Analysis of the bottom of the spectrum of Schrödinger operators with magnetic potentials and applications

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1. Introduction

In an open set $\Omega \subset \mathbb{R}^n$, (more generally on a compact or non compact, with or without boundary) 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: $u_{/\partial\Omega} = 0$,
or
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

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

2. Localization of the groundstate: semi-classically
3. Multiplicity of the lowest eigenvalue

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

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, Helffer-Mohamed, Kwek-Pan

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

Solid state physics
See Bellissard, Helffer-Sjöstrand..

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

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 $n = 2$, the inequality

$$h \int_\Omega B(x)dx \leq ||\nabla_{h,A} u||^2 \, , \; \forall u \in C_0^\infty(\Omega) \, ,$$

with $\nabla_{h,A} = h\nabla - iA$, gives an immediate result. 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 $\Omega = \mathbb{R}^n$ 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 :

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

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!! Moreover, when $n \geq 3$, the essential spectrum is $\mathbb{R}$.

Conjecture

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

Question

Do we have magnetic wells for Pauli ??

Decay estimates

(Initially Agmon, Lithner)

In the semiclassical regime
Helffer-Sjöstrand, Simon, Helffer-Mohamed,..., Helffer-Morame
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.

When a boundary is involved, we will meet

$$|u_h(x)| \sim\leq C \exp -d(x, \partial\Omega)/\sqrt{Ch}) \ .$$

and sometimes we will have to measure the decay inside the boundary.

When $|B|$ has a degenerate minimum, it is interesting to analyze the decay inside the submanifold where $|B|$ is minimum.

Connexion with Schrödinger with degenerate wells (Helffer-Sjöstrand).

In the examples below the well is the circle $x^2 + y^2 = 1$.

- Miniwells :

$$h^2(D_x^2 + D_y^2) + (1 + x^2)(1 - x^2 - y^2)^2 \ .$$

  The well is $x^2 + y^2 = 1$ and the miniwells are $(0, \pm 1)$.
- Uniformly degenerate wells :

$$h^2(D_x^2 + D_y^2) + (1 - x^2 - y^2)^2 \ .$$

  The well is $x^2 + y^2 = 1$ and invariant by rotation.

Agmon estimates.

The Agmon distance d_V associated to the metric

$$(V - E)_+ dx^2 \ .$$

Basic identity :

$$\begin{aligned} &\mathrm{Re}\ \langle \exp -2\tfrac{\Phi}{h} \Delta_{h,A,V}\, u \mid u \rangle \\ = &\,|| \exp \tfrac{\Phi}{h} \nabla_{h,A} u ||^2 + \textstyle\int (V - |\nabla \Phi|^2) \exp \tfrac{2\Phi}{h} |u|^2 \ . \end{aligned}$$

Main idea for Dirichlet:

$\Delta_{h,A} + V$ is rather well understood by

$$-h^2 \Delta + V + h ||\sigma_B|| \ .$$

When $V = 0$, the groundstate is localized near the minima of $||\vec{B}||$.

When $V = hV_1$, one should compare the effect of V_1 and $||\sigma_B||$.

Main idea for Neumann:

Completely different !! When $V = 0$ and σB is constant (not zero), the groundstate is localized at the boundary (effective potential $\Theta_0 ||\sigma_B||$ with $0 < \Theta_0 < 1$)!! There is a different effective potential at the boundary.

Models

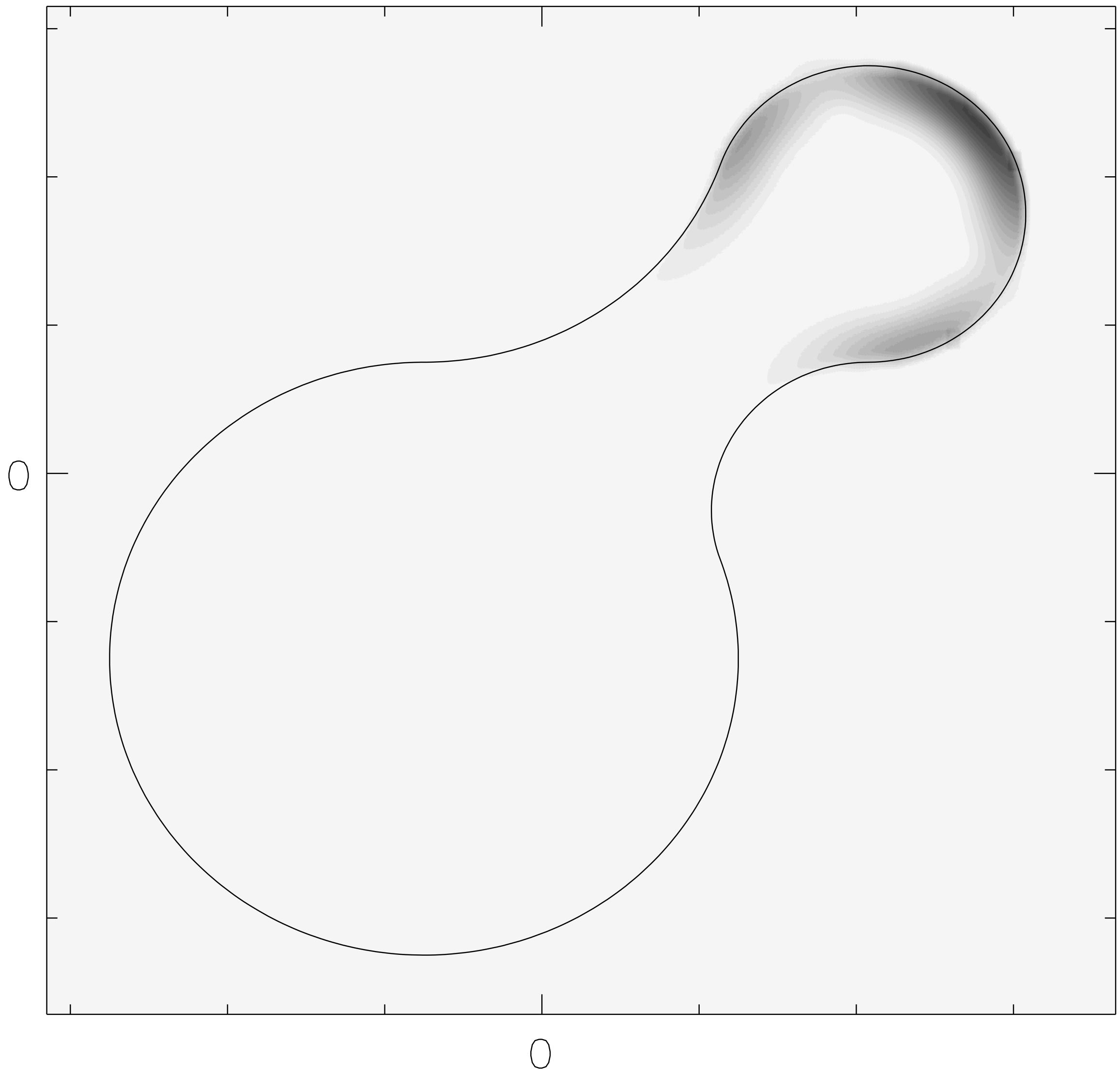
One part of the analysis is based on spectral properties of models :

- $D_t^2 + t^2$ on $\mathbb{R}$ (analysis of the model in $\mathbb{R}^2$)
- $H^{Neu}(\rho) := D_t^2 + (t - \rho)^2$, on $\mathbb{R}^+$, with Neumann condition at 0 (analysis of the model in $\mathbb{R}^2_+$).
- $D_t^2 + D_s^2 + (t\cos\theta - s\sin\theta - \rho)^2$ on $\mathbb{R}^{2,+}$, with Neumann condition at $t = 0$ (analysis of the model in $\mathbb{R}^3_+$).
- $D_u^2 + (u^2 - \rho)^2$ on $\mathbb{R}$ (Montgomery's model).
- $D_s^2 + (D_t - s)^2$ 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.



When B is constant ($\neq 0$), the groundstate is localized at the points of maximal curvature.

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 :

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

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:

- New Hardy estimates for Bohm-Aharonov hamiltonians: Laptev-Weidl, Balinsky, Christ-Fu... The simplest prototype is

$$\int_{\mathbb{R}^2} \frac{|u(x)|^2}{|x|^2}\, dx \leq (\min_{k\in\mathbb{Z}} |k-\Psi|)^{-2} \int_{\mathbb{R}^2} |(\nabla + iA)u(x)|^2\, dx\ ,$$
$$\forall u \in C_0^\infty(\mathbb{R}^2 \setminus 0)\ ,$$

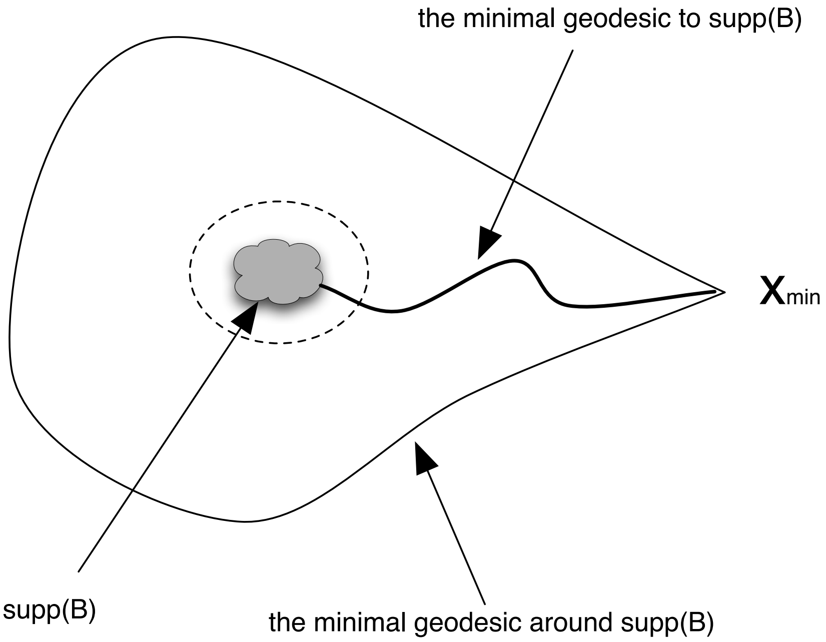
where $A = \frac{\Psi}{r^2}(-y, x)$, so Ψ is the circulation of A around a small positively oriented circle centered at 0.

- 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 $\lambda_{min}(D_{h,A}^2 + V) \leq \lambda_{min}(\Delta_{h,0,V})$,

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

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). 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

1. when $||B||$ has a non degenerate strictly positive minimum, (Helffer-Mohamed, Helffer-Morame) (expansion : $\inf ||B||\, h + \gamma_2 h^2 + o(h^2)$)
2. when $||B||$ vanishes at a point, along a closed curve. (Montgomery, Helffer-Mohamed, Kwek-Pan)

Typically, the model considered by Montgomery was 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 above, see also questions in hypoanalyticity (Helffer, Pham The Lai-Robert, Christ.....) (this is related to the non-hypoanalyticity of $D_t^2 + (t^2 D_x - D_y)^2$ in $\mathbb{R}^3$.)

More recently, a contribution of Kwek-Pan should be mentioned. Although not detailed, this seems to come back to models of the type :

$$(hD_t)^2 + (\gamma(s)t^2 - hD_s)^2 \ .$$

This time, $\gamma(s) \neq 0$ is not constant and there is a localization of the ground state near the minima of $|\gamma|$. The bottom of the spectrum is given by

$$\mu_1(h) = h^{\frac{4}{3}}(\min |\gamma|^{\frac{1}{3}})\hat{\nu}_0 + \mathcal{O}(h^{\frac{5}{3}}) \ ,$$

where

$$\hat{\nu}_0 = \inf_{\rho} \sigma(D_t^2 + (t^2 - \rho)^2) \ .$$

This model will also appear in the analysis of the Neumann problem (n=3).

Expected (Helffer-Morame, work in progress):
$\mu_1(h) \sim h^{\frac{4}{3}}(\min |\gamma|^{\frac{1}{3}})\mu_0 + \nu_1 h^{\frac{5}{3}} + h^{\frac{11}{6}} \sum_{\ell \geq 0} \delta_\ell h^{\frac{\ell}{6}}$.

Neumann when $n = 2$

Bernoff-Sternberg, Lu-Pan, Del Pino-Sternberg, Helffer-Morame, Fournais-Helffer.

Theorem

The groundstate of the Neumann realization satisfies

$$\mu^{(1)}(h) = \Theta_0 h - 2\kappa_{max} M_3 h^{\frac{3}{2}} + \mathcal{O}(h^{\frac{7}{4}}) \ . \tag{1}$$

Here κ_{max} = maximal curvature, $M_3 > 0$ universal constant. For the upper bound, we construct (after Bernoff-Sternberg) in a neighborhood of a point of maximal curvature ($s = 0$ defining this point), the solution takes the form :

$$\begin{aligned} u := \phi(h^{-\frac{1}{2}}t) \exp -\gamma h^{-\frac{1}{4}} s^2 \cdot \\ \exp i h^{-1}[\Phi_0(s,t) + h^{\frac{1}{2}}\Phi_1(s,t)]\chi(s,t) \end{aligned} \tag{2}$$

Remark

$\mathcal{O}(h^{\frac{7}{4}})$ is optimal. The coefficient of $h^{\frac{7}{4}}$ should be related to the second derivative of the curvature at the points of maximal curvatures. (See Bernoff-Sternberg).

Hope (Fournais-Helffer work in progress: Grushin problem or Feshbach projection method leading to a reeduction at the boundary):

$$\mu^{(1)}(h) = \Theta_0 h - 2\kappa_{max} M_3 h^{\frac{3}{2}} + \gamma h^{\frac{7}{4}} + h^{\frac{15}{8}} \sum_{j\geq 0} \alpha_j h^{\frac{j}{8}} .$$

and information on the splitting !

Neumann when $n = 3$

It has been observed by Lu-Pan, that the ground state u^h is localized (as $h \to 0$) near the boundary $\partial\Omega$ but more precisely on the set :

$$\Gamma_{\vec{B}} = \{x \in \partial\Omega \mid \langle \vec{B} \mid N(x) \rangle = 0 \} \ , \tag{3}$$

where $N(x)$ is the normal at x to $\partial\Omega$, that is the set of points in $\partial\Omega$ where $\vec{B}$ is tangent.
It is natural to assume that :

$$\Gamma_{\vec{B}} \text{ is a regular submanifold of } \partial\Omega \ , \tag{4}$$

which will be oriented on each component. At each point x of $\Gamma_{\vec{B}}$, we define the normal curvature along $\vec{B}$ by :

$$\kappa_{n,B}(x) := \ K_x(T(x) \wedge N(x) \ , \ \frac{\vec{B}}{||\vec{B}||}) \ , \tag{5}$$

where K denotes the second fundamental form on the surface $\partial\Omega$ and $T(x)$ is the unit oriented tangent vector to $\Gamma_{\vec{B}}$ at x.

It is natural to assume that :

$$\kappa_{n,B} \neq 0 \ , \quad \text{on } \Gamma_H \ . \tag{6}$$

The last generic assumption is :

The set of points where $\vec{B}$ is tangent to $\Gamma_{\vec{B}}$ is isolated. (7)

On $\Gamma_{\vec{B}}$:

$$\tilde{\gamma}_0(x) = (\tfrac{1}{2})^{\frac{2}{3}}\hat{\nu}_0\delta_0^{\frac{1}{3}}\left(|\kappa_{n,B}(x)|^{\frac{2}{3}}\left(\delta_0 + (1-\delta_0)|\langle T(x) \mid \tfrac{\vec{B}}{|\vec{B}|}\rangle|^2\right)^{\frac{1}{3}}\right) , \tag{8}$$

where $\hat{\nu}_0 > 0$ and $\delta_0 \in]0,1[$ are universal constants attached to spectral invariants related to two model Hamiltonians respectively defined on $\mathbb{R}$ and $\mathbb{R}^+$. $\hat{\nu}_0$ is indeed

$$\hat{\nu}_0 = \inf_\rho \inf \sigma(D_s^2 + (s^2 - \rho)^2) .$$

The minimum of this function, which plays the role of effective curvature, is an important invariant :

$$\hat{\gamma}_0 = \inf_{x\in\Gamma_{\vec{B}}} \tilde{\gamma}_0(x) . \tag{9}$$

Main theorem (Pan, Helffer-Morame) is :

Theorem.
Under the previous assumptions, there exists $\eta > 0$ and $\hat{\gamma}_0 > 0$ such that :

$$\inf\ \sigma(P^{h,N}_{A,\Omega}) = b\Theta_0 h + \hat{\gamma}_0 b^{\frac{2}{3}} h^{\frac{4}{3}} + \mathcal{O}(h^{\eta+\frac{4}{3}})\ , \tag{10}$$

where $\hat{\gamma}_0$ is defined in (9).

Comment:
One can hope a corresponding exponential localization at the points of $\Gamma_{\vec{B}}$, where the infimum of $\tilde{\gamma}_0$ is attained.

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.

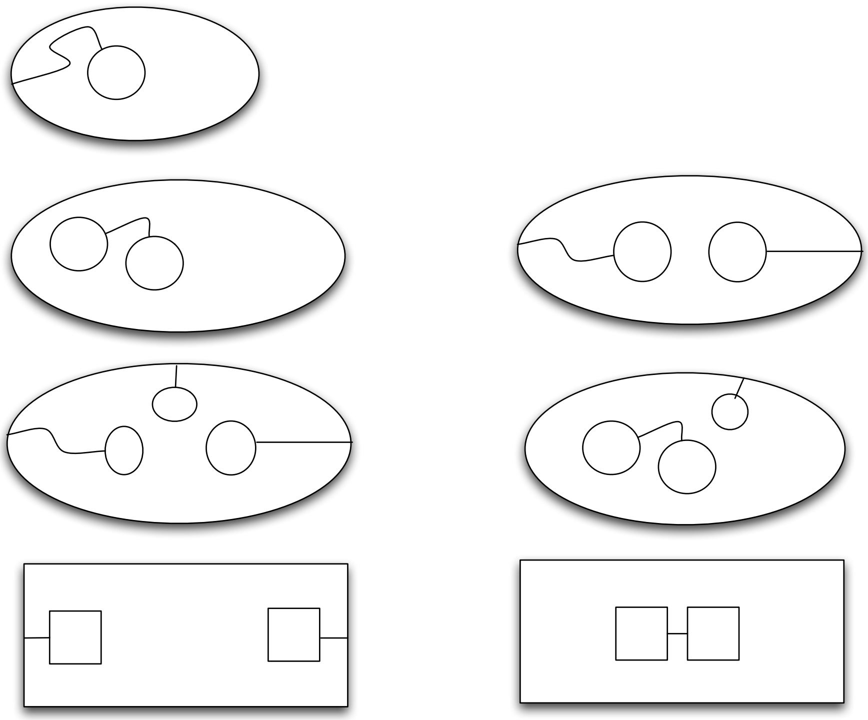
$$\Theta := \frac{1}{2\pi} \int_\sigma \omega_A \ .$$

(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 $\Theta \not\in \mathbb{Z} + \frac{1}{2}$, ≤ 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 $\Theta \not\in \mathbb{Z} + \frac{1}{2}$.
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 and 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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