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

Bernard Helffer

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1 Introduction

Our aim is to describe in these notes 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.

The reader 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spectral theory, Reed-Simon is more than enough and the reader can also look at [LB] (in french) or to the notes of an unpublished course [Hel7].

We will sometimes give detailed proofs but in other cases we will just give some hints and refer to the original references or, in the case when semi-classical analysis is involved, to the books [Hel1] and [DiSj]. Other references 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 [Hel3, Hel4], Mohamed-Raikov [MoRa], [Hel5] 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) [Ma2].

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 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 conclude by two applications to the analysis of 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. After the bibliography, we have added (mainly at te attention of the students), a few appendices on basic topics in spectral theory and propose also typical exercises illustrating the subject.

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2 On the Schrödinger operators 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^∞ vector field on $\overline{\Omega}$, corresponding to the so called magnetic potential, and V (which may depend[1] 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 :

$$\vec{B} = (B^1, B^2, B^3) = (B_{23}, -B_{13}, B_{12}) \ . \tag{2.3}$$

All these objects can be defined more generally on a Riemannian manifold (with notions like connections, curvature, ...) but it is outside the aim of

[1] Typically, one can meet $V(x; h) = V_0(x) + hV_1(x)$.

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 $P_{h,A,V,\Omega}$. The open set Ω can be bounded or the whole space $\mathbb{R}^n$. Many physically interesting situations correspond to $n = 2, 3$. In the case of a bounded 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 :

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

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 and 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 :

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

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

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

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

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

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

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

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

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

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

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

In the general case, if the operator is semi-bounded on $C_0^\infty(\mathbb{R}^n)$ in the sense of (2.5), it has been proved by Simader [Sima] (see also [Hel7]) 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 :

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

2.3 Spectral theory

All the operators introduced above are selfadjoint. If one denotes by P one of these operators, one can analyze its 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 $\operatorname{Ker}(P-\lambda)$. 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 (which is 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 correspond to an eigenvalue or to the bottom of the essential spectrum.
Using the MiniMax characterization (see appendix B), this bottom is determined by

$$\inf(\sigma(P_{h,A,V})) = \inf_{u \in \mathcal{V} \setminus 0} Q_{h,A,V}(u)/||u||^2 \,, \tag{2.14}$$

where $\mathcal{V}$ denotes the form domain of the quadratic form $Q_{h,A,V}$.
It is consequently enough, in order to determine if the bottom corresponds to an eigenvalue, to find a non trivial u in the form domain $\mathcal{V}$, 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).

Example 2.1 .
Let us consider $P_{h,V} := -h^2\Delta + V$ 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 P_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 $\phi_h(x) = \exp -\frac{\lambda}{h}|x - x_{min}|^2$ and $\lambda > 0$, the quotient $\frac{<P_h\phi_h,\phi_h>}{||\phi_h||^2}$ tends as $h \to 0$ to $V(x_{min}) < 0$.
Actually, we can produce a arbitrary number N of eigenvalues below the essential spectrum, under the condition that $0 < h \leq h_N$.

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 2.2 .
There exists a constant L_m, such that, for any V such that $V_- \in L^{\frac{m}{2}}(\mathbb{R}^m)$, and if $m \geq 3$, the number N_- of strictly negative eigenvalues of $P_V = -\Delta + V$ is finite and bounded by

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

This shows that we could have, when $m \geq 3$, examples of negative potentials V (which are not identically zero) and such that the corresponding Schrödinger operator P_V has no eigenvalues. A sufficient condition is indeed

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

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-Rozenbljum) 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 2.3 *(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 $P=-\Delta+V$ 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.

Remark 2.4
Note that these estimates are also true, with the same constants, with $-\Delta$ replaced by $-\Delta_A=\sum_{j=1}^n(D_{x_j}-A_j)^2$. But this is not a consequence of the direct comparison of $-\Delta+V$ and $-\Delta_A+V$, but it comes simply from the fact that the proof for the case without magnetic field can be extended with the same constants.

Remark 2.5
If we reinsert the semi-classical parameter by looking at $P_{h,V}=-h^2\Delta+V$ one can establish (Helffer-Robert [HeRo2]) under suitable assumptions on V the asymptotic estimate

$$\sum_{\lambda_j<0}(-\lambda_j)^s \sim C_{s,n}h^{-n}\int_{V<0}(-V)^{\frac{n}{2}+s}dx\ . \tag{2.20}$$

The effect of a magnetic field is also discussed in this paper and in [LaWe]. Note that in this case the semi-classical Laplacian $-h^2\Delta$ is replaced by

$$-\Delta_{h,A}=-(h\nabla-iA)^2\ , \tag{2.21}$$

and that the main term is independent of the magnetic potential.

2.5 Diamagnetism

Everything being universal in this discussion, we take $h=1$. By Kato's inequality (cf for example [CFKS]), which says that, for all $u\in H^1_{loc}$, for all j,

$$|\partial_j|u||\leq|(\partial_j-iA_j)u|\ ,\ a.e.\ , \tag{2.22}$$

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 :

$$\inf \ \mathrm{Sp} \ \left(P^D_{A,\Omega} + V\right) \geq \inf \ \mathrm{Sp} \ \left(-\Delta^D_\Omega + V\right) \ , \tag{2.23}$$

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

$$\inf \ \mathrm{Sp} \ \left(P^N_{A,\Omega} + V\right) \geq \inf \ \mathrm{Sp} \ \left(-\Delta^N_\Omega + V\right) \ , \tag{2.24}$$

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

Proposition 2.6
Let λ_A be the ground state of P_A, 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 on the circulation of $\vec{A}$ along any closed path.
Let us just present an heuristic proof (see for example [Hel2] for a rigourous proof or [Hel1] in connection with the Bohm-Aharonov effect) which permits to understand this last point. For $u \in H^1$, one can write $u = \rho \exp i\phi$. One has :

$$|(\nabla - iA)u|^2 = |\nabla \rho|^2 + \rho^2 |\nabla \phi - A|^2 \ .$$

If we apply this identity to $u = u_A$ where u_A is a normalized ground state, we obtain :

$$\begin{array}{ll} \lambda_A & = \int_\Omega \left(|(\nabla - iA)u_A|^2 + V|u_A|^2\right) \ dx \\ & = \int_\Omega \left(|\nabla \rho_A|^2 + V|\rho_A|^2\right) dx + \int_\Omega \ \rho_A^2 |\nabla \phi - A|^2 \ dx \\ & \geq \lambda_0 + \int_\Omega \left(\rho_A^2 |\nabla \phi - A|^2\right) dx \ . \end{array}$$

When $\lambda_A = \lambda_0$, we get $\nabla \phi = A$, which implies the various statements. One immediatly deduces that ω_A is closed and due to the fact that ϕ is defined modulo 2π, we get

$$\frac{1}{2\pi} \int_\gamma \omega_A \in \mathbb{Z} \tag{2.25}$$

on any closed path γ.
Conversely, if this condition is satisfied, the multivalued function ϕ defined by :

$$\phi(x) = \int_{\gamma(x_0, x)} \omega_A \ ,$$

where $\gamma(x_0, x)$ is a path in Ω joining x_0 and x, permits to define the C^∞ function on Ω

$$\Omega \ni x \mapsto U(x) = \exp -i\phi(x) \ . \tag{2.26}$$

The associated multiplication operator U gives a the unitary equivalence with the problem with $A = 0$.

Remark 2.7
It is instructive to look at the model of the circle and at the magnetic Laplacian $-(\frac{d}{d\theta} - ia)^2$, where a is a real constant corresponding to the magnetic potential. So the magnetic field is zero and the spectrum can be easily found to be described by the sequence $(n-a)^2$ $(n \in \mathbb{Z})$ with corresponding eigenvectors $\theta \mapsto \exp in\theta$.
We immediately see that, confirming the general statement, the ground state energy, which is equal to $\mathrm{dist}\,(a, \mathbb{Z})^2$, increases when a magnetic potential is introduces. We also observe that the multiplicity of the groundstate is 1 except when $d(a, \mathbb{Z}) = \frac{1}{2}$. We note finally that if we take $\lambda = 1$, the number of eigenvalues which is strictly less than 1, is 1 for $a = 0$, and 2 for $a \in]0, 1[$. This illustrates our previous comment on Cwickel-Lieb-Rozenblium in Remark 2.4.

2.6 Very rough estimates for the Dirichlet realization

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

$$||\nabla_{h,A} u||^2 = \langle P_{h,A,\Omega} u \mid u \rangle \geq h \int_\Omega B(x) |u(x)|^2 dx \ , \ \forall u \in C_0^\infty(\Omega) \ , \tag{2.27}$$

which is interesting only if assuming $B \geq 0$.
Here the basic point is to observe that :

$$hB(x) = \frac{1}{i} [h\partial_{x_1} - iA_1, h\partial_{x_2} - iA_2] \ . \tag{2.28}$$

We then write

$$hB(x) u(x)\, \bar{u}(x) = \frac{1}{i} (X_1 X_2 u)(x)\, \bar{u}(x) - \frac{1}{i} (X_2 X_1 u)(x)\, \bar{u}(x) \ ,$$

with $X_j = h\partial_{x_j} - iA_j$.
Integrating over Ω and performing the integration by parts :

$$h \int_\Omega B(x) |u(x)|^2 dx = -\frac{1}{i} \langle X_1 u \mid X_2 u \rangle + \frac{1}{i} \langle X_2 u \mid X_1 u \rangle \ .$$

It remains then to use Cauchy-Schwarz Inequality.
This leads for the Dirichlet realization and when $B(x) \geq 0$, to the easy but useful estimate :

$$\inf \sigma(P^D_{h,A}) \geq h \inf_{x\in\overline{\Omega}} B(x) := hb \;. \tag{2.29}$$

Note that the converse is asymptotically (as $h \to 0$) true. The proof is rather easy. 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

$$u(x; h) := b^{\frac{1}{4}} h^{-\frac{1}{2}} \exp -\rho\sqrt{b}\frac{|x|^2}{h}\chi(x) \;,$$

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 and to $h = 1$:

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

with

$$u_\rho(y) = b^{\frac{1}{4}} \exp -\rho\sqrt{b}y^2 \;. \tag{2.30}$$

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 :

$$\inf \sigma(P^D_{h,A}) \leq hb + \mathcal{O}(h^{\frac{3}{2}}) \;. \tag{2.31}$$

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

Theorem 2.8 .
The smallest eigenvalue $\lambda^{(1)}(h)$ of the Dirichlet realization $P^D_{h,A,\Omega}$ of $P_{h,A,\Omega}$ satisfies :

$$\frac{\lambda^{(1)}(h)}{h} = b + o(1) \;. \tag{2.32}$$

[2]We leave to the reader the proof for the case when the minimum of $|B(x)|$ is attained at the boundary. One can for example take a sequence of Gaussians centered at a sequence of points tending to one point of the boundary, where B takes its minimum. This affects only the remainder term.

Let us state the theorem in the more general case (cf [Mel], [Ho] (Vol. III, Chapter 22.3) and [HelMo2]). Let us extend at each point B_{jk} as an antisymmetric matrix (more intrinsically, this is the matrix of the two-form σ_B). Then the eigenvalues of iB are real and one can see that if λ is an eigenvalue 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 define

$$\mathrm{Tr}^+ B(x) = \sum_{\lambda_j(x)>0} \lambda_j(x) \; . \tag{2.33}$$

The extension of the previous result is then :

Theorem 2.9 .
The smallest eigenvalue $\lambda^{(1)}(h)$ of the Dirichlet realization $P^D_{h,A,\Omega}$ of $P_{h,A,\Omega}$ satisfies :

$$\frac{\lambda^{(1)}(h)}{h} = \inf_{x\in\Omega} \mathrm{Tr}^+(B(x)) + o(1) \; . \tag{2.34}$$

The idea for the proof 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, with $\partial_j = \partial/\partial x_j$, for $n = 2d$, the model

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

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

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

with

$$\sum_{j=1}^{d} |b_j| = \mathrm{Tr}^+ B \; .$$

2.7 Magnetic bottles

This problematic in mathematical physics was introduced by Avron-Herbst-Simon [AHS] and then discussed by many authors including Colin de Verdière and Helffer-Mohamed [HelMo1](see later Kondratiev-Mazya-Shubin [KoMaSh] and references therein). The question was to analyze the question of compact resolvent when there is no electric field. In the case of dimension 2 the previous trivial inequality (2.27) shows that in the case of $\Omega = \mathbb{R}^2$ and if $B(x) \to +\infty$ as $|x| \to +\infty$, then the magnetic Schrödinger operator has 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. The folk theorem that the condition $|B(x)| \to +\infty$ is sufficient is wrong when the dimension is larger than 3. Counterexamples have been given by Dufresnoy and Iwatsuka. This shows that it is in some sense necessary to control the variation of B in suitable balls. We just mention here the following result of [HelMo1]. Let us introduce, for any $k \geq 0$,

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

Theorem 2.10
Suppose that $\Omega = \mathbb{R}^n$ and that there exists $r \geq 0$ and C such that :

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

Then $P_A = -\Delta_A$ has 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 (2.27) which gives a comparison between selfadjoint operators in the form (for any $\rho \in [0, 1]$)

$$P^D_{h,A} \geq \rho(P^D_{h,A}) + (1-\rho)hB(x)\ . \tag{2.35}$$

The operator on the right hand side of (2.35) 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 optimize over ρ a rough lower bound for the operator :

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

We shall show as quite preliminary result the following proposition, which improves Theorem 2.8 :

Proposition 2.11 .
Under the condition that $x \mapsto B(x)$ is ≥ 0, analytic and strictly larger that $b = \inf_{x\in\Omega} B(x)$ at the boundary, then there exist $\vartheta > 0$ and $C > 0$ such that :

$$\lambda^{(1)}(h) - bh \geq \frac{1}{C} h^{1+\frac{1}{\vartheta}}\ , \tag{2.36}$$

where $b = \inf_{x\in\mathbb{R}^2} B(x)$.

Proof :
We use the Lieb-Thirring bounds for the Schrödinger operator $-\Delta + V_\epsilon$ (see (2.19) and [BeHeVe]) with $V_\epsilon(x) = \frac{1}{2\epsilon}(B(x)-b)$ and $\epsilon = \rho h$.
This gives[3], for any $\lambda > 0$,

$$\sum_{\lambda_j(\epsilon)<\lambda} (\lambda - \lambda_j(\epsilon)) \leq C \int_{V_\epsilon(x)<\lambda} (\lambda - V_\epsilon(x))^2 dx\ .$$

where $\lambda_j(\epsilon)$ denotes the sequence of eigenvalues of $-\Delta + V_\epsilon$.
We now take $\lambda = 2(\lambda_1(\epsilon)+\eta)$ with $\eta > 0$ and get :

$$\lambda_1(\epsilon) + \eta \leq 4C(\lambda_1(\epsilon)+\eta)^2 \left(\int_{V_\epsilon < 2(\lambda_1(\epsilon)+\eta)} dx\right)\ .$$

This gives

$$\frac{1}{4C} \leq (\lambda_1(\epsilon)+\eta) \left(\int_{V_\epsilon < 2(\lambda_1(\epsilon)+\eta)} dx\right)\ ,$$

for any $\eta > 0$. Taking the limit $\eta \to 0$, we obtain first that $\lambda_1(\epsilon) > 0$ and

$$\frac{1}{4C} \leq \lambda_1(\epsilon) \left(\int_{V_\epsilon < 2\lambda_1(\epsilon)} dx\right)\ .$$

[3]We actually apply the inequality with $(V_\epsilon - \lambda)$ replaced by $(V_\epsilon - \lambda)_-$ and combine with the minimax principle.

We now use the analyticity assumption, the set $\{V_\epsilon < 2\lambda_1(\epsilon)\}$ is the set $\{B(x)-b < 2(\epsilon\lambda_1(\epsilon))\}$. But it is easy to show by using Gaussian quasimodes as in Example 2.1, that $(\epsilon\lambda_1(\epsilon))$ tends to zero, as $\epsilon \to 0$. But the measure of $\{B(x)-b<\mu\}$ as $\mu \to 0^+$ is of order μ^ϑ for some $\vartheta > 0$, if $B(x)$ is analytic (see, for this standard result which can be shown for example via Lojaciewicz inequalities, [BeHeVe]).
So we get :

$$\frac{\epsilon}{4C} \leq C(\epsilon\lambda_1(\epsilon))^{1+\vartheta} \; .$$

Coming back to our initial problem, we finally obtain that : $\forall \rho \in]0, \frac{1}{2}]$,

$$\lambda^{(1)}(h) - (1-\rho)hb \geq \frac{h}{C}(\rho h)^{\frac{1}{1+\vartheta}} \; .$$

This can be rewritten in the form :

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

or

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

If we take $\rho = \gamma h^{\frac{1}{\vartheta}}$ and γb small enough, we get (2.36) for h small enough.

Remark 2.12 .
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 2.13 .
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 the theory of 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 of the strong magnetic field (h being fixed) case. 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 bottom 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 The case of $\mathbb{R}^2$

We would like to analyze the spectrum of P_{BA_0} more shortly denoted by :

$$S_B := (D_{x_1} - \frac{B}{2}x_2)^2 + (D_{x_2} + \frac{B}{2}x_1)^2 \ . \tag{3.3}$$

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 selfadjoint 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 U_1 is defined, for $f \in L^2(\mathbb{R}^2)$ by

$$U_1 f = \exp iB\frac{x_1x_2}{2} f \; . \tag{3.4}$$

It satisfies

$$S_B U_1 f = U_1 S_B^1 f \; , \; \forall f \in \mathcal{S}(\mathbb{R}^2) \; , \tag{3.5}$$

with

$$S_B^1 := (D_{x_1})^2 + (D_{x_2} + Bx_1)^2 \; . \tag{3.6}$$

Remark 3.1 .

U_1 is a very special case of what is called a gauge transform. More generally, as was done in the proof of Proposition 2.6 (see (2.26)), we can consider $U = \exp i\phi$, where $\exp i\phi$ 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 has constant coefficients with respect to the x_2-variable, we perform a partial Fourier transform with respect to the x_2 variable

$$U_2 = \mathcal{F}_{x_2 \mapsto \xi_2} \; , \tag{3.7}$$

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

$$S_B^2 := (D_{x_1})^2 + (\xi_2 + Bx_1)^2 \; . \tag{3.8}$$

We now introduce a third unitary transform U_3

$$(U_3 f)(y_1, \xi_2) = f(x_1, \xi_2) \; , \quad \text{with } y_1 = x_1 + \frac{\xi_2}{B} \; , \tag{3.9}$$

and we obtain the operator

$$S_B^3 := D_y^2 + B^2 y^2 \; , \tag{3.10}$$

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 $f \in L^2(\mathbb{R}_{\xi_2})$ (with $||f|| = 1$), 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 eigenspace can be given by vectors $e_j(\xi_2)|B|^{\frac{1}{4}}\ \phi_n(|B|^{\frac{1}{2}} y)$ where e_j ($j \in \mathbb{N}$) is a basis of $L^2(\mathbb{R})$.
We have consequently an empty discrete spectrum and the bottom of the spectrum (which is also the bottom of the essential spectrum) is B. The eigenvalues (which are of infinite mutiplicity!) are usually called Landau levels.

3.3 Towards the analysis of $\mathbb{R}^{2,+}$: 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. For $\xi \in \mathbb{R}$, we consider the Neumann realization $H^{N,\xi}$ in $L^2(\mathbb{R}^+)$ associated with the operator $D_x^2 + (x - \xi)^2$. It is easy to see that the operator has compact resolvent and that the lowest eigenvalue $\mu(\xi)$ of $H^{N,\xi}$ is simple. For the second point, the following simple argument can be used. Suppose by contradiction that the eigenspace is of dimension 2. Then, we can find in this eigenspace an eigenstate 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 L^2-normalized eigenstate. The minimax characterization shows that $\xi \mapsto \mu(\xi)$ is a continuous function. It is a little more work (see Kato [Ka] or the proof below) to show that the function is C^∞ (and actually analytic). 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 (see (3.12) or (3.18)). It is a little more difficult to show that

$$\lim_{\xi \to +\infty} \mu(\xi) = 1 \, . \tag{3.11}$$

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 $x \mapsto \phi_\xi(x)$, 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 quantity $\inf_{\xi \in \mathbb{R}} \inf \mathrm{Sp}\,(H^{N,\xi})$ 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 (Dauge-Helffer [DaHe] motivated by a question of C. Bolley (see [BoHe]))

$$\mu'(\xi) = -[\mu(\xi) - \xi^2]\varphi_\xi(0)^2 \, . \tag{3.12}$$

To get (3.12), 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 (3.12), it comes that, for any critical point ξ_c of μ in $\mathbb{R}^+$

$$\mu''(\xi_c) = 2\xi_c \varphi_{\xi_c}^2(0) > 0 \, . \tag{3.13}$$

So the critical points are necessarily non degenerate local minima. It is then easy to deduce, observing that $\lim_{\xi \to -\infty} \mu(\xi) = +\infty$ and $\lim_{\xi \to +\infty} \mu(\xi) = 1$, that there exists a unique minimum $\xi_0 > 0$ such that

$$\Theta_0 = \inf_\xi \mu(\xi) = \mu(\xi_0) < 1 \, . \tag{3.14}$$

Moreover

$$\Theta_0 = \xi_0^2 \, . \tag{3.15}$$

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

Around the Feynman-Hellmann formula.
Let us give additional remarks on the properties of $\xi \mapsto \mu(\xi)$ and $\varphi_\xi(\cdot)$ which are related to the Feynman-Hellmann formula. We differentiate with respect to ξ the identity[4] :

$$H^N(\xi)\varphi(\cdot;\xi) = \mu(\xi)\varphi(\cdot;\xi)\ . \tag{3.16}$$

We obtain :

$$(\partial_\xi H^N(\xi) - \mu'(\xi))\varphi(\cdot;\xi) + (H^N(\xi) - \mu(\xi))(\partial_\xi\varphi)(\cdot;\xi) = 0\ . \tag{3.17}$$

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

$$\mu'(\xi) = \langle(\partial_\xi H^N(\xi)\varphi_\xi \mid \varphi_\xi\rangle = -2\int_0^{+\infty}(t-\xi)|\varphi_\xi(t)|^2 dt\ . \tag{3.18}$$

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

$$\begin{aligned} &\langle(\partial_\xi H^N(\xi) - \mu'(\xi))\varphi(\cdot;\xi) \mid (\partial_\xi\varphi)(\cdot;\xi)\rangle \\ &\quad + \langle(H^N(\xi) - \mu(\xi))(\partial_\xi\varphi)(\cdot;\xi) \mid (\partial_\xi\varphi)(\cdot;\xi)\rangle = 0\ . \end{aligned} \tag{3.19}$$

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

$$\begin{aligned} &\langle(\partial_\xi H^N(\xi_0)\varphi(\cdot;\xi_0) \mid \partial_\xi\varphi)(\cdot;\xi_0)\rangle \\ &\quad + \langle(H^N(\xi_0) - \mu(\xi_0))(\partial_\xi\varphi)(\cdot;\xi_0) \mid (\partial_\xi\varphi)(\cdot;\xi_0)\rangle = 0\ . \end{aligned} \tag{3.20}$$

We observe that the second term is positive (and with some extra work coming back to (3.17) strictly positive) :

$$\langle(\partial_\xi H^N(\xi_0))\varphi(\cdot;\xi_0) \mid \partial_\xi\varphi)(\cdot;\xi_0)\rangle < 0\ . \tag{3.21}$$

Let us differentiate one more (3.17) with respect to ξ.

$$\begin{aligned} &2(\partial_\xi H^N(\xi) - \mu'(\xi))\partial_\xi\varphi(\cdot;\xi) \\ &+(H^N(\xi) - \mu(\xi))(\partial_\xi^2\varphi)(\cdot;\xi) \\ &+(\partial_\xi^2 H^N(\xi) - \mu''(\xi))\varphi(\cdot;\xi) = 0\ . \end{aligned} \tag{3.22}$$

Taking the scalar product with φ_ξ and $\xi = \xi_0$, we obtain from (3.21) that

$$\mu''(\xi_0) = 2 + \langle(\partial_\xi H^N(\xi_0)\varphi(\cdot;\xi_0) \mid \partial_\xi\varphi)(\cdot;\xi_0)\rangle < 2\ . \tag{3.23}$$

[4] 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.

Proposition 3.2
The eigenvalue $\mu(\xi)$ and the corresponding eigenvector ϕ_ξ are of class C^∞ with respect to ξ.

Proof :
This result (actually the analyticity) is proved in the book of Kato [Ka]. We give here an alternative proof for illustrating how the Grushin's method works. As usual, it is enough to show that, for any k and any $\xi_1 \in \mathbb{R}$, the map $\xi \mapsto \mu(\xi)$ is C^k in some neighborhood of a point ξ_1.
Step 1 :
We recall that $\mu(\xi)$ is simple. Let φ_{ξ_1} the normalized eigenvector attached to $\mu(\xi_1)$. Let us denote by $\varphi^*_{\xi_1}$ the orthogonal projection on φ_{ξ_1}. The domain of the operator can be seen as

$$D(H^N(\xi)) = \{u \in B^2(\mathbb{R}^+) \mid u'(0) = 0\}\ ,$$

where $B^2(\mathbb{R}^+) = \{u \in L^2(\mathbb{R}^+) \mid x^\alpha D_x^\beta u \in L^2(\mathbb{R}^+) \text{ for } |\alpha| + |\beta| \leq 2\}$, and we observe that it is independent of ξ. We sometimes use the notation $D(H^N(\xi)) = B^{2,N}(\mathbb{R}^+)$, when considered as an Hilbert space. We will use a variant of the so called Grushin's method. Let us introduce the unbounded operator on $L^2(\mathbb{R}^+) \times \mathbb{C}$

$$M_0 : = \begin{pmatrix} H^N(\xi_1) - \mu(\xi_1) & \varphi_{\xi_1} \\ \varphi^*_{\xi_1} & 0 \end{pmatrix}$$

with domain $D(H^N(\xi_1)) \times \mathbb{C}$. Actually, it is better to consider it as a bounded operator from $B^{2,N}(\mathbb{R}^+) \times \mathbb{C}$ into $L^2(\mathbb{R}^+) \times \mathbb{C}$
Let us show that this is actually an isomorphism. By elementary algebra, we get that the inverse is

$$R_0 = \begin{pmatrix} E_0 & E_0^+ \\ E_0^- & E_0^{+-} \end{pmatrix},$$

with :

$$E_0 = \left((H^N(\xi_1) - \mu(\xi_1))_{|\varphi^\perp_{\xi_1}}\right)^{-1}\ , \tag{3.24}$$

$$E_0^+ = \varphi_{\xi_1}\ , \tag{3.25}$$

$$E_0^- = \varphi^*_{\xi_1}\ , \tag{3.26}$$

$$E_0^{+-} = 0\ . \tag{3.27}$$

Step 2 :
Let us now introduce

$$M(\xi,\mu) = \begin{pmatrix} H^N(\xi)-\mu & \varphi_{\xi_1} \\ \varphi^*_{\xi_1} & 0 \end{pmatrix}.$$

Let us show that the inversibility is stable when ξ remains near ξ_1, and μ remains near $\mu(\xi_1)$. We observe that :

$$\begin{aligned} M(\xi,\mu) &= M_0 + \begin{pmatrix} (H(\xi)-H(\xi_1))-(\mu-\mu(\xi_1)) & 0 \\ 0 & 0 \end{pmatrix} \\ &= M_0 \left(\mathrm{Id} + R_0 \begin{pmatrix} (H^N(\xi)-H^N(\xi_1))-(\mu-\mu(\xi_1)) & 0 \\ 0 & 0 \end{pmatrix}\right). \end{aligned}$$

But the map $\xi \mapsto H^N(\xi)$ is continuous from $\mathbb{R}$ into $\mathcal{L}(B^{2,N}, L^2)$. So the result is clear and the inverse can be given for (ξ,μ) close to $(\xi_1,\mu(\xi_1))$, by the convergent Neumann series :

$$M(\xi,\mu)^{-1} = \sum_{j\in\mathbb{N}} (-1)^j \left(R_0 \begin{pmatrix} (H(\xi)-H(\xi_1))-(\mu-\mu(\xi_1)) & 0 \\ 0 & 0 \end{pmatrix}\right)^j R_0. \tag{3.28}$$

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 3.3
For any k, there exists a neighborhood of $(\xi_1,\mu(\xi_1))$, such that the inverse of $M(\xi,\mu)$ exists and is a C^k map with values in $\mathcal{L}(L^2\times\mathbb{C}\,,\,B^{2,N}\times\mathbb{C})$.

Proof of Lemma 3.3 :
It is clear that

$$(\xi,\mu) \mapsto T(\xi,\mu) = R_0 \begin{pmatrix} (H(\xi)-H(\xi_1))-(\mu-\mu(\xi_1)) & 0 \\ 0 & 0 \end{pmatrix} \tag{3.29}$$

is C^∞. Let us also observe that :

$$M(\xi,\mu)^{-1} = \sum_{j\in\mathbb{N}} (-1)^j T^j(\xi,\mu) R_0\,, \tag{3.30}$$

for (ξ,μ) near $(\xi_1,\mu(\xi_1))$ and that we can get the convergence is C^k.
Consider

$$r(\xi,\mu) = (H(\xi) - H(\xi_1)) - (\mu - \mu(\xi_1))\ .$$

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

$$\begin{array}{rcl} \partial_\xi r(\xi,\mu) & = & \partial_\xi H(\xi) = -2(t-\xi) \\ \partial_\mu r(\xi,\mu) & = & -1. \end{array} \tag{3.31}$$

In view of (3.30), we will estimate $T(\xi,\mu)^j$:

$$\begin{array}{rl} \left(R_0 \begin{pmatrix} r(\xi,\mu) & 0 \\ 0 & 0 \end{pmatrix}\right)^j & = \left(\begin{pmatrix} E_0 & \varphi_{\xi_1} \\ \varphi^*_{\xi_1} & 0 \end{pmatrix} \begin{pmatrix} r(\xi,\mu) & 0 \\ 0 & 0 \end{pmatrix}\right)^j \\ & = \begin{pmatrix} (E_0 r(\xi,\mu))^j & 0 \\ (\varphi^*_{\xi_1} r(\xi,\mu))(E_0 r(\xi,\mu))^{j-1} & 0 \end{pmatrix}. \end{array} \tag{3.32}$$

So

$$M(\xi,\mu)^{-1} = \textstyle\sum_{j\in\mathbb{N}} (-1)^j \begin{pmatrix} (E_0 r(\xi,\mu))^j & 0 \\ (\varphi^*_{\xi_1} r(\xi,\mu))(E_0 r(\xi,\mu))^{j-1} & 0 \end{pmatrix} R_0\,. \tag{3.33}$$

It is then easy that each term is C^∞ and that, k being fixed, everything converges in C^k in a suitable neighborhood of $(\xi_1,\mu(\xi_1))$.

Lemma 3.4
For (ξ,μ) in a neighborhood of $(\xi_1,\mu(\xi_1))$. μ is an eigenvalue of $H^N(\xi)$ if and only if $E^{+-}(\xi,\mu) = 0$.
Moreover, $E^+(\xi,\mu)$ is then an eigenstate of $H^N(\xi)$ with eigenvalue μ.

Proof of Lemma 3.4 :
Again this is simple linear algebra. Expressing that $R(\xi,\mu)$ is the inverse of $M(\xi,\mu)$ gives :

$$E(\xi,\mu)(H(\xi)-\mu) + E^+(\xi,\mu)\varphi^*_{\xi_1} = \mathrm{Id} \tag{3.34}$$
$$E^-(\xi,\mu)\varphi_{\xi_1} = 1 \tag{3.35}$$
$$E(\xi,\mu)\varphi_{\xi_1} = 0 \tag{3.36}$$
$$E^-(\xi,\mu)(H(\xi)-\mu) + E^{+-}(\xi,\mu)\varphi^*_{\xi_1} = 0 \tag{3.37}$$
$$(H(\xi)-\mu)E(\xi,\mu) + \varphi_{\xi_1}E^-(\xi,\mu) = \mathrm{Id} \tag{3.38}$$
$$\varphi^*_{\xi_1}E^+_{\xi,\mu} = 1 \tag{3.39}$$
$$(H(\xi)-\mu)E^+(\xi,\mu) + \varphi_{\xi_1}E^{+-}(\xi,\mu) = 0 \tag{3.40}$$
$$\varphi^*_{\xi_1}E(\xi,\mu) = 0. \tag{3.41}$$

Taking the composition of $E^+(\xi,\mu)$ with (3.37) on the left, we get

$$E^+(\xi,\mu)E^-(\xi,\mu)(H(\xi)-\mu)+E^{+-}(\xi,\mu)E^+(\xi,\mu)\varphi^*_{\xi_1}=0\,,$$

so

$$E^+(\xi,\mu)\varphi^*_{\xi_1}=-\frac{E^+(\xi,\mu)E^-(\xi,\mu)(H(\xi)-\mu)}{E^{+-}(\xi,\mu)}. \tag{3.42}$$

This quantity (3.42) is well defined if $E^{+-}(\xi,\mu)\neq 0$. So using (3.34) et(3.42) we get,

$$(H(\xi)-\mu)^{-1}=E(\xi,\mu)-\frac{E^+(\xi,\mu)E^-(\xi,\mu)}{E^{+-}(\xi,\mu)}. \tag{3.43}$$

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 (3.40), $E^+(\xi,\mu)$ is an eigenvector as soon that $E^+(\xi,\mu)$ is different from 0. But $E^+\,(\xi_1,\mu(\xi_1))=E_0^+=\varphi_{\xi_1}$ 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 $(\xi_1,\mu(\xi_1)$. But by elementary computations, we have

$$E^{+-}(\xi,\mu)=\sum_{j\geq 1}(-1)^j(\varphi^*_{\xi_1}r(\xi,\mu))(E_0r(\xi,\mu))^{j-1}\varphi_{\xi_1}\,. \tag{3.44}$$

The derivatives at $(\xi_1,\mu(\xi_1))$ are easily computed as :

$$\begin{aligned}
\partial_\xi E^{+-}(\xi_1,\mu(\xi_1)) &= -\varphi^*_{\xi_1}\partial_\xi r(\xi_1,\mu(\xi_1))\varphi_{\xi_1} && (3.45)\\
&= 2\int_{\mathbb{R}^+}(t-\xi_1)\varphi^2_{\xi_1}(t)\,dt && (3.46)\\
\partial_\mu E^{+-}(\xi,\mu(\xi_1)) &= -1. && (3.47)
\end{aligned}$$

In particular $(\partial_\mu E)^{+-}(\xi_1,\mu(\xi_1))\neq 0$ and the implicit function theorem leads to :

Lemma 3.5
For any k, there exists $\eta>0$ and a C^k map $\tilde\mu$ on $]\xi_1-\eta,\xi_1+\eta[$ such that

$$\forall\xi\in]\xi_1-\eta,\xi_1+\eta[,\ \forall\mu\in]\mu(\xi_1)-\eta,\mu(\xi_1)+\eta[,\ E^{+-}(\xi,\mu)=0\Longleftrightarrow\mu=\tilde\mu(\xi).$$

We then obtain a C^k 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_1. By uniqueness, we get that for $|\xi-\xi_1|$ small enough $\tilde\mu(\xi)=\mu(\xi)$.

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

$$\inf \sigma(S_B^{N,\mathbb{R}^{2,+}}) = |B| \inf \mu(\xi) = \Theta_0 |B| \ . \tag{3.48}$$

Similarly, for the Dirichlet realization, we find (See Problem E.13, for details) :

$$\inf \sigma(S_B^{D,\mathbb{R}^{2,+}}) = |B| \inf_{\xi \in \mathbb{R}} \lambda(\xi) = |B| \ . \tag{3.49}$$

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 :

$$\lim_{\alpha \to 0} \frac{\mu^{corn}(\alpha)}{\alpha} = \frac{1}{\sqrt{3}} \ . \tag{3.50}$$

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

$$\mu^{corn}(\alpha) \leq \frac{\alpha}{\sqrt{3 + \alpha^2}} \ , \tag{3.51}$$

which gives (3.50) 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 :

$$\lambda^{(1)}(b, D(0,R)) - b \sim 2^{\frac{3}{2}}\pi^{-\frac{1}{2}}b^{\frac{3}{2}}R\exp(-\frac{bR^2}{2}) . \tag{3.52}$$

The Neumann case is treated in the paper by Baumann-Phillips-Tang [BaPhTa] (Theorem 6.1, p. 24) (see also [PiFeSt] and [HelMo3]) who prove the

Proposition 3.7

$$\mu^{(1)}(b, D(0,R)) = \Theta_0 b - 2M_3\,\frac{1}{R}\,b^{\frac{1}{2}} + \mathcal{O}(1) . \tag{3.53}$$

Here we recall that Θ_0 was introduced in (3.14), 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 changing $\frac{1}{R}$ into $-\frac{1}{R}$ (with a weaker control of the remainder term). 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. Except some aspects related to magnetic fields, this part is very standard and we refer to [CFKS, Hel1, DiSj] for a more complete description of the results.

4.1 Upper bounds

4.1.1 The case of the one dimensional Schrödinger operator

We start with the simplest one-well problem:

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

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

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

with [5]

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

[5] 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 $u_1^h(x)$.

which can be obtained recursively by

$$u_n^1 = c_n(\frac{d}{dy} - \sqrt{\frac{v''(0)}{2}} y) u_{n-1}^1 \,,$$

where c_n is a normalization constant.
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. Note here that the H^1-norm of this function over the complementary of a neighborhood of 0 is exponentially small as $h \to 0$.
We now get

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

The coefficients corresponding to the commutation of $P_{h,v}$ 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, observing that

$$|v(x) - \frac{1}{2} v''(0) x^2| \leq C |x|^3 \,, \quad \text{for } |x| \leq 1 \,,$$

as $\mathcal{O}(h^{\frac{3}{2}})$. Then the spectral theorem gives the existence for $P_{h,v}$ 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

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

4.1.2 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 diagonalizing 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 by $h\sum_j \sqrt{\frac{\lambda_j}{2}} + \mathcal{O}(h^{\frac{3}{2}})$ as in the one-dimensional case.

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 [Si] and also [CFKS]) (another approach is described in [Hel1] and another variant in [DiSj]). The reader can look at Chapter 11 of [CFKS].

Given a covering of $\mathbb{R}^n$, by balls of radius R $B(x^j, R)$ $(j \in \mathcal{J})$ and a corresponding partition of unity, such that, for an R-independent constant,

$$\begin{array}{l} \sum_{j\in\mathcal{J}} (\phi_j^R)^2 = 1\ ,\\ \sum_{\ell=1}^n \sum_{j\in\mathcal{J}} |D_{x_\ell}\phi_j^R|^2 \leq \frac{C}{R^2}\ , \end{array} \tag{4.10}$$

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

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

We can in addition assume that either the balls are centered at the minima of V (denoted by x_{j_k}, $k \in \mathcal{K}$), or that the balls are at a distance at least $\frac{1}{C}R$ of these minima.
In the first case, using the fact that the minimas of V are non degenerate, we get :

$$|\langle P_{h,V}\phi_j^R u \mid \phi_j^R u\rangle \geq \frac{R^2}{C}||\phi_j^R u||^2 \ .$$

In the second case, we observe that :

$$|\,\langle P_{h,V}\phi_j^R u \mid \phi_j^R u\rangle - \langle P_{h,V}^k \phi_j^R u \mid \phi_j^R u\rangle\,| \leq CR^3 ||\phi_j^R u||^2 \ ,$$

where $P_{h,V}^k$ is the quadratic approximation model at the minimum x^{j_k} (replace V by its quadratic approximation $V^k(x) = \inf V + \frac{1}{2}\langle V''(x^{j_k})(x - x^{j_k} \mid (x - x^{j_k}\rangle)$ if the ball is centered at the minimum.

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

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

where the infimum is over the various minima x^{j_k} (assumed to be non degenerate) and $\mu_1(h, x^{j_k})$ denotes the lowest eigenvalue of the harmonic approximation at x^{j_k} $P_{h,V}^k$.
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

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

where A_j^0 is a linear magnetic potential attached to the constant magnetic field $B_{jk} = B_{jk}(0)$,

$$A_j^0(x) = \frac{1}{2}\left(\sum_k B_{jk}x_k\right) \ ,$$

so that in a suitable gauge (note that by a linear gauge, one can first reduce to the case when $A(0) = 0$) is such that $A(x) - A^0(x) = \mathcal{O}(|x|^2)$.

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

$$h\left(\sum_{j=1}^{n}(D_{y_j} - A_j^0)^2 + \frac{1}{2}\langle V''(0)y \mid y\rangle\right) \ ,$$

whose spectrum can be determined explicitely (see [Mel], [Ho] (Vol III) and more specifically for this case [Mat]). One then get easily the upper bound.

2-dimensional harmonic oscillator.

Let us treat the 2-dimensional case as an exercice. We start from

$$D_{x_1}^2 + (D_{x_2} + Bx_1)^2 + \frac{\lambda_1}{2}x_1^2 + \frac{\lambda_2}{2}x_2^2 \ .$$

A partial Fourier transform, leads to

$$D_{x_1}^2 + (\xi_2 + Bx_1)^2 + \frac{\lambda_1}{2}x_1^2 + \frac{\lambda_2}{2}D_{\xi_2}^2 \ .$$

A dilation leads to the standard Schrödinger operator

$$D_t^2 + D_s^2 + (\sqrt{\frac{\lambda_2}{2}}s + Bt)^2 + \frac{\lambda_1}{2}t^2 \ .$$

So we have proved the isospectrality of the initial operator to a standard Schrödinger operator, with potential

$$V^{new}(s,t) = (\sqrt{\frac{\lambda_2}{2}}s + Bt)^2 + \frac{\lambda_1}{2}t^2$$

Its groundstate is immediately computed as

$$\lambda(B) = \sqrt{\lambda(0)^2 + B^2} \text{ with } \lambda(0) = \left(\sqrt{\lambda_1} + \sqrt{\lambda_2}\right)/\sqrt{2}\,.$$

On this explicit formula, one immediately sees the diamagnetic effect announced in Subsection 2.5 and also that

$$\lambda(B) - |B| \leq \lambda(0)\,,$$

which is more specific of the quadratic case.

Lower bounds.
The lower bound is obtained similarly once we have observed that

$$\begin{aligned} &\mathrm{Re}\,\langle P_{h,A,V}u \mid u\rangle \\ &\quad = \textstyle\sum_j \langle P_{h,A,V}\phi_j^R u \mid \phi_j^R u\rangle - h^2 \sum_{j,\ell} |||D_{x_\ell}\phi_j^R|u||^2\,. \end{aligned} \tag{4.13}$$

4.3.2 Magnetic wells

We would like to describe the rather generic case when $B(z) \in C^\infty(\overline{\Omega})$ satisfies, for some $z_0 \in \Omega$:

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

and we assume that the minimum is non degenerate :

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

We introduce in this case the notation :

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

Theorem 4.1 .
If $A \in C^\infty(\overline{\Omega};\mathbb{R}^2)$, *and if the hypotheses (4.14) and (4.15) are satisfied, then*

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

The detailed proof can be found in [HelMo3]. 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 [Mon] in connexion with subriemannian geometry. We will discuss a toy model of this type when presenting the Grushin's method.

4.4 Higher order expansion

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

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

that we can rewrite, using the Taylor expansion at 0 of V_0 and V_1 by formal expansions :

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

This approach was developed by B. Simon [Si] and variants have been also described by Helffer-Mohamed [HelMo2].
We can then find a complete expansion by recursion. One can look for a formal quasimode in the form $h^{-\frac{n}{4}}\left(\sum_{j\in\mathbb{N}} h^{\frac{j}{2}}\phi_j(x/\sqrt{h})\right)$ associated to an approximate eigenvalue $\sum_{j\in\mathbb{N}}\alpha_j h^j$ and determine the α_j's and ϕ_j's by recursion.

Another idea will be to introduce a Grushin's problem. This will be explained in Section 5. A third idea is to construct WKB expansions (see Section 6).

5 Grushin's problem and higher expansions

This method (as initiated by Grushin [Gru] and Sjöstrand [Sj] in the context of hypoellipticity) is also called the Feschbach's projection method (and is analogous to what is done in bifurcation theory under the name of Lyapounov-Schmidt reduction)(see also Combes [Co] and Martinez [Ma2] in the context of the Born-Oppenheimer approximation). This was also applied in the context of Solid State Physics in [HelSj8]. We have already seen how to use it in the analysis of the model on $\mathbb{R}^+$. We will present two other 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 $y \mapsto V(h^{\frac{1}{2}}y)$ at 0, the operator $h\,H(h)$, with

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

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

$$P_0 := H_0 - \mu_0 \,, \tag{5.5}$$

R_0^+ is the operator in $\mathcal{L}(\mathbb{R}, L^2(\mathbb{R}^n))$ defined by :

$$\lambda \mapsto \lambda \psi_0(y) \,, \tag{5.6}$$

and R_0^- is defined in $\mathcal{L}(L^2(\mathbb{R}^n),\mathbb{R})$ by

$$f \mapsto (R_0^- f) = \int_{\mathbb{R}^n} f(y)\psi_0(y)\, dy \; . \tag{5.7}$$

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

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

We also verify that :

$$R_0^- R_0^+ = I \; , \; R_0^+ R_0^- = \Pi_0 \; , \tag{5.8}$$

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

$$(\Pi_0 f)(y) = (\int_{\mathbb{R}^n} f(y)\psi_0(y) dy)\psi_0(y) \; . \tag{5.9}$$

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

$$\mathcal{E}_0 = \begin{pmatrix} E_0 & R_0^+ \\ R_0^- & 0 \end{pmatrix} \; , \tag{5.10}$$

where

$$E_0 := (I - \Pi_0)(P_0)^{-1}(I - \Pi_0) \; . \tag{5.11}$$

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

$$\mathcal{P}(z) = \begin{pmatrix} (P-z) & R_0^+ \\ R_0^- & 0 \end{pmatrix} \; , \tag{5.12}$$

with $P = H(h) - \mu_0$ being considered in a weak sense as a perturbation of P_0 :

$$P \sim P_0 + \sum_{j \geq 1} h^{\frac{j}{2}} T_{j+2} = P_0 + \delta P \; , \tag{5.13}$$

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 $\mathcal{E}(z)$

$$\mathcal{E}(z) = \begin{pmatrix} E(z) & E^+(z) \\ E^-(z) & E^\pm(z) \end{pmatrix} , \tag{5.14}$$

The main "standard result" is that $(P-z)$ is invertible if $E^\pm(z)$ is invertible. This is immediately seen, say for the right inverse, by starting of :

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

which in particular reads

$$\begin{array}{l} (P-z)E(z) + R_0^+ E^-(z) = I , \\ (P-z)E^+(z) + R_0^+ E^\pm(z) = 0 , \\ R_0^- E(z) = 0 , \\ R_0^- E^+ = I . \end{array} \tag{5.15}$$

We shall use this in the following form :
If $z(h)$ is such that $E^\pm(z(h)) = 0$ (or is very small) then the pair $(z(h), E^+(z(h))$, gives an (approximate) eigenvector of P associated to the (approximate) eigenvalue $z(h)$. Just use the second line of (5.15). Moreover the fourth line gives $||E^+|| \geq 1$.
Very formally, if $E^\pm(z)$ is not 0, then $(P-z)$ has an inverse given by :

$$(P-z)^{-1} = E(z) - E^+(z) E^\pm(z)^{-1} E^-(z) . \tag{5.16}$$

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 :

$$\mathcal{E}(z) = \mathcal{E}_0(z) \left(\sum_{j=0}^{+\infty} (-1)^j \mathcal{K}^j \right) .$$

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

$$E^{\pm}(z) \sim \sum_{j=1}^{+\infty} (-1)^j R_0^- [(\delta P - z) E_0]^{j-1} [(\delta P - z) R_0^+] \, . \tag{5.17}$$

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

$$z(h) \sim \sum_{\ell \geq 1} z_\ell h^{\frac{\ell}{2}} \, , \tag{5.18}$$

and the quasimode in the form

$$\phi(y,h) \sim \sum_{\ell \geq 0} \phi_\ell(y) h^{\frac{\ell}{2}} \, , \tag{5.19}$$

in order to solve

$$E^{\pm}(z(h)) \sim 0 \, . \tag{5.20}$$

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, T_3 being odd) to ψ_0, we get

$$E^{\pm}_{\frac{1}{2}}(z) = -z_1 \, . \tag{5.21}$$

So we get $z_1 = 0$.

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

$$\begin{aligned} E_1^{\pm}(z) &= R_0^- (T_4 - z_2) R_0^+ + R_0^- T_3 E_0 T_3 R_0^+ \\ &= R_0^- T_4 R_0^+ + R_0^- T_3 E_0 T_3 R_0^+ - z_2 \, , \end{aligned} \tag{5.22}$$

and leads to the determination of z_2.

The recursion argument
We can continue by recursion. We first analyze the case $k = 2p$ even. For the coefficient of $h^{\frac{k}{2}}$ in the expansion of $E^{\pm}(z(h))$, we get

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

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 for j odd, the fact that E_0 respects the parity and the recursion argument, 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 expansion of the corresponding eigenvector (except if the potential is assumed to be even).

5.2 Grushin's approach for the construction of quasimodes of the Montgomery's approach

We now look at another example called the Montgomery's example [Mon, HelMo3, Hel3, KwPa]. This model corresponds to the case when the magnetic field vanishes non uniformly along a line. 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 creates 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 :

$$H(h) := D_t^2 + (h^{\frac{1}{6}} D_x - t^2(1 + \gamma_1 h^{\frac{1}{3}} x^2))^2 . \tag{5.23}$$

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

$$\mathcal{P}_0 = \begin{pmatrix} P_0 & R_0^+ \\ R_0^- & 0 \end{pmatrix} , \tag{5.24}$$

where

$$\begin{array}{l} P_0 := D_t^2 + (t^2-\xi_0)^2 - \mu_0 \ , \\ P_0\psi_0 = 0, \psi_0 > 0 \ , \ ||\psi_0||_{L^2(\mathbb{R})} = 1 \ , \\ (R_0^+\varphi)(t,x) = \psi_0(t)\varphi(x) \ , \\ (R_0^- f)(x) = \int_{\mathbb{R}} f(t,x)\psi_0(t)dt \ . \end{array} \tag{5.25}$$

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

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

We also verify that :

$$R_0^- R_0^+ = I_{L^2(\mathbb{R})} \ , \ R_0^+ R_0^- = \Pi_0 \ , \tag{5.26}$$

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

$$(\Pi_0 f)(x,t) = (\int f(t,x)\psi_0(t)dt)\psi_0(t) \ . \tag{5.27}$$

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

$$\mathcal{E}_0 = \left(\begin{array}{cc} E_0 & R_0^+ \\ R_0^- & 0 \end{array} \right) \ , \tag{5.28}$$

where

$$E_0 := (I-\Pi_0)(D_t^2 + (t^2-\xi_0)^2 - \mu_0)^{-1}(I-\Pi_0) \ . \tag{5.29}$$

As for the preceding case, the idea is now to consider the more general operator $\mathcal{P}(z)$:

$$\mathcal{P}(z) = \left(\begin{array}{cc} (P-z) & R_0^+ \\ R_0^- & 0 \end{array} \right) \ , \tag{5.30}$$

with

$$P = P_0 + h^{\frac{1}{6}} P_1 + h^{\frac{1}{3}} P_2 + h^{\frac{1}{2}} P_3 + h^{\frac{2}{3}} P_4 = P_0 + \delta P \ , \tag{5.31}$$

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

$$\begin{array}{ll} P_1 & = 2(\xi_0 - t^2)D_x \ , \\ P_2 & = D_x^2 - 2\gamma_1(\xi_0-t^2)t^2x^2 \ , \\ P_3 & = -\gamma_1 t^2(D_x\cdot x^2 + x^2\cdot D_x) \ , \\ P_4 & = t^4x^4 \ . \end{array} \tag{5.32}$$

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.
We now proceed like in the previous subsection but note now that $E^{\pm}$ is no longer a scalar but an (unbounded) operator on $L^2(\mathbb{R}_x)$. So we are now looking for $z(h)$ such that $E^{\pm}(z(h)$ is (approximately) non injective. We are here looking for an expansion

$$z(h) \sim \sum_{j\geq 1} z_j h^{\frac{j}{6}} \ ,$$

and we expand $\mathcal{E}(z)$ in powers of $h^{\frac{j}{6}}$.

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

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

Observing that $(\xi_0 - t^2)\psi_0(t)$ (see (E.9) in Problem E.16) is orthogonal to ψ_0 we get

$$E^{\pm}_{\frac{1}{6}}(z) = z_1 \ . \tag{5.33}$$

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 :

$$\begin{array}{ll} E^{\pm}_{\frac{1}{3}}(z) & = z_2 - R_0^- P_2 R_0^+ + R_0^- P_1 E_0 P_1 R_0^+ \\ & = z_2 - R_0^- D_x^2 R_0^+ + 2R_0^-(\xi_0 - t^2)\gamma_1 x^2 t^2 R_0^+ \\ & \quad +4R_0^-(\xi_0 - t^2) E_0 (\xi_0 - t^2) R_0^+ D_x^2 \\ & = z_2 - \frac{1}{2}\hat{\nu}''(\rho_0) D_x^2 - 2\gamma_1 R_0^-(\xi_0 - t^2)\gamma_1 x^2 t^2 R_0^+ x^2 \ . \end{array} \tag{5.34}$$

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 Introduction

We develop another approach for constructing approximate solutions and establish the existence of a complete expansion for the groundstate energy of a Schrödinger operator. Unfortunately (see however [HelSj7] and [MaSo]) the extension to the case with magnetic field is only partial. More precisely Helffer-Sjöstrand [HelSj7] show that such a construction is possible under analytic assumptions and for a sufficiently small magnetic field and Martinez-Sordoni [MaSo] are able to relax the second assumption at the price of constructing another type of solution.

6.2 WKB construction

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

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

for the Schrödinger equation

$$P_{h,V} = -h^2\Delta + V(x;h) \;,$$

in the neighborhood of a non degenerate minimum of the potential V_0 defined on $\mathbb{R}^p$.

This is one form of what is called a WKB solution (Other solutions are of the type $a(x,h)\exp i\frac{\phi_0(x)}{h}$ and will not be considered here). 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

$$E(h) \sim \sum_{j=0}^{\infty} E_j \; h^j$$

such that

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

After a straightforward computation, we get

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

We reorder the left hand side as a formal series in powers of h and then write that each coefficient in the expansion vanishes. This leads first to

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

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

$$\begin{array}{lll}
(\mathrm{T_1}) & 2\nabla\phi_0(x)\cdot\nabla a_0 + (V_1+\Delta\phi_0 - E_1)a_0 & = 0\ ,\\
(\mathrm{T_2}) & 2\nabla\phi_0(x)\cdot\nabla a_1 + (V_1+\Delta\phi_0 - E_1)a_1 & = \Delta a_0 + E_2 a_0,\\
\cdot & & \\
\cdot & & \\
(\mathrm{T_{k+1}}) & 2\nabla\phi_0(x)\cdot\nabla a_k + (V_1+\Delta\phi_0 - E_1)a_k & = \sum_{j=2}^k E_j\, a_{k+1-j}\\
& & \quad + \Delta a_{k-1}\ +\ E_{k+1}\,a_0\ .
\end{array} \quad (6.3)$$

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

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

which vanishes at 0 (and this determines $E_0 = 0 = \min V_0$), a function $c = (V_1 + \Delta\phi_0 - E_1)$ 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

$$Xu + cu = f$$

with $u(0) = 1$ and $f = 0$ in the case of (T_1) and with $u(0) = 0$ and $f(0) = 0$ in the other case.
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.

6.3 Warm up: 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 constraint that ϕ_0 should be positive. 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.

6.4 The general case

We explain the situation in the case when V_0 is quadratic

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

and $V_1(x)$ is 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

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

we get the equation

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

and we can take A has the positive root of $\frac{1}{2}\mathrm{Hess}\, V_0$, 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 :

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

The existence near a local minimum of a local solution of the eikonal equation $|\nabla \phi|^2 = V - \inf V$ in general having the same quadratic expansion (see also Exercise E.11) is a consequence of the stable manifold theorem (see [AbRo]), which is applied in the neighborhood of the hyperbolic point $(x_{min}, 0)$ to the vector field $\xi \cdot \nabla_\xi + \nabla_x V \cdot \nabla_x$ which is the Hamiltonian flow H_q associated with the Hamiltonian $(x,\xi) \mapsto q(x,\xi) = \xi^2 - V(x)$.

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 :

$$\left(\sum_{j=1}^{p} \mu_j x_j \partial_{x_j}\right) x^\alpha = (\sum_{j=1}^{p} \mu_j \alpha_j) x^\alpha \ ,$$

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).
Once we have solved the equation at the level of formal expansions at the origin, we are reduced to the solvability of the equation for flat functions.

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

with $c(0)=0$ and $\mu_j = \sqrt{\frac{\lambda_j}{2}}$.
We observe that, for g such that $g(0)=0$, the function $\Phi(g)(x)$

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

is well defined and that :

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

We can reduce to the case $c=0$ by first taking $u = \exp \Phi(c)\, v$. The function v satisfies :

$$(\sum_j \mu_j x_j \partial_{x_j}) v(x) = g(x) \ ,$$

with $g = \exp -\Phi(c)\, f$, for which the solution is

$$v = \Phi(g) \ .$$

The general situation in the general case is explained in Helffer[6] [Hel1] or in Dimassi-Sjöstrand [DiSj]) (and of course in [HelSj1]) .

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

6.5 Application

The construction of these WKB solutions give an alternative way for obtaining eigenvalues expansions modulo $\mathcal{O}(h^\infty)$. As in the "generalized" harmonic approximation method, we deduce indeed 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 [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 the family ψ_h lives (resp. fully lives) in a closed set U 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[7] $\overline{\lim}_{h\to 0}\lambda(h) \leq E < \inf \sigma_{ess}(P_{h,V}) - \epsilon_0$ (for ϵ_0) 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

[7] This is in particular the case when $\liminf_{|x|\to+\infty} V(x) > \inf V$.

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.

Once we have determined a closed set U, where ψ_h fully lives (and hopefully the smallest), it is interesting to discuss the behavior of ψ_h outside U, and to measure how small ψ_h decays in this region.

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 $-h^2 \frac{d^2}{dx^2} + x^2$ 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 $P_{h,A,V}$.

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

$$\begin{array}{l} \int_\Omega |\nabla_{h,A}(\exp \frac{\phi}{h}\, u)|^2 \; dx + \int_\Omega (V - |\nabla\phi|^2) \exp \frac{2\phi}{h}\; |u|^2 \; dx = \\ \quad \mathrm{Re}\; \left(\int_\Omega \exp \frac{2\phi}{h}\; (P_{h,A,V} u)(x) \cdot \bar{u}(x) \; dx \right) \; . \end{array} \tag{7.1}$$

Proof :
In the case when ϕ is a $C^2(\bar{\Omega})$- function and $A = 0$, this is an immediate consequence of the Green-Riemann formula :

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

This gives in particular :

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

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 $v, w \in H^1_0(\Omega)$.

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 $\nabla\phi_\epsilon = \nabla\chi_\epsilon \star \phi$. In the case when A is not zero, we have in addition to use

$$\int_\Omega \nabla_{h,A} v \cdot \overline{\nabla_{h,A} w}\; dx = -\int_\Omega \Delta_{h,A} v \cdot \bar{w}\, dx - h \int_{\partial\Omega} (h\partial v/\partial n - i\vec{A}\cdot\vec{n}v)\bar{w}\; d\sigma_{\partial\Omega}\;. \tag{7.4}$$

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 degenerate 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 :

$$d_{(V-E)_+}(x,y) = \inf_{\gamma \in \mathcal{C}^{1,pw}([0,1];x,y)} \int_0^1 [(V(\gamma(t)) - E)_+]^{\frac{1}{2}} |\gamma'(t)| dt\;, \tag{7.5}$$

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

$$\mathcal{C}^{1,pw}([0,1];x,y) = \{\gamma \in \mathcal{C}^{1,pw}([0,1];\mathbb{R}^n)\;,\; \gamma(0) = x\;,\; \gamma(1) = y\}\;. \tag{7.6}$$

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
$$|d(x',y) - d(x,y)| \leq d(x',x)\;,\; \forall x,x',y \in \mathbb{R}^m\;. \tag{7.7}$$

-
$$|\nabla_x d(x,y)|^2 \leq (V-E)_+(x)\;, \tag{7.8}$$
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 $P_{h,V} u_h = \lambda_h u_h$ then the identity (7.1) gives roughly that $\exp \frac{\phi}{h} \, u_h$ 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 $\exp \left(\sup_{\Omega \setminus \Omega_1} \frac{\phi(x)}{h} \right)$. 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

$$\exp (1 - \epsilon) \frac{d(x)}{h} \ u_h = \mathcal{O}(\exp \frac{\epsilon}{h}) \ , \tag{7.9}$$

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

$$\lim \inf_{|x| \to \infty} V > \inf V = 0 \tag{7.10}$$

and

$$V(x) > 0 \ \text{ for } |x| \neq 0 \ . \tag{7.11}$$

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

$$P_{h,V} u_h = \lambda_h u_h \;, \tag{7.12}$$

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

$$||\nabla_{h,A}(\exp \frac{d}{h} \cdot u_h)||_{L^2(K)} + || \exp \frac{d}{h} \cdot u_h||_{L^2(K)} \leq C_{\epsilon,K} \exp \frac{\epsilon}{h} \;, \tag{7.13}$$

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] (see Exercise E.14).

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
- $P_h = -\Delta_{h,A} + V - \lambda_h$.

Let

$$\Omega_\delta^+ = \{x \in \Omega \;,\; V(x) > \delta\} \;,\; \Omega_\delta^- = \{x \in \Omega \;,\; V(x) \leq \delta\} \;.$$

We deduce from (7.1)

$$\begin{aligned} &\int_\Omega |\nabla_{h,A}(\exp \tfrac{\phi}{h} u_h)|^2 dx + \int_{\Omega_\delta^+} (V - \lambda_h - |\nabla\phi|^2) \exp \tfrac{2\phi}{h} |u_h|^2 \, dx \\ &\qquad \leq \sup_{x \in \Omega_\delta^-} |V(x) - \lambda_h - |\nabla \phi|^2| \left(\int_{\Omega_\delta^-} \exp \tfrac{2\phi}{h} |u_h|^2 \, dx \right) \;. \end{aligned}$$

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

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

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

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

and finally

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

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 but 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 $x \mapsto \mathrm{Tr}^+(B(x))$. This is due to (2.27) in the case $n = 2$ ($B(x)$ of constant sign) and to their extensions. The Agmon distance will be attached to $h\left[\mathrm{Tr}^+(B(x)) - \inf_x \mathrm{Tr}^+(B(x))\right] dx^2$.
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 :

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

outside a neighborhood of the magnetic well, that is the set of points where $\mathrm{Tr}^+(B(x)) = \inf_x \mathrm{Tr}^+(B(x)$. We will come back to this in Section 9.

8 On some questions coming from the superconductivity

8.1 Introduction

Let us start by giving a physical presentation of the question and postpone the " mathematical translation of the question". This problem is described in all the basic books in physics (see for example Saint-James-De Gennes [SdG]).

More recently, a lot of articles appear which are devoted to this question. For mentioning some, let us cite the contributions by Bernoff-Sternberg [BeSt], which remain at a formal level, the nice paper by Bauman-Philips-Tang [BaPhTa] treating in detail the case of the disk and the papers by Giorgi-Phillips [GioPh], Lu-Pan [LuPa1, LuPa2, LuPa3, LuPa4, LuPa5] and Del Pino-Fellmer-Sternberg [PiFeSt] for a mathematically rigorous analysis in general domains.

Let us describe the mathematical problem. It is naturally posed for domains in $\mathbb{R}^3$, but for cylindrical domains in $\mathbb{R}^3$, it is natural (but not completely justified mathematically) to consider a functional which is defined in a domain $\Omega \in \mathbb{R}^2$, where Ω is the sectionof the cylinder. This explains why we consider models in $\mathbb{R}^2$. The behavior of the sample can be read on the properties of the minimizers $(\psi, \mathcal{A})$ in $H^1(\Omega;\mathbb{C}) \times H^1(\mathbb{R}^2;\mathbb{R}^2)$ of the Ginzburg-Landau functional $\mathcal{G}$:

$$\hat{\mathcal{G}}(\psi\ ,\ \mathcal{A}) = \int_\Omega \{|(\nabla - i\kappa\mathcal{A})\psi|^2 + \frac{\kappa^2}{2}(|\psi|^2-1)^2\}\ dx + \kappa^2 \int_{\mathbb{R}^2} |\mathrm{rot}\,\mathcal{A} - \mathcal{H}|^2\ dx\ . \tag{8.1}$$

Here Ω is a regular bounded set, ψ is called the order parameter and $\mathcal{A}$ is a magnetic potential defined on $\mathbb{R}^n$. $\mathcal{H}$ is a magnetic vector field when $n = 3$ and is called the external magnetic field or the applied magnetic field. In the case $n = 2$, we identify this magnetic field to a function (thinking that it is the intensity of a magnetic field vector, which is parallel to the axis of the cylinder). It is initially defined on $\mathbb{R}^n$ but in the case when Ω is simply connected, one can reduce everything to Ω and consider the functional

$$\mathcal{G}(\psi\,,\ \mathcal{A}) = \int_\Omega \{|(\nabla - i\kappa\mathcal{A})\psi|^2 + \frac{\kappa^2}{2}(|\psi|^2-1)^2\}\ dx + \kappa^2 \int_{\Omega} |\mathrm{rot}\,\mathcal{A} - \mathcal{H}|^2\ dx\ . \tag{8.2}$$

Here we will always assume that Ω is connected and simply connected.

The parameter κ is a characteristic of the sample. Traditionnally one makes the distinction between the type 1 materials corresponding to κ small and the type 2 materials corresponding to κ large. Mathematically, this leads to analyze various asymptotic regimes like $\kappa \to 0$ or $\kappa \to +\infty$. This is this last case which will be analyzed here. In order to measure the dependence on the size of the external magnetic field, we write $\mathcal{H} = \sigma H_e$.

As Ω is bounded, the existence of a minimizer is rather standard. The minimizer should satisfy the Euler-Lagrange equation, which is called in this context the Ginzburg-Landau system [SdG]). It is well known that there exists a unique vector field $\mathbf{F}$ on Ω such that

$$\mathrm{rot}\,\mathbf{F} = H_e \quad \text{and} \quad \mathrm{div}\,\mathbf{F} = 0 \quad \text{in } \Omega, \quad \mathbf{F}\cdot\nu = 0 \quad \text{on } \partial\Omega.$$

We observe that $(0, \sigma\mathbf{F})$ is a trivial critical point of the functional $\mathcal{G}$. It is therefore natural to discuss in function of σ, if this pair is a local or a global minimizer. As σ is large, one can show [GioPh] that this solution is effectively the unique global minimizer. One says that in this case the superconductivity is destroyed. In other words, the order parameter is identically zero in Ω. It is then natural to try to follow the property of the minimizers when decreasing

σ starting from $+\infty$ and to determine when the trivial solution (also called the normal solution) is no more a global minimum or a local minimum.

8.2 Critical fields and Schrödinger with magnetic field

This leads (**assuming that H_e is constant and of intensity one**) to the definition

$$H_{C_3}(\kappa) = \inf\{\sigma > 0 : (0, \sigma\mathbf{F}) \text{ is the unique global minimizer of } \mathcal{G}\}. \quad (8.3)$$

So $H_{C_3}(\kappa)$ is the bottom of the set

$$\mathcal{N}(\kappa) := \{\sigma > 0 : (0, \sigma\mathbf{F}) \text{ is the unique global minimizer of } \mathcal{G}\}\ . \quad (8.4)$$

The first result that we would like to mention is essentially due to Lu-Pan (cf also Bauman-Phillips-Tang [BaPhTa] for the case of the disk). These theorems are related to the analysis of the Neuman realization of $-(\nabla - i\mathcal{A})^2$. It is useful to observe the strong connexions between the critical field $H_{C_3}(\kappa)$ and the smallest eigenvalue $\mu^{(1)}(\mathcal{A})$ of this realization. One first observes the following elementary lemma (cf [LuPa1]) :

Lemma 8.1 .

- *If $\mu^{(1)}(\kappa\sigma\mathbf{F}) < \kappa^2$, then $\mathcal{G}$ has a non trivial minimizer.*
- *If $\mathcal{G}$ has a non trivial minimizer $(\psi_{\kappa,\sigma}, \mathcal{A}_{\kappa,\sigma})$ then $\mu^{(1)}(\kappa\mathcal{A}_{\kappa,\sigma}) < \kappa^2$.*

Let us give the proof which is easy and enlightning. For the first statement, it is easy to see that if u_1 is a normalized eigenfunction associated with $\mu^{(1)}(\kappa\sigma\mathbf{F})$ and if we consider the pair $(\lambda u_1, \sigma\mathbf{F})$ has for $0 < |\lambda|$ small enough an energy which is strictly less than the energy of the normal solution $(0, \mathbf{F})$. We have indeed

$$\mathcal{G}(\lambda u_1, \sigma\mathbf{F}) - \mathcal{G}(0, \sigma F) = |\lambda|^2(\mu^{(1)}(\kappa\sigma\mathbf{F}) - \kappa^2) + |\lambda|^4 \int_\Omega |u_1(x)|^4\, dx\ .$$

For the second statement, we observe that

$$\mu^{(1)}(\kappa\mathcal{A}_{\kappa,\sigma})||\psi_{\kappa,\sigma}||^2 = ||(\nabla_{\kappa\mathcal{A}_{\kappa,\sigma}}\psi_{\kappa,\sigma}||^2 \leq \kappa^2||\psi_{\kappa,\sigma}||^2 + \mathcal{G}(\psi_{\kappa,\sigma}, \mathcal{A}_{\kappa,\sigma}) - \mathcal{G}(0, \sigma\mathbf{F})\ .$$

This gives the inequality with $\leq$ instead of $<$. A finer analysis, observing that $\int |\psi_{\kappa,\sigma}|^4\ dx > 0$ if $\psi_{\kappa,\sigma}$ is not trivial, gives the stronger result. The lemma is proved.

Remark 8.2
The previous proof gives also an upper bound for the infimum of the Ginzburg-Landau functional $\mathcal{G}(\psi, A)$. Optimizing with respect to λ in the proof of the previous lemma gives indeed :

$$\inf \mathcal{G}(\psi, A) \leq \frac{\kappa^2|\Omega|}{2} - \frac{1}{4}\,\frac{(\mu^{(1)}(\kappa\sigma\mathbf{F}) - \kappa^2)^2}{\int |u_1(x)|^4\,dx}\ .$$

Remark 8.3
The second important remark is that $\psi_{\kappa,\sigma}$ is, using the first Ginzburg-Landau equation, a solution of :

$$-(h\nabla - i\frac{\mathcal{A}_{\kappa,\sigma}}{\sigma})^2\psi_{\kappa,\sigma} + V_{\kappa,\sigma}\psi_{\kappa,\sigma} - \frac{1}{\sigma^2}\psi_{\kappa,\sigma} = 0\ , \tag{8.5}$$

where

$$h = 1/(\kappa\cdot\sigma)\ ,\ V_{\kappa,\sigma} = \sigma^{-2}|\psi_{\kappa,\sigma}|^2\ .$$

If one shows by a priori estimates that $\frac{\mathcal{A}_{\kappa,\sigma}}{\sigma}$ is near $\mathbf{F}$ and that $\psi_{\kappa,\sigma}$ is small in L^∞ in the asymptotic regime considered here (properties established mainly in [LuPa4] and improved in [HePa]), it is not too surprising to think that the analysis which will be presented in the next section of the ground state of $-(h\nabla - i\mathbf{F})^2$ as $h \to 0$ will still be valid for the order parameter corresponding to the minimizer.

Remark 8.4
All these questions are still the object of active researches. Natural questions are :

- *Has, for κ large enough, the equation in σ*

  $$\mu^{(1)}(\kappa\sigma\mathbf{F}) = \kappa^2\ ,$$

  a unique solution ?

- *Is this unique solution $H_{C_3(\kappa)}$?*

We refer to [FoHel2, FoHel3] for the most recent results around the analysis of this third critical field.

9 Main results on semi-classical bottles and proofs

9.1 Introduction

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

$$b < b' \,, \tag{9.1}$$

is satisfied, where we used the notations :

$$\inf_{x\in\bar{\Omega}} |B(x)| = b \,,\; \inf_{x\in\partial\Omega} |B(x)| = b' \,. \tag{9.2}$$

9.2 Main results

We recall that we have given a rough asymptotic estimate for the Dirichlet realization in dimension 2 (see Theorem 2.8) 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 9.1

$$\lim_{h\to 0} \frac{1}{h} \inf \sigma(P^N_{h,A,\Omega}) = \min(b, \Theta_0 b') \,. \tag{9.3}$$

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 (2.27) 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 (9.1) 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 (2.32) is not correct in general).

One important theorem that we would like to present is

Theorem 9.2 .
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 9.3 .
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].
In the Dirichlet case, the inequality (2.27) 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

$$B(x) > 0 \,. \tag{9.4}$$

9.3 Upper bounds

The upper bounds are based on the construction of suitable quasimodes. Gaussians can be used in the case when $b < \Theta_0 b'$. In the case when $\Theta_0 b' < b$ one should use trial functions obtained by mulitplying a boundary tangential Gaussian by a "normal" solution constructed with the help of the first eigenfunction of the model on $\mathbb{R}^+$ (see Subsection 3.3). This leads to :

$$\mu^{(1)}(h) \leq \min(b, \Theta_0 b')\, h + o(h) \,, \tag{9.5}$$

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].

9.4 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,

$$\sum_j |\chi_j^h|^2 = 1 \,, \tag{9.6}$$

$$\sum_j |\nabla \chi_j^h|^2 \leq C\, \epsilon_0^{-2}\, h^{-2\rho} \,, \tag{9.7}$$

and

$$\mathrm{supp}(\chi_j^h) \subset Q_j = B(z_j, \epsilon_0\, h^\rho) \,, \tag{9.8}$$

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 :

$$\text{either } \mathrm{supp}\, \chi_j \cap \partial\Omega = \emptyset \,, \;\; \text{either } z_j \in \partial\Omega \,. \tag{9.9}$$

According to the two alternatives in (9.9), we can decompose the sum in (9.6) 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 :

$$q_h^N(u) = \sum_j q_h(\chi_j^h u) - h^2 \sum_j || \, |\nabla \chi_j^h| \, u \, ||^2 \ , \ \forall u \in H^1(\Omega) \ . \tag{9.10}$$

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

$$q_{h,A}^N(u) = \int_\Omega |h\nabla u - iAu|^2 \, dx \ , \tag{9.11}$$

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 (see [Mel], [Ho]).
If $a_{h,A}^N$ is the associated sesquilinear form, (9.10) is the consequence of the identity, for any function $\chi \in C^\infty(\bar{\Omega})$ and any $u \in H^1(\Omega)$:

$$q_{h,A}^N(\chi u) = \text{ Re } a_{h,A}^N(u, \chi^2 u) + h^2 || \, |\nabla \chi| u \, ||^2_{L^2(\Omega)} \ . \tag{9.12}$$

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 $D(P_{h,A,\Omega}^N) := \{v \in H^2(\Omega) \mid \nu \cdot (h\partial - iA)u_{/\partial\Omega} = 0\}$:

$$q_{h,A}^N(\chi u) = \text{ Re } \langle P_{h,A,\Omega}^N \, u \mid \chi^2 u \rangle_{L^2(\Omega)} + h^2 || \, |\nabla \chi| \, u \, ||^2_{L^2(\Omega)} \ . \tag{9.13}$$

We can rewrite the right hand side of (9.10) as the sum of three (types of) terms.

$$q_h(u) = \sum_{int} q_h(\chi_j^h u) + \sum_{bnd} q_h(\chi_j^h u) - h^2 \sum_j || \, |\nabla \chi_j^h| \, u \, ||^2 \ , \ \forall u \in H^1(\Omega) \ . \tag{9.14}$$

For the last term in the right hand side of (9.14), we get using (9.7) :

$$h^2 \sum_j || \, |\nabla \chi_j^h| \, u \, ||^2 \leq C \, h^{2-2\rho} \, \epsilon_0^{-2} \, ||u||^2 \ . \tag{9.15}$$

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 (9.14) can be estimated from below by using (2.27). The support of $\chi_j^h u$ is indeed contained in Ω. So we have :

$$\sum_{int} q_h(\chi_j^h u) \geq h \sum_{int} \int B(x)|\chi_j^h u|^2 \, dx \, . \tag{9.16}$$

The second term in the right hand side of (9.14) 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 $B(z, 2C\epsilon_0 h^\rho)$ $q_{h,A}(u)$ 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 (cf (2.1)). Let us emphasize that C is independent of j. Let us also introduce for the next formula : $A_j^{lin} := \frac{1}{2}(B(z_j)(-x_2, x_1))$.
By comparison in each ball with the constant magnetic field case, we get, for any $\epsilon > 0$,

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

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

$$q_{h,A}(\chi_j^h u) \geq (1 - Ch^{2\theta}\epsilon^2 - C\epsilon_0 h^\rho) h\Theta_0 \int B(z_j)|\chi_j^h u|^2\, dx - Ch^{4\rho-2\theta}\epsilon^{-2}||\chi_j^h u||^2\ . \tag{9.17}$$

We now put together all the estimates and obtain :

$$\begin{array}{ll} q_{h,A}(u) & \geq h \sum_{int} \int B(x)|\chi_j^h u|^2 dx \\ & \quad +(1 - Ch^{2\theta}\epsilon^2 - C\epsilon_0 h^\rho) h\Theta_0 \sum_{bnd} \int B(z_j)|\chi_j^h u|^2\, dx \\ & \quad -Ch^{4\rho-2\theta}\epsilon^{-2} \sum_{bnd} ||\chi_j^h u||^2 \\ & \quad -C\epsilon_0^{-2}\, h^{2-2\rho}||u||^2\ . \end{array} \tag{9.18}$$

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 :

$$q_{h,A}(u) \geq \left(\min(b, \Theta_0 b')h - Ch^{\frac{5}{4}}\right) ||u||^2\ . \tag{9.19}$$

So, taking $u = u_h^1$, where u_h^1 is a groundstate, we obtain from (9.19) :

Proposition 9.4 .
There exist constants $C > 0$ and $h_0 > 0$ such that, for all $h \in]0, h_0]$:

$$\mu^{(1)}(h) \geq (\min(b, \Theta_0 b'))\, h - Ch^{\frac{5}{4}}\ . \tag{9.20}$$

But for the control of the decay, we need also to take in (9.18) $\rho = \frac{1}{2}$, $\theta = \frac{1}{8}$, $\epsilon = 1$ and ϵ_0 large. This gives an estimate which may look weaker but will be more efficient.

Proposition 9.5 .
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 :

$$\begin{array}{ll} q_{h,A}(u) & \geq h \sum_{int} \int B(x) |\chi_j^h u|^2 dx \\ & -C(\epsilon_0) h \sum_{bnd} \int |\chi_j^h u|^2 \, dx \\ & -\frac{Ch}{\epsilon_0^2} \sum_{int} \int |\chi_j^h u|^2 dx \, . \end{array} \tag{9.21}$$

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

9.5 Agmon's estimates

We first observe that if Φ is a real and uniformly Lipschitzian function and if u is in the domain of the Neumann realization of $P_{h,A}$, then we have by a simple integration by part (see (7.1) and replace ϕ/h by $\phi/\sqrt{h}$) :

$$\begin{array}{l} \ \mathrm{Re}\ \langle P_{h,A} u \mid \exp \frac{2\Phi}{h^{\frac{1}{2}}} u \rangle \\ = \mathrm{Re}\ \langle (\frac{h}{i}\nabla - A) u \mid (\frac{h}{i}\nabla - A) \exp \frac{2\Phi}{h^{\frac{1}{2}}} u \rangle \\ = \langle (\frac{h}{i}\nabla - A) \exp \frac{\Phi}{h^{\frac{1}{2}}} u \mid (\frac{h}{i}\nabla - A) \exp \frac{\Phi}{h^{\frac{1}{2}}} u \rangle - h || |\nabla\Phi| \exp \frac{\Phi}{h^{\frac{1}{2}}} u||^2 \\ = q_{h,A}(\exp \frac{\Phi}{h^{\frac{1}{2}}} u) - h|| |\nabla \Phi| \exp \frac{\Phi}{h^{\frac{1}{2}}} u||^2 \, . \end{array} \tag{9.22}$$

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

$$\mu^{(1)}(h) || \exp \frac{\Phi}{h^{\frac{1}{2}}} u||^2 = q_{h,A}(\exp \frac{\Phi}{h^{\frac{1}{2}}} u) - h|| |\nabla\Phi| \exp \frac{\Phi}{h^{\frac{1}{2}}} u||^2 \, . \tag{9.23}$$

It remains to reimplement the previous inequality in this new one and to use the upper bound (9.5).

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 9.5. We first write :

$$\begin{array}{ll} q_{h,A}(\exp \frac{\Phi}{h^{\frac{1}{2}}} u) & \geq h \sum_{int} \int B(x) | \exp \frac{\Phi}{h^{\frac{1}{2}}} \chi_j^h u|^2 dx \\ & -C(\epsilon_0) h \sum_{bnd} \int |\chi_j^h \exp \frac{\Phi}{h^{\frac{1}{2}}} u|^2 \, dx \\ & -\frac{Ch}{\epsilon_0^2} \sum_{int} \int | \exp \frac{\Phi}{h^{\frac{1}{2}}} \chi_j^h u|^2 dx \, . \end{array} \tag{9.24}$$

Let us consider the case when

$$\Theta_0 b' < b \,. \tag{9.25}$$

The inequality (9.5) becomes :

$$\mu^{(1)}(h) \leq \Theta_0 \, b \, h + o(h) \,. \tag{9.26}$$

Using (9.22), we finally obtain :

$$\left((b - \Theta_0 b') - o(1) - \frac{C}{\epsilon_0^2} - \alpha^2\right) \sum_{int} \int |\exp \frac{\Phi}{h^{\frac{1}{2}}} \chi_j^h u|^2 dx \leq C(\epsilon_0) \sum_{bnd} \int |\chi_j^h u|^2 \, dx \,. \tag{9.27}$$

Taking ϵ_0 large enough,, h_0 small enough and $\alpha < \sqrt{b - \Theta_0 b'}$, we finally obtain the existence of C such that, for $h \in]0, h_0]$, the estimate :

$$|| \exp \frac{\alpha \, d(x, \partial\Omega)}{h^{\frac{1}{2}}} \; u_h || \leq C ||u_h|| \,, \tag{9.28}$$

is satisfied.
This gives the elements of the proof for the following theorem ([LuPa2, HelMo3] and [PiFeSt]) :

Theorem 9.6 .
Undre condition (9.25)*, there exists $C > 0$, $\alpha > 0$, such that if u_h is the ground state of $P^N_{A,h,\Omega}$, then :*

$$|| \exp \frac{\alpha \, d(x, \partial\Omega)}{h^{\frac{1}{2}}} \; u_h(x) ||_{H^1(\Omega)} \leq C ||u_h||_{L^2} \,. \tag{9.29}$$

Note that the condition (9.25) is always satisfied when B is constant because $b = b'$ and $\Theta_0 < 1$.

Remark 9.7 .
On the contrary, when $b < \Theta_0 b'$ the ground state decays exponentially outside neighborhoods of points where $B(x) = b$. Note that in this case the boundary condition does not affect the localization of the ground state or the asymptotics of the ground state energy (exponentially small effect). The decay is then estimated by the weight $\exp -\frac{\alpha_0 d_{B-b}(x)}{\sqrt{h}}$

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A Variations around the spectral theorem

We just come back to the way one can deduce from the existence of quasimodes 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 [ReSi] or Lévy-Bruhl [LB]). 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

$$\eta = \langle \psi \mid A\psi \rangle \in]\alpha, \beta[$$

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 Distance between true and approximate eigenspaces

There is a need to generalize this lemma to more general situations and have an information on the corresponding eigenspaces. We follow here the presentation of [DiSj].

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[8] 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

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

[8] First observe that

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

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 :

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

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 :

$$A\psi_j = \mu_j \psi_j + r_j \ , \ \textit{with} \ . \tag{A.9}$$

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

$$\vec{d}(E, F) \leq (\sum_j ||r_j||^2)^{\frac{1}{2}} / (a(\lambda_S^{min})^{\frac{1}{2}}) \ , \tag{A.10}$$

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

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

Hence

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

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

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

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 for the localization of the eigenvalue

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 also proven that, for ϵ small enough, $\vec{d}(E, F) = \vec{d}(F, E) < 1$.

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

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

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

$$\langle Au \mid u\rangle \geq 0 \; , \; \forall u \in D(A) \; . \tag{B.1}$$

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

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

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

and, for $n \geq 2$,

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

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).

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.5 .
Let A be a selfadjoint semibounded operator of domain $D(A) \subset \mathcal{H}$. Let us introduce

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

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.6 .
In the case when the operator has 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.7 .
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.8 .
Under the same assumption as in Proposition B.7, if a is below the bottom of the essential spectrum of A, then A has at least n eigenvalues (counted with multiplicity).

Exercise B.9 .
In continuation of Example 2.1, show that for any $\epsilon > 0$ and any N, there exists $h_0 > 0$ such that for $h \in]0, h_0]$, $P_{h,V}$ 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.5 is obtained by

Theorem B.10 .
Let A be a selfadjoint semibounded operator and $Q(A)$ its form domain [9] . Then

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

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[10]

$$\langle Au \mid u >\leq \langle Bu \mid u\rangle \,,\ \forall u \in Q(B)\,,$$

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

then

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

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

Example B.11 *(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 $P_{A,V} = -\Delta_A + V$ is less or equal to the N-th eigenvalue of the Dirichlet realization. The proof is immediate if we observe the inclusion of the form domains.

Example B.12 *(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 $H^1_0(\Omega_1)$ with a subspace of $H^1_0(\Omega_2)$ by just an extension by 0 in $\Omega_2 \setminus \Omega_1$.
Other applications appear in Problems E.8 and E.13 (questions 3 and 4).

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 exist $a \in]0,1[$ and C with :

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

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 subsets $\mathcal{K} \subset \mathbb{R}^m$.

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. There are other extensions in case with boundary (see [Bon]).

D Classical Laplace methods

We recall the basic result concerning Laplace integrals. It is modelled on the stationary phase theorem :

Theorem D.1 .
Let Φ be a real C^∞ phase defined on the closed unit ball $\bar{B}(0,1)$ in $\mathbb{R}^n$ 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 on $\bar{B}(0,1)$ 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

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

The proof is rather simple (and actually simpler than for the stationary phase theorem 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: $\Phi(x) = \sum_{j=1}^n y_j^2 =: \hat{\Phi}(y)$.

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 has 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

$$I_{2k} = \int_{-\infty}^{+\infty} t^{2k} \exp -t^2 dt \ ,$$

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 $\mathbb{R}^n$.
We finish with the statement of the Morse Lemma.

Lemma D.2 .
Let $f(x)$ be a real valued C^∞ function in a neighborhood of 0 in $\mathbb{R}^n$. Assume that $(\nabla f)(0) = 0$ and that $A = (\mathrm{Hess}\, f)(0)$ is non-singular. Then there exists a C^∞ map in a neighborhood of 0 such that :

$$f(x) = f(0) + \langle Az \mid z \rangle / 2 \ ,$$

and

$$z = x + \mathcal{O}(|x|^2) \ .$$

The proof is standard (see [Ho]).

E Exercises in Spectral Theory

Exercise E.1 *(selfadjointness and compactness).*
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 has 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 *(magnetic bottles).*
Show that the selfadjoint extension in $L^2(\mathbb{R}^2)$ *of*

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

has compact resolvent.

Exercise E.3 *(Witten laplacians).*
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* $C_0^\infty(\mathbb{R}^m)$ $-\Delta + 2\nabla\phi\cdot\nabla$. *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 : $\int_{\mathbb{R}^m} \exp -2\phi(x)\ dx < +\infty$. *Show that its lowest eigenvalue is simple and determine a corresponding eigenvector.*

Exercise E.4 *(Quasimodes).*
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.5 [11]
Let V *be in* $C_0^\infty(\mathbb{R}^m)$ $(m = 1, 2)$. *Show that the essential spectrum of* $P_V =$

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

$-\Delta + V$ is $[0, +\infty[$.
Let us assume in addition that

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

Find $\psi \in D(P_V)$ such that

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

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 $P_V = -\Delta + V$ has a negative eigenvalue.

Problem E.6 .
Let us consider in $\mathbb{R}^2$ the disk $\Omega := D(0, R)$ and the Dirichlet realization in Ω of the Schrödinger operator

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

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 has 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

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

and establishing the following properties.

- *For $h > 0$, let us denote by $x \mapsto u_1(x\,;\,h)$ an L^2-normalized eigenfunction associated with $\lambda_1(h)$. Show that the family $u_1(\cdot\,;\,h)$ $(0 < h \leq 1)$ 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*

$$\lim_{n\to+\infty} u_1(\cdot\,;\,h_n) = u_\infty$$

  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.7 *(Minimax and perturbation).*
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 : $\langle H_\epsilon u_\epsilon \mid u_\epsilon \rangle_{L^2(\mathbb{R})}$.
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.8 *(Harmonic oscillator in a symmetric interval).*
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 :*

$$||x u_a||_{L^2(]-a,+a[)} \leq C \,.$$

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

Problem E.9 *(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.10 *(Alternative WKB expansion)*
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.11 *(Formal solution of the eikonal equation)*
Solve the eikonal equation $|\nabla \Phi|^2 = V - \inf V$ near a non degenerate minimum of V formally in the sense of formal expansions $\Phi \sim \sum a_\alpha (x - x_{min})^\alpha$, i.e. modulo flat functions at the minimum.

Problem E.12 *(semi-classical analysis and Airy operator)*
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 has 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

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

Problem E.13 *(Schrödinger operator in $\mathbb{R}^2_+$ with Dirichlet conditions). 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 $Q := D^2_{y_1} + (y_1 - y_2)^2$ 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, 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 $\Sigma^D(P)$.*

Exercise E.14 *(Decay at $\pm\infty$)*
Using Agmon's inequalities, show that any eigenfunction of $-\frac{d^2}{dx^2} + x^4$ decays exponentially as $|x| \to +\infty$.

Exercise E.15 *(Decay at $+\infty$)*
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.16 *(The Montgomery's toy model)*
One would like to analyze 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 has 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^1_β the corresponding L^2-normalized strictly positive eigenvector. Admitting that $\beta \mapsto u^1_\beta$ is of class C^1 in a suitable sense, show that

$$\lambda_1'(\beta) = -2 \int (t^2 - \beta)(u^1_\beta)^2(t) dt \ . \tag{E.9}$$

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