On magnetic wells in the semi-classical limit.

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Introduction

In the last 35 years, the specialists in semi-classical analysis get new spectral questions for the Schrödinger operator with magnetic field coming from Physics. Some of them are also related to complex analysis.

We would like to present some of these problems and their solutions.

This involves mathematically a fine analysis of the bottom of the spectrum for Schrödinger operators with magnetic fields.

The boundary condition (namely the Neumann condition) could play a basic role..

Many results are presented in the books of Helffer [He1] (1988) and Fournais-Helffer [FH2] (2010) (see also a recent course by N. Raymond). The results discussed today were obtained in collaboration with J. Sjöstrand, A. Morame, and for the most recent Y. Kordyukov.

Other results have been obtained recently by Fournais-Persson, N. Raymond, Dombrowski-Raymond, Popoff, Raymond-Vu-Ngoc. There is a huge litterature on the counting function and connected spectral quantities. We mainly look in this talk at the bottom of the spectrum but not only to the first eigenvalues.

Main goals

Our main object of interest is the Laplacian with magnetic field on a complete manifold, but in this talk we will mainly consider, except for specific toy models, a magnetic field

$$\beta = \text{ curl } \mathbf{A}$$

on a regular domain $\Omega \subset \mathbb{R}^d$ ($d = 2$ or $d = 3$) associated with a magnetic potential $\mathbf{A}$ (vector field on Ω), which (for normalization) satisfies :

$$\text{div } \mathbf{A} = 0 \,.$$

We start from the closed quadratic form Q_h

$$W_0^{1,2}(\Omega) \ni u \mapsto Q_h(u) := \int_\Omega |(-ih\nabla + \mathbf{A})u(x)|^2 \, dx. \tag{1}$$

Let $\mathcal{H}^D(\mathbf{A}, h, \Omega)$ be the self-adjoint operator associated to Q_h and let $\lambda_1^D(\mathbf{A}, h, \Omega)$ be the corresponding groundstate energy. Motivated by various questions we consider the connected problems in the asymptotic $h \to +0$.

Pb 1 Determine the structure of the bottom of the spectrum : gaps, typically between the first and second eigenvalue.

Pb2 Find an effective Hamiltonian which through standard semi-classical analysis can explain the scomplete pectral picture including tunneling.

We will present results which are

- either rather generic
- or non generic but strongly motivated by physics.

The case when the magnetic field is constant

The first results are known from Landau at the beginning of the Quantum Mechanics) analysis of models with constant magnetic field β.
In the case in $\mathbb{R}^d$ ($d = 2, 3$), the models are more explicitly

$$h^2 D_x^2 + (hD_y - x)^2 \,,$$

($\beta(x, y) = 1$) and

$$h^2 D_x^2 + (hD_y - x)^2 + h^2 D_z^2 \,,$$

($\beta(x, y, z) = (0, 0, 1)$) and we have:

$$\inf \sigma(\mathcal{H}(\mathbf{A}, h, \mathbb{R}^d)) = h|\beta| \,.$$

Let us now look at perturbations of this situation.

The effect of an electric potential

2D with some electric one well potential (Helffer-Sjöstrand (1987)).

First we add an electric potential.

$$h^2 D_x^2 + (hD_y - x)^2 + V(x,y)\,.$$

V creating a well at a minimum of V : $(0,0)$. (V tending to $+\infty$ at ∞).

Harmonic approximation in the non-degenerate case:

$$h^2 D_x^2 + (hD_y - x)^2 + \frac{1}{2} < (x,y) | \mathrm{Hess}\, V(0,0) | (x,y)) \,.$$

$$\lambda_1(h) \sim \alpha h \,.$$

The electric potential plays the dominant role and determines the localization of the ground state. As mentioned to us by E. Lieb, this computation is already done by Fock.

2D with some weak electric potential (Helffer-Sjöstrand (1990)).

$$h^2 D_x^2 + (hD_y - x)^2 + h^2 V(x,y)\,.$$

Close to the first Landau level h, the spectrum is given (modulo $\mathcal{O}(h^{\frac{5}{2}})$) by the h-pseudo-differential operator on $L^2(\mathbb{R})$

$$h + h^3 V^w(x, hD_x) + h^2\,(\,\mathrm{Tr}\ \mathrm{Hess}\,V)^w\,(x, hD_x)$$

Here, for a given h-dependent symbol p on $\mathbb{R}^2$, $p^w(x, hD_x; h))$ denotes the operator

$$(p^w(x, hD_x)u)(x) = (2\pi h)^{-1} \int e^{\frac{i}{h}(x-y)\cdot\xi} p(\frac{x+y}{2}, \xi; h) u(y) dy d\xi\,.$$

Purely magnetic effects in the case of a variable magnetic field

We introduce

$$b = \inf_{x \in \overline{\Omega}} |\beta(x)| \,, \tag{2}$$

$$b' = \inf_{x \in \partial\Omega} |\beta(x)| \,. \tag{3}$$

Theorem 1 : rough asymptotics for h small

$$\lambda_1^D(\mathbf{A}, h, \Omega) = hb + o(h) \tag{4}$$

The Neumann case is quite important in the case of Superconductivity.

$$\lambda_1^D(\mathbf{A}, h, \Omega) = h \inf(b, \Theta_0 b') + o(h) \tag{5}$$

with $\Theta_0 \in]0,1[$.
This is not discussed in this talk.

The consequences are that a ground state is localized as $h \to +0$ for Dirichlet, at the points of $\overline{\Omega}$ where $|\beta(x)|$ is minimum,
All the results of localization are obtained through semi-classical Agmon estimates (as Helffer-Sjöstrand [HS1, HS2] or Simon [Si] have done in the eighties for $-h^2\Delta + V$ or for the Witten Laplacians (Witten, Helffer-Sjöstrand, Helffer-Klein-Nier, Helffer-Nier, Le Peutrec,...) .

The case of $\mathbb{R}^n$ or the interior case

2D case

If

$$b < \inf_{x \in \partial\Omega} |\beta(x)| \,,$$

the asymptotics are the same (modulo an exponentially small error) as in the case of $\mathbb{R}^d$: no boundary effect.
In the case of $\mathbb{R}^d$, we assume

$$b < \liminf_{|x| \to +\infty} |\beta(x)| \,.$$

We assume in addition (generic)

Assumption A

- There exists a unique point $x_{min} \in \Omega$ such that $b = |\beta(x_{min})|$.
- $b > 0$
- This minimum is non degenerate.

We get in $2D$ (Helffer-Morame (2001), Helffer-Kordyukov [HK6] (2009))

Theorem 2

$$\lambda_1^D(\mathbf{A}, h) = bh + \Theta_1 h^2 + o(h^2)\,. \tag{6}$$

where $\Theta_1 = a^2/2b$.

Here

$$a = \mathrm{Tr}\left(\frac{1}{2}\mathrm{Hess}\,\beta(x_{min})\right)^{1/2}\,.$$

The previous statement can be completed in the following way.

$$\lambda_j^D(\mathbf{A}, h) \sim h \sum_{\ell \geq 0} \alpha_{j,\ell} h^{\frac{\ell}{2}} , \tag{7}$$

with

- $\alpha_{j,0} = b$,
- $\alpha_{j,1} = 0$,
- $\alpha_{j,2} = \frac{2d^{1/2}}{b}(j-1) + \frac{a^2}{2b}$,
- $d = \det\left(\frac{1}{2}\mathrm{Hess}\,\beta(x_{min})\right)^{1/2}$.

In particular, we get the control of the splitting $\sim \frac{2d^{1/2}}{b}$.
Note that behind these asymptotics, two harmonic oscillators are present as we see in the sketch. Recent improvments (Helffer-Kordyukov and Raymond–Vu-Ngoc) show that no odd powers of $h^{\frac{1}{2}}$ actually occur.

Interpretation with some effective Hamiltonian

Look at the bottom of the spectrum of

$$h\left(\beta^w(x, hD_x) + h\gamma^w(x, hD_x, h^{\frac{1}{2}})\right) .$$

This gives the result modulo $\mathcal{O}(h^2)$, hence it was natural to find a direct proof of this reduction (which is in the physical litterature is called the lowest Landau level approximation).

Sketch of the initial quasimode proof.

The toy model is

$$h^2 D_x^2 + \left(hD_y - b(x + \frac{1}{3}x^3 + xy^2)\right)^2 .$$

We obtain this toy model by taking a Taylor expansion of the magnetic field centered at the minimum and chosing a suitable gauge.

Sketch of the initial quasimode proof.

The toy model is

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We obtain this toy model by taking a Taylor expansion of the magnetic field centered at the minimum and chosing a suitable gauge.
The second point is to use a blowing up argument $x = h^{\frac{1}{2}} s$, $y = h^{\frac{1}{2}} t$.
Dividing by h this leads (taking $b = 1$) to

$$D_s^2 + (D_t - s + h(\frac{1}{3}s^3 + st^2))^2 .$$

Partial Fourier transform

$$D_s^2 + (\tau - s + h(\frac{1}{3}s^3 + s(D_\tau)^2)^2\,,$$

and translation

$$D_s^2 + \left((-s + h\left(\frac{1}{3}(s+\tau)^3 + (s+\tau)(D_\tau - D_s)^2\right)\right)^2\,.$$

Expand as $\sum_j L_j h^j$, with

- $L_0 = D_s^2 + s^2\,,$
- $L_1 = -\frac{2}{3}s(s+\tau)^3 - s(s+\tau)(D_\tau - D_s)^2 - (s+\tau)(D_\tau - D_s)^2 s\,.$

The second harmonic oscillator appears in the τ variable by considering

$$\phi \mapsto \langle u_0(s), L_1(u_0(s)\phi(\tau))\rangle_{L^2(\mathbb{R}_s)}\,.$$

The recent improvments

In 2013, Helffer-Kordyukov on one side, and Raymond–Vu-Ngoc on the other side reanalyze the problem with two close but different points of view.

The proof of Helffer-Kordyukov is based on

- A change of variable :
- Normal form near a point (the minimum of the magnetic field)
- Construction of a Grushin's problem

This approach is local near the point where the intensity of the magnetic field is assumed to be minimum.

A change of variable

After a gauge transform, we assume that $A_1 = 0$ and $A_2 = A$. We just take :

$$x_1 = A(x, y), \quad y_1 = y$$

In these coordinates the magnetic field reads

$$B = dx_1 \wedge dy_1 \,.$$

Normal form through metaplectic transformations

After the change of variables, gauge transformation, partial Fourier transform, and at the end a dilation, we get

$$T^h_{new}(x,y,D_x,D_y;h) = h\sum_{k=0}^{2} h^{k/2}\,\widetilde{T}_k(x,y,D_x,hD_y,h), \qquad (8)$$

where:

$$\begin{aligned}\widetilde{T}_0(x,y,D_x,hD_y;h) =&(B^2+A_y^2)(h^{\frac12}x+y,hD_y-h^{\frac12}D_x)D_x^2\\ &+A_y(h^{\frac12}x+y,hD_y-h^{\frac12}D_x)D_x x\\ &+xA_y(h^{\frac12}x+y,hD_y-h^{\frac12}D_x)D_x+x^2\,,\end{aligned}$$

Note that $A_y(0,0)=0$ and $B(0,0)=b_0$.

The Grushin problem

Our Grushin problem takes the form

$$\mathcal{P}_h(z) = \begin{pmatrix} h^{-1} T^h_{new} - b_0 - z & R_- \\ R_+ & 0 \end{pmatrix} \tag{9}$$

where T^h_{new} was introduced above, the operator $R_- : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R}^2)$ is given by

$$R_- f(x,y) = H_0(x) f(y)\,, \tag{10}$$

H_0 being the normalized first eigenfunction of the harmonic oscillator

$$T = b_0^2 D_x^2 + x^2\,,$$

and the operator $R_+ : \mathcal{S}(\mathbb{R}^2) \to \mathcal{S}(\mathbb{R})$ is given by

$$R_+ \phi(y) = \int H_0(x) \phi(x,y) dx\,. \tag{11}$$

One can show that in a suitable sense, this system is invertible:

$$\mathcal{E}(z,h) = \begin{pmatrix} E(z,h) & E_- \\ E_+ & \epsilon_\pm(z,h) \end{pmatrix}$$

Here $\epsilon_\pm(z,h)$ is an h-pseudodifferential operator on $L^2(\mathbb{R}_y)$. At least formally, we have

$$z \in \sigma(T^h_{new}) \text{ if and only if } 0 \in \sigma(\epsilon_\pm(z,h))\,.$$

Although not completely correct, think that

$$\epsilon_\pm(z,h) = \epsilon_\pm(0,h) - z\,.$$

Here we follow Helffer-Sjöstrand (Harper) for the $1D$-problem and Fournais-Helffer ((2D)-Neumann).
Suppose that we have found $z = z(h)$ (possibly admitting an expansion in powers of h) and a corresponding approximate 0-eigenfunction $u_h^{qm} \in C^\infty(\mathbb{R})$ of the operator $\epsilon_\pm(z)$

$$\epsilon_\pm(z) u_h^{qm} = \mathcal{O}(h^\infty)\,,$$

such that the frequency set of u_h^{qm} is non-empty and contained in Ω.

Here we use our right inverse and write:

$$\mathcal{P}_h(z) \circ \mathcal{E}_h(z) \sim I\,, \tag{12}$$

with $\mathcal{E}_h(z)$ as above .
In particular it reads:

$$(T^h_{new} - b_0 - z(h))\epsilon_-(z) + R_-\epsilon_\pm(z) \sim 0\,. \tag{13}$$

The quasimode for our problem is simply $\epsilon_-(z)u_h^{qm}$:

$$(T^h_{new} - h^{-1}\lambda_h)\epsilon_-(z)u_h^{qm} = \mathcal{O}(h^\infty)\,,$$

where $\lambda_h = h(b_0 + z(h))$. The structure of $\epsilon_-(z)$ gives a meaning to this expression.
We recover the previous results on quasi-modes but have extended it to excited states.

The converse

This time we start from the eigenfunction u_h of H^h associated with $\lambda_h \in [hb_0, h(b_0 + \epsilon_0)]$ for $\epsilon_0 > 0$ as above.
The rewriting of H^h leads to an associated eigenfunction u_h of T^h_{new} associated with $h^{-1}\lambda_h$ The aim is to construct an approximate eigenfunction for the operator $\epsilon_\pm(z)$ with $z(h) = \frac{1}{h}(\lambda_h - hb_0)$. Formally, the left inverse of $\mathcal{P}_h(z)$ leads to

$$\mathcal{E}_h(z) \circ \mathcal{P}_h(z) \sim I \,. \tag{14}$$

We extract from this the identity:

$$\epsilon_+(z)(T_{new}h - h^{-1}\lambda_h) + \epsilon_\pm(z)R_+ \sim 0\,. \qquad (15)$$

Hence

$$u_h^{qm} = R_+\widetilde{u}_h$$

should be the candidate for an approximate 0-eigenfunction for $\epsilon_\pm(z)$:

$$\epsilon_\pm(z)u_h^{qm} = \mathcal{O}(h^\infty).$$

Birkhoff normal form

The proof of Raymond–Vu-Ngoc is reminiscent of Ivrii's approach (see his book in different versions) and uses a Birkhoff normal form. This approach seems to be semi-global but involves more general symplectomorphisms and their quantification.
We consider the h-symbol of the Schrödinger operator with magnetic potential A:

$$H(x,y,\xi,\eta) = |\xi - A_1(x,y)|^2 + |\eta - A_2(x,y)|^2 \,.$$

Theorem (Ivrii—Raymond–Vu-Ngoc)

$\exists$ a symplectic diffeomorphism Φ defined in an open set $\widetilde{\Omega} \subset \mathbb{C}_{z_1} \times \mathbb{C}_{z_2}$ with value in $T^*\mathbb{R}^2$ which sends $z_1 = 0$ into the surface $H = 0$ and such that

$$H \circ \Phi(z_1, z_2) = |z_1|^2 f(z_2, |z_1|^2) + \mathcal{O}(|z_1|^\infty)\,,$$

where f is smooth.
Moreover, the map

$$\Omega \ni (x, y) \mapsto \phi(x, y) := \Phi^{-1}(x, y, \mathbf{A}(x, y)) \in \{\{0\} \times \mathbb{C}_{z_2}\} \cap \widetilde{\Omega}$$

is a local diffeomorphism and

$$f(\phi(x, y), 0) = B(x, y)\,.$$

The statement in Ivrii is Proposition 13.2.11, p. 1218 (in a version of 2012). Unfortunately, there are many misprints.
We have reproduced above the statement as in Raymond–Vu-Ngoc.

Quantum version (after Raymond–Vu-Ngoc

Theorem

For h small enough, there exists a global Fourier-Integral operator $\mathcal{U}_h$ (essentially unitary modulo $\mathcal{O}(h^\infty)$) such that

$$\mathcal{U}_h^* \mathcal{H} \mathcal{U}_h = \mathcal{I}_h \, F_h + R_h \,,$$

where

$$I_h = -h^2 \frac{d^2}{dx_1^2} + x_1^2 \,,$$

F_h is a classical h-pseudodifferential operator which commutes with I_h, and R_h is a remainder (with $\mathcal{O}(h^\infty)$ property in the important region).
More precisely, the restriction to the invariant space $H_n \otimes L^2(\mathbb{R}_{x_2})$ (H_n is the n-th eigenfunction) can be seen as a h-pseudodifferential operator in the x_2 variable, whose principal symbol is B.

In Ivrii, the relevant statement seems Theorem 13.2.8.

3D case

The problem is partially open (Helffer-Kordyukov [HK8]) in the $3D$ case. What the generic model should be is more delicate. The toy model is

$$h^2 D_x^2 + (hD_y - x)^2 + (hD_z + (\alpha zx - P_2(x,y)))^2$$

with $\alpha \neq 0$, P_2 homogeneous polynomial of degree 2 where we assume that the linear forms $(x,y,z) \mapsto \alpha z - \partial_x P_2$ and $(x,y,z) \mapsto \partial_y P_2$ are linearly independent. We hope to prove :

$$\lambda_1^D(\mathbf{A}, h) = bh + \Theta_{\frac{1}{2}} h^{\frac{3}{2}} + \Theta_1 h^2 + o(h^2)\,. \tag{16}$$

A generic case in $\mathbb{R}^3$

The toy model is

$$h^2 D_x^2 + (hD_y - x)^2 + (hD_z + (\alpha zx - P_2(x,y)))^2$$

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$$\lambda_1^D(\mathbf{A}, h) = bh + \Theta_{\frac{1}{2}} h^{\frac{3}{2}} + \Theta_1 h^2 + o(h^2)\,. \tag{17}$$

More generally, let $M = \mathbb{R}^3$ with coordinates $X = (X_1, X_2, X_3) = (x, y, z)$. and let $\mathbf{A}$ be an 1-form, which is written in the local coordinates as

$$\mathbf{A} = \sum_{j=1}^{3} A_j(X)\, dX_j \,.$$

We are interested in the semi-classical analysis of the Schrödinger operator with magnetic potential $\mathbf{A}$:

$$H^h = \sum_{j=1}^{3} \left(hD_{X_j} - A_j(X) \right)^2 \,.$$

The magnetic field β is given by the following formula

$$\beta = B_1\, dy \wedge dz + B_2\, dz \wedge dx + B_3\, dx \wedge dy\,.$$

We will also use the trace norm of $\beta(x)$:

$$|\beta(X)| = \left[\sum_{j=1}^{3} |B_j(X)|^2\right]^{1/2}\,.$$

Put

$$b = \min\{|\beta(X)|\,:\, X \in \mathbb{R}^3\}$$

and assume that there exist a (connected) compact domain K and a constant $\epsilon_0 > 0$ such that

$$|\beta(X)| \geq b + \epsilon_0, \quad x \notin K\,. \tag{18}$$

Suppose that:

$$b > 0\,, \tag{19}$$

and that there exists a unique minimum $X_0 \in K \subset \mathbb{R}^3$ such that $|B(X_0)| = b_0$, which is non-degenerate:

$$C^{-1}|X - X_0|^2 \leq |\beta(X)| - b \leq C|X - X_0|^2\,. \tag{20}$$

Main statement

Choose an orthonormal coordinate system in $\mathbb{R}^3$ such that the magnetic field at X_0 is $(0,0,b)$. Denote

$$d = \det \mathrm{Hess}\,|\beta(X_0)|\,, \quad a = \frac{1}{2}\frac{\partial^2|\beta|}{\partial z^2}(X_0)\,.$$

Denote by $\lambda_1(H^h) \leq \lambda_2(H^h) \leq \lambda_3(H^h) \leq \dots$ the eigenvalues of the operator H^h in $L^2(\mathbb{R}^3)$ below the essential spectrum.

Theorem (Helffer-Kordyukov) (2011)

Under current assumptions,

$$\lambda_j(H^h) \leq hb + h^{3/2}a^{1/2} + h^2 \left[\frac{1}{b} \left(\frac{d}{2a} \right)^{1/2} (j-1) + \nu_2 \right] + C_j h^{9/4} \,,$$

where ν_2 is some specific spectral invariant.

The theorem is based on a construction of quasimodes. The lower bound is open.

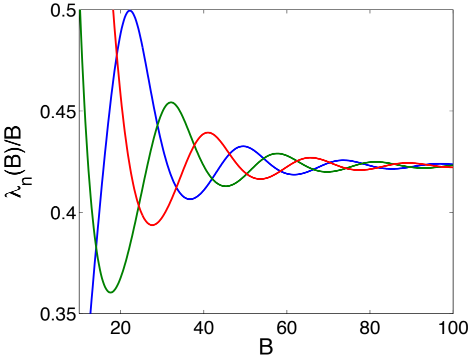
One can expect to find an effective hamiltonian using either ideas of Raymond-Vu-Ngoc or normal forms constructed by V. Ivrii.

Interpretation:

$$h^2 D_z^2 + h|\beta|^w(x, hD_x, z) + \dots .$$

Tunneling with magnetic fields

Essentially no results known (except Helffer-Sjöstrand (Pise)) and this last result is not a "pure magnetic effect".
There are however a few models where one can "observe" this effect in particular in domains with corners ([BDMV]) (numerics with some theoretical interpretation, see also Fournais-Helffer (book [FH1]) and Bonnaillie (PHD)).



The figure describes the graph of $\frac{\lambda_n(h)}{h}$ as a function of $B = h^{-1}$ for the equilateral triangle and for $n = 1, 2, 3$. Notice that $\Theta_0 \approx 0.59$ is, as expected, larger than $\lim_{h \to +\infty} \frac{\lambda_n(h)}{h}$, which corresponds to the groundstate energy of the Schrödinger operator with constant magnetic field equal to 1 in a sector of aperture $\frac{\pi}{3}$.

Other toy models

$$\text{Example 1}: h^2 D_x^2 + (hD_y - a(x))^2 + y^2 .$$

This model is rather artificial (and not purely magnetic) but by Fourier transform, it is unitary equivalent to

$$h^2 D_x^2 + (\eta - a(x))^2 + h^2 D_\eta^2 ,$$

which can be analyzed because it enters in the category of the miniwells problem treated in Helffer-Sjöstrand [HS1] (the fifth). We have indeed a well given by $\beta = a(x)$ which is unbounded but if we assume a varying curvature $\beta(x)$ (with $\liminf |\beta(x)| > \inf |\beta(x)|$) we will have a miniwell localization. A double well phenomenon can be created by assuming $\beta = a'$ even.

Example 2 : $h^2 D_x^2 + (hD_y - a(x))^2 + y^2 + V(x)\,.$

Here one can measure the explicit effect of the magnetic field by considering

$$h^2 D_x^2 + h^2 D_\eta^2 + (\eta - a(x))^2 + V(x)\,.$$

Example 3:
One can also imagine that in the main (2D)-example, as presented before, we have a magnetic double well, and that a tunneling effect could be measured using the effective $(1D)$-hamiltonian : $\beta(x, hD_x)$ assuming that b is holomorphic with respect to one of the variables .
(inspired by discussions with V. Bonnaillie-Noël and N. Raymond.)

Example 4:
Also open is the case considered in Fournais-Helffer (Neumann problem with constant magnetic field in (2D)-domains) [FH1].

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