{2}\frac{(E_1 - \phi_0''(t))}{\phi_0'(t)}\ .$$

All the other equations have the same structure and can be solved using the variation of constants.

6.3 The general case

We explain the situation in the quadratic case

$$V_0(x) = \frac{1}{2}(\sum_j \lambda_j x_j^2)\ ,$$

and $V_1(x)$ general.

Determination of the phase.
The phase should satisfy

$$|\nabla\phi_0|^2 = V_0\ , \tag{6.4}$$

If we look for ϕ_0 has a quadratic form

$$\phi_0(x) = \frac{1}{2}\langle Ax\ ,\ x\rangle\ ,$$

we get the equation

$$A^2 = \frac{1}{2}\mathrm{Hess}\, V_0\ ,$$

and we can take A has the positive root of $\frac{1}{2}\text{Hess}\, V_0$, which was assumed to be strictly positive.

Note that without assuming that V_0 is quadratic, one gets at a critical point x_c of V_0 the following necessary relation (by differentiating two times the eiconal equation) for the solution ϕ_0 :

$$(\text{Hess}\, \phi_0(x_c))^2 = \frac{1}{2}\text{Hess}\, V_0(x_c)\ .$$

Solving formally (in powers of x^α) the transport equation.
For each transport equation, we expand the amplitudes as formal series at 0. We observe that :

$$\sum \mu_j x_j \partial_{x_j} x^\alpha = (\sum_j \mu_j \alpha_j) x^\alpha\ ,$$

and it is then easy to solve the transport equation by recursion, observing that $c(x)x^\alpha$ is a formal series vanishing at order $|\alpha| + 1$.

Solving in spaces of flat functions (integration along bicharacteristics).

$$(\sum_j \mu_j x_j \partial_{x_j} - c(x))u(x) = f(x)\ ,$$

with $c(0) = 0$ and $\mu_j = \sqrt{\frac{\lambda_j}{2}}$.
Reduction to $c = 0$. We observe that, for g flat at 0, the function

$$x \mapsto \int_{-\infty}^{0} g(\exp \mu_1 t\, x_1, \dots, \exp \mu_n t\, x_n)\ dt$$

is well defined and that :

$$(\sum_j \mu_j x_j \partial_{x_j})(\int_{-\infty}^{0} g(\exp \mu_1 t\, x_1, \dots, \exp \mu_n t\, x_n) dt = g(x)\ .$$

The general situation in the general case is explained in Helffer[5] [Hel1] or in Dimassi-Sjöstrand [DiSj]) (and of course in [HelSj1]) .

[5] Note that the simplification in the exposition proposed therein through to Sternberg's linearization theorem is not true in full generality.

6.4 Application

Eigenvalues expansions modulo $\mathcal{O}(h^\infty)$. As in the "generalized" harmonic approximation method, we deduce complete expansions. The advantage, which is not developed here is that the WKB solution is in the neighborhood of the minimum a good a pproximation of the corresponding eigenvector.

7 Decay of the eigenfunctions and applications

7.1 Introduction

As we have already seen when comparing the spectrum of the harmonic oscillator and of the Schrödinger operator, it could be quite important to know **a priori** how the eigenfunction attached to an eigenvalue $\lambda(h)$ decays in the classically forbidden region (that is the set of the x's such that $V(x) > \lambda(h)$). The Agmon's [Ag] estimates give a very efficient way to control such a decay. We refer to [Hel1] or to the original papers of Helffer-Sjöstrand [HelSj1] or Simon [Si] for details and complements.

Let us start with very weak notions of localization. For a family $h \mapsto \psi_h$ of L^2-normalized functions defined in Ω, we will say that ψ_h lives (resp. fully lives) in a closed set of $\overline{\Omega}$ if for any neighborhood $\mathcal{V}(U)$ of U,

$$\lim_{h\to 0}\int_{\mathcal{V}(U)\cap\Omega} |\psi_h|^2 dx > 0 \;,$$

respectively

$$\lim_{h\to 0}\int_{\mathcal{V}(U)\cap\Omega} |\psi_h|^2 dx = 1 \;.$$

For example one expects that the groundstate of the Schrödinger operator $-h^2\Delta + V(x)$ fully lives in $V^{-1}(\inf V)$. Similarly, one expects that if $\overline{\lim}_{h\to 0}\lambda(h) \leq E < \inf \sigma_{ess}(S_{h,V})$ and ψ_h is an eigenvector associated to $\lambda(h)$, then ψ_h will fully live in $V^{-1}(]-\infty, E])$. This is the way one can understand that in the semi-classical limit the quantum mechanics should recover the classical mechanics.

Of course the above is very heuristic but there are more accurate mathematical notions like the frequency set (see [Ro]) permitting to give a mathematical formulation to the above vague statements.

In this section, we will discuss the behavior of ψ_h outside the region where ψ_h fully lives (the smallest U such that ψ_h has the above property).

To illustrate the discussion, one can start with the very explicit example of the harmonic oscillator. The ground state $x \mapsto ch^{-\frac{1}{4}} \exp -\frac{x^2}{h}$ of $-h^2d^2+x^2$ lives at 0 and is exponentially decaying in any interval $[a,b]$ such that $0 \notin [a,b]$. This is this type of result that we will recover but WITHOUT having an explicit expression for ψ_h.

7.2 Energy inequalities

The main but basic tool is a very simple identity attached to the Schrödinger operator

$$S_h = -h^2\Delta + V$$

Proposition 7.1 *:*
Let Ω be a bounded open domain in $\mathbb{R}^m$ with C^2 boundary. Let $V \in C^0(\bar{\Omega};\mathbb{R})$ and ϕ a real valued lipschitzian function on $\bar{\Omega}$. Then, for any $u \in C^2(\bar{\Omega};\mathbb{R})$ with $u_{/\partial\Omega} = 0$, we have

$$\begin{array}{l} h^2 \int_\Omega |\nabla(\exp\phi/h\ u)|^2\ dx + \int_\Omega (V - |\nabla\phi|^2) \exp 2\phi/h\ u^2\ dx = \\ \quad \int_\Omega \exp 2\phi/h\ (S_h u)(x)\cdot u(x)\ dx\ . \end{array} \tag{7.1}$$

Proof:
In the case when ϕ is a $C^2(\bar{\Omega})$- function, this is an immediate consequence of the Green-Riemann formula

$$\int_\Omega \nabla v \cdot \nabla w dx = -\int_\Omega \Delta v \cdot w\, dx - \int_{\partial\Omega} (\partial v/\partial n) w d\sigma_{\partial\Omega}\ . \tag{7.2}$$

This gives in particular :

$$\int_\Omega \nabla v \cdot \nabla w dx = -\int_\Omega \Delta v \cdot w\, dx\ , \tag{7.3}$$

for all $v, w \in C^2(\bar{\Omega})$ such that $w_{/\partial\Omega} = 0$ or $(\partial v/\partial n)_{/\partial\Omega} = 0$.
This can actually be extended to $v, w \in H_0^1(\Omega)$.
To treat the general case, we just write ϕ as a limit as $\epsilon \to 0$ of $\phi_\epsilon = \chi_\epsilon \star \phi$ where $\chi_\epsilon(x) = \chi(\frac{x}{\epsilon})\,\epsilon^{-m}$ is the standard mollifier and we remark that $\nabla\phi$ is almost everywhere the limit of $\nabla\phi_\epsilon = \nabla\chi_\epsilon \star \phi$.

7.3 The Agmon distance

The Agmon metric attached to an energy E and a potential V is defined as $(V-E)_+ dx^2$ where dx^2 is the standard metric on $\mathbb{R}^n$. This metric is degenerated and is identically 0 at points living in the "classical" region: $\{x \mid V(x) \leq E\}$. Associated to the Agmon metric, we define a natural distance

$$(x, y) \mapsto d_{(V-E)_+}(x, y)$$

by taking the infimum :

$$d_{(V-E)_+}(x,y) = \inf_{\gamma \in \mathcal{C}^{1,pw}([0,1];x,y)} \int_0^1 [(V(\gamma(t)) - E)_+]^{\frac{1}{2}} |\gamma'(t)| dt \;, \tag{7.4}$$

where $\mathcal{C}^{1,pw}([0,1];x,y)$ is the set of the piecewise (pw) C^1 paths in $\mathbb{R}^n$ connecting x and y

$$\mathcal{C}^{1,pw}([0,1];x,y) = \{\gamma \in \mathcal{C}^{1,pw}([0,1];\mathbb{R}^n) \;,\; \gamma(0) = x \;,\; \gamma(1) = y\} \;. \tag{7.5}$$

When there is no ambiguity, we shall write more simply $d_{(V-E)_+} = d$.
Similarly to the Euclidean case, we obtain the following properties

- Triangular inequality

$$|d(x',y) - d(x,y)| \leq d(x',x) \;,\; \forall x, x', y \in \mathbb{R}^m \;. \tag{7.6}$$

-

$$|\nabla_x d(x,y)|^2 \leq (V - E)_+(x) \;, \tag{7.7}$$

  almost everywhere.

We observe that the second inequality is satisfied for any derived distance like

$$d(x,U) = \inf_{y \in U} d(x,y) \;.$$

The most useful case will be the case when U is the set $\{x \mid V(x) \leq E\}$. In this case $d(x,U)$ measures the distance to the classical region. All these notions being expressed in terms of metrics, they can be easily extended on manifolds.

7.4 Decay of eigenfunctions for the Schrödinger operator.

When u_h is a normalized eigenfunction of the Dirichlet realization in Ω satisfying $S_h u_h = \lambda_h u_h$ then the identity (7.1) gives roughly that $\exp \phi/h \; u_h$ is well controlled (in L^2) in a region

$$\Omega_1(\epsilon_1, h) = \{x \mid V(x) - |\nabla\phi(x)|^2 - \lambda_h > \epsilon_1 > 0\} \;,$$

by $\exp\left(\sup_{\Omega\setminus\Omega_1}\phi(x)/h\right)$. The choice of a suitable ϕ (possibly depending on h) is related to the Agmon metric $(V-E)_+\, dx^2$, when $\lambda_h \to E$ as $h \to 0$. The typical choice is $\phi(x) = (1-\epsilon)d(x)$ where $d(x)$ is the Agmon distance to the "classical" region $\{x \mid V(x) \leq E\}$. In this case we get that the eigenfunction is localized inside a small neighborhood of the classical region and we can measure the decay of the eigenfunction outside the classical region by

$$\exp(1-\epsilon)d(x)/h\; u_h = \mathcal{O}(\exp\epsilon/h)\;, \tag{7.8}$$

for any $\epsilon > 0$.
More precisely we get for example the following theorem

Theorem 7.2 *:*
Let us assume that V is C^∞, semibounded and satisfies

$$\lim \inf_{|x|\to\infty} V > \inf V = 0 \tag{7.9}$$

and

$$V(x) > 0 \;\text{ for } |x| \neq 0\;. \tag{7.10}$$

Let u_h be a (family of L^2-) normalized eigenfunctions such that

$$S_V(h)u_h = \lambda_h u_h\;, \tag{7.11}$$

with $\lambda_h \to 0$ as $h \to 0$. Then for all ϵ and all compact $K \subset \mathbb{R}^m$, there exists a constant $C_{\epsilon,K}$ such that for h small enough

$$||\nabla(\exp d/h\cdot u_h)||_{L^2(K)} + ||\exp d/h\cdot u_h||_{L^2(K)} \leq C_{\epsilon,K}\exp\epsilon/h \tag{7.12}$$

where $x \to d(x)$ is the Agmon distance between x and 0 attached to the Agmon metric $V\cdot dx^2$.

Useful improvements in the case when $E = \min V$ and when the minima are non degenerate can be obtained by controlling more carefully with respect to h, what is going on near the minima. It is also possible to control the eigenfunction at ∞. This was actually the initial goal of S. Agmon [Ag]

Proof:
Let us choose some $\epsilon > 0$. We shall use the identity (7.1) with

- V replaced by $V - \lambda_h$,

- $\phi = (1-\delta) d(x,U)$, with δ small enough possibly depending on ϵ,
- $u = u_h$, and
- $S_h = -h^2\Delta + V - \lambda_h$.

Let
$$\Omega_\delta^+ = \{x \in \Omega \;,\; V(x) > \delta\} \;,\; \Omega_\delta^- = \{x \in \Omega \;,\; V(x) \leq \delta\} \;.$$
We deduce from (7.1)
$$\begin{array}{l} h^2 \int_\Omega |\nabla (\exp \frac{\phi}{h} u_h)|^2 dx + \int_{\Omega_\delta^+} (V - \lambda_h - |\nabla \phi|^2) \exp \frac{2\phi}{h}\, u_h^2 \; dx \\ \qquad \leq \sup_{x\in \Omega_\delta^-} |V(x) - \lambda_h - |\nabla\phi|^2| \left(\int_{\Omega_\delta^-} \exp \frac{2\phi}{h}\, u_h^2 \; dx \right) \;. \end{array}$$

Then, for some constant C independent of $h \in]0,h_0]$ and $\delta \in]0,1]$, we get

$$\begin{array}{l} h^2 \int_\Omega |\nabla (\exp \frac{\phi}{h} u_h)|^2 dx + \int_{\Omega_\delta^+} (V - \lambda_h - |\nabla \phi|^2) \exp \frac{2\phi}{h}\, u_h^2 \; dx \\ \qquad \leq C \cdot \left(\int_{\Omega_\delta^-} \exp \frac{2\phi}{h}\, u_h^2 \; dx \right) \;. \end{array}$$

Let us observe now that on Ω_δ^+ we have (with $\phi = (1-\delta)d(\cdot,U)$)
$$V - \lambda_h - |\nabla \phi|^2 \geq (2-\delta)\delta^2 + o(1) \;.$$
Choosing $h(\delta)$ small enough, we then get for any $h \in]0, h(\delta)]$
$$V - \lambda_h - |\nabla \phi|^2 \geq \delta^2 \;.$$

This permits to get the estimate
$$\begin{array}{l} h^2 \int_\Omega |\nabla (\exp \frac{\phi}{h} u_h)|^2 dx + \delta^2 \int_{\Omega_\delta^+} \exp \frac{2\phi}{h}\, u_h^2 \; dx \\ \qquad \leq C \cdot \left(\int_{\Omega_\delta^-} \exp \frac{2\phi}{h}\, u_h^2 \; dx \right) \;, \end{array}$$

and finally
$$\begin{array}{l} h^2 \int_\Omega |\nabla (\exp \frac{\phi}{h} u_h)|^2 dx + \delta^2 \int_{\Omega} \exp \frac{2\phi}{h}\, u_h^2 \; dx \\ \qquad \leq \tilde{C} \cdot \exp \frac{a(\delta)}{h} \;, \end{array}$$

where $a(\delta) = 2 \sup_{x\in\Omega_\delta^-} \phi(x)$. We now observe that $\lim_{\delta\to 0} a(\delta) = 0$ and the end of the proof is then easy.

Remark 7.3 *: When V has a unique non degenerate minimum the estimate can be improved when $\lambda_h \in [0, C_0 h]$, by taking $\delta = Ch$, for some $C \geq 1$ and $\phi = d - Ch \inf(\log(\frac{d}{h}), \log C)$. We observe indeed that V, d and $|\nabla d|^2$ are equivalent in the neighborhood of the well.*

Applications:
As a first corollary, we can compare different Dirichlet problems corresponding to different open sets Ω_1 and Ω_2 containing a unique well U attached to an energy E. If for example $\Omega_1 \subset \Omega_2$, one can prove the existence of a bijection b between the spectrum of $S_{(h,\Omega_1)}$ in an interval $I(h)$ tending (as $h \to 0$) to E and the corresponding spectrum of $S_{(h,\Omega_2)}$ such that $|b(\lambda) - \lambda| = \mathcal{O}(\exp -S/h)$ (under a weak assumption on the spectrum at $\partial I(h)$). S is here any constant such that

$$0 < S < d_{(V-E)_+}(\partial\Omega_1, U) .$$

This can actually be improved (using more sophisticated perturbation theory) as $\mathcal{O}(\exp -2S/h)$.

Remark 7.4
It can be useful to extend the properties of the eigenvectors to the decay properties of the kernel of the resolvent of the operator. The reader is invited to look in [DiSj].

7.5 The case with magnetic fields

7.5.1 The case with V.

When V satisfies the previous assumptions, the first result [HelSj7] is that that the addition of a magnetic potential can only improve the decay. This is in the same spirit of the property of diamagnetism. The main reason (with the extension to the case with magnetic field of the Green-Riemann formula) is that we can replace the inequality (7.1) by

$$\begin{aligned} &\int_\Omega |\nabla_{h,A}(\exp\phi/h\ u)|^2\,dx + \int_\Omega (V - |\nabla\phi|^2)\exp 2\phi/h\ |u|^2\,dx = \\ &\qquad \mathrm{Re}\ \left(\int_\Omega \exp 2\phi/h\ (P_{A,h,V}u)(x)\cdot \bar{u}(x)\,dx\right)\ , \end{aligned} \tag{7.13}$$

which is valid for u in the domain of the Dirichlet or Neumann realization of $P_{A,h,V}$.

7.5.2 The case without electric potential

In this case, there is no hope to use the result for V, which does not create any localization. The idea is that the role previously played by $V(x)$ is replaced by $h|B(x)|$ (or more generally to $x \mapsto \operatorname{Tr}_+(B(x))$. This is due to (2.23) in the case $n = 2$ ($B(x)$ of constant sign) and to their extensions. The Agmon distance will be attached to $h\,(\operatorname{Tr}_+(B(x)) - \inf_x \operatorname{Tr}_+(B(x)))\,dx^2$.
The proof is in two steps: treatment of the case with constant magnetic field and then partition of unity for controlling the comparison with this case.
This explains, due to the presence of h before $|B|$, that the decay is measured through a weight in $\exp -\frac{\phi}{\sqrt{h}}$, where ϕ should satisfy :

$$|\nabla\phi|^2 \leq \operatorname{Tr}_+(B(x)) - \inf_x \operatorname{Tr}_+(B(x))\ ,$$

outside a neighborhood of the magnetic well, that is the set of points where $\operatorname{Tr}_+(B(x)) = \inf_x \operatorname{Tr}_+(B(x)$.

8 Application to the superconductivity

8.1 Introduction

The analysis of the superconductivity is based on the analysis of a functional. In the analysis of the stabilty of some minimizers (called the normal solution), one is immediately let to the spectral analysis of the Neumann realization of a Schrödinger opeerator with magnetic fields. We will mainly discuss a theorem by Lu-Pan. As we said one motivation comes from superconductivity but this is also one of the basic problems in the literature in mathematical physics in connexion with semi-classical problems (h being in this context the Planck constant). If one can naturally refer to Kato and, at the end of the seventie's to Avron-Herbst-Simon [AHS] or Combes-Schrader-Seiler [CSS] for the mathematical analysis of the problem, the implementation of semi-classical techniques for the analysis of the ground state appears first in [HelSj7] and then in [HelMo2]. Very roughly, it is shown in [HelMo2] that, if $\Omega = \mathbb{R}^n$, $h|\mathrm{Curl}\, A(x)|$ plays the role of an effective electric potential. By this we mean that the anlysis of the operator : $-h^2\Delta + h|B(x)|$, can give a good information for the localization of the ground state. The boundary case was less analyzed. Of course the case of the Dirichlet realization does not lead to really new phenomena in comparison with the case $\Omega = \mathbb{R}^n$, at least if the condition

$$b < b' \;, \tag{8.1}$$

is satisfied, where we used the notations :

$$\inf_{x\in\bar{\Omega}} |B(x)| = b \;,\; \inf_{x\in\partial\Omega} |B(x)| = b' \;. \tag{8.2}$$

8.2 Main results

We recall that we have given a rough asymptotic estimate for the Dirichlet realization in dimension 2 (see Theorem 2.4) and that by the minimax this gives an upper bound in the case of Neumann. The first "rough" theorem for Neumann is the following :

Theorem 8.1

$$\lim_{h\to 0} \frac{1}{h} \inf \sigma(P^N_{A,h,\Omega}) = \min(b, \Theta_0 b') \;. \tag{8.3}$$

The points where the minima of $|B|$ are sometimes called magnetic wells for the energy b. The decay of the ground state outside the wells can be estimated (cf [Br], [HeNo2]) as a function of the Agmon distance associated to the so called Agmon metric $(|B|-b)dx^2$, where dx^2 denotes the euclidean metric. Note that this metric is degenerate.
We recall that this estimate is very easy to get from (2.23) in the special case when $n=2$ and when the magnetic field has a constant sign. Here $\langle \cdot \mid \cdot \rangle$ denotes the scalar product in $L^2(\Omega)$ and $|| \cdot ||$ the corresponding norm.
In the general case. one can get a similar result but with a remainder in $\mathcal{O}(h^{\frac{5}{4}})||u||^2$ (cf [HelMo3], Theorem 3.1).

As in the case when $A=0$ but an electric potential V is added, it is possible to discuss the various asymptotics in function of the properties of B near the minima (cf [HelMo2, HelMo3, Mon, Sh, Ue1, Ue2] or more recently [KwPa]). As we shall see later, this property is no more true in the case of the Neumann realization. The infimum b of $|B(x)|$on $\bar{\Omega}$ is not necessarily the right quantity for analyzing the bottom of the spectrum as (8.1) is satisfied. Of course, by direct comparison of the variational spaces corresponding to Dirichlet and Neumann, one knows that the smallest eigenvalue $\mu^{(1)}(h)$ of the Neumann realization $P^N_{h,A,\Omega}$ of $P_{h,A,\Omega}$ is bounded from above by $\lambda^{(1)}(h)$ (but the lower bound (2.26) is not correct in general).

One important theorem that we would like to present is

Theorem 8.2 .
If the magnetic field is constant and not zero, then any ground state corresponding to the Neumann realization is localized as $h \to 0$ near the boundary of Ω.

This theorem is general and does not depend on the dimension.

These two theorems are not satisfactory in the sense that they are not necessarily optimal. In the case $n=2$, we can state [HelMo3]

Theorem 8.3 .
Let us assume that $n=2$. If the magnetic field is constant and not zero, then any ground state corresponding to the Neumann realization is localized as $h \to 0$ near the boundary of Ω at the points of maximal curvature.

This gives the general answer for the case of dimension 2. The case of dimension 3 was more difficult and only solved quite recently [HelMo4, HelMo5].

Although the methods of proof can also lead to localization results for the ground state (see [HelMo3], [HelMo4], [HelMo5]) or more generally for minimizers of the Ginzburg-Landau functional (see [LuPa1]-[LuPa5], [HePa]), but this will not be discussed here. This is actually explored in [Pan3].

8.3 About the proofs

In the Dirichlet case, the inequality (2.23) was (at least when the condition $B(x) > 0$ is satisfied) the starting point of the analysis of the decay. This is no more the case when Neumann boundary conditions are assumed, but we can keep the general strategy as developed in [HelMo3].
We assume that Ω is a bounded, regular open set and that

$$B(x) > 0 \,. \tag{8.4}$$

8.4 Upper bounds

Using suitable quasimodes (Gaussians and in the case of the boundary tangential Gaussians multiplied by a "normal" solution constructed with the help of the first eigenfunction of the model on $\mathbb{R}^+$), one can get :

$$\mu^{(1)}(h) \leq \min(b, \Theta_0 b')\, h + C\, h^{\frac{5}{4}} \,, \tag{8.5}$$

Note that Lu-Pan give the weaker :

$$\mu^{(1)}(h) \leq \min(b, \Theta_0 b')\, h + o(h) \,, \tag{8.6}$$

which is enough for the analysis of the decay. Note also that the upper bound involving $b = \inf B$ can also be obtained by using [HelMo3].

8.5 Lower bounds

Let $0 \leq \rho \leq 1$. We first claim that there exists C such that, for any $\epsilon_0 > 0$, we can, by scaling a standard partition of unity of $\mathbb{R}^2$, and by restricting it to $\overline{\Omega}$, find a partition of unity χ_j^h satisfying in Ω,

$$\sum_j |\chi_j^h|^2 = 1 \,, \tag{8.7}$$

$$\sum_j |\nabla \chi_j^h|^2 \leq C\, \epsilon_0^{-2}\, h^{-2\rho} \,, \tag{8.8}$$

and

$$\operatorname{supp}(\chi_j^h) \subset Q_j = B(z_j, \epsilon_0\, h^\rho)\ , \tag{8.9}$$

where $B(c,r)$ denotes the open disc in $\mathbb{R}^2$ of center c and radius r. Moreover, we can add the property that :

$$\text{either}\ \operatorname{supp}\chi_j \cap \partial\Omega = \emptyset\ ,\quad \text{either}\ z_j \in \partial\Omega\ . \tag{8.10}$$

According to the two alternatives in (8.10), we can decompose the sum in (8.7) in the form :

$$\sum = \sum_{int} + \sum_{bnd}\ ,$$

where "int" is in reference to the j's such that $z_j \in \Omega$ and "bnd" is in reference to the j's such that $z_j \in \partial\Omega$.

The second point is to implement this partition of unity in the following way :

$$q_h^N(u) = \sum_j q_h(\chi_j^h u) - h^2 \sum_j ||\, |\nabla\chi_j^h|\, u\, ||^2\ ,\ \forall u \in H^1(\Omega)\ . \tag{8.11}$$

Here q_h^N (or $q_{h,A}^N$, if we want to keep the reference to the magnetic potential) denotes the quadratic form :

$$q_{h,A}^N(u) = \int_\Omega |h\nabla u - iAu|^2\, dx\ , \tag{8.12}$$

and we recall that $||\ \cdot\ ||$ denotes the L^2-norm in Ω.
This formula is usually called IMS formula (see [CFKS]) but is actually much older.
If $a_{h,A}^N$ is the associated sesquilinear form, (8.11) is the consequence of the identity, for any function $\chi \in C^\infty(\bar\Omega)$ and any $u \in H^1(\Omega)$:

$$q_{h,A}^N(\chi u) = \operatorname{Re} a_{h,A}^N(u, \chi^2 u) + h^2 ||\, |\nabla\chi| u\, ||^2_{L^2(\Omega)}\ . \tag{8.13}$$

We will also use later the property that, for any function $\chi \in C^\infty(\bar\Omega)$ and any u in the domain of $P_{h,A,\Omega}^N$, that is for any u in the space $D(P_{h,A,\Omega}^N) := \{v \in H^2(\Omega)\ |\ \nu\cdot(\partial - iA)u_{/\partial\Omega} = 0\}$:

$$q_{h,A}^N(\chi u) = \operatorname{Re} \langle P_{h,A,\Omega}^N\, u\ |\ \chi^2 u\rangle_{L^2(\Omega)} + h^2 ||\, |\nabla\chi|\, u\, ||^2_{L^2(\Omega)}\ . \tag{8.14}$$

We can rewrite the right hand side of (8.11) as the sum of three (types of) terms.

$$q_h(u) = \sum_{int} q_h(\chi_j^h u) + \sum_{bnd} q_h(\chi_j^h u) - h^2 \sum_j || \, |\nabla \chi_j^h| \, u \, ||^2 \;,\; \forall u \in H^1(\Omega) \;. \tag{8.15}$$

For the last term in the right hand side of (8.15), we get using (8.8) :

$$h^2 \sum_j || \, |\nabla \chi_j^h| \, u \, ||^2 \leq C \, h^{2-2\rho} \, \epsilon_0^{-2} \, ||u||^2 \;. \tag{8.16}$$

This measures the price to pay when using a fine partition of unity : If ρ is large, the error is big as $h^{2-2\rho}$. We shall see later what could be the best choice of ρ or of ϵ_0 for our various problems (note that the play with ϵ_0 large will be only interesting when $\rho = \frac{1}{2}$).

The first term in the right hand side of (8.15) can be estimated from below by using (2.23). The support of $\chi_j^h u$ is indeed contained in Ω. So we have :

$$\sum_{int} q_h(\chi_j^h u) \geq h \sum_{int} \int B(x) |\chi_j^h u|^2 \, dx \;. \tag{8.17}$$

The second term in the right hand side of (8.15) is the more delicate and corresponds to the specificity of the Neumann problem. We have to find a lower bound for $q_h(\chi_j^h u)$ for some j such that $z_j \in \partial\Omega$. We emphasize that z_j depends on h, so we have to be careful in the control of the uniformity.
Let z be a point in $\partial\Omega$. The boundary being regular, we can, by a change of coordinates in a small neighborhood of this point, rewrite the form $q_{h,A}$ for u's with support in this neighborhood of z :

$$q_{h,A}(u) = \int_{\tilde{x}_2 > 0} \sum g^{k,\ell}(\tilde{x}) (ih\partial_{\tilde{x}_k} \tilde{u} + A_k(\tilde{x})\tilde{u}) \cdot \overline{(ih\partial_{\tilde{x}_\ell} \tilde{u} + A_\ell(\tilde{x})\tilde{u})} \det(g(\tilde{x})) \, d\tilde{x} \;.$$

Here we can assume that the new cordinates of z are $(0,0)$ and we can also assume that the matrix g is the identity at z :

$$g^{k,\ell}(0) = \delta_{k,\ell} \;.$$

Of course g depends on z, but all the estimates we could need on the derivatives of g will be uniform in z.
The game is now to compare for u's with support in a ball of the type $B(z, 2C\epsilon_0 h^\rho)$ $q_{h,A}$ with the quadratic form :

$$q_{h,\tilde{A}}(\tilde{u}) = \int_{x_2>0} |(ih\partial_{x_1} - \frac{1}{2}B(z)x_2)u|^2 + |(ih\partial_{x_2} + \frac{1}{2}B(z)x_1)u|^2\, dx\ .$$

We have omitted for simplicity the tilde's in the right hand side. The comparison is not direct but as an intermediate step, we have to use a gauge transformation (multiplication by $\exp -i\frac{\phi_j}{h}$) associated to a C^∞ function ϕ_j such that :

$$\omega_A = \omega_{A_{new,j}} - d\phi_j\ ,$$

with

$$A_{new,j}(z_j) = 0\ ,$$
$$|A_{new,j}(x) - \frac{1}{2}(B(z_j)(-x_2, x_1))| \leq C|x|^2\ .$$

In this formula, ω_A is the one-form attached to the vector field A : $\omega_A := A_1 dx_1 + A_2 dx_2$. Let us emphasize that C is independent of j. Let us also introduce for the next formula : $A_j^{lin} := \frac{1}{2}(B(z_j)(-x_2, x_1))$.
Following line by line the computations of [HelMo3], we get :

$$\begin{array}{ll} q_{h,A}(\chi_j^h u) & \geq (1 - Ch^{2\theta}\epsilon^2 - C\epsilon_0 h^\rho) q^h[A_j^{lin}](\exp -\frac{i}{h}\phi_j \chi_j^h u) - Ch^{-2\theta}\epsilon^{-2} |||x|^2 \chi_j^h u||^2 \\ & \geq (1 - Ch^{2\theta}\epsilon^2 - C\epsilon_0 h^\rho) q^h[A_j^{lin}](\exp -\frac{i}{h}\phi_j \chi_j^h u) - Ch^{4\rho-2\theta}\epsilon^{-2} ||\chi_j^h u||^2\ . \end{array}$$

We can now use the result concerning the half -plane in order to get :

$$q_{h,A}(\chi_j^h u) \geq (1 - Ch^{2\theta}\epsilon^2 - C\epsilon_0 h^\rho) h\Theta_0 \int B(z_j)|\chi_j^h u|^2\, dx - Ch^{4\rho-2\theta}\epsilon^{-2}||\chi_j^h u||^2\ . \tag{8.18}$$

We now put together all the estimates and obtain :

$$\begin{array}{ll} q_{h,A}(u) & \geq h \sum_{int} \int B(x)|\chi_j^h u|^2 dx \\ & \quad +(1 - Ch^{2\theta}\epsilon^2 - C\epsilon_0 h^\rho) h\Theta_0 \sum_{bnd} \int B(z_j)|\chi_j^h u|^2\, dx \\ & \quad -Ch^{4\rho-2\theta}\epsilon^{-2} \sum_{bnd} ||\chi_j^h u||^2 \\ & \quad -C\epsilon_0^{-2}\, h^{2-2\rho}||u||^2\ . \end{array} \tag{8.19}$$

We have now to optimize our choices of ρ, θ and ϵ, ϵ_0. If we just want to get a lower bound of the spectrum, we can first write :

$$\begin{array}{ll} q_{h,A}(u) & \geq h \min(b, \Theta_0 b')\, ||u||^2 \\ & \quad - \left(Ch^{2\theta+1}\epsilon^2 + C\epsilon_0 h^{\rho+1} + Ch^{4\rho-2\theta}\epsilon^{-2} + C\epsilon_0^{-2} h^{2-2\rho}\right) ||u||^2\ . \end{array}$$

Taking $\rho = \frac{3}{8}$, $\theta = \frac{1}{8}$, $\epsilon = \epsilon_0 = 1$, we get :

$$q_{h,A}(u) \geq \left(\min(b, \Theta_0 b')h - Ch^{\frac{5}{4}}\right) ||u||^2 \,. \tag{8.20}$$

So, taking $u = u_h^1$, where u_h^1 is a groundstate, we obtain from (8.20) :

Proposition 8.4 .
There exist constants $C > 0$ and $h_0 > 0$ such that, for all $h \in]0, h_0]$:

$$\mu^{(1)}(h) \geq (\min(b, \Theta_0 b')\,)\, h - Ch^{\frac{5}{4}} \,. \tag{8.21}$$

But for the control of the decay, we need also to take in (8.19) $\rho = \frac{1}{2}$, $\theta = \frac{1}{8}$, $\epsilon = 1$ and ϵ_0 large. This gives an estimate which may look weaker but will be more efficient.

Proposition 8.5 .
There exists C and h_0 and, for all $\epsilon_0 > 0$, there exists $C(\epsilon_0)$ such that, for $h \in]0, h_0]$, the following inequality :

$$\begin{array}{rl} q_{h,A}(u) & \geq h \sum_{int} \int B(x)|\chi_j^h u|^2 dx \\ & -C(\epsilon_0) h \sum_{bnd} \int |\chi_j^h u|^2 \, dx \\ & -\frac{Ch}{\epsilon_0^2} \sum_{int} \int |\chi_j^h u|^2 dx \,. \end{array} \tag{8.22}$$

is satisfied, for all $u \in H^1(\Omega)$.

8.6 Agmon's estimates

We continue to follow the proof given in [HelMo3] and will explain the modifications needed in order to treat Neumann problems.
We first observe that if Φ is a real and uniformly Lipschitzian function and if u is in the domain of the Neuman realization of $P_{h,A}$, then we have by a simple integration by part (see (8.13)) :

$$\begin{array}{l} \mathrm{Re}\,\langle P_{h,A} u, \exp \frac{2\Phi}{h^{\frac{1}{2}}} u\rangle \\ = \ \mathrm{Re}\,\langle (\frac{h}{i}\nabla - A)u, (\frac{h}{i}\nabla - A) \exp \frac{2\Phi}{h^{\frac{1}{2}}} u\rangle \\ = \langle (\frac{h}{i}\nabla - A) \exp \frac{\Phi}{h^{\frac{1}{2}}} u, (\frac{h}{i}\nabla - A) \exp \frac{\Phi}{h^{\frac{1}{2}}} u\rangle - h|||\nabla\Phi| \exp \frac{\Phi}{h^{\frac{1}{2}}} u||^2 \\ = q_h[A](\exp \frac{\Phi}{h^{\frac{1}{2}}} u) - h|||\nabla\Phi| \exp \frac{\Phi}{h^{\frac{1}{2}}} u||^2 \,. \end{array} \tag{8.23}$$

We now take $u = u_h$ an eigenfunction attached to the lowest eigenvalue $\mu^{(1)}(h)$. This gives :

$$\mu^{(1)}(h)||\exp\frac{\Phi}{h^{\frac{1}{2}}}u||^2 = q_{h,A}(\exp\frac{\Phi}{h^{\frac{1}{2}}}u) - h|||\nabla\Phi|\exp\frac{\Phi}{h^{\frac{1}{2}}}u||^2\ . \tag{8.24}$$

It remains to reimplement the previous inequality in this new one and to use the upper bound (8.5).

Let us take $\Phi(x) = \alpha\max(d(x,\partial\Omega), h^{\frac{1}{2}})$, where $\alpha > 0$ has to be determined. Let us use Proposition 8.5. We first write :

$$\begin{array}{rl} q_{h,A}(\exp\frac{\Phi}{h^{\frac{1}{2}}}u) & \geq h\sum_{int}\int B(x)|\exp\frac{\Phi}{h^{\frac{1}{2}}}\chi_j^h u|^2 dx \\ & -C(\epsilon_0)h\sum_{bnd}\int|\chi_j^h\exp\frac{\Phi}{h^{\frac{1}{2}}}u|^2\,dx \\ & -\frac{Ch}{\epsilon_0^2}\sum_{int}\int|\exp\frac{\Phi}{h^{\frac{1}{2}}}\chi_j^h u|^2 dx\ . \end{array} \tag{8.25}$$

Let us first consider the case $B(x) = b$. The inequality (8.5) becomes :

$$\mu^{(1)}(h) \leq \Theta_0\, b\, h + C\, h^{\frac{5}{4}}\ . \tag{8.26}$$

Using (8.23), we finally obtain :

$$(b(1-\Theta_0) - Ch^{\frac{1}{4}} - \frac{C}{\epsilon_0^2} - \alpha^2)\sum_{int}\int|\exp\frac{\Phi}{h^{\frac{1}{2}}}\chi_j^h u|^2 dx \leq C(\epsilon_0)\sum_{bnd}\int|\chi_j^h u|^2\,dx\ . \tag{8.27}$$

Taking ϵ_0 large enough and

$$\alpha < \sqrt{b(1-\Theta_0)}$$

we finally obtain the estimate :

$$||\exp\alpha\frac{d(x,\partial\Omega)}{h^{\frac{1}{2}}}u_h|| \leq C||u_h||\ , \tag{8.28}$$

for some new constant $C > 0$.

Note that we just need a weak upper bound of $\mu^{(1)}(h)$ in order to make the argument correct. In particular, the remainder $C\,h^{\frac{1}{4}}$ in (8.27) can be replaced by $o(1)$ without changing the argument. This is the upper bound obtained in [LuPa2].

Let us now show how to go from an L^2-estimate to an L^∞-estimate. Using (8.24), we first get :

$$q_{h,A}(\exp \frac{\Phi}{h^{\frac{1}{2}}} u) \leq C\, h || \exp \frac{\Phi}{h^{\frac{1}{2}}} u||^2 \; . \tag{8.29}$$

This gives, together with (8.28), an estimate in H^1 norm. Coming back to the second order differential equation satisfied by $\exp \frac{\Phi}{h^{\frac{1}{2}}} u$ and using that Φ is constant near the boundary[6], we can use the regularity of the Neumann problem for getting a control in H^2. This gives finally (through the Sobolev injection theorem) the proof in the constant magnetic field case of the following theorem :

Theorem 8.6 .
Let us assume that the condition :

$$\Theta_0 b' < b \; , \tag{8.30}$$

is satisfied.
There exists $C > 0$, $\alpha > 0$ and $\nu \in \mathbb{R}$, such that if u_h is the ground state of $P^N_{A,h,\Omega}$, then :

$$\exp \alpha \frac{d(x, \partial\Omega)}{h^{\frac{1}{2}}} |u_h(x)| \leq C h^{-\nu} ||u_h||_{L^2} \; , \; \forall x \in \Omega \; . \tag{8.31}$$

The condition (8.30) is always satisfied when B is constant because $b = b'$ and $\Theta_0 < 1$ ([PiFeSt]).

The proof when B is not constant is essentially the same. The inequality (8.27) becomes :

$$\left(b - \Theta_0 b' - o(1) - \frac{C}{\epsilon_0^2} - \alpha^2\right) \sum_{int} \int | \exp \frac{\Phi}{h^{\frac{1}{2}}} \chi_j^h u|^2 dx \leq C(\epsilon_0) \sum_{bnd} \int |\chi_j^h u|^2 \, dx \; . \tag{8.32}$$

We can then conclude in the same way (modulo the proof of (8.5) which will be given later.

Remark 8.7 .
On the contrary, when $b < \Theta_0 b'$ the ground state decays exponentially outside neighborhoods of points where $B(x) = b$.

[6] Actually, we need first to use a regularized Φ in order to make the argument rigorous. Another way, would be to use L^p estimates.

9 Splitting between the two first eigenvalues

We will be only very brief on this part but this was one of the main motivation (before we get this application to superconductivity) for a careful analysis of the decay of the eigenfunctions.
The control of the decay of the eigenfunctions has also immediate consequences on the splitting. To understand what is needed, let us recall the following classical formula for the splitting which is nothing else than a version of the minimax principle applied to the orthogonal of $\mathbb{R}\cdot u_1$,

$$
\lambda_2 - \lambda_1 = \inf_{\left\{\begin{array}{c}\phi\,;\ \phi\in C_0^\infty\,,\\ \int \phi(x)\,u_1^{(m)}(x)^2\,dx = 0\end{array}\right\}} \left[\left(\int |h\nabla\phi|^2\, u_1^{(m)}(x)^2\,dx\right) / \left(\int |\phi|^2\, u_1^{(m)}(x)^2\,dx\right)\right] . \tag{9.1}
$$

Here $u_1^{(m)}$ denotes the first normalized eigenfunction of the Schrödinger operator. The estimates about the splitting are then deduced from a good choice of ϕ and from a precise information on the decay of $u_1^{(m)}$ in suitable domains.
Let us consider the double well situation. The potential v is symmetric and has two non degenerate minima. We now choose a function ϕ in C_0^∞ which satisfies

$$
\phi(x) = -\phi(-x)
$$

and

$$
\phi = 1
$$

in a neighborhood of the critical point x_c of V. We recall also that the first eigenfunction is even

$$
u_1^{(m)}(x) = u_1^{(m)}(-x) .
$$

We have used here that the first eigenvalue is simple and that the first eigenfunction can be chosen strictly positive (Perron-Frobenius argument).
As a consequence we have effectively

$$
\int \phi(x) u_1^{(m)}(x)^2 dx = 0 .
$$

We observe also using the Agmon estimates that

$$
\int \phi(x)^2 u_1^{(m)}(x)^2\, dx = 1 + \mathcal{O}(\exp -\frac{S}{h}) ,
$$

and that

$$\int |\nabla\phi(x)|^2 u_1^{(m)}(x)^2 dx = \mathcal{O}(\exp -\frac{S}{h}) ,$$

for some $S > 0$. Coming back to the formula giving the splitting we obtain

$$\lambda_2 - \lambda_1 = \mathcal{O}(\exp -\frac{S}{h}) . \tag{9.2}$$

In the situation of a symmetric double well, we have consequently two eigenvalues whose difference is exponentially small.

Remark 9.1 *:*
According to the result concerning the decay of the first eigenfunction, show that S can be seen as any real number such that

$$S < d_{(V-E)_+}(x_c, -x_c) .$$

Remark 9.2 *:*
In some generic cases, one can actually give a more precise estimate for the splitting in the form

$$\lambda_2 - \lambda_1 = h^{\frac{1}{2}} A_m(h)(\exp -\frac{S_m}{h}) , \tag{9.3}$$

where S_m is the Agmon's distance between the two wells and $A_m(h)$ is a non zero function admitting an expansion of the type $A_m(h) \sim \sum_j a_{m,j} h^j$. This involves the approximation of the eigenfunction of reference one-well problem by WKB solutions and the use of the Laplace integral method.

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A Variations around the spectral theorem

We just come back to the way one can deduce from the existence of quasi-modes information on the spectrum of a selfadjoint operators.

A.1 Spectral Theorem

We refer for this part to any standard book in Spectral Theory (for example Reed-Simon or Lévy-Bruhl). We recall only that if $\lambda \notin \mathrm{Sp}\,(A)$, then

$$||(A-\lambda)^{-1}|| \leq \frac{1}{d(\lambda, \mathrm{Sp}\,(A))}\ . \tag{A.1}$$

This implies immediately that if there exists $\psi \in D(A)$ and $\eta \in \mathbb{R}$ such that $||\psi|| = 1$ and $||(A-\eta)\psi|| \leq \epsilon$, then there exists $\lambda \in \mathrm{Sp}\,(A)$ such that $d(\lambda, \eta) \leq \epsilon$. We emphasize here that there is no assumption of discreteness of the spectrum.

A.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 let $\epsilon = ||(A-\eta)\psi||$. Then it is easy to show that :

$$\eta - \frac{\epsilon^2}{\beta - \eta} \leq \lambda \leq \eta + \frac{\epsilon^2}{\eta - \alpha}\ . \tag{A.2}$$

For the proof we can reduce to the case when $\eta = 0$ and simply observe that $(A-\alpha)(A-\lambda)$ and $(A-\beta)(A-\lambda)$ are positive operators. We can then apply this positivity property for the vector ψ. Note that this gives an additional information, only if ϵ is small enough, more precisely

$$\epsilon^2 \leq (\beta - \eta)(\eta - \alpha)\ . \tag{A.3}$$

A.3 Extensions

There is a need to generalize this lemma to more general situations.

Let E and F be closed subspaces in a Hilbert space $\mathcal{H}$. Let Π_E and Π_F be the orthogonal projections on E and F respectively. We can then define the non-symmetric distance $\vec{d}(E,F)$ as

$$\vec{d}(E,F) = \sup_{x\in E\,,\,||x||=1} d(x,F)\ . \tag{A.4}$$

This can be recognized as

$$\vec{d}(E,F) = \sup_{x\in E\,,\,||x||=1} ||x - \Pi_F x|| = ||(I-\Pi_F)_{|\,E}|| = ||\Pi_E - \Pi_F\Pi_E||\ . \tag{A.5}$$

Observing that $||A|| = ||A^*||$ in $\mathcal{L}(\mathcal{H})$ we finally get :

$$\vec{d}(E,F) = ||\Pi_E - \Pi_F\Pi_E|| = ||\Pi_E - \Pi_E\Pi_F||\ . \tag{A.6}$$

It is easy from the first definition[7] to verify that :

$$\vec{d}(E,G) \leq \vec{d}(E,F) + \vec{d}(F,G)\ . \tag{A.7}$$

Note that $\vec{d}(E,F) = 0$ if and only if $E \subset F$.
We then have the following lemmas

Lemma A.1
If $\vec{d}(E,F) < 1$, then $(\Pi_F)_{|E}\ :\ E \mapsto F$ is injective and $(\Pi_E)_{|F}$ has a bounded right inverse.

The injectivity is easy. If $x \in E$ and $\Pi_F x = 0$, we get

$$||x|| = ||x - \Pi_F x|| \leq \vec{d}(E,F)||x||\ ,$$

which implies $x = 0$.
On the other hand, if $x \in E$, we look for $y = \Pi_F z$, $z \in E$, such that $x = \Pi_E y = \Pi_E\Pi_F z$. Writing this as :

$$x = (I - (\Pi_E\Pi_F - I))z = (I - (\Pi_E\Pi_F - \Pi_E))z\ ,$$

we get that if $\vec{d}(E,F) < 1$ then

$$z = (I - (\Pi_E\Pi_F - \Pi_E))^{-1}x\ .$$

So the right inverse is given by :

$$(\Pi_E)^{-1,r}_{|F} = \Pi_F(I - (\Pi_E\Pi_F - \Pi_E))^{-1}\ . \tag{A.8}$$

[7] First observe that

$$d(x,G) \leq d(x,F) + \vec{d}(F,G)||\Pi_F x||\ .$$

Lemma A.2
If $\vec{d}(E,F) < 1$ and $\vec{d}(F,E) < 1$, then $(\Pi_F)_{|E}$ and $(\Pi_E)_{|F}$ are bijective and $\vec{d}(E,F) = \vec{d}(F,E)$.

Proof.
We have
$$\vec{d}(E,F)^2 = \sup_{x\in E\ ,\ ||x||_E=1} (1 - ||(\Pi_F)_{|\,E}x||^2)\ .$$
This implies
$$\inf_{x\in E\ ,\ ||x||_E=1} ||(\Pi_F)_{|\,E}x||^2 = 1 - \vec{d}(E,F)^2\ .$$
This implies that $(\Pi_F)_{|\,E}$ is injective with bounded left inverse. Similarly, its adjoint is $(\Pi_E)_{|\,F}$ and has the same property. It follows that they are bijective and have the same norm. The same property is true for their inverse. But the last identity can be written as
$$||(\Pi_F)_{|\,E}^{-1}||^{-2} = 1 - \vec{d}(E,F)^2\ ,$$
and we have similarly
$$||(\Pi_E)_{|\,F}^{-1}||^{-2} = 1 - \vec{d}(F,E)^2\ ,$$
This achieves the proof of the lemma.

Proposition A.3
Let A be a selfadjoint operator in a Hilbert space $\mathcal{H}$. Let $I \subset \mathbb{R}$ be a compact interval and let ψ_j ($j = 1,\dots,N$) N linearly independent vectors in $\mathcal{H}$ and μ_j ($j = 1,\dots,N$) in I such that :
$$A\psi_j = \mu_j\psi_j + r_j\ ,\ \textit{with}\ ||r_j|| \le \epsilon\ . \tag{A.9}$$
Let $a > 0$ and assume that $\mathrm{Sp}\,(A)\cap[(I + B(0,2a)) \setminus I] = \emptyset$. Then if E is the space spanned by the ψ_j's and if F is the eigenspace associated to $\mathrm{Sp}\,(A)\cap I$, we have
$$\vec{d}(E,F) \le (N^{\frac{1}{2}}\epsilon)/(a(\lambda_S^{min})^{\frac{1}{2}})\ , \tag{A.10}$$
where λ_S^{min} is the smallest eigenvalue of the $N\times N$ matrix : $S := (\langle\psi_i \mid \psi_j\rangle)_{ij}$.

Proof.
Let $\lambda \in \mathbb{C} \setminus (\{\mu_1,\dots,\mu_N\} \cup \mathrm{Sp}\,(A))$. Let $I = [\alpha,\beta]$. Then by assumption :
$$(A-\lambda)\psi_j = (\mu_j - \lambda)\psi_j + r_j\ ,$$

which can be written as :

$$(A-\lambda)^{-1}\psi_j = (\mu_j-\lambda)^{-1}\psi_j - (A-\lambda)^{-1}(\mu_j-\lambda)^{-1}r_j \ . \tag{A.11}$$

If γ_R is the oriented boundary of $(I+B(0,a))\times i[-R,+R]$, we have :

$$\Pi_F\psi_j = \frac{1}{2i\pi}\int_{\gamma_R}(\mu_j-\lambda)^{-1}\psi_j d\lambda - \frac{1}{2i\pi}\int_{\gamma_R}(A-\lambda)^{-1}(\mu_j-\lambda)^{-1}r_j d\lambda \ .$$

The first integral of the right hand side is equal to ψ_j and the second one tends as $R\to+\infty$ to

$$\frac{1}{2i\pi}\int_{\beta+a-i\infty}^{\beta+a+i\infty}(A-\lambda)^{-1}(\mu_j-\lambda)^{-1}r_j d\lambda - \frac{1}{2i\pi}\int_{\alpha-a-i\infty}^{\alpha-a+i\infty}(A-\lambda)^{-1}(\mu_j-\lambda)^{-1}r_j d\lambda \ .$$

With $\lambda=\beta+a+it$ or $\lambda=\alpha-a+it$, we have

$$||(A-\lambda)^{-1}(\mu_j-\lambda)^{-1}r_j|| \leq \frac{\epsilon}{a^2+t^2} \ .$$

Hence

$$||\Pi_F\psi_j-\psi_j|| \leq \frac{\epsilon}{\pi}\int_{-\infty}^{+\infty}\frac{1}{a^2+t^2}dt = \frac{\epsilon}{a} \ .$$

Now if $u=\sum_j \alpha_j\psi_j \in E$, then

$$||u||^2 = \langle S\alpha \mid \alpha\rangle \geq \lambda_S^{min}||\alpha||^2 \ .$$

So

$$||\Pi_F u - u|| \leq \sum_j |\alpha_j|||\Pi_F\psi_j-\psi_j|| \leq ||\alpha||\frac{\epsilon N^{\frac{1}{2}}}{a} \leq \frac{\epsilon N^{\frac{1}{2}}}{a(\lambda_S^{min})^{\frac{1}{2}}}||u|| \ .$$

The proposition follows.

Remark A.4
If Sp $(A)\cap I$ *is discrete of finite multiplicity and if the right hand side above is strictly less than* 1*, then we conclude that* A *has at least* N *eigenvalues in* I*.*

A.4 Another improvment

We only consider the case when $N = 1$ (and in this case this is essentially a variant of Temple's inequality, see for more general situations the book [Hel1] p. 38-39) and suppose that we have shown that for some normalized ψ generating the one dimensional vector space E, we have

$$(A - \mu)\psi = r \ ,$$

with $||r|| \leq \epsilon$.
We assume that we have applied the previous proposition and that we have proven that $\vec{d}(E, F) = \vec{d}(F, E) = \mathcal{O}(\epsilon) < 1$.

Of course we get by the spectral theorem that for the unique eigenvalue λ in I, we have $|\lambda - \mu| \leq C\epsilon$, but what we would like to show is that the approximation is actually much better, i.e. of order $\mathcal{O}(\epsilon)^2$.

If λ is the eigenvalue and if $v := \pi_F \psi$, we start from the identity :

$$\lambda = \langle Av \mid v \rangle / \langle v \mid v \rangle \ .$$

So we now write

$$\lambda - \mu = \langle (A - \mu)v \mid v \rangle / \langle v \mid v \rangle \ ,$$

that we would like to compare with the quantity $\langle (A - \mu)\psi \mid \psi \rangle$ which will be in many examples explicitely computable. Let us estimate the difference. Using the projection π_F, we obtain :

$$||v||^2 = ||\psi||^2 - ||v - \psi||^2$$

which leads to the estimate :

$$|\, ||v||^2 - 1 \,| \leq d(E, F)^2 \ .$$

In the same way, we observe that :

$$\langle (A - \mu)v \mid v \rangle = \langle (A - \mu)\psi \mid \psi \rangle - \langle (A - \mu)(v - \psi) \mid (v - \psi) \rangle$$

which leads to the estimate :

$$\langle (A - \mu)v \mid v \rangle = \langle (A - \mu)\psi \mid \psi \rangle - \langle r \mid (v - \psi) \rangle$$

and finally to

$$|\langle (A-\mu)v \mid v\rangle - \langle (A-\mu)\psi \mid \psi\rangle| \leq \epsilon d(E,F)\ .$$

This leads to

$$|\lambda - \mu| \leq \frac{1}{1-d(E,F)^2}\epsilon d(E,F)\ , \tag{A.12}$$

Remark A.5
Compare with what is given by Temple's inequality.

B Variational characterization of the spectrum

B.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.

B.2 On positivity

We first recall the following definition

Definition B.1 .
Let A be a symmetric operator. We say that A is positive (and we write $A \geq 0$), if

$$< Au, u > \geq 0 \ , \ \forall u \in D(A) \ . \tag{B.1}$$

The following proposition relates the positivity with the spectrum

Proposition B.2 .
Let A be a selfadjoint operator. Then $A \geq 0$ if and only if $\sigma(A) \subset [0, +\infty[$.

Example B.3 .
Let us consider the Schrödinger operator $P := -\Delta + V$, with $V \in C^\infty$ and semi-bounded, then

$$\sigma(P) \subset [\inf V, +\infty[\ . \tag{B.2}$$

B.3 Variational characterization of the discrete spectrum

Theorem B.4 .
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

$$\lambda^1 = \inf_{\phi \in D(A), \phi \neq 0} ||\phi||^{-2} < A\phi, \phi > , \tag{B.3}$$

$$\lambda^2 = \inf_{\phi \in D(A) \cap K_1^\perp, \phi \neq 0} ||\phi||^{-2} < A\phi, \phi > , \tag{B.4}$$

and, for $n \geq 2$*,*

$$\lambda^n = \inf_{\phi \in D(A) \cap K_{n-1}^\perp, \phi \neq 0} ||\phi||^{-2} < A\phi, \phi > , \tag{B.5}$$

where

$$K_j = \oplus_{i \leq j} \; Ker \; (A - \lambda^i) \; .$$

One can prove actually that, if the right hand side of (B.3) is strictly below Σ, then, the spectrum below Σ is not empty, and the lowest eigenvalue is given by (B.3).

Example B.5 .
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 $V(x_{min}) < 0$.

B.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 B.6 .
Let A be a selfadjoint semibounded operator of domain $D(A) \subset \mathcal{H}$. Let us introduce

$$\mu_n(A) = \sup_{\psi_1, \psi_2, \ldots, \psi_{n-1}} \inf_{\left\{ \begin{array}{l} \phi \in [span(\psi_1, \ldots, \psi_{n-1})]^\perp ; \\ \phi \in D(A) \; and \; ||\phi|| = 1 \end{array} \right\}} \langle A\phi \mid \phi \rangle_{\mathcal{H}} \; . \tag{B.6}$$

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 B.7 .
In the case when the operator is with compact resolvent, case (b) does not occur and the supremum in (B.6) is a maximum. Similarly the infimum is a minimum. This explains the traditional terminology " Max-Min principle" for this theorem.

Note that the proof gives also the following proposition

Proposition B.8 .
Suppose that there exists a *and an* n*-dimensional subspace* $V \subset D(A)$ *such that*

$$\langle A\phi \mid \phi \rangle \leq a||\phi||^2 \ , \ \forall \phi \in V \ , \tag{B.7}$$

is satisfied. Then we have the inequality :

$$\mu_n(A) \leq a \ . \tag{B.8}$$

Corollary B.9 .
Under the same assumption as in Proposition B.8, if a *is below the bottom of the essential spectrum of* A*, then* A *has at least* n *eigenvalues (counted with multiplicity).*

Exercise B.10 .
In continuation of Example B.5, 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*.*

A first natural extension of Theorem B.6 is obtained by

Theorem B.11 .
Let A be a selfadjoint semibounded operator and $Q(A)$ its form domain [8] *.*
Then

$$\mu_n(A) = \sup_{\psi_1,\psi_2,\ldots,\psi_{n-1}} \inf_{\left\{\begin{array}{l}\phi \in [span(\psi_1,\ldots,\psi_{n-1})]^\perp ; \\ \phi \in Q(A) \text{ and } ||\phi|| = 1\end{array}\right\}} \langle A\phi \mid \phi\rangle_{\mathcal{H}} \,. \tag{B.9}$$

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 $\mathcal{S}(\mathbb{R})$ 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[9]

  $$< Au, u > \leq < Bu, u > \,,\; \forall u \in Q(B) \,,$$

  then

  $$\mu_n(A) \leq \mu_n(B) \,.$$

  Similar conclusions occur if we have $D(B) \subset D(A)$.

Example B.12 *(Comparison between Dirichlet and Neumann).*
Let Ω be a bounded regular connected open set in $\mathbb{R}^m$. Then the N-th eigenvalue of the Neumann realization of $-\Delta_A + V$ 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.

[8]associated by completion with the form $u \mapsto \langle u|Au\rangle_{\mathcal{H}}$ initially defined on $D(A)$.
[9]It is enough to verify the inequality on a dense set in $Q(B)$.

Example B.13 *(monotonicity with respect to the domain).*
Let $\Omega_1 \subset \Omega_2 \subset \mathbb{R}^m$ two bounded regular open sets. Then the $n-th$ eigenvalue 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 $\Omega_2 \setminus \Omega_1$.

C Essential spectrum and Persson's Theorem

We refer to [Ag] for proofs and generalizations.

Theorem C.1 .
Let V be a real-valued potential such that, there exists $a \in]0,1[$ and C such that :

$$||Vu||^2 \leq a||\Delta u||^2 + C||u||^2 \ , \ \forall u \in C_0^\infty(\mathbb{R}^m) \ , \tag{C.1}$$

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

$$\inf \sigma_{ess}(H) = \Sigma(H) \ , \tag{C.2}$$

where

$$\Sigma(H) := \sup_{\mathcal{K} \subset \mathbb{R}^m} \left[\inf_{||\phi||=1} \{ < \phi, H\phi > \ | \ \phi \in C_0^\infty(\mathbb{R}^m \setminus \mathcal{K}) \} \right] \ , \tag{C.3}$$

where the supremum is over all compact subset $\mathcal{K} \subset \mathbb{R}^m$.

Essentially this is a corollary of Weyl's Theorem and the property that

$$\sigma_{ess}(H) = \sigma_{ess}(H + W) \ , \tag{C.4}$$

for any regular potential W with compact support.

D Classical Laplace methods

We recall very simple results concerning Laplace integrals and which are the main tool for getting asymptotic expansions. The first one is modelled on the stationary phase theorem:

Theorem D.1 .
Let Φ be a real C^∞ phase defined in a neighborhood $\mathcal{V}$ of the closure of the ball $B(0,1)$ in $\mathbb{R}^m$ such that

- $\Phi \geq 0$ *on* $B(0,1)$ *;* $\Phi > 0$ *on* $\partial B(0,1)$,
- $\Phi(0) = \nabla\Phi(0) = 0$,
- Φ *has a unique non degenerate minimum at* 0.

Let a be a C^∞ function defined in $\mathcal{V}$ and let us consider the Laplace integral

$$I(a,\Phi;h) = \int_{B(0,1)} a(x)\ \exp -\Phi(x)/h\ dx\ ,$$

where $h \in]0,h_0]$. Then, as h tends to 0, $I(a,\Phi;h)$ has the following asymptotic behavior

$$I(a,\Phi;h) \sim h^{\frac{n}{2}} \sum_j \alpha_j \cdot h^j\ , \tag{D.1}$$

with

$$\alpha_0 = (2\pi)^{\frac{n}{2}} \cdot a(0)\ (\det \operatorname{Hess} \Phi(0))^{-\frac{1}{2}}\ . \tag{D.2}$$

The proof is rather simple (and actually simpler than for an oscillatory integral). The assumptions permit to reduce modulo exponentially small contributions (in $\mathcal{O}(\exp -\epsilon_0/h)$ for some $\epsilon_0 > 0$) to an arbitrarily small neighborhood of 0. We can then use the Morse Lemma (see below) in order to write in new coordinates: $\Phi(x) = \sum y_j^2 =: \hat{\Phi}(y)$. We are then reduced to the study of $I(b,\hat{\Phi};h)$ which is easy by taking the Taylor expansion of b at 0. We have indeed, if b is with compact support

$$\begin{aligned} h^{-\frac{1}{2}} \int_{-\infty}^{+\infty} b(y) \exp -\frac{y^2}{h} dy &\sim \sum \frac{1}{\alpha!} b^\alpha(0) h^{-\frac{1}{2}} \int_{-\infty}^{+\infty} y^\alpha \exp -\frac{y^2}{h} dy \\ &\sim \sum_{k\in\mathbb{N}} \frac{1}{(2k)!} b^{2k}(0) h^k I_{2k}\ , \end{aligned}$$

with

$$I_{2k} = \int t^{2k} \exp -t^2 dt\ ,$$

which is explicitly computable by integration by parts (note that $I_{2k} = \frac{2k-1}{2} I_{2k-2}$). We leave to the reader the control of the remainder.

We are then reduced to the computation of very explicit integrals associated with gaussian measures on $\mathbb{R}^n$.

Lemma D.2 *(The Morse Lemma) .*
Let $f(x,y)$ ($x \in \mathbb{R}^n, y \in \mathbb{R}^N$) be a real valued C^∞ function in a neighborhood of $(0,0)$. Assume that $(\nabla_x f)(0,0) = 0$ and that $A = (\mathrm{Hess}_{xx} f)(0,0)$ is non-singular. Then the equation $f'_x(x,y) = 0$ determines in a neighborhood of 0 a C^∞ function $x(y)$ with $x(0) = 0$ and we have in a neighborhood of 0

$$f(x,y) = f(x(y),y) + \langle Az|z\rangle/2$$

where $z = x - x(y) + \mathcal{O}(|x - x(y)|)(|x| + |y|)$ is a C^∞ function of (x,y) at $(0,0)$.

The proof is standard.

E Exercises in Spectral Theory

Exercise E.1 .
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. $V(x) = (x_1 - x_2)^2$.

Determine 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 E.2 .
Show that the selfadjoint extension in $L^2(\mathbb{R}^2)$ *of*

$$T := -\left(\frac{d}{dx_1} - ix_2x_1^2\right)^2 - \frac{d^2}{dx_2^2} + x_2^2\ ,$$

is with compact resolvent.

Exercise E.3 .
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* $|\lambda_1(a) - 1|$*.*
In order to get finer results, one can try to find a formal solution at $\pm\infty$ *in the form* $\exp \frac{x^2}{2} |x|^\rho \sum_{j\geq 0} c_j |x|^{-j}$*.*

Exercise E.4 .
Let ϕ *be a* C^2*- function on* $\mathbb{R}^m$ *such that* $|\nabla\phi(x)| \to +\infty$ *as* $|x| \to +\infty$

and with uniformly bounded second derivatives. Let us consider the differential operator on $C_0^\infty(\mathbb{R}^2)$ $-\Delta + 2\nabla\phi\cdot\nabla$. *We consider this operator as an unbounded operator on* $\mathcal{H} = L^2(\mathbb{R}^m, \exp -2\phi\, dx)$. *Show that it admits a selfadjoint extension and that its spectrum is discrete.*
We assume in addition that : $\int_{\mathbb{R}^m} \exp -2\phi dx < +\infty$. *Show that its lowest eigenvalue is simple and determine a corresponding eigenvector.*

Exercise E.5 .
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 :*

$$\Theta_0 < \sqrt{1 - \frac{2}{\pi}}\ .$$

Problem E.6 [10]
Let V *be in* $C_0^\infty(\mathbb{R}^m)$ $(m = 1, 2)$. *Show that the essential spectrum of* $S_1 = -\Delta + V$ *is* $[0, +\infty[$.
Let us assume in addition that

$$\int_{\mathbb{R}^m} V(x)\, dx < 0\ . \tag{E.1}$$

Find $\psi \in D(S_1)$ *such that*

$$< S_1\psi, \psi >_{L^2(\mathbb{R}^m)} < 0\ .$$

When $m = 1$, *consider the family* $\psi_a = \exp -a|x|$, $a > 0$, *and, when* $m = 2$, $\psi_a(x) = \exp -\frac{1}{2}|x|^a$, $a > 0$.
Deduce that $S_1 = -\Delta + V$ *has a negative eigenvalue.*

Problem E.7 .
Let us consider in the disk of $\mathbb{R}^2$ $\Omega := D(0, R)$ *the Dirichlet realization of the Schrödinger operator*

$$S(h) := -\Delta + \frac{1}{h^2}V(x)\ , \tag{E.2}$$

[10] These counterexamples come back (when $m = 1$ to Avron-Herbst-Simon [AHS] and when $m = 2$ to Blanchard-Stubbe [BS]).

where V is a C^∞ potential on $\bar{\Omega}$ satisfying :

$$V(x) \geq 0 \,. \tag{E.3}$$

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

$$h^2 \lambda_1(h) \geq \epsilon \,. \tag{E.4}$$

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 $h > 0$,

$$\lambda_1(h) \leq C \,. \tag{E.5}$$

One can use the study of the Dirichlet realization of $-\Delta$ in ω.
e) Let us assume that :

$$V > 0 \text{ almost everywhere in } \Omega \,. \tag{E.6}$$

Show that, under this assumption :

$$\lim_{h \to 0} \lambda_1(h) = +\infty \,. \tag{E.7}$$

One could proceed by contradiction supposing that there exists C such that

$$\lambda_1(h) \leq C \,,\ \forall h \text{ such that } 1 \geq h > 0 \,. \tag{E.8}$$

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 $(n \in \mathbb{N})$ 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 explicit 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 E.8 .
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 E.9 .
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 $a \to +\infty$.

Problem E.10 *(Avron-Herbst [CFKS])*
The aim of this problem is to analyze the spectra of the operators

$$H_\pm := -\frac{d^2}{dx^2} + q(x)^2 \pm q'(x) \ ,$$

where $q(x)$ *is a polynomial :*

$$q(x) = x^m + \sum_{j=0}^{m-1} a_j x^j \ .$$

a) Show that these operators are with compact resolvent if and only if $m \geq 1$.
b) Observing that

$$H_\pm = (\frac{d}{dx} \pm q(x))(-\frac{d}{dx} \pm q(x)) \ ,$$

discuss the kernel of $H_\pm$ *in function of* m.
c) Observing that

$$H_\pm(\frac{d}{dx} \pm q(x)) = (\frac{d}{dx} \pm q(x))H_\mp \ ,$$

show that H_+ *and* H_- *have the same spectrum except possibly* 0.
d) Treat completely the case $m = 1$.
e) We assume now that $q(x) = x + gx^2$ *with* $g \neq 0$. *Show that the corresponding operators are unitary equivalent (up to a multiplicative factor) to semiclassical Schrödinger operator.*
f) Show that in this case H_+ *and* H_- *are unitary equivalent.*
g) Show that there exists a unique eigenvalue $\lambda(g)$ *which is* $o(1)$ *as* $g \to 0$.
h) Show that this eigenvalue is actually exponentially small.
i) (More difficult) Find an equivalent of $\lambda(g)$ *in the form*

$$\lambda(g) \sim \alpha |g|^k \exp -\frac{S}{g^2}$$

for suitable $\alpha > 0$, $k \in \mathbb{R}$ *and* $S > 0$.

Exercise E.11

By mimicking the WKB construction given in the course, show that, near the minimum of V_0 (which is assumed to be non degenerate), there exists a WKB solution $u^{wkb}(x,h)$ of the operator $-h^2\Delta + V_0(x)$ in the form

$$u^{wkb}(x,h) := \exp -\frac{\phi(x;h)}{h}$$

with

$$\phi(x;h) \sim \sum_j h^j \phi_j(x)$$

attached to a "formal" eigenvalue $E(h) \sim \sum_j E_j h^j$.

The reader can try a direct proof or to explore the link between this WKB solution and the WKB solution described in the course.

Exercise E.12

Solve the eikonal equation $|\nabla\Phi|^2 = V - \inf V$ near a non degenerate minimum of V formally in the sense: modulo flat function at the minimum.

Problem E.13

One would like to understand the problem on $\mathbb{R}^+$ given by the Dirichlet realization $P^D(h)$ of

$$P(h) := -h^2\frac{d^2}{dx^2} + v(x)\ ,$$

with $v'(x) \geq c > 0$ on $\overline{\mathbb{R}^+}$.

a) Show that the operator is with compact resolvent.

b) We first analyze the case $v(x) = x$, $h = 1$ (In this case the operator is called the Airy operator $A(x, D_x)$). Show that, for the Dirichlet realization A^D of A in $\mathbb{R}^+$, there exists a sequence $(\mu_j)_{j\in\mathbb{N}^*}$ of eigenvalues tending to ∞. Show that the lowest one μ_1 is strictly positive. What is the form domain $Q(A^D)$ of the Airy operator?

c) Show that the corresponding eigenfunctions u_j are in $C^\infty(\overline{\mathbb{R}^+})$.

d) Show that the eigenvalues are of multiplicity 1.

e) We admit that

$$\begin{aligned} D(A^D) &= \{u \in H^1_0(\mathbb{R}^+) \cap H^2(\mathbb{R}^+); xu \in L^2(\mathbb{R}^+)\} \\ &= \{u \in H^1_0(\mathbb{R}^+)\ ,\ x^{\frac{1}{2}}u \in L^2(\mathbb{R}^+)\ ,\ A(x,D_x)u \in L^2(\mathbb{R}^+)\}\ . \end{aligned}$$

Show that the eigenvectors are in $\mathcal{S}(\overline{\mathbb{R}^+})$.

Another approach could be to analyze the Fourier transform of χu_j where χ

is equal to 1 *for* x *large and is equal to* 0 *in a neighborhood of* 0.
f) Describe the spectrum of $A^D(x, hD_x)$ *for any* $h > 0$.
g) We come back to the general case. Transpose for $P^D(h)$ *what was done for the one-well problem via the harmonic approximation, the harmonic oscillator being replaced by the Airy operator. The student can use if needed that* $(A^D(x, D_x) - \mu_1)$ *is a bijection from* $\mathcal{S}_0(\overline{\mathbb{R}^+}) \cap \{\mathbb{R}u_1\}^\perp$ *onto* $\mathcal{S}(\overline{\mathbb{R}^+}) \cap \{\mathbb{R}u_1\}^\perp$ *where*

$$\mathcal{S}_0(\overline{\mathbb{R}^+}) = \{u \in \mathcal{S}(\overline{\mathbb{R}^+}) \text{ s. t. } u(0) = 0\} .$$

Problem E.14 .
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* $\alpha \in \mathbb{R}$.

5. *Show that* $\alpha \mapsto \lambda(\alpha)$ *is a continuous function on* $\mathbb{R}$.

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 $\mathbb{R}^+$ of a function in $\mathcal{S}(\mathbb{R})$. Let, for $\alpha \in \mathbb{R}$, T_α be the distribution in $\mathcal{D}'(\mathbb{R}^+ \times \mathbb{R})$ 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 E.15 .
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 $a \to +\infty$.

Exercise E.16
Using Agmon's inequalities, show that any eigenfunction of $-\frac{d^2}{dx^2} + x^4$ *decays exponentially at* ∞.

Exercise E.17
Using refined Agmon estimates, analyze the decay of the groundstate of the Dirichlet realization of $-h^2 \frac{d^2}{dx^2} + v(x)$ *on* $\mathbb{R}^+$, *under the assumption that* $v' > \delta \geq 0$.

Problem E.18
One would like some spectral properties of the family of operators :

$$P_\beta = D_t^2 + (t^2 - \beta)^2 \; .$$

a) Define the Friedrichs extension starting of $C_0^\infty(\mathbb{R})$ *and show that the operator is with compact resolvent.*
b) We denote by $\lambda_1(\beta)$ *the smallest eigenvalue of* P_β. *Show that* $\beta \mapsto \lambda_1(\beta)$ *is a continuous function of* β.
c) Show that as $\beta \leq 0$, $\beta \mapsto \lambda_1(\beta)$ *is a monotone function of* β.
d) Analyze the behavior of $\lambda_1(\beta)$ *as* $\beta \to -\infty$. *Find first the universal lower bound :*

$$\lambda_1(\beta) \geq \beta^2 \; .$$

e) Using a scaling and a semiclassical analysis, give an asymptotics of $\lambda_1(\beta) - \beta^2$ *as* $\beta \to -\infty$.
e) Using a scaling and a semiclassical analysis, give an asymptotics of $\lambda_1(\beta)$ *as* $\beta \to +\infty$.
f) Show that as $\beta \to +\infty$, $\lambda_2(\beta)$, *the second eigenvalue, has the same asymptotics as* $\lambda_1(\beta)$.
g) Give the asymptotics of $\lambda_3(\beta)$ *as* $\beta \to +\infty$.
h) Find an upperbound, as accurate as possible, for $\lambda_2(\beta) - \lambda_1(\beta)$.
i) Show that $\beta \mapsto \lambda_1(\beta)$ *has at least one minimum over* $\mathbb{R}$, *which belongs to* $[0, +\infty[$.
j) One admits that $\beta \mapsto \lambda_1(\beta)$ *is of class* C^1 *and simple. Let* u_β^1 *the corresponding* L^2*-normalized strictly positive eigenvector. Admitting that* $\beta \mapsto u_\beta^1$ *is of class* C^1, *show that*

$$\lambda'(\beta) = -2 \int (t^2 - \beta)(u_\beta^1)^2(t)\,dt \; .$$

Deduce that the minimum should be in $]0, +\infty[$.