

# Path integrals and the essential self-adjointness of differential operators on noncompact manifolds

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**Abstract** We consider Schrödinger operators on possibly noncompact Riemannian manifolds, acting on sections in vector bundles, with locally square integrable potentials whose negative part is in the underlying Kato class. Using path integral methods, we prove that under geodesic completeness these differential operators are essentially self-adjoint on  $C_0^\infty$ , and that the corresponding operator closures are semibounded from below. These results apply to nonrelativistic Pauli–Dirac operators that describe the energy of Hydrogen type atoms on Riemannian 3-manifolds.

## 1 Introduction

A classical result from B. Simon’s seminal paper [27] states that a Schrödinger operator of the form  $-\Delta + V$  in the Euclidean space  $\mathbb{R}^m$ , with  $V : \mathbb{R}^m \rightarrow \mathbb{R}$  a locally square integrable potential, is essentially self-adjoint on  $C_0^\infty(\mathbb{R}^m)$ , if the negative part of  $V$  is in the Kato class  $\mathcal{K}(\mathbb{R}^m)$ . Note here that this fact is closely related to quantum physics, in the sense that the Coulomb potential  $V(x) = -1/|x|$  is in the above class. Having in mind that all of the above data can be defined on any Riemannian manifold, we are interested in the following question in this paper:

*To what extent can Simon’s result be extended to Schrödinger type operators acting on sections in vector bundles over possibly noncompact Riemannian manifolds?*

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Apart from a pure academic interest, this question is also particularly motivated by the observation that it is possible to model [9, 16] nonrelativistic atomic Hamiltonians on any nonparabolic Riemannian 3-manifold (which have to be  $\text{spin}^{\mathbb{C}}$ , if the electron’s spin is taken into account; in particular, the vector-valued case becomes particularly interesting from this point of view, see Sect. 3 below). This abstraction is desirable from the physics point of view, since one would like to understand deeply which properties of the Euclidean space  $\mathbb{R}^3$  actually guarantee certain spectral properties of quantum systems, or other important results such as the stability of matter [23]. In these situations, the corresponding potential terms are always locally square integrable, and with some control on the underlying Riemannian structure, their negative parts are in the underlying Kato class, so that we basically are in the initial situation.

Before we can formulate our main result, we have to introduce some notation:

Let  $M$  denote a smooth connected Riemannian manifold without boundary. The geodesic distance on  $M$  will be written as  $d(x, y)$ , and  $K_r(x)$  will stand for the open geodesic ball with radius  $r$  around  $x$ , and

$$(0, \infty) \times M \times M \longrightarrow (0, \infty), (t, x, y) \longmapsto p(t, x, y)$$

will stand for the minimal positive heat kernel on  $M$ .

If  $F \rightarrow M$  is a smooth Hermitian vector bundle, then, abusing the notation in the usual way,  $|\bullet|_x$  stands for the norm and the operator norm corresponding to  $(\bullet, \bullet)_x$  on each (finite-dimensional) fiber  $F_x$ , and the scalar product and norm corresponding to the Hilbert space  $\Gamma_{L^2}(M, F)$  will be written as  $(\bullet, \bullet)$  and  $\|\bullet\|$ , respectively, that is,

$$(f_1, f_2) = \int_M (f_1(x), f_2(x))_x \text{vol}(dx), \|f\|^2 = \int_M |f(x)|_x^2 \text{vol}(dx). \tag{1}$$

If  $\tilde{F} \rightarrow M$  is a second bundle as above and if

$$P: \Gamma_{C_0^\infty}(M, F) \longrightarrow \Gamma_{C_0^\infty}(M, \tilde{F})$$

is a linear differential operator, then we denote with  $P^\dagger$  the formal adjoint of  $P$  with respect to (1). In particular, the Laplace–Beltrami operator on  $M$  is given in this sense as  $-\Delta = d^\dagger d$ . The symbol  $\nabla^{TM}$  will denote the Levi-Civita connection, and if nothing else is said, the (co-)tangent bundle of  $M$  will be equipped with the Hermitian structure corresponding to the underlying Riemannian metric of  $M$ . These data will be implicitly complexified, whenever necessary.

Let  $E \rightarrow M$  be a smooth Hermitian vector bundle, let  $\nabla$  be a Hermitian covariant derivative in  $E$  and let  $V: M \rightarrow \text{End}(E)$  be a potential, that is,  $V$  is a measurable section in  $\text{End}(E)$  such that  $V(x): E_x \rightarrow E_x$  is self-adjoint for almost every (a.e.)  $x \in M$ . Furthermore, let  $\mathcal{K}(M)$  denote the class of Kato functions<sup>1</sup> on  $M$ . Our main result reads as follows:

**Theorem 1.1** *Let  $M$  be geodesically complete, let  $|V| \in L^2_{\text{loc}}(M)$  and assume that  $V$  admits a decomposition  $V = V_1 - V_2$  into potentials  $V_j \geq 0$  with  $|V_2| \in \mathcal{K}(M)$ . Then the operator  $\nabla^\dagger \nabla / 2 + V$  is essentially self-adjoint on  $\Gamma_{C_0^\infty}(M, E)$  and its closure is semibounded from below.*

Note that the decomposition  $V = V_1 - V_2$  into nonnegative potentials need not be the canonic one given by  $V = V^+ - V^-$ , which can be defined through the fiberwise spectral calculus of  $E$ .

<sup>1</sup> See Sect. 3.5 for the definition of  $\mathcal{K}(M)$  and for criteria for functions to be in  $\mathcal{K}(M)$ .

Before we explain the strategy of the proof of Theorem 1.1, some remarks are in order:

*Remark 1.2* (a) Theorem 1.1 is disjoint from the various results on essential self-adjointness for operators of the form  $\nabla^\dagger \nabla / 2 + V$  that have been obtained in [1]. The point here is that, in general, Kato potentials need not satisfy the inequality (2.2) from [1], i.e., for every compact  $K \subset M$  there are numbers  $0 < a_K < 1, b_K > 0$  such that

$$\left( \int_K |V_2(x)|_x^2 |u(x)|^2 \text{vol}(dx) \right)^{1/2} \leq a_K \|\Delta u\| + b_K \|u\| \tag{2}$$

for any  $u \in C_0^\infty(M)$ . However, it should be noted that the main strength of the results of [1] lies in the fact that the authors have considered *arbitrary* first order elliptic differential operators instead of  $\nabla$ . It would certainly be an interesting problem to see to what extent our probabilistic techniques below can be extended to cover the latter situation, which has first been considered in [22].

(b) Of course, taking  $E = M \times \mathbb{C}$  and  $\nabla = d + i\beta$  with  $\beta \in \Omega_{\mathbb{R}}^1(M)$ , we can deal with *smooth* magnetic potentials within our framework. In this scalar situation, the analogue of Theorem 1.1 can be easily deduced from (a slight variation of) Theorem 1 in [13], where the authors can even allow magnetic potentials with possibly strong local singularities. We refer the reader to [17] for the scalar situation in Euclidean space.

Let us now explain the strategy (which is partially motivated by [27] and [13]) of the proof of Theorem 1.1, which is given in full detail in the following Sect. 3.5. To this end, we assume for the rest of this section that  $V$  is as in Theorem 1.1. Then by the main result of [14], it is always possible to define the form sum  $H_V$  corresponding to the Friedrichs realization of  $\nabla^\dagger \nabla / 2$  and  $V$  *without any additional assumptions on  $M$*  (see Theorem 2.6 below). The main advantage of this observation is that, unlike in usual essential-self-adjointness proofs, instead of directly proving that  $\nabla^\dagger \nabla / 2 + V$  is essentially self-adjoint on  $\Gamma_{C_0^\infty}(M, E)$ , we will prove that the latter space is an operator core for  $H_V$  (this is the content of Theorem 2.14; Theorem 1.1 itself follows directly from the latter result, which is summarized in Corollary 2.15). In particular, we will use the full spectral calculus given by  $H_V$ .

Having said this, the first step in the proof of this operator core property will be to deduce the following smoothing property (see Proposition 2.11 below):

$$\text{For any } t > 0 \text{ one has } e^{-tH_V} [\Gamma_{L^2}(M, E)] \subset \Gamma_{L^\infty_{\text{loc}}}(M, E). \tag{3}$$

This result will be derived from the path integral formula

$$e^{-tH_V} f(x) = \mathbb{E} \left[ \mathbb{1}_{\{t < \zeta(x)\}} \mathcal{Y}_t^x \parallel_t^{x,-1} f(B_t(x)) \right], \tag{4}$$

where  $B(x)$  is a Brownian motion starting in  $x$  with lifetime  $\zeta(x)$ , where

$$\parallel_t^x : E_x \longrightarrow E_{B_t(x)}$$

is the corresponding stochastic parallel transport with respect to  $\nabla$ ,  $\parallel_t^{x,-1} = \parallel_t^{x,*}$  its inverse, and where

$$\mathcal{Y}_t^x : E_x \longrightarrow E_x$$

is the path ordered exponential<sup>2</sup>

$$\begin{aligned} \gamma_t^x - \mathbf{1} &= \sum_{k=1}^{\infty} (-1)^k \int_{t\Delta_k} \parallel_{s_1}^{x,-1} V(B_{s_1}(x)) \parallel_{s_1}^x \dots \parallel_{s_k}^{x,-1} V(B_{s_k}(x)) \parallel_{s_k}^x ds_1 \dots ds_k \quad (5) \end{aligned}$$

(details on these processes and on formula (4), which is one of the main results of [15], are included in the following section). Again, (3) and (4) are valid *without any additional assumptions on M*.

*Remark 1.3* Note that it is not possible to deduce (3) directly by Sobolev embedding theorems for  $\dim M > 3$ , which is the main motivation for the introduction of path integral techniques in this context.

In a next step, we will use finite speed propagation methods to deduce the following result:

$$\begin{aligned} &\text{The set } D(H_V) \cap \{f \mid f \text{ has a compact support}\} \\ &\text{is an operator core for } H_V, \text{ if } M \text{ is geodesically complete.} \quad (6) \end{aligned}$$

To be precise, we will actually prove a Davies–Gaffney inequality (see Proposition 2.13) for approximations of  $H_V$  and use the fact that this inequality always implies (is in fact equivalent) to finite speed of propagation by the results of [3]. Then one can use a variant of Chernoff’s theorem (see Lemma B.1) to deduce (6). The fact that we use finite speed propagation methods in this context has been particularly motivated by the scalar situation that has been considered in [13], where the authors apply this method in a similar way. As has been noted in [13], this technique avoids the usage of second order cut-off functions, which do not seem to be available without additional control on the underlying Riemannian structure.

As a next step one can combine (6) with (3) to deduce the following fact:

$$\begin{aligned} &\text{The set } D(H_V) \cap \Gamma_{L_{\text{loc}}}^{\infty}(M, E) \cap \{f \mid f \text{ has a compact support}\} \\ &\text{is an operator core for } H_V, \text{ if } M \text{ is geodesically complete.} \quad (7) \end{aligned}$$

Then, we shall use the self-adjointness of  $H_V$  to deduce that the elements  $f$  of the set (7) satisfy  $\nabla^{\dagger} \nabla f \in \Gamma_{L^2}(M, E)$ . Finally, if  $M$  is geodesically complete we can use a (local) result on Friedrichs mollifiers to prove that  $\Gamma_{C_0^{\infty}}(M, E)$  is an operator core for  $H_V$ , by showing that  $\Gamma_{C_0^{\infty}}(M, E)$  is dense in (7) with respect to the graph norm corresponding to  $H_V$ .

This paper is organized as follows: In Sect. 2, we first recall some facts about Kato potentials. The rest of Sect. 2 is completely devoted to the proof of Theorem 1.1. In Sect. 3, we apply Theorem 1.1 in the context of Hydrogen type problems on Riemannian 3-manifolds, which was originally the main motivation for this paper. It seems as if this result has not been stated yet in this form in the literature even for the Euclidean  $\mathbb{R}^3$  (though it should be known in this case). Finally, in the appendix, we have included a fact about Friedrichs mollifiers, an abstract variant of Chernoff’s finite speed of propagation theorem on vector bundles, and some facts about path ordered exponentials that we will need in our probabilistic considerations.

<sup>2</sup> Here,  $t\Delta_k = \{0 \leq s_1 \leq \dots \leq s_k \leq t\} \subset \mathbb{R}^k$  denotes the  $t$ -scaled  $k$ -simplex for any  $k \in \mathbb{N}, t \geq 0$ .

## 2 Kato potentials and the proof of Theorem 1.1

Let us first clarify that in this section,

*M will always be a smooth connected Riemannian manifold without boundary,  $E \rightarrow M$  a smooth Hermitian vector bundle,  $\nabla$  a Hermitian covariant derivative in  $E$ , and  $V : M \rightarrow \text{End}(E)$  a potential.*

By the usual abuse of notation, we will denote the quadratic form corresponding to a symmetric sesquilinear form in some Hilbert space with the same symbol. The symbol  $H_0$  stands for the Friedrichs realization of  $\nabla^\dagger \nabla / 2$ , that is,  $H_0$  is the nonnegative self-adjoint operator in  $\Gamma_{L^2}(M, E)$  which corresponds to the closure  $q_{H_0}$  of the quadratic form given by the symmetric nonnegative operator  $\nabla^\dagger \nabla / 2$ , defined initially on  $\Gamma_{C^\infty}(M, E)$ . Note the well-known:

*Remark 2.1* If  $M$  is geodesically complete, then one has

$$\begin{aligned} D(q_{H_0}) &= \{f|f \in \Gamma_{L^2}(M, E), \nabla f \in \Gamma_{L^2}(M, E \otimes T^*M)\}, \\ q_{H_0}(f, h) &= \frac{1}{2} \int_M (\nabla f(x), \nabla h(x))_x \text{vol}(dx), \end{aligned} \tag{8}$$

and  $\Gamma_{C^\infty}(M, E)$  is an operator core for  $H_0$ , and one has

$$D(H_0) = \{f|f, \nabla^\dagger \nabla f \in \Gamma_{L^2}(M, E)\}, \quad H_0 f = \frac{1}{2} \nabla^\dagger \nabla f. \tag{9}$$

Next, we remark that  $V$  defines a quadratic form in  $\Gamma_{L^2}(M, E)$  by setting

$$\begin{aligned} D(q_V) &= \{f|f \in \Gamma_{L^2}(M, E), (Vf, f) \in L^1(M)\}, \\ q_V(f) &= \int_M (V(x)f(x), f(x))_x \text{vol}(dx). \end{aligned} \tag{10}$$

We will often require a global Kato assumption on some negative part of  $V$ . Before recalling some facts on Kato functions, let us first introduce some notation: Let  $\mathcal{M} := (\Omega, \mathcal{F}, \mathcal{F}_*, \mathbb{P})$  be a filtered probability space which satisfies the usual assumptions. We assume that  $\mathcal{M}$  is chosen in a way such that  $\mathcal{M}$  carries an appropriate family of Brownian motions

$$B(x) : [0, \zeta(x)) \times \Omega \longrightarrow M, x \in M,$$

where  $\zeta(x) : \Omega \rightarrow [0, \infty]$  is the lifetime of  $B(x)$ . We will freely use the fact

$$\mathbb{P}\{B_t(x) \in N, t < \zeta(x)\} = \int_N p(t, x, y) \text{vol}(dy) \text{ for any measurable } N \subset M$$

in the following.

Now a measurable function  $w : M \rightarrow \mathbb{C}$  is said to be in the *Kato class*  $\mathcal{K}(M)$  of  $M$ , if

$$\lim_{t \rightarrow 0^+} \sup_{x \in M} \mathbb{E} \left[ \int_0^t 1_{\{s < \zeta(x)\}} |w(B_s(x))| ds \right] = 0, \text{ which is equivalent to} \tag{11}$$

$$\lim_{t \rightarrow 0^+} \sup_{x \in M} \int_0^t \int_M p(s, x, y) |w(y)| \text{vol}(dy) ds = 0. \tag{12}$$

The local Kato class  $\mathcal{K}_{\text{loc}}(M)$  is defined in the obvious way,

$$\mathcal{K}_{\text{loc}}(M) := \{w | 1_K w \in \mathcal{K}(M) \text{ for all compact } K \subset M\} \supset \mathcal{K}(M),$$

and generally,  $\mathcal{K}_{\text{loc}}(M)$  may depend on the Riemannian structure of  $M$ .

For future reference, we note:

**Lemma 2.2** (a) *One has  $\mathcal{K}(M) \subset L^1_{\text{loc}}(M)$  and  $L^\infty(M) \subset \mathcal{K}(M)$ .*  
 (b) *For any  $w \in L^1_{\text{loc}}(M)$  and a.e.  $x \in M$  one has*

$$\mathbb{P}\{w(B_\bullet(x)) \in L^1_{\text{loc}}[0, \zeta(x)]\} = 1. \tag{13}$$

(c) *For any  $w \in \mathcal{K}_{\text{loc}}(M)$  and all  $x \in M$  one has*

$$\mathbb{P}\{w(B_\bullet(x)) \in L^1_{\text{loc}}[0, \zeta(x)]\} = 1.$$

(d) *For any  $w \in \mathcal{K}(M)$ ,  $t \geq 0$ , one has*

$$\sup_{x \in M} \mathbb{E} \left[ 1_{\{t < \zeta(x)\}} e^{\int_0^t |w(B_s(x))| ds} \right] < \infty. \tag{14}$$

*Proof* Part (a) is an elementary result which is included in [14], and the parts (b)–(d) are included in Prop. 2.4 and Prop. 2.5 in [15]. □

Let us now point out that [14] that one always has

$$L^\infty(M) \subset \mathcal{K}(M) \subset L^1_{\text{loc}}(M),$$

but with some control on the Riemannian structure of  $M$ , one can easily produce a large class of Kato functions. To this end, we first note the following highly nontrivial self-improvement result of on-diagonal upper estimates for  $p(t, x, y)$ , which will be very useful in the following:

**Theorem 2.3** *Assume that there is a  $C > 0$  and a  $t_0 \in (0, \infty]$  such that*

$$\sup_{x \in M} p(t, x, x) \leq \frac{C}{t^{\dim M/2}} \text{ for all } 0 < t \leq t_0.$$

*Then there are  $C_1, C_2 > 0$  such that*

$$\sup_{x, y \in M} p(t, x, y) \leq \frac{C_1}{t^{\dim M/2}} e^{-d(x, y)^2 / (C_2 t)} \text{ for all } 0 < t \leq t_0.$$

The reader may find a proof of this result in [12] (see Theorem 1.1 therein for a more general result).

For any  $p \geq 1$  let  $L^p_{\text{u,loc}}(M)$  denote the space of uniformly locally  $p$ -integrable functions on  $M$ , that is, a measurable function  $v : M \rightarrow \mathbb{C}$  is in  $L^p_{\text{u,loc}}(M)$ , if and only if

$$\sup_{x \in M} \int_{K_1(x)} |v(y)|^p \text{vol}(dy) < \infty. \tag{15}$$

Note the simple inclusions

$$L^p(M) \subset L^p_{\text{u,loc}}(M) \subset L^p_{\text{loc}}(M).$$

Now one has the following result:

**Proposition 2.4** *Let  $p$  be such that  $p \geq 1$  if  $m = 1$ , and  $p > m/2$  if  $m \geq 2$ .*

(a) *If there is  $C > 0$  and a  $t_0 > 0$  such that*

$$\sup_{x \in M} p(t, x, x) \leq \frac{C}{t^{\dim M/2}} \text{ for all } 0 < t \leq t_0, \tag{16}$$

then one has

$$L^p(M) + L^\infty(M) \subset \mathcal{K}(M). \tag{17}$$

(b) *Let  $M$  be geodesically complete, and assume that there are constants  $C_1, \dots, C_6, t_0 > 0$  such that for all  $0 < t \leq t_0, x, y \in M, r > 0$  one has*

$$\text{vol}(K_r(x)) \leq C_1 r^{\dim M} e^{C_2 r}$$

and

$$\frac{C_3}{t^{\dim M/2}} e^{-C_4 d(x,y)^2/t} \leq p(t, x, y) \leq \frac{C_5}{t^{\dim M/2}} e^{-C_6 d(x,y)^2/t}.$$

Then one has

$$L^p_{u,\text{loc}}(M) + L^\infty(M) \subset \mathcal{K}(M). \tag{18}$$

*Proof* (a) Indeed, Theorem 2.3 implies the existence of a  $\tilde{C} > 0$  such that for all  $0 < t \leq t_0$  one has<sup>3</sup>

$$\sup_{x,y \in M} p(t, x, y) \leq \frac{\tilde{C}}{t^{\dim M/2}}.$$

Now we can directly apply Proposition 2.8 in [14] (the corresponding proof is elementary and essentially only uses Hölder’s inequality).

(b) We can use Theorem 3.3 from [21] with  $\nu := m, \beta := 2, V(r) := C_1 r^m e^{C_2 r}, \Phi_1(s) := C_3 e^{-C_4 s^2}, \Phi_2(s) := C_5 e^{-C_6 s^2}$  to deduce the asserted inclusion (keeping  $L^\infty(M) \subset \mathcal{K}(M)$  in mind). Indeed, one just has to note that

$$\int_1^\infty \frac{\max(r^m e^{C_2 r}, r^m) e^{-C_6 r^2}}{r} dr = \int_1^\infty e^{C_2 r} r^{m-1} e^{-C_6 r^2} dr < \infty, \tag{19}$$

which is obvious. □

*Remark 2.5* Let us note that (16) is satisfied, for example, if  $M$  is geodesically complete with Ricci curvature bounded from below and a positive injectivity radius (see example [21], p. 110). The reader may find these and several other aspects on Kato functions in [14] and, particularly, in [21].

The following result is also included in [14]. It shows that, remarkably, one can always define the form sum of  $H_0$  and  $V$  under the following very weak assumptions on  $V$ :

**Theorem 2.6** *Let  $V$  be such that there is a decomposition  $V = V_1 - V_2$  into potentials  $V_j \geq 0$  with  $|V_1| \in L^1_{\text{loc}}(M)$  and  $|V_2| \in \mathcal{K}(M)$ . Then one has*

$$D(q_{H_0} + q_V) = D(q_{H_0}) \cap D(q_{V_1}), \tag{20}$$

and  $q_{H_0} + q_V$  is a densely defined, closed and semibounded from below quadratic form in  $\Gamma_{L^2}(M, E)$ .

<sup>3</sup> Of course this inequality can also be deduced with an elementary argument.

In the situation of Theorem 2.6, the form sum  $H_0 \dot{+} V$  will be denoted with  $H_V$ , that is,  $H_V$  is the self-adjoint semibounded from below operator corresponding to  $q_{H_0} + q_V$ .

*Remark 2.7* In the situation of Theorem 2.6, assume that  $M$  is geodesically complete. Then Proposition 2.14 in [14] states that  $\Gamma_{C_0^\infty}(M, E)$  is a form core for  $H_V$ .

Let us add the following simple observation:

**Lemma 2.8** *Let  $|V| \in L^2_{\text{loc}}(M)$  and assume that there is a decomposition  $V = V_1 - V_2$  into potentials  $V_j \geq 0$  with  $|V_2| \in \mathcal{K}(M)$ . Furthermore, let  $\tilde{H}_{V,\min}$  denote the operator  $\nabla^\dagger \nabla / 2 + V$  with domain of definition  $\Gamma_{C_0^\infty}(M, E)$ , and let  $H_{V,\min} := \overline{\tilde{H}_{V,\min}}$ . Then one has  $H_{V,\min} \subset H_V$ .*

*Proof* Since  $H_V$  is closed, it is sufficient to prove  $\tilde{H}_{V,\min} \subset H_V$ . But if  $f \in \Gamma_{C_0^\infty}(M, E)$ ,  $h \in \mathcal{D}(q_{H_V})$ , then  $f \in \mathcal{D}(q_{H_V})$  and we have

$$q_{H_V}(f, h) = \frac{1}{2} \langle \nabla^\dagger \nabla f, h \rangle + \langle Vf, h \rangle, \tag{21}$$

so  $f \in \mathcal{D}(H_V)$  and  $H_V f = \frac{1}{2} \nabla^\dagger \nabla f + Vf$ . □

As we have already remarked in the introduction, an essential step in the proof of Theorem 1.1 will be to deduce an  $L^2 \rightsquigarrow L^\infty_{\text{loc}}$  smoothing property of the Schrödinger semigroup

$$(e^{-tH_V})_{t \geq 0} \subset \mathcal{L}(\Gamma_{L^2}(M, E)),$$

which will be deduced from a path integral formula for  $e^{-tH_V}$ . In order to formulate the latter formula in our geometric context, for any  $t \geq 0$  the stochastic parallel transport with respect to  $(B(x), \nabla)$  will be written as a pathwise unitary map

$$\parallel_t^x : E_x \longrightarrow E_{B_t(x)}, \quad \text{defined in } \{t < \zeta(x)\} \subset \Omega.$$

Now Theorem 2.11 in [15] states the following Feynman–Kac type path integral formula:

**Theorem 2.9** *In the situation of Theorem 2.6, for a.e.  $x \in M$ , there is a unique process*

$$\mathcal{Y}^x : [0, \zeta(x)) \times \Omega \longrightarrow \text{End}(E_x)$$

which satisfies

$$\frac{d\mathcal{Y}_t^x}{dt} = -\mathcal{Y}_t^x (\parallel_t^{x,-1} V(B_t(x)) \parallel_t^x), \quad \mathcal{Y}_0^x = \mathbf{1} \tag{22}$$

pathwise in the weak sense, and for any  $f \in \Gamma_{L^2}(M, E)$ ,  $t \geq 0$ , a.e.  $x \in M$  one has

$$e^{-tH_V} f(x) = \mathbb{E} \left[ \mathbf{1}_{\{t < \zeta(x)\}} \mathcal{Y}_t^x \parallel_t^{x,-1} f(B_t(x)) \right]. \tag{23}$$

*Remark 2.10* The set of  $x$  for which  $\mathcal{Y}^x$  exists is, by definition, equal to the set  $x$  for which one has (13) for  $w = |V|$ , and if  $x$  is in this set, then the asserted formula (5) from the introduction follows from Lemma C.1.

We will use (23) to deduce:

**Proposition 2.11** *In the situation of Theorem 2.6, one has*

$$e^{-tH_V} [\Gamma_{L^2}(M, E)] \subset \Gamma_{L^\infty_{\text{loc}}}(M, E) \quad \text{for any } t > 0. \tag{24}$$



*Remark 2.12* Note that Lemma 2.2, Theorem 2.6, Theorem 2.9, and Proposition 2.11 are all valid without any further assumptions on the Riemannian structure of  $M$ .

*Proof of Proposition 2.11* We define scalar potentials  $v_j : M \rightarrow [0, \infty)$ ,  $v : M \rightarrow \mathbb{R}$  by

$$v_1(\bullet) := \min \sigma(V_1(\bullet)), v_2(\bullet) := \max \sigma(V_2(\bullet)), v(\bullet) := v_1(\bullet) - v_2(\bullet).$$

Let  $x$  be such that (13) holds for  $w = |V_1|$  and  $w = |V_2|$ . Then  $\mathcal{Y}^x$  exists, and  $V \geq v\mathbf{1}$ , Lemma C.1 and  $-v \leq v_2$  imply

$$\begin{aligned} |\mathcal{Y}_t^x|_x \mathbf{1}_{\{t < \zeta(x)\}} &\leq e^{-\int_0^t v(B_s(x)) ds} \mathbf{1}_{\{t < \zeta(x)\}} \\ &\leq e^{\int_0^t v_2(B_s(x)) ds} \mathbf{1}_{\{t < \zeta(x)\}} \mathbb{P}\text{-a.s. for any } t \geq 0, \end{aligned}$$

so that for any  $t > 0$  one has

$$\begin{aligned} &\left| \mathbb{E} \left[ \mathbf{1}_{\{t < \zeta(x)\}} \mathcal{Y}_t^x \parallel_t^{x,-1} f(B_t(x)) \right] \right|_x \\ &\leq \mathbb{E} \left[ \mathbf{1}_{\{t < \zeta(x)\}} e^{\int_0^t v_2(B_s(x)) ds} |f(B_t(x))|_{B_t(x)} \right] \\ &\leq \sqrt{\mathbb{E} \left[ \mathbf{1}_{\{t < \zeta(x)\}} e^{2 \int_0^t v_2(B_s(x)) ds} \right]} \sqrt{\mathbb{E} \left[ \mathbf{1}_{\{t < \zeta(x)\}} |f(B_t(x))|_{B_t(x)}^2 \right]} \\ &= \sqrt{\mathbb{E} \left[ \mathbf{1}_{\{t < \zeta(x)\}} e^{2 \int_0^t v_2(B_s(x)) ds} \right]} \sqrt{\int_M |f(y)|_y^2 p(t, x, y) \text{vol}(dy)}. \end{aligned} \tag{25}$$

Since for any  $h \in L^1(M)$ , the function

$$M \longrightarrow \mathbb{C}, z \longmapsto \int_M h(y) p(t, z, y) \text{vol}(dy)$$

is in  $C^\infty(M)$  (see Theorem 7.19 in [11]), we can use (14) with  $w = v_2$  to deduce that for any compact  $K \subset M$  one has

$$\sup_{z \in K} \left( \mathbb{E} \left[ \mathbf{1}_{\{t < \zeta(z)\}} e^{2 \int_0^t v_2(B_s(z)) ds} \right] \int_M |f(y)|_y^2 p(t, z, y) \text{vol}(dy) \right) < \infty,$$

so that, in view of (25), the assignment

$$x \longmapsto \mathbb{E} \left[ \mathbf{1}_{\{t < \zeta(x)\}} \mathcal{Y}_t^x \parallel_t^{x,-1} f(B_t(x)) \right]$$

defines an element of  $\Gamma_{\text{loc}}(M, E)$ , and (24) is implied by the path integral formula from Theorem 2.9. □

Next, we are going to deduce a finite propagation speed result, which will be used later on to prove that the compactly supported elements of  $D(H_V)$  are an operator core for  $H_V$  under geodesic completeness. The essential observation is that finite speed of propagation is always implied by a Davies–Gaffney type inequality, through a Paley–Wiener type theorem [3]. As we have already remarked in the introduction, we have borrowed this method from [13].

**Proposition 2.13** *Let  $M$  be geodesically complete.*

- (a) *If  $V$  is bounded, then there is a constant  $D > 0$  such that for all open sets  $U_1, U_2 \subset M$ , all  $f_1, f_2 \in \Gamma_{L^2}(M, E)$  with  $\text{supp}(f_j) \subset U_j$  and all  $t > 0$  one has*

$$|\langle e^{-tH_V} f_1, f_2 \rangle| \leq e^{Dt} e^{-d(U_1, U_2)^2/(4t)} \|f_1\| \|f_2\|. \tag{26}$$

(b) Let  $V$  be as in Theorem 2.6 and assume  $H_V \geq 0$ . Then for any compactly supported  $f \in \Gamma_{L^2}(M, E)$  and any  $t > 0$ , the section  $\cos(t\sqrt{H_V})f$  has a compact support.

*Proof* (a) Under the assumption that  $V$  is bounded and nonnegative, we are going to prove (26) with  $D = 0$ , which of course proves the assertion. To this end, we are going to use the well-known exponential-weight method, that goes back to [10] (see also [3]): Let  $q : M \rightarrow \mathbb{R}$  be a bounded Lipschitz function with  $|dq| \leq C$  a.e. in  $M$ . For any  $f \in \Gamma_{C_0^\infty}(M, E)$ , Lemma 2.8 and the Sobolev product rule

$$\nabla(e^{2q}e^{-tH_V}f) = de^{2q} \otimes e^{-tH_V}f + e^{2q}\nabla e^{-tH_V}f \tag{27}$$

imply

$$\begin{aligned} & \frac{d}{dt} \|e^q e^{-tH_V} f\|^2 \\ &= -2\Re \langle \nabla^\dagger \nabla e^{-tH_V} f, e^{2q} e^{-tH_V} f \rangle - 2 \langle V e^{-tH_V} f, e^{2q} e^{-tH_V} f \rangle \\ &= -2\Re \langle e^q \nabla e^{-tH_V} f, e^q dq \otimes e^{-tH_V} f \rangle - 2 \|e^q \nabla e^{-tH_V} f\|^2 \\ & \quad - 2 \langle V e^{-tH_V} f, e^{2q} e^{-tH_V} f \rangle. \end{aligned} \tag{28}$$

Using Cauchy–Schwarz on the fibers for the first term and  $V \geq 0$  for the last term, the latter expression can be estimated by

$$\begin{aligned} & \leq 2 \int_M e^{q(x)} |\nabla e^{-tH_V} f(x)|_x e^{q(x)} |dq(x)|_x |e^{-tH_V} f(x)|_x \text{vol}(dx) \\ & \quad - 2 \|e^q \nabla e^{-tH_V} f\|^2, \end{aligned} \tag{29}$$

which, using  $XY \leq X^2 + Y^2/4$ , is

$$\leq \frac{1}{2} \|e^q |dq| e^{-tH_V} f\|^2 \leq \frac{C^2}{2} \|e^q e^{-tH_V} f\|^2. \tag{30}$$

Thus, setting  $\mathcal{E}_{f,q}(t) := \|e^q e^{-tH_V} f\|^2$ , putting everything together and using Gronwall, we arrive at

$$\mathcal{E}_{f,q}(t) \leq e^{C^2 t/2} \mathcal{E}_{f,q}(0). \tag{31}$$

Now let  $U_1, U_2$  be disjoint, let  $f \in \Gamma_{C_0^\infty}(M, E)$  with  $\text{supp}(f) \subset U_2$ , and let  $a > 0$ . Then the function  $q := ad(\bullet, U_2)$  is bounded and Lipschitz with  $|dq| \leq a$  a.e. in  $M$  and (31) implies

$$\begin{aligned} & \|1_{U_1} e^{-tH_V} f\|^2 \\ & \leq e^{-ad(U_1, U_2)} e^{a^2 t/2} \mathcal{E}_{f,q}(0) \\ & = e^{-ad(U_1, U_2)} e^{a^2 t/2} \int_{U_2} |f(x)|_x^2 e^{ad(x, U_2)} \text{vol}(dx) \\ & = e^{-ad(U_1, U_2)} e^{a^2 t/2} \|f\|^2, \end{aligned} \tag{32}$$

so that by choosing  $a$  appropriately

$$\|1_{U_1} e^{-tH_V} f\| \leq e^{-d(U_1, U_2)^2/(4t)} \|f\|, \tag{33}$$

which carries over to  $f_2$  by a density argument. Finally, we have

$$|\langle e^{-tH_V} f_1, f_2 \rangle| = |\langle f_1, 1_{U_1} e^{-tH_V} f_2 \rangle| \leq e^{-d(U_1, U_2)^2/(4t)} \|f_1\| \|f_2\| \tag{34}$$

by Cauchy–Schwarz and (33), and everything is proved.

(b) It is sufficient to prove that for any  $U_j, f_j$  as in (a) and any  $0 < s < d(U_1, U_2)$  one has

$$\langle \cos(s\sqrt{H_V}) f_1, f_2 \rangle = 0. \tag{35}$$

Indeed, the latter implies that if  $\text{supp}(f) \subset K_r(x)$  for some  $r > 0, x \in M$ , then for any  $t > 0$  one has

$$\text{supp}(\cos(t\sqrt{H_V}) f) \subset \overline{K_{r+t}(x)}, \tag{36}$$

and the latter set is compact by the geodesic completeness of  $M$ . It remains to prove (35).

If  $V$  is bounded and  $H_V \geq 0$ , then (35) follows directly from (a): Indeed, one can use the same arguments as those in the proof of theorem 3.4 in [3] to see this. Essentially, one has to use a variant of the Paley–Wiener theorem, which has to be applied to an appropriately rescaled version of the analytic function  $z \mapsto \langle e^{-zH_V} f_1, f_2 \rangle, \text{Re } z > 0$ .

Next, we assume that  $V$  is locally integrable and bounded from below with  $H_V \geq 0$ . Then putting  $V_n := \min(V, n)$  for  $n \in \mathbb{N}$  (in the sense of the fiberwise spectral calculus of  $E$ ) we find by the above that (35) is satisfied for  $V$  replaced with  $V_n$ , but monotone convergence of quadratic forms (see the proof of theorem 2.11 in [15]) gives  $H_{V_n} \rightarrow H_V$  as  $n \rightarrow \infty$  in the strong resolvent sense, which implies (35).

Finally, if  $V$  is as in Theorem 2.14 and  $H_V \geq 0$ , let us set  $V_n := \max(-n, V)$ . Then each  $V_n$  is locally integrable and bounded from below with  $H_{V_n} \geq 0$  and again everything follows from the above and monotone convergence of quadratic forms (this is also included in the proof of theorem 2.11 in [15]). □

Now we are in the position to prove the main result of this paper:

**Theorem 2.14** *Let  $M$  be geodesically complete, let  $|V| \in L^2_{\text{loc}}(M)$  and assume that  $V$  has a decomposition  $V = V_1 - V_2$  into potentials  $V_j \geq 0$  with  $|V_2| \in \mathcal{K}(M)$ . Then  $\Gamma_{C_0^\infty}(M, E)$  is an operator core for  $H_V$  and one has*

$$\mathbf{D}(H_V) = \{f | f, (\nabla^\dagger \nabla + V)f \in \Gamma_{L^2}(M, E)\}. \tag{37}$$

*Proof* We have to prove that  $\Gamma_{C_0^\infty}(M, E)$  is dense in  $\mathbf{D}(H_V)$  with respect to the graph  $\|\bullet\|_{H_V}$ . This will be proven in four steps:

(I) *If  $\chi \in C_0^\infty(M)$  and  $f \in \mathbf{D}(H_V)$ , then  $\chi f \in \mathbf{D}(H_V)$  and*

$$H_V(\chi f) = \chi H_V f - \nabla_{(d\chi)^\sharp} f - \frac{1}{2}(\Delta\chi)f. \tag{38}$$

Here,  $(d\chi)^\sharp$  denotes the vector field corresponding to the 1-form  $d\chi$  (with respect to the underlying Riemannian metric).

We first note that the Sobolev product rule

$$\nabla(\chi f) = (d\chi) \otimes f + \chi \nabla f \tag{39}$$

[which is applicable in view of (8) and (20)] shows that  $\chi f$  is in  $\mathbf{D}(q_{H_V})$ , so that in order to prove  $\chi f \in \mathbf{D}(H_V)$ , it is sufficient to construct a  $u \in \Gamma_{L^2}(M, E)$  such that

$$q_{H_V}(\chi f, h) = \langle u, h \rangle \tag{40}$$

for all  $h \in D(q_{H_V})$ , where then  $H_V(\chi f)$  is given by  $u$ . To this end, we calculate

$$\begin{aligned} q_{H_V}(\chi f, h) &= \frac{1}{2} \langle \nabla(\chi f), \nabla h \rangle + \langle V(\chi f), h \rangle \\ &= \frac{1}{2} \langle \nabla f, \nabla(\chi h) \rangle - \frac{1}{2} \langle \nabla f, (d\chi) \otimes h \rangle + \frac{1}{2} \langle (d\chi) \otimes f, \nabla h \rangle + \langle Vf, \chi h \rangle \\ &= \langle H_V f, \chi h \rangle - \langle \nabla_{(d\chi)^\sharp} f, h \rangle + \frac{1}{2} \langle (d^\dagger d\chi) f, h \rangle, \end{aligned}$$

where we have used (39) in the second equality, and  $f \in D(H_V)$  together with an integration by parts formula (Lemma 8.8 in [1]) and the Sobolev product rule

$$\nabla^\dagger(\alpha \otimes f) = (d^\dagger \alpha) f - \nabla_{\alpha^\sharp} f$$

for (sufficiently) smooth 1-forms  $\alpha$  in the third equality. In particular, we found a candidate  $u$  in (40) and it has the desired form as in (38). □

(II) *The space*

$$D^0(H_V) := D(H_V) \cap \{f \mid f \text{ has a compact support}\}$$

is dense in  $D(H_V)$  with respect to  $\|\bullet\|_{H_V}$ .

*Proof* By adding a constant, we can assume that  $H_V \geq 0$ . But then the result readily follows from combining Proposition 2.13 with Lemma B.1. □

(III) *The space*

$$D_{\infty, \text{loc}}^0(H_V) := D^0(H_V) \cap \Gamma_{L^\infty, \text{loc}}(M, E)$$

is dense in  $D^0(H_V)$  with respect to  $\|\bullet\|_{H_V}$ .

*Proof* Let  $f \in D^0(H_V)$  and take  $r > 0$ ,  $y \in M$  with  $\text{supp}(f) \subset K_r(y)$ . Furthermore, pick a  $\chi \in C_0^\infty(M)$  with  $\chi = 1$  in  $K_{r+1}(y)$  and set  $f_t := \chi e^{-tH_V} f$  for any  $t > 0$ . Then Proposition 2.11 implies  $f_t \in D_{\infty, \text{loc}}^0(H_V)$  and clearly  $\|f_t - f\| \rightarrow 0$  as  $t \rightarrow 0+$ . Furthermore, (I) implies  $H_V(\chi f) = H_V f$  and also

$$\begin{aligned} H_V(f_t - f) &= \chi H_V e^{-tH_V} f - \nabla_{(d\chi)^\sharp} e^{-tH_V} f - \frac{1}{2} (\Delta \chi) e^{-tH_V} f - \chi H_V f \\ &\quad + \nabla_{(d\chi)^\sharp} f + \frac{1}{2} (\Delta \chi) f. \end{aligned}$$

Now it is easily seen that  $\|H_V(f_t - f)\| \rightarrow 0$  as  $t \rightarrow 0+$ . □

(IV)  $\Gamma_{C_0^\infty}(M, E)$  is dense in  $D_{\infty, \text{loc}}^0(H_V)$  with respect to  $\|\bullet\|_{H_V}$  and one has

$$D(H_V) = \{f \mid f, (\nabla^\dagger \nabla + V)f \in \Gamma_{L^2}(M, E)\}. \tag{41}$$

*Proof* Let  $f \in D_{\infty, \text{loc}}^0(H_V)$ . By Lemma 2.8 and the self-adjointness of  $H_V$  we have  $H_V \subset H_{V, \text{min}}^*$ , but it is well-known that (see for example p.644 in [1])

$$D(H_{V, \text{min}}^*) = \{f \mid f, (\nabla^\dagger \nabla + V)f \in \Gamma_{L^2}(M, E)\}.$$

In particular  $D_{\infty, \text{loc}}^0(H_V) \subset D(H_{V, \text{min}}^*)$  implies  $w := \nabla^\dagger \nabla f + Vf \in \Gamma_{L^2}(M, E)$ . As  $f$  is locally bounded with a compact support, one also has  $Vf \in \Gamma_{L^2}(M, E)$ , so that

$\nabla^\dagger \nabla f = w - Vf \in \Gamma_{L^2}(M, E)$ . But now the assertion follows directly from Proposition A.1, which is in fact a local result (and which again heavily uses that  $f$  is locally bounded with a compact support).

Finally, (41) simply follows from the essential self-adjointness of  $\tilde{H}_{V,\min}$ , which follows from (II) and the by now proven fact that  $\Gamma_{C_0^\infty}(M, E)$  is an operator core for  $H_V$ . □

We immediately get:

**Corollary 2.15** *Theorem 1.1 holds, that is, under the assumptions of Theorem 2.14, the operator  $\nabla^\dagger \nabla / 2 + V$  is essentially self-adjoint on  $\Gamma_{C_0^\infty}(M, E)$ , and its closure is semibounded from below.*

*Proof* Combining Theorem 2.14 with Lemma 2.8 immediately gives  $H_{V,\min} = H_{V,\min}^* = H_V$ . □

### 3 Application to Hydrogen type problems on Riemannian 3-manifolds

In this section, we shall explain a typical application of Theorem 1.1: The essential self-adjointness of nonrelativistic Hamiltonians corresponding to hydrogen type atoms, with the electron’s spin is taken into account. To this end, let us first explain what the analogues of the Coulomb potential and the Pauli operator are in a general curved setting. Here, we are going to follow [16] closely.

*Throughout Sect. 3, we will assume that  $M$  is a smooth connected Riemannian 3-manifold without boundary.*

Firstly, we want to point out that “nonparabolicity” is the appropriate setting that admits natural analogues of the Coulomb potential:

**Definition 3.1** The Riemannian manifold  $M$  is called *nonparabolic*, if one has

$$\int_0^\infty p(t, x, y) dt < \infty \quad \text{for some (any) } x, y \in M \text{ with } x \neq y.$$

Then

$$G: M \times M \longrightarrow (0, \infty], G(x, y) := \int_0^\infty p(t, x, y) dt$$

is called the *Coulomb potential* on  $M$ .

It should be noted that nonparabolicity always implies noncompactness. The essential point for the interpretation of  $G$  as the Coulomb potential is that  $M$  is nonparabolic, if and only if  $M$  admits a positive Green’s function, and then  $G$  is the minimal positive Green’s function (see [16] and the references therein for these facts). The following criterion can be easily deduced from Theorem 2.3:

**Lemma 3.2** *Assume that there is a  $C > 0$  such that for all  $t > 0$  one has*

$$\sup_{x \in M} p(t, x, x) \leq Ct^{-3/2}. \tag{42}$$

Then  $M$  is nonparabolic and there is a  $\tilde{C} > 0$  with

$$G(x, y) \leq \frac{\tilde{C}}{d(x, y)} \quad \text{for all } x, y \in M. \tag{43}$$

Next, we will explain the natural analogues of the Pauli-operator in our general setting. To this end, we give ourselves a *Pauli-Dirac structure*  $(c, \nabla)$  on  $M$  in the sense of [16], that is, with a smooth Hermitian vector bundle  $E \rightarrow M$  with  $\text{rank } E = 2$ ,

$$c: T^*M \longrightarrow \text{End}(E)$$

is a Clifford multiplication<sup>4</sup> and  $\nabla$  is a Clifford connection<sup>5</sup> with respect to  $c$ .

*Remark 3.3* The existence of a Pauli-Dirac structure on  $M$  is a topological restriction, namely,  $M$  admits a Pauli-Dirac structure, if and only if  $M$  is a  $\text{spin}^{\mathbb{C}}$  manifold. This fact has also been explained in [16].

The *Pauli-Dirac operator*  $\mathcal{D}(c, \nabla)$  with respect to  $(c, \nabla)$  is defined by

$$\mathcal{D}(c, \nabla) := c \circ \nabla: \Gamma_{C_0^\infty}(M, E) \longrightarrow \Gamma_{C_0^\infty}(M, E),$$

which is a linear first order differential operator with  $\mathcal{D}(c, \nabla)^\dagger = \mathcal{D}(c, \nabla)$ . If  $(e_j)$  is some smooth local orthonormal frame for  $TM$ , then one has  $\mathcal{D}(c, \nabla) = \sum_j c(e_j^*) \nabla_{e_j}$ . Furthermore,  $\mathcal{D}(c, \nabla)^2$  is a generalized Laplacian on  $M$  which is given by the following Lichnerowicz formula:

**Lemma 3.4** *The differential form  $\text{tr}[\nabla^2]/i \in \Omega^2(M)$  is real-valued and closed, and one has*

$$\mathcal{D}(c, \nabla)^2 = \nabla^\dagger \nabla + \frac{1}{4} \text{scal}(\bullet) \mathbf{1} + \frac{1}{2} \sum_{i < j} \text{tr}[\nabla^2](e_i, e_j) c(e_i^*) c(e_j^*). \tag{44}$$

The last lemma makes it plausible [see also Remark 3.6 (b) below] to call  $\mathcal{D}(c, \nabla) := \mathcal{D}(c, \nabla)^2$  the *Pauli-Dirac operator* with respect to  $(c, \nabla)$ .

Clearly, if one has (42), then  $G(\bullet, y)$  exists and is locally square integrable for any  $y \in M$ , and for any such  $y$  and  $\kappa \geq 0$  one can consider the operator

$$\tilde{H}(c, \nabla; \kappa, y) := \mathcal{D}(c, \nabla) - \kappa G(\bullet, y) \mathbf{1}$$

in  $\Gamma_{L^2}(M, E)$  with domain of definition  $\Gamma_{C_0^\infty}(M, E)$ , which gives rise to a symmetric operator. Let us furthermore define the smooth potential

$$V(c, \nabla) := \frac{1}{4} \text{scal}(\bullet) \mathbf{1} + \frac{1}{2} \sum_{i < j} \text{tr}[\nabla^2](e_i, e_j) c(e_i^*) c(e_j^*). \tag{45}$$

<sup>4</sup> A Clifford multiplication  $c$  is a morphism of smooth vector bundles such that for all  $\alpha \in \Omega^1(M)$  one has

$$c(\alpha) = -c(\alpha)^*, c(\alpha)^* c(\alpha) = |\alpha|^2.$$

<sup>5</sup> A Clifford connection is a Hermitian connection with the following property: for all  $\alpha \in \Omega^1(M)$  and all  $X \in \Gamma_{C_0^\infty}(M, TM)$ ,  $\psi \in \Gamma_{C_0^\infty}(M, E)$  one has

$$\nabla_X(c(\alpha)\psi) = c(\nabla_X^{\text{TM}}\alpha)\psi + c(\alpha)\nabla_X\psi.$$

With these preparations, Theorem 1.1 has the following important consequence:

**Theorem 3.5** *Assume that  $M$  is geodesically complete with (42) and that  $V(c, \nabla)$  admits a decomposition*

$$V(c, \nabla) = V_1(c, \nabla) - V_2(c, \nabla)$$

*into potentials  $V_j(c, \nabla) \geq 0$  with  $|V_2(c, \nabla)| \in \mathcal{K}(M)$ . Then for any  $\kappa \geq 0$  and  $y \in M$ , the operator  $\tilde{H}(c, \nabla; \kappa, y)$  is essentially self-adjoint and its closure  $H(c, \nabla; \kappa, y)$  is semibounded from below.*

*Proof* Using (43) and Proposition 2.4 (a), one easily checks that Theorem 1.1 can be applied with

$$V := \frac{1}{4} \text{scal}(\bullet) \mathbf{1} + \frac{1}{2} \sum_{i < j} \text{tr}[\nabla^2](e_i, e_j) c(e_i^*) c(e_j^*) - \kappa G(\bullet, y) \mathbf{1},$$

which proves the claim. □

*Remark 3.6* (a) Let

$$S(c, \nabla) := \int_M \left\| \left\| \frac{1}{4} \text{scal}(\bullet) \mathbf{1} + \frac{1}{2} \sum_{i < j} \text{tr}[\nabla^2](e_i, e_j) c(e_i^*) c(e_j^*) \right\| \right\|_x^2 \text{vol}(dx) \in [0, \infty],$$

where  $\| \bullet \|_x$  stands for the fiberwise Hilbert–Schmidt norm. Using  $| \bullet |_x \leq \| \bullet \|_x$  and Proposition 2.4 (a), one sees that the assumption on  $V(c, \nabla)$  in Theorem 3.5 is obviously satisfied under (42), if  $S(c, \nabla) < \infty$ . This variant of Theorem 3.5 has been deduced in [16] with completely different methods, namely, using results of [1] (which rely on pure PDE methods).

(b) In the situation of Theorem 3.5, the operator  $H(c, \nabla; \kappa, y)$  can be interpreted [16] as the nonrelativistic Hamiltonian corresponding to an atom with one electron and a nucleus with  $\sim \kappa$  protons, where the electron’s spin has been taken into account and the nucleus is considered as fixed in  $y$  with respect to the electron. Here, in view of Lemma 3.4, the underlying magnetic field is given by  $\text{tr}[\nabla^2]/i \in \Omega^2(M)$ . In particular, the above mentioned assumption  $S(c, \nabla) < \infty$  is reasonable from the physics point of view, for it corresponds in a certain sense to a “finite magnetic self-energy” [it is essential for this interpretation to take the Hilbert–Schmidt norm in the definition of  $S(c, \nabla)$ ].

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### Appendix A. Friedrichs mollifiers

We record the following result on Friedrichs mollifiers here. Let  $M$  be a smooth connected Riemannian manifold without boundary,  $E \rightarrow M$  a smooth Hermitian vector bundle,  $\nabla$  a Hermitian covariant derivative in  $E$ , and  $V : M \rightarrow \text{End}(E)$  a potential.

**Proposition A.1** *Let  $|V| \in L^2_{\text{loc}}(M)$  and assume that  $f \in \Gamma_{\text{loc}}^\infty(M, E)$  is compactly supported with  $\nabla^\dagger \nabla f \in \Gamma_{\text{loc}}^2(M, E)$  in the sense of distributions. Then there is a sequence  $(f_n)_{n \in \mathbb{N}} \subset \Gamma_{\text{C}_0^\infty}(M, E)$  such that*

$$\begin{aligned} \lim_{n \rightarrow \infty} \|f_n - f\| &= 0, \\ \lim_{n \rightarrow \infty} \|\nabla^\dagger \nabla f_n - \nabla^\dagger \nabla f\| &= 0, \\ \lim_{n \rightarrow \infty} \|V f_n - V f\| &= 0. \end{aligned}$$

*Remark A.2* Note that one indeed has  $f \in \Gamma_{L^2}(M, E)$ , which follows from  $f \in \Gamma_{\text{loc}}^\infty(M, E)$  and the fact that  $f$  has a compact support. Furthermore,  $\nabla^\dagger \nabla f \in \Gamma_{L^2}(M, E)$  follows from  $\nabla^\dagger \nabla f \in \Gamma_{L^2_{\text{loc}}}(M, E)$  and the fact that  $\nabla^\dagger \nabla f$  has a compact support.

*Proof of Proposition 4.3* Since most of the arguments should be well-known, we only sketch the proof. Let  $m := \dim M$  and let  $d$  be the fiber dimension of  $E$ . Since  $f$  is compactly supported, we can use a partition of unity argument to assume that  $f$  is supported in a relatively compact coordinate domain  $U \subset M$  (which is identified with an open subset of  $\mathbb{R}^m$ ) such that there is a smooth orthonormal frame for  $E$  over  $U$ , and we denote the components of  $f$  in this frame with  $f^{(1)}, \dots, f^{(d)}$ . Now take some  $0 \leq j_r \in C_0^\infty(\mathbb{R}^m)$  with  $j(z) = 0$  for  $|z| \geq 1$  and

$$\int_{\mathbb{R}^m} j(z) dz = 1.$$

For  $r > 0$  let  $j_r \in C_0^\infty(\mathbb{R}^m)$  be given by  $j_r(z) = r^{-m} j(r^{-1}z)$ . Let  $r > 0$  be small enough in the following such that the functions

$$x \mapsto \int_{\mathbb{R}^m} j_r(x - y) f^{(i)}(y) dy, \quad i = 1, \dots, d, \tag{46}$$

define an element

$$f_r \in \Gamma_{\text{C}_0^\infty}(U, E) \subset \Gamma_{\text{C}_0^\infty}(M, E).$$

Since the sections  $f_r - f$  and  $\nabla^\dagger \nabla f_r - \nabla^\dagger \nabla f$  are compactly supported, the convergence

$$\lim_{r \rightarrow 0^+} \|f_r - f\| = 0 \tag{47}$$

follows from Lemma 5.13 (ii) in [1], and

$$\lim_{r \rightarrow 0^+} \|\nabla^\dagger \nabla f_r - \nabla^\dagger \nabla f\| = 0$$

follows from the  $L^2_{\text{loc}}$ -version of Proposition 5.14 in [1], which can be proven with analogous arguments. Note that so far we have only used that  $f$  is locally square integrable with a compact support.

The local boundedness assumption on  $f$  comes into play as follows: Namely, this assumption combined with the compact support assumption implies that  $f$  is actually *bounded* and so (46) implies

$$|f_r(x)|_x \leq \|f\|_\infty \quad \text{for all } x, r. \tag{48}$$



Since [in view of (47)] we may assume that  $f_r \rightarrow f$  a.e. in  $M$ , and since  $f_r$  has a compact support, the required convergence

$$\lim_{r \rightarrow 0^+} \|Vf_r - Vf\| = 0$$

now follows from (48) and dominated convergence. □

### Appendix B. Finite speed of propagation

The following lemma is usually referred to as Chernoff’s finite speed of propagation method [2]. Let  $M$  be a smooth connected Riemannian manifold without boundary, and let  $E \rightarrow M$  be a smooth Hermitian vector bundle.

**Lemma B.1** *Let  $S$  be a self-adjoint nonnegative operator in  $\Gamma_{L^2}(M, E)$ . Assume furthermore that  $D^0(S)$ , the compactly supported elements of  $D(S)$ , are dense in  $\Gamma_{L^2}(M, E)$  and that for any  $f \in D^0(S)$  and any  $t > 0$ , the section  $\cos(t\sqrt{S})f$  has a compact support. Then  $D^0(S)$  is an operator core for  $S$ .*

*Proof* The proof is a straightforward generalisation of the proof of Theorem 3 in [13]. □

### Appendix C. Path ordered exponentials

In the following lemma, we collect some known facts about path ordered exponentials for the convenience of the reader:

**Lemma C.1** *Let  $\mathcal{H}$  be a finite dimensional Hilbert space, let  $T \in (0, \infty]$  and let  $F \in L^1_{loc}([0, T], \mathcal{L}(\mathcal{H}))$ . Then the following assertions hold:*

(a) *There is a unique weak (=  $AC_{loc}$ ) solution  $Y : [0, T] \rightarrow \mathcal{L}(\mathcal{H})$  of the ordinary initial value problem*

$$\frac{d}{dt}Y(t) = Y(t)F(t), Y(0) = \mathbf{1}. \tag{49}$$

(b) *For any  $0 \leq t < T$  one has*

$$Y(t) = \mathbf{1} + \sum_{k=1}^{\infty} \int_{0 \leq s_1 \leq \dots \leq s_k \leq t} F(s_1) \dots F(s_k) ds_1 \dots ds_k. \tag{50}$$

(c) *If  $F(\bullet)$  is Hermitian a.e. in  $[0, T]$  and if there exists a real-valued function  $c \in L^1_{loc}[0, T]$  such that for all  $v \in \mathcal{H}$  it holds that*

$$\langle F(\bullet)v, v \rangle_{\mathcal{H}} \leq c(\bullet)\|v\|^2_{\mathcal{H}} \quad \text{a.e. in } [0, T],$$

*then one has*

$$\|Y(t)\|_{\mathcal{H}} \leq e^{\int_0^t c(s)ds} \quad \text{for all } 0 \leq t < T.$$

*Proof* See [7] and the Appendix C of [15]. □

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