

# Semi-classical analysis for magnetic Schrödinger operators and applications : old and new.

Conference in honor of M. Shubin for his 65 birthday

Bernard Helffer (Univ Paris-Sud and CNRS)

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In the last decade, the specialists in semi-classical analysis get new spectral questions for the Schrödinger operator with magnetic field coming from Physics : more specifically from the theory of superconductivity and from the theory of liquid crystals.

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.

The old results are presented in [FH4] or in [He1]. The recent results presented here are obtained in collaboration with A. Morame, S. Fournais, Y. Kordyukov, X. Pan .. or by N. Raymond, S. Fournais and M. Persson. Many are works in progress.

This is also a subject in which M. Shubin has recent contributions

- ▶ in collaboration with Kordyukov and Mathai [KMS, MS] in connection with  $K$ -theory and the question of existence of gaps in the spectrum,
- ▶ and in collaboration with Maz'ya in connection with the question of magnetic bottles but we will be more semi-classical.

There is a huge literature on the counting function and connected spectral quantities. We only look in this talk at the bottom.

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

$$\beta = \operatorname{curl} \mathbf{F}$$

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

$$\operatorname{div} \mathbf{F} = 0, \quad \mathbf{F} \cdot N_{\partial\Omega} = 0,$$

where  $N(x)$  is the unit interior normal vector to  $\partial\Omega$ .

We start from the closed quadratic form  $Q_B$

$$W^{1,2}(\Omega) \ni u \mapsto Q_B(u) := \int_{\Omega} |(-i\nabla + B\mathbf{F})u(x)|^2 dx. \quad (1)$$

Let  $\mathcal{H}^N(\mathbf{BF}, \Omega)$  be the self-adjoint operator associated to  $Q_B$ .  
 $\mathcal{H}^N(\mathbf{BF}, \Omega)$  is the differential operator  $(-i\nabla + \mathbf{BF})^2$  with domain

$$\{u \in W^{2,2}(\Omega) : N \cdot \nabla u|_{\partial\Omega} = 0\} .$$

When  $\Omega$  is bounded, the operator  $\mathcal{H}^N(\mathbf{BF}, \Omega)$  has compact resolvent and we introduce

$$\lambda_1^N(\mathbf{BF}, \Omega) := \inf \text{Spec } \mathcal{H}^N(\mathbf{BF}, \Omega) . \quad (2)$$

One could also look at the Dirichlet realization  $\mathcal{H}^D(\mathbf{BF}, \Omega)$  with domain

$$\{u \in W^{2,2}(\Omega) : u|_{\partial\Omega} = 0\} .$$

and to the corresponding groundstate energy  $\lambda_1^D(\mathbf{BF}, \Omega)$ .

Motivated by various questions we consider the two connected problems in the asymptotic  $B \rightarrow +\infty$ .

**Pb 1** Find an accurate estimate of the groundstate energy

$$B \mapsto \lambda_1^{DorN}(B\mathbf{F}, \Omega).$$

**Pb 2** Find where a corresponding ground state is living as  $B$  tends to  $\infty$ .

**Pb 3** More generally determine the structure of the bottom of the spectrum : gaps.

We will present results which are

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

The first results (Lu-Pan) are based on the old (for the case of  $\mathbb{R}^d$ ) analysis of models with constant magnetic field  $\beta$  :

## 1. The case in $\mathbb{R}^d$ ( $d = 2, 3$ )

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

## 2. The case in the half space $\mathbb{R}_+^d$



$$\inf \sigma(\mathcal{H}^N(\mathbf{BF}, \mathbb{R}_+^2)) = \Theta_0 B|\beta| ,$$



$$\inf \sigma(\mathcal{H}^N(\mathbf{BF}, \mathbb{R}_+^3)) = \varsigma(\vartheta) B|\beta| ,$$

where  $\vartheta$  is the angle between  $\beta$  and  $N$ ,



$$\inf \sigma(\mathcal{H}^D(\mathbf{BF}, \mathbb{R}_+^d)) = B|\beta| .$$

The main points are



$$0 < \Theta_0 < 1. \quad (3)$$

▶ For the case  $d = 3$

$$\Theta_0 = \varsigma\left(\frac{\pi}{2}\right) \leq \varsigma(\theta) \leq \varsigma(0) = 1. \quad (4)$$

▶  $\vartheta \mapsto \varsigma(\vartheta)$  is decreasing on  $[0, \frac{\pi}{2}]$ .

From this, we get

1. The bottom of the spectrum for Neumann in the half space is below the problem in  $\mathbb{R}^d$ .
2. In the  $3D$  case, the bottom of the spectrum is minimal when  $\beta$  is tangent to the boundary.

We introduce

$$b = \inf_{x \in \bar{\Omega}} |\beta(x)|, \quad (5)$$

$$b' = \inf_{x \in \partial\Omega} |\beta(x)|, \quad (6)$$

and, for  $d = 2$ ,

$$b'_2 = \Theta_0 \inf_{x \in \partial\Omega} |\beta(x)|, \quad (7)$$

and, for  $d = 3$ ,

$$b'_3 = \inf_{x \in \partial\Omega} |\beta(x)| \varsigma(\theta(x)) \quad (8)$$

## Theorem 1 : rough asymptotics

$$\lambda_1^N(B\mathbf{F}, \Omega) = B \min(b, b'_d) + o(B), \quad (9)$$

$$\lambda_1^D(B\mathbf{F}, \Omega) = Bb + o(B) \quad (10)$$

Particular case, if  $|\beta(x)| = 1$ , then

$$\min(b, b'_d) = b'_d = \Theta_0. \quad (11)$$

The consequences for Pb 2 are that a ground state is localized as

$B \rightarrow +\infty$ ,

- ▶ for Dirichlet, at the points of  $\overline{\Omega}$  where  $|\beta(x)|$  is minimum,
- ▶ for Neumann,
  - ▶ if  $b < b'_d$ , at the points of  $\Omega$  where  $|\beta(x)|$  is minimum  
(no difference with Dirichlet).
  - ▶ if  $b > b'_d$  at the points of  $\partial\Omega$  where  $|\beta(x)|\varsigma(\theta(x))$  is minimum.

In particular, if  $|\beta(x)| = 1$ , we are, for Neumann, in the second case, hence the groundstate is localized at the boundary.

Moreover, when  $d = 3$ , the groundstate is localized at the point where  $\beta(x)$  is tangent to the boundary.

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  $-h^2\Delta + V$ ).

The semi-classical parameter is  $h = B^{-1}$ .

If

$$b < \inf_{x \in \partial\Omega} |\beta(x)| \text{ for Dirichlet}$$

or if

$$b < b' \text{ for Neumann,}$$

the asymptotics are the same (modulo an exponentially small error).

If we assume in addition

### Assumption A

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

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

## Theorem 2

$$\lambda_1^D(BF) = bB + \Theta_1 + o(1). \quad (12)$$

where  $\Theta_1$  is computed from the Hessian of  $\beta$  at the minimum.

The toy model is

$$D_x^2 + \left( D_y - bB \left( x + \frac{1}{3}x^3 + xy^2 \right) \right)^2.$$

The problem is still open (Helffer-Kordyukov [HK7], work in preparation) in the  $3D$  case. What we should call the generic model is more delicate. The toy model is

$$D_x^2 + (D_y - Bx)^2 + (D_z + B(\alpha z x - P_2(x, y)))^2$$

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 :

$$\lambda_1^D(\mathbf{BF}) = bB + \Theta_{\frac{1}{2}} B^{\frac{1}{2}} + \Theta_1 + o(1). \quad (13)$$

## The case of hypersurface wells

Here is the typical model on  $\mathbb{R} \times \mathbb{S}^1$ .

$$D_t^2 + \left( D_s - B[a_1 - b_0 t - \frac{1}{6}\beta_2(s)t^3] \right)^2.$$

The magnetic field is  $b_0 + \frac{1}{2}\beta_2(s)t^2$ .

If we suppose  $\beta_2(s) > 0$  and  $b_0 > 0$ , the magnetic field admits its minimum on  $t = 0$ .

We have two extreme cases :

- ▶  $\beta_2(s) = \text{Const.}$  (circle action), which leads to the analysis of the family of operators

$$D_t^2 + \left( n - B[a_1 - b_0 t - \frac{1}{2}\beta_2 t^3] \right)^2 .$$

The detailed analysis is open.

- ▶  $\beta_2$  admits a unique minimum.

$$D_t^2 + \left( D_s - B[a_1 - b_0 t - \frac{1}{6}b_3(1 + s^2)t^3] \right)^2$$

This is considered in [HK6] (upper bounds). Two harmonic oscillators are involved !

## The case $b = 0$

There are also many results for the case when  $b = 0$  (Montgomery, Helffer-Mohamed, Pan-Kwek, Helffer-Kordyukov ....).

Here is the typical model on  $\mathbb{R} \times \mathbb{S}^1$ .

$$D_t^2 + \left( D_s - B[a_1 + \frac{1}{2}\beta_1(s)t^2] \right)^2 .$$

The magnetic field is  $\beta_1(s)t$  and vanish on  $t = 0$ .

Again, we have two extreme cases :

- ▶  $\beta_1(s) = \text{Const.} > 0$  (circle action), which leads to the analysis of the family of operators

$$D_t^2 + \left( n - B[a_1 + \frac{1}{2}\beta_1 t^2] \right)^2 .$$

This is the Montgomery operator. A recent key result [He2] is that the ground state energy  $\nu(\rho)$  of the Montgomery operator  $D_t^2 + (t^2 - \rho)^2$  admits a unique minimum  $\hat{\nu}_0$  which is non degenerate.

- ▶  $\beta_1$  admits a unique minimum. This analyzed in Helffer-Kordyukov [HK5].

We describe recent results of N. Raymond in the  $2D$ -case. This time we assume that

### Assumption B

- ▶  $\Theta_0 b' := b'_2 < b$
- ▶  $\partial\Omega \ni x \mapsto |\beta(x)|$  has a unique non degenerate minimum.

## Theorem 3

$$\lambda_1^N(B\mathbf{F}) = b'_2 B + \Theta_{\frac{1}{2}} B^{\frac{1}{2}} + o(B^{\frac{1}{2}}). \quad (14)$$

where

$$\Theta_{\frac{1}{2}} = -\frac{k_0 + k_1}{2} C_1 - \Theta_0 \xi_0 \frac{\partial_\nu \beta}{b'} + \sqrt{3C_1} \Theta_0^{\frac{3}{4}} \sqrt{\alpha} \quad (15)$$

with

$$\alpha = \frac{1}{b'} \frac{\partial^2 \beta}{\partial s^2}$$

and  $k_0$  is the curvature at the minimum and  $k_1 = k_0 - \frac{\partial_\nu \beta}{b'}$ , all the derivatives being computed at the minimum..

In particular cases, there were results by Aramaki.

Concerning Pb 2, the ground state is localized at the minimum.

In the constant magnetic field case, which plays a special role in superconductivity, one needs to go further !

In the two dimensional case, it was proved by DelPino-Felmer-Sternberg-Lu-Pan-Helffer-Morame the

#### Theorem 4

$$\lambda_1(B) = \Theta_0 B - \widehat{k}_0 B^{\frac{1}{2}} + o(B^{\frac{1}{2}}), \quad (16)$$

where  $\widehat{k}_0$  is proportional to the maximal curvature of the boundary.

Concerning Pb 2, we have localization at the point of maximal curvature.

In the case of the disk (first considered by Bauman-Phillips-Tang, then by Helffer-Morame (2001) and Fournais-Helffer (2009))

Let us consider the  $3D$ -situation.

We assume

### Assumption C1

The set of boundary points where  $\beta$  is tangent to  $\partial\Omega$ , i.e.

$$\Gamma := \{x \in \partial\Omega \mid \beta \cdot N(x) = 0\}, \quad (17)$$

is a regular submanifold of  $\partial\Omega$  :

$$d^T(\beta \cdot N)(x) \neq 0, \quad \forall x \in \Gamma. \quad (18)$$

We also assume that

## Assumption C2

The set of points where  $\beta$  is tangent to  $\Gamma$  is finite.

These assumptions are rather generic and for instance satisfied for ellipsoids.

We have the following two-term asymptotics of  $\lambda_1(B)$  (due to Helffer-Morame- Pan).

### Theorem 5

If  $\Omega$  and  $\beta$  satisfy C1-C2, then as  $B \rightarrow +\infty$

$$\lambda_1^N(B) = \Theta_0 B + \hat{\gamma}_0 B^{\frac{2}{3}} + \mathcal{O}(B^{\frac{2}{3}-\eta}),$$

for some  $\eta > 0$ .

## In Formula

$$\lambda_1(B) = \Theta_0 B + \widehat{\gamma}_0 B^{\frac{2}{3}} + o(B^{\frac{2}{3}}). \quad (19)$$

$\Theta_0 \in ]0, 1[$ ,  $\delta_0 \in ]0, 1[$  are spectral quantities and  $\widehat{\gamma}_0$  is defined by

$$\widehat{\gamma}_0 := \inf_{x \in \Gamma} \widetilde{\gamma}_0(x), \quad (20)$$

where

$$\widetilde{\gamma}_0(x) := 2^{-2/3} \widehat{\nu}_0 \delta_0^{1/3} |k_n(x)|^{2/3} \left(1 - (1 - \delta_0) |T(x) \cdot \beta|^2\right)^{1/3}. \quad (21)$$

Here  $T(x)$  is the oriented, unit tangent vector to  $\Gamma$  at the point  $x$  and

$$k_n(x) = |d^T(\beta \cdot N)(x)|.$$

Quite recently, S. Fournais and M. Persson have obtained a rather complete expansion in the case of the ball [FP] modulo  $o(1)$ . The next terms involve  $\sum_{j \geq 3} \Theta_j B^{1-\frac{j}{6}}$  and an explicit oscillatory term of order  $O(1)$ .

In the case when  $|B(x)|$  is constant, X. Pan gives a probably accurate two terms upper bound like in the case when the magnetic field is constant.

A more generic case which is considered by N. Raymond [Ray3] is to consider the case when  $\partial\Omega \ni x' \mapsto \sigma(\vartheta(x'))|\beta(x')|$  admits a non degenerate minimum. In this case, he obtains a (probably) optimal upper bound and a candidate for the splitting given by an effective harmonic oscillator corresponding to a quantization of the Hessian of this function.

## De Gennes model

The spectral analysis is based in particular on the analysis of the family

$$H(\xi) = D_t^2 + (t + \xi)^2, \quad (22)$$

on the half-line (Neumann at 0) whose lowest eigenvalue  $\mu(\xi)$  admits a unique minimum at  $\xi_0 < 0$ .

So our two universal constants attached to the problem on  $\mathbb{R}^+$  can be now defined by :

The first one is

$$\Theta_0 = \mu(\xi_0) . \quad (23)$$

It corresponds to the bottom of the spectrum of the Neumann realization in  $\mathbb{R}_+^2$  (with  $B = 1$ ).

Note that

$$\Theta_0 \in ]0, 1[ .$$

The second constant is

$$\delta_0 = \frac{1}{2} \mu''(\xi_0) , \quad (24)$$

-  S. Agmon, *Lectures on exponential decay of solutions of second order elliptic equations: bounds on eigenfunctions of N-body Schrodinger operators*, Princeton Univ. Press, NJ, 1982.
-  P. Bauman, D. Phillips, and Q. Tang.  
Stable nucleation for the Ginzburg-Landau system with an applied magnetic field.  
Arch. Rational Mech. Anal. 142 (1998), p. 1-43.
-  P. Bauman, M. Calderer, C. Liu and D. Phillips, *The phase transition between chiral nematic and smectic A\* liquid crystals*, Arch. Rational Mech. Anal. 165 (2002), 161-186.
-  S. Fournais and B. Helffer, *On the third critical field in Ginzburg-Landau theory*, Comm. Math. Phys., **266** (2006), 153-196.

-  S. Fournais and B. Helffer, *Strong diamagnetism for general domains and applications*, Ann. Inst. Fourier 2008.
-  S. Fournais and B. Helffer, *On the Ginzburg-Landau critical field in three dimensions*, arXiv:math-ph/0703047v1, March 2007. To appear in CPAM (2008).
-  S. Fournais and B. Helffer, *Spectral methods in surface superconductivity*. Book.
-  S. Fournais and M. Persson.  
Strong diamagnetism for the ball in three dimension.  
Preprint 2009.
-  B. Helffer.  
Analysis of the bottom of the spectrum of Schrödinger operators with magnetic potentials and applications.

European Congress of Mathematics, Stockholm, European Math. Society p. 597-618 (2005).



B. Helffer.

The Montgomery operator revisited.

To appear in Colloquium Mathematicum.



B. Helffer and Y. Kordyukov.

Semi-classical asymptotics and gaps in the spectra of periodic Schrödinger operators with magnetic wells.

Transactions of the American Math. Society 360 (3), p. 1681-1694 (2008).



B. Helffer and Y. Kordyukov. Spectral gaps for periodic Schrödinger operators with hypersurface magnetic wells. in MATHEMATICAL RESULTS IN QUANTUM MECHANICS. Proceedings of the QMath10 Conference. Moieciu, Romania

10 - 15 September 2007, edited by Ingrid Beltita, Gheorghe Nenciu and Radu Purice (Institute of Mathematics 'Simion Stoilow' of the Romanian Academy, Romania). Worldscientific.



B. Helffer and Y. Kordyukov.

The periodic magnetic Schrödinger operators: spectral gaps and tunneling effect.

Proceedings of the Stecklov Math. Institute, volume 261 (2008).



B. Helffer and Y. Kordyukov.

Spectral gaps for periodic Schrödinger operators with hypersurface at the bottom : Analysis near the bottom.

To appear in JFA (2009).



B. Helffer and Y. Kordyukov.

## Semiclassical analysis of Schrödinger operators with magnetic wells.



B. Helffer and Y. Kordyukov.  
2D generic (in preparation)



B. Helffer and Y. Kordyukov.  
3D generic (in preparation)



B. Helffer and A. Morame, *Magnetic bottles in connection with superconductivity*, J. Functional Anal., **185** (2001), 604-680.



B. Helffer and A. Morame, *Magnetic bottles for the Neumann problem: the case of dimension 3*, Proceedings of the Indian Academy of Sciences-Mathematical Sciences, **112**: (1) (2002), 71-84.

-  B. Helffer and A. Morame, *Magnetic bottles for the Neumann problem: curvature effects in the case of dimension 3 - (general case)*, Ann. Sci. Ecole Norm. Sup. **37** (1) (2004), 105-170.
-  B. Helffer and X. B. Pan, *Reduced Landau-de Gennes Functional and Surface Smectic State of Liquid Crystals* Submitted (2008).
-  B. Helffer and J. Sjöstrand,  
six papers on multiple wells in the semi-classical limit  
1983-1986.
-  B. Helffer and J. Sjöstrand.  
Effet tunnel pour l'équation de Schrödinger avec champ  
magnétique,  
Ann. Scuola Norm. Sup. Pisa, Vol XIV, 4 (1987) p. 625-657.
-  Y. Kordyukov, V. Mathai, and M. Shubin.

Equivalence of projections in semi-classical limit and a vanishing theorem for higher traces in  $K$ -theory.

J. Reine Angew. LMath. 581 (2005) 193-236.



K. Lu and X. B. Pan, *Estimates of the upper critical field for the Ginzburg-Landau equations of superconductivity*, Physica D, **127** : (1-2) (1999), 73-104.



K. Lu and X. B. Pan, *Surface nucleation of superconductivity in 3-dimension*, J. Diff. Equations, **168** (2000), 386-452.



V. Mathai and M. Shubin.

Semi-classical asymptotics and gaps in the spectra of magnetic Schrödinger operators.

Geometriae Dedicata 91 (2002), 155-173.



R. Montgomery, *Hearing the zero locus of a magnetic field*.  
Comm. Math. Phys. **168** (3) (1995), 651-675.

-  X. B. Pan, *Landau-de Gennes model of liquid crystals and critical wave number*, Comm. Math. Phys., **239** (1-2) (2003), 343-382.
-  X. B. Pan, *Superconductivity near critical temperature*, J. Math. Phys., **44** (2003), 2639-2678.
-  X. B. Pan, *Surface superconductivity in 3-dimensions*, Trans. Amer. Math. Soc., **356** (10) (2004), 3899-3937.
-  X. B. Pan, *Landau-de Gennes model of liquid crystals with small Ginzburg-Landau parameter*, SIAM J. Math. Anal., **37** (5) (2006), 1616-1648.
-  X. B. Pan, *An eigenvalue variation problem of magnetic Schrödinger operator in three-dimensions*, preprint May 2007.

-  X. B. Pan, *Analogies between superconductors and liquid crystals: nucleation and critical fields*, in: *Asymptotic Analysis and Singularities*, Advanced Studies in Pure Mathematics, Mathematical Society of Japan, Tokyo, **47-2** (2007), 479-517.
-  X. -B. Pan. and K.H. Kwek, *Schrödinger operators with non-degenerately vanishing magnetic fields in bounded domains*. Transactions of the AMS **354** (10) (2002), p. 4201-4227.
-  N. Raymond.  
Uniform spectral estimates for families of Schrödinger operators with magnetic field of constant intensity and applications. To appear in Cubo 11 (2009).
-  N. Raymond,

Sharp asymptotics for the Neumann Laplacian with variable magnetic field : case of dimension 2.

[Annales Henri Poincaré 10 \(1\), p. 95-122 \(2009\).](#)



N. Raymond,

Upper bound for the lowest eigenvalue of the Neumann Laplacian with variable magnetic field in dimension 3.

[June 2009 \(submitted\).](#)



B. Simon,

Series of four papers in the eighties.