

Course notes for
‘Théorie spectrale et analyse non-linéaire’
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1 Abstract of the course

1.1 Introduction

Our aim is to describe in these notes how the techniques of the well-developed semi-classical theory can be applied to provide a precise solution to some problems in the theory of superconductivity. From a spectral point of view the problem is that of the bottom of the spectrum of the Schrödinger operator with magnetic fields.

The reader is supposed to have a good knowledge of elementary spectral analysis, of Hilbertian analysis and of the theory of distributions (Sobolev spaces). For the spectral theory, the books by Reed and Simon [ReSi] is more than enough and the reader can also look at [LB] (in french) or to the notes of an unpublished course [Hel7].

When Schrödinger operators with magnetic fields are concerned, one 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 [Ro2], Kolokoltsov [Ko] (in connection with results of the Maslov's school) and A. Martinez (in the spirit of microlocal analysis) [Ma] .

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 depend¹ on \hbar) a $C^\infty(\overline{\Omega})$ real valued function, corresponding to the so called electric potential, and let $\hbar > 0$ is a small parameter (playing the role of the Planck constant, or in other contexts of the inverse of the intensity of the magnetic field). The vector \vec{A} corresponds more intrinsically to a 1-form

$$\omega_A = \sum_j A_j dx_j . \quad (2.1)$$

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

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

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 with a magnetic vector \vec{B} , by the Hodge map :

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

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

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

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

¹Typically, one can meet $V(x; \hbar) = V_0(x) + \hbar V_1(x)$.

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 taking the so-called Friedrichs extension associated with the quadratic form :

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

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

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

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

$$\mathcal{V}^D(\Omega) = H_0^1(\Omega),$$

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

$$D(P_{h,A,V}^D) = H_0^1(\Omega) \cap H^2(\Omega).$$

The Neumann realization

The Neumann realization corresponds to taking the Friedrichs extension of the quadratic form :

$$C^\infty(\overline{\Omega}; \mathbb{C}) \ni u \mapsto Q_{h,A,V,\Omega}^N(u) := \int_{\Omega} (|\nabla_{h,A}u|^2 + V(x)|u(x)|^2) dx, \quad (2.6)$$

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

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

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

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

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

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

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

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

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 in general. When $V \geq -C$, it is easy to characterize the form domain which is

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

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. The original proof is for the case without magnetic field, but we prove below that one can modify it to accomodate the magnetic case also. The essential self-adjointness means that the Friedrichs extension is the unique selfadjoint extension in $L^2(\mathbb{R}^n)$ starting from $C_0^\infty(\mathbb{R}^n)$ and the domain $D(P_{h,A,V})$ satisfies in this case :

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

We include here the proof of essential self-adjointness.

Theorem 2.1. *Suppose that $P = -(\nabla - iA)^2 + V$ is semibounded on $C_0^\infty(\mathbb{R}^n)$ and that $V \in C^0(\mathbb{R}^n)$, $A \in C^1(\mathbb{R}^n)$. Then P is essentially self-adjoint.*

Proof.

We may assume, since P is semibounded, that

$$\langle u | Pu \rangle \geq \|u\|^2, \quad \forall u \in C_0^\infty(\mathbb{R}^n). \quad (2.13)$$

This inequality extends by density to functions $u \in H_{\text{comp}}^1(\mathbb{R}^n)$ (the H^1 functions of compact support)

$$\|\nabla_A u\|^2 + \int_{\mathbb{R}^n} V(x)|u(x)|^2 dx \geq \|u\|^2, \quad \forall u \in H_{\text{comp}}^1(\mathbb{R}^n). \quad (2.14)$$

According to the general criterion of essential selfadjointness it suffices to verify that the range $R(P)$ is dense. Suppose that $f \in L^2(\mathbb{R}^n)$ is such that

$$\langle f | Pu \rangle = 0, \quad \forall u \in C_0^\infty(\mathbb{R}^n). \quad (2.15)$$

We have to show that $f = 0$.

We first observe that (2.15) implies that $(-\nabla - iA)^2 + V)f = 0$ in the sense of distributions. Standard elliptic regularity theory for the laplacian implies that $f \in H_{\text{loc}}^2(\mathbb{R}^n)$.

We now introduce a family of cut-off functions, ζ_k , by

$$\zeta_k(x) := \zeta(x/k), \quad \forall k \in \mathbb{N}, \quad (2.16)$$

where $\zeta \in C_0^\infty(\mathbb{R}^n)$ satisfies $0 \leq \zeta \leq 1$, $\zeta = 1$ on $B(0, 1)$ and $\text{supp } \zeta \subset B(0, 2)$. For any $u \in C_0^\infty(\mathbb{R}^n)$ we have the identity

$$\begin{aligned} & \int \overline{\nabla_A(\zeta_k f)} \cdot \nabla_A(\zeta_k u) dx + \int \zeta_k^2 V(x) \overline{f(x)} u(x) dx \\ &= \langle f | P(\zeta_k^2 u) \rangle + \int |\nabla \zeta_k(x)|^2 \overline{f(x)} u(x) dx \\ &+ \int \zeta_k(x) \nabla \zeta_k(x) \cdot [\overline{f(x)} \nabla_A u(x) - u(x) \overline{\nabla_A f(x)}] dx \end{aligned} \quad (2.17)$$

When f satisfies (2.15) we get

$$\begin{aligned} & \int \overline{\nabla_A(\zeta_k f)} \cdot \nabla_A(\zeta_k u) dx + \int \zeta_k^2 V(x) \overline{f(x)} u(x) dx \\ &= \int |\nabla \zeta_k(x)|^2 \overline{f(x)} u(x) dx \\ &+ \int \zeta_k(x) \nabla \zeta_k(x) \cdot [\overline{f(x)} \nabla_A u(x) - u(x) \overline{\nabla_A f(x)}] dx. \end{aligned} \quad (2.18)$$

This formula can be extended to functions $u \in H_{\text{loc}}^1$, in particular, we can take $u = f$ and obtain

$$\begin{aligned}
& \|\nabla_A(\zeta_k f)\|^2 + \int \zeta_k^2 V(x) |f(x)|^2 dx \\
&= \text{Re} \left\{ \|\nabla_A(\zeta_k f)\|^2 + \int \zeta_k^2 V(x) |f(x)|^2 dx \right\} \\
&= \int |\nabla \zeta_k(x)|^2 |f(x)|^2 dx .
\end{aligned} \tag{2.19}$$

Using (2.14), (2.19) and taking the limit $k \rightarrow \infty$, we get

$$\begin{aligned}
\|f\|^2 &= \lim_{k \rightarrow \infty} \|\zeta_k f\|^2 \\
&\leq \limsup_{k \rightarrow \infty} \left(\|\nabla_A(\zeta_k f)\|^2 + \int_{\mathbb{R}^n} V(x) |\zeta_k(x) f(x)|^2 dx \right) \\
&= \limsup_{k \rightarrow \infty} \int |\nabla \zeta_k(x)|^2 |f(x)|^2 dx = 0.
\end{aligned} \tag{2.20}$$

This finishes the proof of the theorem. ■

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

$$\sigma_{\text{ess}}(P) = \sigma(P) \setminus \sigma_d(P) . \tag{2.21}$$

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 C), this bottom is determined by

$$\inf(\sigma(P_{h,A,V})) = \inf_{u \in \mathcal{V} \setminus \{0\}} Q_{h,A,V}(u)/\|u\|^2, \quad (2.22)$$

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

$$Q_{h,A,V}(u) < \inf(\sigma_{ess}(P_{h,A,V}))\|u\|^2. \quad (2.23)$$

An easy case when (2.23) is satisfied is when $\sigma_{ess}(P_{h,A,V}) = \emptyset$, corresponding to the case when P has 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 D).

Example 2.2. .

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 $\frac{\langle P_h \phi_h | \phi_h \rangle}{\|\phi_h\|^2}$ tends as $h \rightarrow 0$ to $V(x_{min}) < 0$.

Actually, we can produce an 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 2.3. .

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

bounded by

$$N_- \leq L_m \int_{\{x \mid V(x) < 0\}} (-V(x))^{\frac{m}{2}} dx . \quad (2.24)$$

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

$$N(\lambda) = \#\{\lambda_j < \lambda \mid \lambda_j \in \sigma(P)\} , \quad (2.25)$$

each eigenvalue being counted with multiplicity.

In this situation, it is useful to have either universal estimates (Cwikel-Lieb-Rozenbljum) or semiclassical asymptotics (see Robert [Ro2] or Ivrii [Iv]).

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

$$N^s(\lambda) = \sum_{j: \lambda_j < \lambda} (\lambda - \lambda_j)^s . \quad (2.26)$$

Theorem 2.4. (see [LieTh])

For all n, s with $\frac{n}{2} + s > 1$, there exists a constant C , such that, if V satisfies $V_- \in L^{\frac{n}{2}+s}(\mathbb{R}^n)$, then the eigenvalues of $P = -\Delta + V$ satisfy

$$\sum_{j: \lambda_j < 0} (-\lambda_j)^s \leq C \int_{\{V < 0\}} (-V)^{\frac{n}{2}+s} dx . \quad (2.27)$$

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 2.5.

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 2.6.

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

$$\sum_{j:\lambda_j < 0} (-\lambda_j)^s \sim C_{s,n} h^{-n} \int_{\{V < 0\}} (-V)^{\frac{n}{2}+s} dx . \quad (2.28)$$

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

$$-\Delta_{h,A} = -(h\nabla - iA)^2 , \quad (2.29)$$

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

2.5 Diamagnetism

Everything being universal in this discussion, we take $h = 1$. For Schrödinger operators, the inclusion of a magnetic field raises the energy. That is the consequence of the following basic inequality.

Theorem 2.7 (Diamagnetic inequality).

Let $A : \mathbb{R}^n \rightarrow \mathbb{R}^n$ be in $L^2_{\text{loc}}(\mathbb{R}^n)$ and suppose that $f \in L^2(\mathbb{R}^n)$, is such that $(\nabla + iA)f \in L^2(\mathbb{R}^n)$. Then $|f| \in H^1(\mathbb{R}^n)$ and

$$|\nabla|f|| \leq |(\nabla + iA)f| \quad (2.30)$$

in the sense of distributions.

In the proof we will clearly need to differentiate the absolute value. We state this result as a proposition.

Proposition 2.8.

Suppose that $f \in L^1_{\text{loc}}(\mathbb{R}^n)$ with $\nabla f \in L^1_{\text{loc}}(\mathbb{R}^n)$. Then also $\nabla|f| \in L^1_{\text{loc}}(\mathbb{R}^n)$ and with the notation

$$\text{sign } z = \begin{cases} \frac{\bar{z}}{|z|}, & z \neq 0 \\ 0, & z = 0, \end{cases} \quad (2.31)$$

we have

$$\nabla|f|(x) = \text{Re} \{ \text{sign}(f(x)) \nabla f(x) \}. \quad (2.32)$$

In particular,

$$|\nabla|f|| \leq |\nabla f|.$$

Proof of Proposition 2.8.

Suppose first that $u \in C^\infty(\mathbb{R}^n)$ and define $|z|_\epsilon = \sqrt{|z|^2 + \epsilon^2} - \epsilon$, for $z \in \mathbb{C}$ and $\epsilon > 0$. Then $|u|_\epsilon \in C^\infty(\mathbb{R}^n)$ and

$$\nabla|u|_\epsilon = \frac{\operatorname{Re}(\bar{u}\nabla u)}{\sqrt{|u|^2 + \epsilon^2}}. \quad (2.33)$$

Let now f be as in the proposition and define f_δ as the convolution $f_\delta = f * \rho_\delta$ with ρ_δ being a standard approximation of the unity for convolution. Explicitly, we take a $\rho \in C_0^\infty(\mathbb{R}^n)$ with

$$\rho \geq 0, \quad \int_{\mathbb{R}^n} \rho(x) dx = 1,$$

and define $\rho_\delta(x) := \delta^{-n}\rho(x/\delta)$, for $x \in \mathbb{R}^n$ and $\delta > 0$. Then $f_\delta \rightarrow f$, $|f_\delta| \rightarrow |f|$ and $\nabla f_\delta \rightarrow \nabla f$ in $L^1_{\text{loc}}(\mathbb{R}^n)$ as $\delta \rightarrow 0$.

Take a test function $\phi \in C_0^\infty(\mathbb{R}^n)$. We may extract a subsequence $\{\delta_k\}_{k \in \mathbb{N}}$ (with $\delta_k \rightarrow 0$ for $k \rightarrow \infty$) such that $f_{\delta_k}(x) \rightarrow f(x)$ for almost every $x \in \operatorname{supp} \phi$. We restrict our attention to this subsequence. For simplicity of notation we omit the k from the notation and write $\lim_{\delta \rightarrow 0}$ instead of $\lim_{k \rightarrow \infty}$.

We now calculate, using dominated convergence and (2.33)

$$\begin{aligned} \int (\nabla \phi)|f| dx &= \lim_{\epsilon \rightarrow 0} \int (\nabla \phi)|f|_\epsilon dx \\ &= \lim_{\epsilon \rightarrow 0} \lim_{\delta \rightarrow 0} \int (\nabla \phi)|f_\delta|_\epsilon dx \\ &= - \lim_{\epsilon \rightarrow 0} \lim_{\delta \rightarrow 0} \int \phi \frac{\operatorname{Re}(\bar{f}_\delta \nabla f_\delta)}{\sqrt{|f_\delta|^2 + \epsilon^2}} dx \end{aligned}$$

Using the pointwise convergence of $f_\delta(x)$ and $\|\nabla f_\delta - \nabla f\|_{L^1(\operatorname{supp} \phi)} \rightarrow 0$, we can take the limit $\delta \rightarrow 0$ and get

$$\int (\nabla \phi)|f| dx = - \lim_{\epsilon \rightarrow 0} \int \phi \frac{\operatorname{Re}(\bar{f} \nabla f)}{\sqrt{|f|^2 + \epsilon^2}} dx. \quad (2.34)$$

Now, $\phi \nabla f \in L^1(\mathbb{R}^n)$ and $\frac{\bar{f}(x)}{\sqrt{|f|^2 + \epsilon^2}} \rightarrow \operatorname{sign} f(x)$ as $\epsilon \rightarrow 0$, so we get (2.32) from (2.34) by dominated convergence. ■

Proof of Theorem 2.7.

Since $A \in L^2_{\text{loc}}(\mathbb{R}^n)$ and $f \in L^2(\mathbb{R}^n)$, the assumption $(\nabla + iA)f \in L^2(\mathbb{R}^n)$ implies that $\nabla f \in L^1_{\text{loc}}(\mathbb{R}^n)$. Therefore, we can use Proposition 2.8 to conclude that (2.32) holds for f . Since $\text{Re} \{ \text{sign}(f) i A f \} = 0$, we can rewrite (2.32) as

$$\nabla |f| = \text{Re} \{ \text{sign}(f) (\nabla + iA) f \}, \quad (2.35)$$

and therefore, since $|z| \geq |\text{Re}(z)|$ for all $z \in \mathbb{C}$, we get (2.30). ■

Using Theorem 2.7 we now get, by the variational characterization of the ground state energy, the comparison for Dirichlet eigenvalues,

$$\inf \sigma (P_{A,\Omega}^D + V) \geq \inf \sigma (-\Delta_{\Omega}^D + V). \quad (2.36)$$

Also a similar result is true in the case of Neumann boundary conditions :

$$\inf \sigma (P_{A,\Omega}^N + V) \geq \inf \sigma (-\Delta_{\Omega}^N + V), \quad (2.37)$$

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

Proposition 2.9.

Suppose that $\Omega \subset \mathbb{R}^2$ is simply connected. 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 rigorous proof or [Hel1] in connection with the Aharonov-Bohm 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 :

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

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

$$\frac{1}{2\pi} \int_{\gamma} \omega_A \in \mathbb{Z} \quad (2.38)$$

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

$$\Omega \ni x \mapsto U(x) = \exp(-i\phi(x)) . \quad (2.39)$$

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

Remark 2.10.

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 $\text{dist}(a, \mathbb{Z})^2$, increases when a magnetic potential is introduced. 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 the Cwickel-Lieb-Rozenblum inequality in Remark 2.5.

As discussed above, the diamagnetic inequality (2.30) implies that ground state energies go up when a magnetic field is applied. Consider a fixed A and the ground state energy $e_1(B)$ of the operator $(\nabla - iBA)^2 + V$ (either in a domain and with boundary conditions, or on \mathbb{R}^n). One can now ask the more general question of whether the function $B \mapsto e_1(B)$ is monotone non-decreasing. This is generally not true, see Erdős [Er2] for a counterexample. However, for large B positive results can be obtained.

We consider the Neumann operator $P_{1,BA,V}^N$ in a domain Ω and assume that Ω, V are such that $P_{1,BA,V}^N$ has compact resolvent for all (sufficiently large) $B > 0$. So the spectrum of $P_{1,BA,V}^N$ consists of a sequence of eigenvalues (of finite multiplicity) tending to infinity, in particular, the degeneracy of the ground state is finite. Let $B \in \mathbb{R}$ and let n be the degeneracy of the ground state $\mu_1(B)$. By analytic perturbation theory (see for instance [Ka] or [ReSi, Chapter XII]), there exists $\epsilon > 0$, n analytic functions

$$(B - \epsilon, B + \epsilon) \ni \beta \mapsto \phi_j(\beta) \in H^2(\Omega) \setminus \{0\} ,$$

for $j = 1, \dots, n$, and n analytic functions

$$(B - \epsilon, B + \epsilon) \ni \beta \mapsto E_j(\beta) \in \mathbb{R} ,$$

such that

$$\begin{aligned} P_{1,\beta A,V}^N \phi_j(\beta) &= E_j(\beta) \phi_j(\beta) , \\ E_j(B) &= \mu_1(B) . \end{aligned}$$

We may choose ϵ sufficiently small in order to have the existence (but not necessarily the uniqueness) of $j_+, j_- \in \{1, \dots, n\}$ such that

$$\begin{aligned} \text{For } \beta > B: \quad E_{j_+}(\beta) &= \min_{j \in \{1, \dots, n\}} E_j(\beta) \\ \text{For } \beta < B: \quad E_{j_-}(\beta) &= \min_{j \in \{1, \dots, n\}} E_j(\beta) . \end{aligned} \quad (2.40)$$

Define the left and right derivatives of $\mu_1(B)$:

$$\mu'_{1,\pm}(B) := \lim_{\epsilon \rightarrow 0_{\pm}} \frac{\mu_1(B + \epsilon) - \mu_1(B)}{\epsilon} . \quad (2.41)$$

Proposition 2.11.

For all $B \in \mathbb{R}$, the one-sided derivatives $\mu'_{1,\pm}(B)$ exist and satisfy

$$\mu'_{1,\pm}(B) = -2 \operatorname{Re} \langle \phi_{j_{\pm}} | A \cdot (-i\nabla - BA) \phi_{j_{\pm}} \rangle .$$

Proof.

Clearly, $\mu'_{1,\pm}(B) = E'_{j_{\pm}}(B)$. We will prove that

$$E'_{j_{\pm}}(B) = -2 \operatorname{Re} \langle \phi_{j_{\pm}} | A \cdot (-i\nabla - BA) \phi_{j_{\pm}} \rangle .$$

But this result is just first order perturbation theory (Feynman-Hellman). ■

Theorem 2.12.

Suppose that Ω is bounded with smooth boundary. Let g be a function such that for all $\epsilon \in (-1, 1)$ we have

$$|g(\beta + \epsilon) - g(\beta)| \rightarrow 0 \quad (2.42)$$

as $\beta \rightarrow \infty$.

Suppose that A, V are smooth functions and that Ω, A, V are such that there exists $\alpha \in \mathbb{R}$ such that $\mu_1(B) = \alpha B + g(B) + o(1)$, as $B \rightarrow +\infty$. Then the limits $\lim_{B \rightarrow \infty} \mu'_{1,+}(B)$ and $\lim_{B \rightarrow \infty} \mu'_{1,-}(B)$ exist and

$$\lim_{B \rightarrow \infty} \mu'_{1,+}(B) = \lim_{B \rightarrow \infty} \mu'_{1,-}(B) = \alpha . \quad (2.43)$$

Remark 2.13.

Let $\gamma \in [0, 1)$, then $g(\beta) = \beta^\gamma$ satisfies (2.42). Thus, if there exist powers $\gamma_1, \dots, \gamma_m \in [0, 1)$ and $\alpha, \alpha_1, \dots, \alpha_m \in \mathbb{R}$, such that (as $B \rightarrow \infty$),

$$\mu_1(B) = \alpha B + \sum_{j=1}^m \alpha_j B^{\gamma_j} + o(1),$$

then Proposition 2.12 implies that

$$\lim_{B \rightarrow \infty} \mu'_{1,\pm}(B) = \alpha .$$

Proof of Theorem 2.12.

Clearly², for all B , we have $\mu'_{1,+}(B) \leq \mu'_{1,-}(B)$. So it suffices to prove that

$$\alpha \leq \liminf_{B \rightarrow \infty} \mu'_{1,+}(B) , \quad (2.44)$$

$$\limsup_{B \rightarrow \infty} \mu'_{1,-}(B) \leq \alpha . \quad (2.45)$$

Let $\epsilon > 0$. Then

$$\begin{aligned} \mu'_{1,+}(B) &= -2 \operatorname{Re} \langle \phi_{j_+}(B) | A \cdot (-i\nabla - BA) \phi_{j_+}(B) \rangle \\ &= \frac{1}{\epsilon} \langle \phi_{j_+}(B) | (P_{1,(B+\epsilon)A,V}^N - P_{1,BA,V}^N - \epsilon^2 A^2) \phi_{j_+}(B) \rangle . \end{aligned}$$

²Using the fact that μ_{j_\pm} is an analytic choice of the eigenvalues in a neighborhood of B ,

Therefore, the variational principle implies

$$\mu'_{1,+}(B) \geq \frac{\mu_1(B + \epsilon) - \mu_1(B)}{\epsilon} - \epsilon \|A\|_{L^\infty(\Omega)}^2.$$

By assumption there exists a function $f : \mathbb{R}_+ \rightarrow \mathbb{R}_+$, with $\lim_{\beta \rightarrow \infty} f(\beta) = 0$, and such that

$$|\mu_1(\beta) - (\alpha\beta + g(\beta))| \leq f(\beta).$$

Thus,

$$\mu'_{1,+}(B) \geq \alpha + \frac{g(B + \epsilon) - g(B)}{\epsilon} - \frac{f(B) + f(B + \epsilon)}{\epsilon} - \epsilon \|A\|_{L^\infty(\Omega)}^2. \quad (2.46)$$

Therefore, (using (2.42))

$$\liminf_{B \rightarrow \infty} \mu'_{1,+}(B) \geq \alpha - \epsilon \|A\|_{L^\infty(\Omega)}^2.$$

Since $\epsilon > 0$ was arbitrary, this finishes the proof of (2.44).

The proof of (2.45) is similar (taking $\epsilon < 0$ reverses the inequalities) and is omitted. ■

2.6 Kato's inequality and consequences

In order to obtain stronger results on essential self-adjointness than Theorem 2.1 a useful tool is the so-called Kato inequality. We present it in the magnetic version. For the applications to self-adjointness questions we refer to [ReSi, Vol.2, Section X.4].

Theorem 2.14 (Kato's magnetic inequality).

Let $A \in C^1(\mathbb{R}^n, \mathbb{R}^n)$. Then, for all $f \in L^1_{\text{loc}}(\mathbb{R}^n)$ with $(\nabla - iA)^2 f \in L^2_{\text{loc}}(\mathbb{R}^n)$ we have the inequality

$$\Delta|f| \geq \text{Re} \{ \text{sign}(f)(\nabla - iA)^2 f \}, \quad (2.47)$$

where $\text{sign } f$ was defined in (2.31).

The proof uses the derivative of the absolute value

Theorem 2.15 (Kato's inequality).

Let $f \in L^1_{\text{loc}}(\mathbb{R}^n)$ such that $\Delta f \in L^1_{\text{loc}}(\mathbb{R}^n)$. Then we have the inequality

$$\Delta|f| \geq \text{Re} \{ \text{sign}(f) \Delta f \}, \quad (2.48)$$

in the sense of distributions, where $\text{sign} f$ was defined in (2.31).

The proof of Theorem 2.15 follows the same steps as the proof of Proposition 2.8. That is, one first considers smooth functions f and the regularized absolute value $|z|_\epsilon = \sqrt{|z|^2 + \epsilon^2} - \epsilon$ and calculates directly. One then considers a sequence f_δ of smooth approximations to f . Taking first δ and then ϵ to zero one obtains the desired inequality. We leave the details to the reader (see [ReSi, Vol.2, Section X.4]).

Proof of Theorem 2.14.

We only give the proof under the extra regularity assumption, $A \in C^2(\mathbb{R}^n)$. In that case the assumption $(\nabla - iA)^2 f \in L^2_{\text{loc}}(\mathbb{R}^n)$ and standard elliptic regularity implies that $f \in H^2_{\text{loc}}(\mathbb{R}^n)$, in particular that

$$\Delta f, \nabla f \in L^1_{\text{loc}}(\mathbb{R}^n). \quad (2.49)$$

Suppose now that u is smooth. Then we can calculate as follows, using $|z|_\epsilon = \sqrt{|z|^2 + \epsilon^2} - \epsilon$,

$$\nabla|u|_\epsilon = \frac{\text{Re} \{ \bar{u} \nabla u \}}{\sqrt{|u|^2 + \epsilon^2}} = \frac{\text{Re} \{ \bar{u} (\nabla + iA) u \}}{\sqrt{|u|^2 + \epsilon^2}}. \quad (2.50)$$

We therefore find

$$\begin{aligned} \sqrt{|u|^2 + \epsilon^2} \Delta|u|_\epsilon &= \text{div} (\sqrt{|u|^2 + \epsilon^2} \nabla|u|_\epsilon) - |\nabla|u|_\epsilon|^2 \\ &= \text{Re} \{ \bar{\nabla} u (\nabla + iA) u + \bar{u} \text{div} ((\nabla + iA) u) \} - |\nabla|u|_\epsilon|^2 \\ &= |(\nabla + iA) u|^2 - |\nabla|u|_\epsilon|^2 \\ &\quad + \text{Re} \{ iA \bar{u} (\nabla + iA) u + \bar{u} \text{div} ((\nabla + iA) u) \} \end{aligned} \quad (2.51)$$

By (2.50), $|(\nabla + iA) u|^2 \geq |\nabla|u|_\epsilon|^2$, so (2.51) implies that, for smooth u ,

$$\Delta|u|_\epsilon \geq \text{Re} \frac{\bar{u} (\nabla + iA)^2 u}{\sqrt{|u|^2 + \epsilon^2}}. \quad (2.52)$$

The end of the proof now follows the same lines as the proof of Proposition 2.8, i.e. (2.52) holds for suitably smoothened versions f_δ of f . By taking the limit $\delta \rightarrow 0$ followed by the limit $\epsilon \rightarrow 0$, in the sense of distributions, one arrives at (2.47).

If one only knows that $A \in C^1$, it is not immediate to conclude (2.49). The details in this case can be found in [ReSi, Vol.2, Section X.4]. \blacksquare

2.7 Very rough estimates for the Dirichlet realization

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

$$\|\nabla_{h,A}u\|^2 = \langle P_{h,A,\Omega}u \mid u \rangle \geq h \int_{\Omega} B(x)|u(x)|^2 dx, \quad \forall u \in C_0^\infty(\Omega), \quad (2.53)$$

which is interesting only if assuming $B \geq 0$.

Here the basic point is to observe that :

$$hB(x) = i[h\partial_{x_1} - iA_1, h\partial_{x_2} - iA_2]. \quad (2.54)$$

We then write

$$hB(x)u(x)\bar{u}(x) = i(X_1X_2u)(x)\bar{u}(x) - i(X_2X_1u)(x)\bar{u}(x),$$

with $X_j = h\partial_{x_j} - iA_j$.

Integrating over Ω and performing the integration by parts :

$$h \int_{\Omega} B(x)|u(x)|^2 dx = -i\langle X_1u \mid X_2u \rangle + i\langle X_2u \mid X_1u \rangle.$$

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 :

$$\inf \sigma(P_{h,A}^D) \geq h \inf_{x \in \bar{\Omega}} B(x) := hb. \quad (2.55)$$

Note that the converse is asymptotically (as $h \rightarrow 0$) 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

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

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 $h = 1$:

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

with

$$u_\rho(y) = b^{\frac{1}{4}} \exp\left(-\rho\sqrt{b}y^2\right). \quad (2.56)$$

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 :

$$\inf \sigma(P_{h,A}^D) \leq hb + \mathcal{O}(h^{\frac{3}{2}}). \quad (2.57)$$

So we have proved³ (in the 2-dimensional case) :

Theorem 2.16. .

The smallest eigenvalue $\lambda^{(1)}(h)$ of the Dirichlet realization $P_{h,A,\Omega}^D$ of $P_{h,A,\Omega}$ satisfies :

$$\frac{\lambda^{(1)}(h)}{h} = b + o(1). \quad (2.58)$$

Exercise 2.17.

Show that (for Dirichlet) in the case when the magnetic field is constant, one has

$$\frac{\lambda^{(1)}(h)}{h} = b + \mathcal{O}\left(\exp - \frac{S}{h}\right), \quad (2.59)$$

for some $h > 0$.

Hint.

Take a centered gaussian which is as far as possible from the boundary.

³We 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 Theorem 2.16 in a 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

$$\mathrm{Tr}^+ B(x) = \sum_{j:\lambda_j(x)>0} \lambda_j(x) . \quad (2.60)$$

The extension of the previous result is then :

Theorem 2.18. .

The smallest eigenvalue $\lambda^{(1)}(h)$ of the Dirichlet realization $P_{h,A,\Omega}^D$ of $P_{h,A,\Omega}$ satisfies :

$$\frac{\lambda^{(1)}(h)}{h} = \inf_{x \in \Omega} \mathrm{Tr}^+(B(x)) + o(1) . \quad (2.61)$$

The idea for the proof is to first treat the constant field case, and then to make a partition of unity. For the constant field 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

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

with

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

2.8 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 (2.53) which gives a comparison between selfadjoint operators in the form (for any $\rho \in [0, 1]$)

$$P_{h,A}^D \geq \rho(P_{h,A}^D) + (1 - \rho)hB(x) . \quad (2.62)$$

The operator on the right hand side of (2.62) 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 :

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

Remark 2.19.

According to the diamagnetic inequality, we will instead look for a lower bound of the lowest eigenvalue of the Dirichlet realization of the operator

$$-\rho h^2 \Delta + (1 - \rho)hB(x) .$$

This leads to the following proposition, which improves Theorem 2.16 :

Proposition 2.20. .

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

$$\lambda^{(1)}(h) - bh \geq \frac{1}{C} h^{1+\frac{1}{\vartheta}} , \quad (2.63)$$

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

Proof.

We use Remark 2.19 for some $\rho \in]0, \frac{1}{2}]$. We observe that for any ρ , we have

$$\lambda^{(1)}(h) \geq \rho h^2 \lambda_1(\epsilon) + (1 - \rho)hb ,$$

where $\lambda_1(\epsilon)$ is the lowest eigenvalue of the Schrödinger operator $-\Delta + V_\epsilon$ (see (2.27) and [BeHeVe]) with $V_\epsilon(x) = \frac{1}{2\epsilon}(B(x) - b)$ and $\epsilon = \rho h$.

We now apply the Lieb-Thirring bounds for $-\Delta + V_\epsilon$. This gives⁴, for any $\lambda > 0$,

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

⁴We actually apply the inequality with $(V_\epsilon - \lambda)$ replaced by $(V_\epsilon - \lambda)_-$ and combine with the minimax principle.

where $\lambda_j(\epsilon)$ denotes the sequence of eigenvalues of $-\Delta + V_\epsilon$. Note that the fact that we consider the first moment instead of the counting function is due to the fact that we would like to avoid the unfortunate condition on the dimension appearing in the Cwikel-Lieb-Rozenblum estimate.

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 $\eta \rightarrow 0$, we obtain first that $\lambda_1(\epsilon) > 0$ and

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

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 2.2, that $(\epsilon\lambda_1(\epsilon))$ tends to zero, as $\epsilon \rightarrow 0$. But the measure of $\{B(x) - b < \mu\}$ as $\mu \rightarrow 0^+$ 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 (2.63) for h small enough. ■

Remark 2.21. .

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 2.22.

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 this is optimal.

3 Models with constant magnetic field in dimension 2

Before we 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 for particular 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

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

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 :

$$P_{h,bA_0} = h^2 P_{1,bA_0/h}. \quad (3.2)$$

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 :

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

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

$$U_1 f = \exp(iB \frac{x_1 x_2}{2}) f . \quad (3.4)$$

It satisfies

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

with

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

Remark 3.1. .

U_1 is a very special case of what is called a gauge transformation. More generally, as was done in the proof of Proposition 2.9 (see (2.39)), 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 $\tilde{A} = A + \text{grad } \phi$. Here we observe that $B := \text{curl } A = \text{curl } \tilde{A}$. The associated magnetic field is unchanged in a gauge transformation. We are discussing in our example the very special (but important!) case 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

$$U_2 = \mathcal{F}_{x_2 \mapsto \xi_2} , \quad (3.7)$$

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

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

We now introduce a third unitary transform U_3

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

and we obtain the operator

$$S_B^3 := D_y^2 + B^2 y^2 , \quad (3.10)$$

operating on $L^2(\mathbb{R}_{y,\xi_2}^2)$.

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 multiplicity!) 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 $\mu(\xi) \rightarrow +\infty$ as $\xi \rightarrow -\infty$. 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

$$\lim_{\xi \rightarrow +\infty} \mu(\xi) = 1 . \quad (3.11)$$

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 $\xi \rightarrow +\infty$. 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 $\xi \rightarrow +\infty$ 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 us to the observation that the infimum of the spectrum, $\inf_{\xi \in \mathbb{R}} \inf \sigma(H^{N,\xi})$, is actually a minimum [DaHe] and strictly 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]))

$$\mu'(\xi) = -[\mu(\xi) - \xi^2]\varphi_\xi(0)^2 . \quad (3.12)$$

To get (3.12), we observe that, if $\tau > 0$, then

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

Observing that

$$\varphi'_{\xi+\tau}(\tau) = \varphi''_\xi(0)\tau + \mathcal{O}(\tau^2)$$

as $\tau \rightarrow 0$, and using the equation satisfied by φ_ξ , we can take the limit $\tau \rightarrow 0$ to get the formula.

Remark 3.2.

In the case of the Dirichlet realization, we have a similar formula :

$$\lambda'(\xi) = -((\varphi_\xi^D)'(0))^2 ,$$

where φ_ξ^D is the ground state of the Dirichlet realization and this shows immediately the monotonicity. Note that $(\varphi_\xi^D)'(0) \neq 0$ (by Cauchy uniqueness

theorem), so λ' is strictly negative.

This formula is actually a particular case of a general formula (called Rellich's Formula) for the Dirichlet realization of Schrödinger operator.

From (3.12), it follows that, for any critical point ξ_c of μ in \mathbb{R}^+

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

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

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

Moreover

$$\Theta_0 = \xi_0^2 . \quad (3.15)$$

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 identity⁵ :

$$H^N(\xi)\varphi(\cdot; \xi) = \mu(\xi)\varphi(\cdot; \xi) . \quad (3.16)$$

We obtain :

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

Taking the scalar product with φ_{ξ} in $L^2(\mathbb{R}^+)$, we obtain the so-called Feynman-Hellmann Formula

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

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

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

⁵We 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 of writing the differentiation.

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

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

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

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

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

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

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

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

Proposition 3.3.

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].

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 :

$$\inf \sigma(S_B^{N, \mathbb{R}^{2,+}}) = |B| \inf \mu(\xi) = \Theta_0 |B| . \quad (3.24)$$

Similarly, for the Dirichlet realization, we find (See Problem F.7, for details) :

$$\inf \sigma(S_B^{D, \mathbb{R}^{2,+}}) = |B| \inf_{\xi \in \mathbb{R}} \lambda(\xi) = |B| . \quad (3.25)$$

3.5 The case of a 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. Bonnaille 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 $\Omega_\alpha : \{(x_1, x_2) \in \mathbb{R}^2 \mid |x_2| \leq \text{tg}(\frac{\alpha}{2})x_1\}$. 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 :

$$\lim_{\alpha \rightarrow 0} \frac{\mu^{corn}(\alpha)}{\alpha} = \frac{1}{\sqrt{3}}. \quad (3.26)$$

Computing the energy of the quasimode u_α (following an idea of Bonnaille-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

$$\mu^{corn}(\alpha) \leq \frac{\alpha}{\sqrt{3+\alpha^2}}, \quad (3.27)$$

which gives (3.26) above (the lower bound is more difficult). This also answers the question of 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 boundary conditions was considered by L. Erdős in connection with an isoperimetric inequality [Er1]. By using the techniques of [BoHe], one can then show [HelMo3] the following proposition which is a small improvement of his result

Proposition 3.4. .

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

$$\lambda^{(1)}(b, D(0, R)) - b \sim 2^{\frac{3}{2}} \pi^{-\frac{1}{2}} b^{\frac{3}{2}} R \exp(-\frac{bR^2}{2}). \quad (3.28)$$

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 3.5.

$$\mu^{(1)}(b, D(0, R)) = \Theta_0 b - 2M_3 \frac{1}{R} b^{\frac{1}{2}} + \mathcal{O}(1) . \quad (3.29)$$

Here we recall that Θ_0 was introduced in (3.14), and that $M_3 > 0$ is a universal constant. Notice that an improvement of (3.29) has been obtained in [FoHel3].

Remark 3.6.

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 techniques for analyzing the ground-state energy (also called lowest eigenvalue or principal eigenvalue) of a Schrödinger operator in the case when 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:

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

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

Let us assume that

$$v''(0) > 0. \quad (4.2)$$

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

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

This means that we replace the potential v by its quadratic approximation at 0, namely $\frac{1}{2}v''(0)x^2$, and consider the associated Schrödinger operator.

Using the dilation $x = h^{\frac{1}{2}}y$, we observe that this operator is unitarily equivalent to

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

Consequently, the eigenvalues are given by

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

and the corresponding eigenfunctions are

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

with ⁶

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

which can be obtained recursively by

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

where c_n is a normalization constant.

We now return to the full operator $P_{h,v}$. For simplicity we will only consider 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 $h \rightarrow 0$.

We now get

$$\left(P_{h,v} - h \cdot \sqrt{\frac{v''(0)}{2}} \right) u_1^{h,app} = \mathcal{O}(h^{\frac{3}{2}}). \quad (4.8)$$

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 estimated, observing that

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

as $\mathcal{O}(h^{\frac{3}{2}})$. The spectral theorem applied to (4.8) gives the existence of an eigenvalue $\lambda(h)$ of $P_{h,v}$ such that

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

⁶We 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 $u_1^h(x)$.

In particular, we get the inequality

$$\lambda_1(h) \leq h \cdot \sqrt{\frac{v''(0)}{2}} + C h^{\frac{3}{2}}. \quad (4.9)$$

Combining with other techniques, one can actually prove that

$$\left| \lambda_1(h) - h \cdot \sqrt{\frac{v''(0)}{2}} \right| \leq C \cdot h^{\frac{3}{2}} \quad (4.10)$$

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 of 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 [Sim2] 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,

$$\begin{aligned} \sum_{j \in \mathcal{J}} (\phi_j^R)^2 &= 1, \\ \sum_{\ell=1}^n \sum_{j \in \mathcal{J}} |D_{x_\ell} \phi_j^R|^2 &\leq \frac{C}{R^2}, \end{aligned} \quad (4.11)$$

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

$$\begin{aligned} \langle P_{h,V} u \mid u \rangle &= \sum_j \langle P_{h,V} \phi_j^R u \mid \phi_j^R u \rangle - h^2 \sum_{j,\ell} \| |D_{x_\ell} \phi_j^R| u \|^2 \\ &\geq \sum_j \langle P_{h,V} \phi_j^R u \mid \phi_j^R u \rangle - C \frac{h^2}{R^2} \|u\|^2. \end{aligned} \quad (4.12)$$

We now suppose $R \in]0, 1]$. We can in addition assume that either the balls are centered at the minima of V (denoted by x^{jk} , $k \in \mathcal{K}$), or that the balls are at a distance at least $\frac{1}{C}R$ of these minima.

In the first case, 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^{jk} , i.e. the operator obtained by replacing V by its quadratic approximation

$$V^k(x) = \inf V + \frac{1}{2} \langle V''(x^{jk})(x - x^{jk} \mid (x - x^{jk}),$$

if the ball is centered at the minimum.

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

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

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 $\frac{R^2}{C} = \frac{h^{\frac{4}{5}}}{C}$, which is dominant in comparison with h as $h \rightarrow 0$. We then get the lower bound

$$\lambda_1(h) \geq \inf V + h(\inf_k \mu_1(h, x^{j_k})) - Ch^{\frac{6}{5}}, \quad (4.13)$$

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 [Sim2]). 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

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

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 $A(0) = 0$)

$$A(x) - A^0(x) = \mathcal{O}(|x|^2).$$

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

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

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

2-dimensional harmonic oscillator.

Let us treat the 2-dimensional case as an exercise. 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

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

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

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

Its groundstate is immediately computed as

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

In 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 (paramagnetic inequality).

The fact that this last inequality (which says that the groundstate energy of the Pauli operator is lower than in the case without magnetic field) cannot be extended for more general situations has been shown by Avron-Simon and Helffer using the Aharonov-Bohm effect.

Lower bounds.

The lower bound is obtained similarly once we have observed that

$$\begin{aligned} \operatorname{Re} \langle P_{h,A,V} u \mid u \rangle \\ = \sum_j \langle P_{h,A,V} \phi_j^R u \mid \phi_j^R u \rangle - h^2 \sum_{j,\ell} \| |D_{x_\ell} \phi_j^R| u \|^2 . \end{aligned} \quad (4.14)$$

We have then, for the balls containing the minima, to replace the magnetic potential by its affine approximation at the momentum and to control the remainder. Note that there is a “small” additional difficulty (of the same type as for the manifold case) for controlling the term corresponding to the approximation of the magnetic potential.

Let us more precisely describe what is going on. A new control is only necessary for the balls centered at one of the minima. The idea is that the harmonic approximation at the minimum (we choose one of the minima, take coordinates such that 0 is the minimum of V , so $V(0) = \nabla V(0) = 0$) has to be replaced by

$$P_h^{app,0} := \sum_{\ell} (hD_{x_\ell} - A_\ell^{lin}(x))^2 + \frac{1}{2} \operatorname{Hess} V(0) x \cdot x .$$

We recall from the previous paragraph that this spectrum is known and equal to h times the spectrum computed for $h = 1$, as immediately seen by the dilation $x = \sqrt{h}y$.

After a gauge transformation, we can assume that

$$A(x) - A^{lin}(x) = \mathcal{O}(|x|^2)$$

and note that the magnetic field attached to $A^{lin}(x)$ is the value of the magnetic field attached to A at 0.

We now take $R = h^{\frac{2}{5}}$ and write

$$\begin{aligned} \langle P_{h,A,V} \phi_j^R u \mid \phi_j^R u \rangle \geq & \langle P^{app,0} \phi_j^R u \mid \phi_j^R u \rangle - Ch^{\frac{6}{5}} \|\phi_j^R u\|^2 \\ & - \left| \int |(A(x) - A^{lin}(x)) \phi_j^R u| \cdot |(h\nabla - iA^{lin}(x)) \phi_j^R u| dx \right| . \end{aligned}$$

This leads first (omitting the reference to R which is now chosen) to

$$\begin{aligned} \langle P_{h,A,V} \phi_j u \mid \phi_j u \rangle \geq \\ \langle P^{app,0} \phi_j u \mid \phi_j u \rangle - Ch^{\frac{6}{5}} \|\phi_j u\|^2 - Ch^{\frac{4}{5}} \|\phi_j u\| \cdot \|(h\nabla - iA^{lin}(x)) \phi_j u\| dx . \end{aligned}$$

Using then Cauchy-Schwarz with some (to be determined) weight $\rho(h)$, we obtain

$$\begin{aligned}
& \langle P_{h,A,V} \phi_j u \mid \phi_j u \rangle \\
& \geq \langle P_{app,0} \phi_j u \mid \phi_j u \rangle - Ch^{\frac{6}{5}} \|\phi_j u\|^2 \\
& \quad - Ch^{\frac{4}{5}} \left(\frac{1}{\rho(h)^2} \|\phi_j u\|^2 + \rho(h)^2 \|(h\nabla - iA^{lin}(x))\phi_j u\|^2 \right) \\
& \geq (1 - h^{\frac{4}{5}} \rho(h)^2) \langle P_{app,0} \phi_j u \mid \phi_j u \rangle - Ch^{\frac{6}{5}} \|\phi_j u\|^2 - Ch^{\frac{4}{5}} \frac{1}{\rho(h)^2} \|\phi_j u\|^2 .
\end{aligned}$$

The choice of $\rho(h) = h^{-\frac{1}{5}}$ leads to

$$\langle P_{h,A,V} \phi_j^R u \mid \phi_j^R u \rangle \geq (1 - h^{\frac{2}{5}}) \langle P_{app,0} \phi_j^R u \mid \phi_j^R u \rangle - Ch^{\frac{6}{5}} \|\phi_j^R u\|^2 .$$

We are now essentially in the same situation as in the case without magnetic field.

4.3.2 Magnetic wells

We would like to describe a case where no electric potential is present. We consider the rather generic case when $B(z) \in C^\infty(\bar{\Omega})$ satisfies, for some $z_0 \in \Omega$:

$$B(z) > b := B(z_0) > 0, \quad \forall z \in \bar{\Omega} \setminus \{z_0\}, \quad (4.15)$$

and we assume that the minimum is non degenerate :

$$\text{Hess } B(z_0) > 0 . \quad (4.16)$$

We introduce in this case the notation :

$$a = \text{Tr} \left(\frac{1}{2} \text{Hess } B(z_0) \right)^{1/2} . \quad (4.17)$$

Theorem 4.1. .

If $A \in C^\infty(\bar{\Omega}; \mathbb{R}^2)$, and if the hypotheses (4.15) and (4.16) are satisfied, then

$$\mu(h) = [b + \frac{a^2}{2b}h]h + o(h^2) . \quad (4.18)$$

The detailed proof can be found in [HelMo3]. It is based on the analysis of the simpler model where near 0

$$B(z) = b + \alpha x^2 + \beta y^2. \quad (4.19)$$

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

$$A_1(z) = 0 \quad \text{and} \quad A_2(z) = bx + \frac{\alpha}{3}x^3 + \beta xy^2. \quad (4.20)$$

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 connection with subriemannian geometry.

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 [Sim2] 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. A third idea is to construct WKB expansions. This will not be detailed in this course.

5 Decay of the eigenfunctions and applications

5.1 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 [Sim2] 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 $\bar{\Omega}$ if for any neighborhood $\mathcal{V}(U)$ of U ,

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

respectively

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

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, if⁷ $\lim_{h \rightarrow 0} \lambda(h) \leq E < \inf \sigma_{ess}(P_{h,V}) - \epsilon_0$ (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 should recover the classical mechanics.

Of course the above is very heuristic but there are more accurate mathematical notions like the frequency set (see [Ro2]) 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 $-h^2 \frac{d^2}{dx^2} + x^2$

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

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 .

5.2 Energy inequalities

The main but basic tool is a very simple identity attached to the Schrödinger operator $P_{h,A,V}$.

Proposition 5.1. :

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

$$\int_{\Omega} |\nabla_{h,A}(\exp \frac{\phi}{h} u)|^2 dx + \int_{\Omega} (V - |\nabla\phi|^2) \exp \frac{2\phi}{h} |u|^2 dx = \operatorname{Re} \left(\int_{\Omega} \exp \frac{2\phi}{h} (P_{h,A,V}u)(x) \cdot \overline{u(x)} dx \right). \quad (5.1)$$

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 :

$$\int_{\Omega} \nabla v \cdot \nabla \bar{w} dx = - \int_{\Omega} \Delta v \cdot \bar{w} dx - \int_{\partial\Omega} (\partial v / \partial n) \bar{w} d\sigma_{\partial\Omega}. \quad (5.2)$$

This gives in particular :

$$\int_{\Omega} \nabla v \cdot \nabla \bar{w} dx = - \int_{\Omega} \Delta v \cdot \bar{w} dx, \quad (5.3)$$

for all $v, w \in C^2(\bar{\Omega})$ such that $w|_{\partial\Omega} = 0$ or $(\partial v / \partial n)|_{\partial\Omega} = 0$.

This can actually be extended to $v, w \in H_0^1(\Omega)$.

We then observe (we treat the case when $A = 0$) :

$$\begin{aligned} \operatorname{Re} \int \exp \frac{2\phi}{h} (-h^2 \Delta u) \cdot \bar{u} dx &= \operatorname{Re} \int (h \nabla u) \cdot \overline{(h \nabla \exp \frac{2\phi}{h} u)} dx \\ &= \operatorname{Re} \int ((h \nabla - \nabla \phi) \exp \frac{\phi}{h} u) \cdot \overline{(h \nabla + \nabla \phi) \exp \frac{\phi}{h} u} dx \\ &= \int |(h \nabla \exp \frac{\phi}{h} u)|^2 dx - \int |\nabla \phi|^2 |\exp \frac{\phi}{h} u|^2 dx. \end{aligned}$$

The case when A is not zero is treated similarly.

To treat more general ϕ 's, we just write ϕ as a limit as $\epsilon \rightarrow 0$ of $\phi_{\epsilon} = \chi_{\epsilon} \star \phi$

where $\chi_\epsilon(x) = \chi(\frac{x}{\epsilon}) \epsilon^{-m}$ is the standard mollifier and we remark (this is a standard result about Lipschitz functions) 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

$$\int_{\Omega} \nabla_{h,A} v \cdot \overline{\nabla_{h,A} w} dx = - \int_{\Omega} \Delta_{h,A} v \cdot \bar{w} dx - h \int_{\partial\Omega} (h\partial v/\partial n - i\vec{A} \cdot \vec{n}v) \bar{w} d\sigma_{\partial\Omega} . \quad (5.4)$$

Remark 5.2.

This identity is adapted to the Dirichlet realization. We will need a similar identity for the Neumann realization. In this case, we will instead of the condition $u|_{\partial\Omega} = 0$ take the Neumann (magnetic) condition.

5.3 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 :

$$d_{(V-E)_+}(x, y) = \inf_{\gamma \in \mathcal{C}^{1,pw}([0,1];x,y)} \int_0^1 [(V(\gamma(t)) - E)_+]^{\frac{1}{2}} |\gamma'(t)| dt , \quad (5.5)$$

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

$$\mathcal{C}^{1,pw}([0,1];x,y) = \{\gamma \in \mathcal{C}^{1,pw}([0,1];\mathbb{R}^n) , \gamma(0) = x , \gamma(1) = y\} . \quad (5.6)$$

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

$$|d(x', y) - d(x, y)| \leq d(x', x) , \forall x, x', y \in \mathbb{R}^m . \quad (5.7)$$

$$|\nabla_x d(x, y)|^2 \leq (V - E)_+(x) , \quad (5.8)$$

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.

5.4 Decay of eigenfunctions for the Schrödinger operator.

When u_h is a normalized eigenfunction of the Dirichlet realization in Ω satisfying $P_{h,A,V}u_h = \lambda_h u_h$ then the identity (5.1) 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 $\lambda_h \rightarrow E$ as $h \rightarrow 0$. 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

$$\exp(1 - \epsilon) \frac{d(x)}{h} u_h = \mathcal{O}(\exp \frac{\epsilon}{h}) , \quad (5.9)$$

for any $\epsilon > 0$.

More precisely we get for example the following theorem

Theorem 5.3. :

Let us assume that V is C^∞ , semibounded and satisfies

$$\lim_{|x| \rightarrow \infty} \inf V > \inf V = 0 \quad (5.10)$$

and

$$V(x) > 0 \text{ for } |x| \neq 0 . \quad (5.11)$$

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

$$P_{h,A,V}u_h = \lambda_h u_h , \quad (5.12)$$

with $\lambda_h \rightarrow 0$ as $h \rightarrow 0$. 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

$$\|\nabla_{h,A}(\exp \frac{d}{h} \cdot u_h)\|_{L^2(K)} + \|\exp \frac{d}{h} \cdot u_h\|_{L^2(K)} \leq C_{\epsilon,K} \exp \frac{\epsilon}{h} , \quad (5.13)$$

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

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

Proof:

Let us choose some $\epsilon > 0$. We shall use the identity (5.1) 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
- $P_{h,A,V}$ replaced by $-\Delta_{h,A} + V - \lambda_h$.

Let

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

We deduce from (5.1)

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

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

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

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

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

and finally

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

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

Remark 5.4.

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 $h \rightarrow 0$) 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 $\mathcal{O}(\exp -2S/h)$.

Let us just give a hint about the proof. If $(u_h^{(2)}, \lambda_h^{(2)})$ is a family of spectral pairs of the Dirichlet realization of the Schrödinger in Ω_2 . Then if χ is a cutoff function with compact support in Ω_1 , which is equal to 1 on a neighborhood of U , then we can use $\chi u_h^{(2)}$ as a quasimode. We observe indeed that

$$(-\Delta_{h,A} + V - \lambda_h^{(2)})(\chi u_h^{(2)}) = -2(\nabla\chi) \cdot (\nabla_{h,A} u_h^{(2)}) - h^2(\Delta\chi)u_h^{(2)}.$$

Then the choice of χ and the Agmon estimates on $u_h^{(2)}$ permit to show that the right hand side is exponentially small as stated.

Remark 5.5.

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].

5.5 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 $x \mapsto \text{Tr}^+(B(x))$). This is due to (2.53) in the case $n = 2$ ($B(x)$ of constant sign) and to their extensions. The Agmon distance will be attached to $h [\text{Tr}^+(B(x)) - \inf_x \text{Tr}^+(B(x))] dx^2$.

The proof is in two steps: treatment of the case with constant magnetic field and then partition of unity for controlling the comparison with this case.

This explains, due to the presence of h before $|B|$, that the decay is measured through a weight in $\exp -\frac{\phi}{\sqrt{h}}$, where ϕ should satisfy :

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

outside a neighborhood of the magnetic well, that is the set of points where $\text{Tr}^+(B(x)) = \inf_x \text{Tr}^+(B(x))$. We will come back to this in Section 7.

6 On some questions coming from superconductivity

6.1 Introduction to the problem in superconductivity

This problem is physically described in all the basic books in physics (see for example Saint-James-De Gennes [SdG]). 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 paper by Bauman-Phillips-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, and more recent contributions by Helffer-Morame [HelMo3, HelMo4, HelMo5], Fournais-Helffer [FoHel1, FoHel2, FoHel3], Bonnaillie [Bon]

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 section of 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 (ψ, \mathcal{A}) in $H^1(\Omega; \mathbb{C}) \times H^1(\mathbb{R}^2; \mathbb{R}^2)$ of the Ginzburg-Landau functional \mathcal{G} :

$$\hat{\mathcal{G}}(\psi, \mathcal{A}) = \int_{\Omega} \{ |(\nabla - i\kappa\mathcal{A})\psi|^2 + \frac{\kappa^2}{2} (|\psi|^2 - 1)^2 \} dx + \kappa^2 \int_{\mathbb{R}^2} |\text{curl } \mathcal{A} - \mathcal{H}|^2 dx . \quad (6.1)$$

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

$$\mathcal{G}(\psi, \mathcal{A}) = \int_{\Omega} \{ |(\nabla - i\kappa\mathcal{A})\psi|^2 + \frac{\kappa^2}{2} (|\psi|^2 - 1)^2 \} dx + \kappa^2 \int_{\Omega} |\text{curl } \mathcal{A} - \mathcal{H}|^2 dx . \quad (6.2)$$

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

The parameter κ is a characteristic of the sample. Traditionally one makes the distinction between Type I materials, corresponding to κ small, and the Type II materials, corresponding to large κ . Mathematically, this leads to the analysis of various asymptotic regimes like $\kappa \rightarrow 0$ or $\kappa \rightarrow +\infty$. It is this last case that 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, we will prove this existence in the next section. The minimizer should satisfy the Euler-Lagrange equation, which is called in this context the Ginzburg-Landau system [SdG].

This equation reads

$$\left. \begin{aligned} (\nabla - i\kappa\mathcal{A})^2\psi &= -\kappa^2(1 - |\psi|^2)\psi \\ \text{curl}^2\mathcal{A} &= -\frac{i}{2\kappa}(\bar{\psi}\nabla\psi - \psi\nabla\bar{\psi}) - |\psi|^2\mathcal{A} \end{aligned} \right\} \quad \text{in } \Omega; \quad (6.3a)$$

$$\left. \begin{aligned} (\nabla_{\kappa\mathcal{A}}\psi) \cdot \nu &= 0 \\ \text{curl}\mathcal{A} - \mathcal{H} &= 0 \end{aligned} \right\} \quad \text{on } \partial\Omega. \quad (6.3b)$$

Here, for $\mathcal{A} = (A_1, A_2)$, $\text{curl}\mathcal{A} = \partial_{x_1}A_2 - \partial_{x_2}A_1$, and

$$\text{curl}^2\mathcal{A} = (\partial_{x_2}(\text{curl}\mathcal{A}), -\partial_{x_1}(\text{curl}\mathcal{A})).$$

Notice that the weak formulation of (6.3) is

$$\text{Re} \int_{\Omega} \overline{(\nabla - i\kappa\mathcal{A})\phi} \cdot (\nabla - i\kappa\mathcal{A})\psi - \kappa^2(1 - |\psi|^2)\bar{\phi}\psi \, dx = 0, \quad (6.4a)$$

$$\int_{\Omega} (\text{curl}\alpha)(\text{curl}\mathcal{A} - \mathcal{H}) \, dx = \frac{i}{\kappa} \int_{\Omega} \text{Im}(\bar{\psi}(\nabla - i\kappa\mathcal{A})\psi) \alpha \, dx, \quad (6.4b)$$

for all $(\phi, \alpha) \in H^1(\Omega) \times H^1(\Omega; \mathbb{R}^2)$.

Due to the gauge invariance of the functional, it is better to restrict (without loss of generality) to the smaller set $H^1(\Omega, \mathbb{C}) \times H_{\text{div}}^1(\Omega)$, where

$$H_{\text{div}}^1(\Omega) = \left\{ \mathcal{V} = (V_1, V_2) \in H^1(\Omega)^2 \mid \text{div}\mathcal{V} = 0 \text{ in } \Omega, \mathcal{V} \cdot \nu = 0 \text{ on } \partial\Omega \right\}. \quad (6.5)$$

The space $H_{\text{div}}^1(\Omega)$ inherits the topology (norm) from $H^1(\Omega; \mathbb{R}^2)$.

The analysis of the system (6.3) can be performed by PDE techniques. We note that this system is (weakly) non linear, that $H^1(\Omega)$ is compactly

imbedded in $L^6(\Omega)$ and that, if $\operatorname{div} A = 0$, $\operatorname{curl}^2 \mathcal{A} = (-\Delta A_1, -\Delta A_2)$. One can show in particular that the solution in $H^1(\Omega, \mathbb{C}) \times H_{\operatorname{div}}^1(\Omega)$ of this “elliptic” system is actually, when Ω is regular, in $C^\infty(\overline{\Omega})$.

It is well known that there exists a unique vector field \mathbf{F} in $H_{\operatorname{div}}^1(\Omega)$ such that

$$\begin{aligned} \operatorname{curl} \mathbf{F} &= H_e \quad \text{and} \quad \operatorname{div} \mathbf{F} = 0, \quad \text{in } \Omega, \\ \mathbf{F} \cdot \nu &= 0 \quad \text{on } \partial\Omega. \end{aligned}$$

We observe that $(0, \sigma \mathbf{F})$ is a trivial critical point of the functional \mathcal{G} , i.e. a trivial solution of the Ginzburg-Landau system. It is therefore natural to discuss as a function of σ , whether this pair is a local or a global minimizer. When σ is large, one can show [GioPh] (see Subsection 6.3) 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.

In the analysis, we will need the following standard result (see for example [Tem]) on the curl-div system

Proposition 6.1.

If Ω is bounded, regular and simply connected, then curl defines an isomorphism from $H_{\operatorname{div}}^1(\Omega)$ onto $L^2(\Omega)$.

6.2 Existence of a minimizer

Using the discussion in the previous section it is natural to impose the condition that $\mathcal{A} \in H_{\operatorname{div}}^1(\Omega)$.

Theorem 6.2. *Suppose that Ω is bounded and simply connected with smooth boundary. For all $\kappa \in \mathbb{R}$ and $\mathcal{H} \in L^2(\Omega)$, the functional \mathcal{G} on $H^1(\Omega) \times H_{\operatorname{div}}^1(\Omega)$ has a minimizer.*

Proof.

Let $(\psi_n, \mathcal{A}_n) \in H^1(\Omega) \times H_{\operatorname{div}}^1(\Omega)$ be a minimizing sequence, i.e.

$$\lim_{n \rightarrow \infty} \mathcal{G}(\psi_n, \mathcal{A}_n) = \inf_{(\psi, \mathcal{A}) \in H^1(\Omega) \times H_{\operatorname{div}}^1(\Omega)} \mathcal{G}(\psi, \mathcal{A}). \quad (6.6)$$

Step 1. $\{(\psi_n, \mathcal{A}_n)\}$ is bounded in $H^1(\Omega) \times H^1(\Omega)$.

By using that \mathcal{G} is the sum of three positive terms, we get the existence of a constant $E_0 > 0$ such that

$$T_n \leq E_0, \quad (6.7)$$

where T_n is any of the three terms

$$\int_{\Omega} |(\nabla - i\kappa\mathcal{A}_n)\psi_n|^2 dx, \quad \int_{\Omega} (|\psi_n|^2 - 1)^2 dx, \quad \int_{\Omega} |\operatorname{curl}\mathcal{A}_n - \mathcal{H}|^2 dx.$$

Since \mathcal{H} is a fixed function in $L^2(\Omega)$ and $\operatorname{div}\mathcal{A}_n = 0$, we get from Proposition 6.1 that \mathcal{A}_n is uniformly bounded in $H^1(\Omega)$.

Notice, using Cauchy-Schwarz and the inequality $2ab \leq \epsilon a^2 + \epsilon^{-1}b^2$ for any $\epsilon > 0$, that

$$\begin{aligned} \int_{\Omega} (|\psi_n|^2 - 1)^2 dx &= \int_{\Omega} |\psi_n|^4 - 2|\psi_n|^2 + 1 dx \\ &\geq \|\psi_n\|_4^4 - 2\|\psi_n\|_4^2 \sqrt{|\Omega|} \geq \frac{1}{2}\|\psi_n\|_4^4 - 2|\Omega|. \end{aligned}$$

Therefore, ψ_n is uniformly bounded in $L^4(\Omega)$, and therefore—using again the Cauchy-Schwarz inequality—in $L^2(\Omega)$.

The boundedness of \mathcal{A}_n in $H^1(\Omega)$ implies, by the Sobolev embedding theorem, that \mathcal{A}_n is uniformly bounded in $L^4(\Omega)$. Combined with the L^4 -bound on ψ_n this gives uniform boundedness of $\mathcal{A}_n\psi_n$ in $L^2(\Omega)$. So, considering the uniform bound,

$$\int_{\Omega} |\nabla\psi_n - i\kappa\mathcal{A}_n\psi_n|^2 dx \leq E_0,$$

this implies that $\{\psi_n\}_n$ is uniformly bounded in $H^1(\Omega)$.

Step 2. A weak limit is a minimizer.

We now extract a subsequence, again denoted by $\{(\psi_n, \mathcal{A}_n)\}$, converging weakly in $H^1(\Omega) \times H^1(\Omega)$ to some $(\psi, \mathcal{A}) \in H^1(\Omega) \times H^1(\Omega)$. Of course, by passage to the limit

$$\operatorname{div}\mathcal{A} = 0, \quad \text{in } \Omega$$

in the sense of distributions. Furthermore, since the inclusion $H^1(\Omega) \rightarrow H^s(\Omega)$ is compact for all $s < 1$ and the restriction $H^s(\Omega) \rightarrow L^2(\partial\Omega)$ is continuous for all $s > 1/2$, we also get

$$\mathcal{A} \cdot \nu = 0, \quad \text{on } \partial\Omega.$$

Thus $\mathcal{A} \in H_{\text{div}}^1(\Omega)$. We can estimate,

$$\begin{aligned} \int_{\Omega} |\text{curl } \mathcal{A} - \mathcal{H}|^2 dx &= \lim_n \langle \text{curl } \mathcal{A} - \mathcal{H} | \text{curl } \mathcal{A}_n - \mathcal{H} \rangle_{L^2 \times L^2} \\ &\leq \|\text{curl } \mathcal{A} - \mathcal{H}\|_2 \liminf_n \|\text{curl } \mathcal{A}_n - \mathcal{H}\|_2. \end{aligned}$$

Therefore,

$$\int_{\Omega} |\text{curl } \mathcal{A} - \mathcal{H}|^2 dx \leq \liminf_n \int_{\Omega} |\text{curl } \mathcal{A}_n - \mathcal{H}|^2 dx. \quad (6.8)$$

The same type of calculation gives that

$$\int_{\Omega} |(\nabla - i\kappa\mathcal{A})\psi|^2 dx \leq \liminf_n \int_{\Omega} |(\nabla - i\kappa\mathcal{A}_n)\psi_n|^2 dx. \quad (6.9)$$

The compactness of the Sobolev embedding $H^1(\Omega) \rightarrow L^p(\Omega)$, for $p = 2, 4$ implies that

$$\int_{\Omega} (|\psi|^2 - 1)^2 dx = \lim_n \int_{\Omega} (|\psi_n|^2 - 1)^2 dx. \quad (6.10)$$

Combining (6.6) with (6.8), (6.9) and (6.10) shows that (ψ, \mathcal{A}) is a minimizer.

■

6.3 The result of Giorgi-Phillips

Let us give a rather simple proof of this result.

The first important property is

Proposition 6.3.

If (ψ, \mathcal{A}) is a minimizer of \mathcal{G} , then for (almost) all $x \in \Omega$,

$$|\psi(x)| \leq 1. \quad (6.11)$$

Sketch of a proof via the maximum principle.

Assuming the regularity of the minimizer (up to the boundary), we can apply

the Maximum principle to the function $u(x) = |\psi(x)|^2$. We observe that u satisfies⁸

$$\frac{1}{2}\Delta u + \kappa^2 u(1 - u) = |\nabla_{\kappa\mathcal{A}}\psi|^2. \quad (6.12)$$

This equation is a direct consequence of the first Ginzburg-Landau equation. We multiply it by $\bar{\psi}$ and take the real part. The formula is then a consequence of the identity

$$\operatorname{Re} (\Delta_{\kappa\mathcal{A}}\psi \cdot \bar{\psi}) = \frac{1}{2}\Delta(|\psi|^2) - |(\nabla - i\kappa\mathcal{A})\psi|^2,$$

with $\Delta_{\kappa\mathcal{A}} = (\nabla - i\kappa\mathcal{A})^2$.

This in particular implies :

$$\frac{1}{2}\Delta u + \kappa^2 u(1 - u) \geq 0. \quad (6.13)$$

Now if u admits a maximum which is > 1 then we get a contradiction as follows. If this maximum is attained at one point of Ω , we have indeed $\Delta u \leq 0$ and $\kappa^2 u(1 - u) < 0$ in contradiction with (6.13). If the maximum was attained at the boundary, we should use in addition the fact that u satisfies the usual Neumann boundary condition.

Instead of giving the necessary justifications for the above proof, we prefer the following attractive short argument from [DGP].

Proof of Proposition 6.3.

With the notation $[t]_+ = \max(t, 0)$, we define $\Omega_+ := \{x \in \Omega : |\psi(x)| > 1\}$, and the following functions on Ω_+ ,

$$f := \frac{\psi}{|\psi|}, \quad \tilde{\psi} := [|\psi| - 1]_+ f.$$

Notice that $[t]_+ = \frac{t+|t|}{2}$, so applying Proposition 2.8 twice, we see that

$$[|\psi| - 1]_+ \in H^1(\Omega), \quad \text{and} \quad \nabla[|\psi| - 1]_+ = 1_{\Omega_+} \nabla[|\psi| - 1]_+ = 1_{\Omega_+} \nabla|\psi|.$$

⁸Here we cheat a little because we do not control in detail a possible problem near the zeroes of ψ . But this is not a deep problem because we have to show here that u can not be too large so the zero set of u cannot be a problem.

Let $\chi \in C^\infty(\mathbb{R})$ be increasing and satisfy,

$$\chi(t) = 0 \text{ on } t \leq 1/4, \quad \chi(t) = 1 \text{ on } t \geq 3/4,$$

and define

$$G(z) = \chi(|z|) \frac{z}{|z|}, \quad \tilde{f} := G(\psi).$$

Then, since G is smooth with bounded derivatives, the chain rule gives that $\tilde{f} \in H^1(\Omega)$ (see for instance [LiLo, Theorem 6.16]). Furthermore, $\psi = [|\psi| - 1]_+ \tilde{f}$, so

$$(\nabla - iA)\tilde{\psi} = 1_{\Omega_+} \tilde{f} \nabla |\psi| + [|\psi| - 1]_+ (\nabla - iA)\tilde{f}$$

Now, clearly,

$$1_{\Omega_+} (\nabla - iA)\psi = 1_{\Omega_+} (\nabla - iA)(|\psi|\tilde{f}) = 1_{\Omega_+} \{ \tilde{f} \nabla |\psi| + |\psi| (\nabla - iA)\tilde{f} \}$$

So therefore,

$$\operatorname{Re} \left\{ \overline{(\nabla - iA)\tilde{\psi}} \cdot (\nabla - iA)\psi \right\} = 1_{\Omega_+} \left(|\nabla |\psi||^2 + (|\psi| - 1)|\psi| |(\nabla - iA)\tilde{f}|^2 \right).$$

Here we used that on Ω_+ , we have $|f| = |\tilde{f}| = 1$, and therefore

$$f \nabla \bar{f} + \bar{f} \nabla f = \nabla |f|^2 = 0,$$

so $1_{\Omega_+} f \nabla \bar{f}$ takes values in $i\mathbb{R}^2$.

Thus we have, by the weak form of the first Ginzburg-Landau equation, and the support of $\tilde{\psi}_\epsilon$

$$\begin{aligned} 0 &= \operatorname{Re} \left\{ \int_{\Omega} \overline{(\nabla - iA)\tilde{\psi}} (\nabla - iA)\psi + \tilde{\psi} (|\psi|^2 - 1)\psi \, dx \right\} \\ &= \int_{\Omega_+} |\nabla |\psi||^2 + (|\psi| - 1)|\psi| |(\nabla - iA)\tilde{f}|^2 + (1 + |\psi|)(|\psi| - 1)^2 |\psi| \, dx. \end{aligned}$$

Since the integrand is non-negative, we easily conclude that Ω_+ has measure zero. \blacksquare

We now assume that we have a **non normal** minimizer for \mathcal{G} . This means that

$$\mathcal{G}(\psi, \mathcal{A}) \leq \frac{\kappa^2}{2} |\Omega| \tag{6.14}$$

and

$$\int_{\Omega} |\psi|^2 dx > 0. \quad (6.15)$$

Condition (6.14) implies the following inequality :

$$\int_{\Omega} |(\nabla - i\kappa\mathcal{A})\psi|^2 dx + \kappa^2 \int_{\Omega} |\operatorname{curl} \mathcal{A} - \mathcal{H}|^2 dx \leq \kappa^2 \int_{\Omega} |\psi(x)|^2 dx. \quad (6.16)$$

We will now show that this last inequality will permit the control of $\int_{\Omega} |(\nabla - i\kappa\sigma\mathbf{F})\psi|^2 dx$.

Without loss of generality, we can assume that \mathcal{A} satisfies the additional condition

$$\operatorname{div} \mathcal{A} = 0 \text{ in } \Omega, \quad \mathcal{A} \cdot \nu = 0 \text{ on } \partial\Omega. \quad (6.17)$$

We now use the result Proposition 6.1 on the curl-div system to conclude that there exists a constant C_{Ω} such that

$$\|\mathcal{V}\|_{L^2}^2 \leq C_{\Omega} \|\operatorname{curl} \mathcal{V}\|_{L^2(\Omega)}^2, \quad \forall \mathcal{V} \in H_{div}^1(\Omega). \quad (6.18)$$

We now compare $\int_{\Omega} |(\nabla - i\kappa\sigma\mathbf{F})\psi|^2$ and $\int_{\Omega} |(\nabla - i\mathcal{A})\psi|^2$. A trivial estimate is

$$\int_{\Omega} |(\nabla - i\kappa\sigma\mathbf{F})\psi|^2 \leq 2\|(\nabla - i\kappa\mathcal{A})\psi\|^2 + 2\kappa^2\|(\mathcal{A} - \sigma\mathbf{F})\psi\|^2. \quad (6.19)$$

Implementing (6.11) and (6.18) gives

$$\int_{\Omega} |(\nabla - i\kappa\sigma\mathbf{F})\psi|^2 \leq 2 \int_{\Omega} |(\nabla - i\kappa\mathcal{A})\psi|^2 + 2C_{\Omega}\kappa^2\|\operatorname{curl}(\mathcal{A} - \sigma\mathbf{F})\|^2. \quad (6.20)$$

This leads to

$$\int_{\Omega} |(\nabla - i\kappa\sigma\mathbf{F})\psi|^2 \leq (2 + 2C_{\Omega})\kappa^2 \int_{\Omega} |\psi|^2 dx. \quad (6.21)$$

But ψ satisfies (6.15), so we finally obtain

$$\mu^{(1)}(\sigma\kappa\mathbf{F}) \leq (2 + 2C_{\Omega})\kappa^2. \quad (6.22)$$

But we will see in the next section, by semi-classical techniques that there exists $C_0(\Omega) > 0$ and $h_0(\Omega) > 0$ such that if

$$\sigma\kappa \geq \frac{1}{h_0}, \quad (6.23)$$

then

$$\mu^{(1)}(\sigma\kappa\mathbf{F}) \geq \frac{1}{C_0(\Omega)}\sigma\kappa. \quad (6.24)$$

So we have shown that if, for some pair (κ, σ) satisfying (6.23), a non normal minimizer exists then

$$\sigma < (2 + 2C_\Omega)C_0(\Omega)\kappa.$$

This can be reformulated in the following way

Theorem 6.4 (Giorgi-Phillips).

Suppose that $\mathcal{H} = \sigma H_e$, where $H_e > 0$, in the definition of the Ginzburg-Landau functional. If Ω is simply connected, there exists a constant $C(\Omega) > 0$ such that if

$$\sigma > C(\Omega) \max\left(\kappa, \frac{1}{\kappa}\right),$$

then \mathcal{G} has as unique minimizer (up to gauge transform) the normal solution $(0, \sigma\mathbf{F})$.

Remark 6.5.

We emphasize that the result is true for any $\kappa > 0$. But as $t = \kappa\sigma$ tends to 0, $\mu^{(1)}(t\mathbf{F})$ is $\mathcal{O}(t^2)$. We will analyze this question in the next subsection. As observed in [GioPh], one can improve the theorem, assuming $\kappa \leq 1$ by saying that there exists $C(\Omega)$ such that if $\sigma > C(\Omega)$, then \mathcal{G} has as unique minimizer (up to gauge transform) the normal solution $(0, \sigma\mathbf{F})$.

Remark 6.6.

The fact that $\text{curl}\mathbf{F}$ is constant does not play an important role. A weaker assumption of non vanishing of $\text{curl}\mathbf{F}$ will be enough for showing that as $\sigma \rightarrow +\infty$ the unique minimizer is the normal solution. See Remark 2.22.

6.4 Perturbation theory and analysis of the weak κ situation

In this subsection, we present some results of X. Pan [Pan3] (see also Bolley-Helffer for the analysis of a 1-dimensional reduced model).

If \mathcal{A} satisfies the two conditions $\mathcal{A} \cdot \nu = 0$ on $\partial\Omega$ and $\text{div}\mathcal{A} = 0$ in Ω , the domain the Schrödinger realization is fixed and the dependence with respect to κ is analytic. We can then apply Kato's theory (analytic perturbation theory) to the analysis of the groundstate energy. For $\kappa = 0$, $\Delta_{\mathcal{A}}$ is simply

the Neumann realization of the Laplacian in Ω . The groundstate energy is 0 and this is an eigenvalue of multiplicity 1 (Ω is assumed to be connected). The associated eigenfunction can be chosen as

$$\varphi_0 = \frac{1}{|\Omega|^{\frac{1}{2}}} . \quad (6.25)$$

We consequently know that, for κ small ($\kappa \in] -\kappa_0, +\kappa_0[$) enough, the groundstate eigenvalue remains simple and admits the expansion

$$\mu^{(1)}(\kappa\mathcal{A}) \sim \sum_{j \geq 1} \kappa^j \mu_j ,$$

as $\kappa \rightarrow 0$.

But the diamagnetic inequality immediatly implies that $\mu_1 = 0$. So we know that

$$\mu^{(1)}(\kappa\mathcal{A}) \sim \sum_{j \geq 2} \kappa^j \mu_j , \quad (6.26)$$

and it is interesting to compute μ_2 .

This can be done by using formal expansions in the following way. We look for an eigenvalue admitting expansion (6.26) and an eigenfunction

$$\varphi^{(1)}(\kappa\mathcal{A})(x) \sim \sum_{j \geq 0} \kappa^j \varphi_j . \quad (6.27)$$

Moreover, we actually do not loose in generality by adding the condition that φ_j is orthogonal to φ_0 for $j \geq 1$. This can be rewritten in the form

$$\int_{\Omega} \varphi_j dx = 0 ,$$

for $j = 1, \dots, n$.

We now write formally that

$$-\Delta_{\kappa\mathcal{A}} \varphi^{(1)}(\kappa\mathcal{A}) - \mu^{(1)}(\kappa\mathcal{A}) \varphi^{(1)}(\kappa\mathcal{A}) \sim 0 . \quad (6.28)$$

We note that with our choice of gauge

$$-\Delta_{\kappa\mathcal{A}} = -\Delta + 2i\kappa\mathcal{A} \cdot \nabla + \kappa^2 |\mathcal{A}|^2 .$$

We denote by \mathcal{R}_0 the operator defined by

$$\mathcal{R}_0 := \Pi_0 \Delta^{-1} \Pi_0 ,$$

where Π_0 is the projector on the first eigenfunction.

Computing the coefficients of each powers of κ in (6.28), we get the equations (we just write the first equations....). The coefficient of κ^0 is 0. Let us look as the coefficient of κ

$$-\Delta \varphi_1 = -2i\mathcal{A}\nabla \varphi_0 = 0 . \quad (6.29)$$

We can consequently choose $\varphi_1 = 0$.

Let us now look at the coefficient of κ^2 . Taking account of the previous equation, we obtain :

$$-\Delta \varphi_2 - \mu_2 \varphi_0 + |\mathcal{A}|^2 \varphi_0 = 0 . \quad (6.30)$$

This equation can be solved if and only if

$$\mu_2 = \int_{\Omega} |\mathcal{A}|^2 dx .$$

This gives the value of μ_2 , which is non zero iff the magnetic field curl A is non identically 0. We are also very happy to verify that μ_2 is positive, as predicted by the diamagnetic inequality. For this value of μ_2 , one can then define φ_2 by

$$\varphi_2 := \frac{1}{|\Omega|^{\frac{1}{2}}} \mathcal{R}_0 |\mathcal{A}|^2 .$$

It is easy to see that one can continue to solve uniquely the equations. The necessary condition for solving determines indeed at each step μ_j .

Remark 6.7.

In the previous subsection, we can apply this result with κ replaced by $\kappa\sigma$, and \mathcal{A} replaced by \mathbf{F} . In this case, we note that one solution $\sigma(\kappa)$ of $\mu(\sigma\kappa\mathbf{F}) = \kappa^2$, admits the expansion (for κ small)

$$\sigma(\kappa) \sim \sum_j \sigma_j \kappa^j ,$$

with

$$\sigma_0 = \mu_2^{-\frac{1}{2}} , \quad \mu_2 = \int_{\Omega} |\mathbf{F}|^2 dx .$$

6.5 Critical fields and Schrödinger operators with magnetic field

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

$$H_{C_3}(\kappa) = \inf\{\sigma > 0 : (0, \sigma \mathbf{F}) \text{ is the unique global minimizer of } \mathcal{G}\}. \quad (6.31)$$

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

$$\mathcal{N}(\kappa) := \{\sigma > 0 : (0, \sigma \mathbf{F}) \text{ is the unique global minimizer of } \mathcal{G}\}. \quad (6.32)$$

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 Neumann realization of $-(\nabla - i\mathcal{A})^2$. It is useful to observe the strong connections 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 6.8. .

- 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 enlightening. 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 $(\lambda u_1, \sigma\mathbf{F})$ we get, for $0 < |\lambda|$ small enough, an energy which is strictly less than the energy of the normal solution $(0, \mathbf{F})$. We have indeed

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

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 6.9.

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

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

Remark 6.10.

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

$$-(h\nabla - i\frac{\mathcal{A}_{\kappa, \sigma}}{\sigma})^2 \psi_{\kappa, \sigma} + V_{\kappa, \sigma} \psi_{\kappa, \sigma} - \frac{1}{\sigma^2} \psi_{\kappa, \sigma} = 0, \quad (6.33)$$

where

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

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 $h \rightarrow 0$ will still be valid for the order parameter corresponding to the minimizer.

Remark 6.11.

All these questions are still the object of active research. Natural questions are :

- Does the equation in σ ,

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

have a unique solution for κ large enough?

- Is this unique solution the critical field $H_{C_3(\kappa)}$?

Notice that Theorem 2.12 can be used to give an affirmative answer to the first question if one can prove a sufficiently precise asymptotic expansion for the lowest eigenvalue $\mu^{(1)}(\kappa\sigma\mathbf{F})$. We refer to [FoHel2, FoHel3] for the most recent results around the analysis of this third critical field.

7 Main results on semi-classical bottles and proofs

7.1 Introduction

If one can naturally refer to Kato and, at the end of the seventies'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 $\Omega = \mathbb{R}^n$, $h|\text{curl } A(x)|$ plays the role of an effective electric potential. By this we mean that the analysis 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

$$b < b' , \tag{7.1}$$

is satisfied, where we used the notations :

$$\inf_{x \in \Omega} |B(x)| = b , \quad \inf_{x \in \partial\Omega} |B(x)| = b' . \tag{7.2}$$

7.2 Main results

We recall that we have given a rough asymptotic estimate for the Dirichlet realization in dimension 2 (see Theorem 2.16) 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 7.1.

$$\lim_{h \rightarrow 0} \frac{1}{h} \inf \sigma(P_{h,A,\Omega}^N) = \min(b, \Theta_0 b') . \tag{7.3}$$

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 (2.53) in the special case

when $n = 2$ and when the magnetic field has a constant sign. Here $\langle \cdot | \cdot \rangle$ 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, Shi, 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 $\overline{\Omega}$ is not necessarily the right quantity for analyzing the bottom of the spectrum as (7.1) 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 $P_{h,A,\Omega}^N$ of $P_{h,A,\Omega}$ is bounded from above by $\lambda^{(1)}(h)$ (but the lower bound (2.58) is not correct in general).

One important theorem that we would like to present is

Theorem 7.2. .

If the magnetic field is constant and not zero, then any ground state corresponding to the Neumann realization is localized as $h \rightarrow 0$ 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 7.3. .

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 $h \rightarrow 0$ 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 (2.53) 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

$$B(x) > 0 . \tag{7.4}$$

7.3 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 multiplying 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). More precisely, we can take near one point x_0 of the boundary, where $|B(x)| = b'$, a system of coordinates $x \mapsto (s, t)$ such that $t(x)$ denotes the distance to the boundary and $s(x)$ is a parametrization of the boundary with $s(x_0) = 0$. In these coordinates, the “principal part” will look like

$$h^2 D_t^2 + (h D_s - b't)^2$$

on the half plane $t > 0$. (It is better to think that we should consider $S^1 \times]0, t_0]$ with Neumann at $t = 0$ and Dirichlet at $t = t_0$).

The first guess in order to have a lower energy is to look for

$$(t, s) \mapsto h^{-\frac{1}{4}} e^{i\rho_0 \frac{s}{\sqrt{h}}} u_0(h^{-\frac{1}{2}} \beta t)$$

where $\mathbb{R}^+ \ni v \mapsto u_0(v)$ is the eigenvalue for the half-line model with $\xi = \xi_0$ and magnetic field equal to 1 (β and ρ_0 being suitably chosen) in order to get the minimal energy (for the moment it is an L^∞ -eigenfunction).

This leads to

$$\beta^2 D_v^2 + \left(\rho_0 - \frac{b'}{\beta} v\right)^2 u_0 = \Theta_0 b' v .$$

So we should take the pair (β, ρ_0) with $\beta = \sqrt{b'}$ and $\rho_0 = \xi_0 \beta$.

It then remains to localize the candidate in the s variable closely to $s = 0$ and to localize in the t direction with a cut-off function $t \mapsto \chi(t)$ with compact support in $[0, t_0)$ and to localize in the s direction with a function $s \mapsto \chi_0(s)$ with support in a neighborhood of 0. So the trial function that we choose (for an h independent constant and for $\alpha > 0$ arbitrary) is

$$\phi_0(t, s; h) = C h^{-\frac{5}{16}} \chi(t) \chi_0(s) \exp -\alpha \frac{s^2}{h^{\frac{1}{4}}} \exp \left(i \xi_0 \sqrt{b'} \frac{s}{\sqrt{h}} \right) u_0 \left((b'/h)^{\frac{1}{2}} t \right) .$$

Computing the energy of this trial function, this leads to :

$$\mu^{(1)}(h) \leq \min(b, \Theta_0 b') h + o(h) , \quad (7.5)$$

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].

7.4 Lower bounds

Let $0 \leq \rho \leq 1$. We first claim that there exists C such that, for any $\delta_0 > 0$, 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 ,

$$\sum_j |\chi_j^h|^2 = 1 , \quad (7.6)$$

$$\sum_j |\nabla \chi_j^h|^2 \leq C \delta_0^{-2} h^{-2\rho} , \quad (7.7)$$

and

$$\text{supp}(\chi_j^h) \subset Q_j = B(z_j, \delta_0 h^\rho) , \quad (7.8)$$

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 :

$$\text{either } \text{supp } \chi_j \cap \partial\Omega = \emptyset , \text{ either } z_j \in \partial\Omega . \quad (7.9)$$

According to the two alternatives in (7.9), we can decompose the sum in (7.6) 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 :

$$q_h^N(u) = \sum_j q_h(\chi_j^h u) - h^2 \sum_j \| |\nabla \chi_j^h| u \|^2 , \quad \forall u \in H^1(\Omega) . \quad (7.10)$$

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

$$q_{h,A}^N(u) = \int_{\Omega} |h\nabla u - iAu|^2 dx , \quad (7.11)$$

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, (7.10) is the consequence of the identity, for any function $\chi \in C^\infty(\bar{\Omega})$ and any $u \in H^1(\Omega)$:

$$q_{h,A}^N(\chi u) = \operatorname{Re} a_{h,A}^N(u, \chi^2 u) + h^2 \|\nabla \chi |u|\|_{L^2(\Omega)}^2 . \quad (7.12)$$

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

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

we have

$$q_{h,A}^N(\chi u) = \operatorname{Re} \langle P_{h,A,\Omega}^N u \mid \chi^2 u \rangle_{L^2(\Omega)} + h^2 \|\nabla \chi |u|\|_{L^2(\Omega)}^2 . \quad (7.13)$$

We can rewrite the right hand side of (7.10) as the sum of three (types of) terms.

$$q_h(u) = \sum_{int} q_h(\chi_j^h u) + \sum_{bnd} q_h(\chi_j^h u) - h^2 \sum_j \|\nabla \chi_j^h |u|\|^2 , \quad \forall u \in H^1(\Omega) . \quad (7.14)$$

For the last term in the right hand side of (7.14), we get using (7.7) :

$$h^2 \sum_j \|\nabla \chi_j^h |u|\|^2 \leq C h^{2-2\rho} \delta_0^{-2} \|u\|^2 . \quad (7.15)$$

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 δ_0 for our various problems (note that the play with δ_0 large will be only interesting when $\rho = \frac{1}{2}$).

The first term in the right hand side of (7.14) can be estimated from below by using (2.53). The support of $\chi_j^h u$ is indeed contained in Ω . So we have :

$$\sum_{int} q_h(\chi_j^h u) \geq h \sum_{int} \int B(x) |\chi_j^h u|^2 dx . \quad (7.16)$$

The second term in the right hand side of (7.14) 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 coordinates 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 $B(z, 2C\delta_0 h^\rho)$ $q_{h,A}(u)$ 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

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

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,

$$\begin{aligned} q_{h,A}(\chi_j^h u) &\geq (1 - Ch^{2\theta} - C\delta_0 h^\rho) q^h[A_j^{lin}](\exp\{-\frac{i}{h}\phi_j\}\chi_j^h u) \\ &\quad - Ch^{-2\theta} \| |x|^2 \chi_j^h u \|^2 \\ &\geq (1 - Ch^{2\theta} - C\delta_0 h^\rho) q^h[A_j^{lin}](\exp\{-\frac{i}{h}\phi_j\}\chi_j^h u) \\ &\quad - Ch^{4\rho-2\theta} \|\chi_j^h u\|^2 . \end{aligned}$$

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

$$q_{h,A}(\chi_j^h u) \geq (1 - Ch^{2\theta} - C\delta_0 h^\rho) h\Theta_0 \int B(z_j) |\chi_j^h u|^2 dx - Ch^{4\rho-2\theta} \|\chi_j^h u\|^2 . \quad (7.17)$$

We now put together all the estimates and obtain :

$$\begin{aligned} q_{h,A}(u) &\geq h \sum_{int} \int B(x) |\chi_j^h u|^2 dx \\ &\quad + (1 - Ch^{2\theta} - C\delta_0 h^\rho) h\Theta_0 \sum_{bnd} \int B(z_j) |\chi_j^h u|^2 dx \\ &\quad - Ch^{4\rho-2\theta} \sum_{bnd} \|\chi_j^h u\|^2 \\ &\quad - C\delta_0^{-2} h^{2-2\rho} \|u\|^2 . \end{aligned} \quad (7.18)$$

We have now to optimize our choices of ρ , θ and δ_0 . If we just want to get a lower bound of the spectrum, we can first write :

$$q_{h,A}(u) \geq h \min(b, \Theta_0 b') \|u\|^2 - (Ch^{2\theta+1} + C\delta_0 h^{\rho+1} + Ch^{4\rho-2\theta} + C\delta_0^{-2} h^{2-2\rho}) \|u\|^2 .$$

Taking $\rho = \frac{3}{8}$, $\theta = \frac{1}{8}$, $\delta_0 = 1$, we get :

$$q_{h,A}(u) \geq \left(\min(b, \Theta_0 b') h - Ch^{\frac{5}{4}} \right) \|u\|^2 . \quad (7.19)$$

So, taking $u = u_h^1$, where u_h^1 is a groundstate, we obtain from (7.19) :

Proposition 7.4. .

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

$$\mu^{(1)}(h) \geq (\min(b, \Theta_0 b')) h - Ch^{\frac{5}{4}} . \quad (7.20)$$

But for the control of the decay, we need also to take in (7.18) $\rho = \frac{1}{2}$, $\theta = \frac{1}{8}$, and δ_0 large. This gives an estimate which may look weaker but will be more efficient.

Proposition 7.5.

There exists C and h_0 and, for all $\delta_0 > 0$, there exists $C(\delta_0)$ such that, for $h \in]0, h_0]$, the following inequality :

$$\begin{aligned} q_{h,A}(u) &\geq h \sum_{int} \int B(x) |\chi_j^h u|^2 dx \\ &\quad - C(\delta_0) h \sum_{bnd} \int |\chi_j^h u|^2 dx \\ &\quad - \frac{Ch}{\delta_0^2} \sum_{int} \int |\chi_j^h u|^2 dx . \end{aligned} \quad (7.21)$$

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

7.5 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 (5.1) and replace ϕ/h by ϕ/\sqrt{h}) :

$$\begin{aligned} &\text{Re} \langle P_{h,A} u \mid \exp \frac{2\Phi}{h^{\frac{1}{2}}} u \rangle \\ &= \text{Re} \langle (\frac{h}{i} \nabla - A) u \mid (\frac{h}{i} \nabla - A) \exp \frac{2\Phi}{h^{\frac{1}{2}}} u \rangle \\ &= \langle (\frac{h}{i} \nabla - A) \exp \frac{\Phi}{h^{\frac{1}{2}}} u \mid (\frac{h}{i} \nabla - A) \exp \frac{\Phi}{h^{\frac{1}{2}}} u \rangle - h \|\nabla \Phi\| \exp \frac{\Phi}{h^{\frac{1}{2}}} u \|^2 \\ &= q_{h,A}(\exp \frac{\Phi}{h^{\frac{1}{2}}} u) - h \|\nabla \Phi\| \exp \frac{\Phi}{h^{\frac{1}{2}}} u \|^2 . \end{aligned} \quad (7.22)$$

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

$$\mu^{(1)}(h) \|\exp \frac{\Phi}{h^{\frac{1}{2}}} u\|^2 = q_{h,A}(\exp \frac{\Phi}{h^{\frac{1}{2}}} u) - h \|\nabla \Phi\| \exp \frac{\Phi}{h^{\frac{1}{2}}} u \|^2 . \quad (7.23)$$

It remains to reimplement the previous inequality in this new one and to use the upper bound (7.5).

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 7.5. We first write :

$$\begin{aligned} q_{h,A}(\exp \frac{\Phi}{h^{\frac{1}{2}}} u) &\geq h \sum_{int} \int B(x) |\exp \frac{\Phi}{h^{\frac{1}{2}}} \chi_j^h u|^2 dx \\ &\quad - C(\delta_0) h \sum_{bnd} \int |\chi_j^h \exp \frac{\Phi}{h^{\frac{1}{2}}} u|^2 dx \\ &\quad - \frac{Ch}{\delta_0^2} \sum_{int} \int |\exp \frac{\Phi}{h^{\frac{1}{2}}} \chi_j^h u|^2 dx . \end{aligned} \quad (7.24)$$

Let us consider the case when

$$\Theta_0 b' < b . \quad (7.25)$$

The inequality (7.5) becomes :

$$\mu^{(1)}(h) \leq \Theta_0 b' h + o(h) . \quad (7.26)$$

Using (7.22), we now obtain :

$$\begin{aligned} \left((b - \Theta_0 b') - o(1) - \frac{C}{\delta_0^2} - \alpha^2 \right) \sum_{int} \int |\exp(\frac{\Phi}{h^{\frac{1}{2}}}) \chi_j^h u|^2 dx \\ \leq C(\delta_0) \sum_{bnd} \int |\chi_j^h u|^2 dx . \end{aligned} \quad (7.27)$$

Taking δ_0 large enough,, h_0 small enough and $\alpha < \sqrt{b - \Theta_0 b'}$, we finally get the existence of C such that, for $h \in]0, h_0]$, the estimate :

$$\| \exp \frac{\alpha d(x, \partial\Omega)}{h^{\frac{1}{2}}} u_h \| \leq C \| u_h \| , \quad (7.28)$$

is satisfied.

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

Theorem 7.6. .

Under condition (7.25), there exists $C > 0$, $\alpha > 0$, such that if u_h is the ground state of $P_{A,h,\Omega}^N$, then :

$$\| \exp \frac{\alpha d(x, \partial\Omega)}{h^{\frac{1}{2}}} u_h(x) \|_{H^1(\Omega)} \leq C \| u_h \|_{L^2} . \quad (7.29)$$

Note that the condition (7.25) is always satisfied when B is constant because $b = b'$ and $\Theta_0 < 1$.

Remark 7.7. .

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 $\exp -\frac{\alpha_0 d_{B=b}(x)}{\sqrt{h}}$, where $d_{B=b}$ is the Agmon distance to the minima of $B(x)$ for the potential $B(x) - b$.

A Discussion about reduced spaces and gauge invariance

The first remark is that given $\widehat{\mathcal{A}}$ on an open set $\widehat{\Omega}$, one can always find a gauge transform such that :

$$\operatorname{div} \widehat{\mathcal{A}} = 0 \text{ in } \widehat{\Omega}, \widehat{\mathcal{A}} \cdot \nu \text{ on } \partial\widehat{\Omega}. \quad (\text{A.1})$$

The proof is standard and very simple. Given a general $\widehat{\mathcal{A}}$, we look for $\widehat{\varphi}$ such that :

$$\operatorname{div} (\widehat{\mathcal{A}} + \operatorname{grad} \widehat{\varphi}) = 0, (\widehat{\mathcal{A}} + \nabla \widehat{\varphi}) \cdot \nu \text{ on } \partial\widehat{\Omega}. \quad (\text{A.2})$$

This reads

$$\Delta \widehat{\varphi} = -\operatorname{div} \widehat{\mathcal{A}} \text{ in } \widehat{\Omega}, \partial_\nu \widehat{\varphi} = -\widehat{\mathcal{A}} \cdot \nu \text{ on } \partial\widehat{\Omega}. \quad (\text{A.3})$$

This is a non-homogeneous Neumann problem, whose solution is unique if we add the condition that

$$\int_{\widehat{\Omega}} \widehat{\varphi} dx = 0. \quad (\text{A.4})$$

The proof can be in two steps. We first reduce to the homogeneous case by choosing $\widehat{\psi}$ in $\widehat{\Omega}$ such that

$$\partial_\nu \widehat{\psi} = \widehat{\mathcal{A}} \cdot \nu \text{ on } \partial\widehat{\Omega}. \quad (\text{A.5})$$

Then $\widehat{\chi} = \widehat{\varphi} + \widehat{\psi}$, should be a solution of

$$\Delta \widehat{\chi} = \operatorname{div} \widehat{\mathcal{A}} + \Delta \widehat{\psi}, \partial_\nu \widehat{\chi} = 0 \text{ on } \partial\widehat{\Omega}.$$

This last equation can be solved if the right hand side is orthogonal to constants, that is, if

$$\int_{\widehat{\Omega}} (\operatorname{div} \widehat{\mathcal{A}} + \Delta \widehat{\psi}) dx = 0.$$

But this is an immediate consequence of (A.5). We then find the unique solution $\widehat{\chi}$ by adding the condition

$$\int_{\widehat{\Omega}} \widehat{\chi} dx = \int_{\widehat{\Omega}} \widehat{\psi} dx.$$

Remark A.1.

We note that in this proof the simplyconnectedness of $\widehat{\Omega}$ is not used.

B Variations around the spectral theorem

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

B.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 $\lambda \notin \sigma(A)$, then

$$\|(A - \lambda)^{-1}\| \leq \frac{1}{d(\lambda, \sigma(A))}. \quad (\text{B.1})$$

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 $\lambda \in \sigma(A)$ such that $d(\lambda, \eta) \leq \epsilon$. We emphasize here that there is no assumption of discreteness of the spectrum.

B.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

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

and let

$$\epsilon = \|(A - \eta)\psi\|.$$

Then it is easy to show that :

$$\eta - \frac{\epsilon^2}{\beta - \eta} \leq \lambda \leq \eta + \frac{\epsilon^2}{\eta - \alpha}. \quad (\text{B.2})$$

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

$$\epsilon^2 \leq (\beta - \eta)(\eta - \alpha). \quad (\text{B.3})$$

B.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

$$\vec{d}(E, F) = \sup_{x \in E, \|x\|=1} d(x, F) . \quad (\text{B.4})$$

This can be recognized as

$$\vec{d}(E, F) = \sup_{x \in E, \|x\|=1} \|x - \Pi_F x\| = \|(I - \Pi_F)|_E\| = \|\Pi_E - \Pi_F \Pi_E\| . \quad (\text{B.5})$$

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

$$\vec{d}(E, F) = \|\Pi_E - \Pi_F \Pi_E\| = \|\Pi_E - \Pi_E \Pi_F\| . \quad (\text{B.6})$$

It is easy from the first definition⁹ to verify that :

$$\vec{d}(E, G) \leq \vec{d}(E, F) + \vec{d}(F, G) . \quad (\text{B.7})$$

Note that $\vec{d}(E, F) = 0$ if and only if $E \subset F$.

We then have the following lemmas

Lemma B.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

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

⁹First 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 :

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

Lemma B.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 B.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 :

$$A\psi_j = \mu_j\psi_j + r_j, \text{ with.} \quad (\text{B.9})$$

Let $a > 0$ and assume that $\sigma(A) \cap [(I + B(0, 2a)) \setminus I] = \emptyset$. Then if E is the space spanned by the ψ_j 's and if F is the eigenspace associated to $\sigma(A) \cap I$, we have

$$\vec{d}(E, F) \leq \left(\sum_j \|r_j\|^2 \right)^{\frac{1}{2}} / (a(\lambda_S^{\min})^{\frac{1}{2}}), \quad (\text{B.10})$$

where λ_S^{\min} is the smallest eigenvalue of the $N \times N$ matrix : $S := (\langle \psi_i | \psi_j \rangle)_{ij}$.

Proof.

Let $\lambda \in \mathbb{C} \setminus (\{\mu_1, \dots, \mu_N\} \cup \sigma(A))$. Let $I = [\alpha, \beta]$. Then by assumption :

$$(A - \lambda)\psi_j = (\mu_j - \lambda)\psi_j + r_j,$$

which can be written as :

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

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 $R \rightarrow +\infty$ 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 B.4.

If $\sigma(A) \cap I$ 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 .

B.4 Another improvement 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 explicitly 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

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

C Variational characterization of the spectrum

C.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.

C.2 On positivity

We first recall the following definition

Definition C.1. .

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

$$\langle Au \mid u \rangle \geq 0, \quad \forall u \in D(A). \quad (\text{C.1})$$

The following proposition relates the positivity with the spectrum

Proposition C.2. .

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

Example C.3. .

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

$$\sigma(P) \subset [\inf V, +\infty[. \quad (\text{C.2})$$

C.3 Variational characterization of the discrete spectrum

Theorem C.4. .

Let A be a selfadjoint semibounded operator. Let $\Sigma := \inf \sigma_{\text{ess}}(A)$ and let us consider $\sigma(A) \cap]-\infty, \Sigma[$, described as a sequence (finite or infinite) of eigenvalues that we write in the form

$$\lambda^1 < \lambda^2 < \dots < \lambda^n \dots .$$

Then we have

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

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

and, for $n \geq 2$,

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

where

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

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

C.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 C.5. .

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

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

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 C.6. .

In the case when the operator has compact resolvent, case (b) does not occur and the supremum in (C.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 C.7. .

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

$$\langle A\phi | \phi \rangle \leq a \|\phi\|^2, \quad \forall \phi \in V, \quad (\text{C.7})$$

is satisfied. Then we have the inequality :

$$\mu_n(A) \leq a . \quad (\text{C.8})$$

Corollary C.8. .

Under the same assumption as in Proposition C.7, if a is below the bottom of the essential spectrum of A , then A has at least n eigenvalues (counted with multiplicity).

Exercise C.9. .

In continuation of Example 2.2, 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 C.5 is obtained by

Theorem C.10. .

Let A be a selfadjoint semibounded operator and $Q(A)$ its form domain ¹⁰ . Then

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

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, $Q(B) \subset Q(A)$ and¹¹

$$\langle Au | u \rangle \leq \langle Bu | u \rangle , \quad \forall u \in Q(B) ,$$

then

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

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

¹⁰associated by completion with the form $u \mapsto \langle u | Au \rangle_{\mathcal{H}}$ initially defined on $D(A)$.

¹¹It is enough to verify the inequality on a dense set in $Q(B)$.

Example C.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 C.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 $H_0^1(\Omega_1)$ with a subspace of $H_0^1(\Omega_2)$ by just an extension by 0 in $\Omega_2 \setminus \Omega_1$.

Other applications appear in Problems F.4 and F.7 (questions 3 and 4). Note that this monotonicity result is wrong for the Neumann problem.

D Essential spectrum and Persson's Theorem

We refer to [Ag] for proofs and generalizations.

Theorem D.1. .

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

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

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

$$\inf \sigma_{ess}(H) = \Sigma(H), \quad (\text{D.2})$$

where

$$\Sigma(H) := \sup_{\mathcal{K} \subset \mathbb{R}^m} \left[\inf_{\|\phi\|=1} \{ \langle \phi | H\phi \rangle \mid \phi \in C_0^\infty(\mathbb{R}^m \setminus \mathcal{K}) \} \right], \quad (\text{D.3})$$

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

$$\sigma_{ess}(H) = \sigma_{ess}(H + W), \quad (\text{D.4})$$

for any regular potential W with compact support. There are other extensions in case with boundary (see [Bon]).

E Boundary coordinates.

Let Ω be a smooth, simply-connected domain in \mathbb{R}^2 . Let $\gamma : \mathbb{R}/|\partial\Omega| \rightarrow \partial\Omega$ be a parametrization of the boundary with $|\gamma'(s)| = 1$ for all s . Let $\nu(s)$ be the unit vector, normal to the boundary, pointing inward at the point $\gamma(s)$. We choose the orientation of the parametrization γ to be counter-clockwise, so

$$\det(\gamma'(s), \nu(s)) = 1 .$$

The curvature $k(s)$ of $\partial\Omega$ at the point $\gamma(s)$ is now defined by

$$\gamma''(s) = k(s)\nu(s) .$$

The map Φ defined in the introduction,

$$\begin{aligned} \Phi : \mathbb{R}/|\partial\Omega| \times (0, t_0) &\rightarrow \Omega , \\ (s, t) &\mapsto \gamma(s) + t\nu(s) , \end{aligned} \tag{E.1}$$

is clearly a diffeomorphism, when t_0 is sufficiently small, with image

$$\Phi(\mathbb{R}/|\partial\Omega| \times (0, t_0)) = \{x \in \Omega \mid \text{dist}(x, \partial\Omega) < t_0\} =: \Omega_{t_0} .$$

Furthermore, $t(\Phi(s, t)) = t$.

If \vec{A} is a vector field on Ω_{t_0} with $B = \text{curl } \vec{A}$ we define the associated fields in (s, t) -coordinates by

$$\tilde{A}_1(s, t) = (1 - tk(s))\vec{A}(\Phi(s, t)) \cdot \gamma'(s) , \quad \tilde{A}_2(s, t) = \vec{A}(\Phi(s, t)) \cdot \nu'(s) , \tag{E.2}$$

$$\tilde{B}(s, t) = B(\Phi(s, t)) . \tag{E.3}$$

Then $\partial_s \tilde{A}_2 - \partial_t \tilde{A}_1 = (1 - tk(s))\tilde{B}$. Furthermore, for all $u \in W^{1,2}(\Omega_{t_0})$, we have, with $v = u \circ \Phi$,

$$\begin{aligned} \int_{\Omega_{t_0}} |(-i\nabla - \vec{A})u|^2 dx & \tag{E.4} \\ &= \int \left\{ (1 - tk(s))^{-2} \left| (-i\partial_s - \tilde{A}_1)v \right|^2 + \left| (-i\partial_t - \tilde{A}_2)v \right|^2 \right\} (1 - tk(s)) ds dt , \\ \int_{\Omega_{t_0}} |u(x)|^2 dx &= \int |v(s, t)|^2 (1 - tk(s)) ds dt . \end{aligned}$$

Lemma E.1.

Suppose Ω is a bounded, simply connected domain with smooth boundary and let t_0 be the constant from (E.1). Then there exists a constant $C > 0$ such that, if \vec{A} is a vector potential in Ω with

$$\operatorname{curl} \vec{A} = 1 \quad \text{on } \partial\Omega, \quad (\text{E.5})$$

and with \tilde{A} defined as in (E.2), then there exists a gauge function $\varphi(s, t)$ on $\mathbb{R}/|\partial\Omega| \times (0, t_0)$ such that

$$\bar{A}(s, t) = \begin{pmatrix} \bar{A}_1(s, t) \\ \bar{A}_2(s, t) \end{pmatrix} := \tilde{A} - \nabla_{(s,t)}\varphi = \begin{pmatrix} \gamma_0 - t + \frac{t^2 k(s)}{2} + t^2 b(s, t) \\ 0 \end{pmatrix}, \quad (\text{E.6})$$

where

$$\gamma_0 = \frac{1}{|\partial\Omega|} \int_{\Omega} \operatorname{curl} \vec{A} \, dx,$$

and b satisfies the estimate,

$$\|b\|_{L^\infty(\mathbb{R}/|\partial\Omega| \times (0, \frac{t_0}{2}))} \leq C \|\operatorname{curl} \vec{A} - 1\|_{C^1(\Omega_{t_0})}. \quad (\text{E.7})$$

Furthermore, if $[s_0, s_1]$ is a subset of $\mathbb{R}/|\partial\Omega|$ with $s_1 - s_0 < |\partial\Omega|$, then we may choose φ on $(s_0, s_1) \times (0, t_0)$ such that

$$\bar{A}(s, t) = \begin{pmatrix} \bar{A}_1(s, t) \\ \bar{A}_2(s, t) \end{pmatrix} := \tilde{A} - \nabla_{(s,t)}\varphi = \begin{pmatrix} -t + \frac{t^2 k(s)}{2} + t^2 b(s, t) \\ 0 \end{pmatrix}, \quad (\text{E.8})$$

with b still satisfying the estimate (E.7).

Proof.

Notice first that

$$\int_0^{|\partial\Omega|} A_1(s, 0) \, ds = \int_0^{|\partial\Omega|} \vec{A} \cdot \gamma'(s) \, ds = \int_{\Omega} \operatorname{curl} \vec{A} \, dx.$$

Let us write

$$\nu = \operatorname{curl} \vec{A} - 1, \quad \tilde{\nu}(s, t) = \nu(\Phi(s, t)), \quad \tilde{\nu}' = \frac{\tilde{\nu}}{t}.$$

Then $\|\tilde{\nu}'\|_{L^\infty} \leq C\|\nu\|_{C^1(\Omega_{t_0})}$ and

$$\partial_s \tilde{A}_2 - \partial_t \tilde{A}_1 = (1 - tk(s))(1 + t\tilde{\nu}') .$$

Define

$$\varphi(s, t) = \int_0^t \tilde{A}_2(s, t') dt' + \left(\int_0^s \tilde{A}_1(s', 0) ds' - s\gamma_0 \right) . \quad (\text{E.9})$$

Then φ is a well-defined continuous function on $\mathbb{R}/|\partial\Omega| \times (0, t_0)$. We pose $\bar{A} = \tilde{A} - \nabla\varphi$ and find

$$\begin{aligned} \bar{A}(s, t) &= \begin{pmatrix} \bar{A}_1(s, t) \\ \bar{A}_2(s, t) \end{pmatrix} = \begin{pmatrix} \bar{A}_1(s, t) \\ 0 \end{pmatrix} , \\ \partial_t \bar{A}_1(s, t) &= -(\partial_s \tilde{A}_2 - \partial_t \tilde{A}_1) = -(1 - tk(s))(1 + t\tilde{\nu}') , \\ \bar{A}_1(s, 0) &= \gamma_0 . \end{aligned}$$

Therefore,

$$\bar{A}_1(s, t) = \gamma_0 - t + \frac{t^2 k(s)}{2} - \int_0^t t'(1 - t'k(s))\tilde{\nu}'(s, t') dt' ,$$

and we get (E.6) by applying l'Hôpital's rule to the integral.

In the case where we only consider a part $(s_0, s_1) \times (0, t_0)$ of the ring $\mathbb{R}/|\partial\Omega| \times (0, t_0)$, we have trivial topology and therefore any two vector fields generating the same magnetic field are gauge equivalent. Therefore the constant term, γ_0 , can be omitted. From a more practical point of view, one can see that we can omit the term $s\gamma_0$ in (E.9) since we do not need to ensure the periodicity of the function φ .

■

F Exercises in Spectral Theory

Exercise F.1. (*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 upper bound for $\Theta_0 = \inf_{\xi} \mu(\xi)$ where $\mu(\xi)$ is the smallest eigenvalue of $P_0(\xi)$. Following the book of the physicist Kittel, one can proceed by minimizing $\langle P_0(\xi)\phi(\cdot; \rho) | \phi(\cdot; \rho) \rangle$ 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 F.2. ¹²

Let V be in $C_0^{\infty}(\mathbb{R}^m)$ ($m = 1, 2$). Show that the essential spectrum of $P_V = -\Delta + V$ is $[0, +\infty[$.

Let us assume in addition that

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

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

$$\langle P_V \psi | \psi \rangle_{L^2(\mathbb{R}^m)} < 0.$$

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 F.3. .

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

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

¹²These counterexamples come back (when $m = 1$ to Avron-Herbst-Simon [AHS] and when $m = 2$ to Blanchard-Stubbe [BS]).

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

$$V(x) \geq 0 . \quad (\text{F.3})$$

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 $h \rightarrow 0$. Show that $h \rightarrow \lambda_1(h)$ is monotonically increasing.

c) Let us assume that $V > 0$ on $\overline{\Omega}$; show that there exists $\epsilon > 0$ such that

$$h^2 \lambda_1(h) \geq \epsilon . \quad (\text{F.4})$$

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 $h > 0$,

$$\lambda_1(h) \leq C . \quad (\text{F.5})$$

One can use the study of the Dirichlet realization of $-\Delta$ in ω .

e) Let us assume that :

$$V > 0 \text{ almost everywhere in } \Omega . \quad (\text{F.6})$$

Show that, under this assumption :

$$\lim_{h \rightarrow 0} \lambda_1(h) = +\infty . \quad (\text{F.7})$$

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

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

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 $n \rightarrow +\infty$ and $u_\infty \in L^2(\Omega)$ such that

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

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

$$\lambda_1(h) \geq \frac{1}{Ch} .$$

Justify the answer by illustrating the arguments by examples and counterexamples.

Problem F.4. (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 $a \rightarrow +\infty$. One can use a suitable construction of approximate eigenvectors.

(d) What is the behavior of $\lambda_1(a)$ as $a \rightarrow 0$. One can use the change of variable $x = ay$ and analyze the limit $\lim_{a \rightarrow 0} a^2 \lambda_1(a)$.

(e) Let $\mu_1(a)$ be the smallest eigenvalue of the Neumann realization in $] -a, +a[$. Show that $\mu_1(a) \leq \lambda_1(a)$.

(f) Show that, if u_a is a normalized eigenfunction associated with $\mu_1(a)$, then there exists a constant C such that, for all $a \geq 1$, we have :

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

(g) Show that, for u in $C^2([-a, +a])$ and χ in $C_0^2([-a, +a])$, we have :

$$-\int_{-a}^{+a} \chi^2 u''(t) u(t) dt = \int_{-a}^{+a} |(\chi u)'(t)|^2 dt - \int_{-a}^{+a} \chi'(t)^2 u(t)^2 dt .$$

(h) Using this identity with $u = u_a$, a suitable χ which should be equal to 1 on $[-a + 1, a - 1]$, the estimate obtained in (f) and the minimax principle, show that there exists C such that, for $a \geq 1$, we have :

$$\lambda_1(a) \leq \mu_1(a) + Ca^{-2} .$$

Deduce the limit of $\mu_1(a)$ as $a \rightarrow +\infty$.

(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 F.5. (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

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

discuss the kernel of H_\pm in function of m .

- c) Observing that

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

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 $g \rightarrow 0$.

- 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 $S > 0$.

Problem F.6. (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

$$\begin{aligned} D(A^D) &= \{u \in H_0^1(\mathbb{R}^+) \cap H^2(\mathbb{R}^+); xu \in L^2(\mathbb{R}^+)\} \\ &= \{u \in H_0^1(\mathbb{R}^+), x^{\frac{1}{2}}u \in L^2(\mathbb{R}^+), A(x, D_x)u \in L^2(\mathbb{R}^+)\}. \end{aligned}$$

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

Another approach could be to analyze the Fourier transform of χu_j where χ is equal to 1 for x large and is equal to 0 in a neighborhood of 0.

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

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

Problem F.7. (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 $Q := D_{y_1}^2 + (y_1 - y_2)^2$ in $\mathbb{R}^+ \times \mathbb{R}$.
3. We first consider the following family of Dirichlet problems associated with the family of differential operators : $\alpha \mapsto H(\alpha)$ defined on $]0, +\infty[$ by :

$$H(\alpha) = D_t^2 + (t - \alpha)^2.$$

Compare with the Dirichlet realization of the harmonic oscillator in $] - \alpha, +\infty[$.

4. Show that the lowest eigenvalue $\lambda(\alpha)$ of $H(\alpha)$ is a monotonic function of $\alpha \in \mathbb{R}$.
5. Show that $\alpha \mapsto \lambda(\alpha)$ is a continuous function on \mathbb{R} .
6. Analyze the limit of $\lambda(\alpha)$ as $\alpha \rightarrow -\infty$.
7. Analyze the limit of $\lambda(\alpha)$ as $\alpha \rightarrow +\infty$.
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 $\mathcal{D}'(\mathbb{R}^+ \times \mathbb{R})$ defined 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 $\Sigma^D(P)$.*

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