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Confining quantum particles with a purely magnetic field

Yves Colin de Verdière* & Françoise Truc†

April 18, 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 behavior 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.

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*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

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1 Introduction

The problem

Let us consider a particle in a domain Ω in \mathbb{R}^d ($d \geq 2$) in the presence of a magnetic field B . We will always assume that the topological boundary $\partial\Omega := \bar{\Omega} \setminus \Omega$ of Ω 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 behavior of $B(x)$ as x tends to $\partial\Omega$ which ensure that the magnetic operator H_A is essentially self-adjoint on $C_0^\infty(\Omega)$. These conditions will not depend on the gauge A , but only on the field B . One could have called such pairs (Ω, 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 ionized plasma which is heated is confined thanks to magnetic fields.

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 generalizes 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. The regularity conditions on the direction of the magnetic field was introduced in the important paper [3] 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 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.

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 to 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, $\forall u \in C_o^\infty(\Omega)$, the quadratic form h_A satisfies the quite optimal bound

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

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 $|B(x)|_{\text{sp}} \geq (1 + \eta)D(x)^{-2}$ where $\eta > 0$ and D is the distance to the boundary of Ω .

We study then examples in the following cases:

- The domain Ω 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)
- Monopoles and dipoles in $\Omega = \mathbb{R}^3 \setminus 0$
- For any $\epsilon > 0$ and $d = 2$, we construct, in the unit disk, 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.

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 $|B(x)|_{\text{sp}} \geq CD(x)^{-2}$? We know that the optimal constant lies in the interval $[\sqrt{3}/2, 1]$.

2 Notations and definitions

2.1 The domain Ω

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

Definition 2.1 We will denote by d_R the distance defined on Ω 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 (Ω, d_R) and by $\Omega_\infty = \widehat{\Omega} \setminus \Omega$ the metric boundary of Ω .

We say that Ω is regular if Ω_∞ is compact.

If Ω is regular, $\partial\Omega$ is compact. In fact the identity map of Ω extends to a continuous map π from $\widehat{\Omega}$ onto $\overline{\Omega}$ and $\pi(\Omega_\infty) = \partial\Omega$. $(\widehat{\Omega}, \pi)$ is a “desingularization” 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, Ω 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.

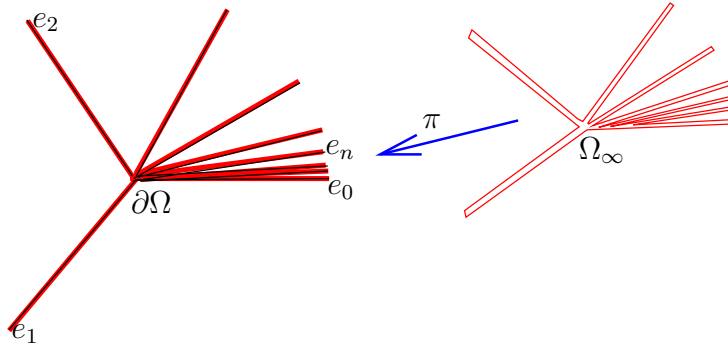


Figure 1: An example where ∂X is compact while X_∞ is not compact

We will use the following regularity property:

Definition 2.2 Let us assume that Ω 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 $C_c^\infty(\Omega)$ the space of complex-valued smooth functions with compact support in Ω .

2.2 The distance to the boundary

2.2.1 The distance function

Let $D(x)$ be, for any $x \in \Omega$, the Riemannian distance to the boundary, given by $D(x) = \min_{y \in \Omega_\infty} d_R(x, y)$.

Lemma 2.3 *The function D is 1-Lipschitz and then almost everywhere differentiable in Ω . At any point x of differentiability of D , we have $|dD(x)| \leq 1$.*

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 neighborhood U of x_0 in \mathbb{R}^d onto an open neighborhood V of 0 in $\mathbb{R}^d_{x_1, x'}$, 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 ϵ -quasi-isometry (see definition in Appendix C) with ϵ 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 $B = b_{12} dx_1 \wedge dx_2 + b_{34} dx_3 \wedge dx_4 + \dots$ with $b_{12} \geq b_{34} \geq \dots > 0$; the sequence b_{12}, b_{34}, \dots is unique: the non-zero eigenvalues of the antisymmetric endomorphism \vec{B} of \mathbb{R}^d associated to $B(x)$ are $\pm i b_{12}, \pm i b_{34}, \dots$.

Definition 2.4 *We define then the spectral norm of B by $|B|_{\text{sp}} := \sum_{j=1}^{\lfloor d/2 \rfloor} b_{2j-1, 2j}$.*

$|B|_{\text{sp}}$ is one half of the trace norm of \vec{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 to B , defined by $\iota(\vec{B})dx \wedge dy \wedge dz = B$.

Remark 2.5 $|B|_{\text{sp}}$ is the infimum of the spectrum of the Schrödinger operator with constant magnetic field B in \mathbb{R}^d .

2.4 Magnetic fields

The *magnetic potential* is a smooth real one-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 two-form $B = dA$. We have $B(x) = \sum_{1 \leq j < k \leq d} b_{jk}(x) dx_j \wedge dx_k$ with $b_{jk}(x) = \partial_j a_k(x) - \partial_k a_j(x)$.

If X is a smooth sub-manifold of \mathbb{R}^d , we will denote by j_X (or j if the context is clear) the embedding $j_X : X \hookrightarrow \mathbb{R}^d$ and, if ω is a differential form on \mathbb{R}^d , by $j^*(\omega)$ the pull-back of ω onto X .

Definition 2.6 *The magnetic connection ∇ is the differential operator defined by*

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

The magnetic Schrödinger operator H_A is defined by

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

The magnetic Dirichlet integral h_A is defined, for $u \in C_o^\infty(\Omega)$, by

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

The operator H_A is formally symmetric on $C_o^\infty(\Omega)$.

Definition 2.7 *We will say that $B = dA$ is a confining field in Ω if H_A is essentially self-adjoint.*

The commutator formula $[\nabla_j, \nabla_k] = -ib_{jk}$ will be very important.

3 Main results

3.1 The results

Let us take H_A with domain $\mathcal{D}(H_A) = C_o^\infty(\Omega)$. 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 Ω 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 Ω_∞ (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 $dA' = dA = B$.

3.2 Remarks

- If Ω 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 $f(x)/|df(x)|$.

- **About optimality**

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

Proposition 3.3 *For any $0 < \alpha < \sqrt{3}/2$, there exists a magnetic field B for which H_A (with $dA = B$) is not essentially self-adjoint and such that $|B|_{\text{sp}}$ grows close to the boundary $\partial\Omega$ as*

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

We prove this proposition in Section 11 in the case $d = 2$, but the proof can be easily generalized 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 Two general lemmas

4.1 Essential self-adjointness depends only on the boundary behavior

Lemma 4.1 *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_o^m (the space of compactly supported H^m functions). So that $\|M(L_1 - ci)^{-1}\| = O(c^{-1})$.

□

This implies that, in order to prove self-adjointness in Ω , we have nothing to do at infinity in \mathbb{R}^d thanks to the results of [14].

4.2 Essential self-adjointness is independent of the choice of a gauge

Lemma 4.2 *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 $C_o^\infty(X)$) 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.

□

5 Agmon estimates

Using Agmon estimates [1], the following statement is derived from [20] in Appendix E:

Theorem 5.1 *Assume that $\partial\Omega$ is compact, and that there exists $c \in \mathbb{R}$ such that, for all $u \in C_o^\infty(\Omega)$, $h_A(u) - \int_\Omega D(x)^{-2}|u(x)|^2 dx \geq c\|u\|^2$. Then, for $E \ll 0$, if v is a weak $L^2(\Omega)$ -solution of $(H_A - E)v = 0$, v vanishes identically and H_A is essentially self-adjoint.*

Reading the proof in [20], one sees that the only property of Ω 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 2.3. The fact that Ω is bounded does not play an important role, only the fact that $\partial\Omega$ is compact is important. The fact that H_A is essentially self-adjoint follows from the criterion (4) of Theorem X.1 in [22].

6 Lower bounds for the magnetic Dirichlet integrals

6.1 Some Lemmas

Lemma 6.1 *For any $u \in C_o^\infty(\Omega)$, we have*

$$h_A(u) \geq |\langle b_{12}u|u \rangle| + |\langle b_{34}u|u \rangle| + \dots .$$

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 12 by 34, 56, \dots .

□

Lemma 6.2 *Let Ω 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 neighborhood U of x_0 in \mathbb{R}^d so that, for any $\phi \in C_o^\infty(U \cap \Omega)$,*

$$h_A(\phi) \geq (1 - \epsilon) \int_U |B(x)|_{\text{sp}} |\phi(x)|^2 dx , \quad (6.1)$$

where $|B(x)|_{\text{sp}}$ is defined in Definition 2.4.

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 $n(x_0) = n_{12} dx_1 \wedge dx_2 + n_{34} dx_3 \wedge dx_4 + \dots$ with $n_{2k-1, 2k} \geq 0$ and $\sum_k n_{2k-1, 2k} = 1$. From Lemma 6.1, we have, for $\phi \in C_o^\infty(\Omega \cap U)$,

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

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

□

Remark 6.3 *The estimate (6.1) is optimal in view of the remark 2.5.*

6.2 The 2-dimensional case

Theorem 6.4 *Let us assume that $\partial\Omega \subset B(O, R)$. If $d = 2$ and if B does not vanish near the boundary, then there exists $c_R \in \mathbb{R}$ so that, $\forall u \in C_o^\infty(\Omega)$,*

$$h_A(u) \geq \int_{\Omega \cap B(O, R)} |B||u|^2 |dx| - c_R \|u\|^2. \quad (6.2)$$

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 Ω_l open sets such that $\Omega_1 \cap \partial\Omega = \emptyset$, $B > 0$ on Ω_2 and $B < 0$ on Ω_3 . We can assume that Ω_2 and Ω_3 are bounded. Take a partition of unity ϕ_j , $j = 1, 2, 3$, so that, for $j = 2, 3$, $\phi_j \in C_o^\infty(\Omega_j)$, and $\sum \phi_j^2 \equiv 1$.

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

$$h_A(u) = \sum_{l=0}^2 h_A(\phi_l u) - \int_{\Omega} \left(\sum_{l=0}^2 |d\phi_l|^2 \right) |u|^2 |dx|. \quad (6.3)$$

with the lower bound of Lemma 6.1 in $\Omega_l \cap \Omega$ for $l = 2, 3$ and the lower bound 0 for Ω_1 .

□

6.3 The case $d > 2$

Theorem 6.5 *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, $\forall u \in C_o^\infty(\Omega)$,*

$$h_A(u) \geq (1 - \epsilon) \int_{\Omega \cap B(O, R)} |B|_{\text{sp}} |u|^2 |dx| - C_{\epsilon, R} \int_{\Omega} |u|^2 |dx|. \quad (6.4)$$

Proof.–

We first choose a finite covering of Ω_∞ by open sets U_l , $l = 1, \dots, N$ of \mathbb{R}^d which satisfies the estimates of Lemma 6.2. We choose then a partition of unity ϕ_l , $l = 0, \dots, N$ with

- For $l \geq 1$, $\phi_l \in C_o^\infty(U_l)$
- ϕ_0 is $C_o^\infty(\Omega)$
- $\sum_l \phi_l^2 \equiv 1$ in Ω
- $\sup \sum_l |d\phi_l|^2 = M$.

Using the estimates given in Lemma 6.2 for $l \geq 1$ and the fact that $\sum_l |d\phi_l|^2$ is bounded by M , we get, using IMS identity (6.3), the inequality (6.4).

□

7 Proof of the main theorems

Using Theorem 5.1, it is enough to show that there exists $c \in \mathbb{R}$ such that, for all $u \in C_o^\infty(\Omega)$,

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

under the assumptions of Theorems 3.1 and 3.2. This is a consequence of Theorem 6.4 for $d = 2$ and Theorem 6.5 for $d > 2$.

8 Polytopes

A polytope is a convex compact polyhedron. Let Ω 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 $i = 1, \dots, d$, $\sum_{j=1}^d n_{ij}^2 = 1$ (normalization) and $n_{i1} \neq 0$ (this last condition can always be satisfied by moving Ω by a generic isometry). We have the

Theorem 8.1 *The operator H_A in Ω with*

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

is essentially self-adjoint.

Proof.–

We have

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

and $D = \min_{1 \leq i \leq N} |L_i|$. So that $B = b_1 dx_1 \wedge dx_2 + \sum_{j=3}^d b_j dx_j \wedge dx_2$ with $b_1 \geq D^{-2}$. We then apply directly Lemma 6.1 and Theorem 5.1. □

9 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 9.1 *Let us assume that the Euler characteristic of $\partial\Omega$ vanishes (we say that Ω is toroidal). Let A_0 be a smooth 1-form on $\bar{\Omega}$ so that the 1-form on $\partial\Omega$ defined by $\omega = j^*(A_0)$ does not vanish, and consider a 1-form A in Ω 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 9.2 *The existence of ω 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 $\bar{\Omega}$. 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 $\beta = a_2 dx_2 + \dots$ and $\omega = a_2(0, x') dx_2 + \dots$ 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 $\bar{\Omega}$.

- 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

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

Therefore we conclude that the hypotheses of Theorem 3.2 are fulfilled. □

Remark 9.3 *From the calculation before, it follows that ω and α are invariant by any gauge transform in $\partial\Omega$.*

Remark 9.4 *If $d = 3$, the magnetic field can be identified with a vector field in Ω . The assumptions of the previous Theorem imply that this field is asymptotic to $-\alpha V^\perp/D^{\alpha+1}$ where V is the vector field associated to ω and V^\perp is deduced from V by a rotation of $\pm\pi/2$ (depending of conventions for the orientation of $\partial\Omega$). It means that 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 spiraling around the field lines and do not cross the boundary. It would be nice to have a precise statement.*

10 Non toroidal domains

10.1 Statement of results

We try to follow the same strategy than in Section 9, but now any 1-form on $X = \partial\Omega$ may have some zeroes. We need the

Definition 10.1 *A 1-form ω on a compact manifold X is generic if ω has a finite number of zeroes and $d\omega$ does not vanish at the zeroes of ω ,*

and we have the

Theorem 10.2 *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 ω ,*

$$|d\omega(m)|_{\text{sp}} > 1 , \tag{10.1}$$

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 Ω such that near X , $A = A_0/D^2$, $B = dA$ is confining in Ω .

We see that the field is more singular than in the toroidal case. We could have taken this highly singular part only near the zeroes of ω .

10.2 Local model

We will work in an adapted chart at a zero of ω . 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 6.1 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 (10.1), that there exists a neighborhood U of the origin and an $\eta > 0$ so that, for any $u \in C_o^\infty(U)$,

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

10.3 Globalization

Near each zero of ω , we take a local chart of \mathbb{R}^d where A is given by the local model. Such a chart is an ϵ -quasi-isometry (see Appendix C) with ϵ as small as one wants. This gives the local estimate near the zeroes of ω . The local estimate outside the zeroes of ω is clear because we have then $|B|_{\text{sp}} \geq C/D^3$ with $C > 0$. We finish the proof of Theorem 10.2 with IMS formula and the local estimates needed in Theorem 5.1.

11 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 11.1 *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, θ) ,

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

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 and reduce the measure $|rdrd\theta|$ to $2\pi dr$ by a change of function: for any function of the type $u(r) = r^{-1/2}v(r)$, $H_A u = r^{-1/2} \left(-\frac{d^2}{dr^2} + V(r) \right) v$, where

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

According to theorem X.10 of [22], we know that the operator $H = -\frac{d^2}{dr^2} + V(r)$ is in the limit circle case at $r = 1$, since, there exists $\epsilon > 0$ with

$$V(r) \leq \left(\frac{3}{4} - \epsilon \right) (r-1)^{-2}$$

near $r = 1$. Let $v(r)$ be an L^2 solution of $(H - E)v = 0$, then $u(r) = r^{-1/2}v(r)$ is also an L^2 solution of $(H_A - E)u = 0$ in Ω .

12 Singular points

12.1 Monopoles

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

Definition 12.1 *The monopole of degree m , $m \in \mathbb{Z} \setminus 0$, is the magnetic field $B_m = (m/2)p^*(\sigma)$ where $p : \mathbb{R}^3 \setminus 0 \rightarrow S^2$ is the radial projection and σ the area form on 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 12.2 *Let us note, for further comparisons, that $|B_m| \geq \frac{|m|}{2}r^{-2}$ where the constant is sharp.*

The flux of B_m through S^2 is equal to $2\pi m$. This is a well-known *quantization 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 ∇_m on Ω with curvature B_m . We first construct L_m and ∇_m on S^2 and then take their pull-backs: ∇_m in a direction tangent to a sphere is the same and ∇_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 S^2 (discussed for example in [27]). Let us denote by λ_1^m the lowest eigenvalue of K_m . The self-adjointness of H_m depends of the value of λ_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] (reproduced in Appendix B), we know that $\lambda_1^m = |m|/2$ so that

Theorem 12.3 *The Schrödinger operator H_m (monopole of degree m) is essentially self-adjoint if and only if $|m| \geq 2$.*

12.2 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 12.4 *If $\lim_{x \rightarrow 0} |x|^2 |B(x)|_{\text{sp}} = +\infty$ and, for any $x \neq 0$, the direction $n(x)$ 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 $|x|^{-1}$.

□

12.3 Multipoles

Let us denote, for $x \in \mathbb{R}^3$, \mathcal{B}_x the monopole with center x : $\mathcal{B}_x = \tau_x^*(B_2)$ with τ_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 12.5 *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 12.4, 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

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

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

□

Remark 12.6 *We do not know if all multipoles of degree ≥ 2 are essentially self-adjoint.*

13 Appendix A: magnetic Schrödinger operators for non exact magnetic fields

Let B be a real valued closed 2–form on $\Omega \subset \mathbb{R}^d$. If $B = dA$ is exact, the magnetic Schrödinger operator is H_A . If B is not exact, we can still construct a magnetic Schrödinger operator M_B (well-defined up to gauge transform if the cohomology $H^1(\Omega, \mathbb{R})$ vanishes) provided that the cohomology class of $B/2\pi$ is integer. Locally, $B = dA$ and M_B coincide with H_A up to (local) gauge transform.

The construction is summarized as follows: under the integrality assumption, there exists an Hermitian line bundle L over Ω with an Hermitian connection ∇ of curvature B . This bundle is unique modulo tensor products with a flat line bundle which is trivial if $H^1(\Omega, \mathbb{Z})$ vanishes. M_B is associated to the quadratic form m_B on $L^2(\Omega, L)$, the space of L^2 sections of L , defined by $m_B(f) = \int_{\Omega} \|\nabla f\|^2 dx$.

14 Appendix B: 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 σ is the area form on S^2 . The metric is the usual Riemannian metric on S^2 :

Theorem 14.1 *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 recognize the spectrum of the Laplace operator on S^2 .

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

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

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

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 ∂_θ^2 which has to be removed. It is enough then to look at the spectral decomposition of Δ_{S^3} using spherical harmonics: the k th eigenspace of Δ_{S^3} is of dimension $(k+1)^2$ and splits into $k+1$ subspaces of dimension $k+1$ corresponding to $m = -k, -k+2, \dots, k$.

15 Appendix C: quasi-isometries

Our previous examples have smooth boundaries (excepting the convex polyhedra (section 8)). In order to build new examples, like non convex polyhedra, one can use quasi-isometries.

Definition 15.1 *Given $0 < c \leq C$, a (c, C) -quasi-isometry of Ω_1 onto Ω_2 is an homeomorphism of $F : \overline{\Omega_1}$ onto $\overline{\Omega_2}$ whose restriction to Ω_1 is a smooth diffeomorphism onto Ω_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 ϵ -quasi-isometry is an $(1 - \epsilon, 1 + \epsilon)$ quasi-isometry.

Lemma 15.2 *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 Ω_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 15.3 *Assuming that, for any $u \in C_o^\infty(\Omega_2)$,*

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

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

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

In other words, we can check that H_{A_1} is essentially self-adjoint from an estimate for h_{A_2} using Theorem 5.1.

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 15.2, we get the estimate.

□

16 Appendix D: Riemannian context

16.1 “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. Now (Ω, g) is a smooth Riemannian manifold. We are interested in cases where (Ω, g) is not complete. Let us recall that g induces on Ω 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 Ω 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, Ω_∞ is in general not equal to the boundary $\partial\Omega$.

The Definition 2.1 is now replaced by:

Definition 16.1 *The Riemannian manifold (Ω, g) is regular if*

1. Ω_∞ is compact
2. For any $\epsilon > 0$, every $x_0 \in \Omega_\infty$ has a neighborhood U so that $U \cap \Omega$ is ϵ -quasi-isometric 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 $\widehat{\Omega}$.

16.2 Magnetic fields on Riemannian manifolds

The magnetic potential is a smooth real valued 1-form A on Ω , 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 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:

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

16.3 Main result

The following result is an extension of Theorem 3.2 to the Riemannian case:

Theorem 16.2 *Let (Ω, 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 Ω_∞ 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 to g_{x_0}), has a limit as $x \rightarrow x_0$, then H_A is essentially self-adjoint on $C_0^\infty(\Omega)$.*

The proof 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} .

17 Appendix E: Agmon-type estimates

We recall here the method used in [20], which still holds for a Schrödinger operator with magnetic potential. We adapt it to the Riemannian case: (Ω, g) is a smooth Riemannian manifold so that Ω_∞ is compact. We define now $D(x)$ for $x \in \Omega$ as the Riemannian distance to Ω_∞ .

Theorem 17.1 Let v be a weak solution of $(H_A - E)v = 0$, and assume that v belongs to $L^2(\Omega)$. Let us assume that there exists a constant $c > 0$ such that, for all $u \in C_0^\infty(\Omega)$,

$$\langle u|(H_A - E)u \rangle - \int_{\{x \in \Omega \mid D(x) \leq 1\}} \frac{|u(x)|^2}{D(x)^2} |dx|_g \geq c\|u\|^2. \quad (17.1)$$

Then $v \equiv 0$.

Proof.–

This theorem is based on the following simple identity ([20])

Lemma 17.2 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

$$\langle fv|(H_A - E)(fv) \rangle = \langle v \mid |df(x)|^2 v \rangle. \quad (17.2)$$

Let us give two numbers ρ and R satisfying respectively $0 < \rho < \frac{1}{2}$ and $1 < R < +\infty$. We will apply identity (17.2) with $f = F(D)$ where $F(u)$ the piecewise smooth function defined by

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

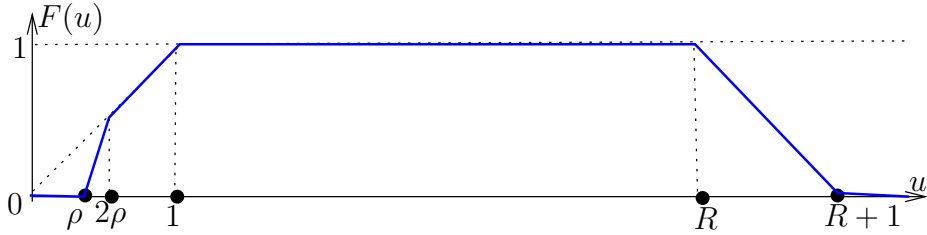


Figure 2: The function F

We have $|df|^2 = F'(D)^2$ almost everywhere. From the inequality (17.1) applied to fv , we get:

$$\langle (H_A - E)(fv) \mid fv \rangle \geq \int_{2\rho \leq D(x) \leq 1} |v|^2 |dx|_g + c\|fv\|^2. \quad (17.3)$$

On the other hand, using the explicit values of df and Equation (17.2), we get:

$$\begin{aligned} \langle (H_A - E)(fv) \mid fv \rangle &\leq 4 \int_{\rho \leq D(x) \leq 2\rho} |v|^2 |dx|_g + \dots \\ &\dots \int_{2\rho \leq D(x) \leq 1} |v|^2 |dx|_g + \int_{R \leq D(x) \leq R+1} |v|^2 |dx|_g. \end{aligned} \quad (17.4)$$

Putting together the inequalities (17.3) and (17.4), we get

$$c\|fv\|^2 \leq 4 \int_{\rho \leq D(x) \leq 2\rho} |v|^2 |dx|_g + \int_{R \leq D(x) \leq R+1} |v|^2 |dx|_g. \quad (17.5)$$

Taking $\rho \rightarrow 0$ and $R \rightarrow +\infty$ in the inequalities (17.5), we get that the L^2 norm of v vanishes.

□

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