



**HAL**  
open science

# Confining quantum particles with a purely magnetic field

Yves Colin de Verdière, Françoise Truc

► **To cite this version:**

Yves Colin de Verdière, Françoise Truc. Confining quantum particles with a purely magnetic field. 2009. hal-00365828v3

**HAL Id: hal-00365828**

**<https://hal.science/hal-00365828v3>**

Preprint submitted on 15 Oct 2009

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# Confining quantum particles with a purely magnetic field

Yves Colin de Verdière\* & Françoise Truc†

October 15, 2009

## Abstract

We consider a Schrödinger operator with a magnetic field (and no electric field) on a domain in the Euclidean space with a compact boundary. We give sufficient conditions on the behaviour of the magnetic field near the boundary which guarantees essential self-adjointness of this operator. From the physical point of view, it means that the quantum particle is confined in the domain by the magnetic field. We construct examples in the case where the boundary is smooth as well as for polytopes; these examples are highly simplified models of what is done for nuclear fusion in tokamacs. We also present some open problems.

## Contents

<b>1</b>	<b>Introduction</b>	<b>2</b>
1.1	The problem . . . . .	2
1.2	Previous works . . . . .	2
1.3	Rough description of our results . . . . .	3
1.4	Open problems . . . . .	3
<b>2</b>	<b>Definitions and background results</b>	<b>4</b>
2.1	The domain $\Omega$ . . . . .	4
2.2	The distance to the boundary . . . . .	4
2.2.1	The distance function . . . . .	4
2.2.2	Adapted charts for smooth boundaries . . . . .	5
2.3	Antisymmetric forms . . . . .	5
2.4	Magnetic fields . . . . .	5
2.5	The Riemannian context . . . . .	6
2.5.1	“Regular” Riemannian manifolds . . . . .	6
2.5.2	Magnetic fields on Riemannian manifolds . . . . .	6
2.6	Essential self-adjointness . . . . .	7
2.6.1	Essentially self-adjoint operators . . . . .	7
2.6.2	Essential self-adjointness depends only on the boundary behaviour . . . . .	7
2.6.3	Essential self-adjointness is independent of the choice of a gauge . . . . .	7
<b>3</b>	<b>Main results</b>	<b>7</b>

---

\*Institut Fourier, Unité mixte de recherche CNRS-UJF 5582, BP 74, 38402-Saint Martin d’Hères Cedex (France), yves.colin-de-verdiere@ujf-grenoble.fr

†Institut Fourier, francoise.truc@ujf-grenoble.fr

<b>4</b>	<b>Proof of the main results</b>	<b>8</b>
4.1	Agmon estimates . . . . .	9
4.2	Quasi-isometries . . . . .	10
4.3	Lower bounds for the magnetic Dirichlet integrals . . . . .	11
4.3.1	Basic magnetic estimates . . . . .	11
4.3.2	The 2-dimensional case . . . . .	11
4.3.3	The case $d > 2$ . . . . .	12
4.4	End of the proof of the main theorems . . . . .	12
<b>5</b>	<b>Examples</b>	<b>12</b>
5.1	Polytopes . . . . .	12
5.2	Examples in domains whose Euler characteristic of the boundary vanishes (“toroidal domains”). . . . .	13
5.3	Non toroidal domains . . . . .	14
5.3.1	Statement of results . . . . .	14
5.3.2	Local model . . . . .	14
5.3.3	Globalisation . . . . .	15
5.4	An example of a non essentially self-adjoint Schrödinger operator with large magnetic field near the boundary . . . . .	15
5.5	Singular points . . . . .	15
5.5.1	Monopoles . . . . .	15
5.5.2	The spectra of the operators $K_m$ , the “spherical Landau levels” . . . . .	16
5.5.3	A general result for $\Omega = \mathbb{R}^d \setminus 0$ . . . . .	17
5.5.4	Multipoles . . . . .	17

# 1 Introduction

## 1.1 The problem

Let us consider a particle in a domain  $\Omega$  in  $\mathbb{R}^d$  ( $d \geq 2$ ) in the presence of a magnetic field  $B$ . We will always assume that the topological boundary  $\partial\Omega := \overline{\Omega} \setminus \Omega$  of  $\Omega$  is compact. At the classical level, if the strength of the field tends to infinity as  $x$  approaches the boundary  $\partial\Omega$ , we expect that the charged particle is confined and never visits the boundary: the Hamiltonian dynamics is complete. At the quantum level the fact that the particle never feels the boundary amounts to saying that the magnetic field completely determines the motion, so there is no need for boundary conditions. At the mathematical level, the problem is to find conditions on the behaviour of  $B(x)$  as  $x$  tends to  $\partial\Omega$  which ensure that the magnetic operator  $H_A$  is essentially self-adjoint (see Section 2.6) on  $C_0^\infty(\Omega)$  (the space of compactly supported smooth functions). These conditions will not depend on the gauge  $A$ , but only on the field  $B$ . One could have called such pairs  $(\Omega, A)$  “magnetic bottles”, but this denomination is already introduced in the important paper [3] for Schrödinger operators with magnetic fields in the whole of  $\mathbb{R}^d$  having compact resolvents. This question may be of technological interest in the construction of tokamacs for the nuclear fusion [30]. The ionised plasma which is heated is confined thanks to magnetic fields.

## 1.2 Previous works

The same problem, concerning scalar (electric) potentials, has been intensively studied. In the many-dimensional case the basic result appears in a paper by B. Simon [24] which generalises results of H. Kalf, J. Walter and U.-V. Schminke (see [15] for a general review). Concerning the magnetic potential, the first general result is by Ikebe and Kato: in [14], they prove self-adjointness in the case of  $\Omega = \mathbb{R}^d$  for

any regular enough magnetic potential. This result was then improved in [25, 26]. Concerning domains with boundary, we have not seen results in the purely magnetic case. A regularity condition on the direction of the magnetic field was introduced in the important paper [3] (Corollary 2.10 p. 853) in order to construct “magnetic bottles” in  $\mathbb{R}^d$ . It was used later in many papers like [5, 7, 28, 29, 9, 10, 11, 4].

In the recent paper [20], G. Nenciu and I. Nenciu give an optimal condition for essential self-adjointness on the electric potential near the boundary of a bounded smooth domain; they use Agmon-type results on exponential decay of eigenfunctions combined with multidimensional Hardy inequalities.

### 1.3 Rough description of our results

As we will see, in the case of a magnetic potential the Agmon-type estimates still hold, whereas the Hardy inequalities cannot be used because there is no separation between kinetic and potential energy. Actually the point is that we need, to apply the strategy of [20], some lower bound on the magnetic quadratic form  $h_A$  associated with the magnetic potential  $A$ . Our main result is as follows: under some continuity assumption on the direction of  $B(x)$  at the boundary, for any  $\epsilon > 0$  and  $R > 0$ , there exists a constant  $C_{\epsilon,R} \in \mathbb{R}$  such that the quadratic form  $h_A$  satisfies the quite optimal bound

$$\forall u \in C_0^\infty(\Omega), \quad h_A(u) \geq (1 - \epsilon) \int_{\Omega \cap \{|x| \leq R\}} |B|_{\text{sp}} |u|^2 |dx| - C_{\epsilon,R} \|u\|^2. \quad (1.1)$$

Here  $|B(x)|_{\text{sp}}$  is a suitable norm on the space of bi-linear antisymmetric forms on  $\mathbb{R}^d$ , called the *spectral norm*. This implies that  $H_A$  is essentially self-adjoint if there exists  $\eta > 0$  so that  $|B(x)|_{\text{sp}} \geq (1 + \eta)D(x)^{-2}$  where  $D$  is the distance to the boundary of  $\Omega$ .

We study then examples in the following cases:

- The domain  $\Omega$  is a polytope
- The boundary  $\partial\Omega$  is smooth and the Euler characteristic  $\chi(\partial\Omega)$  vanishes (toroidal domain)
- The boundary  $\partial\Omega$  is smooth and the Euler characteristic  $\chi(\partial\Omega)$  does not vanish (non toroidal domain)
- The domain  $\Omega$  is  $\mathbb{R}^3 \setminus 0$  and the field is a monopole or a dipole
- The domain  $\Omega$  is the unit disk: for any  $\epsilon > 0$  and  $d = 2$ , we construct an example of a non essentially self-adjoint operator  $H_A$  with  $|B(x)|_{\text{sp}} \sim (\sqrt{3}/2 - \epsilon)D(x)^{-2}$  showing that our bound is rather sharp.

### 1.4 Open problems

The following questions seem to be quite interesting:

- What are the properties of a *classical* charged particle in a confining magnetic box? Are almost all trajectories not hitting the boundary?
- What is the *optimal* constant  $C$  in the estimates  $|B(x)|_{\text{sp}} \geq CD(x)^{-2}$  of our main result 3.2? From our main results and the example in the unit disk given in Section 5.4, we see that the optimal constant lies in the interval  $[\sqrt{3}/2, 1]$ .

## 2 Definitions and background results

In this section, we will give precise definitions and related notations. We will also review some known results with references to the literature.

### 2.1 The domain $\Omega$

In what follows, we will keep the following definitions:  $\Omega$  is an open set in the Euclidean space  $\mathbb{R}^d$  ( $d \geq 2$ ) with a compact topological boundary  $\partial\Omega = \overline{\Omega} \setminus \Omega$ , so that either  $\Omega$  or  $\mathbb{R}^d \setminus \Omega$  is bounded.

**Definition 2.1** We will denote by  $d_R$  the distance defined on  $\Omega$  by the Riemannian metric induced by the Euclidean metric:

$$d_R(x, y) = \inf_{\gamma \in \Gamma_{x,y}} \text{length}(\gamma)$$

where  $\Gamma_{x,y}$  is the set of smooth curves  $\gamma : [0, 1] \rightarrow \Omega$  with  $\gamma(0) = x$ ,  $\gamma(1) = y$ .

We will denote by  $\widehat{\Omega}$  the metric completion of  $(\Omega, d_R)$  and by  $\Omega_\infty = \widehat{\Omega} \setminus \Omega$  the metric boundary of  $\Omega$ .

We say that  $\Omega$  is regular if  $\Omega_\infty$  is compact.

If  $\Omega$  is regular,  $\partial\Omega$  is compact. In fact the identity map of  $\Omega$  extends to a continuous map  $\pi$  from  $\widehat{\Omega}$  onto  $\overline{\Omega}$  and  $\pi(\Omega_\infty) = \partial\Omega$ .  $(\widehat{\Omega}, \pi)$  is a “desingularisation” of  $\overline{\Omega}$ . If  $X = \partial\Omega$  is a compact  $C^1$  sub-manifold or a compact simplicial complex embedded in a piecewise  $C^1$  way,  $\Omega$  is regular.

If  $X = \cup_{n \in \mathbb{N}} [0, 1]e_n$  with  $e_n$  a sequence of unit vectors in  $\mathbb{R}^2$  converging to  $e_0$ , then  $\mathbb{R}^2 \setminus X$  is not regular, even if  $\partial\Omega = X$  is compact.

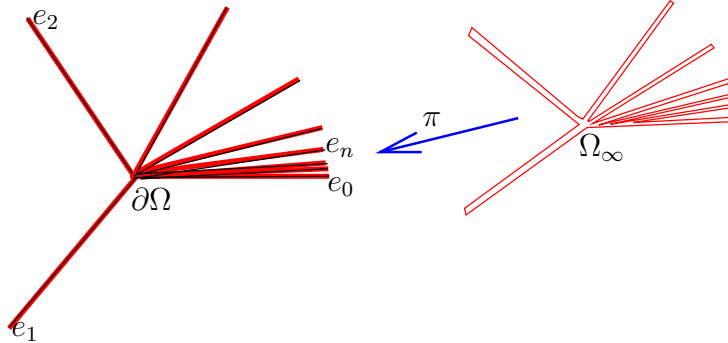


Figure 1: An example where  $\partial X$  is compact while  $X_\infty$  is not compact

We will use the following regularity property:

**Definition 2.2** Let us assume that  $\Omega$  is regular. A continuous function  $f : \Omega \rightarrow \mathbb{C}$  is regular at the boundary if it extends by continuity to  $\widehat{\Omega}$ .

The Lebesgue measure will be  $|dx|$  and we will denote by  $\langle u, v \rangle := \int_{\Omega} u\bar{v}|dx|$  the  $L^2$  scalar product and by  $\|u\|$  the  $L^2$  norm of  $u$ . We will denote by  $C_0^\infty(\Omega)$  the space of complex-valued smooth functions with compact support in  $\Omega$ .

### 2.2 The distance to the boundary

#### 2.2.1 The distance function

**Definition 2.3** Let us denote by  $\hat{d}_R$  the extension of  $d_R$  by continuity to  $\widehat{\Omega}$ . For  $x \in \Omega$ , let  $D(x)$  be the distance to the boundary  $\Omega_\infty$ , given by  $D(x) = \min_{y \in \Omega_\infty} \hat{d}_R(x, y)$ .

**Lemma 2.4** *The function  $D$  is 1-Lipschitz and almost everywhere differentiable in  $\Omega$ . At any point  $x$  of differentiability of  $D$ , we have  $|dD(x)| \leq 1$ .*

The inequality  $|D(x) - D(x')| \leq d_R(x, x')$  follows from the triangle inequality for  $\hat{d}_R$ . The almost everywhere differentiability of Lipschitz functions is the celebrated Theorem of Hans Rademacher [21]; see also [19] p. 65 and [13].

### 2.2.2 Adapted charts for smooth boundaries

Assuming that the boundary is smooth, we can find, for each point  $x_0 \in \partial\Omega$ , a diffeomorphism from an open neighbourhood  $U$  of  $x_0$  in  $\mathbb{R}^d$  onto an open neighbourhood  $V$  of 0 in  $\mathbb{R}_{x_1, x'}$  satisfying:

- $x_1(F(x)) = D(x)$
- The differential  $F'(x_0)$  of  $F$  is an isometry
- $F(U \cap \Omega) = V \cap \{x_1 > 0\}$ .

We will call such a chart an adapted chart at the point  $x_0$ . Such a chart is an  $\epsilon$ -quasi-isometry (see the definition in Section 4.2) with  $\epsilon$  as small as one wants by choosing  $U$  small enough.

## 2.3 Antisymmetric forms

Let us denote by  $\wedge^k \mathbb{R}^d$  the space of real-valued  $k$ -linear antisymmetric forms on the Euclidean space  $\mathbb{R}^d$ . The space  $\wedge^1 \mathbb{R}^d$  is the dual of  $\mathbb{R}^d$ , and it is equipped with the natural Euclidean norm:  $|\sum_{j=1}^d a_j dx_j|^2 = \sum_{j=1}^d a_j^2$ . The space  $\wedge^2 \mathbb{R}^d$  is equipped with the spectral norm: if  $B \in \wedge^2 \mathbb{R}^d$ , there exists an orthonormal basis of  $\mathbb{R}^d$  so that  $B = b_{12} dx_1 \wedge dx_2 + b_{34} dx_3 \wedge dx_4 + \dots + b_{2\bar{d}-1, 2\bar{d}}$  with  $\bar{d} = [d/2]$  and  $b_{12} \geq b_{34} \geq \dots \geq 0$ ; the sequence  $b_{12}, b_{34}, \dots$  is unique: the eigenvalues of the antisymmetric endomorphism  $\tilde{B}$  of  $\mathbb{R}^d$  associated with  $B(x)$  are  $\pm i b_{12}, \pm i b_{34}, \dots, \pm i b_{2\bar{d}-1, 2\bar{d}}$  and 0 if  $d$  is odd.

**Definition 2.5** *We define the spectral norm of  $B$  by  $|B|_{\text{sp}} := \sum_{j=1}^{\bar{d}} b_{2j-1, 2j}$ .*

$|B|_{\text{sp}}$  is one half of the trace norm of  $\tilde{B}$ , hence  $|B|_{\text{sp}}$  is a norm on  $\wedge^2 \mathbb{R}^d$ . If  $d = 2$ ,  $|B|_{\text{sp}} = |B|$ ; if  $d = 3$ ,  $|B|_{\text{sp}}$  is the Euclidean norm of the vector field  $\vec{B}$  associated with  $B$ , defined by  $\iota(\vec{B})dx \wedge dy \wedge dz = B$  where  $\iota(\vec{B})\omega$  is the inner product of the vector field  $\vec{B}$  with the differential form  $\omega$ .

**Remark 2.6**  $|B|_{\text{sp}}$  is the infimum of the spectrum of the Schrödinger operator with constant magnetic field  $B$  in  $\mathbb{R}^d$ .

## 2.4 Magnetic fields

Let us give the basic definitions and notations concerning magnetic fields in a domain  $\Omega$ . The *magnetic potential* is a smooth real 1-form  $A$  on  $\Omega \subset \mathbb{R}^d$ , given by  $A = \sum_{j=1}^d a_j dx_j$ , and the associated *magnetic field* is the 2-form  $B = dA$ ; more explicitly, we have  $B(x) = \sum_{1 \leq j < k \leq d} b_{jk}(x) dx_j \wedge dx_k$  with  $b_{jk}(x) = \partial_j a_k(x) - \partial_k a_j(x)$ .

Let us define now the Schrödinger operator with magnetic field  $B = dA$ :

**Definition 2.7** *The magnetic connection  $\nabla = (\nabla_j)$  is the differential operator defined by*

$$\nabla_j = \frac{\partial}{\partial x_j} - i a_j .$$

The magnetic Schrödinger operator  $H_A$  is defined by

$$H_A = - \sum_{j=1}^d \nabla_j^2 .$$

The magnetic Dirichlet integral  $h_A = \langle H_A \cdot | \cdot \rangle$  is given, for  $u \in C_0^\infty(\Omega)$ , by

$$h_A(u) = \int_{\Omega} \sum_{j=1}^d |\nabla_j u|^2 |dx| .$$

Let us note the commutator formula  $[\nabla_j, \nabla_k] = -ib_{jk}$  which will be very important. From the previous definitions and the fact that the formal adjoint of  $\nabla_j$  is  $-\nabla_j$ , it is clear that the operator  $H_A$  is symmetric on  $C_0^\infty(\Omega)$ .

**Definition 2.8** *We will say that  $B = dA$  is a confining field in  $\Omega$  if  $H_A$  is essentially self-adjoint (see Section 2.6).*

## 2.5 The Riemannian context

### 2.5.1 “Regular” Riemannian manifolds

The context of an Euclidean domain is not the most natural one for our problem. In particular, the “regularity assumption” of Definition 2.1 can easily be extended to the Riemannian context. Let  $(\Omega, g)$  be a smooth Riemannian manifold. We are interested in cases where  $(\Omega, g)$  is not complete. Let us recall that  $g$  induces on  $\Omega$  a distance  $d_g$  defined by  $d_g(x, y) = \inf_{\gamma \in \Gamma_{x,y}} \text{length}(\gamma)$  where  $\Gamma_{x,y}$  is the set of smooth paths  $\gamma : [0, 1] \rightarrow \Omega$  so that  $\gamma(0) = x$ ,  $\gamma(1) = y$ . We will denote by  $\widehat{\Omega}$  the metric completion of  $\Omega$  and by  $\Omega_\infty = \widehat{\Omega} \setminus \Omega$  the metric boundary. In the case where  $\Omega \subset \mathbb{R}^d$  is equipped with the Euclidean Riemannian metric,  $\Omega_\infty$  is in general not equal to the boundary  $\partial\Omega$ .

Definition 2.1 is now replaced by:

**Definition 2.9** *The Riemannian manifold  $(\Omega, g)$  is regular if*

1.  $\Omega_\infty$  is compact
2. For any  $\epsilon > 0$ , every  $x_0 \in \Omega_\infty$  has a neighbourhood  $U$  so that so that  $U \cap \Omega$  is  $\epsilon$ -quasi-isometric (see Definition 4.4) to an open set of  $\mathbb{R}^d$  with an Euclidean metric.

A function  $f : \Omega \rightarrow \mathbb{C}$  is regular at the boundary if it extends by continuity to  $\widehat{\Omega}$ .

### 2.5.2 Magnetic fields on Riemannian manifolds

The magnetic potential is a smooth real valued 1-form  $A$  on  $\Omega$ , the magnetic field is the 2-form  $B = dA$ . The norm  $|B(x)|_{\text{sp}}$  is calculated with respect to the Euclidean metric  $g_{x_0}$ . The magnetic potential defines a connection  $\nabla$  on the trivial line bundle  $\Omega \times \mathbb{C} \rightarrow \Omega$  by  $\nabla_X f = df(X) - iAf$ . The magnetic Dirichlet integral is  $h_A(f) = \int_{\Omega} \|\nabla f\|_g^2 |dx|_g$  where the norm of the 1-form  $\nabla f(x)$  is calculated with the dual Riemannian norm:  $\|\nabla f\|_g^2 = \sum_{ij} g^{ij} \nabla_{\partial_i} f \nabla_{\partial_j} f$  and  $|dx|_g = \theta |dx_1 \cdots dx_d|$  is the Riemannian volume. The magnetic Schrödinger operator is then defined by:

$$H_A f = -\theta^{-1} \sum_{ij} \nabla_{\partial_i} (\theta g^{ij} \nabla_{\partial_j} f) .$$

## 2.6 Essential self-adjointness

In this section, we will review what is an essentially self-adjoint operator and give some easy propositions which we were not able to point in the literature.

### 2.6.1 Essentially self-adjoint operators

Let us recall the following

**Definition 2.10** *A differential operator  $P : C_0^\infty(\Omega) \rightarrow C_0^\infty(\Omega)$  is essentially self-adjoint in  $L^2(\Omega, |dx|)$  if  $P$  is formally symmetric (for any  $u, v \in C_0^\infty(\Omega)$ ,  $\langle Pu|v \rangle = \langle u|Pv \rangle$ ) and the closure of  $P$  is self-adjoint.*

A basic criterion for essential self-adjointness is the following (see criterion (4) of Theorem X.1 and Corollaries in [22]):

**Proposition 2.11** *Let  $P$  be as before and formally symmetric. Let us assume either that*

(1) *there exists  $E \in \mathbb{R}$  so that any solution  $v \in L^2(\Omega)$  of  $(P - E)v = 0$  (in the weak sense of Schwartz distributions) vanishes,*

*or that*

(2) *there exists  $\lambda_\pm \in \mathbb{C}$  with  $\pm \Im(\lambda_\pm) > 0$  so that any solution  $v \in L^2(\Omega)$  of  $(P - \lambda_\pm)v = 0$  (in the weak sense of Schwartz distributions) vanishes.*

*Then  $P$  is essentially self-adjoint.*

### 2.6.2 Essential self-adjointness depends only on the boundary behaviour

**Proposition 2.12** *Let  $X$  be a smooth manifold with a smooth density  $|dx|$ . Let  $L_j$ ,  $j = 1, 2$  be two formally symmetric elliptic differential operators of degree  $m$  on  $L^2(X, |dx|)$  and let us assume that  $L_1$  is essentially self-adjoint and  $L_2 - L_1 = M$  is compactly supported. Then  $L_2$  is essentially self-adjoint.*

*Proof.*– It is enough to show that  $L_2 - ci$  is invertible for  $c$  real and large enough. We have  $L_2 - ci = (\text{Id} + M(L_1 - ci)^{-1})(L_1 - ci)$ . Moreover the domain of  $L_1$  contains  $H_0^m$  (the space of compactly supported  $H^m$  functions). So that  $\|M(L_1 - ci)^{-1}\| = O(c^{-1})$ .  $\square$

### 2.6.3 Essential self-adjointness is independent of the choice of a gauge

**Proposition 2.13** *Let  $X$  be a smooth manifold with a smooth density  $|dx|$ . Let us consider a Schrödinger operator  $H_{A_1}$  and  $A_2 = A_1 + dF$  with  $F \in C^\infty(X, \mathbb{R})$ . Then, if  $H_{A_1}$  is essentially self-adjoint,  $H_{A_2}$  is also essentially self-adjoint.*

*Proof.*– We have formally (as differential operators)

$$H_{A_2} = e^{iF} H_{A_1} e^{-iF} .$$

Hence,  $H_{A_2} - ci = e^{iF} (H_{A_1} - ci) e^{-iF}$ . The domain  $D_2$  of the closure of  $H_{A_2}$  (defined on  $C_0^\infty(X)$ ) is  $e^{iF}$  times the domain  $D_1$  of the closure of  $H_{A_1}$ . The result follows from the fact that  $e^{\pm iF}$  is invertible in  $L^2$  and an isomorphism of the domains.  $\square$

## 3 Main results

Let us take  $H_A$  with domain  $\mathcal{D}(H_A) = C_0^\infty(\Omega)$ . As explained in the introduction, we are looking for growth assumptions on  $|B|_{\text{sp}}$  close to  $\partial\Omega$  ensuring essential self-adjointness of  $H_A$ . We formulate now our main results:



**Theorem 3.1** *Let us take  $d = 2$ . Assume that  $\partial\Omega$  is compact with a finite number of connected components and that  $B(x)$  satisfies near  $\partial\Omega$*

$$|B(x)|_{\text{sp}} \geq (D(x))^{-2}, \quad (3.1)$$

*then the Schrödinger operator  $H_A$  is essentially self-adjoint. This still holds true for any gauge  $A'$  such that  $dA' = dA = B$ .*

**Theorem 3.2** *Let us take  $d > 2$ . Assume that  $\Omega$  is regular and that there exists  $\eta > 0$  such that  $B(x)$  satisfies near  $\partial\Omega$*

$$|B(x)|_{\text{sp}} \geq (1 + \eta) (D(x))^{-2}, \quad (3.2)$$

*and that the functions*

$$n_{jk}(x) = \frac{b_{jk}(x)}{|B(x)|_{\text{sp}}} \quad (3.3)$$

*are regular at the boundary  $\Omega_\infty$  (for any  $1 \leq j < k \leq d$ ) (see Definition 2.2). Then the Schrödinger operator  $H_A$  is essentially self-adjoint. This still holds true for any gauge  $A'$  such that  $dA' = dA = B$ .*

**Remark 3.3** *If  $\Omega$  is defined (locally or globally) by  $\Omega := \{x \in \mathbb{R}^d \mid f(x) > 0\}$  with  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  smooth,  $df(y) \neq 0$  for  $y \in \partial\Omega$ , then  $f(x) \sim |df(x)|D(x)$  for  $x$  close to  $\partial\Omega$ . And we can replace in the estimates (3.2)  $D(x)$  by  $f(x)/|df(x)|$ .*

Theorem 3.2 can be extended to Riemannian manifolds as follows:

**Theorem 3.4** *Let  $(\Omega, g)$  be a regular Riemannian manifold with a magnetic field  $B = dA$ . Let us assume that  $\|B\|_{\text{sp}} \geq (1 + \epsilon)D^{-2}$  near  $\Omega_\infty$  and that, for each  $x_0 \in \Omega_\infty$ , the direction  $n(x)$  of  $B$ , calculated with the metric  $g_{x_0}$  (i.e. using the trivialisation of the tangent bundle associated with  $g_{x_0}$ ), has a limit as  $x \rightarrow x_0$ , then  $H_A$  is essentially self-adjoint on  $C_0^\infty(\Omega)$ .*

The exponent 2 of the leading term in Equations (3.1) and (3.2) is optimal, as shown in the following

**Proposition 3.5** *For any  $0 < \alpha < \sqrt{3}/2$ , there exists a magnetic field  $B$  such that  $H_A$  (with  $dA = B$ ) is not essentially self-adjoint and such that the growth of  $|B|_{\text{sp}}$  near the boundary  $\partial\Omega$  satisfies*

$$|B(x)|_{\text{sp}} \geq \frac{\alpha}{(D(x))^2}.$$

We prove this proposition in Section 5.4 in the case  $d = 2$ , but the proof can be easily generalised to larger dimensions.

As a consequence of this proposition, together with Theorem 3.1 (respectively 3.2), we get that the optimal constant in front of the leading term  $(D(x))^{-2}$  is in  $[\sqrt{3}/2, 1]$ .

Hence we see that the situation for confining magnetic fields is not the same as for confining potentials (for which the optimal constant is  $3/4$ , hence is smaller than  $\sqrt{3}/2$ ).

Indeed this is due to the difference between the Hardy inequalities in the two situations: the term  $1/(4D^2)$  does not appear in the magnetic case, as it does in the case of a scalar potential, where it plays the role of an "additional barrier".

## 4 Proof of the main results

In this Section, we prove Theorems 3.1, 3.2 and 3.4 using the method of [20] which we first review.

## 4.1 Agmon estimates

The following statement is proved, using Agmon estimates [1], in [20]:

**Theorem 4.1** *Assume that  $\partial\Omega$  is compact, and that there exists  $c \in \mathbb{R}$  such that, for all  $u \in C_0^\infty(\Omega)$ ,  $h_A(u) - \int_\Omega D(x)^{-2}|u(x)|^2 dx \geq c\|u\|^2$ . Then  $H_A$  is essentially self-adjoint.*

Reading the proof in [20], one sees that the only property of  $\Omega$  which is used is that the function  $D(x)$  is smooth near the boundary and satisfies  $|dD(x)| \leq 1$ . One can extend the proof to the case where  $\partial\Omega$  is not a smooth manifold by using the properties of the function  $D$  described in Lemma 2.4. The fact that  $\Omega$  is bounded does not play an important role, only the compactness of  $\partial\Omega$  is important. The essential self-adjointness of  $H_A$  results from the Proposition 2.11 and the following

**Theorem 4.2** *Let  $v \in L^2(\Omega)$  be a weak solution of  $(H_A - E)v = 0$ . Let us assume that there exists a constant  $c > 0$  such that, for all  $u \in C_0^\infty(\Omega)$ ,*

$$\langle u|(H_A - E)u \rangle - \int_{\{x \in \Omega \mid D(x) \leq 1\}} \frac{|u(x)|^2}{D(x)^2} dx \geq c\|u\|^2. \quad (4.1)$$

Then  $v \equiv 0$ .

For the reader's convenience, we give here the proof of Theorem 4.2 following the strategy of [20] in a slightly simplified way.

*Proof.*— The proof is based on the following simple identity ([20])

**Lemma 4.3** *Let  $v$  be a weak solution of  $(H_A - E)v = 0$ , and let  $f$  be a real-valued Lipschitz function with compact support. Then*

$$\langle fv|(H_A - E)(fv) \rangle = \langle v \mid |df(x)|^2 v \rangle. \quad (4.2)$$

Let us give two numbers  $\rho$  and  $R$  satisfying respectively  $0 < \rho < \frac{1}{2}$  and  $1 < R < +\infty$ . We will apply identity (4.2) with  $f = F(D)$  where  $F(u)$  the piecewise smooth function defined by

$$F(u) = \begin{cases} 0 & \text{for } u \leq \rho \text{ and for } u \geq R+1 \\ 2(u - \rho) & \text{for } \rho \leq u \leq 2\rho \\ u & \text{for } 2\rho \leq u \leq 1 \\ 1 & \text{for } 1 \leq u \leq R \\ R+1 - u & \text{for } R \leq u \leq R+1 \end{cases}$$

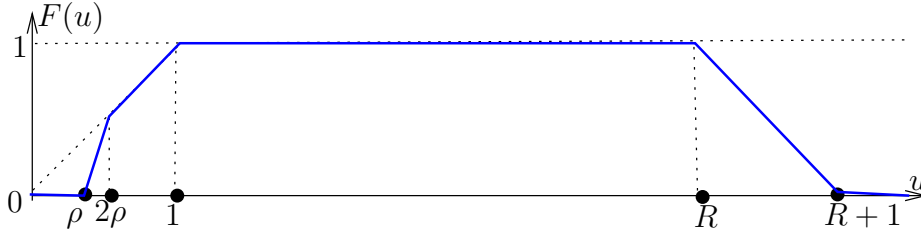


Figure 2: The function  $F$

We have  $|df|^2 = F'(D)^2$  almost everywhere. From the inequality (4.1) applied to  $fv$ , we get:

$$\langle (H_A - E)(fv) \mid fv \rangle \geq \int_{2\rho \leq D(x) \leq 1} |v|^2 dx + c\|fv\|^2. \quad (4.3)$$

On the other hand, using the explicit values of  $df$  and Equation (4.2), we get:

$$\begin{aligned} \langle (H_A - E)(fv) | fv \rangle &\leq 4 \int_{\rho \leq D(x) \leq 2\rho} |v|^2 |dx|_g + \dots \\ \dots \int_{2\rho \leq D(x) \leq 1} |v|^2 |dx|_g &+ \int_{R \leq D(x) \leq R+1} |v|^2 |dx|_g . \end{aligned} \quad (4.4)$$

Putting together the inequalities (4.3) and (4.4), we get

$$c \|fv\|^2 \leq 4 \int_{\rho \leq D(x) \leq 2\rho} |v|^2 |dx|_g + \int_{R \leq D(x) \leq R+1} |v|^2 |dx|_g . \quad (4.5)$$

Taking  $\rho \rightarrow 0$  and  $R \rightarrow +\infty$  in the inequalities (4.5), we get that the  $L^2$  norm of  $v$  vanishes. □

## 4.2 Quasi-isometries

In section 5 we give examples which have smooth boundaries (excepting the convex polyhedra (section 5.1)). In order to build new examples, like non convex polyhedra, one can use quasi-isometries.

**Definition 4.4** *Given  $0 < c \leq C$ , a  $(c, C)$ -quasi-isometry of  $\Omega_1$  onto  $\Omega_2$  is an homeomorphism of  $F : \overline{\Omega_1}$  onto  $\overline{\Omega_2}$  whose restriction to  $\Omega_1$  is a smooth diffeomorphism onto  $\Omega_2$  and such that*

$$\forall x, y \in \overline{\Omega_1}, \quad cd_R(x, y) \leq d_R(F(x), F(y)) \leq Cd_R(x, y) .$$

*An  $\epsilon$ -quasi-isometry is an  $(1 - \epsilon, 1 + \epsilon)$  quasi-isometry.*

**Lemma 4.5** *We have the bounds*

$\|F'\| \leq C$ ,  $\|(F^{-1})'\| \leq c^{-1}$ ,  $|\det(F')| \leq C^d$ ,  $cD_1(x) \leq D_2(F(x)) \leq CD_1(x)$ , where, for  $i = 1, 2$ ,  $D_i(x)$  denotes, for any  $x \in \Omega_i$ , the distances to the boundary  $(\Omega_i)_\infty$ .

We will start with a magnetic potential  $A_2$  in  $\Omega_2$  and define  $A_1 = F^*(A_2)$ . We want to compare the magnetic quadratic forms  $h_{A_2}(u)$  and  $h_{A_1}(u \circ F)$  as well as the  $L^2$  norms. We get:

**Theorem 4.6** *Assuming that, for any  $u \in C_0^\infty(\Omega_2)$ ,*

$$h_{A_2}(u) \geq K \int_{\Omega_2} \frac{|u|^2}{D_2^2} |dx_2| - L \|u\|^2 ,$$

*we have, for any  $v \in C_0^\infty(\Omega_1)$ ,*

$$h_{A_1}(v) \geq K \left(\frac{c}{C}\right)^{d+2} \int_{\Omega_1} \frac{|v|^2}{D_1^2} |dx_1| - Lc^2 \|v\|^2 .$$

In other words, we can check that  $H_{A_1}$  is essentially self-adjoint from an estimate for  $h_{A_2}$  using Theorem 4.1.

*Proof.*— Let us start making the change of variables  $x_2 = F(x_1)$  in the integral  $h_{A_2}(u)$ . Putting  $v = u \circ F$ , we get  $h_{A_2}(u) = \int_{\Omega_1} \|\nabla_{A_1} v(x_1)\|_g^2 |\det(F'(x_1))| |dx_1|$  where  $g$  is the inverse of the pull-back of the Euclidean metric by  $F$ . Using Lemma 4.5, we get the estimate. □

### 4.3 Lower bounds for the magnetic Dirichlet integrals

#### 4.3.1 Basic magnetic estimates

**Lemma 4.7** *For any  $u \in C_0^\infty(\Omega)$ , we have*

$$h_A(u) \geq |\langle b_{12}u|u \rangle| + |\langle b_{34}u|u \rangle| + \cdots + |\langle b_{2\bar{d}-1, 2\bar{d}}u|u \rangle| .$$

*Proof.*– We have

$$|\langle b_{12}u|u \rangle| = |\langle [\nabla_1, \nabla_2]u|u \rangle| \leq 2|\langle \nabla_1 u | \nabla_2 u \rangle| \leq \int_{\Omega} (|\nabla_1 u|^2 + |\nabla_2 u|^2) |dx| .$$

We take the sum of similar inequalities replacing the indices  $(1, 2)$  by  $(3, 4), \dots, (2\bar{d}-1, 2\bar{d})$ .  $\square$

**Lemma 4.8** *Let  $\Omega$  be a regular open set in  $\mathbb{R}^d$ . Let  $x_0 \in \Omega_\infty$  and assume that  $B(x)$  does not vanish near the point  $x_0$  and that the direction of  $B$  is regular near  $x_0$ . Let  $A$  be a local potential for  $B$  near  $x_0$ , then, for any  $\epsilon > 0$ , there exists a neighbourhood  $U$  of  $x_0$  in  $\mathbb{R}^d$  so that, for any  $\phi \in C_0^\infty(U \cap \Omega)$ ,*

$$h_A(\phi) \geq (1 - \epsilon) \int_U |B(x)|_{\text{sp}} |\phi(x)|^2 |dx| , \quad (4.6)$$

where  $|B(x)|_{\text{sp}}$  is defined in Definition 2.5.

*Proof.*– Let us choose  $U$  so that, for all  $x \in U \cap \Omega$ ,  $|n(x) - n(x_0)|_{\text{Eucl}} \leq \epsilon \sqrt{\frac{2}{d(d-1)}}$ , where  $|\sum_{i < j} a_{ij} dx_i \wedge dx_j|_{\text{Eucl}}^2 = \sum_{i < j} a_{ij}^2$ , by applying Definition 2.2 to  $n(x)$  at the point  $x_0$ . We choose orthonormal coordinates in  $\mathbb{R}^d$  so that  $n(x_0) = n_{12} dx_1 \wedge dx_2 + n_{34} dx_3 \wedge dx_4 + \cdots$  with  $n_{2k-1, 2k} \geq 0$  and  $\sum_k n_{2k-1, 2k} = 1$ . From Lemma 4.7, we have, for  $\phi \in C_0^\infty(\Omega \cap U)$ ,

$$h_A(\phi) \geq \int_U |B(x)|_{\text{sp}} (n_{12}(x) + n_{34}(x) + \cdots) |\phi(x)|^2 |dx|$$

and  $n_{12}(x) + n_{34}(x) + \cdots \geq 1 - \epsilon$ , because the Euclidean norm of  $n(x)$  is independent of the orthonormal basis.  $\square$

**Remark 4.9** *The estimate (4.6) is optimal in view of Remark 2.6.*

#### 4.3.2 The 2-dimensional case

**Theorem 4.10** *Let us assume that  $\partial\Omega \subset B(O, R)$  and that  $\partial\Omega$  has a finite number of connected components. If  $d = 2$  and if  $B$  does not vanish near  $\partial\Omega$ , then there exists  $c_R \in \mathbb{R}$  so that,  $\forall u \in C_0^\infty(\Omega)$ ,*

$$h_A(u) \geq \int_{\Omega \cap B(O, R)} |B||u|^2 |dx| - c_R \|u\|^2 . \quad (4.7)$$

*Proof.*– As  $B$  does not vanish near  $\partial\Omega$ , the sign of  $B$  is constant near each connected component of  $\partial\Omega$ . Let us write  $\bar{\Omega} \subset \cup_{l=1}^3 \Omega_l$  with  $\Omega_l$  open sets such that  $\Omega_1 \cap \partial\Omega = \emptyset$ ,  $B > 0$  on  $\Omega_2$  and  $B < 0$  on  $\Omega_3$ . We can assume that  $\Omega_2$  and  $\Omega_3$  are bounded. Take a partition of unity  $\phi_j$ ,  $j = 1, 2, 3$ , so that, for  $j = 2, 3$ ,  $\phi_j \in C_0^\infty(\Omega_j)$ , and  $\sum \phi_j^2 \equiv 1$ .

Now we use the IMS formula (see [23])

$$h_A(u) = \sum_{l=0}^2 h_A(\phi_l u) - \int_{\Omega} \left( \sum_{l=0}^2 |d\phi_l|^2 \right) |u|^2 |dx| . \quad (4.8)$$

with the lower bound of Lemma 4.7 in  $\Omega_l \cap \Omega$  for  $l = 2, 3$  and the lower bound 0 for  $\Omega_1$ .  $\square$

### 4.3.3 The case $d > 2$

**Theorem 4.11** *Let us assume that  $\partial\Omega \subset B(O, R)$ . Assume that  $B = dA$  does not vanish near  $\partial\Omega$  and that the functions  $n_{jk}(x)$  are regular at the boundary  $\partial\Omega$ , then, for any  $\epsilon > 0$ , there exists  $C_{\epsilon, R} > 0$  so that,  $\forall u \in C_0^\infty(\Omega)$ ,*

$$h_A(u) \geq (1 - \epsilon) \int_{\Omega \cap B(O, R)} |B|_{\text{sp}} |u|^2 |dx| - C_{\epsilon, R} \int_{\Omega} |u|^2 |dx|. \quad (4.9)$$

*Proof.*— We first choose a finite covering of  $\Omega_\infty$  by open sets  $U_l$ ,  $l = 1, \dots, N$  of  $\mathbb{R}^d$  which satisfies the estimates of Lemma 4.8. We choose then a partition of unity  $\phi_l, l = 0, \dots, N$  with

- For  $l \geq 1$ ,  $\phi_l \in C_0^\infty(U_l)$
- $\phi_0$  is  $C_0^\infty(\Omega)$
- $\sum_l \phi_l^2 \equiv 1$  in  $\Omega$
- $\sup \sum_l |d\phi_l|^2 = M$ .

Using the estimates given in Lemma 4.8 for  $l \geq 1$  and the fact that  $\sum_l |d\phi_l|^2$  is bounded by  $M$ , we get, using IMS identity (4.8), the inequality (4.9).  $\square$

## 4.4 End of the proof of the main theorems

Using Theorem 4.1, it is enough to show that there exists  $c \in \mathbb{R}$  such that, for all  $u \in C_0^\infty(\Omega)$ ,

$$h_A(u) \geq \int_{\Omega \cap B(O, R)} |D(x)|^{-2} |u(x)|^2 |dx| - c \|u\|^2,$$

under the assumptions of Theorems 3.1 and 3.2. This is a consequence of Theorem 4.10 for  $d = 2$  and Theorem 4.11 for  $d > 2$ .

The proof of Theorem 3.4 is an adaptation of the case of an Euclidean domain. The partition of unity is constructed using only the distance function which has enough regularity. We use also the fact that near each point  $x_0$  of the boundary the metric is quasi-isometrically close to the Euclidean metric  $g_{x_0}$ .

## 5 Examples

### 5.1 Polytopes

A *polytope* is a convex compact polyhedron. Let  $\Omega$  be a polytope given by

$$\Omega = \cap_{i=1}^N \{x \mid L_i(x) < 0\},$$

where the  $L_i$ 's are the affine real-valued functions

$$L_i(x) = \sum_{j=1}^d n_{ij} x_j + a_i.$$

We will assume that, for  $i = 1, \dots, d$ ,  $\sum_{j=1}^d n_{ij}^2 = 1$  (normalisation) and  $n_{i1} \neq 0$  (this last condition can always be satisfied by moving  $\Omega$  by a generic isometry). We have the

**Theorem 5.1** *The operator  $H_A$  in  $\Omega$  with*

$$A = \left( \frac{1}{n_{11}L_1} + \frac{1}{n_{21}L_2} + \cdots \right) dx_2 ,$$

*is essentially self-adjoint.*

*Proof.*– We have

$$B = \left( \frac{1}{L_1^2} + \frac{1}{L_2^2} + \cdots \right) dx_1 \wedge dx_2 + \sum_{j=3}^d b_j dx_j \wedge dx_2 ,$$

and  $D = \min_{1 \leq i \leq N} |L_i|$ . So that  $B = b_{12} dx_1 \wedge dx_2 + \sum_{j=3}^d b_j dx_j \wedge dx_2$  with  $b_{12} \geq D^{-2}$ . We then apply directly Lemma 4.7 and Theorem 4.1.  $\square$

## 5.2 Examples in domains whose Euler characteristic of the boundary vanishes (“toroidal domains”).

Let us assume that  $\partial\Omega$  is a smooth compact manifold of co-dimension 1 and denote by  $j : \partial\Omega \rightarrow \mathbb{R}^d$  the injection of  $\partial\Omega$  into  $\mathbb{R}^d$ . A famous theorem of H. Hopf (see [2, 12]) asserts that there exists a nowhere vanishing tangent vector field to  $\partial\Omega$  (or 1-form) if and only if the Euler characteristic of  $\partial\Omega$  vanishes.

**Theorem 5.2** *Let us assume that the Euler characteristic of  $\partial\Omega$  vanishes (we say that  $\Omega$  is toroidal). Let  $A_0$  be a smooth 1-form on  $\overline{\Omega}$  so that the 1-form on  $\partial\Omega$  defined by  $\omega = j^*(A_0)$  does not vanish, and consider a 1-form  $A$  in  $\Omega$  defined, near  $\partial\Omega$ , by  $A = A_0/D^\alpha$ . We assume that either  $\alpha > 1$ , or  $\alpha = 1$  with the additional condition that for any  $y \in \partial\Omega$ ,  $|\omega(y)| > 1$ . Then  $H_A$  is essentially self-adjoint.*

**Remark 5.3** *The existence of  $\omega$  is provided by the topological assumption on  $\partial\Omega$ . This works if  $\Omega \subset \mathbb{R}^3$  is bounded by a 2-torus. It is the case for tokamacs.*

*Proof.*– We will apply Theorem 3.2. We have to check:

- The uniform continuity of the direction of the magnetic field or the extension by continuity to  $\overline{\Omega}$ . It has to be checked locally near the boundary  $\partial\Omega$ . We will use an adapted chart (see section 2.2.2).

In these local coordinates we write  $A_0 = a_1 dx_1 + \beta$  with  $\beta = a_2 dx_2 + \cdots + a_d dx_d$  and  $\omega = a_2(0, x') dx_2 + \cdots + a_d(0, x') dx_d$  so we get

$$B = d \left( \frac{A_0}{x_1^\alpha} \right) = \frac{x_1 dA_0 - \alpha dx_1 \wedge \beta}{x_1^{\alpha+1}} .$$

Thus we get that the direction of  $B$  is equivalent as  $x_1 \rightarrow 0^+$  to that of  $dx_1 \wedge \omega$  which is non vanishing and continuous on  $\overline{\Omega}$ .

- The lower bound (3.2)  $|B|_{\text{sp}} \geq (1 + \eta)D^{-2}$  near  $\partial\Omega$ . The norm of  $B$  near the boundary is given, as  $x \rightarrow y$  by

$$|B(x)|_{\text{sp}} \sim \alpha |\omega(y)| / D^{\alpha+1} .$$

Therefore we conclude that the hypotheses of Theorem 3.2 are fulfilled.  $\square$

**Remark 5.4** *The asymptotic behaviour of  $B(x)$  as  $x \rightarrow \partial\Omega$  is*

$$B(x) \sim -\frac{\alpha dx_1 \wedge \omega(y)}{D^{\alpha+1}}.$$

*It follows that  $\omega$  and  $\alpha$  depend only of  $B$  and are invariant by any gauge transform in  $\Omega$ .*

**Remark 5.5** *If  $d = 3$ , the magnetic field  $B$  can be identified with a vector field  $\vec{B}$  in  $\Omega$  defined by*

$$\iota(\vec{B}) dx_1 \wedge dx_2 \wedge dx_3 = B$$

*as in Section 2.3. Using the induced Riemannian structure, we can identify any 1-form  $\omega$  on  $\partial\Omega$  with a vector field  $\vec{\omega}$ . Moreover  $\partial\Omega$  is oriented by any 2-form  $\Sigma = \iota(\nu)dx_1 \wedge dx_2 \wedge dx_3$  with  $\nu$  any outgoing vector field near  $\partial\Omega$ . Using the previous identifications, the asymptotic behaviour of  $\vec{B}$  near  $\partial\Omega$  is given by*

$$\vec{B} \sim \alpha r(\vec{\omega})/D^{\alpha+1},$$

*where  $r$  is the rotation by  $+\pi/2$  in the tangent space to  $\partial\Omega$ .*

*It means that  $\vec{B}$  is very large near  $\partial\Omega$  and parallel to  $\partial\Omega$ . From the point of view of classical mechanics, the trajectories of the charged particle are spiralling around the field lines and do not cross the boundary. It would be nice to have a precise statement.*

## 5.3 Non toroidal domains

### 5.3.1 Statement of results

We try to follow the same strategy than in Section 5.2, but now we will allow the 1-form  $\omega$  on  $X = \partial\Omega$  to have some zeroes. This is forced by the topology if the Euler characteristic of  $\partial\Omega$  does not vanish. We need the

**Definition 5.6** *A 1-form  $\omega$  on a compact manifold  $X$  is generic if  $\omega$  has a finite number of zeroes and  $d\omega$  does not vanish at the zeroes of  $\omega$ .*

We have the

**Theorem 5.7** *Let  $\Omega \subset \mathbb{R}^d$  with a smooth compact boundary  $X = \partial\Omega$ . Let  $A_0$  be a smooth 1-form in  $\mathbb{R}^d$  so that  $\omega = j_X^*(A_0)$  is generic. We assume also that, at each zero  $m$  of  $\omega$ ,*

$$|d\omega(m)|_{\text{sp}} > 1, \tag{5.1}$$

*where the norm  $|d\omega(m)|_{\text{sp}}$  is calculated in the space of anti-symmetric bi-linear forms on the tangent space  $T_m\partial\Omega$ . Then, if  $A$  is a 1-form in  $\Omega$  such that near  $X$ ,  $A = A_0/D^2$ ,  $B = dA$  is confining in  $\Omega$ .*

We see that the field need to be more singular than in the toroidal case. We could have taken this highly singular part only near the zeroes of  $\omega$ .

### 5.3.2 Local model

We will work in an adapted chart at a zero of  $\omega$ . We take  $A = A_0/x_1^2$  with  $j^*(A_0) = \omega$ , we have:  $A_0 = a_1 dx_1 + \beta$  and  $\beta(0) = 0$ .

We have

$$B = \frac{d\omega}{x_1^2} + dx_1 \wedge \rho + o(x_1^{-1}).$$

Applying the basic estimates of Lemma 4.7 in some orthonormal coordinates in  $\mathbb{R}^{d-1}$  so that  $d\omega(0) = b_{23}dx_2 \wedge dx_3 + \dots$ , we see, using the assumption (5.1), that there exists a neighbourhood  $U$  of the origin and an  $\eta > 0$  so that, for any  $u \in C_0^\infty(U)$ ,

$$h_A(u) \geq (1 + \eta) \int_U \frac{|u|^2}{x_1^2} |dx| .$$

### 5.3.3 Globalisation

Near each zero of  $\omega$ , we take a local chart of  $\mathbb{R}^d$  where  $A$  is given by the local model. Such a chart is an  $\epsilon$ -quasi-isometry (see 4.4) with  $\epsilon$  as small as one wants. This gives the local estimate near the zeroes of  $\omega$ . The local estimate outside the zeroes of  $\omega$  is clear because we have then  $|B|_{\text{sp}} \geq C/D^3$  with  $C > 0$ : this follows from the estimates in Section 5.2 with  $\alpha = 2$ . We finish the proof of Theorem 5.7 with IMS formula and the local estimates needed in Theorem 4.1.

## 5.4 An example of a non essentially self-adjoint Schrödinger operator with large magnetic field near the boundary

Let us consider the 1-form defined on  $\Omega = \{(x, y) \in \mathbb{R}^2 \mid x^2 + y^2 = r^2 < 1\}$  by  $A = \alpha(xdy - ydx)/(r-1)$  where  $0 < \alpha < \sqrt{3}/2$ . The magnetic potential  $A$  is invariant by rotations. Then

**Theorem 5.8** *The operator  $H_A$  is not essentially self-adjoint.*

The corresponding magnetic field  $B$  writes  $B(x, y) = \frac{\alpha(r-2)}{(r-1)^2} dx \wedge dy$ , and, near the boundary,  $|B(x)| \sim \alpha/(D(x))^2$ . We have, in polar coordinates  $(r, \theta)$ ,

$$H_A = -\frac{\partial^2}{\partial r^2} - \frac{1}{r} \frac{\partial}{\partial r} - \frac{2i\alpha r}{r-1} \frac{\partial}{\partial \theta} + \frac{\alpha^2 r^2}{(r-1)^2} .$$

Hence the operator  $H_A$  splits as a sum  $\sum_{m \in \mathbb{Z}} H_{A,m}$  where  $H_{A,m}$  acts on functions  $e^{im\theta} f(r)$ . We will look at the  $m = 0$  component: Theorem 5.8 follows from the

**Lemma 5.9** *If  $0 < \alpha < \sqrt{3}/2$ , on the Hilbert space  $L^2(]0, 1[, r dr)$ , the operator*

$$H = -\frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} + \frac{\alpha^2 r^2}{(r-1)^2}$$

*is in the limit circle case near  $r = 1$  and hence is not essentially self-adjoint.*

*Proof.*— Let  $U$  be the unitary transform  $U : u \rightarrow r^{1/2}u$  from  $L^2(]0, 1[, r dr)$  onto  $L^2(]0, 1[, dr)$ . Then  $K = UHU^{-1}$  is given by

$$-\frac{d^2}{dr^2} - \frac{1}{4r^2} + \frac{\alpha^2 r^2}{(r-1)^2} .$$

$K$  is known to be in the limit circle case at  $r = 1$  (Theorem X.10 in [22].) □

## 5.5 Singular points

### 5.5.1 Monopoles

We will first discuss the case of monopoles in  $\mathbb{R}^3$ . Here  $\Omega$  is  $\mathbb{R}^3 \setminus 0$ .



**Definition 5.10** *The monopole of degree  $m$ ,  $m \in \mathbb{Z} \setminus 0$ , is the magnetic field  $B_m = (m/2)p^*(\sigma)$  where  $p : \mathbb{R}^3 \setminus 0 \rightarrow \mathbb{S}^2$  is the radial projection and  $\sigma$  the area form on  $\mathbb{S}^2$ . In coordinates*

$$B_m = \frac{m}{2} \frac{xdy \wedge dz + ydz \wedge dx + zdx \wedge dy}{(x^2 + y^2 + z^2)^{3/2}} .$$

**Remark 5.11** *Let us note, for comparisons with the case where  $\partial\Omega$  is of codimension 1, that  $|B_m|_{\text{sp}} = \frac{|m|}{2}r^{-2}$ .*

The flux of  $B_m$  through  $\mathbb{S}^2$  is equal to  $2\pi m$ . This is a well-known *quantisation condition* which is needed in order to build a quantum monopole. In order to define the Schrödinger operator  $H_m$ , we first introduce an Hermitian complex line bundle  $L_m$  with an Hermitian connexion  $\nabla_m$  on  $\Omega$  with curvature  $B_m$ . We first construct  $L_m$  and  $\nabla_m$  on  $\mathbb{S}^2$  and then take their pull-backs:  $\nabla_m$  in a direction tangent to a sphere is the same and  $\nabla_m$  vanishes on radial directions. We have, using spherical coordinates,

$$H_m = -\frac{\partial^2}{\partial r^2} - \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} K_m ,$$

where  $K_m$  is the angular Schrödinger operator on  $\mathbb{S}^2$  (discussed for example in [27]). Let us denote by  $\lambda_1^m$  the lowest eigenvalue of  $K_m$ . The self-adjointness of  $H_m$  depends of the value of  $\lambda_1^m$ . As a consequence of Weyl's theory for Sturm-Liouville equations,  $H_m$  is essentially self-adjoint if and only if  $\lambda_1^m \geq 3/4$ . From [17, 18, 27] (sketched in Section 5.5.2), we know that  $\lambda_1^m = |m|/2$  so that

**Theorem 5.12** *The Schrödinger operator  $H_m$  (monopole of degree  $m$ ) is essentially self-adjoint if and only if  $|m| \geq 2$ .*

### 5.5.2 The spectra of the operators $K_m$ , the “spherical Landau levels”

These spectra are computed in [17, 18] and in the PhD thesis [27]. We sketch here the calculus. Recall that  $K_m$  is the Schrödinger operator with magnetic field  $m\sigma/2$  where  $\sigma$  is the area form on  $\mathbb{S}^2$ . The metric is the usual Riemannian metric on  $\mathbb{S}^2$ :

**Theorem 5.13** *The spectrum of  $K_m$  is the sequence*

$$\lambda_k = \frac{1}{4} (k(k+2) - m^2) , \quad k = |m|, |m| + 2, \dots ,$$

*with multiplicities  $k+1$ . In particular, the ground state  $\lambda_{|m|}$  of  $K_m$  is  $|m|/2$ , with multiplicity  $|m|+1$ . The ground state is exactly the norm of the magnetic field.*

If  $m = 0$ , the reader will recognise the spectrum of the Laplace operator on  $\mathbb{S}^2$ .

We start with the sphere  $\mathbb{S}^3$  with the canonical metric. Looking at  $\mathbb{S}^3 \subset \mathbb{C}^2$ , we get an free isometric action of  $\mathbb{S}_\theta^1$  on  $\mathbb{S}^3$ :  $\theta.(z_1, z_2) = e^{i\theta}(z_1, z_2)$ . The quotient manifold is  $\mathbb{S}^2$  with  $1/4$  times the canonical metric; the volume  $2\pi^2$  of  $\mathbb{S}^3$  divided by  $2\pi$  is  $\pi$  which is one fourth of  $4\pi$ .

The quotient map  $\mathbb{S}^3 \rightarrow \mathbb{S}^2$  is the Hopf fibration, a  $\mathbb{S}^1$ -principal bundle. The sections of  $L_m$  over  $\mathbb{S}^2$  are identified with the functions on  $\mathbb{S}^3$  which satisfy  $f(\theta z) = e^{im\theta} f(z)$ . With this identification of the sections of  $L_m$ , we have

$$K_m = \frac{1}{4} (\Delta_{\mathbb{S}^3} - m^2) ,$$

where  $1/4$  comes from the fact that the quotient metric is  $1/4$  of the canonical one and  $m^2$  from the action of  $\partial_\theta^2$  which has to be removed. It is enough then to look at the spectral decomposition of  $\Delta_{\mathbb{S}^3}$  using spherical harmonics: the  $k$ th eigenspace of  $\Delta_{\mathbb{S}^3}$  is of dimension  $(k+1)^2$  and splits into  $k+1$  subspaces of dimension  $k+1$  corresponding to  $m = -k, -k+2, \dots, k$ .

### 5.5.3 A general result for $\Omega = \mathbb{R}^d \setminus 0$

In this section  $\Omega = \mathbb{R}^d \setminus 0$  and  $B$  is singular at the origin.

**Theorem 5.14** *If  $\lim_{x \rightarrow 0} |x|^2 |B(x)|_{\text{sp}} = +\infty$  and, for any  $x \neq 0$ , the direction  $n(tx)$  has a limit as  $t \rightarrow 0^+$ , then  $M_B$  is essentially self-adjoint*

*Proof.*— The proof is essentially the same as the proof of Theorem 3.2 except that in the application of IMS method, we have to take a conical partition of unity whose gradients can only be bounded by  $|x|^{-1}$ .  $\square$

### 5.5.4 Multipoles

Let us denote, for  $x \in \mathbb{R}^3$ ,  $\mathcal{B}_x$  the monopole with centre  $x$ :  $\mathcal{B}_x = \tau_x^*(B_2)$  with  $\tau_x$  the translation by  $x$  and  $B_2$  the monopole with  $m = 2$ . If  $P\left(\frac{\partial}{\partial x}\right)$  is a homogeneous linear differential operator of degree  $n$  on  $\mathbb{R}^3$  with constant coefficients, we define  $B_P = P(\mathcal{B}_x)_{x=0}$ . Then  $B_P$  is called a multipole of degree  $n$ . All multipoles are exact! It is a consequence of the famous Cartan's formula: if  $P$  is of degree 1, hence a constant vector field,

$$B_V = \mathcal{L}_V \mathcal{B}_0 = d(\iota(V)\mathcal{B}_0) .$$

A multipole of degree 1 is called a dipole; viewed from very far away, the magnetic field of the earth looks like a dipole.

**Theorem 5.15** *If  $B_V = dA_V$  is a dipole,  $H_{A_V}$  is essentially self-adjoint.*

*Proof.*— Because  $B_V$  is homogeneous of degree  $-\alpha = -3$ , it is enough, using 5.14, to show that  $B_V$  does not vanish.  $V$  is a constant vector field, hence up to a dilatation, we can take  $V = \partial/\partial z$ . We have

$$B_{\partial/\partial z} = \frac{d}{dt}\Big|_{t=0} \frac{xdy \wedge dz + ydz \wedge dx + (z-t)dx \wedge dy}{(x^2 + y^2 + (z-t)^2)^{3/2}} ,$$

which gives

$$B_{\partial/\partial z} = \frac{3xzd y \wedge dz + 3y z d z \wedge dx + (2z^2 - x^2 - y^2)dx \wedge dy}{(x^2 + y^2 + z^2)^{5/2}} .$$

The form  $B_{\partial/\partial z}$  does not vanish in  $\Omega$ .  $\square$

**Remark 5.16** *We do not know if all multipoles of degree  $\geq 2$  are essentially self-adjoint.*

## References

- [1] S. Agmon. *Lectures on exponential decay of solutions of second-order elliptic equations*, Mathematical Notes **29**, Princeton University Press (1982).
- [2] P. Alexandroff & H. Hopf. *Topologie. Band I*, Chelsea Publishing Co., Bronx, N. Y., (1972).
- [3] J. Avron, I. Herbst & B. Simon. *Schrödinger operators with magnetic fields*, Duke. Math. J. **45** (1978), 847-883.
- [4] A. Balinsky, A. Laptev & A. Sobolev. *Generalized Hardy Inequality for the Magnetic Dirichlet Forms*, Journal of Statistical Physics **116** (2004), 507-521.
- [5] Y. Colin de Verdière. *L'asymptotique de Weyl pour les bouteilles magnétiques*, Commun. Math. Phys. **105** (1986), 327-335.

- [6] H. Cycon, R. Froese, W. Kirsch & B. Simon. *Schrödinger Operators with Application to Quantum Mechanics and Global Geometry*, Texts and Monographs in Physics, Springer-Verlag (1987).
- [7] A. Dufresnoy. *Un exemple de champ magnétique dans  $\mathbb{R}^{\nu}$* , Duke. Math. J. **50** (1983), 729-734.
- [8] N. Dunford & J. T. Schwartz. *Linear operator II. Spectral Theory*, John Wiley & sons, New York (1971).
- [9] L. Erdős & J. P. Solovej. *Semiclassical eigenvalue estimates for the Pauli operator with strong nonhomogeneous magnetic fields, I* Duke. Math. J. **96** (1999), 127-173.
- [10] L. Erdős & J. P. Solovej. *Magnetic Lieb-Thirring inequalities with optimal dependence on the field strength*, Journ. Stat. Phys. **116** (2004), 475-506.
- [11] L. Erdős & J. P. Solovej. *Magnetic Lieb-Thirring inequalities for the 3-dimensional Pauli operator with a strong nonhomogeneous magnetic fields*, Ann. Henri Poincaré **5** (2004), 671-745.
- [12] V. Guillemin & A. Pollack. *Differential topology*, Prentice-Hall Inc., Englewood Cliffs, N.J., (1974).
- [13] J. Heinonen. *Lectures on Lipschitz analysis*, Report. University of Jyväskylä, Department of Mathematics and Statistics, **100** (2005). <http://www.math.jyu.fi/tutkimus/ber.html>
- [14] T. Ikebe & T. Kato. *Uniqueness of the self-adjoint extension of singular elliptic differential operators*, Arch. Rational Mech. Anal. **9** (1962), 77–92.
- [15] H. Kalf, U-V. Schminke, J. Walter & R. Wüst. *On the spectral theory of Schrödinger and Dirac operators with strongly singular potentials*, Lecture Notes in Mathematics **448** (1975), 182-226.
- [16] B. Kostant. *Quantization and unitary representations*. Lecture Notes in Maths (Springer) **170** (1970), 87–208.
- [17] R. Kuwabara. *On spectra of the laplacian on vector bundles*. Jour. Math. Tokushima Univ. **16** (1982), 1–23.
- [18] R. Kuwabara. *Spectrum of the Schrödinger operator on a line bundle over complex projective spaces*. Tohoku Math. Jour. **40** (1988), 199-211.
- [19] C. B. Morrey. *Multiple Integrals in the Calculus of Variations*. Springer (1966).
- [20] G. Nenciu & I. Nenciu. *On confining potentials and essential self-adjointness for Schrödinger operators on bounded domains in  $\mathbb{R}^n$* , [arXiv 0811.2982v1](https://arxiv.org/abs/0811.2982v1)
- [21] H. Rademacher. *Über partielle und totale differenzierbarkeit von Funktionen mehrerer Variablen und über die Transformation der Doppelintegrale*, Math. Ann. **79**, (1919), 340–359.
- [22] M. Reed & B. Simon. *Methods of Modern mathematical Physics II*, New York Academic Press, (1975).
- [23] I. Sigal. *Geometrical methods in the Quantum Many Body Problem, Nonexistence of very negative ions*, Commun. Math. Phys. **85** (1982) 309–324.

- [24] B. Simon. *Essential Self-adjointness for Schrödinger operators with singular potentials: A generalized Kalf-Walter-Schminke theorem*, Arch. Rational Mech. Analysis, **52** (1973), 44-48.
- [25] B. Simon. *Schrödinger operators with singular magnetic vector potentials*. Math. Z. **131** (1973), 361–370.
- [26] M. Shubin. *The essential Self-adjointness for Semi-bounded Magnetic Schrödinger operators on Non-compact Manifolds*, J. Func. Anal. **186** (2001), 92-116.
- [27] N. Toriki-Hamza. *Stabilité des valeurs propres et champ magnétique sur une variété riemannienne et sur un graphe*, PhD thesis, Grenoble University (1989).
- [28] F. Truc. *Trajectoires bornées d'une particule soumise à un champ magnétique linéaire*, Annales de l'IHP (Physique théorique), **64** (1996), 127-154.
- [29] F. Truc. *Semi-classical asymptotics for magnetic bottles*, Asympt. Anal. **15** (1997), 385-395.
- [30] <http://en.wikipedia.org/wiki/Tokamak>