On Schrödinger operator with magnetic fields (Old and New)

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1. Introduction

In an open set $\Omega \subset \mathbb{R}^n$, we consider the Schrödinger operator with magnetic field:

$$\Delta_{h,A,V} = \sum_j (hD_{x_j} - A_j)^2 + V$$

where h is a possibly small > 0 parameter (semi-classical limit), ω_A, called magnetic potential (sometimes identified with a vector $\vec{A}$), is the 1-form

$$\omega_A = \sum_j A_j(x)dx_j \; , \; \vec{A} = (A_1, \cdots, A_n)$$

and V is a C^∞ potential.

Boundary conditions:
Dirichlet Condition: $u_{/\partial\Omega} = 0$,
Neumann Condition: $(\vec{n} \cdot (h\nabla - i\vec{A})u)_{/\partial\Omega} = 0$.
No condition, if $\Omega = \mathbb{R}^n$ (essentially selfadjoint).

Basic object: the **magnetic field (2-form)**

$$\sigma_B = d\omega_A$$

When $n = 2$, identification with a function : $\sigma_B = B\, dx_1 \wedge dx_2$.
When $n = 3$: $\sigma_B = \sum_{i<j} B_{ij} dx_i \wedge dx_j$, can be identified with a vector (by the Hodge map) $\vec{B}$.

For the analysis, it is important to realize that

$$B_{jk} = \frac{1}{ih}[hD_{x_j} - A_j, hD_{x_k} - A_k]\ .$$

The "brackets" technique will play an important role.

Gauge invariance : $(u, A) \mapsto (u \exp -i\frac{\phi}{h}, A + d\phi)$.

This implies same σ_B. Converse partially true (topology of Ω!!).

Mathematical questions

Selfadjointness: Kato,...
Mathematical foundations: Avron-Herbst-Simon,....

Some of the questions (personal choice!!) are :

1. When Ω is unbounded, is the operator with compact resolvent ? Determination of the essential spectrum.

2. Dependence of the ground state energy on A, on h, on the geometry of Ω (holes, points of maximal curvature, corners).

3. Localization of the groundstate: semi-classically, at infinity.

All these questions are already interesting without magnetic potential.

The two last questions are specific from the case with magnetic field !!

1. Multiplicity of the lowest eigenvalue

   (When $A = 0$, we know that the lowest eigenvalue (if it exists) is simple)

2. Nodal sets.

   (When $A = 0$, we know that the corresponding ground state (eigenvector) is strictly positive)

Motivations

In addition to their intrinsic interest, these mathematical questions are strongly motivated by :

Atomic physics
See Lieb-Solovej-Yngason

Geometry
Magnetic field in correspondence with curvature,
$\nabla - iA$ in correspondence with connections.
See Montgomery,...

Complex analysis
See Demailly, Fu-Straube, Christ-Fu...

Solid state physics
See Bellissard,..

Superconductivity
See Del Pino-Fellmer-Sternberg, Lu-Pan, Helffer-Morame.

Compactness of the resolvent and essential spectrum

It is not necessary that $V \to +\infty$:

$$-\Delta + x_1^2 x_2^2 \text{ is with compact resolvent.}$$

Avron-Herbst-Simon (magnetic bottles). Helffer-Nourrigat (nilpotent techniques), Robert, Simon, Helffer-Mohamed.... When $n = 2$,

$$h \int_\Omega B(x)dx \leq ||\nabla_A u||^2 \, , \; \forall u \in C_0^\infty(\Omega) \; .$$

More difficult for $n \geq 3$!!

This works for Dirichlet, not for Neumann.
One can iterate with higher order brackets along Kohn's argument. This leads to Helffer-Mohamed Criterion (to look at pure magnetic effect, we assume $V = 0$).

Compactness criterion in the Pure Magnetic Case

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

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

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

Then $-\Delta_A$ *is with compact resolvent.*

Examples :

$$(D_{x_1} - x_2 x_1^2)^2 + (D_{x_2} + x_1 x_2^2)^2$$

(Easy with the above inequality)
but also

$$(D_{x_1} - x_2 x_1^2)^2 + (D_{x_2} - x_1 x_2^2)^2$$

Question : Is there a semi-classical version of this theorem (notion of magnetic wells)? See later.

What about Dirac and Pauli ?

Here: $\Omega = \mathbb{R}^n$ (n=2,3).

Dirac operator :

$$D_{h,A} = \sum_j \sigma_j (hD_{x_j} - A_j)^2$$

on $L^2(\Omega, \mathbb{C}^k)$ $(k = 2$ if $n = 2$, $k = 4$ if $n = 3)$, where the σ_j's are the Pauli matrices:

$$\sigma_j \sigma_k + \sigma_k \sigma_j = 2\delta_{jk}$$

$$D_{h,A}^2 := \text{ Pauli Operator}$$

Under the same assumptions, Helffer-Nourrigat-Wang have shown that Dirac and Pauli are not with compact resolvent!!

Conjecture

The pure magnetic Dirac operator is never with compact resolvent !!

Decay estimates

- At infinity:
Brummelhuis, Helffer-Nourrigat, Erdös, Martinez-Sordoni, Nakamura

- In the semiclassical regime:
Helffer-Sjöstrand, Helffer-Mohamed,... cf Superconductivity

Two types of results:
Type 1: it decays at least like when $A = 0$ (connected to diamagnetism)

$$|u_h(x)| \sim\leq C \exp -d_V(x, V^{(-1)}(\min V))/h \; .$$

This is rather optimal (as $A = 0$)
Type 2: The magnetic field is itself creating the decay (for example when $V = 0$).

$$|u_h(x)| \sim\leq C \exp -d_B(x, |B|^{(-1)}(\min |B|))/\sqrt{Ch}) \; .$$

This is NOT optimal.

Agmon estimates.

The Agmon distance d_V associated to the metric $(V-E)_+ dx^2$.
Basic identity :

$$\text{Re } \langle \exp -2\frac{\Phi}{h} \Delta_{h,A,V}\, u \mid u \rangle = || \exp \frac{\Phi}{h} \nabla_{h,A} u ||^2 + \int (V - |\nabla \Phi|^2) \exp \frac{2\Phi}{h} |u|^2 \, .$$

Main idea for Dirichlet: $\Delta_{h,A} + V$ is rather well understood by $-h^2\Delta + V + h||B||$.
When $V = 0$, the groundstate is localized near the minima of $||\sigma_B||$.

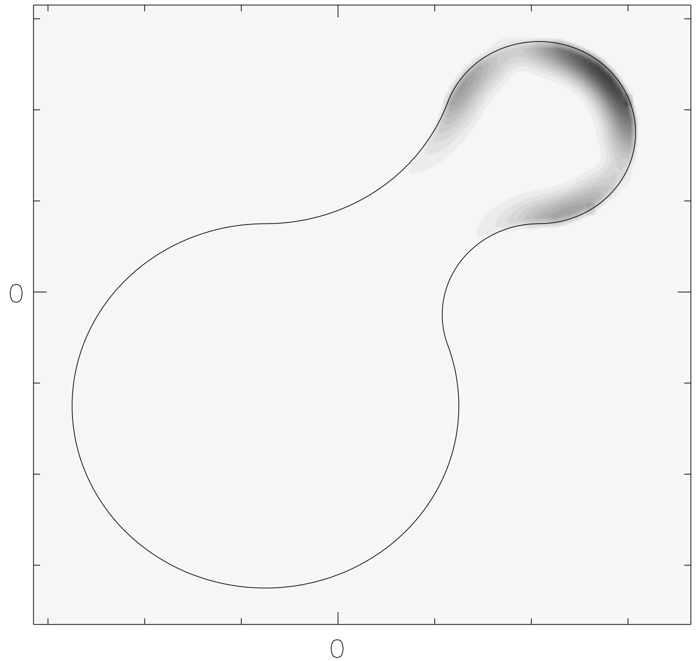
For Neumann, this is completely different !! When $V = 0$ and σ_B is constant (not zero), the groundstate is localized at the boundary (effective potential $\Theta_0|B|$ with $0 < \Theta_0 < 1$)!! There is a different effective potential at the boundary.

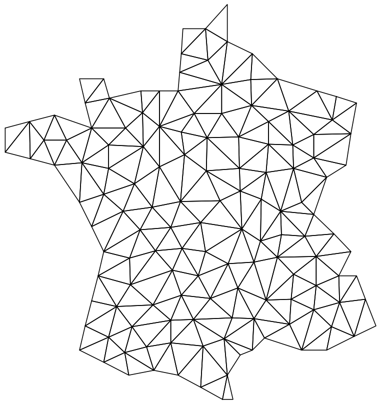
One part of the analysis is based on spectral properties of models :

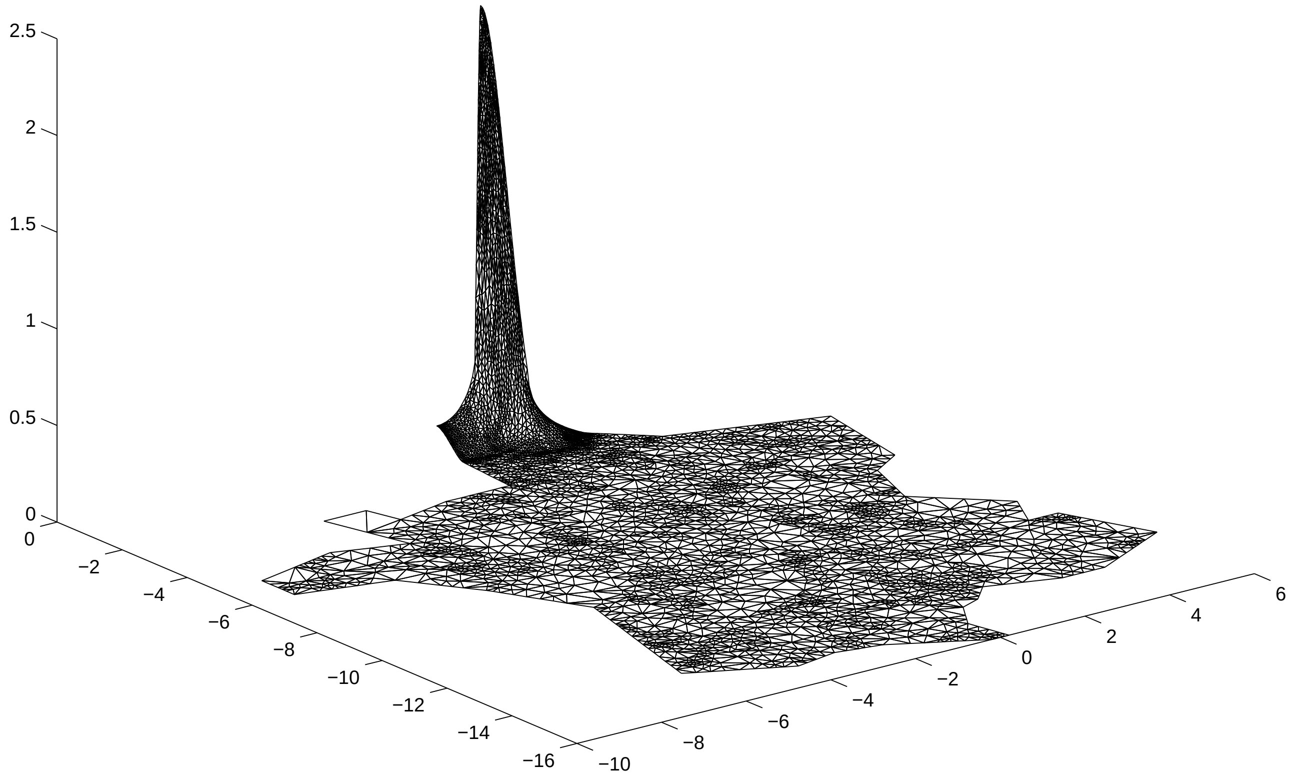
- $D_t^2 + t^2$ on $\mathbb{R}$
- $H^{Neu}(\rho) := D_t^2 + (t-\rho)^2$, on $\mathbb{R}^+$, with Neumann condition at 0.
- $D_t^2 + D_s^2 + (t\cos\theta - s\sin\theta - \rho)^2$ on $\mathbb{R}^{2,+}$, with Neumann condition at $t = 0$.
- $D_u^2 + (u^2 - \rho)^2$ on $\mathbb{R}$.
- $D_s^2 + (D_t - s)^2$ in an infinite sector of angle α (Neumann).

The questions are: bottom of the spectrum, infimum over ρ (for example $\Theta_0 = \inf_\rho \inf \sigma(H^{Neu}(\rho))$) , infimum over θ, dependence on α.

Application: Localization at the boundary, localization at the points of maximal curvature ($n = 2$), localization at the points where the magnetic field (seen as a vector) is tangent at the boundary ($n = 3$), at the corners (Jadallah, Bonnaillie). Below: a numerical computation by Hornberger for the maximal curvature effect.



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6

Diamagnetism, paramagnetism in the semi-classical regime.

We know (Kato's inequality) that the ground state energies (=lowest eigenvalues) satisfy

$$\lambda_{h,A,V} \geq \lambda_{h,0,V} \ .$$

A simple result (Lavine-O'Caroll (heuristic), Helffer) is that :

$$\lambda_{h,A,V} = \lambda_{h,0,V} \text{ if and only if } \begin{cases} \sigma_B = 0 \\ \frac{1}{2\pi} \int_\gamma \omega_A \in \mathbb{Z}, \forall \text{ path } \gamma \ . \end{cases}$$

It is interesting to measure **quantitatively** $\lambda_{h,A,V} - \lambda_{h,0,V}$, especially in the case when $\sigma_B = 0$. This is called the Bohm-Aharonov effect for bounded states.

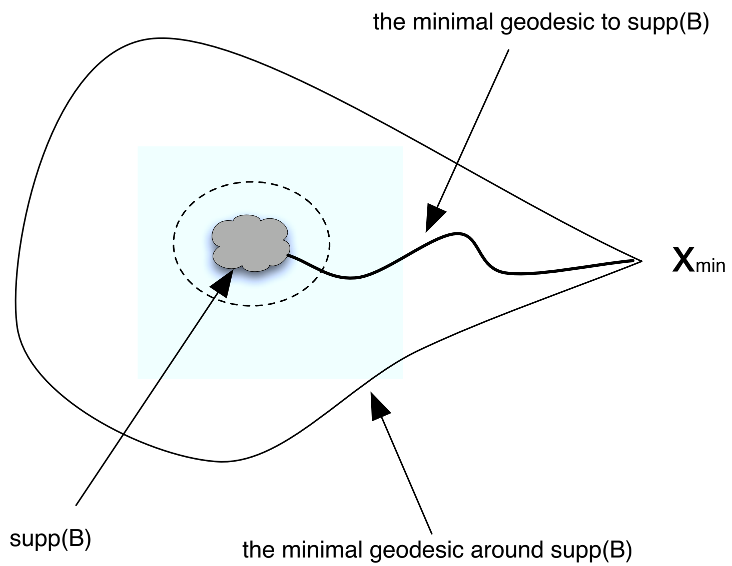
Two techniques:

- Hardy inequality (Laptev-Weidl, Christ-Fu),
- semi-classical analysis: Comparison between direct effects and, in the case of "holes" or high electric barriers on the support of B, flux effects.

Roughly :

$$\lambda_{h,A,V} - \lambda_{h,0,V} \sim (1 - \cos\frac{\Phi}{h}) a(h) \exp -\frac{S_0}{h} + b(h) \exp -\frac{2S_1}{h} \ ,$$

where S_0 is the Agmon length of the shortest touristical path (around the support of σ_B), and S_1 is the Agmon distance to the support of B. Here V is a one well potential (having a minimum at x_{min}) which is "large" (possibly infinite) on the support of σ_B.



For the paramagnetism.
We come back to Pauli.

Question:
Do we have $\lambda_{min}(D^2_{h,A} + V) \leq \lambda_{min}(\Delta_{h,0,V})$,

$$\text{with } D^2_{h,A} = \Delta_{h,A} \otimes I + h \sum_j \sigma_j \vec{B}_j$$

Counterexamples (Avron-Simon (radial example), Helffer (by semi-classical analysis), Christ-Fu).
In Helffer's example $S_0 < 2S_1$, the term $h\sigma \cdot \vec{B}$ perturbes the spectrum in comparison with the magnetic Schrödinger operator by $\mathcal{O}(\exp -\frac{2S_1}{h})$.

Semi-classical estimates for the splitting of Dirac (with V): B. Parisse.

Can we hear the zero locus...

Formulation due to R. Montgomery (in reference to M. Kac), extension by Helffer-Mohamed.

We have already mentioned that for Dirichlet ($V = 0$), the ground state is localized near the minimum of $||B||$.

Asymptotics of the ground state energy (substitute for the harmonic approximation) can be given when $||B||$ has a non degenerate strictly positive minimum, or when $||B||$ vanishes at a point, along a closed curve. Typically, the model is locally $(hD_t)^2 + (t^2 - hD_s)^2$, which is related to the spectral analysis of $D_t^2 + (t^2 - \rho)^2$ in $\mathbb{R}$ (See also Kwek-Pan).

See above, see also questions in hypoanalyticity (Helffer, Pham The Lai-Robert, Christ.....)

Nodal sets and multiplicity

Let us consider the case of an annulus like symmetric domain in $\mathbb{R}^2$ and the Dirichlet case with 0-magnetic field.

$$\Theta := \frac{1}{2\pi} \int_\sigma \omega_A \ .$$

(Normalized flux in the hole = circulation along a simple path around the hole).

Theorem. • *$\Theta \mapsto \lambda(\Theta)$ is 1-periodic, $\lambda(-\Theta) = \lambda(\Theta)$.*

- *The multiplicity is 1 for $\Theta \notin \mathbb{Z} + \frac{1}{2}$, ≤ 2 for $\Theta = \mathbb{Z} + \frac{1}{2}$. $[0, \frac{1}{2}] \ni \Theta \mapsto \lambda(\Theta)$ is monotonic.*

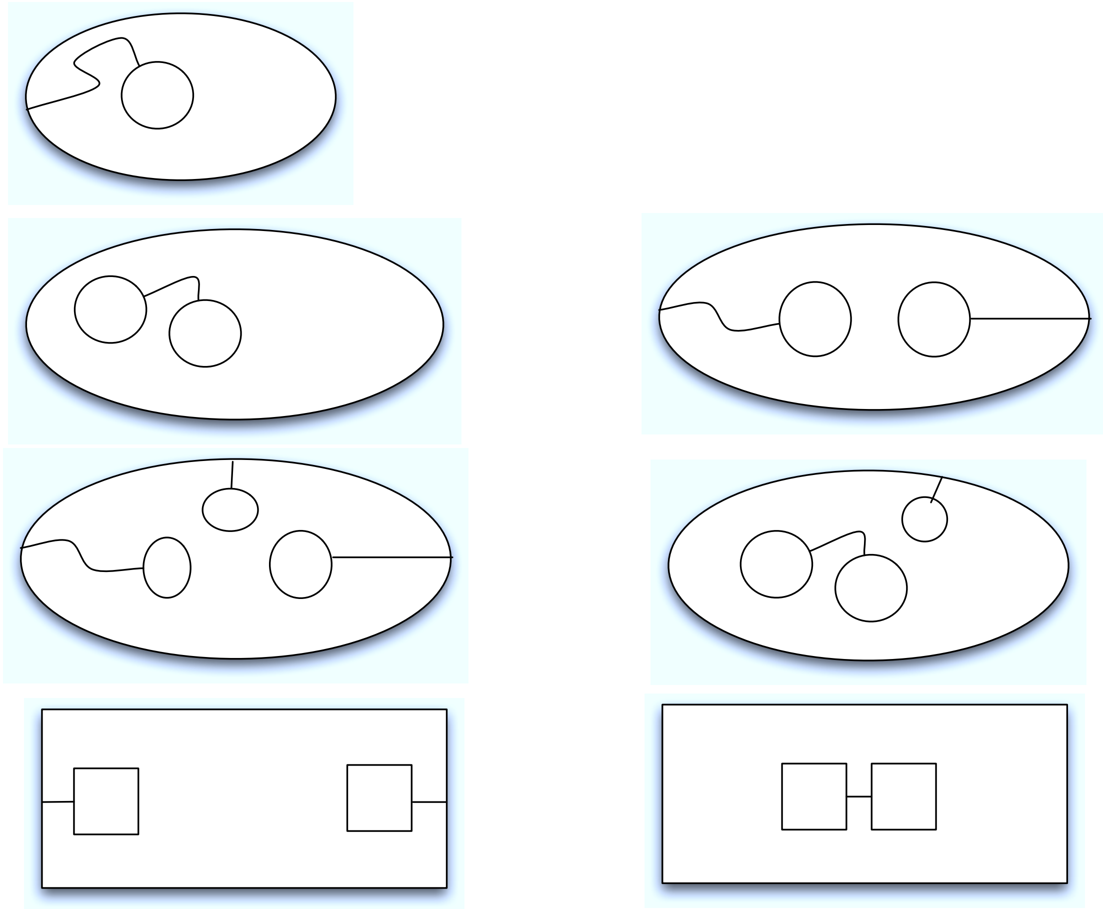
- *The zero set is empty for $\Theta \notin \mathbb{Z} + \frac{1}{2}$.*

- *For $\Theta = \mathbb{Z} + \frac{1}{2}$, there is a basis of the groundstate eigenspace such that the nodal set is one line joining the two components of the boundary.*

Papers by subsets of $\{$ Helffer, Maria or Thomas Hoffmann-Ostenhof, Nadirashvili, Owen$\}$

Extensions for many holes, Schrödinger with periodic potentials...

Below we give (after H-HO-HO-O) a qualitative picture (not computed!!) describing the possible topological structure of the nodal lines for the groundstate in domains with holes and with normalized flux $1/2$. Note that there are very few "quantitative" results, except by semiclassical analysis ($\frac{1}{2}+\frac{1}{2}=1$) (see above) or for very symmetric situation by analyzing singular limits of domains (see below R. Joly-G. Raugel).



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