Essential self-adjointness for magnetic Schrödinger operators on non-compact manifolds

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Abstract

We give a condition of essential self-adjointness for magnetic Schrödinger operators on non-compact Riemannian manifolds with a given positive smooth measure which is fixed independently of the metric. This condition is related to the classical completeness of a related classical hamiltonian without magnetic field. The main result generalizes the result by I. Oleinik [46, 47, 48], a shorter and more transparent proof of which was provided by the author in [59]. The main idea, as in [59], consists in an explicit use of the Lipschitz analysis on the Riemannian manifold and also by additional geometrization arguments which include a use of a metric which is conformal to the original one with a factor depending on the minorant of the electric potential.

We also prove a magnetic version of the A. Povzner theorem [49] on essential self-adjointness of semi-bounded Schrödinger operators, as well as its generalization to manifolds.

1 Introduction

Let (M, g) be a Riemannian manifold (i.e. M is a C^∞-manifold, (g_{jk}) is a Riemannian metric on M), $\dim M = n$. We will always assume that M is connected. We will also assume that we are given a *positive smooth measure* $d\mu$ i.e. a measure which has a C^∞ positive density $\rho(x)$ with respect to the Lebesgue measure $dx = dx^1 \dots dx^n$ in any local coordinates $x^1, \dots, x^n$, so we will write $d\mu = \rho(x)dx$. This measure may be completely independent of the Riemannian metric, but may of course coincide with the canonical measure $d\mu_g$ induced by the metric (in this case $\rho = \sqrt{g}$ where $g = \det(g_{jk})$, so locally $d\mu_g = \sqrt{g}dx$).

The main purpose of this paper is to study essential self-adjointness of magnetic Schrödinger operators in $L^2(M) = L^2(M, d\mu)$.

Denote $\Lambda^p_{(k)}(M)$ the set of all k-smooth (i.e. of the class C^k) complex-valued p-forms on M. We will write $\Lambda^p(M)$ instead of $\Lambda^p_{(\infty)}(M)$. A *magnetic potential* is a real-valued 1-form $A \in \Lambda^1_{(1)}(M)$. So in local coordinates $x^1, \dots, x^n$ it can be written as

$$A = A_j dx^j,$$

where $A_j = A_j(x)$ are real-valued C^1-functions of the local coordinates, and we use the standard Einstein summation convention.

The usual differential can be considered as a first order differential operator

$$d : C^\infty(M) \longrightarrow \Lambda^1(M).$$

We will also need a deformed differential

$$d_A : C^\infty(M) \longrightarrow \Lambda^1_{(1)}(M), \qquad u \mapsto du + iuA,$$

where $i = \sqrt{-1}$.

The Riemannian metric (g_{jk}) and the measure $d\mu$ induce an inner product in the spaces of smooth forms with compact support in a standard way. In particular, this inner product on functions has the form

$$(u, v) = \int_M u\bar{v} d\mu,$$

where the bar over v means the complex conjugation.

For smooth forms $\alpha = \alpha_j dx^j, \beta = \beta_k dx^k$ denote

$$\langle \alpha, \beta \rangle = g^{jk} \alpha_j \beta_k,$$

where (g^{jk}) is the inverse matrix to (g_{jk}). So the result $\langle \alpha, \beta \rangle$ is a scalar function on M. Then for α, β with compact support we have

$$(\alpha, \beta) = \int_M \langle \alpha, \bar{\beta} \rangle d\mu,$$

where

$$\bar{\beta} = \bar{\beta}_k dx^k.$$

Using the inner products in spaces of smooth functions and forms with compact support we can define the completions of these spaces. They are Hilbert spaces which we will denote $L^2(M)$ for functions and $L^2\Lambda^1(M)$ for 1-forms. These spaces depend on the choice of the metric (g_{jk}) and the measure $d\mu$. However we will skip this dependence in the notations of the spaces for simplicity of notations. This will not lead to a confusion because both metric and measure will be fixed through the whole paper unless indicated otherwise.

The corresponding local spaces will be denoted $L^2_{loc}(M)$ and $L^2_{loc}\Lambda^1(M)$ respectively. These spaces do not depend on the metric or measure. For example $L^2_{loc}(M)$ consists of all functions $u : M \to \mathbb{C}$ such that for any local coordinates $x^1, \dots, x^n$ defined in an open set $U \subset M$ we have $u \in L^2$ with respect to the Lebesgue measure $dx^1 \dots dx^n$ on any compact subset in U.

Formally adjoint operators to the differential operators with sufficiently smooth coefficients are well defined through the inner products above. In particular, we have an operator

$$d_A^* : \Lambda^1_{(1)}(M) \longrightarrow C(M),$$

defined by the identity

$$(d_A u, \omega) = (u, d_A^* \omega), u \in C_c^\infty(M), \omega \in \Lambda^1_{(1)}(M).$$

(Here $C_c^\infty(M)$ is the set of all C^∞ functions with compact support on M.)

Therefore we can define the magnetic Laplacian Δ_A (with the potential A) by the formula

$$-\Delta_A = d_A^* d_A : C^\infty(M) \longrightarrow C(M).$$

Now the main object of our study will be the *magnetic Schrödinger operator*

$$H = H_{A,V} = -\Delta_A + V, \tag{1.1}$$

where $V \in L^\infty_{loc}(M)$ i.e. V is a locally bounded measurable function which is called *electric potential*. We will always assume V to be real-valued. Then H becomes a symmetric operator in $L^2(M)$ if we consider it on the domain $C_c^\infty(M)$. In this paper we will discuss conditions on V (at infinity) which guarantee that this operator is essentially self-adjoint in $L^2(M)$ (which means that its closure in $L^2(M)$ is a self-adjoint operator).

Note that for $A = 0$ the operator Δ_A becomes a generalized Laplace-Beltrami operator Δ on scalar functions on M and it can be locally written in the form

$$\Delta u = \frac{1}{\rho} \frac{\partial}{\partial x^j} (\rho g^{jk} \frac{\partial u}{\partial x^k}). \tag{1.2}$$

The operator $H_{A,V}$ with $A = 0$ becomes a generalized Schrödinger operator

$$H_{0,V} = -\Delta + V. \tag{1.3}$$

Recent results by I. Oleinik [46, 47, 48] provided the most advanced essential self-adjointness condition for $H_{0,V}$ which is directly connected to the classical completeness of a related hamiltonian system. (I. Oleinik considered the case $d\mu = d\mu_g$ only but his arguments work for arbitrary $d\mu$ without any changes.) A simpler and more transparent proof of the I. Oleinik's result was given in [59]. In the present paper we extend the result of I. Oleinik to the case of magnetic Schrödinger operators $H_{A,V}$ using a modification of arguments given in [59]. The result is that the essential self-adjointness for $H_{A,V}$ holds under the same condition on (M, g) and V as was imposed in the I. Oleinik's theorem, and with no additional condition at infinity on the magnetic potential A.

The importance of the essential self-adjointness of H becomes clear if we turn to the quantum mechanics and try to use the differential expression (1.1) to produce a quantum observable (a Hamiltonian) associated with this expression: a self-adjoint operator in $L^2(M)$ which extends $H|_{C_c^\infty(M)}$. Essential self-adjointness means that such an extension exists and is unique. This in turn implies the existence and uniqueness of the solution of the following Cauchy problem for the evolutionary Schrödinger equation:

$$\frac{1}{i} \frac{\partial \psi(t)}{\partial t} = H\psi(t),\ \psi(0) = \psi_0 \in C_c^\infty(M),\ \psi(t) \in L^2(M) \text{ for all } t \in \mathbb{R}.$$

(See e.g. [2], Ch.VI, Sect.1.7.) Here H is applied to ψ in the sense of distributions and the derivative in t is taken in the norm sense.

In case when this existence and uniqueness holds, it is natural to say that we have *quantum completeness* for the corresponding quantum system. If for example the uniqueness does not hold, we need some extra data to construct a Hamiltonian, e.g. boundary conditions etc.

Let us also consider the classical system, which corresponds to the quantum Hamiltonian $H_{0,V}$, i.e. the Hamiltonian system with the Hamiltonian

$$h(p,x) = |p|^2 + V(x) \tag{1.4}$$

in the cotangent bundle T^*M (with the standard symplectic structure). Here p is considered as a cotangent vector at the point $x \in M$, $|p|$ means the length of p with respect to the metric induced by g on T^*M. In local coordinates $(x^1, \dots, x^n)$ we have

$$|p|^2 = g^{ij}(x)p_i p_j, \text{ where } p = p_j dx^j \in T^*_x M.$$

In the coordinates $(x^1, \dots, x^n, p_1, \dots, p_n)$ the hamiltonian system has the form

$$\frac{dx^i}{dt} = \frac{\partial h}{\partial p_i}, \ \frac{dp_i}{dt} = -\frac{\partial h}{\partial x^i}, \ i = 1, \dots, n. \tag{1.5}$$

Let us assume for a moment that $V \in C^2(M)$, so the local Hamiltonian flow associated with the classical Hamiltonian (1.4) is well defined. Let us say that the system is *classically complete* if all the hamiltonian trajectories, i.e. solutions of (1.5), with arbitrary initial conditions are defined for all values of t. Usually it is more natural to require that they are defined for almost all initial conditions (in the phase space T^*M), but this distinction will not play any role in our considerations, though it is relevant if we want to treat potentials with local singularities (e.g. Coulomb type potentials).

We refer to Reed and Simon [51] for a more detailed discussion about classical and quantum completeness.

In the future we will assume that

$$V(x) \geq -Q(x) \text{ for all } x \in M, \tag{1.6}$$

where Q is a real-valued function which is positive and somewhat more regular than V itself.

For any $x, y \in M$ denote by $d_g(x,y)$ the distance between x and y induced by the Riemannian metric g.

Now we can formulate the main result which generalizes the result of I. Oleinik [47] (see also [59]):

Theorem 1.1 *Assume that $A \in \Lambda^1_{(1)}(M)$, V satisfies (1.6) where $Q(x) \geq 1$ for all $x \in M$ and the following conditions are satisfied:*

(a) The function $Q^{-1/2}$ is globally Lipschitz i.e.

$$|Q^{-1/2}(x) - Q^{-1/2}(y)| \leq C d_g(x,y), \ x, y \in M, \tag{1.7}$$

(*b*) $\int^{\infty} Q^{-1/2} ds = \infty,$

where the integral is taken along any parametrized curve (with a parameter $t \in [a, \infty)$), such that it goes out to infinity (i.e. leaves any compact $K \subset M$ starting at some value of the parameter t), ds means the arc length element associated with the given metric g.

Then the operator $H_{A,V}$ given by (1.1) is essentially self-adjoint.

Remark 1. The requirement (b) is related to the classical completeness of the system with the Hamiltonian $|p|^2 - Q(x)$ if we additionally assume that $Q \in C^2(M)$. To illustrate this assume for simplicity that $M = \mathbb{R}^n$ and the metric g is the standard flat metric on $\mathbb{R}^n$. Now assume that (b) is satisfied. Then along the classical trajectory of the Hamiltonian $|p|^2 - Q(x)$ we have

$$|p|^2 - Q(x) = E = const.$$

It follows that

$$dt = \frac{ds}{|\dot{x}|} = \frac{ds}{2|p|} = \frac{ds}{2\sqrt{E + Q(x)}},$$

hence the classical completeness for the Hamiltonian $|p^2| - Q(x)$ follows from the condition (b).

Remark 2. If we assume that $Q \in C^2(M)$ then the condition (b) is equivalent to the geodesic completeness of the Riemannian metric $\tilde{g}$ given by $\tilde{g}_{ij} = Q^{-1} g_{ij}$ (so $\tilde{g}$ is conformal to the original metric g).

Note also that (b) implies that the original metric g is also complete because $Q \geq 1$.

Remark 3. The requirement (a) in the theorem does not impose any serious restrictions on the growth of Q at infinity, but rather restricts oscillations of Q. Indeed, we can equivalently rewrite (a) in the form of the following estimate:

$$|dQ| \leq 2CQ^{3/2},$$

where $|dQ|$ means the length of the cotangent vector dQ as above. Arbitrary tower of exponents

$$e^r, e^{e^r}, e^{e^{e^r}} \ldots,$$

satisfies this estimate. (Here $r = r(x) = d_g(x, x_0)$ with a fixed $x_0 \in M$.)

Imposing appropriate conditions on V sometimes leads to the equivalence of the conditions of classical and quantum completeness (in case $A = 0$). An example of such situation was provided by A. Wintner [74] in case $n = 1$, with the restrictions which mean that the derivatives of V are small compared with V itself. However some conditions are indeed necessary even in case $n = 1$. This was shown by J. Rauch and M. Reed [50] who refer to unpublished lectures of E. Nelson. Examples given in [50] show that the classical and quantum completeness conditions are independent if no additional restrictions on V are imposed. (See also discussion on classical and quantum completeness in Appendix to Sect.X.1 in the M. Reed and B. Simon book [51].)

Remark 4. The theorem of I. Oleinik (i.e. Theorem 1.1 in case $A = 0$) was extended to the Laplacian on forms of arbitrary degree by M. Braverman [4]. The Braverman result holds for the magnetic Schrödinger operator as well (which is well defined on forms of arbitrary degree), but we restrict ourselves to the case of the operator on functions for the simplicity of exposition.

2 Algebraic preliminaries

We will start by considering the operator d^*, which is formally adjoint to d, so $d^* : \Lambda^1_{(1)}(M) \to C(M)$. This operator is related with the divergence of vector fields. Let v be a smooth vector field on M. Denote by ω_v the 1-form corresponding to v i.e. locally $\omega_v = (\omega_v)_j dx^j$ where

$$(\omega_v)_j = g_{jk}v^k.$$

Vice versa, for any smooth 1-form ω we will denote by v_ω the corresponding vector field, so locally $v_\omega = v_\omega^k \partial/\partial x_k$ where

$$v_\omega^k = g^{kj}\omega_j.$$

Then we will define the divergence of v by the formula

$$\operatorname{div} v = -d^*\omega_v. \tag{2.1}$$

Equivalently we can write

$$d^*\omega = -\operatorname{div} v_\omega. \tag{2.2}$$

A straightforward calculation shows that in local coordinates

$$\operatorname{div} v = \frac{1}{\rho}\frac{\partial}{\partial x^i}(\rho v^i), \quad v = v^i\frac{\partial}{\partial x^i}. \tag{2.3}$$

It follows from (2.1) that $\operatorname{div} v$ (as given by (2.3)) does not depend on the choice of local coordinates but only on the metric and measure. On the other hand (2.3) implies that $\operatorname{div} v$ does not depend on the metric (even though it is not immediately seen from (2.1)).

We have the following Leibniz rule for d^* (or, equivalently, for the divergence):

$$d^*(f\omega) = fd^*\omega - \langle df, \omega\rangle, \quad f \in C^1(M),\ \omega \in \Lambda^1_{(1)}(M). \tag{2.4}$$

For the Laplacian Δ (on functions) we have

$$\Delta u = -d^*du = \operatorname{div}(\nabla u), \qquad u \in C^2(M), \tag{2.5}$$

where ∇u means the gradient of u associated with g, i.e. the vector field which corresponds to du and is given in local coordinates as

$$\nabla u = g^{jk} \frac{\partial u}{\partial x^j} \frac{\partial}{\partial x^k}.$$

Let us identify the magnetic potential A with the multiplication operator

$$A : C^\infty(M) \longrightarrow \Lambda^1_{(1)}(M).$$

Then the formally adjoint operator A^* is a substitution operator of the vector field v_A into 1-forms, or in other words

$$A^*\omega = \langle A, \omega\rangle = g^{jk} A_j \omega_k. \tag{2.6}$$

This gives us a formula for d_A^*:

$$d_A^*\omega = (d^* - iA^*)\omega = -\operatorname{div} v_\omega - i\langle A, \omega\rangle. \tag{2.7}$$

It follows that

$$d_A^*(f\omega) = fd^*\omega - \langle df, \omega\rangle - if\langle A, \omega\rangle, \quad f \in C^1(M),\ \omega \in \Lambda^1_{(1)}(M). \tag{2.8}$$

The following Leibniz rules for d_A^* immediately follow:

$$\begin{aligned} d_A^*(f\omega) &= fd_A^*\omega - \langle df, \omega\rangle, \\ d_A^*(f\omega) &= fd^*\omega - \langle d_A f, \omega\rangle, \end{aligned}$$

where $f,\ \omega$ are as in (2.8).

Using these formulas, we can write an explicit expression for the magnetic Laplacian Δ_A. Namely,

$$\begin{aligned} -\Delta_A u &= d_A^* d_A u = (d^* - iA^*)(du + iAu) \\ &= d^*du - iA^*du + id^*(Au) + A^*Au \\ &= -\Delta u - i\langle A, du\rangle - i \operatorname{div}(uv_A) + \langle A, A\rangle u \\ &= -\Delta u - 2i\langle A, du\rangle + (id^*A + |A|^2)u. \end{aligned}$$

Hence we obtain the following expression for the magnetic Schrödinger operator (1.1):

$$H_{A,V}u = -\Delta u - 2i\langle A, du\rangle + (id^*A + |A|^2)u + Vu. \tag{2.9}$$

On the other hand using the expressions (2.3) and (2.6) for the divergence and the operator A^* we easily obtain that in local coordinates

$$H_{A,V}u = -\frac{1}{\rho}\left(\frac{\partial}{\partial x^j} + iA_j\right)\left[\rho g^{jk}\left(\frac{\partial}{\partial x^k} + iA_k\right)u\right] + Vu, \tag{2.10}$$

or in slightly different notations

$$H_{A,V}u = \frac{1}{\rho}(D_j + A_j)[\rho g^{jk}(D_k + A_k)u] + Vu, \tag{2.11}$$

where $D_j = -i\partial/\partial x_j$.

Remark. A similar operator in $\mathbb{R}^n$ (with $\rho = 1$) was considered by T. Ikebe and T. Kato [29], K. Jörgens [32], M.S.P. Eastham, W.D. Evans and J.B. McLeod [17], A. Devinatz [16] in the space $L^2(\mathbb{R}^n, dx)$ where dx is the standard Lebesgue measure on $\mathbb{R}^n$. The general operator of the form (2.10) on manifolds was studied by H.O.Cordes [13]. In this generality it includes some natural geometric situations (in particular the case $\rho = \sqrt{g}$).

3 Preliminaries on the Lipschitz analysis and the Stokes formula on a Riemannian manifold

Let (M, g) be a Riemannian manifold. A function $f : M \to \mathbb{R}$ is called *a Lipschitz function with a Lipschitz constant* C if

$$|f(x) - f(x')| \le C d_g(x, x'), \quad x, x' \in M. \tag{3.1}$$

It is well known that in this case f is differentiable almost everywhere and

$$|df| \le C \tag{3.2}$$

with the same constant C. Here $|df|$ means the length of the cotangent vector df in the metric associated with g. The corresponding differential df, as well as the partial derivatives of the first order, coincide with the distributional derivatives. Vice versa if $df \in L^\infty(M)$, for the distributional differential $df = (\partial f/\partial x^j)dx^j$, then f can be modified on a set of measure 0 so that it becomes a Lipschitz function.

The estimate (3.2) can be also rewritten in the form

$$|\nabla f| \le C \tag{3.3}$$

(again with the same constant C).

In local form (in open subsets of $\mathbb{R}^n$) these facts are discussed e.g. in the book of V. Mazya [43], Sect.1.1. The correspondence between constants in (3.1), (3.2) and (3.3) is straightforward.

The Lipschitz vector fields, differential forms etc. are defined in an obvious way

The formulas (2.1), (2.2), (2.3), (2.4), (2.7) apply to Lipschitz vector fields and forms instead of smooth ones.

We will also need local Sobolev spaces $W^{m,2}_{loc}$ on M for arbitrary integer m. We need this spaces for functions, vector fields and differential forms. For simplicity let us consider functions first. If $m \ge 0$ then the space $W^{m,2}_{loc}(M)$ consists of functions $u \in L^2_{loc}(M)$ such that their derivatives of the order $\le m$ in local coordinates also belong to L^2_{loc} in these coordinates. (The functions which coincide almost everywhere are identified.) Denote also by $W^{m,2}_{comp}(M)$ the space of functions which belong to $W^{m,2}_{loc}(M)$ and have a compact support.

If $m < 0$ then $W^{m,2}_{loc}(M)$ is a dual space to $W^{-m,2}_{comp}(M)$ and it consists of all distributions which can be locally represented as sums of derivatives of order $\le -m$ of functions from L^2_{loc}.

These definitions obviously extend to vector fields and differential forms.

We will need the Stokes formula, or rather the divergence formula for Lipschitz vector fields v on M in the following simplest form:

Proposition 3.1 *Let $v = v(x)$ be a vector field which is in $W^{1,2}_{comp}$ on M. Then*

$$\int_M \operatorname{div} v \, d\mu = 0.$$

The proof of the Proposition can be easily reduced to the case when v is supported in a domain of local coordinates. After that we can use mollification (regularization) of v to approximate v by smooth vector fields. A more advanced statement which does not require a compact support and includes a boundary integral, can be proved for Lipschitz vector fields ([43], Sect. 6.2).

Again using mollifiers we easily see that the formulas (2.1), (2.2), (2.3), (2.4), (2.7) apply to functions, vector fields and forms from $W^{1,2}_{loc}$ instead of smooth ones.

4 Proof of Theorem 1.1

In this section we will always write H instead of $H_{A,V}$ for simplicity of notations.

Let H_{min} and H_{max} be the minimal and maximal operators associated with the differential expression (1.1) for H in $L^2(M)$. Here H_{min} is the closure of H in $L^2(M)$ from the initial domain $C_c^\infty(M)$, $H_{max} = H^*_{min}$ (the adjoint operator to H_{min} in $L^2(M)$). Clearly

$$\operatorname{Dom}(H_{max}) = \{u \in L^2(M) |\; Hu \in L^2(M)\},$$

where Hu is understood in the sense of distributions.

It follows from the standard functional analysis arguments (see. e.g. [3], Appendix 1), that the essential self-adjointness of H is equivalent to the symmetry of H_{max} which means that

$$(H_{max}u, v) = (u, H_{max}v), \quad u, v \in \operatorname{Dom}(H_{max}). \tag{4.1}$$

To establish the symmetry of H_{max} we need some information about $\operatorname{Dom}(H_{max})$. We will start with a simple lemma establishing necessary local information.

Lemma 4.1 *Assume as before that $A \in \Lambda^1_{(1)}(M)$ and $V \in L^\infty_{loc}(M)$. Then $u \in \operatorname{Dom}(H_{max})$ implies that $u \in W^{2,2}_{loc}(M)$.*

Proof. We will repeat an argument given in [3], Appendix 2, proof of Theorem 2.1.

Assume that $u \in \mathrm{Dom}\,(H_{max})$. Due to (2.9) this means that $u \in L^2(M)$ and

$$-\Delta u - 2i\langle A, du\rangle + (id^*A + |A|^2)u + Vu = f \in L^2(M),$$

where Δu and $\langle A, du\rangle$ are understood in the sense of distributions, so a priori $\Delta u \in W^{-2,2}_{loc}(M)$, $\langle A, du\rangle \in W^{-1,2}_{loc}(M)$. Note also that $(id^*A + |A|^2)u + Vu \in L^2_{loc}(M)$. It follows from the local elliptic regularity theorem applied to $-\Delta$ that $u \in W^{1,2}_{loc}(M)$.

This already implies that $\langle A, du\rangle \in L^2_{loc}(M)$. Applying the local elliptic regularity theorem again we see that $u \in W^{2,2}_{loc}(M)$. □

Remark. Lemma 4.1 is certainly not new, though I had difficulty to find a statement which would exactly imply it. More general equations are considered e.g. by D. Gilbarg and N.S. Trudinger ([21], Theorem 8.10), but with a stronger a priori requirement $u \in W^{1,2}$.

The following key lemma provides necessary global information:

Lemma 4.2 *If $u \in \mathrm{Dom}\,(H_{max})$, then*

$$\int_M Q^{-1}|d_A u|^2 d\mu \le 2[(8C^2+1)\|u\|^2 + \|u\|\cdot\|Hu\|] < \infty. \tag{4.2}$$

Here $\|\cdot\|$ means the norm in $L^2(M)$, and C is the Lipschitz constant for $Q^{-1/2}$ from (1.7).

Proof. Let us choose a Lipschitz function $\phi : M \to \mathbb{R}$, such that ϕ has a compact support and

$$0 \le \phi \le Q^{-1/2}. \tag{4.3}$$

Note that this implies that $\phi \le 1$.

Let us estimate the quantity $I \ge 0$ where

$$I^2 = \int_M \phi^2 |d_A u|^2 d\mu.$$

To this end let us calculate first $d^*(\phi^2\bar{u} d_A u)$ using (2.2), (2.7) and the Leibniz rules from Sect.3:

$$\begin{aligned}
d^*(\phi^2\bar{u}\, d_A u) &= \phi^2\bar{u}\, d^* d_A u - \langle d(\phi^2\bar{u}), d_A u\rangle \\
&= \phi^2\bar{u}\, d^* d_A u - \phi^2\langle d\bar{u}, d_A u\rangle - 2\phi\bar{u}\langle d\phi, d_A u\rangle \\
&= \phi^2\bar{u}\, d_A^* d_A u + \phi^2\bar{u} i\, A^*(d_A u) - \phi^2\langle d\bar{u}, d_A u\rangle - 2\phi\bar{u}\langle d\phi, d_A u\rangle \\
&= \phi^2\bar{u}\, d_A^* d_A u - \phi^2\langle d\bar{u} - i\bar{u}A, d_A u\rangle - 2\phi\bar{u}\langle d\phi, d_A u\rangle \\
&= \phi^2\bar{u}\, d_A^* d_A u - \phi^2|d_A u|^2 - 2\phi\bar{u}\langle d\phi, d_A u\rangle.
\end{aligned}$$

It follows that

$$\phi^2|d_A u|^2 = -d^*(\phi^2\bar{u} d_A u) + \phi^2\bar{u}(d_A^* d_A u) - 2\phi\bar{u}\langle d\phi, d_A u\rangle. \tag{4.4}$$

Replacing $d_A^* d_A u$ by $(H-V)u$, we obtain

$$\begin{aligned}\phi^2|d_Au|^2 &= -d^*(\phi^2\bar{u}d_Au) - 2\phi\bar{u}\langle d\phi, d_Au\rangle + \phi^2\bar{u}\cdot Hu - \phi^2V|u|^2\\ &\le -d^*(\phi^2\bar{u}d_Au) - 2\phi\bar{u}\langle d\phi, d_Au\rangle + \phi^2\bar{u}\cdot Hu + \phi^2Q|u|^2.\end{aligned}$$

(Note that the right hand side of the last equality is real because the left hand side is.)

Let us integrate the inequality over M. Due to (2.2) and the Stokes formula (Proposition 3.1) the integral of the first term in the right hand side vanishes. Taking into account that $0 \le \phi \le 1$ and $\phi^2 Q \le 1$ due to (4.3), we can estimate the integral of the last two terms by $\|u\|(\|u\| + \|Hu\|)$. Now denote by $\tilde{C}$ the Lipschitz constant of ϕ, so that $|d\phi| \le \tilde{C}$. Then we obtain by the Cauchy-Schwarz inequality

$$\begin{aligned}&2\left|\int_M \phi\bar{u}\langle d\phi, d_Au\rangle d\mu\right| =\\ &2\left|\int_M \langle \bar{u}d\phi, \phi d_Au\rangle d\mu\right| \le 2\tilde{C}I\|u\|.\end{aligned}$$

Overall we obtain the inequality

$$I^2 \le 2\tilde{C}I\|u\| + \|u\|(\|u\| + \|Hu\|).$$

Estimating

$$2\tilde{C}I\|u\| \le \frac{1}{2}I^2 + 8\tilde{C}^2\|u\|^2,$$

we arrive at the estimate

$$I^2 \le 2[(8\tilde{C}^2+1)\|u\|^2 + \|u\|\cdot\|Hu\|]. \tag{4.5}$$

Now it is easy to construct a sequence of Lipschitz functions ϕ_k, $k = 1, 2, \dots$, such that ϕ_k satisfies

$$0 \le \phi_k \le Q^{-1/2}, \quad |d\phi_k| \le C + 1/k,$$

(4.3) for any k, $\phi_1 \le \phi_2 \le \dots$, and

$$\lim_{k\to\infty} \phi_k(x) = Q^{-1/2}(x), \quad x \in M.$$

Indeed, take a function $\chi : \mathbb{R} \to \mathbb{R}$, such that $\chi \in C^\infty(\mathbb{R})$, $0 \le \chi \le 1$, $\chi(t) = 1$ if $t \le 1$, $\chi(t) = 0$ if $t \ge 3$, and $|\chi'| \le 1$. Then we can take

$$\phi_k(x) = \chi(k^{-1}d_g(x, x_0))Q^{-1/2}(x),$$

where $x_0 \in M$ is an arbitrary fixed point. The estimate (4.5) holds for ϕ_k with $\tilde{C} = C + 1/k$. Taking the limit as $k \to \infty$, we obtain (4.2). $\square$

Proof of Theorem 1.1. We want to prove that the operator H_{max} is symmetric.

Let us introduce a new metric $\tilde{g}_{ij} = Q^{-1}g_{ij}$ and denote the corresponding distance function by $\tilde{d}$. This means that for any $x, y \in M$

$$\tilde{d}(x,y) = \inf \left\{ \int_\gamma Q^{-1/2} ds |\ \gamma : [0,1] \to M,\ \gamma(0) = x, \gamma(1) = y \right\},$$

where $\gamma \in C^\infty$ and ds means the element of the arc length of γ associated with g. Denote also

$$P(x) = \tilde{d}(x, x_0),$$

where $x_0 \in M$ is fixed. The completeness condition (b) means exactly that

$$P(x) \to \infty \text{ as } x \to \infty,$$

or, equivalently, that the set $\{x|\ P(x) \le t\} \subset M$ is compact for any $t \in \mathbb{R}$.

Clearly, $|dP|_{\tilde{g}} \le 1$, which can be rewritten as

$$|dP|^2 \le Q^{-1}.$$

(Here, as above, $|dP|$ means the length of the cotangent vector dP with respect to the original metric g.)

Now for two functions $u, v \in \operatorname{Dom}(H_{max})$ consider the following integral:

$$I_t = \int_{\{x|\ P(x) \le t\}} \left(1 - \frac{P(x)}{t}\right) (u \cdot \overline{Hv} - \bar{v} \cdot Hu) d\mu.$$

By the dominated convergence theorem we obviously have

$$I_t \to \int_M (u \cdot \overline{Hv} - \bar{v} \cdot Hu) d\mu = (u, Hv) - (Hu, v) \quad \text{as } t \to \infty. \tag{4.6}$$

(Here $(\cdot,\cdot)$ means the scalar product in $L^2(M)$.) Hence the desired symmetry of H_{max} is equivalent to the fact that $I_t \to 0$ as $t \to \infty$ for any $u, v \in \operatorname{Dom}(H_{max})$.

Now note that

$$u \cdot \overline{Hv} - \bar{v} \cdot Hu = \bar{v} \cdot \Delta_A u - u \cdot \overline{\Delta_A v} = u \cdot \overline{d_A^* d_A v} - \bar{v} \cdot d_A^* d_A u. \tag{4.7}$$

Here both terms are locally integrable due to Lemma 4.1.

We claim that the right hand side of (4.7) can be presented as a divergence in the following way:

$$u \cdot \overline{d_A^* d_A v} - \bar{v} \cdot d_A^* d_A u = d^*(u \cdot \overline{d_A v} - \bar{v} \cdot d_A u). \tag{4.8}$$

Indeed, calculating the right hand side by use of the Leibniz rule (2.4) for d^* and formulas for $d_A,\ d_A^*$ from Sect.3, we obtain:

$$\begin{aligned}
& d^*(u \cdot \overline{d_A v} - \bar{v} \cdot d_A u) \\
= \ & (u \cdot \overline{d^* d_A v} - \bar{v} \cdot d^* d_A u) - (\langle du, \overline{d_A v} \rangle - \langle d\bar{v}, d_A u \rangle) \\
= \ & (u \cdot \overline{d^* d_A v} - \bar{v} \cdot d^* d_A u) - (\langle du, \overline{iAv} \rangle - \langle d\bar{v}, iAu \rangle) \\
= \ & (u \cdot \overline{d^* d_A v} - \bar{v} \cdot d^* d_A u) - (\langle d_A u, \overline{iAv} \rangle - \langle \overline{d_A v}, iAu \rangle) \\
= \ & (u \cdot \overline{(d^* d_A v - i\langle A, d_A v \rangle)} - \bar{v} \cdot (d^* d_A u - i\langle A, d_A u \rangle)) \\
= \ & u \cdot \overline{d_A^* d_A v} - \bar{v} \cdot d_A^* d_A u,
\end{aligned}$$

as claimed.

Using (4.8) and the Leibniz rules, we can rewrite the integrand of I_t as

$$\begin{aligned} & \left(1-\frac{P(x)}{t}\right)(u\cdot\overline{Hv}-\bar{v}\cdot Hu) \\ = & \left(1-\frac{P(x)}{t}\right)d^*(u\cdot\overline{d_A v}-\bar{v}\cdot d_A u) \\ = & \ d^*\left[\left(1-\frac{P(x)}{t}\right)(u\cdot\overline{d_A v}-\bar{v}\cdot d_A u)\right]+\frac{1}{t}\left(u\langle dP,\overline{d_A v}\rangle-\bar{v}\langle d_A u, dP\rangle\right). \end{aligned}$$

The integral of the first term in the right hand side (with respect to $d\mu$) vanishes due to Proposition 3.1. Therefore using the Cauchy-Schwarz inequality we obtain

$$\begin{aligned} |I_t| &= \left|\frac{1}{t}\int_{\{x|\ P(x)\le t\}}\left(u\langle dP,\overline{d_A v}\rangle-\bar{v}\langle d_A u, dP\rangle\right)d\mu\right| \\ &= \left|\frac{1}{t}\int_{\{x|\ P(x)\le t\}}\left(u\langle Q^{1/2}dP, Q^{-1/2}\overline{d_A v}\rangle-\bar{v}\langle Q^{-1/2}d_A u, Q^{1/2}dP\rangle\right)d\mu\right| \\ &\le \frac{1}{t}(\|v\|\|Q^{-1/2}d_A u\|+\|u\|\|Q^{-1/2}d_A v\|). \end{aligned}$$

By Lemma 4.2 the right hand side is $O(1/t)$, so $I_t \to 0$ as $t \to \infty$. Due to (4.6) this proves that H_{max} is symmetric i.e. (4.1) holds. This ends the proof of Theorem 1.1. □

5 Semi-bounded operators

The goal of this section is to extend the Povzner theorem on essential self-adjointness of an arbitrary semi-bounded Schrödinger operator (see [49], [23]) to the case of magnetic Schrödinger operators on manifolds. For operators in $\mathbb{R}^n$ and in its open subsets this was done in increasing generality by E. Wienholtz [73], H. Stetkær-Hansen [67] and J. Walter [72]. We will use the method of Wienholtz (explaned also in [23]) when we treat the case of locally bounded potentials V and the method of C. Simader [**?**] for more singular V.

We will start by imposing an additional condition on the manifold (M, g). Denote by $C^1_{comp}(M)$ the set of all C^1 functions with compact support on M.

Definition. Let (M, g) be a Riemannian manifold. We will say that it satisfies *the condition* (B) if (M, g) is complete and there exists a sequence of functions $\phi_N : M \to \mathbb{R}$, $N = 1, 2, \ldots$, with the following properties:

(a) $\phi_N \in C^1_{comp}(M)$ and $\nabla\phi_N \in \mathrm{Lip}\,(M)$, $N = 1, 2, \ldots$;

(b) $0 \le \phi_N(x) \le 1$, $x \in M$, $N = 1, 2, \ldots$;

(c) for every compact $K \subset M$ there exists $N_0 > 0$ such that $\phi_N = 1$ on K

if $N \geq N_0$;

(*d*) $\varepsilon_N := \sup_{x\in M} |\nabla\phi_N(x)| \to 0 \quad as \quad N \to \infty.$

Note that for any complete Riemannian manifold (M, g) it is very easy to construct a sequence of functions $\phi_N \in \mathrm{Lip}\,(M)$, $N = 1, 2, \ldots$, satisfying the conditions (b), (c), (d) above. For example, we can take

$$\phi_N(x) = \chi(N^{-1}\mathrm{dist}(x, x_0)),$$

where $\chi \in C_c^\infty(\mathbb{R})$, $\chi(t) = 1$ if $|t| \leq 1$, and $0 \leq \chi(t) \leq 1$ for all $t \in \mathbb{R}$. However it is not clear how to construct such functions with $\nabla\phi_N \in \mathrm{Lip}\,(M)$ as required in (a). But there are many manifolds where this is easily possible, e.g. the construction above works for $\mathbb{R}^n$, the hyperbolic space, and generally for any manifold with an empty cut-locus, so that the function $x \mapsto \mathrm{dist}(x, x_0)$ is in $C^\infty(M)$ (or even only in $C^2(M)$).

More generally, in the construction above we can replace the distance function $d(x) = \mathrm{dist}(x, x_0)$ by a *regularized distance*: a function $\tilde{d} : M \to \mathbb{R}$ such that $\tilde{d} \geq 0$, $\tilde{d} \in C^1(M)$, $\nabla\tilde{d} \in \mathrm{Lip}_{loc}\,((M))$ and

$$C^{-1}d(x) - C_1 \leq \tilde{d}(x) \leq Cd(x) + C_1$$

with some positive constants C, C_1. Such a function $\tilde{d} \in C^\infty(M)$ can be easily constructed on any manifold of bounded geometry (see e.g. the construction given in [58]). Subtler arguments by J. Cheeger and M. Gromov [10] (which are based on a result of U. Abresch [1] about smoothing of Riemannian metrics, I. Yomdin's theorem which is a quantitative refinement of the Sard Lemma - see [24] , pp. 123–124, and some arguments from [9]), allow to construct such regularized distance on any complete Riemannian manifold with a bounded sectional curvature (without any restrictions on the injectivity radius, which are part of the usual definition of bounded geometry).

Hence, any complete Riemannian manifold with bounded sectional curvature also satisfies the condition (B).

5.1 Locally bounded potentials

For simplicity of exposition we treat the case of locally bounded potentials first, even though a more general result will be established later in this section.

Theorem 5.1 *Let us assume that the manifold (M, g) satisfies the condition (B) above, $A \in \mathrm{Lip}_{loc}(M)$, $V \in L^\infty_{loc}(M)$ and the corresponding magnetic Schrödinger operator $H_{A,V}$ is semi-bounded below on $C_c^\infty(M)$ i.e. there exists a constant $C \in \mathbb{R}$ such that*

$$(H_{A,V}u, u) \geq -C(u, u), \quad u \in C_c^\infty(M). \tag{5.1}$$

Then $H_{A,V}$ is essentially self-adjoint.

Remark. It is also convenient to use the quadratic form

$$h_{A,V}(u,u) = \|d_A u\|^2 + (Vu,u) = \int_M \left(|d_A u|^2 + V|u|^2\right) d\mu. \tag{5.2}$$

Clearly

$$(H_{A,V}u,u) = h_{A,V}(u,u), \quad u \in C_c^\infty(M). \tag{5.3}$$

Proof of Theorem 5.1. We will extend the Wienholtz proof [73] of the Povzner theorem (see also I.M. Glazman [23]).

Note that the smoothness requirements on A, V imply that the operator $H_{A,V}$ is well defined on $C_c^\infty(M)$ and maps this space into $L^2(M)$ (see Sect.3), as well as on $L^2(M)$ (which it maps to the space of distributions on M).

Adding $(C+1)I$ to $H_{A,V}$ we can assume that $H_{A,V} \geq I$ on $C_c^\infty(M)$ i.e.

$$(H_{A,V}u,u) \geq (u,u), \quad u \in C_c^\infty(M), \tag{5.4}$$

or, equivalently,

$$h_{A,V}(u,u) \geq (u,u), \quad u \in C_c^\infty(M). \tag{5.5}$$

If this is true, then it is well known (see e.g. [23]) that the essential self-adjointness of $H_{A,V}$ is equivalent to the fact that the equation

$$H_{A,V}u = 0 \tag{5.6}$$

has no non-trivial solutions in $L^2(M)$ (understood in the sense of distributions).

Assume that u is such a solution. First note that it is in $W^{2,2}_{loc}(M)$ due to Lemma 4.1.

Let us take a cut-off function ϕ_N on M from the definition of the property (B) above.

Then denoting $u_N = \phi_N u$ we see that u_N is in the domain of the minimal operator associated with $H_{A,V}$, hence

$$\|u_N\|^2 \leq (H_{A,V}u_N, u_N). \tag{5.7}$$

Now we will prove an identity which will be useful not only in this proof but in extending the result to singular potentials.

Let us calculate $H_{A,V}(\phi u)$ for arbitrary functions u, ϕ such that $u \in W^{2,2}_{loc}(M)$ and $\phi \in C^1(M)$ has a locally Lipschitz gradient. We will use the Leibniz type formulas from Sect.2. Applying d_A^* to

$$d_A(\phi u) = \phi d_A u + u d\phi,$$

we obtain

$$d_A^* d_A(\phi u) = \phi d_A^* d_A u - 2\langle d\phi, d_A u\rangle + u d^* d\phi,$$

hence

$$H_{A,V}(\phi u) = \phi H_{A,V}u - 2\langle d\phi, d_A u\rangle - u\Delta\phi. \tag{5.8}$$

Now let us additionally assume that ϕ is real-valued and has a compact support. Then multiplying (5.8) by $\phi\bar{u}$ and integrating over M (with respect to the chosen measure $d\mu$ with a positive smooth density) we get

$$(H_{A,V}(\phi u), \phi u) = (\phi H_{A,V}u, \phi u) - 2\int_M [\langle d\phi, du\rangle + 2i\langle A, d\phi\rangle u + u\Delta\phi]\phi\bar{u}d\mu.$$

Adding this formula with the complex conjugate one and dividing by 2, we see that the term with A under the integral sign cancels, so we get:

$$\begin{aligned}(H_{A,V}(\phi u), \phi u) &= \mathrm{Re}\,(\phi H_{A,V}u, \phi u) - \int_M [\langle \phi d\phi, \bar{u}du + ud\bar{u}\rangle + |u|^2\phi\Delta\phi]d\mu \\ &= \mathrm{Re}\,(\phi H_{A,V}u, \phi u) - \int_M [\langle \phi d\phi, d(|u|^2)\rangle + |u|^2\phi\Delta\phi]d\mu \\ &= \mathrm{Re}\,(\phi H_{A,V}u, \phi u) - \int_M \left(|u|^2 d^*(\phi d\phi) + |u|^2\phi\Delta\phi\right) d\mu.\end{aligned}$$

Since

$$d^*(\phi d\phi) = \phi d^* d\phi - \langle d\phi, d\phi\rangle = -\langle d\phi, d\phi\rangle - \phi\Delta\phi,$$

we finally obtain the desired identity

$$(H_{A,V}(\phi u), \phi u) = \mathrm{Re}\,(\phi H_{A,V}u, \phi u) + \int_M |d\phi|^2|u|^2 d\mu. \tag{5.9}$$

To use this identity in our proof assume that $H_{A,V}u = 0$. This implies

$$(H_{A,V}(\phi u), \phi u) = \int_M |d\phi|^2|u|^2 d\mu.$$

Now taking $\phi = \phi_N$ and applying the estimate (5.7), we obtain

$$\|\phi_N u\|^2 \le \int_M |\nabla\phi_N|^2|u|^2 d\mu.$$

In particular, for any compact $K \subset M$ we obtain for $N \ge N_0(K)$:

$$\int_K |u|^2 d\mu \le \int_M |\nabla\phi_N|^2|u|^2 d\mu \le \varepsilon_N \int_M |u|^2 d\mu.$$

If now $u \in L^2(M, d\mu)$, then taking limit as $N \to \infty$, we see that $u = 0$ on K, hence $u \equiv 0$. $\square$

5.2 Singular potentials

Now we will consider the magnetic Schrödinger operators $H_{A,V}$ on Riemannian manifodls (M,g) satisfying the condition (B) formulated at the beginning of Sect. 5. We will still assume that $A \in \mathrm{Lip}_{loc}(M)$ but we will not require that V is locally bounded. Instead we will assume the following:

(H) $V = V_+ + V_-$ where $V_+ \geq 0$, $V_- \leq 0$, $V_+ \in L^2_{loc}(M)$ and $V_- \in L^p_{loc}(M)$ with $p = n/2$ if $n \geq 5$, $p > 2$ if $n = 4$, and $p = 2$ if $n \leq 3$.

Theorem 5.2 *Let the manifold (M,g) satisfy the condition (B), $A \in \mathrm{Lip}_{loc}(M)$, V satisfies the condition (H) above, and the corresponding magnetic Schrödinger operator $H_{A,V}$ is semi-bounded below on $C_c^\infty(M)$. Then $H_{A,V}$ is essentially self-adjoint.*

Proof. 1. Let us choose a relatively compact coordinate neighborhood U in M with coordinates $x^1, \dots, x^n$ which are defined in a neighborhood of $\bar{U}$. Let Δ_0 denote the flat Laplacian in these coordinates. Then due to the standard elliptic estimates the operators $H_{A,0}$ and Δ_0 have equal strength on functions supported in U, i.e. there exists $C > 0$ such that

$$C^{-1}\|\Delta_0 u\| \leq \|H_{A,0}u\| \leq C\|\Delta_0 u\|, \quad u \in C_c^\infty(U). \tag{5.10}$$

Now assume that supp $V_- \subset U$. Then it follows from (H) that V_- has Δ_0-bound $\varepsilon > 0$ for arbitrarily small ε, i.e.

$$\|V_- u\| \leq \varepsilon\|\Delta_0 u\| + C_\varepsilon\|u\|, \quad u \in C^\infty(U). \tag{5.11}$$

Using (5.10) we see that (5.11) is equivalent to a similar estimate with Δ_0 replaced by $H_{A,0}$. We can also remove the requirement supp $V_- \subset U$:

$$\|V_- u\| \leq \varepsilon\|H_{A,0}u\| + C_\varepsilon\|u\|, \quad u \in C^\infty(M); \tag{5.12}$$

this holds whenever $V_- \in L^p_{comp}(M)$ with p as in (H) (with C_ε depending on V_-). To see this, it is enough to split V_- into a sum of non-positive potentials supported in coordinate neighborhoods,

Define $V_-^{(N)}(x) = V_-(x)$ on supp ϕ_N, and $V_-^{(N)}(x) = 0$ otherwise. Then (5.12) holds for $V_-^{(N)}$. It follows from Theorem 1.1 and from the Kato-Rellich perturbation theorem (Theorem X.12 in [51]) that the operator $H_{A,-V_-^{(N)}} = H_{A,0} + V_-^{(N)}$ is essentially self-adjoint.

Now we can use the Kato inequality technique from [36] (see also generalization to operators on manifolds and in sections of vector bundles developed by H. Hess, R. Schrader and D.A. Uhlenbrock [27, 28]), or the perturbation arguments from the proofs of Theorems X.28, X.29 from [51] to prove that the operator $H_N = H_{A,V_+ + V_-^{(N)}} = H_{A,0} + V_+ + V_-^{(N)}$ is essentially self-adjoint for any $N = 1, 2, \dots$.

2. In what follows we will write H instead of $H_{A,V}$. Note that for any fixed $u \in \operatorname{Dom}(H_{max})$

$$|(u, H(\phi_N f))| = |(Hu, \phi_N f)| \le C\|f\|, \quad f \in C_c^\infty(M). \tag{5.13}$$

Similarly to (5.8) we have

$$H(\phi_N f) = \phi_N Hf - 2\langle d\phi_N, d_A f\rangle - f\Delta\phi_N,$$

hence

$$(\phi_N u, Hf) = 2(u, \langle d\phi_N, d_A f\rangle) + (u, f\Delta\phi_N) + (u, H(\phi_N f)),$$

and using (5.13) we conclude that

$$|(\phi_N u, Hf)| \le C\left(\|df\| + \|f\|\right), \quad f \in C_c^\infty(M),$$

with the constant C depending on H and ϕ_N (but not on f). Since the left hand side depends only on the restriction of u to a neigborhood of supp ϕ_N, we can also write

$$|(\phi_N u, H_N f)| \le C\left(\|df\| + \|f\|\right), \quad f \in C_c^\infty(M). \tag{5.14}$$

3. Our next goal is to establish that $\operatorname{Dom}(H_{max}) \subset W^{1,2}_{loc}(M)$. It is enough to prove that (5.14) implies that $\phi_N u \in W^{1,2}_{loc}(M)$. We will repeat the arguments from [62]. Denote $v = \phi_N u$, so $v \in L^2(M)$.

By the standard domination argument we have

$$|(V_-^{(N)} f, f)| \le a\|df\|^2 + C\|f\|^2, \quad f \in C_c^\infty(M), \tag{5.15}$$

with an arbitrarily small $a > 0$ and C depending on a or, equivalently,

$$|(V_-^{(N)} f, f)| \le a\|d_A f\|^2 + C'\|f\|^2, \quad f \in C_c^\infty(M). \tag{5.16}$$

Choosing an arbitrary $\lambda > 0$, we obtain

$$\begin{aligned}((H_N + \lambda)f, f) &= \|d_A f\|^2 + (V_+ f, f) + (V_-^{(N)} f, f) + \lambda\|f\|^2 \\ &\ge (1-a)\|d_A f\|^2 + (\lambda - C')\|f\|^2 \\ &\ge (1-a)\|df\|^2 + (\lambda - C'')\|f\|^2.\end{aligned}$$

Now let us choose here $\lambda > C''$. Taking closure, we see that the estimate (5.16) holds for all f in the domain of the closure of H_N understood as the operator with the domain $C_c^\infty(M)$. It is a standard fact that this closure coincides with $H_N^{**} = (H_N^*)^*$. However since H_N is essentially self-adjoint, we have $H_N^{**} = H_N^*$ and the domain $D_N = \operatorname{Dom}(H_N^{**})$ coincides with the domain of the corresponding maximal operator H_N^*, i.e. with the set of all $f \in L^2(M)$ such that $H_N f \in L^2(M)$ where $H_N f$ is understood in the sense of distributions. In particular, (5.17) holds for all $f \in D_N$.

Clearly, H_N is semibounded below. Therefore for sufficiently large $\lambda > 0$ the operator $H_N^* : D_N \to L^2(M)$ is bijective. Hence for any $\phi \in C_c^\infty(M)$ supported in the domain of some local cordinates $x^1, \dots, x^n$, and for any $j \in \{1, \dots, n\}$ we can find $f_j \in D_N$ such that $(H_N + \lambda)f_j = \partial_j^* \phi$ where $\partial_j = \partial/\partial x^j$ and ∂_j^* means the formally adjoint operator with respect to the inner product induced by the Riemannian measure in the choosen coordinate neighborhood. It follows that for any $\varepsilon > 0$

$$(5.17) \qquad |((H_N + \lambda)f_j, f_j)| = |(\partial_j^* \phi, f_j)| = |(\phi, \partial_j f_j)| \le \frac{\varepsilon}{2}\|\partial_j f_j\|^2 + \frac{1}{2\varepsilon}\|\phi\|^2.$$

Combining (5.17) and (5.17) we obtain

$$(5.18) \qquad \|df_j\| + \|f_j\| \le C'\|\phi\|,$$

with C' independent of ϕ. Now taking $f = f_j$ in (5.14) we obtain

$$(5.19) \qquad |(v, \partial_j^* \phi)| \le C''\|\phi\|.$$

This implies that $\partial_j v \in W^{1,2}_{loc}$ in the coordinate neighborhood. Choosing a covering of M by such coordinate neighborhoods we see that $v = \phi_N u \in W^{1,2}_{loc}(M)$. Since N was arbitrary, we see that $u \in W^{1,2}_{loc}(M)$.

4. Let us start with the identity (5.9) which was established in the case of a locally bounded V for all $u \in W^{2,2}_{loc}(M)$ and real-valued compactly supported ϕ with a Lipschitz gradient. Let us try to relax the requirement on u first, still assuming that $V \in L^\infty_{loc}(M)$. We claim that (5.9) makes sense and holds for any $u \in W^{1,2}_{loc}(M)$. Indeed, both sides of (5.9) make perfect sense for any such u if we understand the inner products as dualities between $W^{-1,2}_{loc}(M)$ and $W^{1,2}_{comp}(M)$. To prove this identity for an arbitrary $u \in W^{1,2}_{loc}(M)$ we just need to approximate u by functions from $C_c^\infty(M)$ in the $W^{1,2}$-norm in a neighborhood of supp ϕ.

This argument works also if instead of the local boundedness of V we assume that $V \in L^p_{loc}(M)$ where p is the same as in the condition (H). Indeed, the Sobolev inequality gives a continous imbedding of $W^{1,2}_{loc}(M)$ into $L^q_{loc}(M)$ where $q \le 2n/(n-2)$ if $n \ge 3$ and $q < \infty$ if $n = 2$. For any $u \in W^{1,2}_{loc}(M)$ we have then $|u|^2 \in L^{q/2}_{loc}(M)$ and the last space is in a continuos dualily with $L^p_{comp}(M)$ (by the usual integration) due to the Hölder inequality. Therefore in this case we can again prove the identity (5.9) for any $u \in W^{1,2}_{loc}(M)$ taking approximations by functions from $C_c^\infty(M)$.

So it remains to remove requirement $V_+ \in L^p_{loc}(M)$ for $n \ge 4$ replacing it by the inclusion $V_+ \in L^2_{loc}(M)$. This can be done as follows. Let us fix functions $u \in W^{1,2}_{loc}(M)$ and $\phi \in C^1_{comp}(M)$ with a locally Lipschitz gradient. Then regularize V_+, replacing it by $V_+^{(k)}(x) = V_+(x)$ if $V_+(x) \le k$, and $V_+^{(k)}(x) = k$ if $V_+(x) > k$; here $k = 1, 2, \dots$. Then the identity (5.9) holds with $V^{(k)} = V_+^{(k)} + V_-$ instead of V because $V^{(k)} \in L^p_{loc}(M)$. But now we can take limit as

$k \to \infty$. The only terms depending on k in (5.9) will be two identical terms

$$\int_M V_+^{(k)} |\phi u|^2 d\mu$$

in the left and right hand sides. This integral obviously has a limit (possibly $+\infty$) because the integrand converges monotonically. By the Beppo Levi theorem this limit equals

$$\int_M V_+ |\phi u|^2 d\mu, \tag{5.20}$$

so taking $k \to \infty$ we see that (5.9) holds for V.

If we ony require that $u \in W^{1,2}_{loc}(M)$, then both sides of (5.9) can possibly be $+\infty$. If we know however that $u \in \mathrm{Dom}\,(H_{max})$ then the right han side is finite (which in fact just means the finitenes of the integral (5.20)). Then the left hand side in finite too.

5. Using the identity (5.9) wich is now established for all $u \in \mathrm{Dom}\,(H_{max})$, we can finish the proof of Theorem 5.2 by repeating the arguments of the proof of Theorem 5.1 which follow after this identity. $\square$

Remark. The requirement on p in the condition (H) is almost optimal. Indeed, we must require that $V \in L^2_{loc}(M)$ if we wish $H_{A,V}$ to be defined on $C_c^\infty(M)$. This is the only requirement which imposed for $n \leq 3$; the requirement $p > 2$ in case $n = 4$ is only slightly worse. As to the requirement $p = n/2$ in case $n \geq 5$, it can not be replaced by $p = n/2 - \varepsilon$ with $\varepsilon > 0$. This was shown by B. Simon even in $\mathbb{R}^n$ and without magnetic field (see [65] or [51], Example 4 in Ch.X.2): the operator $-\Delta - \alpha/|x|^2$ on $C_c^\infty(\mathbb{R}^n)$ with a real parameter α is bounded from below if an only if $\alpha \leq (n-1)(n-3)/4 + 1/4$ and essentially self-adjoint if and only if $\alpha \leq (n-1)(n-3)/4 - 3/4$. However the requirement $V_- \in L^p_{loc}(M)$ can be replaced by weaker requirements formulated in less explicite terms, e.g. Stummel classes and domination requirements (see e.g. [62]).

6 Examples and further comments

In this section we will provide several examples, further results and relevant bibliographical comments (by necessity incomplete).

1. Let us comment about the *gauge invariance* for the magnetic Schrödinger operators. It is easy to see that if we replace A by $A' = A + d\phi$ with a real-valued $\phi \in C^1(M)$, such that $\nabla\phi \in \mathrm{Lip}_{loc}\,(M)$, then we have

$$H_{A',V} = e^{-i\phi} H_{A,\phi} e^{i\phi}, \tag{6.1}$$

both for minimal and maximal operators defined by the expression $H_{A,V}$. Therefore it is clear that being essentially self-adjoint is a gauge invariant property, i.e. it does not change under any gauge transformation $A \mapsto A + d\phi$. This well known observation was extended by H. Leinfelder [39] to a very general class of operators and gauge transformations with minimal regularity conditions. He considers the case $M = \mathbb{R}^n$ (with the standard metric) but his arguments are easily extended to the case of arbitrary Riemannian manifolds, so we will formulate the result for the general case. Let us consider a class $\mathcal{L}_2(M)$ which consists of operators $H_{A,V}$ on a Riemannian manifold (M, g) with $A \in L^4_{loc}(M)$, $d^*A \in L^2_{loc}$ and $V \in L^2_{loc}(M)$. Assume further that we have two operators $H_{A,V}, H_{A',V} \in \mathcal{L}_2(M)$ and $A' = A + d\phi$ where ϕ is a distribution on M. Then the essential self-adjointness properties for A and A' are equivalent.

If M has vanishing cohomology $H^1(M, \mathbb{R})$ (e.g. if M is simply-connected) then the gauge invariance above means that the essential self-adjointness depends in fact on the magnetic field $B = dA$ (which is a 2-form or a de Rham current of degree 2) and not on the magnetic potential A itself.

2. Let us give some particular cases of Theorem 1.1.

Theorem 6.1 *Let (M, g) be a complete Riemannian manifold. Then the magnetic Laplacian $\Delta_A = -d_A^* d_A$ is essentially self-adjoint in $L^2(M, d\mu)$ for any magnetic potential $A \in \Lambda^1_{(1)}(M)$ and any positive smooth measure $d\mu$.*

Proof. Take $Q(x) \equiv 1$ and use Theorem 1.1. □

Theorem 6.1 generalizes the classical theorem by M. Gaffney [20] which corresponds to the case when $A = 0$ and $d\mu = d\mu_g$.

Note however that in fact the proof of Theorem 1.1 uses some elements of the Gaffney's proof.

N.N. Ural'ceva [71] and S.A. Laptev [38] provided examples of elliptic operators in $L^2(\mathbb{R}^n, dx)$ of the form

$$\frac{\partial}{\partial x^j}\left(g^{jk}(x)\frac{\partial}{\partial x^k}\right)$$

(with smooth positive definite matrices (g^{jk})) which are not essentially self-adjoint due to the fact that the coefficients g^{jk} are "rapidly growing". In these examples the inverse matrix (g_{jk}) is vice versa "rapidly decaying", which implies that $\mathbb{R}^n$ with the metric (g_{jk}) is not complete.

Theorem 6.2 *Let (M, g) be a complete Riemannian manifold with a positive smooth measure $d\mu$, $A \in \Lambda^1_{(1)}(M)$, $V \in L^\infty_{loc}(M)$, and $V(x) \geq -C$, $x \in M$, with a constant C. Then the magnetic Schrödinger operator $H = -\Delta_A + V(x)$ is essentially self-adjoint.*

In case when $M = \mathbb{R}^n$ (with the standard metric and measure) and $A = 0$ this result was established independently by T. Carleman [8] and K. Friedrichs [19], and the Carleman proof is reproduced in the book of I.M. Glazman [23], Theorem 34 in Sect.3. In this case the requirement $V \in L^\infty_{loc}$ can be completely removed, i.e. replaced by $V \in L^2_{loc}(\mathbb{R}^n)$, as was shown by T. Kato [36] (see also [51], Sect. X.4). This can be done with the help of the Kato inequality

$$\Delta|u| \geq \mathrm{Re}[(\mathrm{sgn}\, u)\Delta u],$$

for any $u \in L^1_{loc}$ such that $\Delta u \in L^1_{loc}$. Here $\mathrm{sgn}\, u(x) = \overline{u(x)}/|u(x)|$ if $u(x) \neq 0$ and 0 if $u(x) = 0$. Some non-positive perturbations can be allowed as well. For example, it is sufficient to require that $V = V_1 + V_2$ where $V_1 \in L^2_{loc}$, $V_1 \geq 0$, and V_2 is bounded with respect to $-\Delta$ with the $-\Delta$-bound $a < 1$. In particular, it is sufficient to assume that

$$V_+ = \max(V, 0) \in L^2_{loc}, \quad V_- = \min(V, 0) \in L^p + L^\infty,$$

where $p = 2$ if $n \leq 3$; $p > 2$ if $n = 4$, and $p = n/2$ if $n \geq 5$. The work by T. Kato was partially motivated by the paper of B. Simon [65] who proved the essential self-adjointness under an additional restriction compared with [36]. The reader may consult Chapters X.4, X.5 in M. Reed and B. Simon [51] for more references, motivations and a review.

It is actually sufficient to require only that the operator H_{min} is semi-bounded below, as was suggested by I.M. Glazman and proved by A.Ya. Povzner [49]. Another proof was suggested by E. Wienholtz [73] and also reproduced in [23].

Though the completeness requirement looks natural in case of semi-bounded operators, sometimes it can be relaxed and incompletness may be compensated by a specific behavior of the potential (see e.g. A.G. Brusentsev [6] and also the references there).

The following theorem in case $M = \mathbb{R}^n$ with the standard metric and measure and with $A = 0$ is due to D.B. Sears (see e.g. [57, 69, 3]), who followed an idea of an earlier paper by E.C. Titchmarsh.

Theorem 6.3 *Let us fix $x_0 \in M$ and denote $r = r(x) = d_g(x, x_0)$. Assume that $A \in \Lambda^1_{(1)}(M)$ and $V(x) \geq -Q(r)$ where $Q(r) \geq 1$ for all $r \geq 0$,*

$$\int_0^\infty \frac{dr}{\sqrt{Q(r)}} = \infty, \tag{6.2}$$

and one of the following two conditions is satisfied:

(a) $Q^{-1/2}$ is globally Lipschitz, i.e.

$$|Q^{-1/2}(r) - Q^{-1/2}(r')| \leq C|r - r'|, \quad r, r' \in [0, \infty); \tag{6.3}$$

(b) Q is monotone increasing.

Then the operator (1.1) is essentially self-adjoint.

Proof. Under condition (a) this theorem clearly follows from Theorem 1.1.

Now assume that (b) is satisfied. Then we can follow F.S. Rofe-Beketov [52] to reduce this to the case when in fact (a) is satisfied. It is enough to construct a new function $\tilde{Q}$, such that $\tilde{Q}(r) \geq Q(r)$ for all $r \geq 0$ and $\tilde{Q}$ satisfies both (6.2) and (a). To this end we can define $\tilde{Q}(n) = Q(n+1)$, $n = 0, 1, 2, \ldots$, and then extend $\tilde{Q}^{-1/2}$ to the semi-axis $[0, \infty)$ by linear interpolation, i.e. take

$$\tilde{Q}^{-1/2}(\alpha n + (1-\alpha)(n+1)) = \alpha \tilde{Q}^{-1/2}(n) + (1-\alpha)\tilde{Q}^{-1/2}(n+1),$$

where $0 \leq \alpha \leq 1$, $n = 0, 1, \ldots$. It is easy to see that $\tilde{Q}$ satisfies the desired conditions. □

Remark 1. F.S. Rofe-Beketov [53] proved in case $M = \mathbb{R}^n$ (with the standard metric and measure0 and $A = 0$ that the local inequality $V(x) \geq -Q(x)$ can be replaced by an operator inequality

$$H \geq -\varepsilon\Delta - Q(x)$$

with a constant $\varepsilon > 0$. This allows in particular some potentials which are unbounded below. I. Oleinik [48] noticed that this result can be carried over to the case of manifolds as well.

Remark 2. F.S. Rofe-Beketov [52] noticed that if in Theorem 6.3 we have $Q(r) < \infty$ for all $r \geq 0$ and Q satisfies (6.3), then we can always replace Q by another function $Q_1 \in C^\infty$ such that Q_1 also satisfies all the conditions (including (a) with a possibly bigger Lipschitz constant).

Indeed, it suffices to construct a globally Lipschitz C^∞ function $Q_1 : [0, \infty) \to [1, \infty)$ so that $Q(r)/2 \leq Q_1(r) \leq 2Q(r)$ for all $r \geq 0$. To this end we can first mollify $Q^{-1/2}$ on each of the overlapping intervals $[0, 4], [2, 6], [6, 10], \ldots,$ by convolution with a positive smooth probability measure supported in a small neighborood of 0. This neighborhood should depend on the chosen interval to insure the desired inequalities. Note that the convolution does not change the Lipschitz constant. Then we can use a partition of unity on $[0, \infty)$ such that it is subordinated to the covering of $[0, \infty)$ by the intervals above and consists of functions which have uniformly bounded derivatives of any fixed order (e.g. translations of an appropriately fixed C^∞ function). Using such partition of unity to glue locally mollified function $Q^{-1/2}$ we arrive to the desired approximation $Q_1^{-1/2}$.

Remark 3. Another Sears-type result was obtained by T. Ikebe and T. Kato [29] where magnetic Schrödinger operators in $\mathbb{R}^n$ (with the standard metric and measure) with possibly locally singular potentials were considered. The allowed local singularities are most naturally described by the Stummel type conditions first introduced by F. Stummel [68]; see also E. Wienholtz [73], E. Nelson [45], K. Jörgens [32], G. Hellwig [26], T. Kato [36], B. Simon [65], H. Kalf and F.S. Rofe-Beketov [34] and references there for other results on operators with singular potentials. In particular a recent paper by H. Kalf and F.S. Rofe-Beketov [34] contains most general results which provide the essential self-adjointness of a Schrödinger operator in $\mathbb{R}^n$ under the condition that the operator is locally self-adjoint and appropriate Sears type conditions at infinity are imposed.

Remark 4. B.M. Levitan [42] gave a new proof of Theorem 6.3 (in case $M = \mathbb{R}^n$ with the standard metric and measure and with $A = 0$). His proof uses the wave equation and the finite propagation speed argument. Similar arguments were later used by A.A. Chumak [12], P. Chernoff [11] and T. Kato [37] to prove essential self-adjointness in a somewhat different context. A.A. Chumak considered semi-bounded Schrödinger operators on complete Riemannian manifolds. P. Chernoff proves in particular the essential self-adjointness for the powers of such operators as well as Dirac operators, whereas T. Kato extends the arguments and results to the powers H^m, $m = 1, 2, \dots,$ (in $\mathbb{R}^n$) under the condition that $H \geq -a - b|x|^2$ with some constants a, b.

Note however that the self-adjointness of the powers of the Laplacian on a complete Riemannian manifold was first established by H.O. Cordes [13] without finite propagation speed argument. (See also the book [14] for a variety of results on essential self-adjointness of semi-bounded Schrödinger-type operators on manifolds and their powers.)

There are many results on self-adjointness of more general higher order operators – see e.g. M. Schechter [55] for operators in $\mathbb{R}^n$ (and also for similar L^p results in $\mathbb{R}^n$) and also M. Shubin [58] for operators on manifolds of bounded geometry, as well as F.S. Rofe-Beketov [54] and references there.

3. Now we will formulate a result generalizing a theorem of I. Oleinik [48] (who considered the case $d\mu = d\mu_g$ and $A = 0$) which shows that in fact it is sufficient to restrict the behavior of the potential V only on some sequence of layers or shells which eventually surround all the points in M. The motivation of this result is obvious from the classical point of view this is obvious because the classical completeness can be guaranteed if the classical particle escaping to infinity spends infinite time already inside the layers. The first result of this kind in case $n = 1$ is due to P. Hartman [25], and further generalizations were obtained in one-dimensional case by R. Ismagilov [30] (higher order operators), and in case $M = \mathbb{R}^n$ by M.G. Gimadislamov [22], F.S. Rofe-Beketov [53], M.S.P. Eastham, W.D. Evans, J.B. McLeod [17] and A. Devinatz [16] (the last two references also include magnetic field terms).

Theorem 6.4 *Let $\{\Omega_k | \, k = 0, 1, \dots, \}$ be a sequence of open relatively compact subsets with smooth boundaries in M, $\overline{\Omega_k} \subset \Omega_{k+1}$, $\cup_k \Omega_k = M$. Denote $T_k = \Omega_{2k+1} \setminus \overline{\Omega_{2k}}$, and let h_k be the minimal thickness of the layer T_k, i.e. $h_k = \mathrm{dist}_g(\Omega_{2k}, M \setminus \Omega_{2k+1})$. Assume that $A \in \Lambda^1_{(1)}(M)$ and*

$$V(x) \geq -C\gamma_k, \; x \in T_k, \quad k = 0, 1, \dots, \tag{6.4}$$

where $C > 0$, $\gamma_k \geq 1$, and

$$\sum_{k=0}^{\infty} \min\{h_k^2, h_k \gamma_k^{-1/2}\} = \infty. \tag{6.5}$$

Then the operator (1.1) is essentially self-adjoint.

Proof. Following F.S. Rofe-Beketov [53] and I. Oleinik [48] we will construct a minorant Q for the potential V, so that the conditions (a) and (b) in Theorem 1.1 are satisfied.

We will start by constructing for any $k = 0, 1, \ldots$, a function $Q_k \geq 0$ on M such that $Q_k = +\infty$ on $M \setminus T_k$, then assemble $Q^{-1/2}$ as a linear combination of the functions $Q_k^{-1/2}$.

Denote for any $x \in M$

$$\delta_{2k}(x) = \mathrm{dist}_g(x, \Omega_{2k}), \quad \delta_{2k+1}(x) = \mathrm{dist}_g(x, M \setminus \Omega_{2k+1}), \quad k = 0, 1, \ldots.$$

For $p = 2k, 2k+1$ introduce sets

$$\Omega'_p = \{x |\, \delta_p(x) \leq h_k/4\}$$

and functions $\delta'_p : M \to [0, \infty)$,

$$\delta'_p(x) = \mathrm{dist}_g(x, M \setminus \Omega'_p).$$

Now define

$$Q_k^{-1/2}(x) = h_k^{-1}, \quad x \in M \setminus (\Omega'_{2k} \cup \Omega'_{2k+1}),$$

and

$$Q_k^{-1/2}(x) = h_k^{-1} \delta_p(x)(\delta_p(x) + \delta'_p(x))^{-1}, \quad x \in \Omega'_p,$$

where $p = 2k$ or $2k+1$. Clearly $0 \leq Q_k^{-1/2}(x) \leq h_k^{-1}$ on M and $Q_k^{-1/2}(x) = 0$ if $x \notin T_k$.

Let us evaluate the Lipschitz constant for $Q_k^{-1/2}$. To this end denote $f(s,t) = s/(s+t)$, and observe that the absolute values of both partial derivatives of f in s and t are bounded by $(s+t)^{-1}$ if $s, t \geq 0$, $s + t > 0$. Also both δ_p and δ'_p are Lipschitz with the Lipschitz constant 1. Now note that it is easily follows from the triangle inequality that

$$\delta_p(x) + \delta'_p(x) \geq h_k/4, \quad x \in M.$$

Hence by the chain rule we see that

$$|\nabla(Q_k^{-1/2})| \leq 2h_k^{-1} \cdot 4h_k^{-1} = 8h_k^{-2}.$$

Hence the Lipschitz constant of $Q_k^{-1/2}$ does not exceed $8h_k^{-2}$.

Now let us define

$$Q^{-1/2}(x) = \sum_{k=0}^{\infty} a_k Q_k^{-1/2},$$

where we will adjust the coefficients $a_k \geq 0$ so that all the conditions are satisfied. Let us list these conditions turn by turn.

(a) We need the condition $V \geq -Q$ to be satisfied which will be guaranteed if $-C\gamma_k \geq -Q(x)$, $x \in T_k$. This is equivalent to $Q_k^{-1/2} \leq (C\gamma_k)^{-1/2}$, $k = 0, 1, \ldots$, and will be guaranteed if $a_k h_k^{-1} \leq (C\gamma_k)^{-1/2}$ or

$$a_k \leq C^{-1/2} h_k \gamma_k^{-1/2}. \tag{6.6}$$

(b) The Lipschitz constant of $Q^{-1/2}$ is evaluated by $8 \sup_k (a_k h_k^{-2})$, so for $Q^{-1/2}$ to be Lipschitz it is sufficient to have

$$a_k \leq C_1 h_k^2 \tag{6.7}$$

with some constant $C_1 > 0$.

(c) At last we need the condition (b) of Theorem 1.1 to be satisfied. Note that the minimal thickness of the internal layer $T_k' = M \setminus (\Omega_{2k}' \cup \Omega_{2k+1}')$ is at least $h_k/2$, and $Q^{-1/2} = a_k h_k^{-1}$ in T_k'. It follows that the condition (b) in Theorem 1.1 will be satisfied if we require

$$\sum_{k=0}^{\infty} a_k = \infty. \tag{6.8}$$

Now taking $C_1 = C^{-1/2}$ we can choose

$$a_k = C^{-1/2} \min\{h_k^2, h_k \gamma_k^{-1/2}\},$$

so the conditions (6.6), (6.7) will be automatically satisfied. The condition (6.8) will be satisfied if we require the condition (6.5) to hold. □

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