BROWNIAN MOTION AND THE FEYNMAN-KAC FORMULA ON RIEMANNIAN MANIFOLDS

BATU GÜNEYSU

1. Introduction

Given a potential $w : \mathbb{R}^m \to \mathbb{R}$ and defining the *Schrödinger operator* $-\Delta + w$ in the Hilbert space $L^2(\mathbb{R}^m)$ of square-integrable functions $\Psi : \mathbb{R}^m \to \mathbb{C}$, in quantum physics one is interested in the unitary group

$$e^{-it(-\Delta+w)} \in \mathscr{L}(L^2(\mathbb{R}^m)), \quad \text{where } \Delta := \sum_{j=1}^m \partial_j^2 \text{ and } i := \sqrt{-1}.$$

Given an initial value $\Psi_0 \in L^2(\mathbb{R}^m)$ which is in the domain of definition of $-\Delta + w$, the Hilbert space valued function

$$[0,\infty) \ni t \longmapsto \Psi(t) := e^{-it(-\Delta+w)}\Psi_0 \in L^2(\mathbb{R}^m)$$

uniquely solves the Schrödinger equation

$$(d/dt)\Psi(t) = -i(-\Delta + w)\Psi(t), \quad \Psi(0) = \Psi_0$$

in the sense of Hilbert-space valued differentiable functions. Richard Feynman discovered in this PhD thesis 1948 the intuitive representation

$$e^{-it(-\Delta+w)}\Psi_0(x) = \frac{1}{Z(t)} \int_{\{\gamma:[0,\infty)\to\mathbb{R}^m,\gamma(0)=x\}} e^{-i\int_0^t w(\gamma(s))ds}\Psi_0(\gamma(t))e^{-i\int_0^t |\dot\gamma(s)|^2 ds} D^x(\gamma),$$

where $Z(t)$ is a certain normalization constant, where D^x is some sort of Lebesgue measure on the space of paths on $\mathbb{R}^m$ starting x and $\int_0^t |\dot\gamma(s)|^2 ds$ is the energy of such a path γ.

Unfortunately, one can *prove* that D^x does not exist[1], and of course many paths do not have a finite energy. In addition, strictly speaking one has $Z(t) = 0$.

On the other hand, switching from it to t, although each factor is problematic, by some 'miracle' the product

$$dP_t^x(\gamma) := \frac{1}{Z(t)} e^{-\int_0^t |\dot\gamma(s)|^2 ds} \cdot D^x(\gamma)$$

turns out to be well-defined in a sense that can be made precise. The point is that $e^{-\int_0^t |\dot\gamma(s)|^2 ds}$ is damping and can absorb some of the infinities of $D^x/Z(t)$, while $e^{-\int_0^t |\dot\gamma(s)|^2 ds}$ was oscillating and could not do that.

[1] There exists no nontrivial translation invariant measure on an infinite dimensional Banach space.

In fact, P^x_t turns out to be induced from a genuine probability measure P^x on the space of continuous paths $\gamma : [0,\infty) \to \mathbb{R}^m$ with $\gamma(0) = x$, which is called the *Wiener measure*. Furthermore, any process in $\mathbb{R}^m$ whose law is P^x is called a *Brownian motion on* $\mathbb{R}^m$ *with starting point* x.

Being equipped with this observation, given a Brownian motion $X^x : [0,\infty)\times\Omega \to \mathbb{R}^m$ with starting point x, which is defined on some probability space (Ω, P), it turns that the unique solution of the *heat semigroup* $e^{-t(-\Delta+w)} \in \mathscr{L}(L^2(\mathbb{R}^m))$, which with $\Psi(t) := e^{-t(-\Delta+w)}\Psi_0$ uniquely solves

$$(d/dt)\Psi(t) = -(-\Delta + w)\Psi(t), \quad \Psi(0) = \Psi_0$$

in the sense of Hilbert-space valued functions, admits the completely well-defined representation

$$e^{-t(-\Delta+w)}\Psi_0(x) = \int_\Omega e^{-\int_0^t w(X^x(s))ds}\Psi_0(X^x(t))dP,$$

which is the famous *Feynman-Kac formula.*

In this lecture course we are going to address the following questions:

- What is the precise definition of $-\Delta+w$ as a genuine (unbounded) self-adjoint operator in the Hilbert space $L^2(\mathbb{R}^m)$ which is bounded from below? This is a somewhat complicated problem, as in quantum physics, one has to deal with nonsmooth and unbounded potentials w such as the Coulomb potential $w(x) = -1/|x|$.
- What is the precise definition of Brownian motion in $\mathbb{R}^m$? This is closely related to the existence of the Wiener measure; which turns out to be induced in a sense that can be made precise by the Gauss-Weierstrass function

$$p : (0,\infty)\times\mathbb{R}^m\times\mathbb{R}^m \longrightarrow [0,\infty), \quad p(t, x, y) := (4\pi t)^{-m/2}e^{-\frac{|x-y|^2}{4t}}.$$

- What happens if we replace $\mathbb{R}^m$ with an open subset of $\mathbb{R}^m$ or more generally with an Riemannian manifold (and the Lebesgue measure with the Riemannian volume measure)? In fact, we are going to treat all the above problems from the very beginning on arbitrary (possibly noncompact) Riemannian manifolds. The essential observation here is that the Gauss-Weierstrass is the integral kernel of the heat semigroup ('heat kernel'),

$$e^{-t(-\Delta)}\Psi_0(x) = \int_{\mathbb{R}^m} p(t, x, y)\Psi_0(y)dy.$$

Note that in particular $p(t, x, y)$ is a fundamental solution of the heat equation in $\mathbb{R}^m$ in the sense that

$$\partial_t p(t, x, y) = -\Delta_x p(t, x, y), \quad \lim_{t\to 0+} p(t, \bullet, y) = \delta_y.$$

Thus, replacing Δ with the Laplace-Beltrami operator on a Riemannian manifold and the Lebsgue measure dy with the Riemannian volume measure, we will be interested in the *heat kernel* of a Riemannian manifold. In fact, proving its existence and its properties that guarantee the existence of the Wiener measure (or equivalently Brownian motion) on an arbitrary Riemannian manifold will be the main challenge of the course.

- The final part of the course will be devoted to the proof of the Feynman-Kac formula on an arbitrary Riemannian manifold.

We close this section with a brief historical account on the connection between Brownian motion and the heat equation: in 1827 the botanist Brown was watching small test particles (pollen,...) in suspended in a fluid medium (water,...) in a body $M \subset \mathbb{R}^3$ and was shocked by the fact that the pollen is moving. Having started with pollen, his first conclusion was that pollen is alive, until he repeated the experiment with other test particles that he was sure of not being alive. His observations were that the trajectory X of each test particle was random and independent of the trajectory of any other test particle (so wlog we can consider one test particle). This leads to the idea that X should be what we call today a stochastic process, that is, a map

$$X : [0,\infty) \times (\Omega, \mathscr{F}, P) \longrightarrow M,$$

where $(\Omega, \mathscr{F}, P)$ is a probability space. Here, the set Ω contains the random parameters and for each fixed $\omega \in \Omega$, the map

$$X(\omega) : [0,\infty) \longrightarrow M$$

is called a (random) path of the process. Then Brown observed that the expected displacement of the test particle was a decreasing function of its size and of viscosity of the medium, which increasing with the temperature of the medium.
Let

$$u(\cdot,\cdot,y) : (0,\infty) \times M \longrightarrow [0,\infty), \quad (t,x,y) \longmapsto u(t,x,y)$$

denote the probability density of X, assuming that X starts in some $y \in M$. In other words, the probability of finding X in $A \subset M$ at the time t is given by

$$P\{X_t \in A\} = \int_A u(t,x,y)dy.$$

It was then Einstein who derived in 1905 that this density solves the heat equation

$$\partial_t u(t,x,y) = -D\Delta_x u(t,x,y),$$

where the diffusion constant $D > 0$ of the system is given by

$$\frac{kT}{6\pi\nu R},$$

where k is the Boltzmann constant, T the temperature of the medium, ν its viscosity and R the radius of the test particle. Assuming that $u(t,x,y)$ behaves like the three dimensional Gauss-Weierstrass function, one can then easily derive the fundamental relation

$$\int_\Omega |X_t^j - y^j|^2 dP \approx D \cdot t, \tag{1}$$

for the average square displacement, which explains all observations of Brown. The stochastic process underlying the random trajectory of a test particle as above is precisely a *Brownian motion.*

Einstein's conclusion was that the medium consists of very small particles (which we would call molecules today), subject to some random kinematics, which bombard the larger test particles and lead to their random movement. The above fundamental relation (1) was confirmed in an experiment by Perrin in 1908 for which he received the Nobel price later. Note that all of this is roughly 20 years before quantum mechanics, and so these results can be thought of as a first confirmation of the atomic structure of matter.

2. Linear operators in Banach and Hilbert spaces

2.1. **Motivation.** We collect here some facts on linear operators. For a detailed discussion of the (standard) results below, we refer the reader to [39, 29, 23].

This section is motivated by the following observations from linear algebra: assume a linear operator T in a (say) complex *finite dimensional* Hilbert space $\mathscr{H} \cong \mathbb{C}^l$ is given. Then for every $\psi_0 \in \mathscr{H}$ there is a unique solution $\Psi : [0,\infty) \to \mathscr{H}$ of the 'heat equation'

$$(d/dt)\Psi(t) = -T\Psi(t), \quad \Psi(0) = \Psi_0.$$

In fact, we can simply set $\Psi(t) = e^{-tT}\Psi_0$, with

$$e^{-tT} = \sum_{j=0}^{\infty}(-tT)^j/j!$$

the matrix exponential series. Now if $\mathscr{H}$ is infinite dimensional (in our case this will the Hilbert space of square integrable functions on a Riemannian manifold), for T's one is interested in (in our case: the Laplace-Beltrami operator), the exponential series will never converge. The way out of this is provided by the following observation: assume in the above finite dimensional situation that T is *self-adjoint.* Then, as T is diagonalizable, one has

$$T = \int_{\{\lambda\in\mathbb{R}:\ \lambda \text{ is an eigenvalue of } T\}} \lambda \ P_T(d\lambda) := \sum_{\{\lambda\in\mathbb{R}:\ \lambda \text{ is an eigenvalue of } T\}} \lambda P_T(\lambda) \tag{2}$$

with $P_T(\lambda)$ the projection onto the eigenspace of λ. Given a function $f : \mathbb{R} \to \mathbb{C}$ (like $f(r) = e^{-tr}$!), the above formula suggests to define a linear operator $f(T)$ in $\mathscr{H}$ by setting

$$f(T) := \int_{\{\lambda\in\mathbb{R}:\ \lambda \text{ is an eigenvalue of } T\}} f(\lambda) \ P_T(d\lambda) := \sum_{\{\lambda\in\mathbb{R}:\ \lambda \text{ is an eigenvalue of } T\}} f(\lambda) P_T(\lambda). \tag{3}$$

For $f(r) = e^{-tr}$ this definition is equivalent to using the matrix exponential.

By John von Neumann's spectral theorem, it turns out that given any self-adjoint operator T in a possibly infinite dimensional Hilbert space there exists a unique projection-valued measure P_T such that one has

$$T = \int \lambda \ dP_T(\lambda),$$

and using the above observations this fact leads to satisfactory solution theory of the abstract heat equation induced by T. The purpose of this section is to explain these facts im detail. Before that, let us list some issues that are supposed to motivate some of the following definitions:

- a self-adjoint operator $T : \mathscr{H} \to \mathscr{H}$ in a Hilbert space is automatically bounded (= continuous). However, the operators we will be interested in (like the Laplace-Beltrami operator) turn out to be never bounded. The way out of this is consider linear operators $T : \mathrm{Dom}(T) \to \mathscr{H}$ that are defined on a (typically dense) subspace $\mathrm{Dom}(T) \subset \mathscr{H}$, called the *domain of definition of* T. Thus: any self-adjoint operator T in $\mathscr{H}$ with $\mathrm{Dom}(T) = \mathscr{H}$ is automatically bounded, the self-adjoint operators of interest are not bounded (and so cannot be defined everyhwere). Although self-adjoint operators are not bounded, they turn out to satisfy a weaker useful property, namely they are *closed*.
- In infinite dimensions, it is often easier to define a self-adjoint operator via symmetric sesquilinear forms. Note that in finite dimensions, given any symmetric sesquilinear form
$$Q : \mathscr{H} \times \mathscr{H} \longrightarrow \mathbb{C}$$
there exists a unique self-adjoin operator $T_Q : \mathscr{H} \to \mathscr{H}$ such that
$$Q(\Psi_1, \Psi_2) = \langle T_Q \Psi_1, \Psi_2 \rangle .$$
In the infinite dimensional case, again domain of definition questions arise and, in particular, one needs the sesqulinear form to be bounded from below in a certain sense in order that it induces a self-adjoint operator (which is then also bounded from below).
- In infinite dimensions, the actual definition of the adjoint of an operator (and thus of self-adjointness) is a bit subtle, which is due to the above mentioned domain of definition problems. In particular, we will distinguish symmetric operators from self-adjoint ones, noting that an everywhere defined operator is self-adjoint if any only if it is symmetric, and so this distinction is not needed in finite dimensions.

2.2. **Facts about linear operators in Banach and Hilbert spaces.** Classical references for the topics of this section are [40, 23].

We understand all our normed spaces to be over $\mathbb{C}$. As we have explained above, it is essential to require a linear operator T between Banach spaces $\mathscr{B}_1$ and $\mathscr{B}_2$ to be only defined on a subspace $\mathrm{Dom}(T) \subset \mathscr{B}_1$, called its *domain of definition*, so that T is actually a linear map $T : \mathrm{Dom}(T) \to \mathscr{B}_2$. Its image or *range* $\mathrm{Ran}(T) \subset \mathscr{B}_2$ is defined to be the linear space of all $f_2 \in \mathscr{B}_2$ for which there exists $f_1 \in \mathrm{Dom}(T)$ with $Tf_1 = f_2$. Its *kernel* $\mathrm{Ker}(T)$ is given by all $f \in \mathrm{Dom}(T)$ with $Tf = 0$.

Such a linear operator T is called *bounded*, if there exists a constant $C \geq 0$ such that $\|Tf\| \leq C \|f\|$ for all $f \in \mathrm{Dom}(T)$, and the smallest such C is called the operator norm of T and denotes by $\|T\|$. Boundedness of T is equivalent to its continuity as a map between normed spaces (considered as metric and thus topological spaces in the usual way). If

$\mathrm{Dom}(T)$ is dense, then T can be uniquely extended to a bounded linear map $\mathscr{B}_1 \to \mathscr{B}_2$, which will be denoted with the same symbol again. The linear space of bounded linear operators is denoted by $\mathscr{L}(\mathscr{B}_1, \mathscr{B}_2)$ and becomes a Banach space itself with the above operator norm. One sets

$$\mathscr{L}(\mathscr{B}_1) := \mathscr{L}(\mathscr{B}_1, \mathscr{B}_1).$$

Theorem 2.1 (Closed graph theorem). *A linear operator T from $\mathscr{B}_1$ to $\mathscr{B}_2$ is bounded, if and only if its graph*

$$\{(f_1, f_2) \in \mathrm{Dom}(T) \times \mathscr{B}_2 : Tf_1 = f_2\} \subset \mathscr{B}_1 \times \mathscr{B}_2$$

is closed.

We also record:

Theorem 2.2 (Uniform boundeness principle). *For a subset $A \subset \mathscr{L}(\mathscr{B}_1, \mathscr{B}_2)$ the following conditions are equivalent:*

- *for all $f \in \mathscr{B}_1$ there exists a constant $C_f \geq 0$ with $\|Tf\| \leq C_f$ for all $T \in A$.*
- *there exists a constant $C \geq 0$ with $\|T\| \leq C$ for all $T \in A$.*

Let $\mathscr{H}$ be a separable complex Hilbert space. The underlying scalar product, which is assumed to be antilinear in its first slot, will be simply denoted by $\langle \bullet, \bullet \rangle$, and the induced norm (as well as the induced operator norm) is denoted by $\|\bullet\|$.

Theorem 2.3 (Riesz-Fischer's duality theorem). *Assume $T \in \mathscr{L}(\mathscr{H}, \mathbb{C})$, that is, T is a linear continuous functional on $\mathscr{H}$. Then there exists a unique $f_T \in \mathscr{H}$ such that for all $h \in \mathscr{H}$ one has*

$$T(h) = \langle f_T, h \rangle .$$

The map $T \mapsto f_T$ induces an anti-linear isometric isomorphism between $\mathscr{L}(\mathscr{H}, \mathbb{C})$ and $\mathscr{H}$.

If $\tilde{\mathscr{H}}$ is another seperable complex Hilbert space case and R is a densely defined linear operator from $\mathscr{H}$ to $\tilde{\mathscr{H}}$, then the *adjoint* R^* of R is a linear operator from $\tilde{\mathscr{H}}$ to $\mathscr{H}$ which is defined as follows: $\mathrm{Dom}(R^*)$ is given by all $f \in \tilde{\mathscr{H}}$ for which there exists $f^* \in \mathscr{H}$ such that

$$\langle f^*, h \rangle = \langle f, Rh \rangle \quad \text{ for all } h \in \mathrm{Dom}(R),$$

and then $R^* f := f^*$.

In the sequel, let S and T be arbitrary linear operators in $\mathscr{H}$. Firstly, T is called *an extension of* S (symbolically $S \subset T$), if $\mathrm{Dom}(S) \subset \mathrm{Dom}(T)$ and $Sf = Tf$ for all $f \in \mathrm{Dom}(S)$.

If S is densely defined, then S is called *symmetric*, if $S \subset S^*$ and *self-adjoint* if $S = S^*$. Clearly, self-adjoint operators are symmetric. Note for the symmetry of only needs to check that it is densely defined

$$\langle Sf_1, f_2 \rangle = \langle f_1, Sf_2 \rangle$$

for all $f_1, f_2 \in \mathrm{Dom}(S)$. Checking self-adjointness is a tricky business for unbounded operators, while checking symmetry is very easy:

Example 2.4. Assume $U \subset \mathbb{R}^m$ is open and the operator $S := -\Delta = -\sum_{j=1}^m \partial_j^2$ in the complex Hilbert space $L^2(U)$ is given the domain of definition $\mathrm{Dom}(S) := C_c^\infty(U)$. Then S is symmetric: for all $f_1, f_2 \in \mathrm{Dom}(S) = C_c^\infty(U)$ by Stokes' Theorem one has

$$\langle Sf_1, f_2\rangle = \int_U \overline{(-\Delta) f_1} f_2 dx$$

$$= \int_U (\nabla f_1, \nabla f_2) dx + \text{a boundary term that vanishes because } f_j \text{ is compactly supported in } U$$

$$= \int_U \overline{f_1}(-\Delta) f_2 dx = \langle f_1, Sf_2\rangle \,.$$

This operator is not self-adjoint (in general it has many self-adjoint extensions; in case $U = \mathbb{R}^m$ it has precisely one self-adjoint extension; exercises).

The operator S is called *semibounded* (from below), if there exists a constant $C \geq 0$ such that for all $f \in \mathrm{Dom}(S)$ one has

$$\langle Sf, f\rangle \geq -C \left\| f \right\|^2 , \tag{4}$$

or in short: $S \geq -C$. Since $\mathscr{H}$ is assumed to be complex, semibounded operators are automatically symmetric (by complex polarization).

S is called *closed*, if whenever $(f_n) \subset \mathrm{Dom}(S)$ is a sequence such that $f_n \to f$ for some $f \in \mathscr{H}$ and $Sf_n \to h$ for some $h \in \mathscr{H}$, then one has $f \in \mathrm{Dom}(S)$ and $Sf = h$.

S is called *closable*, if it has a closed extension. In this case, S has a smallest closed extension $\overline{S}$, which is called the *closure of* S. The closure $\overline{S}$ is determined as follows: $\mathrm{Dom}(\overline{S})$ is given by all $f \in \mathscr{H}$ for which there exists a sequence $(f_n) \subset \mathrm{Dom}(S)$ such that $f_n \to f$ and such that (Sf_n) converges, and then $\overline{S}f := \lim_n Sf_n$.

Adjoints of densely defined operators are closed, so that that symmetric operators are closable; self-adjoint operators are closed. Bounded operators are always closed by the closed graph theorem.

If S is densely defined and closable, then S^* is densely defined and $S^{**} = \overline{S}$.

If T is symmetric, then T is called *essentially self-adjoint*, if $\overline{T}$ is self-adjoint. Then $\overline{T}$ is the unique self-adjoint extension of T.

We record:

Theorem 2.5. *Assume that S is semibounded (in particular, symmetric) with $S \geq -C$ for some constant $C \geq 0$. Then S is essentially self-adjoint, if and only if there exists $z \in \mathbb{C} \setminus [-C, \infty)$ such that* $\mathrm{Ker}((S - z)^*) = \{0\}$.

The *resolvent set* $\rho(S)$ is defined to be the set of all $z \in \mathbb{C}$ such that $S - z$ is invertible as a linear map $\mathrm{Dom}(S) \to \mathscr{H}$ and $(S - z)^{-1}$ is in addition bounded as a linear operator from $\mathscr{H}$ to $\mathscr{H}$. If S is closed and $(S - z)$ invertible, then $(S - z)^{-1}$ is automatically bounded by the closed graph theorem. The *spectrum* $\sigma(S)$ of S is defined as the complement $\sigma(S) := \mathbb{C} \setminus \rho(S)$. Resolvent sets of closed operators are open, therefore spectra of closed operators are always closed.

A number $z \in \mathbb{C}$ is called an *eigenvalue of* S, if $\mathrm{Ker}(S-z) \neq \{0\}$. In this case, $\dim \mathrm{Ker}(S-z)$ is called the *multiplicity* of z, and each $f \in \mathrm{Ker}(S-z) \setminus \{0\}$ is called an *eigenvector of S corresponding to z*. Of course each eigenvalue is in the spectrum. The eigenvalues of a symmetric operator are real, and the eigenvectors corresponding to different eigenvalues of a symmetric operator are orthogonal. A simple result that reflects the subtlety of the notion of a "self-adjoint operator" when compared to that of a"symmetric operator" is the following: A symmetric operator in $\mathscr{H}$ is self-adjoint, if and only if its spectrum is real. If S is self-adjoint, then $S \geq -C$ for a constant $C \geq 0$ is equivalent to $\sigma(S) \subset [-C, \infty)$ (cf. Satz 8.26 in [40]).

The *essential spectrum* $\sigma_{\mathrm{ess}}(S) \subset \sigma(S)$ of S is defined to be the set of all eigenvalues λ of S such that either λ has an infinite multiplicity, or λ is an accumulation point of $\sigma(S)$. Then the *discrete spectrum* $\sigma_{\mathrm{dis}}(S) \subset \sigma(S)$ is defined as the complement

$$\sigma_{\mathrm{dis}}(S) := \sigma(S) \setminus \sigma_{\mathrm{ess}}(S).$$

As every isolated point in the spectrum of a self-adjoint operator is an eigenvalue (cf. Folgerung 3, p. 191 in [39]), it follows that in case of S being self-adjoint, the set $\sigma_{\mathrm{dis}}(S)$ is precisely the set of all isolated eigenvalues of S that have a finite multiplicity.

Let $\tilde{\mathscr{H}}$ be another complex separable Hilbert space. We recall that given $q \in [1, \infty)$, some $K \in \mathscr{L}(\mathscr{H}, \tilde{\mathscr{H}})$ is called

- *compact*, if for every orthonormal sequence (e_n) in $\mathscr{H}$ and every orthonormal sequence (f_n) in $\tilde{\mathscr{H}}$ one has $\langle Ke_n, f_n \rangle \to 0$ as $n \to \infty$
- *q-summable* (or an element of the *q-th Schatten class of operators $\mathscr{H} \to \tilde{\mathscr{H}}$*), if for every (e_n), (f_n) as above one has

$$\sum_n |\langle Ke_n, f_n \rangle|^q < \infty.$$

Let us denote the class of compact operators with $\mathscr{J}^{\infty}(\mathscr{H}, \tilde{\mathscr{H}})$ and the q-th Schatten class with $\mathscr{J}^{q}(\mathscr{H}, \tilde{\mathscr{H}})$, with the convention $\mathscr{J}^{\bullet}(\mathscr{H}) := \mathscr{J}^{\bullet}(\mathscr{H}, \mathscr{H})$. These are linear spaces with

$$\mathscr{J}^{q_1}(\mathscr{H}, \tilde{\mathscr{H}}) \subset \mathscr{J}^{q_2}(\mathscr{H}, \tilde{\mathscr{H}}) \quad \text{for all } q_2 \in [1, \infty], \text{ with } q_1 \leq q_2,$$

and one has inclusions of the type $\mathscr{J}^{q} \circ \mathscr{L} \subset \mathscr{J}^{q}$, $\mathscr{L} \circ \mathscr{J}^{q} \subset \mathscr{J}^{q}$ for all $q \in [1, \infty]$, and $\mathscr{J}^{q_1} \circ \mathscr{J}^{q_2} \subset \mathscr{J}^{q_3}$ if $1/q_1 + 1/q_2 = 1/q_3$ with $q_j \in [1, \infty)$.
For obvious reasons, $\mathscr{J}^{1}$ is called the *trace class*, and moreover $\mathscr{J}^{2}$ is called the *Hilbert-Schmidt class.*

Example 2.6. A bounded operator K in $L^2(X, \mu)$-space is Hilbert-Schmidt, if (and only if) it is an integral operator with a square integrable integral kernel, that is, if

$$Kf(x) = \int k(x, y) f(y) d\mu(y)$$

for some $k \in L^2(X \times X, \mu \otimes \mu)$. This follows from evaluating

$$\sum_n |\langle Ke_n, f_n \rangle|^2$$

explicitly using Parseval's identity.

Let us now turn towards the formulation of the spectral theorem (I will follow [40] here):

Definition 2.7. A *spectral resolution* P on $\mathscr{H}$ is a map $P : \mathbb{R} \to \mathscr{L}(\mathscr{H})$ such that

- for every $\lambda \in \mathbb{R}$ one has $P(\lambda) = P(\lambda)^*$, $P(\lambda)^2 = P(\lambda)$ (that is, each $P(\lambda)$ is an orthogonal projection onto its image)
- P is monotone in the sense that $\lambda_1 \leq \lambda_2$ implies $\mathrm{Ran}(P(\lambda_1)) \subset \mathrm{Ran}(P(\lambda_2))$
- P is right-continuous in the strong topology[2] of $\mathscr{L}(\mathscr{H})$
- $\lim_{\lambda \to -\infty} P(\lambda) = 0$ and $\lim_{\lambda \to \infty} P(\lambda) = \mathrm{id}_{\mathscr{H}}$, both in the strong sense.

It follows that for every $f \in \mathscr{H}$, the function

$$\lambda \mapsto \langle P(\lambda)f, f \rangle = \|P(\lambda)f\|^2$$

is right-continuous and increasing. Thus by the usual Stieltjes construction[3] it induces a Borel measure on $\mathbb{R}$, which will be denoted by $\langle P(d\lambda)f, f \rangle$. This measure has the total mass

$$\langle P(\mathbb{R})f, f \rangle = \|f\|^2 .$$

Given such P and a Borel function $\phi : \mathbb{R} \to \mathbb{C}$, the set

$$D_{P,\phi} := \left\{ f \in \mathscr{H} : \int_{\mathbb{R}} |\phi(\lambda)|^2 \langle P(d\lambda)f, f \rangle < \infty \right\}$$

is a dense linear subspace of $\mathscr{H}$ (cf. Satz 8.8 in [40]), and accordingly one can define a linear operator $\phi(P)$ with $\mathrm{Dom}(\phi(P)) := D_{P,\phi}$ in $\mathscr{H}$ by mimicking the complex polarization identity,

$$\begin{aligned} \langle \phi(P)f_1, f_2 \rangle := \; & (1/4) \int_{\mathbb{R}} \phi(\lambda) \; \langle P(d\lambda)(f_1 + f_2), f_1 + f_2 \rangle \\ & -(1/4) \int_{\mathbb{R}} \phi(\lambda) \; \langle P(d\lambda)(f_1 - f_2), f_1 - f_2 \rangle \\ & +(\sqrt{-1}/4) \int_{\mathbb{R}} \phi(\lambda) \; \left\langle P(d\lambda)(f_1 - \sqrt{-1}f_2), f_1 - \sqrt{-1}f_2 \right\rangle \\ & -(\sqrt{-1}/4) \int_{\mathbb{R}} \phi(\lambda) \; \left\langle P(d\lambda)(f_1 + \sqrt{-1}f_2), f_1 + \sqrt{-1}f_2 \right\rangle , \end{aligned}$$

where $f_1, f_2 \in \mathrm{Dom}(\phi(P))$. Every spectral measure induces the following "calculus":

[2] $T_n \to T$ strongly in $\mathscr{L}(\mathscr{H})$ means that $T_n f \to Tf$ for all $f \in \mathscr{H}$; this is weaker that convergence in the operator norm toppology, which means that $\|T_n - T\| \to 0$.

[3] Given a right-continuous and increasing function $F : \mathbb{R} \to \mathbb{R}$ there exists precisely one measure μ_F on $\mathbb{R}$ such that for all $b > a$ one has $\mu_F((a, b]) = F(b) - F(a)$.

Theorem 2.8. *Let P be a spectral resolution on $\mathscr{H}$, and let $\phi:\mathbb{R}\to\mathbb{C}$ be a Borel function. Then:*
(i) *One has $\phi(P)^*=\overline{\phi}(P)$; in particular, $\phi(P)$ is self-adjoint, if and only if ϕ is real-valued.*
(ii) *One has $\|\phi(P)\|\leq \sup_{\mathbb{R}}|\phi|\in[0,\infty]$.*
(iii) *If $\phi\geq -C$ for some constant $C\geq 0$, then one has $\phi(P)\geq -C$.*
(iv) *If $\phi':\mathbb{R}\to\mathbb{C}$ is another Borel function, then*

$$\phi(P)+\phi'(P)\subset(\phi+\phi')(P),\ \mathrm{Dom}(\phi(P)+\phi'(P))=\mathrm{Dom}((|\phi|+|\phi'|)(P))$$

and

$$\phi(P)\phi'(P)\subset(\phi\phi')(P),\quad \mathrm{Dom}(\phi(P)\phi'(P))=\mathrm{Dom}((\phi\phi')(P))\cap\mathrm{Dom}(\phi');$$

in particular, if ϕ' is bounded, then

$$\begin{aligned}&\phi(P)+\phi'(P)=(\phi+\phi')(P),\\&\phi(P)\phi'(P)=(\phi\phi')(P).\end{aligned}$$

(v) *For every $f\in\mathrm{Dom}(\phi(P))$ one has*

$$\|\phi(P)f\|^2=\int_{\mathbb{R}}|\phi(\lambda)|^2\left\langle P(d\lambda)f,f\right\rangle.$$

One variant of the spectral theorem is:

Theorem 2.9. *For every self-adjoint operator S in $\mathscr{H}$ there exists precisely one spectral resolution P_S on $\mathscr{H}$ such that $S=\mathrm{id}_{\mathbb{R}}(P_S)$. The operator P_S is called* the spectral resolution of S, *and it has the following additional properties:*

- *P_S is concentrated on the spectrum of S in the sense that for every Borel function $\phi:\mathbb{R}\to\mathbb{C}$ one has*
$$\phi(P_S)=(1_{\sigma(S)}\cdot\phi)(P_S)$$
- *if $\phi:\mathbb{R}\to\mathbb{R}$ is continuous, then $\sigma(\phi(P_S))=\overline{\phi(\sigma(S))}$*
- *if $\phi,\phi':\mathbb{R}\to\mathbb{R}$ are Borel functions, then one has the transformation rule $(\phi\circ\phi')(P_S)=\phi(P_{\phi'(P_S)})$.*

In view of these results, given a self-adjoint operator S in $\mathscr{H}$, the calculus of Theorem 2.8 applied to $P=P_S$ is usually referred to as the *spectral calculus of S*. Likewise, given a Borel function $\phi:\mathbb{R}\to\mathbb{C}$ one sets

$$\phi(S):=\phi(P_S).$$

Note that we have

$$\left\langle\phi(S)f,f\right\rangle=\int_{\sigma(S)}\phi(\lambda)\left\langle P_S(d\lambda)f,f\right\rangle$$

or in short

$$\phi(S)=\int_{\sigma(S)}\phi(\lambda)\ P_S(d\lambda)$$

and for ϕ the identity,

$$S=\int_{\sigma(S)}\lambda\ P_S(d\lambda),$$

which is the promised variant of (2) and (3).

Remark 2.10. Let S be a self-adjoint operator in $\mathscr{H}$.
1. The spectral calculus of S is compatible with all functions of S that can be defined "by hand". For example, for every $z \in \mathbb{C} \setminus \mathbb{K}$ one has $\phi(S) = (S - z)^{-1}$ with $\phi(\lambda) := 1/(\lambda - z)$, or $S^n = \phi(S)$ with $\phi(\lambda) := \lambda^n$.
2. If S is a semibounded operator and $z \in \mathbb{C}$ is such that $\Re z < \min \sigma(S)$, then the spectral calculus (together with a well-known Laplace transformation formula for functions) shows that for every $b > 0$ one has the following formula for $f_1, f_2 \in \mathscr{H}$:

$$\left\langle (S - z)^{-b} f_1, f_2 \right\rangle = \frac{1}{\Gamma(b)} \int_0^\infty s^{b-1} \left\langle e^{zs} e^{-sS} f_1, f_2 \right\rangle ds. \tag{5}$$

3. If $S \geq -C$ for some constant $C \geq 0$, then the collection $(e^{-tS})_{t \geq 0}$ forms a strongly continuous self-adjoint semigroup of bounded operators (contractive, if one can pick $C = 0$), and one has the abstract smoothing effect

$$\mathrm{Ran}(e^{-tS}) \subset \bigcap_{n \in \mathbb{N}_{\geq 1}} \mathrm{Dom}(S^n) \quad \text{ for all } t > 0.$$

Moreover, for every $\psi_0 \in \mathscr{H}$ the path

$$[0, \infty) \ni t \longmapsto \psi(t) := e^{-tS} \psi_0 \in \mathscr{H}$$

is the uniquely determined continuous path with $\psi(0) = \psi_0$ which is differentiable in $(0, \infty)$ and satisfies there the *abstract heat equation*

$$(d/dt)\psi(t) = -S\psi(t).$$

This will be an exercise.
4. If $S \geq -C$ for some constant $C \geq 0$ and if $e^{-tS} \in \mathscr{J}^2(\mathscr{H})$ for some $t > 0$, then S has a purely discrete spectrum (so the spectrum consists of countably many eigenvalues having a finite multiplicity) and if one ennumerates the eigenvalues in an increasing way and counting multiplicity, (λ_n), then one has $-C \leq \lambda_0 < \lambda_1 \nearrow \infty$ if $\mathscr{H}$ is infinite dimensional.

Example 2.11. Assume on a sigma-finite measurable space (X, μ) we are given a measurable function $\psi : X \to \mathbb{C}$. Then the associated maximally defined multiplication in $L^2(X, \mu)$ is given by

$$\mathrm{Dom}(M_\psi) := \{f \in L^2(X, \mu) : \psi f \in L^2(X, \mu)\}, \quad M_\psi f(x) := \psi(x) f(x).$$

M_ψ is bounded from below, if and only if $\psi \geq C$ μ-a.e. for some $C \in \mathbb{R}$ and bounded, if and only $|\psi| \leq c$ μ-a.e. for some $c \geq 0$. Moreover, M_ψ is always closed, and a point $z \in \mathbb{C}$ lies in the spectrum if and only if for all $\epsilon > 0$ one has

$$\mu\{x \in X : |\psi(x) - z| < \epsilon\} > 0.$$

and z is an eigenvalue, if and only if

$$\mu\{x \in X : \psi(x) = z\} > 0.$$

The operator M_ψ is self-adjoint if only if $\psi(x) \in \mathbb{R}$ for μ-a.e. $x \in X$. In the latter case, concerning the spectral calculus, one has $\phi(M_\psi) = M_{\phi \circ \psi}$. Some of these statements will

be proved in the exercises.
Using the spectral theorem one can show that every self-adjoint operator is unitarily equivalent to a self-adjoint multiplication operator on some finite measure space. Here, a linear operator V between two Hilbert spaces is called *unitary*, if it is bijective with $V^{-1} = V^*$ and two linear operators are called *unitarily equivalent*, if there exits a unitary operator V with $B = V^*AV$.

We now collect some basic facts about possibly unbounded sesquilinear forms on Hilbert spaces. Unless otherwise stated, all statements below can be found in section VI of T. Kato's book [23].
Let again $\mathscr{H}$ be a complex separable Hilbert space. A *sesquilinear form* Q on $\mathscr{H}$ is understood to be a map

$$Q : \mathrm{Dom}(Q) \times \mathrm{Dom}(Q) \longrightarrow \mathbb{C},$$

where $\mathrm{Dom}(Q) \subset \mathscr{H}$ is a linear subspace called the *domain of definition of* Q, such that Q is antilinear[4] in its first slot, and linear in its second slot. The *quadratic form* induced by Q is simply the map

$$Q : \mathrm{Dom}(Q) \longrightarrow \mathbb{C}, \mapsto f \longmapsto Q(f,f).$$

Let Q and Q' be sesquilinear forms on $\mathscr{H}$ in this section.
Q' is called an *extension of* Q, symbolically $Q \subset Q'$, if $\mathrm{Dom}(Q) \subset \mathrm{Dom}(Q')$ and if both forms coincide on $\mathrm{Dom}(Q)$.
Q is called *symmetric*, if $Q(f_1, f_2) = Q(f_2, f_1)^*$, and *semibounded (from below)*, if its quadratic form is real-valued with and there exists a constant $C \geq 0$ such that

$$Q(f,f) \geq -C \left\| f \right\|^2 \quad \text{for all } f \in \mathrm{Dom}(Q), \tag{6}$$

symbolically $Q \geq -C$. Again by complex polarization, every semibounded form is automatically symmetric (as the quadratic form is real-valued).
Following Kato, given a sequence $(f_n) \subset \mathrm{Dom}(Q)$ and $f \in \mathscr{H}$ we write $f_n \underset{Q}{\longrightarrow} f$ as $n \to \infty$, if one has $f_n \to f$ in $\mathscr{H}$ and in addition

$$Q(f_n - f_m, f_n - f_m) \to 0 \quad \text{as } n, m \to \infty.$$

Then Q is called *closed*, if $f_n \underset{Q}{\longrightarrow} f$ implies that $f \in \mathrm{Dom}(Q)$. A semibounded Q is closed, if and only if for some/every $C \geq 0$ with $Q \geq -C$ the scalar product on $\mathrm{Dom}(Q)$ given by

$$\left\langle f_1, f_2 \right\rangle_{Q,C} = (1 + C) \left\langle f_1, f_2 \right\rangle + Q(f_1, f_2) \tag{7}$$

[4] We warn the reader, however, that in [23] the forms are assumed to be antilinear in their second slot; thus, if $Q(f_1, f_2)$ is a form in our sense, the theory from [23] has to be applied to the complex conjugate form $Q(f_1, f_2)^*$.

turns $\mathrm{Dom}(Q)$ into a Hilbert space. Futhermore, for a semibounded $Q \geq -C$ its closedness is equivalent to the lower-semicontinuity of the function

$$\mathscr{H} \longrightarrow [-C, \infty], \ f \longmapsto \begin{cases} Q(f,f), & \text{if } f \in \mathrm{Dom}(Q) \\ \infty \quad \text{else.} \end{cases}$$

The form Q is called *closable*, if it has a closed extension. If Q is semibounded and closable, then it has a smallest semibounded and closed extension $\overline{Q}$, which is (well-)defined as follows: $\mathrm{Dom}(\overline{Q})$ is given by all $f \in \mathscr{H}$ that admit a sequence $(f_n) \subset \mathrm{Dom}(Q)$ with $f_n \underset{Q}{\longrightarrow} f$; then one has

$$\overline{Q}(f,h) = \lim_n Q(f_n, h_n), \qquad \text{where } f_n \underset{Q}{\longrightarrow} f,\ h_n \underset{Q}{\longrightarrow} h.$$

If Q is closed, then a linear subspace $D \subset \mathrm{Dom}(Q)$ is called a *core* of Q, if $\overline{Q|_D} = Q$.

Proposition 2.12. *If Q and Q' are semibounded and closed, then $Q + Q'$ is semibounded and closed on its natural domain of definition.*

The following notions will be convenient:

Definition 2.13. Let Q be symmetric. If $\mathrm{Dom}(Q) \subset \mathrm{Dom}(Q')$, then Q' is called

- *Q-bounded with bound* < 1, if there exist constants $\delta \in [0,1)$, $A \in [0,\infty)$ such that

$$|Q'(f,f)| \leq A \|f\|^2 + \delta Q(f,f) \quad \text{ for every } f \in \mathrm{Dom}(Q), \tag{8}$$

- *infinitesimally Q-bounded*, if for every $\delta \in [0,\infty)$ there exists a constant $A = A_\delta \in [0,\infty)$ with (8).

The next result from perturbation theory is the famous KLMN (Kato-Lax-Lions-Milgram-Nelson) theorem and will allow us to consider perturbations of Laplacians by potentials later on:

Theorem 2.14. *Let Q be semibounded and closed, and let Q' be symmetric and Q-bounded with bound < 1. Then $Q + Q'$ is semibounded and closed on its natural domain* $\mathrm{Dom}(Q) \cap \mathrm{Dom}(Q') = \mathrm{Dom}(Q)$*. Moreover, every form core of Q is also one of $Q + Q'$, and for every constant $c \geq 0$ with $Q \geq -c$ and every A, δ as in (8) one has the explicit lower bound*

$$Q + Q' \geq -(1-\delta)c - A.$$

Using the spectral calculus one defines:

Definition 2.15. Given a self-adjoint operator S in $\mathscr{H}$, the (densely defined and symmetric) sesquilinear form Q_S in $\mathscr{H}$ given by $\mathrm{Dom}(Q_S) := \mathrm{Dom}(\sqrt{|S|})$ and

$$Q_S(f_1, f_2) := \left\langle \sqrt{|S|} f_1, \sqrt{|S|} f_2 \right\rangle$$

is called the *form associated with S*.

The following fundamental result links the world of densely defined, semibounded, closed forms with that of semibounded self-adjoint operators (cf. Theorem VIII.15 in [29] for this exact formulation):

Theorem 2.16. *For every self-adjoint semibounded operator S in $\mathscr{H}$, the form Q_S is densely defined, semibounded and closed. Conversely, for every densely defined, closed and semibounded sesquilinear form Q in $\mathscr{H}$, there exists precisely one self-adjoint semibounded operator S_Q in $\mathscr{H}$ such that $Q = Q_{S_Q}$. The operator S_Q will be called* the operator associated with Q.

The correspondence $S \mapsto Q_S$ has the following additional properties:

Theorem 2.17. *Let Q be densely defined, closed and semibounded. Then:*

- *S_Q is the uniquely determined self-adjoint and semibounded operator in $\mathscr{H}$ such that* $\mathrm{Dom}(S_Q) \subset \mathrm{Dom}(Q)$ *and*
$$\langle S_Q f_1, f_2\rangle = Q(f_1, f_2) \ \ \textit{for all } f_1 \in \mathrm{Dom}(S_Q),\ f_2 \in \mathrm{Dom}(Q).$$
- $\mathrm{Dom}(S_Q)$ *is a core of Q; some $f_1 \in \mathrm{Dom}(Q)$ is in $\mathrm{Dom}(S_Q)$, if and only if there exists $f_2 \in \mathscr{H}$ and a core D of Q with*
$$Q(f_1, f_3) = \langle f_2, f_3\rangle \qquad \textit{for all } f_3 \in D,$$
and then $S_Q f_1 = f_2$.
- *One has*
$$\mathrm{Dom}(Q) = \left\{ h \in \mathscr{H} :\ \lim_{t\to 0+} \left\langle \frac{h - e^{-tS_Q}h}{t}, h \right\rangle < \infty \right\},$$
$$Q(h,h) = \lim_{t\to 0+} \left\langle \frac{h - e^{-tS_Q}h}{t}, h \right\rangle.$$
- *One has the variational principle*

$$\min \sigma(S_Q) = \inf\{Q(f,f) :\ f \in \mathrm{Dom}(Q),\ \|f\| = 1\} \tag{9}$$
$$= \inf\{\langle S_Q f, f\rangle :\ f \in \mathrm{Dom}(S_Q),\ \|f\| = 1\}. \tag{10}$$

Notation 2.18. If Q, Q' are symmetric, we write $Q \geq Q'$, if and only if $\mathrm{Dom}(Q) \subset \mathrm{Dom}(Q')$ and $Q(f,f) \geq Q'(f,f)$ for all $f \in \mathrm{Dom}(Q)$.

The Friedrichs extension of a semibounded operator can be defined as follows:

Example 2.19. Let $S \geq -C$ be a symmetric (in particular, a densely defined) and semibounded operator in $\mathscr{H}$. Then the form $(f_1, f_2) \mapsto \langle S f_1, f_2\rangle$ with domain of definition $\mathrm{Dom}(S)$ is closable, and of course the closure $\tilde{Q}_S$ of that form is densely defined and semibounded. The operator S_F associated with $\tilde{Q}_S$ is called the *Friedrichs realization of S*. The operator S_F can also be characterized as follows: S_F is the uniquely determined self-adjoint semibounded extension of S with domain of definition $\subset \mathrm{Dom}(\tilde{Q}_S)$. Let $\mathscr{M}_C(S)$ denote the class of all self-adjoint extensions of S which are $\geq -C$. Thus we have $S_F \in \mathscr{M}_C(S)$, and in addition the following maximality property holds:
$$T \in \mathscr{M}_C(S) \quad \Rightarrow \quad Q_T \leq \tilde{Q}_S.$$

In particular, S_F has the smallest bottom of spectrum $\min \sigma(S_F)$ among all operators in $\mathscr{M}_C(S)$. This is Krein's famous result on the characterization of semibounded extensions [1] [24].

Remark 2.20. Let U be an open subset of $\mathbb{R}^m$.
1. The *fundamental lemma of distribution theory* states that given $f_1, f_2 \in L^1_{\mathrm{loc}}(U)$ one has $f_1 = f_2$ a.e., if and only if one has

$$\int_U \overline{f_1}\phi = \int_U \overline{f_2}\phi$$

for all smooth comactly supported functions ϕ on U.
2. Given $f \in L^1_{\mathrm{loc}}(U)$, $p \in [1, \infty]$, and a partial differential operator P on U with smooth coefficients, one says that $Pf \in L^p_{\mathrm{loc}}(U)$ *in the sense of distributions*, if there exists an $h \in L^p_{\mathrm{loc}}(U)$ such that for all smooth compactly supported functions ϕ on U one has

$$\int_U \overline{f} P^\dagger \phi = \int_U \overline{h}\phi,$$

where $P^\dagger$ denotes the formal adjoint of P. Then $Pf := h$ is uniquely determined and so well-defined by the fundamental lemma of distribution theory. Recall that the formal adjoint of $P = \sum_\alpha P_\alpha \partial^\alpha$ is the differential operator given by $P^\dagger \psi = \sum_\alpha (-1)^\alpha \partial^\alpha (\overline{P_\alpha}\psi)$.

Let us see how the Friedrichs construction can be used to define a self-adjoint realization of the Laplace operator $-\Delta$ in $L^2(U)$, where U is an arbitrary open subset of $\mathbb{R}^m$: consider $-\Delta$ as a linear operator in $L^2(U)$, defined initially on $C^\infty_c(U)$. We have seen above that $-\Delta$ is symmetric; more precisely, for all $f_1, f_2 \in C^\infty_c(U)$ one has

$$\langle (-\Delta) f_1, f_2 \rangle_U = \int_U (\nabla f_1, \nabla f_2),$$

so

$$\langle (-\Delta) f_1, f_1 \rangle = \int_U |\nabla f_1|^2 \geq 0,$$

and $-\Delta \geq 0$ in $L^2(U)$. It follows from the previous example that $-\Delta$ canonically induces a self-adjoint operator $H_U \geq 0$ in $L^2(U)$, called the *Dirichlet-Laplacian* in U. In terms of the Euclidean Sobolev spaces $W^{k,p}(U)$ and $W^{k,p}_0(U)$: one has

$$\mathrm{Dom}(H_U) = \{f \in W^{1,2}_0(U) : \Delta f \in L^2(U)\}, \quad H_U f = -\Delta f,$$

where Δf is understood in the sense of distributions. Here, given $p \in [1, \infty]$, $k \in \mathbb{N}$, the Banach space $W^{k,p}(U)$ is given by all $f \in L^p(U)$ such that $\partial^\alpha f \in L^p(U)$ for all $|\alpha| \leq k$, and $W^{k,p}_0(U)$ denotes the closure of $C^\infty_c(U)$ in $W^{k,p}(U)$.

3. Basic facts on differential operators on Riemann manifolds

Let M be a manifold[5] of dimension m. Recall that a *vector bundle of rank* ℓ is a smooth surjective map of manifolds $\pi : E \to M$ such that for all $x \in M$ the *fiber* $E_x := \pi^{-1}(\{x\}) \subset$

[5]We understand all our manifolds ad bundles to be smooth and without boundary.

E over x is an ℓ-dimensional vector space, and for every $x_0 \in M$ there exists an open neighbourhood U of x_0 and smooth maps $e_1, \dots, e_\ell : U \to E$ such that

- $e_j(x) \in E_x$ for all $x \in U$, $j = 1, \dots, \ell$,
- $e_1(x), \dots, e_\ell(x) \in E_x$ is a basis.

For example, $\pi : E = M \times \mathbb{C}^l \to M$ is a vector bundle ('trivial vector bundle') with π the projection. Or examples come from differential topology: $\pi : TM \to M$ is the tangent bundle, $\pi : T^*M \to M$ the cotangent bundle, and one can forms bundles like $\pi : E_1 \otimes E_2 \to M$, $\pi : E_1 \wedge E_2 \to M$ etc. in a natural way.

Given an open subset $U \subset M$, we denote with $\Gamma_{C^\infty}(U, E)$ the smooth sections of $E \to M$ over U, that is, the linear space (in fact $C^\infty(U)$ left module, where $C^\infty(U) = C^\infty(U, \mathbb{C})$) of all smooth maps $\psi : U \to E$ with $\psi(x) \in E_x$ for all $x \in U$. Likewise, smooth compactly supported sections will be denoted with $\Gamma_{C^\infty_c}(U, E)$. Note that, as we have already done, one can often safely ommit the map π in the notation.

Let $E \to M$, $F \to M$ be vector bundles over M with rank ℓ_0 and rank ℓ_1, respectively. We understand all vector bundles over $\mathbb{C}$ (if not we can complexify; for example, a priori, the tangent bundle $E = TM \to M$ is of course naturally given over $\mathbb{R}$).

In case $E = M \times \mathbb{C}^l \to M$ is a trivial vector bundle, then each fiber E_x is given by $\{x\} \times \mathbb{C}^l$ and we can identify $\Gamma_{C^\infty}(M, E)$ with $C^\infty(M, \mathbb{C}^l)$.

A linear map

$$P : \Gamma_{C^\infty}(M, E) \longrightarrow \Gamma_{C^\infty}(M, F)$$

is called *restrictable*, if for all open $U \subset M$ there exists a linear map

$$P|_U : \Gamma_{C^\infty}(U, E) \longrightarrow \Gamma_{C^\infty}(U, F)$$

with $P|_U \psi|_U = (P\psi)|_U$ for all $\psi \in \Gamma_{C^\infty}(M, E)$.

Definition 3.1. A restrictable linear map

$$P : \Gamma_{C^\infty}(M, E) \longrightarrow \Gamma_{C^\infty}(M, F)$$

is called a (smooth, linear) *partial differential operator of order* $\leq k \in \mathbb{N}_{\geq 0}$, if for any chart $((x^1, \dots, x^m), U)$ of M which admits frames[6] $e_1, \dots, e_{\ell_0} \in \Gamma_{C^\infty}(U, E)$, $f_1, \dots, f_{\ell_1} \in \Gamma_{C^\infty}(U, F)$, and any multi-index[7] $\alpha \in \mathbb{N}^m_k$, there are (necessarily uniquely determined) smooth functions

$$P_\alpha : U \longrightarrow \mathrm{Mat}(\mathbb{C}; \ell_0 \times \ell_1)$$

such that for all $(\phi^{(1)}, \dots, \phi^{(\ell_0)}) \in C^\infty(U, \mathbb{C}^{\ell_0})$ one has

$$P|_U \sum_{i=1}^{\ell_0} \phi^{(i)} e_i = \sum_{j=1}^{\ell_1} \sum_{i=1}^{\ell_0} \sum_{\alpha \in \mathbb{N}^m_k} P_{\alpha ij} \frac{\partial^{|\alpha|} \phi^{(i)}}{\partial x^\alpha} f_j \quad \text{in } U.$$

Any differential operator P satisfies $\mathrm{supp}(P\psi) \subset \mathrm{supp}(\psi)$, that is, P is local.

---

[6]that is, 'frame' means that $e_1(x), \dots, e_{\ell_0}(x)$ is basis of E_x for all $x \in U$

[7]$\mathbb{N}^m_k$ denotes the set of multi-indices $\alpha = (\alpha_1, \dots, \alpha_m) \in (\mathbb{N}_{\geq 0})^m$ such that $\alpha_1 + \dots + \alpha_m \leq k$.

Definition 3.2. Let $k \in \mathbb{N}_{\geq 0}$ and let

$$P : \Gamma_{C^\infty}(M, E) \longrightarrow \Gamma_{C^\infty}(M, F)$$

be a differential operator of order $\leq k$.
a) The (linear k-th order principal) symbol of P is the unique morphism

$$\mathrm{symb}^k_P : (T^*M)^{\odot k} \otimes E \longrightarrow F$$

of vector bundles, where $\odot$ stands for the symmetric tensor product, such that for all $((x^1, \dots, x^m), U)$, $e_1, \dots, e_{\ell_0}$, $f_1, \dots, f_{\ell_1}$ as in Definition 3.1, and all real-valued $\zeta^{(i)}_\alpha \in C^\infty(U)$ (where i runs through $i = 1, \dots, \ell_0$ and α runs through $\alpha \in \mathbb{N}^m$ is such that $\alpha_1 + \cdots + \alpha_m = k$), one has

$$\mathrm{symb}^k_P \left(\sum_{\alpha \in \mathbb{N}^m : \alpha_1 + \cdots + \alpha_m = k} \sum_{i=1}^{\ell_0} \zeta^{(i)}_\alpha dx^\alpha_\odot \otimes e_i \right) = \sum_{\alpha \in \mathbb{N}^m : \alpha_1 + \cdots + \alpha_m = k} \sum_{i=1}^{\ell_0} \sum_{j=1}^{\ell_1} P_{\alpha i j} \zeta^{(i)}_\alpha f_j \quad \text{in } U.$$

b) P is called *elliptic*, if for all $x \in M$, $v \in T^*_x M \setminus \{0\}$, the linear map $\mathrm{symb}^k_{P,x}(v^{\otimes k}) : E_x \to F_x$ is invertible.

Remark 3.3. 1. Keep in mind that (at least locally) an operator P of order $\leq k$ can also be considered as having order $\leq l$ where $l > k$ (set the higher order coefficients $= 0$), and then P can be elliptic as in the k-sense but not in the l-sense. Thus we always have to specify the order of P when we talk about ellipticity.
2. Ellipticity is a local question: it needs to be checked in some chart around x only.

A (smooth) metric h_E on $E \to M$ is by definition a section $h_E \in \Gamma_{C^\infty}(M, E^* \otimes E^*)$, such that h_E is fiberwise a scalar product. Then the datum $(E, h_E) \to M$ is referred to as a *metric vector bundle*. In other words, for every $x \in M$ we have a scalar product $h_E(x) : E_x \times E_x \to \mathbb{C}$ and $h_E(x)$ depends smoothly on x. The trivial vector bundle $M \times \mathbb{C}^l \to M$ is equipped with its canonic smooth metric which is induced by $(z, z') \mapsto \sum_{j=1}^{l} \overline{z_j} z_j$, where $z, z' \in \mathbb{C}^l$.

Definition 3.4. A Riemannian metric on M is by definition a metric g on $TM \to M$, and then the pair (M, g) is called a (smooth) *Riemannian manifold.*

Proposition and definition 3.5. *For any Riemannian metric g on M there exists precisely one Borel measure μ_g on M such that for every chart $((x^1, \dots, x^m), U)$ for M and any Borel set $N \subset U$, one has*

$$\mu_g(N) = \int_N \sqrt{\det(g(x))} dx,$$

where $\det(g(x))$ *is the determinant of the matrix* $g_{ij}(x) := g(\partial_i, \partial_j)(x)$ *and where* $dx = dx^1 \cdots dx^m$ *stands for the Lebesgue integration.*

Proof. Exercise. ∎

The above measure μ_g is called the *Riemannian volume measure* on (M,g). It is a Radon measure with a full topological support in the sense that $\mu_g(U)>0$ for all open nonempty $U\subset M$.

Remark 3.6. That two Borel sections are equal μ_g-a.e. does not depend on a particular choice of g. Thus, given $k\in\mathbb{N}_{\geq 0}$, $q\in[1,\infty]$ we can define a the local Sobolev space $\Gamma_{W^{k,q}_{\mathrm{loc}}}(M,E)$ to be the space of equivalence classes of Borel sections ψ of $E\to M$ such that in every chart $U\subset M$ in which $E\to M$ admits a local frame e_j one has $\psi^{(j)}\in W^{k,q}_{\mathrm{loc}}(U)$, if $\psi=\sum_j\psi^{(j)}e_j$ in U. In particular, we get the local L^q-spaces

$$\Gamma_{L^q_{\mathrm{loc}}}(M,E):=\Gamma_{W^{0,q}_{\mathrm{loc}}}(M,E).$$

The fundamental lemma of distribution theory takes the following form:

Lemma 3.7. *For all $f_1,f_2\in\Gamma_{L^1_{\mathrm{loc}}}(M,E)$ one has $f_1=f_2$ a.e., if and only if there exists a pair (respectively: for all pairs) of metrics (g,h_E) with*

$$\int_M h_E(f_1,\psi)d\mu_g=\int_M h_E(f_2,\psi)d\mu_g\quad\textit{for all }\psi\in\Gamma_{C^\infty_c}(M,E).$$

Proof. $\Rightarrow$: Clear.
$\Leftarrow$: Let $U\subset M$ be a chart which admits an orthonormal frame $e_1,\dots,e_l$ for $(E,h_E)\to M$ (of course M be can covered with such U's) and let ψ be an arbitrary smooth section with a compactl support in U. Then writing $f_j=\sum_i f^i_j e_i$, $j=1,2$, and $\psi=\sum_i\psi^i e_i$ we have

$$\begin{aligned}&\int_U\sum_i\sqrt{\det(g)}\cdot\overline{f^i_1}\psi^i dx=\int_M h_E(f_1,\psi)d\mu_g=\int_M h_E(f_2,\psi)d\mu_g\\&=\int_U\sum_i\sqrt{\det(g)}\cdot\overline{f^i_2}\psi^i dx,\end{aligned}$$

so that by the Euclidean fundamental lemma of distribution theory we have

$$\sqrt{\det(g)}\cdot\overline{f^i_1}=\sqrt{\det(g)}\cdot\overline{f^i_2}$$

a.e. in U, for all i, so $f_1=f_2$ as $\sqrt{\det(g)}>0$.
It is now obvious that these statements are equivalent to: for all pairs (g,h_E) one has.... ■

Now we can prove:

Proposition and definition 3.8. *Assume that g is a Riemannian metric on M and that $(E,h_E)\to M$ and $(F,h_F)\to M$ are metric vector bundles. Then for any differential operator*

$$P:\Gamma_{C^\infty}(M,E)\longrightarrow\Gamma_{C^\infty}(M,F)$$

of order $\leq k$ there is a uniquely determined differential operator

$$P^{g,h_E,h_F}:\Gamma_{C^\infty}(M,F)\longrightarrow\Gamma_{C^\infty}(M,E)$$

of order $\leq k$ which satisfies

$$\int_M h_E\left(P^{g,h_E,h_F}\psi,\phi\right)d\mu_g=\int_M h_F\left(\psi,P\phi\right)d\mu_g$$

for all $\psi\in\Gamma_{C^\infty}(M,F)$, $\phi\in\Gamma_{C^\infty}(M,E)$ with either ϕ or ψ compactly supported. The operator P^{g,h_E,h_F} is called the formal adjoint of P with respect to (g,h_E,h_F). *An explicit local formula for P^{g,h_E,h_F} can be found in the proof.*

Proof. Uniqueness follows from the fundamental lemma of distribution theory. As differential operators are local, it is sufficient to prove the local existence. To this end, in the situation of Definition 3.1, we assume that e_i and f_j are orthonormal with respect to h_E and h_F, respectively. Then an integration by parts shows that

$$P^{g,h_E,h_F}\sum_{j=1}^{\ell_1}\psi^{(i)}f_j:=\frac{1}{\sqrt{\det(g)}}\sum_{i=1}^{\ell_0}\sum_{j=1}^{\ell_1}\sum_{\alpha\in\mathbb{N}_k^m}(-1)^{|\alpha|}\frac{\partial^{|\alpha|}\left(\overline{P_{\alpha ji}}\sqrt{\det(g)}\psi^{(j)}\right)}{\partial x^\alpha}e_i\quad\text{in } U \tag{11}$$

does the job. ■

There is a way to define the action of differential operators on locally integrable functions:

Proposition and definition 3.9. *Given P as above, $f\in\Gamma_{L^1_{\mathrm{loc}}}(M,E)$ and a subspace $A\subset\Gamma_{L^1_{\mathrm{loc}}}(M,F)$ we write $Pf\in A$, if there exists $h\in A$, such that for all triples of metrics (g,h_E,h_F) it holds that*

$$\int_M h_E\left(P^{g,h_E,h_F}\psi,f\right)d\mu_g=\int_M h_F\left(\psi,h\right)d\mu_g\ \ \textit{for all }\psi\in\Gamma_{C^\infty_c}(M,F)\ . \tag{12}$$

Then h is uniquely determined and we set $Pf:=h$. This property is equivalent to (12) being true for some *triple (g,h_E,h_F) of this kind (and is thus independent of the metrics).*

Proof. Clearly h is uniquely determined by the fundamental lemma of distribution theory. It remains to show that if (12) holds for some triple (g,h_E,h_F) then it also holds for any other such triple. This is left as an exercise. ■

Remark 3.10. One says that given $f_n,f\in\Gamma_{L^1_{\mathrm{loc}}}(M,E)$ that $f_n\to f$ in the sense of distributions, if for all $\psi\in\Gamma_{C^\infty_c}(M,E)$ and some pair of metrics (g,h_E) one has

$$\int_M h_E\left(f_n-f,\psi\right)d\mu_g\to 0$$

as $n\to\infty$. Using that ψ is compactly supported one easily checks that this automatically holds for all pairs of metrics (g,h_E). Moreover, distributional limits are uniquely determined. Given P as above, it is clear that $f_n\to f$ in the sense of distributions implies $Pf_n\to Pf$ in the sense of distributions, if $Pf_n,Pf\in\Gamma_{L^1_{\mathrm{loc}}}(M,E)$ (as the action of P is defined by duality).

Lemma 3.11 (Local elliptic regularity)**.** *Assume*

$$P:\Gamma_{C^\infty}(M,E)\longrightarrow\Gamma_{C^\infty}(M,F)$$

is elliptic of order $\leq k$ *and let* $q \in [1,\infty)$. *Then for all* $f \in \Gamma_{L^q_{\mathrm{loc}}}(M,E)$ *with* $Pf \in \Gamma_{L^q_{\mathrm{loc}}}(M,F)$ *one has* $f \in \Gamma_{W^{k,q}_{\mathrm{loc}}}(M,E)$ *if* $q>1$ *and* $f \in \Gamma_{W^{k-1,1}_{\mathrm{loc}}}(M,E)$ *if* $q=1$.

Proof. The $q>1$ is a classical fact by Nirenberg [27] and can be found in many textbooks such as [28]. The $q=1$ case is nonstandard uses Besov spaces. Together with Guidetti and Pallara I have given a proof in [10]. ■

Recall in this context that the local Sobolev embedding implies

$$\bigcap_{l\in\mathbb{N}} \Gamma_{W^{l,p}_{\mathrm{loc}}}(M,E) \subset \Gamma_{C^\infty}(M,E) \quad \text{for all } p \in (1,\infty). \tag{13}$$

Remark 3.12. To give an idea of how ellipticity comes into play in such a result: Assume $M=\mathbb{R}^m$ and $E=F$ are the trivial line bundles $\mathbb{R}^m\times\mathbb{C}\to\mathbb{C}$ (so that P acts on functions and has scalar coefficients). Assume further that $P=\sum_{|\alpha|\leq k} P_\alpha \partial^\alpha$ has constant coefficients. The global Sobolev spaces $W^{k,2}(\mathbb{R}^m)$, $k\in\mathbb{N}$, can be equivalently defined via Fourier transform

$$F : S'(\mathbb{R}^m) \longrightarrow S'(\mathbb{R}^m) \tag{14}$$

mapping between Schwartz distributions:

$$W^{k,2}(\mathbb{R}^m) = \{f \in L^2(\mathbb{R}^m) : \int |Ff(\zeta)|^2(1+|\zeta|^2)^k d\zeta < \infty\}.$$

Recall here that the space of Schwartz functions $S(\mathbb{R}^m)$ is defined to be the space of smooth functions $\phi:\mathbb{R}^m\to\mathbb{C}$ such that

$$p_{\alpha,\beta}(\phi) := \sup_{x\in\mathbb{R}^m} |x^\alpha \partial^\beta \phi(x)| < \infty,$$

which becomes a topologic vector space with the family of seminorms $p_{\alpha,\beta}$, and that the space of Schwartz distributions $S'(\mathbb{R}^m)$ is defined as the space of continuous linear forms on $S(\mathbb{R}^m)$. The Fourier transform is a priori a linear homeomorphism

$$F : S(\mathbb{R}^m) \longrightarrow S(\mathbb{R}^m),$$

which extends to a unitary map

$$F : L^2(\mathbb{R}^m) \longrightarrow L^2(\mathbb{R}^m),$$

and which acts dually to give the linear homeomorphism (14).
Then P defines a continuous map

$$P : W^{k,2}(\mathbb{R}^m) \to L^2(\mathbb{R}^m),$$

which, using that $F^{-1}PF$ is nothing but multiplication by $\zeta \mapsto \sum_{|\alpha|\leq k} P_\alpha \zeta^\alpha$, can be shown to be bijective, if $\sum_{|\alpha|=k} P_\alpha\zeta^\alpha \neq 0$ for all $\zeta \in \mathbb{R}^m\setminus\{0\}$ (this requires some work). So $Pf=g\in L^2(\mathbb{R}^m)$ implies $f=P^{-1}g\in W^{k,2}(\mathbb{R}^m)$.
The case of nonconstant coefficients can be deduced from this result by 'freezing the coefficients' (leading to $\tilde{P}$ with constant coefficients) and estimating the error $P-\tilde{P}$ carefully. Finally, the local manifold case follows from this by a partition of unity argument.

From now on we fix once for all a connected Riemannian manifold $M = (M, g)$ with dimension m.

We are going to ommit the dependence on g in the notation whenever there is no danger of confusion. For example the Riemann volume measure is denoted by μ. In addition, a metric vector bundle is simply depicted by $E \to M$, that is, the dependence on the fiber metrics will be ommited in the notation and the metric on $E \to M$ is simply denoted by $(\cdot, \cdot)$. For all $q \in [1, \infty]$ we get the global[8] Banach space $\Gamma_{L^q}(M, E)$ given by all equivalence classes of Borel sections f of $E \to M$ such that

$$\|f\|_q < \infty,$$

where

$$\|f\|_q := \begin{cases} \inf\{C \geq 0 : |f| \leq C \ \ \mu\text{-a.e.}\}, & \text{if } q = \infty \\ \left(\int_M |f|^q d\mu\right)^{1/q} & \text{else,} \end{cases}$$

and

$$|f| := \sqrt{(f, f)}$$

is the fiberwise norm. The space $\Gamma_{L^2}(M, E)$ becomes a Hilbert space via

$$\langle f_1, f_2 \rangle := \int_M (f_1, f_2) d\mu.$$

With this convention, it makes sense to denote the formal adjoint of a differential operator

$$P : \Gamma_{C^\infty}(M, E) \longrightarrow \Gamma_{C^\infty}(M, F)$$

acting between metric vector bundles simply by

$$P^\dagger : \Gamma_{C^\infty}(M, F) \longrightarrow \Gamma_{C^\infty}(M, E).$$

We record:

Lemma 3.13. *The space $\Gamma_{C^\infty_c}(M, E)$ is dense in $\Gamma_{L^q}(M, E)$ for all $q \in [1, \infty)$. In particular, $C^\infty_c(M)$ is dense in $L^q(M)$.*

Proof. Step 1: $A := \Gamma_{L^q_c}(M, E)$ is dense in $\Gamma_{L^q}(M, E)$.
Proof of step 1: Pick an exhaustion K_n of M with compact sets. Given $f \in \Gamma_{L^q}(M, E)$ set $f_n := 1_{K_n} f \in A$. Then we have

$$\lim_n \int |f_n - f|^q d\mu = \lim_n \int |(1_{K_n} - 1)|^q |f|^q d\mu = 0$$

by dominated convergence.
Step 2: $\Gamma_{C^\infty_c}(M, E)$ is dense in A.
Proof of step 2: Given $f \in A$ cover its support by finitely many charts (U_n) for M which admit an orthonormal frame. Pick a partition of unity $(\phi_n) \subset C^\infty_c(M)$ subordinate to

[8] Unlike the local L^q-spaces considered above, these spaces depend very much on all choices of metrics, unless M is compact!

(U_n). Then $f_n := \phi_n f$ is compactly supported in U_n and L^q thereon. Given arbitrary $\epsilon > 0$, using Friedrichs mollifiers, for each n we can pick $f_{n,\epsilon} \subset \Gamma_{C_c^\infty}(U_n, E)$ with

$$\left\| f_{n,\epsilon} - f_n \right\|_q < \epsilon / 2^{n+1}.$$

Then $f_\epsilon := \sum_n f_{n,\epsilon} \in \Gamma_{C_c^\infty}(M, E)$ and

$$\left\| f_\epsilon - f \right\|_q = \left\| \sum_n f_{n,\epsilon} - \sum_n f_n \right\|_q \leq \sum_n \left\| f_{n,\epsilon} - f_n \right\|_q < \epsilon,$$

completing the proof. ■

4. The Friedrichs realization of the Laplace-Beltrami operator

Since we have fxied g, the tangent bundle $TM \to M$ is by definition a metric bundle, using the isomorphism of vector bundles

$$\sharp : T^*M \longrightarrow TM$$

induced by the fiberwise nondegeneracy of g, we get a metric g^* on $T^*M \to M$ by setting

$$(\alpha, \beta) := (\sharp\alpha, \sharp\beta).$$

Let

$$d : C^\infty(M) \longrightarrow \Omega^1_{C^\infty}(M) := \Gamma_{C^\infty}(M, T^*M)$$

denote the exterior differential. It is a first order differential operator (which does not depend on g) given locally by $df = \sum_i \partial_i f dx^i$.

Definition 4.1. The *Laplace-Beltrami operator* is the second order differential operator given by

$$\Delta := -d^\dagger d : C^\infty(M) \longrightarrow C^\infty(M).$$

Locally one has

$$d^\dagger \alpha = -\frac{1}{\sqrt{\det(g)}} \sum_k \partial_k \Big(\sqrt{\det(g)} \sum_j g^{kj} \alpha_j \Big)$$

if $\alpha = \sum_j \alpha_j dx^j$ and $g^{kj} := (dx^k, dx^j)$. This formula shows

$$\Delta = \frac{1}{\sqrt{\det(g)}} \sum_i \partial_i \Big(\sqrt{\det(g)} \sum_j g^{ij} \partial_j \Big),$$

which can be worked out to give

$$\Delta = \sum_{ij} g^{ij} \partial_i \partial_j + \quad \text{lower order terms},$$

in particular, in each chart U, the symbol of Δ (as an operator of order ≤ 2...!) is given by $g^{ij}(x)\zeta_i\zeta_j$, $x \in U$, $\zeta \in T_xM$. This implies that Δ is elliptic (as g^{ij} is nondegenerate).

Remark 4.2. Local elliptic regularity shows: $f \in L^2_{\mathrm{loc}}(M)$, $\Delta f \in L^2_{\mathrm{loc}}(M)$ implies $f \in W^{2,2}_{\mathrm{loc}}(M)$, in particular, locally all weak partial derivatives of order ≤ 2 of f are in L^2_{loc} (say in each chart). It is a more delicate question to investigate the following GLOBAL question: Does $f \in L^2(M)$, $\Delta f \in L^2(M)$ imply $df \in \Omega^1_{L^2}(M)$? We will come back to this later (geodesic completeness!).

Lemma 4.3. *a) One has*

$$d(f_1 f_2) = f_1 df_2 + f_2 df_1, \tag{15}$$

$$d^\dagger(f\alpha) = f d^\dagger \alpha - (df, \alpha), \tag{16}$$

$$\Delta(f_1 f_2) = f_1 \Delta f_2 + f_2 \Delta f_1 + 2\Re(df_1, df_2), \tag{17}$$

$$\Delta(u \circ f) = (u'' \circ f) \cdot |df|^2 + (u' \circ f) \cdot \Delta f. \tag{18}$$

Proof. Exercise. For example, one can use the above local formulae. ∎

Consider now the densely defined, nonnegative, symmetric sesqulinear form Q' in $L^2(M)$ given by

$$\mathrm{Dom}(Q') = C_c^\infty(M), \quad Q'(f_1, f_2) = \int (df_1, df_2) d\mu.$$

It is induced by the symmetric nonnegative operator $-\Delta$ (with $\mathrm{Dom}(-\Delta) = C_c^\infty(M)$), as we have

$$Q'(f_1, f_2) = \int \overline{-\Delta f_1} f_2 d\mu = \langle -\Delta f_1, f_2 \rangle .$$

By Friedrichs' theorem (cf. Example 2.19), it follows that Q' is closable. Let us describe its closure. To this end, define the global Sobolev space

$$W^{1,2}(M) := \{ f \in L^2(M) : df \in \Omega^1_{L^2}(M) := \Gamma_{L^2}(M, T^*M) \},$$

which is a Hilbert space with scalar product

$$\langle f_1, f_2 \rangle_{W^{1,2}} := \langle f_1, f_2 \rangle + \langle df_1, df_2 \rangle = \int \overline{f_1} f_2 d\mu + \int (df_1, df_2) d\mu.$$

Then we define

$$W^{1,2}_0(M) := \quad \text{closure of } C_c^\infty(M) \text{ with respect to } \|\cdot\|_{W^{1,2}}.$$

Remark 4.4. If $M = \mathbb{R}^m$ (with its Euclidean metric) then one has $W^{1,2}_0(\mathbb{R}^m) = W^{1,2}(\mathbb{R}^m)$, while if M is a bounded open subset U of $\mathbb{R}^m$ then one has $W^{1,2}_0(U) \neq W^{1,2}(U)$. We will come to problems of this kind later on.

Now by Kato's theory it follows that the closure Q of Q' is the closed nonnegative densely defined nonnegative symmetric sesqulinear form given by

$$\mathrm{Dom}(Q) = W^{1,2}_0(M), \quad Q(f_1, f_2) = \int (df_1, df_2) d\mu.$$

By Kato's theory (cf. Theorem 2.17) there exists a uniquely determined self-adjoint nonnegative operator H in $L^2(M)$ such that $\mathrm{Dom}(H) \subset \mathrm{Dom}(Q)$ and

$$\langle H f_1, f_2 \rangle = Q(f_1, f_2) \text{ for all } f_1 \in \mathrm{Dom}(H),\ f_2 \in \mathrm{Dom}(Q).$$

Moreover, some $f_1 \in \mathrm{Dom}(Q)$ is in $\mathrm{Dom}(H)$, if and only if there exists $f_2 \in L^2(M)$ with

$$Q(f_1, f_3) = \langle f_2, f_3 \rangle \qquad \text{for all } f_3 \in C_c^\infty(M),$$

and then $Hf_1 = f_2$. It follows now easily that

$$\mathrm{Dom}(H) = \{f \in W_0^{1,2}(M) : \Delta f \in L^2(M)\}, \quad Hf = -\Delta f.$$

5. Geodesic completeness and the essential self-adjointness of $-\Delta$

This section deals with the following question: under which condition on the geometry of M, that is, on g, is H is the *unique* self-adjoint realization of $-\Delta$?

To this end, for all $x, y \in M$ we define $\varrho(x, y)$ to be the infimum of all $\int_a^b |\dot{\gamma}(s)| ds$ such that $[a, b] \subset \mathbb{R}$ is a closed interval and $\gamma : [a, b] \to M$ is a piecewise smooth curve with $\gamma(a) = x$, $\gamma(b) = y$. Note that $\dot{\gamma}(s) \in T_{\gamma(s)}M$ and

$$\ell(\gamma) := \int_a^b |\dot{\gamma}(s)| ds$$

can be interpreted as the Riemannian length of the curve γ (this notion is, as usual, justified by approximating with 'summing up the lenghtsof polygons approximating the curve' and taking the limit.

Remark 5.1. The main reason why we assume throughout that M is connected is that otherwise the set whose infimum defines $\varrho(x, y)$ could be empty, leading to $\varrho(x, y) = \infty$.

The main properties of

$$\varrho : M \times M \longrightarrow [0, \infty), \quad (x, y) \longmapsto \varrho(x, y)$$

are collected in the following Theorem:

Theorem 5.2. *a) ϱ is a distance on M (the corresponding open balls will simply be denoted with*

$$B(x, r) := \{y : \varrho(x, y) < r\} \subset M$$

in the sequel) and one has

$$\overline{B(x, r)} = \{y : \varrho(x, y) \leq r\}. \tag{19}$$

b) ϱ induces the original topology on M.
c) The following statements are equivalent:
i) M is complete.
ii) All closed bounded subsets of M are compact.
ii') All bounded subsets of M are relatively compact.
iii) M admits a sequence $(\chi_n) \subset C_c^\infty(M)$ of first order cut-off functions*, that is, (χ_n) has the following properties*:

- (C1) $0 \leq \chi_n(x) \leq 1$ *for all* $n \in \mathbb{N}_{\geq 1}$, $x \in M$,
- (C2) *for all compact* $K \subset M$, *there is an* $n_0(K) \in \mathbb{N}$ *such that for all* $n \geq n_0(K)$ *one has* $\chi_n |_K = 1$,
- (C3) $\|d\chi_n\|_\infty \to 0$ *as* $n \to \infty$.

Proof. a) Clearly ϱ is nonnegative and $\varrho(x,x) = 0$. To show the triangle inequality, fix $x, y, z \in M$ and pick a piecewise smooth path γ_1 from x to z and a piecewise smooth path γ_2 from z to y. Let γ be the path from x to y obtained as $\gamma = \gamma_2\gamma_1$ in the obvious sense. Then one has

$$\varrho(x,y) \leq \ell(\gamma) = \ell(\gamma_2) + \ell(\gamma_1),$$

so

$$\varrho(x,y) \leq \varrho(x,z) + \varrho(z,y)$$

follows from minimizing in γ.

To see that ϱ is nondegenerate, we first prove:

Claim: for all $p \in M$ there exists a chart $p \in U \subset M$ and a constant C such that

$$C^{-1}|x-y| \leq \varrho(x,y) \leq C|x-y|$$

for all $x, y \in U$.

Proof of the claim: pick a chart $p \in W$ with coordinates $x^1, \ldots, x^m$ and pick a *Euclidean* ball $V \subset W$ of radius $r > 0$ around p whose closure is included in W. For all $x \in \overline{V}$, $\zeta \in T_xM$ one has

$$|\zeta|^2 := |\zeta|_g^2 = \sum_{ij} g_{ij}(x)\zeta^i\zeta^j, \quad |\zeta|_e^2 = \sum_j (\zeta^j)^2.$$

Since $(g_{ij}(x))_{ij}$ is positive definite and depends continuously on x we find $C > 1$ such that for all $x \in \overline{V}$, $\zeta \in T_xM$ one has

$$C^{-2}\sum_j (\zeta^j)^2 \leq \sum_{ij} g_{ij}(x)\zeta^i\zeta^j \leq C^2 \sum_j (\zeta^j)^2,$$

so

$$C^{-1}|\zeta|_e \leq |\zeta| \leq C|\zeta|_e.$$

For any piecewise smooth path γ which remains in $\overline{V}$ we get

$$C^{-1}\ell_e(\gamma) \leq \ell(\gamma) \leq C\ell_e(\gamma).$$

If $x, y \in V$, then we get

$$\varrho(x,y) \leq \ell(\gamma_{x,y}) \leq C|x-y|,$$

where $\gamma_{x,y}$ is the straight line from x to y.

We are going to show that on U defined as the Euclidean ball in W around p of radius $r/3$ one has the reverse inequality, so that U does the job.

Let $x, y \in U$ and let γ be an arbitrary piecewise smooth curve in M from x to y. If γ stays in V then[9]

$$\ell_e(\gamma) \geq |x-y|$$

and so

$$\ell(\gamma) \geq C^{-1}|x-y|. \tag{20}$$

[9]Here we use that the lenght distance of $x, y \in \mathbb{R}^m$ induced by the Euclidean Riemannian metric is precisely $|x-y|$.

If γ intersects ∂V, pick a point $z \in \partial V$ which is hit by γ and let $\tilde{\gamma}$ denote the part of γ which connects in $\overline{V}$ the point x with z. Thus

$$\ell(\gamma) \geq \ell(\tilde{\gamma}) \geq C^{-1}|x-z| \geq C^{-1}(2r/3) \geq C^{-1}|x-y|.$$

Thus taking $\inf_\gamma$ we get

$$\varrho(x,y) \geq C^{-1}|x-y|,$$

proving the claim.
In order to show that ϱ is nondegenerate, fix distinct $p, x \in M$. Pick a chart U around p and $C > 1$ as in the above claim. If $x \in U$ then clearly $\varrho(x,p) > 0$. If $x \in M \setminus U$ pick $r > 0$ small with $B_e(p,r) \subset U$ (Euclidean ball). Then any curve γ from x to p must hit $\partial B_e(p,r)$, and so $\ell(\gamma) \geq C^{-1}r$ and by taking $\inf_\gamma$ we arrive at $\varrho(x,p) \geq C^{-1}r > 0$. This completes the proof that ϱ is a distance.

The proof of (19) is left as an exercise.
b) It is enough to show that for all $p \in M$ there exists a chart U around p and $R > 0$, $C > 1$ such that for all $r \in (0,R]$ one has

$$B_e(p,C^{-1}r) \subset B(p,r) \subset B_e(p,Cr) \subset U.$$

To this end pick U, C as in the claim and $\epsilon > 0$ small with $B_e(p,\epsilon) \subset U$. Set $R := \epsilon/(2C)$ and let $0 < r \leq R$. If $x \in B_e(p,C^{-1}r)$ we have $x \in U$ and so $x \in B(p,r)$. If we can show that $B(p,r) \subset U$, then clearly $B(p,r) \subset B_e(p,Cr)$. To show that $B(p,r) \subset U$, assume $x \notin U$. Then any curve γ from x to p hits a point $y \in U$ with $|y-p| = \epsilon/2$. Thus we obtain,

$$\ell(\gamma) \geq \varrho(y,p) \geq C^{-1}|y-p| = \epsilon/(2C) \geq r,$$

and taking $\inf_\gamma$ this shows $\varrho(x,p) \geq r$ and so $x \notin B(p,r)$.
c) i) $\Leftrightarrow$ ii): Exercise (a proof which does not use exponential coordinates).
ii) $\Leftrightarrow$ ii'): this is trivial.
i) $\Leftrightarrow$ iii): I sketch a proof: if $M = (M,g)$ is complete, then by a small generalization of Nash's embedding theorem we can pick a smooth embedding $\iota : M \to \mathbb{R}^l$ such that g is the pull-back of the Euclidean metric on $\mathbb{R}^l$ (thus an *isometric embedding*), where $l \geq m$ is large enough, and such that $\iota(M)$ is a closed subset of $\mathbb{R}^l$: note here that the original Nash embedding does not produce a closed image; to correct this, one constructs a new metric $\tilde{g}$ on M, embeds $(M,\tilde{g})$ into some $\mathbb{R}^{l'}$ isometrically via some map $\Psi : M \to \mathbb{R}^{l'}$ and constructs, using that closed balls are compact on (M,g), a map $\phi : M \to \mathbb{R}$, such that

$$\iota := (\Psi, \psi) : M \to \mathbb{R}^l$$

is an isometric embedding of (M,g), where $l := l' + 1$. A detailed explanation of the above construction of ι has been given by O. Mueller in [26].
From here the proof is straightforward: ι is proper, and therefore the composition

$$f : M \longrightarrow \mathbb{R}, \;\; f(x) := \log(1 + |\iota(x)|^2)$$

is a smooth proper function with $|df| \leq 1$, since

$$\tilde{f} : \mathbb{R}^l \longrightarrow \mathbb{R}, \;\; \tilde{f}(v) := \log(1 + |v|^2)$$

is a smooth proper function whose gradient is absolutely bounded by 1. Pick now a sequence $(\varphi_n) \subset C^\infty_{\mathrm{c}}(\mathbb{R})$ of first order cut-off functions on the Eudlidean space $\mathbb{R}$. (For example, let $\varphi : \mathbb{R} \to [0,1]$ be smooth and compactly supported with $\varphi = 1$ near 0, and set $\varphi_n(r) := \varphi(r/n)$, $r \in \mathbb{R}$.) Then $\chi_n(x) := \varphi_n(f(x))$ obviously has the desired properties, in view of the chain rule $d\chi_n(x) = \varphi_n'(f(x))df(x)$.

iii) $\Leftrightarrow$ ii'): Suppose that M admits a sequence $(\chi_n) \subset C^\infty_{\mathrm{c}}(M)$ of first order cut-off functions. Then given $\mathscr{O} \in M$, $r > 0$, we are going to show that there is a compact set $A_{\mathscr{O},r} \subset M$ such that

$$\varrho(x, \mathscr{O}) > r \text{ for all } x \in M \setminus A_{\mathscr{O},r},$$

which implies that any open geodesic ball is relatively compact. To see this, we define $A_{\mathscr{O}} := \{\mathscr{O}\}$, and a number $n_{\mathscr{O},r} \in \mathbb{N}$ large enough such that $\chi_{n_{\mathscr{O},r}} = 1$ on $A_{\mathscr{O}}$ and

$$\sup_{x \in M} \left| d\chi_{n_{\mathscr{O},r}}(x) \right| \leq 1/(r+1). \tag{21}$$

Now let $A_{\mathscr{O},r} := \mathrm{supp}(\chi_{n_{\mathscr{O},r}})$, let $x \in M \setminus A_{\mathscr{O},r}$, and let

$$\gamma : [a,b] \longrightarrow M$$

be a piecewise smooth curve with $\gamma(a) = x$, $\gamma(b) = \mathscr{O}$. Then we have

$$1 = \chi_{n_{\mathscr{O},r}}(\mathscr{O}) - \chi_{n_{\mathscr{O},r}}(x) = \chi_{n_{\mathscr{O},r}}(\gamma(b)) - \chi_{n_{\mathscr{O},r}}(\gamma(a)) = \int_a^b \big(d\chi_{n_{\mathscr{O},r}}(\gamma(s)), \dot{\gamma(s)} \big) ds,$$

where we have used the chain rule. By using (21) and taking $\inf_\gamma \cdots$, we arrive at

$$\varrho(x, \mathscr{O}) \geq r + 1 \text{ for all } x \in M \setminus A_{\mathscr{O},r},$$

as claimed. ■

Now we can prove the following result, which has been first shown by Gaffney, 1954 (from my point of view: much ahead of his time!). We follows a proof given by Strichartz in 1983:

Theorem 5.3. *Assume M is complete. Then the symmetric nonnegative operator $-\Delta$ (defined on $C^\infty_{\mathrm{c}}(M)$) is essentially self-adjoint in $L^2(M)$. As a consequence, it has a unique self-adjoint extension which necessarily coincides with $H \geq 0$.*

Proof. By the abstract functional analytic fact Theorem 2.5, it suffices to show that $\mathrm{Ker}((-\Delta + 1)^*) = \{0\}$. Let

$$f \in \mathrm{Ker}((-\Delta + 1)^*).$$

Unpacking definitions one finds that this is equivalent to $f \in L^2(M)$ and $-\Delta f = -f$, in particular, f is smooth by local elliptic regularity. We pick a sequence (χ_n) of first order cut-off functions. Then by the product rule for d from Lemma 4.3 we have

$$\begin{aligned} &(d(\chi_n f), d(\chi_n f)) \\ &= (df, \chi_n f d\chi_n) + (df, \chi_n^2 df) + |f d\chi_n|^2 + (f d\chi_n, \chi_n df), \end{aligned}$$

which, using

$$(df, d(\chi_n^2 f)) = (df, \chi_n^2 df) + 2(df, f\chi_n d\chi_n),$$

implies

$$|d(\chi_n f)|^2 = (d(\chi_n f), d(\chi_n f))$$
$$= (df, d(\chi_n^2 f)) + |fd\chi_n|^2 - (df, f\chi_n d\chi_n) + (fd\chi_n, \chi_n df).$$

This in turn implies (after adding the complex conjugate of the formula to itself)

$$2|d(\chi_n f)|^2 = 2\Re(df, d(\chi_n^2 f)) + 2|fd\chi_n|^2.$$

Integrating and then integrating by parts in the last equality, we get

$$\int |d(\chi_n f)|^2 d\mu = \Re \int (\chi_n d^\dagger df, \chi_n f) d\mu + \int |fd\chi_n|^2 d\mu.$$

Using $d^\dagger df = -\Delta f = -f$ and

$$\int |d(\chi_n f)|^2 d\mu \geq 0$$

we see

$$\int |\chi_n|^2 |f|^2 d\mu \leq \int |fd\chi_n|^2 d\mu,$$

which implies $\int |f|^2 d\mu = 0$ and thus $f = 0$ by dominated convergence, using the properties of (χ_n).

■

Some remarks are in order:

Remark 5.4. 1. There are some interesting (though not many) incomplete Riemannian manfolds such that $-\Delta$ is essentially self-adjoint.
2. We are going to prove in the exercises that even the Schrödinger operator $-\Delta + V$ in $L^2(M)$ is essentially self-adjoint, if M is complete and $V : M \to \mathbb{R}$ is smooth and bounded from below. Note V has to be real-valued to get a symmetric operator.
3. The ultimate essential self-adjointness result on Riemann manifolds is the following one: assume M is complete and $V \in L^2_{\mathrm{loc}}(M)$ has a little more local regularity ('local Kato class' of M) such that $-\Delta + V$ is bounded from below. Then $-\Delta + V$ is essentially self-adjoint. This result can by applied to get that the Hamilton operator corresponding to a molecule is essentially self-adjoint (so there is no ambiguity concerning the quantum mechanics of matter).
4. Similar essential self-adjointness results hold for operators of the form $\nabla^\dagger \nabla + V$ on metric vector bundles $E \to M$, where ∇ is a metric connection on $E \to M$ and V is a pointwise self-adjoint L^2_{loc}-section of $\mathrm{End}(E) \to M$ (Güneysu/Post; Braverman/Milatovic/Shubin; Lesch). These results are needed at least to deal with molecules in magnetic fields.

6. Some regularity results

Lemma 6.1. *Assume $f_1 \in W^{1,2}_0(M)$, $f_2 \in W^{1,2}(M)$, $\Delta f_2 \in L^2(M)$. Then one has the following integration by parts formula,*

$$\int \overline{f_1} \Delta f_2 d\mu = -\int (df_1, df_2) d\mu.$$

Proof. If f_1 is smooth and compactly supported, then the identity follows immediately from the definition of weak (= distributional) derivatives. It carries over to general f_1's by a trivial density argument. ∎

Note that every $f_2 \in \mathrm{Dom}(H)$ satisfies the above assumption. Often, this is used in the form $f_2 = e^{-tH}h$ for some $h \in L^2(M)$, $t > 0$, as we know that for all $t > 0$,

$$\mathrm{Ran}(e^{-tH}) \subset \bigcap_{n\in\mathbb{N}} \mathrm{Dom}(H^n)$$

by the spectral calculus.

Lemma 6.2. *Given a sequence of smooth functions $\psi_k : \mathbb{R} \to \mathbb{R}$, $k \in \mathbb{N}$, with*

$$\psi_k(0) = 0, \quad \sup_{k\in\mathbb{N}} \sup_{t\in\mathbb{R}} |\psi'_k(t)| < \infty,$$

and a pair of functions $\psi : \mathbb{R} \to \mathbb{R}$, $\varphi : \mathbb{R} \to \mathbb{R}$ with

$$\psi_k \to \psi, \psi'_k \to \varphi$$

pointwise as $k \to \infty$.
a) For every real-valued $f \in W^{1,2}_0(M)$ one has $\psi \circ f \in W^{1,2}_0(M)$ and

$$d(\psi \circ f) = (\varphi \circ f)df.$$

b) For every real-valued $f \in W^{1,2}(M)$ one has $\psi \circ f \in W^{1,2}(M)$ and

$$d(\psi \circ f) = (\varphi \circ f)df.$$

If in addition φ is continuous away from an at most countable set, then $f_n, f \in W^{1,2}(M)$, $f_n \to f$ in $W^{1,2}(M)$ implies $\psi \circ f_n \to \psi \circ f$ in $W^{1,2}(M)$, as $n \to \infty$.
c) For every real-valued $f \in W^{1,2}_{\mathrm{loc}}(M)$ one has $\psi \circ f \in W^{1,2}_{\mathrm{loc}}(M)$ and

$$d(\psi \circ f) = (\varphi \circ f)df.$$

Proof. a) Lemma 5.2 in [8].
b) Theorem 5.7 in [8].
c) This follows from applying b) with M replaced by a relatively compact chart of M. ∎

Denote with $a_+ := \max(0, a) \in [0, \infty)$ the positive part of $a \in \mathbb{R}$ and with $a_- := a_+ - a \in [0, \infty)$ its negative part.

Example 6.3. Given $c \geq 0$ set $\psi(t) := (t - c)_+$,

$$\phi(t) := \begin{cases} 0, & t \leq c, \\ 1, & t > c \end{cases}.$$

Then picking $\psi_1 : \mathbb{R} \to \mathbb{R}$ smooth with

$$\psi_1(t) := \begin{cases} 0, & t - 1 \leq c, \\ 1, & t > c + 2, \end{cases}$$

the sequence $\psi_k(t) := k^{-1}\psi_1(kt)$ satisfies the assumptions of the previous lemma, yielding that for all real-valued $f \in W_0^{1,2}(M)$ (resp. $f \in W^{1,2}(M)$) one has $(f-c)_+ \in W_0^{1,2}(M)$ (resp. $(f-c)_+ \in W^{1,2}(M)$) and the formula

$$d(f-c)_+ = \begin{cases} df, & \text{if } f > c \\ 0, & \text{else} \end{cases}$$

Moreover, $f_n \to f$ in $W^{1,2}(M)$ implies $(f_n - c)_+ \to (f-c)_+$ in $W^{1,2}(M)$.

Let $N \subset M$ be an arbitrary subset. Then a function $f : N \to \mathbb{R}$ on M is called *Lipschitz*, if there exists a constant C such that for all $x, y \in N$ one has

$$|f(x) - f(y)| \leq C\varrho(x,y). \tag{22}$$

Lipschitz functions are continuous, restrictions of Lipschitz functions are again Lipschitz, and for a fixed $x_0 \in M$, the function

$$M \ni x \mapsto \varrho(x, x_0)$$

is Lipschitz. Note also that if $U \subset M$ is open, then with an obvious notation one has

$$\varrho_U(x,y) \geq \varrho(x,y) \quad \text{for all } x, y \in U,$$

so a Lipschitz function $f : U \to \mathbb{R}$ in the above sense is also a Lipschitz function with respect to the Riemannian manifold (U, g_U).

Remark 6.4. The following assertions can be deduced in an elementary way and hold on every metric space: If f, g are Lipschitz, then so is $f+g$, $\min(f,g)$, $\max(f,g)$; the product fg is Lipschitz, if in addition f is bounded on the support of g.
A function $f : M \to \mathbb{R}$ is called *locally Lipschitz*, if for each compact $K \subset M$ there exists a $C = C_K$ with (22) for all $x, y \in K$. The composition of a Lipschitz function with a Lipschitz function on $\mathbb{R}$ is Lipschitz; the composition of a locally Lipschitz function with a locally Lipschitz function on $\mathbb{R}$ is locally Lipschitz.

Lemma 6.5. *a) If $f : M \to \mathbb{R}$ is a Lipschitz function, then $df \in \Omega^1_{L^\infty}(M)$ (as distributions, in the sense of Definition 3.9) and one has $\|df\|_\infty \leq C'$, where C' is the smallest C with (22). If $f : M \to \mathbb{R}$ is locally Lipschitz, then $df \in \Omega^1_{L^\infty_{\mathrm{loc}}}(M)$.*
b) A C^1-function $f : M \to \mathbb{R}$ with $\|df\|_\infty < \infty$ is Lipschitz. In particular, C^1-functions are locally Lipschitz.

Proof. a) This follows from applying the corresponding Euclidean result (Rademacher's theorem) in 'nice charts' like those appearing in the proof of Theorem 5.2, namely, by scaling the charts if necessary, one can can find for each $p \in M$ a chart U with $p \in U$ and

$$(1/2)\delta_{ij} \leq g_{ij}(x) \leq 2\delta_{ij}$$

for all $x \in U$, as bilinear forms (the point is that the constant in this quasi-isometry, $C = 2$, is uniform in each chart. Rademacher's theorem can either be deduced with methods of Analysis 1, by reducing to the $m = 1$ case with a covering argument ('Vitali covering'), using that functions on an interval having a bounded variation are almost

everywhere differentiable by Lebesgue's theorem, or by using a Sobolev embedding theorem (cf. Theorem 3.1, resp. section 4.2 in [14]).
The local statement can be deduced as follows from the above: Assume $N \subset M$ is open and relatively compact and let $f : M \to \mathbb{R}$ be locally Lipschitz. Pick $\phi \in C_c^\infty(M)$ with $\phi = 1$ on N. Then ϕf is globally Lipschitz and so $d(\phi f) \in \Omega^1_{L^\infty}(M)$. Since $f = \phi f$ on N we thus get $df \in \Omega^1_{L^\infty}(N)$.
b) This follows applying the mean value theorem for differentiation in nice charts. ■

Lemma 6.6. *One has $W_c^{1,2}(M) \subset W_0^{1,2}(M)$ (note that $W_c^{1,2}(M)$ does not depend on g, as locally any two Riemannian metrics are equivalent as bilinear forms). In particular, for every compactly supported Lipschitz function $f : M \to \mathbb{R}$ one has $f \in W_0^{1,2}(M)$.*

Proof. Let $h \in W_c^{1,2}(M)$. Covering the support of h with finitely many nice charts, we can assume that M is an open subset of the Euclidean $\mathbb{R}^m$. In this case the assertion follows from Friedrichs mollifiers.
For the second statement, note that f is L^2 (continuous and compactly supported) and df is L^2 (bounded by the previous Lemma and compactly supported), so $f \in W_c^{1,2}(M)$. ■

Lemma 6.7. *One has the product rule $d(f_1 f_2) = f_1 df_2 + f_2 df_1$ if $f_1, f_2 : M \to \mathbb{R}$ are locally Lipschitz. If $\psi : \mathbb{R} \to \mathbb{R}$ is C^1 and $f : M \to \mathbb{R}$ is locally Lipschitz, then $\psi \circ f$ is locally Lipschitz with the chain rule $d(\psi \circ f) = (\psi' \circ f)df$.*

Proof. In view of the cut-off function argument from the proof of Lemma 6.5 b) we can assume that f_1 and f_2 are compactly supported, so that $f_1, f_2 \in W_0^{1,2}(M)$ by the previous lemma. Pick a sequence $(\phi_n) \subset C_c^\infty(M)$ with $\phi_n \to f_1$ in $W^{1,2}(M)$. Since f_1 is bounded, we can assume for the proof that (ϕ_n) is uniformly bounded in $W^{1,2}(M)$ (and so (ϕ_n) is uniformly bounded in $L^2(M)$ and $(d\phi_n)$ is uniformly bounded in $\Omega^1_{L^2}(M)$: indeed, let $C := \|f_1\|_\infty$ and pick $\psi : \mathbb{R} \to \mathbb{R}$ with $\psi(t) = t$ for all t with $|t| \leq C$ and with ψ' bounded. Then by Lemma 6.2 we have $\psi \circ \phi_n \to f_1$, and $(\psi \circ \phi_n)$ is uniformly bounded in $W^{1,2}(M)$. Thus we can pick sequences ϕ_n, θ_n in $C_c^\infty(M)$ which are both uniformly bounded in $W^{1,2}(M)$ and $\phi_n \to f_1$ and $\theta_n \to f_2$ in $W^{1,2}(M)$. Then one easily checks that (a standard $\epsilon/2$ type argument which uses that f_j are bounded) that $\phi_n\theta_n \to f_1 f_2$ in $L^2(M)$, which using Cauchy-Schwarz implies $\phi_n\theta_n \to f_1 f_2$ in the sense of distributions, and so $d(\phi_n\theta_n) \to d(f_1 f_2)$ in the sense of distributions (cf. Remark 3.10).
Similarly, as df_1,df_2 are bounded by Lemma 6.5 a) (since f_j are compactly supported), one can check that $\phi_n d\theta_n \to f_1 df_2$ and $\theta_n d\phi_n \to f_2 df_1$ in $\Omega^1_{L^2}(M)$, and so

$$d(\phi_n\theta_n) = \theta_n(d\phi_n) + \phi_n d\theta_n \to f_2 df_1 + f_1 df_2$$

in $\Omega^1_{L^2}(M)$, which using Cauchy-Schwarz implies $\phi_n\theta_n \to f_2 df_1 + f_1 df_2$ in the sense of distributions. This completes proof.
It remains to prove the asserted chain rule: since C^1-functions are locally Lipschitz, it suffices to prove the formula in each open relatively compact subset of M. In particular, we can assume that f is compactly supported. Furthermore, we can assume that $\psi(0) = 0$ (if not: consider $\tilde{\psi} := \psi - \psi(0)$), and as f is bounded also that ψ is compactly supported

(in particular, ψ' is bounded). Under these assumptions, the chain rule follows trivially from Lemma 6.2. ■

Lemma 6.8. *Assume $f_1 : M \to \mathbb{R}$ is bounded and Lipschitz and $f_2 \in W_0^{1,2}(M)$. Then $f_1 f_2 \in W_0^{1,2}(M)$ and one has the product rule $d(f_1 f_2) = f_1 df_2 + f_2 df_1$.*

Proof. Assume first $f_2 \in C_c^\infty(M)$. Then we have $f_1 f_2$ is compactly supported and Lipschitz, thus in $W_0^{1,2}(M)$, and the product rule holds by the previous lemma.
If $f_2 \in W_0^{1,2}(M)$, then $f_1 f_2 \in L^2(M)$ and $f_1 df_2 + f_2 df_1 \in \Omega^1_{L^2}(M)$, as f_1 and df_1 are bounded. This implies $fg \in W^{1,2}(M)$. Pick a sequence ϕ_n in $C_c^\infty(M)$ such that $\phi_n \to f_2$ in $W^{1,2}(M)$. Then we have $f_1\phi_n \in W_0^{1,2}(M)$ and $f_1\phi_n \to f_1 f_2$ in $L^2(M)$, as f_1 is bounded. Applying the product rule to $f_1\phi_n$ and using that f, df are bounded, one easily finds that also

$$d(f_1\phi_n) \to f_1 df_2 + f_2 df_1.$$

in $\Omega^1_{L^2}(M)$. It follows from these two convergences that $f_1\phi_n \to f_1 f_2$ in $W^{1,2}(M)$ and so $f_1 f_2 \in W_0^{1,2}(M)$, as the latter is a closed subspace of $W^{1,2}(M)$. Finally, $d(f_1\phi_n) \to f_1 df_2 + f_2 df_1$ in $\Omega^1_{L^2}(M)$ implies the corresponding convergence in the sense of distributions (by Cauchy-Schwarz), $f_1\phi_n \to f_1 f_2$ in $L^2(M)$ implies the corresponding convergence in the sense of distributions, and so by Remark 3.10 also $d(f_1\phi_n) \to d(f_1 f_2)$, which also establishes the product formula for $f_1 f_2$. ■

Lemma 6.9. *Assume $f_1 \in W^{1,2}_{\mathrm{loc}}(M)$ and that $f_2 : M \to \mathbb{R}$ is compactly supported and Lipschitz. Then one has $f_1 f_2 \in W_0^{1,2}(M)$ and the product rule applies.*

Proof. Multiplying f_1 with a smooth compactly supported function which is $= 1$ on the support of f_2 we can assume that $f_1 \in W_0^{1,2}(M)$ (cf. Lemma 6.6), in which case the statement follows from the previous lemma. ■

7. Basic properties of the heat kernel

The "heat semigroup"

$$(e^{-tH})_{t\geq 0} \subset \mathscr{L}(L^2(M))$$

is defined by the spectral calculus. It is a strongly continuous and self-adjoint semigroup with

$$\left\|e^{-tH}\right\|_{2,2} \leq 1,$$

where $\left\|\cdot\right\|_{q_1,q_2}$ denotes the operator for linear operators from $L^{q_1}(M)$ to $L^{q_2}(M)$. Moreoever, for every $f \in L^2(M)$ the path

$$[0,\infty) \ni t \longmapsto e^{-tH} f \in L^2(M)$$

is the uniquely determined continuous path

$$[0,\infty) \longrightarrow L^2(M)$$

which is C^1 in $(0,\infty)$ (in the norm topology) with values in $\mathrm{Dom}(H)$ thereon, and which satisfies the abstract "heat equation"

$$(d/dt)e^{-tH} f = -He^{-tH} f, \quad t > 0,$$

subject to the initial condition $e^{-tH}f|_{t=0} = f$. All of the above facts follow from abstract functional analytic results and only rely on the fact that H is self-adjoint and nonnegative. The aim of this section is to show that e^{-tH} is given by an integral kernel

$$e^{-tH}f(x) = \int p(t,x,y)f(y)d\mu(y),$$

such that for fixed x, $(t,y) \mapsto p(t,x,y)$ solves the heat equation

$$\partial_t u(t,y) = \Delta_y u(t,y)$$

with initial condition $u(0,x) = \delta_x$.

Theorem 7.1. *a) There is a unique smooth map*

$$(0,\infty) \times M \times M \ni (t,x,y) \longmapsto p(t,x,y) \in [0,\infty),$$

the heat kernel of H, *such that for all* $t > 0$, $f \in L^2(M)$, *and* μ*-a.e.* $x \in M$ *one has*

$$e^{-tH}f(x) = \int p(t,x,y)f(y)d\mu(y). \tag{23}$$

b) For all $s,t > 0$, $x,y \in M$ *one has*

$$\int p(t,x,y)^2 d\mu(y) < \infty, \tag{24}$$

$$p(t,y,x) = p(t,x,y), \tag{25}$$

$$p(t+s,x,y) = \int p(t,x,z)p(s,z,y)d\mu(z), \tag{26}$$

$$\int p(t,x,z)d\mu(z) \leq 1. \tag{27}$$

c) For any $f \in L^2(M)$, *the function*

$$(0,\infty) \times M \ni (t,x) \longmapsto P_t f(x) := \int p(t,x,y)f(y)d\mu(y) \in \mathbb{C}$$

is smooth and one has

$$\frac{\partial}{\partial t}P_t f(x) = \Delta_x P_t f(x) \quad \textit{for all } (t,x) \in (0,\infty) \times M.$$

d) For all fixed $x \in M$, *the function* $(t,y) \mapsto p(t,x,y)$ *solves the heat equation*

$$\partial_t u(t,y) = \Delta_y u(t,y)$$

in $(0,\infty) \times M$, *with initial condition* $u(0,x) = \delta_x$, *in the sense that*

$$\lim_{t\to 0+} \int p(t,x,y)\phi(y)d\mu(y) = \phi(x) \quad \textit{for all } \phi \in C_c^\infty(M).$$

Proof. Before we come to the proof of the actual statements of Theorem 7.1, let us first establish some auxiliary results.
Step 1: For fixed $t > 0$, there exists a smooth version of $x \mapsto e^{-tH} f(x)$ (which from now on will always be taken).
Proof: To see this, note that for any $n \in \mathbb{N}_{\geq 1}$ one has

$$\mathrm{Dom}(H^n) \subset W^{2n,2}_{\mathrm{loc}}(M),$$

by local elliptic regularity. By the spectral calculus and the local Sobolev embedding (13), this implies

$$\mathrm{Ran}(e^{-tH}) \subset \bigcap_{n \in \mathbb{N}_{\geq 1}} \mathrm{Dom}(H^n) \subset C^\infty(M) \text{ for any } t > 0.$$

Step 2: For any $t > 0$, $U \subset M$ open and relatively compact, the map

$$e^{-tH} : L^2(M) \longrightarrow C_b(U) \tag{28}$$

is a bounded linear operator between Banach spaces, where the space of bounded continuous functions $C_b(U)$ is equipped with its usual uniform norm.
Proof: A priory, this map is algebraically well-defined by step 1. The asserted boundedness follows from the closed graph theorem. Indeed, assume assume $f_n \to f$ in $L^2(M)$ and $e^{-tH} f_n$ converges in $C_b(U)$ to some h. Then $e^{-tH} f_n \to e^{-tH} f$ in $L^2(M)$, thus after possibly picking a subsequence, $e^{-tH} f_n \to e^{-tH} f$ μ-a.e. and so $e^{-tH} f = h$.
Step 3: For fixed $s > 0$, the map

$$L^2(M) \times M \ni (f, x) \longmapsto e^{-sH} f(x) \in \mathbb{C}$$

is jointly continuous.
Proof: Let $U \subset M$ be an arbitrary open and relatively compact subset. Given a sequence

$$((f_n, x_n))_{n \in \mathbb{N}_{\geq 0}} \subset L^2(M) \times U$$

which converges to

$$(f, x) \in L^2(M) \times U,$$

we have

$$\begin{aligned}
&\left|e^{-sH} f_n(x_n) - e^{-sH} f(x)\right| \\
&\leq \left|e^{-sH}[f_n - f](x_n)\right| + \left|e^{-sH} f(x) - e^{-sH} f(x_n)\right| \\
&\leq \left\|e^{-sH}\right\|_{L^2(M), C_b(U)} \|f_n - f\|_2 + \left|e^{-sH} f(x) - e^{-sH} f(x_n)\right| \\
&\ \to 0, \text{ as } n \to \infty,
\end{aligned}$$

by step 2 and step 1.
Step 4: For fixed $\epsilon > 0$ and $f \in L^2(M)$, the map

$$\{\Re > \epsilon\} \times M \ni (z, x) \longmapsto e^{-zH} f(x)$$

is jointly continuous.
Proof: Indeed, this map is equal to the composition of the maps

$$\{\Re > \epsilon\} \times M \xrightarrow{(z,x) \mapsto (e^{-(z-\epsilon)H} f, x)} L^2(M) \times M \xrightarrow{(f,x) \mapsto e^{-\epsilon H} f(x)} \mathbb{C},$$

where the second map is continuous by Step 3. The first map is continuous, since the map

$$\{\Re > 0\} \ni z \longmapsto e^{-zH} f \in L^2(M) \tag{29}$$

is holomorphic. Note that, a priory, (29) is a weakly holomorphic semigroup by the spectral calculus, which is then indeed (norm-) holomorphic by the weak-to-strong differentiability theorem.

Step 5: For any $f \in L^2(M)$, there exists a jointly smooth version $(t,x) \mapsto P_t f(x)$ of $(t,x) \mapsto e^{-tH} f(x)$, which satisfies

$$\frac{\partial}{\partial t} P_t f(x) = \Delta_x P_t f(x). \tag{30}$$

Proof: By Step 4, for arbitrary $f \in L^2(M)$, the map

$$\{\Re > 0\} \times M \ni (z,x) \longmapsto e^{-zH} f(x) \in \mathbb{C}$$

is jointly continuous. It then follows from the holomorphy of (29) that for any open ball B in the open right complex plane which has a nonempty intersection with $(0,\infty)$, for any $t \in B \cap (0,\infty)$, and for *any* $x \in M$, we have Cauchy's integral formula

$$e^{-tH} f(x) = \oint_{\partial B} \frac{e^{-zH} f(x)}{t - z} dz,$$

noting that the holomorphy of (29) a priori only implies Cauchy's integral formula for *almost every* x. Now the claim follows from differentiating under the line integral, observing that for fixed $z \in \{\Re > 0\}$, the map

$$M \ni x \longmapsto e^{-zH} f(x) = e^{-\Re(z)H} \left[e^{-\sqrt{-1}\Im(z)H} f \right](x) \in \mathbb{C}$$

is smooth by Step 1. Finally, the asserted formula (30) follows from the by now proved existence of a smooth version of $(t,x) \mapsto e^{-tH} f(x)$ and the fact that

$$(d/dt) e^{-tH} f = H e^{-tH} f, \ \ t > 0,$$

in the sense of norm differentiable maps $(0,\infty) \to L^2(M)$.

Let us now come to the actual proof of Theorem 7.1.

a) First of all, it is clear that any such heat kernel is uniquely determined (by the fundamental lemma of distribution theory). To see its existence, we start by remarking that for every $x \in M$, $t > 0$, the complex linear functional given by

$$L^2(M) \ni f \longmapsto P_t f(x) \in \mathbb{C}$$

is bounded by Step 2. Thus by Riesz-Fischer's representation theorem, there exists a unique function $p_{t,x} \in L^2(M)$ such that for all $f \in L^2(M)$ one has

$$P_t f(x) = \langle p_{t,x}, f \rangle . \tag{31}$$

Clearly $p_{t,x} \in \mathbb{R}$ for all $y \in M$, for if not, then e^{-tH} would not preserve reality (but it does, as $-\Delta$ is an operator with real-valued coefficients, so H preserves reality and so its heat semigroup). Moreover, it follows immediately from step 5 that $(t,x) \mapsto p_{t,x}$ is weakly smooth. Then, this map is in fact norm smooth as a map $(0,\infty) \times M \to L^2(M)$

by the weak-to-strong differentiability theorem. We claim that the integral kernel which is well-defined by the "regularization"

$$p(t,x,y) := \left\langle p_{t/2,x}, p_{t/2,y} \right\rangle \tag{32}$$

has the desired properties. Firstly, the smoothness of $(t,x,y) \mapsto p(t,x,y)$ follows immediately from the norm smoothness of $(t,x) \mapsto p_{t,x}$ and the smoothness of the Hilbertian pairing $(f,g) \mapsto \langle f,g \rangle$.
Claim 1: One has

$$P_{t+s}f(x) = \int \langle p_{t,z}, p_{s,x} \rangle f(z) d\mu(z)$$

Proof of Claim 1:

$$\begin{aligned} P_{t+s}f(x) &= P_s P_t f(x) \\ &= \langle p_{s,x}, P_t f \rangle \\ &= \langle P_t p_{s,x}, f \rangle \\ &= \int P_t p_{s,x}(z) f(z) d\mu(z) \\ &= \int \langle p_{t,z}, p_{s,x} \rangle f(z) d\mu(z). \end{aligned}$$

Claim 2: For all $t > 0$, the scalar product $\langle p_{s',z}, p_{t-s',x} \rangle$ does not depend on $s' \in (0,t)$.
Proof of Claim 2: Let $r \in (0,s')$. Then using Claim 1 with $f = p_{r,x}$,

$$\begin{aligned} &\langle p_{s',z}, p_{t-s',x} \rangle = P_{s'} p_{t-s',x}(z) = P_r P_{s'-r} p_{t-s',x}(z) \\ &= \int p_{r,z} \langle p_{s'-r,z'}, p_{t-s',x} \rangle d\mu(z') \\ &= P_{t-r} p_{r,z}(x) = \langle p_{t-r,x}, p_{r,z} \rangle = \langle p_{r,z}, p_{t-r,x} \rangle . \end{aligned}$$

Now it follows from Claim 1 that

$$P_t f(x) = \int \left\langle p_{t/2,x}, p_{t/2,y} \right\rangle f(y) d\mu(y) = \int p(t,x,y) f(y) d\mu(y).$$

It remains to show $p(t,x,y) \geq 0$: It will be shown as an exercise (which relies on Lemma 6.2 and Example 6.3!) that $f \leq 1$ implies $P_t f \leq 1$. Thus if $c > 0$ and $f \leq c$ we have $P_t f \leq c$. If $f \geq 0$ we have $-f \leq c$ for all $c > 0$, so that we get $P_t(-f) \leq c$ and taking $c \to 0+$ we have shown that $f \geq 0$ implies $P_t f \geq 0$.
Now note that by the fundamental lemma of distribution theory we have $p_{t,x} = p(t,x,\cdot)$ μ-a.e., and so $p(t,x,\cdot) = p_{t,x} \in L^2(M)$. Thus writing

$$p(t,x,y) = p(t,x,y)_+ - p(t,x,y)_-$$

we get

$$\begin{aligned} &0 \leq P_t(p(t,x,\cdot)_-)(x) = \langle p(t,x,\cdot), p(t,x,\cdot)_- \rangle \\ &= \langle p(t,x,\cdot)_+, p(t,x,\cdot)_- \rangle - \langle p(t,x,\cdot)_-, p(t,x,\cdot)_- \rangle \\ &= - \langle p(t,x,\cdot)_-, p(t,x,\cdot)_- \rangle , \end{aligned}$$

so $\|p(t,x,\cdot)_-\|_2 = 0$ and the claim follows form continuity.

b) We have already shown the asserted square integrability. The symmetry $p(t,y,x) = p(t,x,y)$ follows immediately from

$$p(t,x,y) = \left\langle p_{t/2,x}, p_{t/2,y} \right\rangle .$$

Next, for all $0 < s' < t'$ one has

$$p(t',x,y) = \left\langle p_{s',x}, p_{t'-s',y} \right\rangle ,$$

as the formula holds for $s' = t/2$ and the as the RHS does not depend on s' by Claim 2. So

$$\int p(t,x,z)p(s,z,y)d\mu(z) = \langle p(t,x,\cdot), p(s,y,\cdot)\rangle = \langle p_{t,x}, p_{s,y}\rangle = p(t+s,x,y).$$

It remains to show

$$\int p(t,x,y)d\mu(y) \leq 1.$$

This follows by monotone konvergence from $P_t f \leq 1$ for all $f \leq 1$, by letting f run through $f = 1_{K_n}$ for K_n some compact exhaustion of M.
c) = Step 5 and the proof of part a).
d) For fixed s we set

$$v(t,y) := p(t+s,x,y) = p(t+s,y,x) = \int p(t,y,z)p(s,z,x)d\mu(z) = P_t p(s,\cdot,x)(y),$$

which by Step 5 solves the heat equation in (t,y). It follows that $(t,y) \mapsto v(t-s,y) = p(t,x,y)$ solves the heat equation, too.
Given any self-adjoint semibounded operator $\tilde{H}$ and any $\tilde{\phi} \in \mathrm{Dom}(\tilde{H}^l)$ for some $l \in \mathbb{N}_{\geq 0}$ the spectral calculus implies

$$\left\| e^{-t\tilde{H}}\tilde{\phi} - \tilde{\phi} \right\|_{\tilde{H}^l} := \left\| e^{-t\tilde{H}}\tilde{\phi} - \tilde{\phi} \right\| + \left\| \tilde{H}^l (e^{-t\tilde{H}}\tilde{\phi} - \tilde{\phi}) \right\| \to 0.$$

Applying this with $\tilde{H} = H$, $\tilde{\phi} = \phi$, noting that $\phi \in \mathrm{Dom}(H^l)$ for all l, as ϕ is smooth and compactly supported, we get

$$\left\| e^{-tH}\phi - \phi \right\|_{H^l} \to 0$$

for all l, but by elliptic regularity and the Sobolev embeding theorem, convergence with respect to all $\|\cdot\|_{H^l}$ implies convergence in $C^\infty(M)$ (which is locally uniform convergence of all derivates in charts).

■

8. Strong parabolic maximum principle and its applications

From here on we will closely follow the presentation from Grigor'yan's book [8]. The following result (and all its consequences) relies heavily on our standing assumption that M is connected:

Theorem 8.1. *i) The* strong parabolic minimum principle *holds: assume $I \subset \mathbb{R}$ is an open interval and $0 \leq u \in C^2(I \times M)$ solves*

$$\partial_t u \geq \Delta u.$$

If there exists $(t', x') \in I \times M$ with $u(t', x') = 0$, then one has $u(t, x) = 0$ for all $x \in M$ and all $t \leq t'$.

ii) The strong parabolic maximum principle *holds: assume $I \subset \mathbb{R}$ is an open interval and $0 \geq u \in C^2(I \times M)$ solves*

$$\partial_t u \leq \Delta u.$$

If there exists $(t', x') \in I \times M$ with $u(t', x') = 0$, then one has $u(t, x) = 0$ for all $x \in M$ and all $t \leq t'$

Proof. i) Step 1): *Let $\Omega \subset \mathbb{R} \times M$ be nonempty, open, and relatively compact and assume*[10] *$u \in C^2(\overline{\Omega})$ is such that*

$$\partial_t u \geq \Delta u \quad \text{ in } \Omega.$$

Then one has $\inf_{\overline{\Omega}} u = \inf_{\partial_p \Omega}$, where $\partial_p \Omega$ denotes the parabolic boundary of Ω, which is defined as the complement

$$\partial \Omega \setminus \partial_{\mathrm{top}} \Omega,$$

where $\partial_{\mathrm{top}} \Omega$ denotes the set of all $(t, x) \in \partial \Omega$ which admit an open neighborhood $U \subset M$ of x and $\epsilon > 0$ such that $(t - \epsilon, t) \times U \subset \Omega$. This is called parabolic minimum principle.

Proof of step 1:

WLOG we can assume the strict inequality $\partial_t u > \Delta u$ in Ω (if this is not satisfied, one can replace u by $u_\epsilon := u + \epsilon t$ and take $\epsilon \to 0+$). Let

$$(t_0, x_0) := \mathrm{argmin}_{(s,y) \in \overline{\Omega}} u(s, y).$$

It suffices to show $(t_0, x_0) \in \partial_p \Omega$. Assume the contrary. Then either $(t_0, x_0) \in \Omega$ or $(t_0, x_0) \in \partial_{\mathrm{top}} \Omega$. In both cases there exists a chart U around x_0 and $\epsilon > 0$ such that

$$\Gamma := (t_0 - \epsilon, t_0) \times U \subset \Omega.$$

By the definition of (x_0, t_0), one has

$$t_0 = \mathrm{argmin}_{s \in [t_0 - \epsilon, t_0]} u(s, x_0),$$

and so $\partial_t u(t_0, x_0) \leq 0$. By diagonalizing $g_{ij}(x_0)$ and making the induced coordinate transformation on U, we can assume that the coordinates $(x^1, \ldots, x^m)$ on U satisfy, for some constants, $b_1, \ldots, b_m$,

$$\Delta f(x_0) = \sum_{i=1}^{m} \frac{\partial^2}{(\partial x^i)^2} f(x_0) + \sum_{i=1}^{m} b_i \frac{\partial}{\partial x^i} f(x_0),$$

for all $f \in C^2(U)$. Since

$$x_0 = \mathrm{argmin}_{y \in \overline{U}} u(t_0, y),$$

[10]This means that u is the restriction of C^2-function on M to $\overline{\Omega}$

we have

$$\frac{\partial}{\partial x^i}u(t_0,x_0)=0, \quad \frac{\partial^2}{(\partial x^i)^2}u(t_0,x_0)\geq 0,$$

and so

$$\Delta u(t_0,x_0)\geq 0.$$

This estimate together with $\partial_t u(t_0,x_0)\leq 0$ contradicts $\partial_t u>\Delta u$ in Ω and proves the parabolic minimum principle.

Step 2): *Let V be a chart in M, let $x_0,x_1\in V$ be such that the line connecting x_0 and x_1 lies in V and assume $I\subset\mathbb{R}$ is an open interval and $0\leq u\in C^2(I\times M)$ solves*

$$\partial_t u\geq \Delta u.$$

Then for all $t_0,t_1\in I$ with $t_1>t_0$ and $u(t_0,x_0)>0$ one has $u(t_1,x_1)>0$.

Proof of step 2: Assume WLOG $t_0=0$ and that

- V is relatively compact and its closure is contained in a chart,
- $r>0$ is so small that the $2r$-neighborhood of the line connecting x_0 and x_1 lies in V, and that for $U:=B_e(x_0,r)$ one has

$$\inf_{x\in U}u(0,x)>0.$$

Set

$$\zeta:=\frac{1}{t_1}(x_1-x_0).$$

Then for all $t\in[0,t_1]$ one has $U+t\zeta\in V$. Consider the open tilted cylinder ('schiefer Zylinder')

$$\Gamma:=\{(t,x):t\in(0,t_1),x\in U+t\zeta\}.$$

We are going to show that $u>0$ in $\overline{\Gamma}$ away from the lateral surface of $\overline{\Gamma}$ ('Oberflaeche von $\overline{\Gamma}$ ohne Deckel und Boden'). To this end, pick a function $v\in C^2(\overline{\Gamma})$ such that

(33) $$\partial_t v\leq \Delta v \quad \text{in } \Gamma,$$

(34) $$v=0 \quad \text{on the lateral surface of } \overline{\Gamma} \text{ and } v>0 \text{ elsewhere on } \overline{\Gamma}.$$

Such a function v will be constructed in the exercises. Pick $\epsilon>0$ such that

$$\inf_{x\in U}u(0,x)\geq \epsilon\sup_{x\in U}v(0,x),$$

in particular, $u\geq\epsilon v$ at the bottom $\overline{U}$ of $\overline{\Gamma}$. In particular, $u\geq \epsilon v$ on $\partial_p\Gamma$. Since the function $u-\epsilon v$ satisfies the assumptions of the parabolic minimum principle, one has $u\geq\epsilon v$ in $\overline{\Gamma}$. In light of (34), this implies $u>0$ on $\overline{\Gamma}$ away from the lateral surface of $\overline{\Gamma}$, completing the proof of step 2.

Step 3): *The strong parabolic minimum principle holds:*

Proof of step 3: Given $u(t',x')=0$ for some $(t',x')\in I\times M$, it suffices to prove $u(t,x)=0$ for all $(t,x)\in I\times M$ with $t<t'$. Pick a finite sequence of points $x_0,\dots,x_k$ such such that $x_0=x$, $x_k=x'$ and such that x_i and x_{i+1} lie in the same chart together with line connecting these two points, for all $i=0,\dots,k$ (finally, here we use that M is connected!!).

Picking a finite sequence of times $t = t_0 < \dots t_k = t'$ we can use step 2 k-times to deduce that if $u(t_0, x_0) = u(t, x) > 0$ then also $u(t_1, x_1) > 0$, and so $u(t_2, x_2) > 0$ and so on, yielding finally that $u(t_k, x_k) = u(t', x') > 0$, a contradiction. This completes the proof of the strong parabolic minimum principle.

ii) This follows from applying i) to $-u$. ■

Corollary 8.2. *One has $p > 0$.*

Proof. Assume there exist t', x', y' with $p(t', x', y') = 0$. Then as $(t, y) \mapsto p(t, x', y)$ solves the heat equation one has $p(t, x', y) = 0$ for all $y \in M$ all $t \leq t'$. Pick ϕ smooth compactly supported with $\phi(x') = 1$. Then we have

$$\int p(t, x, y)\phi(y) d\mu(y) \to 0$$

as $t \to 0+$ by $p(t, x', y) = 0$ for all $y \in M$ all $t \leq t'$, while

$$\int p(t, x, y)\phi(y) d\mu(y) \to 1$$

as $t \to 0+$ by Theorem 7.1 d) and $\phi(x') = 1$. ■

Definition 8.3. Given $\alpha \in \mathbb{R}$, a real-valued function $u \in C^2(M)$ is called

- α-*superharmonic*, if $(-\Delta + \alpha)u \geq 0$,
- α-*subharmonic*, if $(-\Delta + \alpha)u \leq 0$,
- α-*harmonic*, if $(-\Delta + \alpha)u = 0$.

In the α-harmonic case we can assume that u is smooth by local elliptic regularity. If $\alpha = 0$, one simply says *superharmonic* (subharmonic) [harmonic], instead of 0-superharmonic, (0-subharmonic) [0-harmonic].

Theorem 8.4 (Strong elliptic minimum/maximum principle)**.** *i) Assume $\alpha \in \mathbb{R}$ and that $u \geq 0$ is α-superharmonic. If there exists x_0 with $u(x_0) = 0$, then one has $u \equiv 0$.*
ii) Assume $\alpha \in \mathbb{R}$ and that $u \leq 0$ is α-subharmonic. If there exists x_0 with $u(x_0) = 0$, then one has $u \equiv 0$.

Proof. i) Apply the strong parabolic minimum principle to $v(t, x) := e^{\alpha t} u(x)$.
ii) Apply i) to $-u$. ■

Corollary 8.5. *i) If u is superharmonic and if there exits x_0 with $u(x_0) = \inf u$, then $u \equiv \inf u$.*
ii) If u is subharmonic and if there exits x_0 with $u(x_0) = \sup u$, then $u \equiv \sup u$.

Proof. i) Apply the strong elliptic minumum principle to $\tilde{u} := u - \inf u$.
ii) Apply i) to $-u$. ■

Example 8.6. Let N be a compact connected manifold (accoring to our convention: smooth without boundary). By picking a Riemannian metric on N, using the Hodge-Theorem and that continuous real-valued functions on a compact space attain their minimum and maximum, we get from the above Corollary

$$\mathsf{H}^0(N) = \{f : \Delta f = 0\} = \{\text{constant real-valued functions on } N\} = \mathbb{R}$$

for the zeroth homology group of N.

Theorem 8.7 (Elliptic minimum/maximum principle)**.** *Let $V \subset M$ be open, relatively compact with ∂V nonempty.*
i) Assume $u \in C^2(V) \cap C(\overline{V})$ is superharmonic, then one has

$$\inf_{\overline{V}} u = \inf_{\partial V} u.$$

ii) Assume $u \in C^2(V) \cap C(\overline{V})$ is subharmonic, then one has

$$\sup_{\overline{V}} u = \sup_{\partial V} u.$$

Proof. i) set $r := \inf_{\overline{V}} u$ and

$$S := \{x \in \overline{V} : u(x) = r\}.$$

It suffices to show that S intersets ∂V. Assume not. Then one has $S \subset V$. We are going to show that the closed set S is open, so $S = M$, a contradiction to $S \subset V \subset M \setminus \partial V$. Let $x \in S \subset V$ and let $N \subset V$ be a connected open nbh of x. Then $u|_N$ attains its minimum in x, and so $u \equiv r$ by the above Corollary. Thus we have shown $N \subset S$, showing that S is open.
ii) Apply i) to $-u$. ■

9. Some spectral theory

In general, both parts of the spectrum (discrete spectrum and essential spectrum) of H can be nonempty and the only thing we know for sure is $\sigma(H) \subset [0, \infty)$, as $H \geq 0$. The following simple result indicated that essential spectrum can only be nonempty on noncompactness M's:

Theorem 9.1. *Assume that for some $t > 0$ one has*

$$\sup_{x \in X} p(t, x, x) < \infty,$$

and that $\mu(M) < \infty$. Then H has a purely discrete spectrum (so the spectrum consists of eigenvalues having finite multiplicity), and if (λ_n) denotes the increasing ennumeration of the eigenvalues with each eigenvalue counted according to its multiplicity, then one has

$$0 \leq \lambda_n \nearrow \infty.$$

Proof. By abstract functional analysis it suffices to show that $P_t = e^{-tH}$ is Hilbert-Schmidt. But the latter is an integral operator, so it suffices to show

$$\int \int p(t, x, y)^2 d\mu(x) d\mu(y) < \infty.$$

Since

$$\int \int p(t, x, y)^2 d\mu(x) d\mu(y) = \int p(t, x, x) d\mu(x),$$

the claim follows from the assumptions. ■

The latter result clearly applies to compact M's (so compact M's have a purely discrete spectrum), but also to some noncompact M's! For example, as we shall see later on (cf. Corollary 9.8 below), the result applies to open relatively compact subsets of an arbitrary Riemannian manifold (so those have a purely discrete spectrum, too). To prove the latter statement, we are going to show

$$p^U(t,x,y) \leq p(t,x,y),$$

where $U \subset M$ is an arbitrary open relatively compact subset and p^U its heat kernel, that is, the heat kernel of the Riemannian manifold $(U, g|_U)$. To this end, we record:

Lemma 9.2. *For all $0 \leq f \in W_0^{1,2}(M)$ there exists a sequence $0 \leq f_k \in C_c^\infty(M)$ with $f_k \to f$ as $k \to \infty$ in $W^{1,2}(M)$.*

Proof. Pick a sequence $h_k \in C_c^\infty(M)$ with $h_k \to f$ in $W^{1,2}(M)$, and pick $\psi : \mathbb{R} \to [0,\infty)$ smooth with $\psi(0) = 0$ and $\sup_t |\psi'(t)| < \infty$. Then $0 \leq \psi \circ h_k \in C_c^\infty(M)$ and $\psi \circ h_k \to \psi \circ f$ in $W^{1,2}(M)$ by Lemma 6.2 (applied with a constant sequence). Thus it suffices to show that there exists a sequence $\psi_k : \mathbb{R} \to [0,\infty)$ smooth with $\psi_k(0) = 0$ and $\sup_{k,t} |\psi_k'(t)| < \infty$ such that $\psi_k \circ f \to f$ in $W^{1,2}(M)$. So this end, let $\phi(t) := 1_{(0,\infty=}(t)$, $\psi(t) := t_+$, $t \in \mathbb{R}$, and pick ψ_k as in Example 6.3. Then for some $C > 0$ we have $|\psi_k(t) - \psi(t)| \leq C|t|$ for all t,k, so that $\psi_k \circ f \to \psi \circ f = f$ in $L^2(M)$ by dominated convergence. Moreover, we have $d(\psi_k \circ f) = (\psi_k' \circ f)df$ by Lemma 6.2 which shows that $d(\psi_k \circ f) \to (\phi \circ f)df = df$ again by dominated convergence. This completes the proof. ∎

Let $U \subset M$ be open and denote by $\tilde{\alpha}$ the trivial extension to M by zero away from U of a function or a 1-form on U. Then we consider $L^2(U)$ as a closed subspace of $L^2(M)$ via the embedding $f \mapsto \tilde{f}$, and likewise we have $\Omega^1_{L^2}(U) \subset \Omega^1_{L^2}(M)$.

Lemma 9.3. *Let $U \subset M$ be open. Then for all $f \in W_0^{1,2}(U)$ one has $\tilde{f} \in W_0^{1,2}(M)$ and $d\tilde{f} = \widetilde{df}$. In particular, $W_0^{1,2}(U) \subset W_0^{1,2}(M)$ is a closed subspace.*

Proof. If $f \in C_c^\infty(U)$ then clearly $\tilde{f} \in C_c^\infty(M)$ with $d\tilde{f} = \widetilde{df}$ by locality of differential operators.
Now let $f \in W_0^{1,2}(U)$ and pick a sequence $f_n \subset C_c^\infty(U)$ with $f_n \to f$ in $W^{1,2}(U)$. Then clearly $\tilde{f}_n \to \tilde{f}$ in $L^2(M)$. Moreover, $\tilde{f}_n$ is Cauchy in $W^{1,2}(M)$, and its limit must be $\tilde{f}$, because $\tilde{f}_n \to \tilde{f}$ in $L^2(M)$. In particular, $d\tilde{f}_n \to d\tilde{f}$ in $\Omega_{L^2}(M)$. On the other hand, we have $df_n \to df \in \Omega_{L^2}(U)$ and so $\widetilde{df_n} \to \widetilde{df} \in \Omega_{L^2}(M)$. In view of $\widetilde{df_n} = d\widetilde{f_n}$, we have ultimately shown $d\tilde{f} = \widetilde{df}$.

∎

The analogous result with $W_0^{1,2}$ replaced by $W^{1,2}$ is wrong: in $\mathbb{R}^m$, one has $1 \in W^{1,2}(B(x_0,1))$ (this is trivial), but $\tilde{1} = 1_{B(x_0,1)} \notin W^{1,2}(\mathbb{R}^m)$ (this requires some work).

Lemma 9.4. *Let $h \in W^{1,2}(M)$. Then there exists $v \in W_0^{1,2}(M)$ with $h \leq v$, if and only if one has $h_+ \in W_0^{1,2}(M)$.*

Proof. Exercise. ∎

Lemma 9.5. *Assume* $0 \leq u \in W^{1,2}(M)$*,* $f \in L^2(M)$ *is real-valued,* $\lambda > 0$*, and that one has* $(-\Delta + \lambda)u \geq f$ *weakly, meaning that*

$$\int u(-\Delta + \lambda)\phi d\mu \geq \int f\phi d\mu \tag{35}$$

for all $0 \leq \phi \in C_c^\infty(M)$*. Then one has* $u \geq (H + \lambda)^{-1}f$*.*

Proof. Write $f = (H + \lambda)(H + \lambda)^{-1}f$ and set $v := (H + \lambda)^{-1}f \in \mathrm{Dom}(H) \subset W_0^{1,2}(M)$. Then one has

$$(-\Delta + \lambda)(v - u) \leq 0$$

weakly, and so

$$(-\Delta + \lambda)h \leq 0$$

weakly, if we set $h := v - u \in W^{1,2}(M)$. Thus, integrating by parts,

$$\int (dh, d\phi)d\mu + \lambda \int h\phi d\mu \leq 0$$

for all $0 \leq \phi \in C_c^\infty(M)$. Since both sided are continuous in the $W^{1,2}$-norm, Lemma 9.2 shows that the the latter inequality holds for all $0 \leq \phi \in W_0^{1,2}(M)$. By Lemma 9.4 we have $0 \leq h_+ \in W_0^{1,2}(M)$, and so

$$\int (dh, dh_+)d\mu + \lambda \int hh_+d\mu = \int (dh, dh_+)d\mu + \lambda \int h_+^2 d\mu \leq 0.$$

By Example 6.3 one has

$$\int (dh, dh_+)d\mu = \int |dh_+|^2 d\mu,$$

and so

$$\int |dh_+|^2 d\mu + \lambda \int h_+^2 d\mu =\leq 0,$$

and so $h_+ = 0$, as $\lambda > 0$. This shows $v - u \leq 0$, and so $v = (H + \lambda)^{-1}f \leq u$. ■

Lemma 9.6. *For all* $\lambda > 0$ *one has* $(H + \lambda)^{-1}f_1 \leq (H + \lambda)^{-1}f_2$*, whenever* $f_1, f_2 \in L^2(M)$ *are such that* $f_1 \leq f_2$*.*

Proof. By linearity we can assume $f_1 = 0$. Using the formula (Laplace-transforms)

$$(r + \lambda)^{-1} = \int_0^\infty e^{-\lambda s}e^{-sr}ds$$

with $r = H$ (spectral calculus) implies

$$(H + \lambda)^{-1}f_2 = \int_0^\infty e^{-\lambda s}P_s f_2 ds \geq 0,$$

where the intregal converges in the L^2-sense, so the claim follows from $P_s f_2 \geq 0$ (which is a consequence of $p(s, x, y) \geq 0$). Note there that on any measure space $0 \leq h_n \to h$ in L^p for some $p \in [1, \infty)$ implies $h \geq 0$. ■

Given $U \subset M$ open, we denote with H^U, P^U, p^U the objects H, P, p which are defined on the Riemannian manifold $(U, g|_U)$. Based on the above auxiliary results we can prove:

Theorem 9.7. *For all open $U \subset M$, $t > 0$, $x, y \in U$ one has $p^U(t,x,y) \leq p(t,x,y)$.*

Proof. It suffices to prove that for all $0 \leq f \in L^2(U)$, $x \in U$, one has

$$\left(\int_U p^U(t,x,y)f(y)d\mu(y) =\right) P_t^U f(x) \leq P_t \tilde{f}(x) \; \left(= \int_U p(t,x,y)f(y)d\mu(y)\right). \tag{36}$$

Step 1: *For all $\lambda > 0$ one has $(H^U+\lambda)^{-1}f \leq (H+\lambda)^{-1}\tilde{f}$.*
Proof of step 1: We have $u := (H+\lambda)^{-1}\tilde{f} \in W_0^{1,2}(M) \subset W^{1,2}(M)$, and this function in ≥ 0 by Lemma 9.6. Clearly, $u|_U \in W^{1,2}(U)$ and $(-\Delta+\lambda)u|_U = f|_U$. Thus, we have

$$(H+\lambda)^{-1}\tilde{f} = u \geq (H^U+\lambda)^{-1}\tilde{f}.$$

from Lemma 9.5.
Step 2: *For all $\lambda > 0$, $k \in \mathbb{N}$, one has $(H^U+\lambda)^{-k}f \leq (H+\lambda)^{-k}\tilde{f}$.*
Proof of step 2: This follows from applying step 1 and Lemma 9.6 (using the latter for M and for U).
Step 3: *One has (36).*
Proof of step 3: By applying the formula $e^{-tr} = \lim_k \left(\frac{k}{t}\right)^k (r+k/t)^{-k}$ for $r = H, H^U$ (spectral calculus), we get the L^2-convergences

$$P_t^U = e^{-tH^U} = \lim_k \left(\frac{k}{t}\right)^k (H^U+k/t)^{-k}, \quad P_t = e^{-tH} = \lim_k \left(\frac{k}{t}\right)^k (H+k/t)^{-k},$$

so that the claim follows from Step 2.

■

Applying the last result with M replaced by V, where $V \subset M$ is open with $U \subset V$, implies that for all $0 \leq f \in L^2(M)$ one has $P_t^U f|_U \leq P_t^V f|_V$, in particular if $(U_j)_{j\in\mathbb{N}}$ is an exhaustion of M with open subsets the limit $\lim_n P_t^{U_n} f|_{U_n}$ exists pointwise. As one might guess, one has that for all $t > 0$ (exercise)

$$P_t^{U_n} f|_{U_n} \nearrow P_t f \quad \mu\text{-a.e.} \tag{37}$$

With some nore efforts, one can prove that the above relation actually holds pointwise (and even in the C^∞), but we will not need this stronger statement.

Corollary 9.8. *For all open relatively compact $U \subset M$ the operator H^U has a purely discrete spectrum.*

Proof. Combine Theorem 9.7 with Theorem 9.1. ■

10. Wiener measure and Brownian motion on Riemannian manifolds

Roughly speaking, one would like to construct Brownian motion $X(x_0)$ on M, starting from $x_0 \in M$, as follows: It should be an M-valued process[11] with continuous paths

$$X(x_0) : [0, \infty) \times \Omega \longrightarrow M, \tag{38}$$

which is defined on some probability space $(\Omega, \mathbb{P}, \mathscr{F})$, and which has the transition probability densities given by $p(t, x, y)$. In other words, given $n \in \mathbb{N}$, a finite sequence of times $0 < t_1 < \cdots < t_n$ and Borel sets $A_1, \dots, A_n \subset M$, setting $\delta_j := t_{j+1} - t_j$ with $t_0 := 0$, we would like the probability of finding the Brownian particle simultaneously in A_1 at the time t_1, in A_2 at the time t_2, and so on, to be given by the quantity

$$\begin{aligned} &\mathbb{P}\{X_{t_1}(x_0) \in A_1, \dots, X_{t_n}(x_0) \in A_n\} \\ &= \int \cdots \int 1_{A_1}(x_1) p(\delta_0, x_0, x_1) \cdots \\ &\qquad \times 1_{A_n}(x_n) p(\delta_{n-1}, x_{n-1}, x_n) d\mu(x_1) \cdots d\mu(x_n), \end{aligned} \tag{39}$$

whenever the particle starts from x_0. Equivalently, one could say that a Brownian motion on M with starting point x_0 is a process with continuous paths (38), such that the finite-dimensional distributions of its law are given by the right-hand side of (39)[12]. In fact, such a path space measure is uniquely determined by its finite-dimensional distributions (cf. Remark 10.8 below). In particular, all Brownian motions should have the same law, which we will call the *Wiener measure* later on.

Ultimately, the above prescriptions indeed turn out to work perfectly well in terms of giving Brownian motion for the Euclidean $\mathbb{R}^m$ or for compact Riemannian manifolds. On the other hand, we see from (39) that, in particular, it is required that for all $t > 0$,

$$\mathbb{P}\{X_t(x_0) \in M\} = \int_M p(t, x_0, y) d\mu(y).$$

Lemma 10.1. *Assume $M = U$ is an open connected subset of the Euclidean $\mathbb{R}^m$ with $\mathbb{R}^m \setminus U$ has a positive measure (for example U could be bounded). Then one has*

$$\int_U p^U(t, x_0, y) dy < 1 \text{ for some (in fact: all) } (t, x_0) \in (0, \infty) \times M. \tag{40}$$

[11] We recall that given two measurable spaces Ω_1 and Ω_2, a map

$$X : [0, \infty) \times \Omega_1 \longrightarrow \Omega_2, \quad (t, \omega) \longmapsto X_t(\omega)$$

is called an Ω_2-*valued process*, if for all $t \geq 0$ the induced map $X_t : \Omega_1 \to \Omega_2$ is measurable. The maps $t \mapsto X_t(\omega)$, with fixed $\omega \in \Omega_1$, are referred to as the *paths of* X.

[12] The law of $X(x_0)$ is by definition the probability measure on the space of continuous paths on M, which is defined as the pushforward of $\mathbb{P}$ under the induced map

$$\Omega \longrightarrow C([0, \infty), M), \ \omega \longmapsto X_\bullet(x_0)(\omega).$$

Proof. One has

$$\int_U p^U(t,x_0,y)dy \le \int_U p(t,x_0,y)dy = \int_{\mathbb{R}^m} p(t,x_0,y)dy - \int_{\mathbb{R}^m\setminus U} p(t,x_0,y)dy,$$

so the claim follows from

$$\int_{\mathbb{R}^m} p(t,x_0,y)dy = \int_{\mathbb{R}^m} \frac{1}{(4\pi t)^{m/2}} e^{-\frac{|x_0-y|^2}{4t}} dy$$

as by (Fourier transform) the Euclidean heat kernel is given by the Gauss-Weierstrass formula

$$p(t,x_0,y) = \frac{1}{(4\pi t)^{m/2}} e^{-\frac{|x_0-y|^2}{4t}}$$

and as one has

$$\int_{\mathbb{R}^m\setminus U} p(t,x_0,y)dy > 0,$$

as $p > 0$ and $\mathbb{R}^m \setminus U$ has positive measure.

■

The above Lemma leads to the conceptual difficulty that the process can leave its space of states with a strictly positive probability and one ends up with:

Definition 10.2. M is called *stochastically complete*, if one has

$$\int_M p(t,x_0,y)d\mu(y) = 1 \quad \text{for all } (t,x_0) \in (0,\infty)\times M.$$

Using the Champman-Kolmogorov equations it is easily checked that M is stochastically complete, if and only if one has

$$\int_M p(t,x_0,y)d\mu(y) = 1 \quad \text{for } \textit{some } (t,x_0) \in (0,\infty)\times M.$$

Remark 10.3. Stochastic completeness is unrelated to geodesic completeness. For example, $\mathbb{R}^m \setminus \{0\}$ is stochastically complete but geodesically incomplete, and there exist geodesically complete and but stochastically incomplete M's. On the other hand, a celebrated result by Yau states that if M is geodesically complete with a Ricci curvature bounded from below by a constant, then M is stochastically complete. In particular, the Euclidean $\mathbb{R}^m$ is stochastically complete (of course this follows, as already observed, also simply from a calculation), and compact M's are stochastically complete.

Since we aim to work on arbitrary Riemannian manifolds, we need to solve the above conceptual problem of stochastic incompleteness. This is done by using the Alexandrov compactification of M. Since it does not cause much extra work, we start by explaining the corresponding constructions in the setting of an arbitrary Polish space, recalling that a topological space is called Polish, if it is separable and if it admits a complete metric which induces the original topology.

Notation 10.4. Given a locally compact Polish space N, we set

$$\widetilde{N} := \begin{cases} N, \text{if } N \text{ is compact} \\ \text{Alexandrov compactification } N \cup \{\infty_N\}, \text{ if } N \text{ is noncompact.} \end{cases}$$

We recall here that ∞_N is any point $\notin N$, and that the topology on $N \cup \{\infty_N\}$ is defined as follows: $U \subset N \cup \{\infty_N\}$ is declared to be open, if and only if either U is an open subset of N or if there exists a compact set $K \subset N$ such that $U = (N \setminus K) \cup \{\infty_N\}$. This construction depends trivially on the choice of ∞_N, in the sense that for any other choice $\infty'_N \notin N$, the canonical bijection $N \cup \{\infty_N\} \to N \cup \{\infty'_N\}$ is a homeomorphism.
We consider the path space $\Omega_N := C([0,\infty), \widetilde{N})$, and thereon we denote (with a slight abuse of notation) the canonically given coordinate process by

$$\mathbb{X} : [0,\infty) \times \Omega_N \longrightarrow \widetilde{N}, \ \ \mathbb{X}_t(\gamma) := \gamma(t).$$

We consider Ω_N a topological space with respect to the topology of uniform convergence on compact subsets, and we equip it with its Borel sigma-algebra $\mathscr{F}^N$.

We fix such a locally compact Polish space N (e.g., a manifold) for the moment. It is well-known that Ω_N as defined above is Polish again. In fact, $\widetilde{N}$ is Polish, and if we pick a bounded metric $\varrho_{\widetilde{N}} : \widetilde{N} \times \widetilde{N} \to [0,1]$ which induces the original topology on $\widetilde{N}$, then

$$\varrho_{\Omega_N}(\gamma_1, \gamma_2) := \sum_{j=1}^{\infty} \max_{0 \leq t \leq j} \varrho_{\widetilde{N}}(\gamma_1(t), \gamma_2(t))$$

is a complete separable metric[13] on Ω_N which induces the original topology (of local uniform convergence). Furthermore, since evaluation maps of the form

$$X_1 \times C(X_1, X_2) \longrightarrow X_2, \ \ (x, f) \longmapsto f(x)$$

are always jointly continuous, if X_1 is locally compact and Hausdorff and if $C(X_1, X_2)$ is equipped with its topology of local uniform convergence, it follows that $\mathbb{X}$ is in fact jointly continuous. In particular, $\mathbb{X}$ is jointly (Borel) measurable.

Notation 10.5. Given a set Ω and a collection $\mathscr{C}$ of subsets of Ω or of maps with domain Ω, the symbol $\langle \mathscr{C} \rangle$ stands for the smallest sigma-algebra on Ω which contains $\mathscr{C}$. Furthermore, whenever there is no danger of confusion, we will use notations such as

$$\{f \in A\} := \{y \in \Omega : f(y) \in A\} \subset \Omega,$$

where $f : \Omega \to \Omega'$ and $A \subset \Omega'$.

[13] In fact, it is easy to see that this is a complete metric which induces the original topology. On the other hand, the proof that this topology is separable is a little tricky. Although it is not so easy to find a precise reference, we believe that these results can be traced back to Kolmogorov.

Definition 10.6. 1. A subset $C \subset \Omega_N$ is called a *Borel cylinder*, if there exist $n \in \mathbb{N}$, $0 < t_1 < \cdots < t_n$ and Borel sets $A_1, \dots, A_n \subset \widetilde{N}$, such that

$$C = \{\mathbb{X}_{t_1} \in A_1, \dots, \mathbb{X}_{t_n} \in A_n\} = \bigcap_{j=1}^{n} \mathbb{X}_{t_j}^{-1}(A_j).$$

The collection of all Borel cylinders in Ω_N will be denoted by $\mathscr{C}^N$.
2. Likewise, given $t \geq 0$, the collection $\mathscr{C}_t^N$ of *Borel cylinders in* Ω_N *up to the time* t is defined to be the collection of subsets $C \subset \Omega_N$ of the form

$$C = \{\mathbb{X}_{t_1} \in A_1, \dots, \mathbb{X}_{t_n} \in A_n\} = \bigcap_{j=1}^{n} \mathbb{X}_{t_j}^{-1}(A_j),$$

where $n \in \mathbb{N}$, $0 < t_1 < \cdots < t_n < t$, and where $A_1, \dots, A_n \subset \widetilde{N}$ are Borel sets.

It is easily checked inductively that both $\mathscr{C}^N$ and $\mathscr{C}_t^N$ are π-systems in Ω_N, that is, both collections are (nonempty and) stable under taking finitely many intersections. The following fact makes $\mathscr{F}^N$ handy in applications:

Lemma 10.7. *One has*

$$\mathscr{F}^N = \left\langle \mathscr{C}^N \right\rangle = \left\langle (\mathbb{X}_s : \Omega_N \longrightarrow \widetilde{N})_{s \geq 0} \right\rangle. \tag{41}$$

Proof. Since for every fixed $s \geq 0$ the map

$$\mathbb{X}_s : \Omega_N \longrightarrow \tilde{N},\ \gamma \longmapsto \gamma(s)$$

is $\mathscr{F}^N$-measurable, it is clear that $\mathscr{C}^N \subset \mathscr{F}^N$, and therefore

$$\left\langle \mathscr{C}^N \right\rangle \subset \mathscr{F}^N.$$

In order to see

$$\mathscr{F}^N \subset \left\langle \mathscr{C}^N \right\rangle,$$

pick a topology-defining metric $\varrho_{\widetilde{N}}$ on $\widetilde{N}$ and denote the corresponding closed balls by $\overline{B_{\widetilde{N}}}(x, r)$. Then, since the elements of Ω_N are continuous, for all $\gamma_0 \in \Omega_N$, $n \in \mathbb{N}$, $\epsilon > 0$ one has

$$\begin{aligned} &\left\{\gamma : \max_{0 \leq t \leq n} \varrho_{\widetilde{N}}(\gamma(t), \gamma_0(t)) \leq \epsilon\right\} \\ &= \bigcap_{0 \leq t \leq n,\ t \text{ is rational}} \left\{\gamma : \gamma(t) \in \overline{B_{\widetilde{N}}}(\gamma_0(t), \epsilon)\right\}, \\ &= \bigcap_{0 < t \leq n,\ t \text{ is rational}} \left\{\gamma : \gamma(t) \in \overline{B_{\widetilde{N}}}(\gamma_0(t), \epsilon)\right\}. \end{aligned}$$

Therefore, sets of the form

$$\left\{\gamma : \max_{0 \leq t \leq n} \varrho_{\widetilde{N}}(\gamma(t), \gamma_0(t)) \leq \epsilon\right\},\quad \gamma_0 \in \Omega_N,\ n \in \mathbb{N},\ \epsilon > 0 \tag{42}$$

are $\langle\mathscr{C}^N\rangle$-measurable. Since the collection of sets of the form (42) generates the topology of local uniform convergence[14], it is clear that the induced Borel sigma-algebra $\mathscr{F}^N$ satisfies $\mathscr{F}^N \subset \langle\mathscr{C}^N\rangle$.
The inclusion

$$\left\langle\mathscr{C}^N\right\rangle \subset \left\langle(\mathbb{X}_s : \Omega_N \longrightarrow \widetilde{N})_{s\geq 0}\right\rangle$$

is clear, since each set in $\mathscr{C}^N$ is a finite intersection of sets of the form $\mathbb{X}_s^{-1}(A)$, $s > 0$, $A \subset \widetilde{N}$ Borel. To see

$$\left\langle(\mathbb{X}_s : \Omega_N \longrightarrow \widetilde{N})_{s\geq 0}\right\rangle \subset \left\langle\mathscr{C}^N\right\rangle,$$

note that for every metric $\varrho_{\widetilde{N}}$ that generates the topology on $\widetilde{N}$, one has

$$\left\langle(\mathbb{X}_s : \Omega_N \longrightarrow \widetilde{N})_{s\geq 0}\right\rangle = \left\langle\left\{\mathbb{X}_s^{-1}\big(\overline{B_{\widetilde{N}}}(x,r)\big) : x \in \widetilde{N}, r > 0, s \geq 0\right\}\right\rangle,$$

with the corresponding closed balls $\overline{B_{\widetilde{N}}}(\dots)$, so that it only remains to prove

$$\mathbb{X}_0^{-1}\big(\overline{B_{\widetilde{N}}}(x,r)\big) \in \left\langle\mathscr{C}^N\right\rangle$$

for all $x \in \widetilde{N}$, $r > 0$. This, however, follows from

$$\mathbb{X}_0^{-1}\big(\overline{B_{\varrho_{\widetilde{N}}}}(x,r)\big) = \big\{\gamma : \lim_{n\to\infty} \varrho_{\widetilde{N}}(\gamma(1/n), x) \leq r\big\},$$

since clearly $\gamma \mapsto \varrho_{\widetilde{N}}(\gamma(1/n), x)$ is a $\langle\mathscr{C}^N\rangle$-measurable function on Ω_N (the pre-image of an interval of the form $[0, R]$ under this map is the cylinder set $\mathbb{X}_{1/n}^{-1}\big(\overline{B_{\widetilde{N}}}(x,R)\big)$). This completes the proof. ■

Remark 10.8. By the above lemma, $\mathscr{C}^N$ is a π-system that generates $\mathscr{F}^N$. It then follows from an abstract measure theoretic result that every finite measure on $\mathscr{F}^N$ is uniquely determined by its values on $\mathscr{C}^N$.

Definition 10.9. Setting

$$\mathscr{F}_t^N := \left\langle(\mathbb{X}_s : \Omega_N \longrightarrow \widetilde{N})_{0\leq s\leq t}\right\rangle \quad \text{for every } t \geq 0,$$

it follows from Lemma 10.7 that

$$\mathscr{F}_*^N := \bigcup_{t\geq 0} \mathscr{F}_t^N$$

becomes a filtration of $\mathscr{F}^N$. It is called the *filtration generated by the coordinate process on* Ω_N.

Precisely as for the second equality in (41), one proves

$$\mathscr{F}_t^N = \left\langle\mathscr{C}_t^N\right\rangle \quad \text{for all } t \geq 0. \tag{43}$$

Particularly important $\mathscr{F}_t^N$-measurable sets are provided by exit times:

[14]To be precise, this collection forms a basis of neighbourhoods of this topology.

Definition 10.10. Given an arbitrary subset $U \subset \widetilde{N}$, we define

$$\zeta_U : \Omega_N \longrightarrow [0,\infty], \qquad \zeta_U := \inf\{t \geq 0 : \mathbb{X}_t \in \widetilde{N} \setminus U\}, \tag{44}$$

and call this map the *the first exit time of* $\mathbb{X}$ *from* U, with $\inf\{...\} := \infty$ in case the set is empty.

There is the following result, which in a probabilistic language means that first exit times from open sets are $\mathscr{F}^N_*$-optional times:[15]

Lemma 10.11. *Assume that* $U \subset \widetilde{N}$ *is open with* $U \neq \widetilde{N}$. *Then one has*

$$\{t < \zeta_U\} \in \mathscr{F}^N_t \quad \text{for all } t \geq 0.$$

Proof. The proof actually only uses that $\mathbb{X}$ has continuous paths and that $\widetilde{N}$ is metrizable: Pick a metric $\varrho_{\widetilde{N}}$ on $\widetilde{N}$ which induces the original topology. Then, since $\tilde{N} \setminus U$ is closed and $\mathbb{X}$ has continuous paths, we have

$$\{t < \zeta_U\} = \bigcup_{n \in \mathbb{N}} \bigcup_{0 \leq s \leq t,\ s \text{ is rational}} \{\varrho_{\widetilde{N}}(\mathbb{X}_s, \tilde{N} \setminus U) \geq 1/n\}.$$

The set on the right-hand side clearly is $\in \mathscr{F}^N_t$, since the distance function to a nonempty set is continuous and thus Borel. ■

We return to our Riemannian setting. In order to apply the above abstract machinery in this case, we have to extend some Riemannian data to the compactification of M (in the noncompact case):

Notation 10.12. Let $\widetilde{\mu}$ denote the Borel measure on $\widetilde{M}$ given by μ if M is compact, and which is extended to ∞_M by setting $\mu(\infty_M) = 1$ in the noncompact case. Then we define a Borel function

$$\widetilde{p} : (0,\infty) \times \widetilde{M} \times \widetilde{M} \longrightarrow [0,\infty)$$

as follows: $\widetilde{p} := p$ if M is compact, and in case M is noncompact, then for $t > 0$, $x, y \in M$ we set

$$\widetilde{p}(t,x,y) := p(t,x,y),\ \widetilde{p}(t,\infty_M,x) := 0,\ \widetilde{p}(t,\infty_M,\infty_M) := 1,$$
$$\widetilde{p}(t,y,\infty_M) := 1 - \int_M p(t,y,z)d\mu(z).$$

It is straightforward to check that the pair $(\widetilde{p},\widetilde{\mu})$ satisfies the Chapman-Kolmogorov equations, that is, for all $s,t > 0$, $x, y \in \widetilde{M}$ one has

$$\int_{\widetilde{M}} \widetilde{p}(t,x,z)\widetilde{p}(s,z,y)d\widetilde{\mu}(z) = \widetilde{p}(s+t,x,y). \tag{45}$$

[15] Let $(\Omega, \mathscr{F})$ be a measure space, and let $\mathscr{F}_* = (\mathscr{F}_t)_{t\geq 0}$ be a filtration of $\mathscr{F}$. Then a map $\tau : \Omega \to [0,\infty]$ is called a $\mathscr{F}_*$*-optional time*, if for all $t \geq 0$ one has $\{t < \tau\} \in \mathscr{F}_t$, and it is called a $\mathscr{F}_*$*-stopping time*, if for all $t \geq 0$ one has $\{t \leq \tau\} \in \mathscr{F}_t$.

Furthermore, one has

$$\int_{\widetilde{M}} \widetilde{p}(t,x,y)d\widetilde{\mu}(y) = 1 \text{ for all } x \in \widetilde{M}, \tag{46}$$

in contrast to the possibility of $\int_M p(t,x,y)d\mu(y) < 1$ in case M is stochastically incomplete. It is precisely the conservation of probability (46) which motivates the above Alexandrov machinery. Since there is no danger of confusion, the following abuse of notation will be very convenient in the sequel:

Notation 10.13. We write $\zeta := \zeta_M$ for the first exist time of the coordinate process $\mathbb{X}$ on Ω_M from $M \subset \widetilde{M}$.

For obvious reasons, ζ is also called the *explosion time* of $\mathbb{X}$. Note also that one has $\zeta > 0$, and that by our previous conventions we have $\zeta \equiv \infty$ if M is compact. The last fact is consistent with the fact that compact Riemannian manifolds are stochastically complete.

The following existence result will be central in the sequel:

Proposition and definition 10.14. *The* Wiener measure $\mathbb{P}^{x_0}$ *with initial point* $x_0 \in M$ *is defined to be the unique probability measure on* $(\Omega_M, \mathscr{F}^M)$ *which satisfies*

$$\begin{aligned}&\mathbb{P}^{x_0}\{\mathbb{X}_{t_1} \in A_1, \dots, \mathbb{X}_{t_n} \in A_n\}\\ &= \int \cdots \int 1_{A_1}(x_1)\widetilde{p}(\delta_0, x_0, x_1) \cdots\\ &\qquad \times 1_{A_n}(x_n)\widetilde{p}(\delta_{n-1}, x_{n-1}, x_n) d\widetilde{\mu}(x_1) \cdots d\widetilde{\mu}(x_n)\end{aligned}$$

for all $n \in \mathbb{N}$, *all finite sequences of times* $0 < t_1 < \cdots < t_n$ *and all Borel sets* $A_1, \dots, A_n \subset \widetilde{M}$, *where* $\delta_j := t_{j+1} - t_j$ *with* $t_0 := 0$. *It has the additional property that*

$$\mathbb{P}^{x_0}\Big(\{\zeta = \infty\} \bigcup \Big\{\zeta < \infty \text{ and } \mathbb{X}_t = \infty_M \text{ for all } t \in [\zeta, \infty)\Big\}\Big) = 1, \tag{47}$$

in other words, the point at infinity ∞_M *is a "trap" for* $\mathbb{P}^{x_0}$*-a.e. path.*[16]

Proof. We will consider the case that M is an open relatively compact subset of a Riemannian manifold.

Step 1: Consider Ω_M^0 the space of *all* maps from $[0, \infty) \to \widetilde{M}$ with the smallest sigma-algebra $\mathscr{F}^{M,0}$ such that with the process

$$\mathbb{X}^0 : [0, \infty) \times \Omega_M^0 \longrightarrow \widetilde{M}, \quad \mathbb{X}_t^0(\gamma) := \gamma(t),$$

[16]It is a trap in the sense that once a path touches ∞_M, it remains there for all times.

the maps $\mathbb{X}^0_t$ are measurable for all $t \geq 0$. Then there exists a unique probability measure $\mathbb{P}^{x_0,0}$ on $(\Omega^0_M, \mathscr{F}^{M,0})$ such that

$$\begin{aligned}&\mathbb{P}^{x_0,0}\{\mathbb{X}^0_{t_1} \in A_1, \dots, \mathbb{X}^0_{t_n} \in A_n\}\\ &= \int \cdots \int 1_{A_1}(x_1)\widetilde{p}(\delta_0, x_0, x_1) \cdots\\ &\qquad \times 1_{A_n}(x_n)\widetilde{p}(\delta_{n-1}, x_{n-1}, x_n) d\widetilde{\mu}(x_1) \cdots d\widetilde{\mu}(x_n).\end{aligned}$$

Proof: Given subsets $G \subset F \subset [0, \infty)$ we get a projection map

$$\pi^F_G : \widetilde{M}^F \longrightarrow \widetilde{M}^G, \quad \gamma \longmapsto \gamma|_G.$$

Let $\mathscr{F}^{M,0}_F$ denote the smallest sigma-algebra such that the maps

$$\pi^F_{\{t\}} : \widetilde{M}^F \to \widetilde{M}^{\{t\}} = \widetilde{M}$$

are measurable. A family probability measures P_F which for every finite subset F of $[0, \infty)$ associates a probability measure P_F on $(\widetilde{M}^F, \mathscr{F}^{M,0}_F)$ is called consistent, if

$$(\pi^F_G)_* P_F = P_G \quad \text{for all finite } G \subset F \subset [0, \infty)$$

Then Kolmogorov's consistency theorem states that there exists a unique probability measure P on $(\widetilde{M}^{[0,\infty)}, \mathscr{F}^{M,0}$ such that

$$(\pi^{[0,\infty)}_F)_* P = P_F \quad \text{for all finite } F \subset [0, \infty).$$

Applying this with P_F given by

$$\begin{aligned}&P_F(B)\\ &= \int \cdots \int 1_B(x_1, \dots, x_n)\widetilde{p}(\delta_0, x_0, x_1) \cdots\\ &\qquad \times \widetilde{p}(\delta_{n-1}, x_{n-1}, x_n) d\widetilde{\mu}(x_1) \cdots d\widetilde{\mu}(x_n).\end{aligned}$$

where $F = \{0 < t_1 < \cdots < t_n\}$ and $B \subset \mathscr{F}^{M,0}_F$ proves the claim. Here, consistency follows from the Chapman-Kolmogorov equations

Step 2: There exists a process

$$\mathbb{Y} : [0, \infty) \times \Omega^0_M \longrightarrow \widetilde{M}$$

which has continuous paths and satisfies $\mathbb{P}^{x_0,0}\{\mathbb{Y}_t = \mathbb{X}^0_t\} = 1$ for all $t \geq 0$.

Proof: Kolmogorov-Chentsov's theorem on the existence of a continuous version of a stochastic process shows that it suffices to show the existence of constants $a, b, C, \epsilon > 0$ such that for all $t, s \geq 0$ with $|t - s| < \epsilon$ one has

$$\int \varrho(\mathbb{X}^0_s, \mathbb{X}^0_t)^a d\mathbb{P}^{x_0,0} \leq C|t - s|^{1+b}.$$

This follows from heat kernel estimates on compact Riemannian manifolds without boundary (Li-Yau heat kernel estimates).

Step 3: one has $\mathscr{F}^M = \mathscr{F}^{M,0} \cap \Omega^M$.
This follows from Lemma 10.7.

Step 3: The actual claim.
Proof: By Step 2,3, the measure $\mathbb{P}^{x_0,0}$ is concentrated on Ω_M, so its restriction to Ω_M does the job. ■

An obvious but nevertheless very important consequence of (47) is that for all $x_0 \in M$ one has

$$\mathbb{P}^{x_0}\{1_{\{t<\zeta\}} = 1_{\{X_t \in M\}}\} = 1. \tag{48}$$

In the sequel, integration with respect to the Wiener measure will often be written as an expectation value,

$$\mathbb{E}^{x_0}\left[\Psi\right] := \int \Psi d\mathbb{P}^{x_0} := \int \Psi(\gamma) d\mathbb{P}^{x_0}(\gamma),$$

where $\Psi : \Omega_M \to \mathbb{C}$ is any appropriate (say, nonnegative or integrable) Borel function. We remark that using monotone convergence, the defining relation of the Wiener measure implies that for all $n \in \mathbb{N}$, all finite sequences of times $0 < t_1 < \cdots < t_n$ and all Borel functions

$$f_1, \dots, f_n : \widetilde{M} \longrightarrow [0, \infty),$$

one has

$$\mathbb{E}^{x_0}\left[f_1(\mathbb{X}_{t_1}) \cdots f_n(\mathbb{X}_{t_n})\right] \tag{49}$$

$$= \int \cdots \int f_1(x_1) \widetilde{p}(\delta_0, x_0, x_1) \cdots$$

$$\times f_n(x_n) \widetilde{p}(\delta_{n-1}, x_{n-1}, x_n) d\widetilde{\mu}(x_1) \cdots d\widetilde{\mu}(x_n), \tag{50}$$

where $\delta_j := t_{j+1} - t_j$ with $t_0 := 0$. In particular, by the very construction of $\widetilde{M}$ and $\widetilde{\mu}$, the above formula in combination with (48) implies

$$\mathbb{E}^{x_0}\left[1_{\{t_1<\zeta\}} f_1(\mathbb{X}_{t_1}) \cdots 1_{\{t_n<\zeta\}} f_n(\mathbb{X}_{t_n})\right] \tag{51}$$

$$= \mathbb{E}^{x_0}\left[1_{\{\mathbb{X}_{t_1} \in M\}} f_1(\mathbb{X}_{t_1}) \cdots 1_{\{\mathbb{X}_{t_n} \in M\}} f_n(\mathbb{X}_{t_n})\right]$$

$$= \int \cdots \int f_1(x_1) p(\delta_0, x_0, x_1) \cdots$$

$$\times f_n(x_n) p(\delta_{n-1}, x_{n-1}, x_n) d\mu(x_1) \cdots d\mu(x_n), \tag{52}$$

therefore quantities that are given by averaging over paths that remain on M until any fixed time can be calculated by genuine Riemannian data on M, as it should be. In the sequel, we will also freely use the following facts:

Remark 10.15. 1. Each of the measures $\mathbb{P}^{x_0}$ is concentrated on the set of paths that start in x_0, meaning that

$$\mathbb{P}^{x_0}\{\mathbb{X}_0 = x_0\} = 1 \quad \text{for all } x_0 \in M,$$

as it should be. To see this, pick a metric $\widetilde{\varrho}$ on $\widetilde{M}$ which induces the topology on $\widetilde{M}$, and set

$$\widetilde{f} := \widetilde{\varrho}(\bullet, x_0) - \widetilde{\varrho}(\infty_M, x_0) \in C(\tilde{M}).$$

As $x_0 \in M$, the very definition of $(\widetilde{p}, \widetilde{\mu})$ implies that for all $t > 0$ one has

$$\int_{\widetilde{M}} \widetilde{p}(t, x_0, y)\widetilde{\varrho}(y, x_0) d\widetilde{\mu}(y) = \int_M p(t, x_0, y)\widetilde{f}|_M(y) d\mu(y) + \widetilde{\varrho}(\infty_M, x_0),$$

which, since $\widetilde{f}|_M$ is a continuous bounded function on M, implies through (49) and the fact that for all $f \in C_b(M)$ one has [8]

$$P_t f \to f \quad \text{locally uniformly as } t \to 0+,$$

the L^1-convergence

$$\mathbb{E}^{x_0}\left[\widetilde{\varrho}(\mathbb{X}_t, x_0)\right] = \int_{\widetilde{M}} \widetilde{p}(t, x_0, y)\widetilde{\varrho}(y, x_0) d\widetilde{\mu}(y) \to 0 \ \text{ as } t \to 0+.$$

Thus we can pick a sequence of strictly positive times a_n with $a_n \to 0$ such that $\widetilde{\varrho}(\mathbb{X}_{a_n}, x) \to 0$ $\mathbb{P}^{x_0}$-a.e., and the claim follows from

$$\widetilde{\varrho}(\mathbb{X}_0, x) \leq \widetilde{\varrho}(\mathbb{X}_0, \mathbb{X}_{a_n}) + \widetilde{\varrho}(\mathbb{X}_{a_n}, x) \quad \text{for all } n \in \mathbb{N}$$

and the continuity of the paths of $\mathbb{X}$.

2. For every Borel set $N \subset M$ with $\mu(N) = 0$ and every $x \in M$, one has

$$\int_0^\infty \int_{\Omega_M} 1_{\{(s',\gamma'):\, \gamma'(s') \in N\}}(s, \gamma) d\mathbb{P}^x(\gamma) ds = \int_0^\infty \int_N p(s, x, y) d\mu(y) ds = 0. \tag{53}$$

This fact follows immediately from the defining relation of the Wiener measure. For the first identity in (53), one also needs Fubini's Theorem, which can be used due to $\mathbb{X}$ being jointly measurable.

3. For each fixed $A \in \mathscr{F}^M$, the map

$$M \longrightarrow [0, 1], \ \ x \longmapsto \mathbb{P}^x(A) \tag{54}$$

is Borel measurable. In fact, this is obvious for $A \in \mathscr{C}^M$ by the defining relation of the Wiener measure, and it holds in general by the monotone class theorem, since $\mathscr{C}^M$ is a π-system which generates $\mathscr{F}^M$, and since the collection of sets

$$\{A : A \in \mathscr{F}^M, \ \ (54) \text{ is Borel measurable}\}$$

forms a monotone Dynkin-system.

The following result is crucial:

Lemma 10.16. *The family of Wiener measures satisfies the following Markov property: For all $x_0 \in M$, all times $t \geq 0$, all $\mathscr{F}^M_t$-measurable functions $\phi : \Omega_M \to [0, \infty)$, and all $\mathscr{F}^M$-measurable functions $\Psi : \Omega_M \to [0, \infty)$, one has*

$$\int \phi(\gamma)\Psi(\gamma(t + \bullet)) d\mathbb{P}^{x_0}(\gamma) = \int \phi(\gamma) \int \Psi(\omega) d\mathbb{P}^{\gamma(t)}(\omega) d\mathbb{P}^{x_0}(\gamma) \in [0, \infty]. \tag{55}$$

Proof. By monotone convergence, it is sufficient to consider the case $\phi = 1_A$, $\Psi = 1_B$ with $A \in \mathscr{F}_t^M$, $B \in \mathscr{F}_M$. Furthermore, for fixed $A \in \mathscr{F}_t^M$, using a monotone class argument as in Remark 10.15.3, it follows that it is sufficient to prove the formula for $B \in \mathscr{C}^M$. Using yet another monotone class argument, it follows that ultimately we have to check the formula only for $\phi = 1_A$, $\Psi = 1_B$ with $A \in \mathscr{C}_t^M$, $B \in \mathscr{C}_M$. So we pick $k, l \in \mathbb{N}$, finite sequences of times $0 < r_1 < \cdots < r_k < t$, $0 < s_1 < \cdots < s_l$, Borel sets

$$A_1, \dots, A_k, B_1, \dots, B_l \subset \widetilde{M}$$

with

$$A = \bigcap_{i=1}^{k} \mathbb{X}_{r_i}^{-1}(A_i), \quad B = \bigcap_{i=1}^{l} \mathbb{X}_{s_i}^{-1}(B_i),$$

and $s_0 := 0$, $r_0 := 0$. Then by the defining relation of the Wiener measure we have

$$\begin{aligned}
&\int 1_A(\gamma) \cdot 1_B(\gamma(t + \bullet)) d\mathbb{P}^{x_0}(\gamma) \\
&= \int 1_{\{\mathbb{X}_{r_1} \in A_1\}} \cdots 1_{\{\mathbb{X}_{r_k} \in A_k\}} 1_{\{\mathbb{X}_{s_1+t} \in B_1\}} \cdots 1_{\{\mathbb{X}_{s_l+t} \in B_l\}} d\mathbb{P}^{x_0} \\
&= \int \cdots \int 1_{A_1}(x_1) \widetilde{p}(r_1 - r_0, x_0, x_1) \cdots 1_{A_k}(x_k) \widetilde{p}(r_k - r_{k-1}, x_{k-1}, x_k) \\
&\times 1_{B_1}(x_{k+1}) \widetilde{p}(s_1 + t - r_k, x_k, x_{k+1}) \cdots \\
&\times 1_{B_l}(x_{k+l}) \widetilde{p}(s_l - s_{l-1}, x_{k+l-1}, x_{k+l}) d\widetilde{\mu}(x_1) \cdots d\widetilde{\mu}(x_{k+l}).
\end{aligned}$$

On the other hand, if for every $y_0 \in \widetilde{M}$ we set

$$\begin{aligned}
\Psi(y_0) := &\int \cdots \int 1_{B_1}(y_1) \widetilde{p}(s_1 - s_0, y_0, y_1) \cdots \\
&\times 1_{B_l}(y_l) \widetilde{p}(s_l - s_{l-1}, y_{l-1}, y_l) d\widetilde{\mu}(y_1) \cdots d\widetilde{\mu}(y_l),
\end{aligned}$$

then by using the defining relation of the Wiener measure for the $d\mathbb{P}^{\gamma(t)}(\omega)$ integration and then using (49), we get

$$\begin{aligned}
&\int 1_A(\gamma) \int 1_B(\omega) d\mathbb{P}^{\gamma(t)}(\omega) d\mathbb{P}^{x_0}(\gamma) \\
&= \int 1_{\{\mathbb{X}_{r_1} \in A_1\}}(\gamma) \cdots 1_{\{\mathbb{X}_{r_k} \in A_k\}}(\gamma) \Psi(\gamma(t)) d\mathbb{P}^{x_0}(\gamma) \\
&= \int \cdots \int 1_{A_1}(z_1) \widetilde{p}(r_1 - r_0, x_0, z_1) \cdots 1_{A_k}(z_k) \widetilde{p}(r_{k-1} - r_k, z_{k-1}, z_k) \\
&\times \widetilde{p}(t - r_k, z_k, z) 1_{B_1}(y_1) \widetilde{p}(s_1 - s_0, z, y_1) \cdots 1_{B_l}(y_l) \widetilde{p}(s_l - s_{l-1}, y_{l-1}, y_l) \\
&\times d\widetilde{\mu}(y_1) \cdots d\widetilde{\mu}(y_l) d\widetilde{\mu}(z_1) \cdots d\widetilde{\mu}(z_k) d\widetilde{\mu}(z),
\end{aligned}$$

which is equal to the above expression for

$$\int 1_A(\gamma) \cdot 1_B(\gamma(t + \bullet)) d\mathbb{P}^{x_0}(\gamma),$$

since by the Chapman-Kolomogorov equation and recalling $s_0 = 0$, we have

$$\int\int \widetilde{p}(t - r_k, z_k, z) 1_{B_1}(y_1)\widetilde{p}(s_1 - s_0, z, y_1) d\widetilde{\mu}(z) d\widetilde{\mu}(y_1)$$
$$= \int \widetilde{p}(t - r_k + s_1, z_k, y_1) 1_{B_1}(y_1) d\widetilde{\mu}(y_1).$$

This completes the proof. ■

Now we are in the position to define Brownian motion on an arbitrary Riemannian manifold:

Definition 10.17. 1. Let $(\Omega, \mathscr{F}, \mathbb{P})$ be a probability space, $x_0 \in M$, and let

$$X(x_0) : [0,\infty) \times \Omega \longrightarrow \widetilde{M}, \quad (t,\omega) \longmapsto X_t(x_0)(\omega)$$

be a continuous process. Then the tuple $(\Omega, \mathscr{F}, \mathbb{P}, X(x_0))$ is called a *Brownian motion on M with starting point x_0*, if the law of $X(x_0)$ with respect to $\mathbb{P}$ is equal to the Wiener measure $\mathbb{P}^{x_0}$. Recall that this means the following: The pushforward of $\mathbb{P}$ with respect to the $\mathscr{F}/\mathscr{F}^M$ measurable[17] map

$$\Omega \longrightarrow \Omega_M, \ \omega \longmapsto \big(t \longmapsto X_t(x_0)(\omega)\big) \tag{56}$$

is $\mathbb{P}^{x_0}$.
2. Assume that $(\Omega, \mathscr{F}, \mathbb{P}, X(x_0))$ is a Brownian motion on M with starting point x_0, and that $\mathscr{F}_* := (\mathscr{F}_t)_{t\geq 0}$ is a filtration of $\mathscr{F}$. Then the tuple $(\Omega, \mathscr{F}, \mathscr{F}_*, \mathbb{P}, X(x_0))$ is called an *adapted Brownian motion on M with starting point* x_0, if $X(x_0)$ is adapted to $\mathscr{F}_* := (\mathscr{F}_t)_{t\geq 0}$ (that is, $X_t(x_0) : \Omega \to \widetilde{M}$ is $\mathscr{F}_t$-measurable for all $t \geq 0$) and if in addition the following Markov property holds: For all times $t \geq 0$, all $\mathscr{F}_t$ measurable functions $\phi : \Omega \to [0,\infty)$, and all Borel functions $\Psi : \Omega_M \to [0,\infty)$, one has

$$\int \phi(\omega)\Psi(X_{t+\bullet}(x_0)(\omega)) d\mathbb{P}(\omega) = \int \phi(\omega) \int \Psi(\gamma) d\mathbb{P}^{X_t(x_0)(\omega)}(\gamma) d\mathbb{P}(\omega).$$

It follows from the above results that a canonical adapted Brownian motion with starting point x_0 is given in terms of the Wiener measure by the datum

$$(\Omega, \mathscr{F}, \mathscr{F}_*, \mathbb{P}, X(x_0)) := (\Omega_M, \mathscr{F}^M, \mathscr{F}^M_*, \mathbb{P}^{x_0}, \mathbb{X}). \tag{57}$$

Having recorded the existence of Brownian motion, we can immediately record the following characterization of the stochastic completeness property that was previously defined by the "parabolic condition"

$$\int_M p(t, x_0, y) d\mu(y) = 1 \quad \text{for all } (t, x_0) \in (0,\infty) \times M:$$

Namely, M is stochastically complete, if and only if for every $x_0 \in M$ and every Brownian motion $(\Omega, \mathscr{F}, \mathbb{P}, X(x_0))$ on M with starting point x_0, one has

$$\mathbb{P}\{X_t(x_0) \in M\} = 1 \quad \textit{for all } t \geq 0,$$

[17]Note that by assumption $X_t(x_0)$ is $\mathscr{F}^M_t$-measurable for all $t \geq 0$, so that indeed (56) is automatically $\mathscr{F}/\mathscr{F}^M$ measurable.

that is, if all Brownian motions remain on M for all times. This observation follows immediately from the defining relation of the Wiener measure.
The second part of Definition 10.17 is motivated by the fact that every Brownian motion has the required Markov property with respect to its own filtration:

Lemma 10.18. *Every Brownian motion $(\Omega, \mathscr{F}, \mathbb{P}, X(x_0))$ on M with starting point x_0 is automatically an $(\mathscr{F}_t^{X(x_0)})_{t\geq 0}$-Brownian motion, where*

$$\mathscr{F}_t^{X(x_0)} := \langle (X_s(x_0))_{0\leq s\leq t} \rangle \,, \quad t \geq 0$$

denotes the filtration of $\mathscr{F}$ which is generated by $X(x_0)$.

Proof. We have to show that given $t \geq 0$, an $\mathscr{F}_t^{X(x_0)}$-measurable function $\phi : \Omega \to [0, \infty)$, and a Borel function $\Psi : \Omega_M \to [0, \infty)$, one has

$$\int \phi(\omega)\Psi(X_{t+\bullet}(x_0)(\omega))d\mathbb{P}(\omega) = \int \phi(\omega) \int \Psi(\gamma)d\mathbb{P}^{X_t(x_0)(\omega)}(\gamma)d\mathbb{P}(\omega).$$

Assume for the moment that we can pick an $\mathscr{F}_t^M$-measurable function $f : \Omega_M \to [0, \infty)$ such that $f(X'(x_0)) = \phi$, where

$$X'(x_0) : \Omega \longrightarrow \Omega_M$$

denotes the induced $\mathscr{F}/\mathscr{F}^M$ measurable map (56). Then, since the law of $X(x_0)$ is $\mathbb{P}^{x_0}$, we can use the Markov property from Lemma 10.16 to calculate

$$\begin{aligned}
&\int \phi(\omega)\Psi(X_{t+\bullet}(x_0)(\omega))d\mathbb{P}(\omega)\\
&= \int f(\omega')\Psi(\omega'(t+\bullet))d\mathbb{P}^{x_0}(\omega')\\
&= \int f(\omega') \int \Psi(\gamma)d\mathbb{P}^{\omega'(t)}(\gamma)d\mathbb{P}^{x_0}(\omega')\\
&= \int f\big(X(x_0)(\omega)\big) \int \Psi(\gamma)d\mathbb{P}^{X_t(x_0)(\omega)}(\gamma)d\mathbb{P}(\omega)\\
&= \int \phi(\omega) \int \Psi(\gamma)d\mathbb{P}^{X_t(x_0)(\omega)}(\gamma)d\mathbb{P}(\omega),
\end{aligned}$$

proving the claim in this case. It remains to prove that one can always "factor" ϕ in the above form. Somewhat simpler variants of such a statement are usually called Doob-Dynkin lemma in the literature. An important point here is that the factoring procedure can be chosen to be positivity preserving. We give a quick proof: Set $X := X(x_0)$, $X' := X'(x_0)$, and assume first that ϕ is a simple function, that is, ϕ is a finite sum $\phi = \sum_j c_j 1_{A_j}$ with constants $c_j \geq 0$ and disjoint sets $A_j \in \mathscr{F}_t^X$. Then by the definition of this sigma-algebra, there exist times $0 \leq s_j \leq t$ and Borel sets $B_j \subset \widetilde{M}$ with $A_j = X_{s_j}^{-1}(B_j)$, such that with $C_j := \mathbb{X}_{s_j}^{-1}(B_j) \in \mathscr{F}_t^M$, the function $f := \sum_j c_j 1_{C_j}$ on Ω_M is nonnegative, $\mathscr{F}_t^M$-measurable, and satisfies $f(X') = \phi$. In the general case, there exists an increasing sequence of nonnegative $\mathscr{F}_t^X$-measurable simple functions ϕ_n on Ω such that $\lim_n \phi_n = \phi$.

By the above, we can pick for each n an $\mathscr{F}_t^M$-measurable nonnegative function f_n on Ω_M with $f_n(X') = \phi_n$. The set

$$\Omega' := \{f_n \text{ converges pointwise }\} \subset \Omega$$

clearly contains the image of X', and it is straighforwardly seen to be $\mathscr{F}_t^M$-measurable. Then $f := \lim_n(f_n 1_{\Omega'})$ has the desired properties. Note that the above proof is entirely measure theoretic and does not use any particular (say, topological) properties of the involved quantities. ■

Definition 10.19. M is called *nonparabolic*, if and only if for all $x, y \in M$ with $x \neq y$ one has the finiteness of the Coulomb potential

$$G(x, y) := \int_0^\infty p(t, x, y)dt.$$

One can easily show that compact M's are always parabolic, and that the Euclidean $\mathbb{R}^m$ is nonparabolic if and only $m \geq 3$. Probabilistically, this property means [9]:

Theorem 10.20. *M is nonparabolic, if and only if every Brownian motion $(\Omega, \mathscr{F}, \mathbb{P}, X(x_0))$ on M with starting point x_0 is transient, in the sense that for every precompact set $U \subset M$ one has*

$$\mathbb{P}\{\textit{there exists } s > 0 \textit{ such that for all } t > s \textit{ one has } X_t(x_0) \notin U\} = 1,$$

that is, if and only if all Brownian motions on M eventually leave each precompact set almost surely.

One can show that if M is geodesically complete with $\mathrm{Ric} \geq 0$, then (M, Ψ) is nonparabolic, if and only if

$$\int_0^\infty \frac{t}{\mu(x, \sqrt{t})} dt < \infty \quad \text{for all } x \in M,$$

11. Feynman-Kac formula

The aim here is to derive a path integral formula for the semigroup $P_t^w := e^{-tH_w} \in \mathscr{L}(L^2(M))$ associated with a Schrödinger operator of the form $H_w := -\Delta + w$, where $w : M \to \mathbb{R}$ is a potential. In case $w = 0$ we simply have,

$$P_t f(x) = \mathbb{E}^x \left[1_{\{t<\zeta\}} f(\mathbb{X}_t)\right],$$

which *is* a path integral formula, as

$$\mathbb{E}^x \left[1_{\{t<\zeta\}} f(\mathbb{X}_t)\right] = \int_{\{t<\zeta\}} f(\gamma(t))d\mathbb{P}^x(\gamma).$$

In the general case, according to Richard Feynman's thesis, we expect a formula of the form

$$P_t^w f(x) = \int_{\{t<\zeta\}} e^{-\int_0^t w(\gamma(s))ds} f(\gamma(t))d\mathbb{P}^x(\gamma) = \mathbb{E}^x \left[1_{\{t<\zeta\}} e^{-\int_0^t w(\mathbb{X}_s)ds} f(\mathbb{X}_t)\right]. \tag{58}$$

Actually, in quantum physics, one is rather interested in the unitary group $e^{-\mathrm{i}tH_w} \in \mathscr{L}(L^2(M))$, which with $\Psi(t) := P^w_{\mathrm{i}t}\Psi$, $\Psi \in L^2(M)$, solves the Schrödinger equation

$$(d/dt)\Psi(t) = -iH^w\Psi(t), \quad \Psi(0) = \Psi.$$

Feynman then 'showed' that (without any mathematical rigour) that

$$e^{-\mathrm{i}tH_w}f(x) = \int_{\{t<\zeta\}} e^{-\mathrm{i}\int_0^t w(\gamma(s))ds} f(\gamma(t)) e^{-\mathrm{i}\int_0^t |\dot\gamma(s)|^2 ds} D^x(\gamma),$$

where D^x is some sort of Riemannian wolume measure on the space of paths on M starting x and $\int_0^t |\dot\gamma(s)|^2 ds$ is the energy of such a path γ. Now one can *prove* that D^x does not exist, and of course many paths do not have a finite energy. On the other hand, switching from it to t, although each factor is problematic, the product

$$e^{-\int_0^t |\dot\gamma(s)|^2 ds} \cdot D^x(\gamma)$$

is well-defined and in fact one has

$$e^{-\int_0^t |\dot\gamma(s)|^2 ds} D^x(\gamma) = dP^x(\gamma)$$

in a sense that can be made precise. The point is that $e^{-\int_0^t |\dot\gamma(s)|^2 ds}$ is damping and can absorb some of the infinities of $D^x(\gamma)$, while $e^{-\int_0^t |\dot\gamma(s)|^2 ds}$ was oscillating and could not do that.

The first issue that has to be attacked is which w's can be dealt with in such a formula. In quantum physics, one has to deal with nonsmooth and unbounded w's such as the Coulomb potential $w(x) = -1/|x|$ for $M = \mathbb{R}^3$. Ultimately, the following class has turned out to be useful:

Definition 11.1. A Borel function $w : M \to \mathbb{R}$ is said to be in the *Kato class* $\mathcal{K}(M)$ of M, if

$$\lim_{t\to 0+} \sup_{x\in M} \int_0^t \mathbb{E}^x\left[1_{\{s<\zeta\}}|w(\mathbb{X}_s)|\right] ds = 0. \tag{59}$$

Note that

$$\int_0^t \mathbb{E}^x\left[1_{\{s<\zeta\}}|w(\mathbb{X}_s)|\right] ds = \int_0^t \int_M p(s,x,y)\,|w(y)|\,d\mu(y)ds$$

Obviously, $\mathcal{K}(M)$ is a real linear space. We are going to show in an exercise that $\mathcal{K}(M) \subset L^1_{\mathrm{loc}}(M)$ and that if $M = \mathbb{R}^3$ with its Euclidean metric then the Coulomb potential $w(x) := -1/|x|$ is in $\mathcal{K}(\mathbb{R}^3)$.

Next, let us record the following simple inequalities:

Lemma 11.2. *For any Borel function $w : M \to \mathbb{C}$ and any $r, t > 0$, one has*

$$\begin{aligned}
&\big(1 - e^{-rt}\big) \sup_{x \in M} \int_0^\infty e^{-rs} \int_M p(s,x,y)|w(y)|d\mu(y)ds \\
&\leq \sup_{x \in M} \int_0^t \int_M p(s,x,y)\,|w(y)|\,d\mu(y)ds \\
&\leq e^{rt} \sup_{x \in M} \int_0^\infty e^{-rs} \int_M p(s,x,y)|w(y)|d\mu(y)ds.
\end{aligned}$$

Proof. For any $x \in M$ we have

$$\begin{aligned}
&\int_0^\infty e^{-rs} \int_M p(s,x,y)|w(y)|d\mu(y)ds \\
&= \sum_{k=0}^\infty \int_{kt}^{t(k+1)} e^{-rs} \int_M p(s,x,y)|w(y)|d\mu(y)ds \\
&= \sum_{k=0}^\infty e^{-rkt} \int_M p(kt,x,z) \int_0^t \int_M e^{-rs} p(s,z,y)|w(y)|d\mu(y)\ ds\ d\mu(z) \\
&\leq \left(\sum_{k=0}^\infty e^{-rkt}\right) \sup_{z \in M} \int_0^t e^{-rs} \int_M p(s,z,y)|w(y)|d\mu(y)ds \\
&= \frac{1}{1 - e^{-rt}} \sup_{z \in M} \int_0^t e^{-rs} \int_M p(s,z,y)|w(y)|d\mu(y)ds,
\end{aligned}$$

from which the claims easily follow. Here, we have used the Chapman-Kolomogorov identity and $\int p(s',x',y')d\mu(y') \leq 1$. ■

Now we continue with a useful characterization of the contractive Dynkin and the Kato class, respectively. In view of

$$(H + r)^{-1} = \int_0^\infty e^{-rs} e^{-sH} ds,$$

and recalling our notation for the Wiener measure (Notation 10.13), the following lemma can be considered a resolvent/semigroup/Brownian motion equivalence-type result. It follows immeadiately from Lemma 11.2 and the heat kernel characterization of the Kato class:

Lemma 11.3. *For a Borel function $w : M \to \mathbb{C}$, the following statements are equivalent:*

i) $w \in \mathcal{K}(M)$.

ii) *One has*

$$\lim_{r \to \infty} \sup_{x \in M} \int_0^\infty e^{-rs} \int_M p(s,x,y)|w(y)|d\mu(y)ds = 0.$$

The following result is again of fundamental importance, since it shows that given a Kato function $w : M \to \mathbb{R}$ one can make sense of $H + w$ as a self-adjoint semibounded operator in the sense of sesquilinear forms, using the KLMN theorem (Theorem 2.14):

Lemma 11.4. *For any $r > 0$, any Borel function $w : M \to \mathbb{C}$, and any $f \in W^{1,2}_0(M)$ one has*

$$\left\| \sqrt{|w|} f \right\|_2^2 \leq \frac{C_r(w)}{2} \|df\|_2^2 + C_r(w) r \|f\|_2^2, \tag{60}$$

where

$$C_r(w) := \sup_{x \in M} \int_0^\infty e^{-rs} \int_M p(s,x,y)|w(y)| d\mu(y) ds \in [0,\infty].$$

Proof. We can assume that w is nonnegative. It suffices to show

$$\left\| \widehat{w^{1/2}} (H + r)^{-1/2} h \right\|_2^2 \leq C_r(w) \|h\|_2^2 \qquad \text{for all } h \in L^2(M), \tag{61}$$

where $\widehat{w^{1/2}} = \widehat{w}^{1/2}$ denotes the maximally defined multiplication operator induced by $w^{1/2}$, that is, $\mathrm{Dom}(\widehat{w^{1/2}})$ is given by those $f \in L^2(M)$ which satisfy $w^{1/2} f \in L^2(M)$. Indeed, once we have established the above estimate, applying it to $h = (H + r)^{1/2} f$ with $f \in W^{1,2}_0(M) = \mathrm{Dom}((H + r)^{1/2})$ proves

$$\left\| \widehat{w^{1/2}} f \right\|_2^2 \leq C_r(w) \left\| (H + r)^{1/2} f \right\|_2^2 = C_r(w) \left\| H^{1/2} f \right\|_2^2 + r C_r(w) \|f\|_2^2,$$

which is nothing but the asserted estimate. So it remains to prove (61). To this end, setting $w_n := \min(w, n) \in L^\infty(M)$, $n \in \mathbb{N}$, and using monotone convergence and $C_r(w_n) \leq C_r(w)$, it is actually sufficient to prove that for all n one has

$$\left\| \widehat{w_n^{1/2}} (H + r)^{-1/2} \right\|_{2,2}^2 \leq C_r(w_n). \tag{62}$$

Since $\widehat{w_n^{1/2}}$ and $(H + r)^{-1/2}$ are self-adjoint and since $\mathscr{L}(L^2(M))$ is a C^*-algebra, one has

$$\begin{aligned}\left\| \widehat{w_n^{1/2}} (H + r)^{-1} \widehat{w_n^{1/2}} \right\|_{2,2} &= \left\| \widehat{w_n^{1/2}} (H + r)^{-1/2} \left(\widehat{w_n^{1/2}} (H + r)^{-1/2} \right)^* \right\|_{2,2} \\ &= \left\| \widehat{w_n^{1/2}} (H + r)^{-1/2} \right\|_{2,2}^2 .\end{aligned}$$

To estimate this expression, let $f_1, f_2 \in L^2(M)$. Using the Laplace transform

$$(H + r)^{-1} = \int_0^\infty e^{-rs} e^{-sH} ds,$$

we get

$$\begin{aligned}
&\left|\left\langle \widehat{w_n^{1/2}}(H+r)^{-1}\widehat{w_n^{1/2}} f_1, f_2\right\rangle\right| \\
&\leq \int_0^\infty \int_M \int_M w_n^{1/2}(x)|f_1(y)|w_n^{1/2}(y)|f_2(x)|p(s,x,y)e^{-rs}d\mu(y)d\mu(x)ds.
\end{aligned}$$

Once we apply Cauchy-Schwarz to the Borel measure

$$d\rho(y,x,s) = p(s,x,y)e^{-rs}d\mu(y)d\mu(x)ds \text{ on } M\times M\times (0,\infty),$$

we therefore get

$$\begin{aligned}
&\left|\left\langle \widehat{w_n^{1/2}}(H+r)^{-1}\widehat{w_n^{1/2}} f_1, f_2\right\rangle\right| \\
&\leq \left(\int_0^\infty \int_M \int_M w_n(x)|f_1(y)|^2 p(s,x,y)e^{-rs}d\mu(y)d\mu(x)ds\right)^{1/2} \\
&\times \left(\int_0^\infty \int_M \int_M w_n(y)|f_2(x)|^2 p(s,x,y)e^{-rs}d\mu(y)d\mu(x)ds\right)^{1/2} \\
&= \left(\int_M \int_0^\infty e^{-rs}\int_M w_n(x)p(s,y,x)d\mu(x)ds|f_1(y)|^2 d\mu(y)\right)^{1/2} \\
&\times \left(\int_M \int_0^\infty e^{-rs}\int_M w_n(y)p(s,x,y)d\mu(y)ds|f_2(x)|^2 d\mu(x)\right)^{1/2} \\
&\leq C_r(w_n)\|f_1\|_2\|f_2\|_2,
\end{aligned}$$

which proves (62). ■

The above result together with Theorem 2.14 immediately implies the following result, which gives a precise definition of the left hand side of the Feynman-Kac formula:

Corollary 11.5. *Assume $w \in \mathcal{K}(M)$. Then the densely defined symmetric sesqui-linear form*

$$C_c^\infty(M)\times C_c^\infty(M) \ni (f_1,f_2) \longmapsto \int (df_1, df_2)d\mu + \int \overline{wf_1}f_2 d\mu \in \mathbb{C}$$

in $L^2(M)$ is semibounded and closable. Its closure Q_w is given by

$$\mathrm{Dom}(Q_w) = W_0^{1,2}(M), \quad Q_w(f_1,f_2) = \int (df_1,df_2)d\mu + \int \overline{wf_1}f_2 d\mu$$

(part of this statement is $\overline{wf_1}f_2 \in L^1(M)$ for all $f_1, f_2 \in W_0^{1,2}(M)$.).

Definition 11.6. Let $w \in \mathcal{K}(M)$. The semibounded self-adjoint operator in $L^2(M)$ induced by Q_w is denoted with H_w and called *the Schrödinger operator induced by the potential w.* The induced heat semigroup $e^{-tH_w} \in \mathscr{L}(L^2(M))$, $t \geq 0$, is called the *Schrödinger semigroup* induced by w.

Note that by functional analysis, given an initial value $\psi_0 \in L^2(M)$, the function

$$\psi : [0,\infty) \longrightarrow L^2(M), \quad \psi(t) := e^{-tH_w}\psi_0$$

is the unique continuous function which is differentiable in $(0,\infty)$ and takes values in $\mathrm{Dom}(H_w)$ thereon, and which solves the heat equation (with heat sinks given by w)

$$(d/dt)\psi(t) = -H_w\psi(t), \quad \psi(0) = \psi_0.$$

That the right hand side of the Feynman-Kac formula is well-defined for perturbations from the Kato class relies on:

Lemma 11.7. *Let $w \in \mathcal{K}(M)$.*
a) For all $x \in M$ one has

$$\mathbb{P}^x \left\{ w(\mathbb{X}_\bullet) \in L^1_{\mathrm{loc}}[0,\zeta) \right\} = 1.$$

b) There are $c_j = c_j(w) > 0$, $j = 1,2$, such that for all $t \geq 0$,

$$\sup_{x\in M} \mathbb{E}^x \left[e^{\int_0^t |w(\mathbb{X}_s)|ds} 1_{\{t<\zeta\}} \right] \leq c_1 e^{tc_2} < \infty. \tag{63}$$

Proof. a) Pick a continuous function $\rho : M \to [0,\infty)$ such that for all $c \in [0,\infty)$ the level sets $\{\rho \in [c,\infty)\}$ are compact. Then the collection of subsets $(U_n)_{n\in\mathbb{N}}$ of M given by

$$U_n := \text{ interior of } \{\rho \in [1/n,\infty)\}$$

forms an exhaustion of M with open relatively compact subsets. For every $n \in \mathbb{N}$, define the first exit times

$$\zeta_n^{(1)} := \zeta_{U_n} : \Omega_M \longrightarrow [0,\infty].$$

Then the sequence $\zeta_n^{(1)}$ *announces* ζ with respect to $\mathbb{P}^x$ for every $x \in M$ in the following sense: There exists a set $\Omega_x \subset \Omega_M$ with $\mathbb{P}^x(\Omega_x) = 1$, such that for all paths $\gamma \in \Omega_x$ one has the following two properties:

- $\zeta_n^{(1)}(\gamma) \nearrow \zeta(\gamma)$ as $n \to \infty$,
- the implication $\zeta(\gamma) < \infty \Rightarrow \zeta_n^{(1)}(\gamma) < \zeta(\gamma)$ holds true for all n.

To see that ζ is indeed announced by $\zeta_n^{(1)}$ in the asserted form, one can simply set

$$\Omega_x := \{\gamma \in \Omega_M : \ \gamma(0) = x\}.$$

Then $\mathbb{P}^x(\Omega_x) = 1$ and the asserted properties follow easily from continuity arguments, since Ω_x is a set of continuous paths that start in x. It follows immediately that $\zeta_n^{(2)} := \min(\zeta_n^{(1)}, n)$ also announces ζ. As a consequence, we have

$$\mathbb{P}^x \left\{ w(\mathbb{X}_\bullet) \in L^1_{\mathrm{loc}}[0,\zeta) \right\} = \mathbb{P}^x \bigcap_{n\in\mathbb{N}} \left\{ \int_0^{\zeta_n^{(2)}} |h(\mathbb{X}_s)|\, ds < \infty \right\}.$$

Now we have

$$\mathbb{E}^x\left[\int_0^{\zeta_n^{(2)}} |w(\mathbb{X}_s)|\, ds\right] \leq \mathbb{E}^x\left[\int_0^{\min(\zeta,n)} |w(\mathbb{X}_s)|\, ds\right]$$
$$= \mathbb{E}^x\left[\int_0^{n} |w(\mathbb{X}_s)|\, 1_{\{s<\zeta\}} ds\right] = \int_0^n \int_M p(s,x,y)\, |w(y)|\, d\mu(y),$$

and this number is finite for all n: indeed, take a $t>0$ with

$$\sup_{x\in M}\int_M \int_0^t p(s,x,y)|w(y)|ds\ d\mu(y) < \infty,$$

which clearly exists by the Kato assumption on w, and pick $l\in\mathbb{N}$ with $n<lt$. Then we can estimate as follows,

$$\sup_{x\in M}\int_M \int_0^n p(s,x,y)|w(y)|ds\ d\mu(y)$$
$$\leq \sup_{x\in M}\int_M \int_0^{lt} p(s,x,y)|w(y)|ds\ d\mu(y)$$
$$\leq \sum_{k=1}^{l}\sup_{x\in M}\int_M \int_0^{t} p((k-1)t+s,x,y)|w(y)|ds\ d\mu(y)$$
$$= \sum_{k=1}^{l}\sup_{x\in M}\int_0^t \int_M p((k-1)t,x,z)\int_M p(s,z,y)|w(y)|d\mu(y)d\mu(z)ds$$
$$\leq \left(\sum_{k=1}^{l}\sup_{x\in M}\int_M p((k-1)t,x,z)d\mu(z)\right)\times$$
$$\times \sup_{z\in M}\int_0^t\int_M p(s,z,y)|w(y)|d\mu(y)ds$$
$$\leq l\sup_{z\in M}\int_0^t\int_M p(s,z,y)|w(y)|d\mu(y)ds < \infty,$$

where we have used the Chapman-Kolomogorov identity and

$$\int p(s',x',y')d\mu(y') \leq 1.$$

b) With $\tilde{M} = M\cup\{\infty_M\}$ the Alexandrov compactification of M, we can canonically extend w to a Borel function $\widetilde{w}:\tilde{M}\to\mathbb{R}$ by setting $\widetilde{w}(\infty_M)=0$. Then one trivially has

$$\mathbb{E}^x\left[e^{\int_0^t|w(\mathbb{X}_s)|ds}1_{\{t<\zeta\}}\right] \leq \mathbb{E}^x\left[e^{\int_0^t|\widetilde{w}(\mathbb{X}_s)|ds}\right]. \tag{64}$$

2. (Khas'minskii's lemma) For any $s\geq 0$, let

$$J(w,s) := \sup_{x\in M}\mathbb{E}^x\left[e^{\int_0^s|\widetilde{w}(\mathbb{X}_r)|dr}\right]\in[0,\infty].$$

Then for every $s > 0$ with

$$D(w,s) := \sup_{x\in M} \mathbb{E}^x \left[\int_0^s |w(\mathbb{X}_r)| \, 1_{\{r<\zeta\}} dr \right] < 1$$

it holds that

$$J(w,s) \leq \frac{1}{1 - D(w,s)}. \tag{65}$$

Proof: One has

$$D(w,s) = \sup_{x\in M} \mathbb{E}^x \left[\int_0^s |\widetilde{w}(\mathbb{X}_r)| \, dr \right].$$

For any $n \in \mathbb{N}$, let

$$s\sigma_n := \Big\{ q = (q_1, \ldots, q_n) : 0 < q_1 < \cdots < q_n < s \Big\} \subset \mathbb{R}^n$$

denote the open scaled simplex. In the chain of equalities

$$\mathbb{E}^x \left[e^{\int_0^s |\widetilde{w}(\mathbb{X}_r)| dr} \right] = 1 + \sum_{n=1}^{\infty} (1/n!) \int_{[0,s]^n} \mathbb{E}^x \left[|\widetilde{w}(\mathbb{X}_{q_1})| \ldots |\widetilde{w}(\mathbb{X}_{q_n})| \right] d^n q$$
$$= 1 + \sum_{n=1}^{\infty} \int_{s\sigma_n} \mathbb{E}^x \left[|\widetilde{w}(\mathbb{X}_{q_1})| \ldots |\widetilde{w}(\mathbb{X}_{q_n})| \right] d^n q$$
$$= 1 + \sum_{n=1}^{\infty} \int_0^s \int_{q_1}^s \cdots \int_{q_{n-1}}^s \mathbb{E}^x \left[|\widetilde{w}(\mathbb{X}_{q_1})| \ldots |\widetilde{w}(\mathbb{X}_{q_n})| \right] d^n q,$$

the first one follows from Fubini's theorem, and the second one from combining the fact that the integrand is symmetric in the wariables q_j with the fact that the number of orderings of a real-walued tuple of length n is $n!$. In particular, by comparison with a geometric series, it is sufficient to prowe that for all natural $n \geq 2$, one has

$$J_n(w,s) := \sup_{x\in M} \int_0^s \int_{q_1}^s \cdots \int_{q_{n-1}}^s \mathbb{E}^x \left[|\widetilde{w}(\mathbb{X}_{q_1})| \ldots |\widetilde{w}(\mathbb{X}_{q_n})| \right] d^n q$$
$$\leq D(w,s) J_{n-1}(w,s). \tag{66}$$

But the Markov property of the family of Wiener measures implies

$$J_n(w,s) = \sup_{x\in M} \int_0^s \int_{q_1}^s \cdots \int_{q_{n-2}}^s \int_{\Omega_M} |\widetilde{w}(\gamma(q_1))| \ldots |\widetilde{w}(\gamma(q_{n-1}))| \times$$
$$\times \int_{\Omega_M} \int_0^{s-q_{n-1}} |\widetilde{w}(\omega(u))| \, du \; d\mathbb{P}^{\gamma(q_{n-1})}(\omega) d\mathbb{P}^x(\gamma) d^{n-1} q$$
$$\leq D(w,s) J_{n-1}(w,s), \tag{67}$$

which prowes Khas'minskii's lemma.

3. Pick $s > 0$ with $D(w,s) < 1$. Then for any $t > 0$ one has

$$J(w,t) \leq \frac{1}{1 - D(w,s)} e^{\frac{t}{s} \log\left(\frac{1}{1-D(w,s)} \right)}.$$

Proof: Pick a large $n \in \mathbb{N}$ with $t < (n+1)s$. Then the Markov property of the family of Wiener measures and Khas'minskii's lemma imply

$$\begin{aligned}
J(w,t) &\leq J(w,(n+1)s)\\
&= \sup_{x\in M}\int_{\Omega_M} e^{\int_0^{ns}|\widetilde{w}(\gamma(r))|dr}\int_{\Omega_M} e^{\int_0^{s}|\widetilde{w}(\omega(r))|dr} d\mathbb{P}^{\gamma(ns)}(\omega)d\mathbb{P}^{x}(\gamma)\\
&\leq \frac{1}{1-D(w,s)}J(w,ns)\\
&= \frac{1}{1-D(w,s)}\times\\
&\quad\times \sup_{x\in M}\int_{\Omega_M} e^{\int_0^{(n-1)s}|\widetilde{w}(\gamma(r))|dr}\int_{\Omega_M} e^{\int_0^{s}|\widetilde{w}(\omega(r))|dr} d\mathbb{P}^{\gamma((n-1)s)}(\omega)d\mathbb{P}^{x}(\gamma)\\
&\leq \dots\ (n\text{-times})\\
&\leq \frac{1}{1-D(w,s)}\left(\frac{1}{1-D(w,s)}\right)^n\\
&\leq \frac{1}{1-D(w,s)}e^{\frac{t}{s}\log\left(\frac{1}{1-D(w,s)}\right)},
\end{aligned}$$

which proves (63) in view of (64). ■

Now we can finally prove:

Theorem 11.8 (Feynman-Kac formula)**.** *Let $w \in \mathcal{K}(M)$. Then for all $t > 0$, $f \in L^2(M)$, μ-a.e. $x \in M$, one has*

$$e^{-tH_w}f(x) = \mathbb{E}^x\left[1_{\{t<\zeta\}}e^{-\int_0^t w(\mathbb{X}_s)ds}f(\mathbb{X}_t)\right]. \tag{68}$$

Proof. Step 1: (68) holds in case $w : M \to \mathbb{R}$ is continuous and bounded.
Proof: Decomposing

$$f = f_1 - f_2 + f_3 - \sqrt{-1}f_4, \quad f_j \geq 0,$$

if necessary, we can and we will assume $f \geq 0$ for the proof. Since w is bounded, it simply acts as a bounded multiplication operator (that will be denoted by the same symbol again). By (51), for every $t > 0$, $n \in \mathbb{N}$ and μ-a.e. $x_0 \in M$, we have

$$\begin{aligned}
&(e^{-(t/n)H}e^{-(t/n)w})^n f(x_0) =\\
&\int\cdots\int \exp\left(-(t/n)\sum_{i=1}^n w(x_i)\right)p(t/n,x_0,x_1)\cdots p(t/n,x_{n-1},x_n)f(x_n)\\
&\times d\mu(x_1)\cdots d\mu(x_n) =\\
&\mathbb{E}^{x_0}\left[1_{\{t<\zeta\}}\exp\left(-(t/n)\sum_{i=1}^n w(\mathbb{X}_{t/n})\right)f(\mathbb{X}_t)\right].
\end{aligned}$$

Since w is continuous, for each fixed continuous path which remains on M until t, the $\exp(\cdots)$-expression represents Riemann sums for $-\int_0^t w(\mathbb{X}_s)ds$. Furthermore, we have

$$1_{\{t<\zeta\}} \exp\left(-(t/n)\sum_{i=1}^n w(\mathbb{X}_{t/n})\right) f(\mathbb{X}_t) \le \exp(t\left\|w\right\|_\infty) 1_{\{t<\zeta\}} f(\mathbb{X}_t),$$

and clearly

$$\mathbb{E}^{x_0}\left[1_{\{t<\zeta\}} f(\mathbb{X}_t)\right] = \int_M p(t,x_0,y)f(y)d\mu(y) < \infty,$$

therefore dominated convergence shows that for μ-a.e. $x_0 \in M$,

$$\lim_{n\to\infty} (e^{-(t/n)H} e^{-(t/n)w})^n f(x_0) = \mathbb{E}^{x_0}\left[1_{\{t<\zeta\}} e^{-\int_0^t w(\mathbb{X}_s)ds} f(\mathbb{X}_t)\right].$$

On the other hand, Trotter's product formula

A semibounded, B bounded, $e^{-t(A+B)} = \lim_{n\to\infty}\left(e^{-(t/n)A}e^{-(t/n)B}\right)^n$ *strongly for all* $t \ge 0$,

gives (after picking a subsequence, if necessary, to turn the L^2-convergence to a μ-a.e. convergence)

$$\lim_{n\to\infty} e^{-(t/n)H} e^{-(t/n)w} f(x_0) = e^{-tH_w} f(x_0) \quad \text{for } \mu\text{-a.e. } x_0,$$

which proves the Feynman-Kac formula in this case.

Step 2: (68) holds in case w is a bounded potential.
Proof: We will use Friedrichs mollifiers to reduce everything to the continous (in fact: smooth) bounded case from step 1. To this end, we pick an atlas $(U_l)_{l\in\mathbb{N}}$ for M such that each U_l is relatively compact. We also take a subordinate partition of unity $\varphi_l \in C_{\mathrm{c}}^\infty(U_l)$. Then

$$w^{(l)} := \varphi_l w : U_l \longrightarrow \mathbb{R}$$

defines a bounded compactly supported function, and using Friedrichs mollifiers we can pick a sequence

$$(w_n^{(l)})_n \subset C_{\mathrm{c}}^\infty(U_l)$$

such that μ-a.e. in U_l we have

$$|w_n^{(l)}| \le \left\|w\right\|_\infty < \infty, \quad w_n^{(l)} \to w^{(l)} \text{ as } n \to \infty.$$

Defining a sequence of smooth potentials

$$w_n := \sum_l \varphi_l w_n^{(l)},$$

one has

$$|w_n| \le \left\|w\right\|_\infty,\ w_n \to w\ \mu\text{-a.e.} \tag{69}$$

It is clear from (69) and dominated convergence that

$$\lim_{n\to\infty} H_{w_n}\psi = H_w\psi \text{ in } L^2(M)$$

for all

$$\psi \in \mathrm{Dom}(H_w) = \mathrm{Dom}(H_{w_n}) = \mathrm{Dom}(H).$$

Thus by the following abstract convergence result for semigroups,
$A_n f \to Af$ for all $f \in \mathrm{Dom}(A) = \mathrm{Dom}(A_n)$, and A, A_n semibounded $\Rightarrow e^{-tA_n} \to e^{-tA}$ strongly for all $t \geq 0$
we have

$$\lim_{n\to\infty} e^{-tH_{w_n}} f = e^{-tH_w} f \;\text{ in } L^2(M).$$

In particular, passing to a subsequence if necessary, we can and we will assume

$$\lim_{n\to\infty} e^{-tH_{w_n}} f(x) = e^{-tH_w} f(x) \quad \text{for } \mu\text{-a.e. } x, \tag{70}$$

so we find

$$e^{-tH_w} f(x) = \lim_{n\to\infty} \mathbb{E}^x \left[1_{\{t<\zeta\}} e^{-\int_0^t w_n(\mathbb{X}_s) ds} f(\mathbb{X}_t) \right] \quad \text{for } \mu\text{-a.e. } x \tag{71}$$

by the already established validity of the covariant Feynman-Kac formula for $e^{-tH_{w_n}} f$. It remains to show that the right-hand side of (71) is equal to

$$\mathbb{E}^x \left[1_{\{t<\zeta\}} e^{-\int_0^t w(\mathbb{X}_s) ds} f(\mathbb{X}_t) \right].$$

To this end, applying (69) together with the elementary inequality

$$\left| e^a - e^b \right| \leq 2 \left| a - b \right| e^{\max(a,b)}, \quad a, b \in \mathbb{R}, \tag{72}$$

shows that one has

$$\begin{aligned} &1_{\{t<\zeta\}} \left| e^{-\int_0^t w(\mathbb{X}_s) ds} - e^{-\int_0^t w_n(\mathbb{X}_s) ds} \right| \\ &\leq 2 \cdot 1_{\{t<\zeta\}} e^{\|w\|_\infty t} \int_0^t \left| w(\mathbb{X}_s) - w_n(\mathbb{X}_s) \right| ds \;\; \mathbb{P}^x\text{-a.s.}, \end{aligned}$$

so using (69) once more with dominated convergence, we find

$$\lim_{n\to\infty} 1_{\{t<\zeta\}} \left| e^{-\int_0^t w_n(\mathbb{X}_s) ds} - e^{-\int_0^t w(\mathbb{X}_s) ds} \right| = 0 \;\; \mathbb{P}^x\text{-a.s.} \tag{73}$$

Finally, we may use (73) and

$$1_{\{t<\zeta\}} e^{-\int_0^t w_n(\mathbb{X}_s) ds} f(\mathbb{X}_t) \leq e^{\|w\|_\infty t} \quad \mathbb{P}^x\text{-a.s.}$$

to deduce (68) from (71) and dominated convergence.

Step 3: (68) holds in case w is bounded from below and Kato.
Proof: By adding a constant if necessary, we can assume $w \geq 0$. Set $w_n := \min(n, w)$, so $|w_n| \leq |w|$. As in the previous step we have

$$\begin{aligned} &1_{\{t<\zeta\}} \left| e^{-\int_0^t w(\mathbb{X}_s) ds} - e^{-\int_0^t w_n(\mathbb{X}_s) ds} \right| \\ &\leq 2 \cdot 1_{\{t<\zeta\}} e^{\int_0^t |w(\mathbb{X}_s)| ds} \int_0^t \left| w(\mathbb{X}_s) - w_n(\mathbb{X}_s) \right| ds \;\; \mathbb{P}^x\text{-a.s.}, \end{aligned}$$

so from dominated convergence

$$1_{\{t<\zeta\}}e^{-\int_0^t w_n(\mathbb{X}_s)ds} \to 1_{\{t<\zeta\}}e^{-\int_0^t w(\mathbb{X}_s)ds} \quad \mathbb{P}^x\text{-a.s.}$$

Furthermore, because $w_n \geq 0$,

$$1_{\{t<\zeta\}}e^{-\int_0^t w_n(\mathbb{X}_s)ds} f(\mathbb{X}_t) \leq 1_{\{t<\zeta\}} f(\mathbb{X}_t) \quad \mathbb{P}^x\text{-a.s. },$$

and

$$\mathbb{E}^x\left[1_{\{t<\zeta\}}f(\mathbb{X}_t)\right] = \int p(t,x,y)f(y)dy < \infty,$$

so

$$\mathbb{E}^x\left[1_{\{t<\zeta\}}e^{-\int_0^t w_n(\mathbb{X}_s)ds} f(\mathbb{X}_t)\right] \to \mathbb{E}^x\left[1_{\{t<\zeta\}}e^{-\int_0^t w(\mathbb{X}_s)ds} f(\mathbb{X}_t)\right]$$

by dominated convergence. On the other hand, we have $w_n \nearrow w$ as $n \to \infty$ and $|w_n| \leq |w|$ so that

$$e^{-tH_{w_n}} \to e^{-tH_w}$$

strongly in $L^2(M)$, and then pointwise a.e. after picking a subsequence, by the following convergence result for forms in combination with dominated convergence:

Let $q, q_1 \leq q_2 \leq \dots$ be a sequence of densely defined, closed and semibounded sesquilinear forms on a common complex separable Hilbert space $\mathscr{H}$ which have the same domain of definition with $q_n \to q$. Then with A_n the operator corresponding to q_n and A the operator corresponding to q, one has

$$e^{-tA_n} \to e^{-tA} \quad \text{strongly as } n \to \infty\text{, for all } t \geq 0.$$

Step 4: (68) holds for w Kato.

Proof: Set $w_n := w_n := \max(-n, w)$. Then $|w_n| \leq |w|$ so that as above one sees

$$1_{\{t<\zeta\}}e^{-\int_0^t w_n(\mathbb{X}_s)ds} \to 1_{\{t<\zeta\}}e^{-\int_0^t w(\mathbb{X}_s)ds} \quad \mathbb{P}^x\text{-a.s.}$$

and

$$\mathbb{E}^x\left[1_{\{t<\zeta\}}e^{-\int_0^t w_n(\mathbb{X}_s)ds} f(\mathbb{X}_t)\right] \to \mathbb{E}^x\left[1_{\{t<\zeta\}}e^{-\int_0^t w(\mathbb{X}_s)ds} f(\mathbb{X}_t)\right]$$

follows from dominated convergence, because

$$1_{\{t<\zeta\}}e^{-\int_0^t w_n(\mathbb{X}_s)ds} f(\mathbb{X}_t) \leq 1_{\{t<\zeta\}}e^{\int_0^t |w(\mathbb{X}_s)|ds} f(\mathbb{X}_t),$$

and

$$\mathbb{E}^x\left[1_{\{t<\zeta\}}e^{\int_0^t |w(\mathbb{X}_s)|ds} f(\mathbb{X}_t)\right] \leq \mathbb{E}^x\left[1_{\{t<\zeta\}}e^{2\int_0^t |w(\mathbb{X}_s)|ds}\right]^{1/2} \mathbb{E}\left[1_{\{t<\zeta\}}f(\mathbb{X}_t)^2\right]^{1/2} < \infty,$$

where

$$\mathbb{E}^x\left[1_{\{t<\zeta\}}f(\mathbb{X}_t)^2\right] = \int p(t,x,y)f(y)^2dy < \infty$$

follows for example from Remark 11.10 below. Furthermore, since $w_n \searrow w$ and $|w_n| \leq |w|$ one has

$$e^{-tH_{w_n}} \to e^{-tH_w}$$

strongly in $L^2(M)$, and then pointwise a.e. after picking a subsequence, by the following convergence result for forms and dominated convergence:

Let $q, q_1 \geq q_2 \geq \dots$ be a sequence of densely defined, closed and semibounded sesquilinear forms on a common complex Hilbert space $\mathscr{H}$ with a common domain of definition with $q_n \to q$. Then with A_n the operator corresponding to q_n and A the operator corresponding to q, one has

$$e^{-tA_n} \to e^{-tA} \text{ strongly in } \mathscr{H} \text{ as } n \to \infty, \text{ for all } t \geq 0.$$

■

Let us prove some simple but important consequences of the Feynman-Kac formula.

Corollary 11.9. *Let $w \in \mathcal{K}(M)$. Then e^{-tH_w} is positivity improving for all $t > 0$. In particular, if $\lambda := \min \sigma(H_w)$ is an eigenvalue of H_w, then λ is simple and there is a unique strictly positive normalized eigenfunction of H_w corresponding to λ.*

Proof. Let $f \in L^2(M) \setminus \{0\}$ be given with $f \geq 0$ μ-a.e. Then $\mu\{f > 0\} > 0$ and we have

$$\mathbb{P}^x\{f(\mathbb{X}_t) > 0, t < \zeta\} = \int_{\{f>0\}} p(t, x, y) d\mu(y) > 0.$$

Since, $\int_0^t w(\mathbb{X}_s) ds \in \mathbb{R}$ $\mathbb{P}^x$-a.s. in $\{t < \zeta\}$, it follows that with

$$\Omega' := \{t < \zeta, e^{-\int_0^t w(\mathbb{X}_s) ds} f(\mathbb{X}_t) > 0\}$$

one has $\mathbb{P}(\Omega') > 0$, thus by the Feynman-Kac formula we arrive at

$$e^{-tH_w} f(x) = \int_{\Omega'} e^{-\int_0^t w(\mathbb{X}_s) ds} f(\mathbb{X}_t) d\mathbb{P}^x > 0 \text{ for } \mu\text{-a.e. } x.$$

The statement on the ground state energy follows from an abstract Perron-Frobenius theorem, which states that the ground state energy of the generator of a positivity improving semigroup has a simple ground state energy and the unique normalized ground state can be chosen strictly positive. ■

Note that, by definition, our Schroedinger semigroups map $L^2(M)$ to $L^2(M)$ boundedly. Analogous L^q-estimates depend partially on the geometry. To this end, for arbitrary $U \subset M$ and $t > 0$, set

$$C_U(t) := \sup_{x \in U, y \in M} p(t, x, y) \in [0, \infty].$$

Remark 11.10. If U is relatively compact, one has $C_U(t) < \infty$ without any assumptions on M at all.
Proof: We have (since the heat kernel is smooth) the a-priori *algebraic* mapping property

$$1_U e^{-sH} : L^1(M) \longrightarrow L^\infty(M), \tag{74}$$

for all $s > 0$, which by the closed graph theorem self-improves in the sense that (74) is in fact a *bounded* operator. Indeed, because of

$$\int p(s, x, y) d\mu(y) \leq 1, \tag{75}$$

we have from Fubini that

$$e^{-sH} : L^1(M) \longrightarrow L^1(M),$$

is bounded, so

$$1_U e^{-sH} : L^1(M) \longrightarrow L^1(M),$$

is bounded. Assume $f_n \to f$ in $L^1(M)$, and $1_U e^{-sH} f_n$ converges to some g in $L^\infty(M)$. Then $1_U e^{-sH} f_n \to 1_U e^{-sH} f$ in $L^1(M)$, so $\lim_n 1_U e^{-sH} f_n = 1_U e^{-sH} f$ almost surely after picking a subsequence, and so $g = 1_U e^{-sH} f$ and (74) is bounded by the closed graph theorem. Let us denote the operator norm of (74) by $B_U(s) < \infty$, for any $s > 0$. Using the Chapman-Kolmogorov equation, an application of this boundedness to $p(t/2, \bullet, y) \in L^1(M)$ and using (75), we find that for all $x \in U$, $y \in M$ one has

$$\begin{aligned} p(t,x,y) &= \left[e^{-\frac{t}{2}H} p(t/2,\bullet,y)\right](x) \leq \sup_{x'\in U} \left[e^{-\frac{t}{2}H} p(t/2,\bullet,y)\right](x') \\ &\leq B_U(t/2) \int_M p(t/2,z,y) d\mu(z) \leq B_U(t/2), \end{aligned}$$

thus we arrive at the bound

$$C_U(t) \leq B_U(t/2) < \infty.$$

For unbounded U's it can happen that $C_U(t) = \infty$. If $C_M(t) < \infty$ for all $t > 0$, then M is called *ultracontractive*. For example Euclidean $\mathbb{R}^m$ or compact M's are obviously ultracontractive.

Given a Kato function $v : M \to [0,\infty)$ and $t \geq 0$ set

$$C_U(v,t) := \sup_{x\in U} \mathbb{E}^x \left[e^{\int_0^t v(\mathbb{X}_s) ds} 1_{\{t<\zeta\}}\right] \in [0,\infty).$$

Theorem 11.11. *Let w be in the Kato class.*
a) For any $t \geq 0$, $q \in [1,\infty]$, and any Borel $U \subset M$ (in particular for $U = M$) one has

$$\left\| 1_U e^{-tH_w} |_{L^q(M)\cap L^2(M)} \right\|_{q,q} \leq C_U(|w|,t) < \infty. \tag{76}$$

b) Let $t > 0$, let $U \subset M$ be a Borel set with $C_U(t/2) < \infty$, let $1 < q < \infty$, and let $1 < q^* < \infty$ be determined by $1/q + 1/q^* = 1$. Then one has

$$\left\| 1_U e^{-tH_w} |_{L^q(M)\cap L^2(M)} \right\|_{q,\infty} \leq C_U\big(q^*|w|,t\big) C_U(t)^{\frac{1}{q}}, \tag{77}$$

and

$$\left\| 1_U e^{-tH_w} |_{L^q(M)\cap L^2(M)} \right\|_{1,q} \leq C_U\big(q|w|,t\big) C_U(t)^{\frac{1}{q^*}}. \tag{78}$$

c) For every $t > 0$ with[18] *$C_M(t/2) < \infty$ and every $1 \leq q_1 \leq q_2 \leq \infty$, one has*

$$\left\| e^{-tH_w} |_{L^{q_1}(M)\cap L^2(M)} \right\|_{q_1,q_2} \leq C_M\big(2|w|,t\big) C_M(t/2)^{\frac{1}{q_1}-\frac{1}{q_2}}. \tag{79}$$

Remark 11.12. 1. It is important to note that if $f \in \mathrm{Dom}(H_w)$ is an eigenfunction of H_w, $H_w f = \lambda f$, then by the spectral calculus one has $f = e^{t\lambda} e^{-tH_w} f$ for all $t \geq 0$, so that the above estimates give parametric L^{q_2}- estimates for L^{q_1}-eigenfunctions!
2. Note that part a) of the theorem does not depend at all on the geometry of M, while part b) depends mildly on the geometry as these estimates can at least be localized (in

[18]Note that such a $t > 0$ need not exist at all.

the sense that one can always take U relatively compact), while part c) depends heavily on the geometry.

For the proof we recall:

Theorem 11.13 (Riesz-Thorin's interpolation theorem). *Let (X,μ) and (Y,ρ) be sigma-finite measure spaces, let $a_0,a_1,b_0,b_1\in[1,\infty]$, and assume that*

$$T: L^{a_0}_{\mu}(X)\cap L^{a_1}_{\mu}(X)\longrightarrow L^{b_0}_{\rho}(Y)\cap L^{b_1}_{\rho}(Y)$$

is a complex linear map. Assume further that there are numbers $C_0,C_1>0$ such that for all $f\in L^{a_0}_{\mu}(X)\cap L^{a_1}_{\mu}(X)$ one has

$$\|Tf\|_{L^{b_0}_{\rho}}\leq C_0\|f\|_{L^{a_0}_{\mu}},\ \ \|Tf\|_{L^{b_1}_{\rho}}\leq C_1\|f\|_{L^{a_1}_{\mu}}.$$

Then for any $r\in[0,1]$, there exists a bounded extension

$$T_{a_r,b_r}\in\mathscr{L}\big(L^{a_r}_{\mu}(X),L^{b_r}_{\rho}(Y)\big)$$

of T, which satisfies

$$\|T_{a_r,b_r}\|_{L^{a_r}_{\mu},L^{b_r}_{\rho}}\leq C_0^{1-r}C_1^{r},\ \ \text{where}\ \frac{1}{a_r}:=\frac{1-r}{a_0}+\frac{r}{a_1},\ \frac{1}{b_r}:=\frac{1-r}{b_0}+\frac{r}{b_1},$$

with the usual conventions $1/\infty:=0$, $1/0:=\infty$.

Proof of Theorem 11.11. Set $w':=-|w|$, so that by the Feynman-Kac formula

$$|e^{-tH_w}f(x)|\leq e^{-tH_{w'}}|f(x)|=\mathbb{E}^x\left[1_{\{t<\zeta\}}e^{\int_0^t|w(\mathbb{X}_s)|ds}|f(\mathbb{X}_t(x))|\right]$$

and it suffices to control $e^{-tH_{w'}}$. In view of the Feynman-Kac formula we define

$$e^{-tH_{w'}}h(x):=\mathbb{E}^x\left[1_{\{t<\zeta\}}e^{\int_0^t|w(\mathbb{X}_s)|ds}h(\mathbb{X}_t(x)|\right],$$

whenever the expectation is well-defined.
a) Let $h\in L^q(M)$.
The case $q=\infty$ follows immediately from the Feynman-Kac formula.
In case $q=1$, let $\bigcup_n B_n=U$ be a relatively compact exhaustion of U. Then we have

$$\begin{aligned}\int_U|e^{-tH_{w'}}h|\cdot 1_{B_n}d\mu&\leq\int_U|h|e^{-tH_{w'}}1_{B_n}d\mu\\ &\leq\left\|1_Ue^{-tH_{w'}}\right\|_{\infty,\infty}\|h\|_1,\end{aligned}$$

where we have used the self-adjointness of $e^{-tH_{w'}}$ for the first inequality, and the case of $q=\infty$ for the inequality. Using monotone convergence, this implies

$$\left\|1_Ue^{-tH_{w'}}h\right\|_1\leq C_U(|w|,t)\|h\|_1.$$

We have shown so far that

$$\max\left(\left\|1_Ue^{-tH_{w'}}\right\|_{1,1},\left\|1_Ue^{-tH_{w'}}\right\|_{\infty,\infty}\right)\leq C_U(|w|,t).$$

In case $1 < q < \infty$, applying Riesz-Thorin's theorem (cf. appendix, Theorem 11.13) with $T = 1_U e^{-tH_{w'}}$, $a_0 = b_0 = 1$, $a_1 = b_1 = \infty$, $C_0 = C_1 = C_U(|w|, t)$, $r = 1 - 1/q$ we get

$$\left\| 1_U e^{-tH_{w'}} \right\|_{q,q} \leq C_U(|w|, t),$$

which completes the proof of part a).

b) Let $h \in L^q(M)$. For any $u > 0$, we have

$$\begin{aligned}
&\left\| 1_U e^{-uH_{w'}} h \right\|_\infty \leq \sup_{x \in U} \mathbb{E}^x \left[1_{\{u<\zeta\}} e^{\int_0^u |w|(\mathbb{X}_r) dr} |h|(\mathbb{X}_u) \right] \\
&\leq \sup_{x \in U} \mathbb{E}^x \left[1_{\{u<\zeta\}} e^{q^* \int_0^u |w|(\mathbb{X}_r(x)) dr} \right]^{1/q^*} \mathbb{E}^x \left[1_{\{u<\zeta\}} |h|^q(\mathbb{X}_u) \right]^{1/q} \\
&\leq C_U(q^*|w|, u)^{1/q^*} \left\| 1_U e^{-uH} \right\|_{1,\infty}^{1/q} \|h\|_q \leq C_U(q^*|w|, u)^{1/q^*} C_U(u)^{1/q} \|h\|_q \,,
\end{aligned}$$

The $L^1 \to L^q$ estimate follows from the above $L^q \to L^\infty$ estimate and a duality argument, namely, for every $u > 0$ we can estimate for every $h \in L^1(M)$ as follows:

$$\begin{aligned}
&\left\| 1_U e^{-uH_{w'}} h \right\|_q \leq \sup_{\psi \in C_c^\infty(M), \|\psi\|_{q^*} \leq 1} \int_U e^{-uH_{w'}} |h| \cdot |\psi| d\mu \\
&= \sup_{\psi \in C_c^\infty(M), \|\psi\|_{q^*} \leq 1} \int_U |h| \cdot e^{-uH_{w'}} |\psi| d\mu \\
&\leq \sup_{\psi \in C_c^\infty(M), \|\psi\|_{q^*} \leq 1} \left\| 1_U e^{-uH_{w'}} |\psi| \right\|_\infty \|h\|_1 \\
&\leq \sup_{\psi \in C_c^\infty(M), \|\psi\|_{q^*} \leq 1} \left\| 1_U e^{-uH_{w'}} \right\|_{q^*,\infty} \|\psi\|_{q^*} \|h\|_1 \\
&\leq \left\| 1_U e^{-uH_{w'}} \right\|_{q^*,\infty} \|h\|_1 \,,
\end{aligned}$$

which by the above can be estimated as

$$\leq C_U(q|w|, u)^{1/q} C_U(u)^{1/q^*} \|h\|_1 \,.$$

c) Throughout, let $h \in L^{q_1}(M)$.

Case $1 = q_1 < q_2 = 2 < \infty$: This follows from part b) applied to $U = M$. Case $1 = q_1 < q_2 = \infty$: We have

$$\begin{aligned}
&\left\| e^{-tH_{w'}} h \right\|_\infty = \left\| e^{-\frac{t}{2} H_{w'}} e^{-\frac{t}{2} H_{w'}} h \right\|_\infty \\
&\leq \left\| e^{-\frac{t}{2} H_{w'}} \right\|_{2,\infty} \left\| e^{-\frac{t}{2} H_{w'}} h \right\|_2 \leq \left\| e^{-\frac{t}{2} H_{w'}} \right\|_{2,\infty} \left\| e^{-\frac{t}{2} H_{w'}} \right\|_{1,2} \|h\|_1 \,,
\end{aligned}$$

which can be estimated by the previous case and part b) as

$$\leq C_M(2|w|, t/2) C_M(t/2) \|h\|_1 \,. \tag{80}$$

Case $1 < q_1 < q_2 = \infty$: Qualitatively, this case is covered by part b). However, being equipped with a global $L^1 \to L^\infty$ estimate, we can use Riesz-Thorin to get an estimate which has "some more uniformity" in $q = q_1$: Indeed, applying Riesz-Thorin with

$$T = e^{-tH_{w'}}, a_0 = 1, b_0 = \infty, a_1 = b_1 = \infty, r = 1 - 1/q_1$$

implies

$$\left\|e^{-tH_{w'}}\right\|_{q_1,\infty} \le \left\|e^{-tH_{w'}}\right\|_{1,\infty}^{1/q_1} \left\|e^{-tH_{w'}}\right\|_{\infty,\infty}^{1-1/q_1},$$

which can be estimated by the above considerations as

$$\le \big(C_M(2|w|,t/2)C_M(t/2)\big)^{1/q_1} C_M(2|w|,t)^{1-1/q_1} \le C_M(2|w|,t)C_M(t/2)^{1/q_1}.$$

Case $1 \le q_1 \le q_2 < \infty$: Applying Riesz-Thorin with

$$T = e^{-tH_{w'}},\ a_0 = 1,\ b_0 = 1,\ a_1 = \frac{q_1(q_2-1)}{q_2-q_1},\ b_1 = \infty,\ r = 1 - 1/q_2$$

gives the bound

$$\left\|e^{-tH_{w'}}\right\|_{q_1,q_2} \le \left\|e^{-tH_{w'}}\right\|_{1,1}^{1/q_1} \left\|e^{-tH_{w'}}\right\|_{a_1,\infty}^{1-1/q_2},$$

and thus

$$\left\|e^{-tH_{w'}}\right\|_{q_1,q_2} \le \left\|e^{-tH_{w'}}\right\|_{1,1}^{1/q_1} \left\|e^{-tH_{w'}}\right\|_{1,\infty}^{1/q_1-1/q_2} \left\|e^{-tH_{w'}}\right\|_{\infty,\infty}^{1-1/q_1}.$$

Combining the last estimate with the previously established estimates, we arrive at

$$\left\|e^{-tH_{w'}}\right\|_{q_1,q_2} \le C_M\big(2|w|,t\big)C_M(t/2)^{\frac{1}{q_1}-\frac{1}{q_2}}.$$

■

Theorem 11.14. *Assume $w \in \mathcal{K}(M)$. Then for all $f \in L^2(M)$, the map*

$$(0,\infty) \times M \ni (t,x) \longmapsto \mathrm{e}^{-tH_w} f(x) \in \mathbb{C}$$

is jointly continuous. (To be precise: there exists a jointly continuous map $(t,x) \mapsto f_t(x) \in \mathbb{C}$ from $(0,\infty) \times M$ to $\mathbb{C}$, such that for all $t > 0$ the μ-equivalence class $\mathrm{e}^{-tH_w} f$ agrees μ-a.e. with f_t.) In particular, all eigenfunctions of H_w are continuous.

We prepare the proof of Theorem 11.14 with the following simple Lemma:

Lemma 11.15. *Let $U \subset M$ be open, and assume that*

(81) $\quad (h_n)_{n\in\mathbb{N}} \subset C_b(U) = C(U) \cap L^\infty(U),\ h \in L^\infty(U),\ \left\|h_n - h\right\|_\infty \to 0$ *as* $n \to \infty$.

Then (h_n) converges uniformly everywhere *in U. In particular, h can be chosen to be continuous.*

Proof. This fact follows from a standard argument which only uses that μ is a Borel measure with a full support: Assume the contrary. Then (h_n) is not a Cauchy sequence with respect to $\|\bullet\|_\infty$. Accordingly, there is an $\epsilon > 0$ such that for all $N \in \mathbb{N}$ one can find natural numbers $n, m \ge N$ and a point $x \in U$ with $|h_n(x) - h_m(x)| > \epsilon$. Thus, since h_n and h_m are continuous, there exists a nonempty open set $U' \subset U$ with $|h_n(x) - h_m(x)| > \epsilon$ for all $x \in U'$. We arrive at $\mu\{|h_n - h_m| > \epsilon\} > 0$, which contradicts the assumption that (h_n) is Cauchy with respect to $\|\bullet\|_\infty$.
The continuous representative $\tilde{h}$ of h is simply given by the $\|\bullet\|_\infty$-limit of the sequence h_n. This completes the proof. ■

Proof of Theorem 11.14. The statement concerning the eigensections is immediately implied by the continuity of the semigroup in $x \in M$, using the spectral calculus.
To show the latter, let us recall that by Theorem 11.11 a), the operator e^{-tH_w} maps bounded functions into bounded functions. This fact will be used several times in the sequel. The proof of the joint continuity of the semigroup in (t,x) will be carried out in three steps:
Step 1: One has

$$\lim_{t\to 0+} \left\|(e^{-tH_w} - e^{-tH})|_{L^2(M)\cap L^\infty(M)}\right\|_{\infty,\infty} = 0.$$

Proof: Let $f \in L^2(M)\cap L^\infty(M)$ and assume $t \leq 1$. Let us define a sequence of bounded potentials by

$$w_n(x) := \begin{cases} \frac{\min(|w(x)|,n)}{|w(x)|} w(x), & \text{if } w(x) \neq 0 \\ 0, \quad \text{else.} \end{cases}$$

Since w_n is bounded, we can use Duhamel's formula

$$e^{-tH_{w_n}} f(x) - e^{-tH} f(x) = \int_0^t e^{-(t-s)H} w_n e^{-sH_{w_n}} f(x) ds,$$

thus using that $e^{-(t-s)H}$ is positivity preserving, we get the first inequality in

$$\begin{aligned}\left|e^{-tH_{w_n}} f(x) - e^{-tH} f(x)\right| &\leq \int_0^t e^{-(t-s)H} \left[|w_n| \cdot \left|e^{-sH_{w_n}} f\right|\right](x) ds \\ \leq \|f\|_\infty \int_0^t e^{-(t-s)H} |w_n|(x) &\left\|e^{-sH_{w_n}}|_{L^2(M)\cap L^\infty(M)}\right\|_{\infty,\infty} ds.\end{aligned}$$

We have

$$\begin{aligned}\left\|e^{-sH_{w_n}}|_{L^2(M)\cap L^\infty(M)}\right\|_{\infty,\infty} &\leq \sup_{x\in M} \mathbb{E}^x \left[e^{\int_0^s |w_n(\mathbb{X}_r)|dr} 1_{\{s<\zeta\}}\right] \\ \leq \sup_{x\in M} \mathbb{E}^x \left[e^{\int_0^s |w(\mathbb{X}_r)|dr} 1_{\{s<\zeta\}}\right] &\leq c_1(|w|) e^{sc_2(|w|)} \leq c_1(|w|) e^{c_2(|w|)} =: c_w,\end{aligned}$$

where we have used Khashminkii's lemma and $s \leq 1$. Therefore, we find

$$\begin{aligned}\left|e^{-tH_{w_n}} f(x) - e^{-tH} f(x)\right| &\leq c_w \|f\|_\infty \int_0^t e^{-(t-s)H} |w_n| ds \\ = c_w \|f\|_\infty \int_0^t \int_M & p(t-s,x,y) |w_n(y)| d\mu(y) ds \\ \leq c_w \|f\|_\infty \int_0^t \int_M & p(s,x,y) |w(y)| d\mu(y) ds.\end{aligned}$$

On the other hand, in view of $w_n \nearrow w$, $|w_n| \leq |w|$, we can use dominated convergence to conclude that $Q_{w_n} \nearrow Q_w$ as $n \to \infty$ in the sense of monotonely increasing quadratic forms, so that (by picking a subsequence of w_n if necessary) we have the first equality in

$$\begin{aligned}&\left|e^{-tH_w}f(x)-e^{-tH}f(x)\right|=\lim_{n\to\infty}\left|e^{-tH_{w_n}}f(x)-e^{-tH}f(x)\right|\\&\leq C_w\left\|f\right\|_\infty\int_0^t\int_M p(s,x,y)|w(y)|d\mu(y)ds,\end{aligned}$$

which tends to 0 as $t\to 0+$ uniformly in x, by the very definition of the Kato class. This completes the proof of step 1.

Step 2: For all fixed $t>0$, $f\in L^2(M)\cap L^\infty(M)$, *the function* $x\mapsto e^{-tH_w}f(x)$ *is continuous.*
Proof: Let $0<s<t$. Recalling that $e^{-sH}e^{-(t-s)H_w}f$ is continuous (in fact, smooth) by local elliptic regularity, a use of the above lemma shows that it is sufficient to prove

$$\left\|e^{-tH_w}f-e^{-sH}e^{-(t-s)H_w}f\right\|_\infty\to 0\ \text{ as } s\to 0+. \tag{82}$$

To this end, we start by observing that for all $0<s<t$ the spectral calculus gives us

$$\begin{aligned}&e^{-tH_w}f-e^{-sH}e^{-(t-s)H_w}f=\left(e^{-tH_w}e^{(t-s)H_w}-e^{-sH}\right)e^{-(t-s)H_w}f\\&=\left(e^{-sH_w}-e^{-sH}\right)e^{-(t-s)H_w}f,\end{aligned}$$

and thus,

$$\begin{aligned}&\left\|e^{-tH_w}f-e^{-sH}e^{-(t-s)H_w}f\right\|_\infty\\&=\left\|\left(e^{-sH_w}-e^{-sH}\right)e^{-(t-s)H_w}f\right\|_\infty\\&\leq\left\|(e^{-sH_w}-e^{-sH})|_{L^2(M)\cap L^\infty(M)}\right\|_{\infty,\infty}\left\|e^{-(t-s)H_w}f\right\|_\infty\\&\leq\left\|(e^{-sH_w}-e^{-sH})|_{L^2(M)\cap L^\infty(M)}\right\|_{\infty,\infty}\left\|e^{-(t-s)H_w}|_{L^2(M)\cap L^\infty(M)}\right\|_{\infty,\infty}\left\|f\right\|_\infty. \qquad (83)\end{aligned}$$

which is

$$\leq C(w,t)\left\|f\right\|_\infty\left\|(e^{-sH_w}-e^{-sH})|_{L^2(M)\cap L^\infty(M)}\right\|_{\infty,\infty}.$$

Now step 1 shows that the above expression tends to 0 as $s\to 0+$, which completes the proof of step 2.

Step 3: For all fixed $t>0$, $f\in L^2(M)$, *the function* $e^{-tH_w}f$ *is continuous.*
Proof: It remains to remove the boundedness condition on f. Let U be an arbitrary open relatively compact subset of M. Then we have

$$e^{-tH_w}\in\mathscr{L}\Big(L^2(M),L^\infty(U)\Big).$$

Thus, setting for $n\in\mathbb{N}$

$$f_n:=\begin{cases}\frac{\min(n,|f|)}{|f|}f, & \text{if } f\neq 0\\ 0, & \text{else}\end{cases}\in L^2(M)\cap L^\infty(M),$$

we have $f_n\to f$ in $L^2(M)$, and $x\mapsto e^{-tH_w}f_n(x)$ is continuous by step 2. Furthermore, $e^{-tH_w}f_n\to e^{-tH_w}f$ in $L^\infty(U)$. Now the claim of step 3 follows from the previous lemma.

Step 4: The full statement. It remains to prove the asserted joint continuity. Note first that for every open relatively compact $U \subset M$ and every $s > 0$, one has

$$e^{-sH_w} \in \mathscr{L}\big(L^2(M), C_b(U)\big), \tag{84}$$

which follows from combining the algebraic mapping property

$$e^{-sH_w} : L^2(M) \longrightarrow C_b(U)$$

(step 3) with the closed graph theorem. Now

$$L^2(M) \times U \ni (f, x) \longmapsto e^{-sH_w} f(x) \in \mathbb{C}$$

is continuous for all $s > 0$: given a sequence

$$((f_n, x_n))_{n\in\mathbb{N}} \subset L^2(M) \times U$$

which converges to

$$(f, x) \in L^2(M) \times U,$$

we have

$$\begin{aligned}
&\big|e^{-sH_w} f_n(x_n) - e^{-sH_w} f(x)\big| \\
&\leq \big|e^{-sH_w}[f_n - f](x_n)\big| + \big|e^{-sH_w} f(x) - e^{-sH_w} f(x_n)\big| \\
&\leq \big\|e^{-sH_w}\big\|_{\mathscr{L}(L^2(M),C_b(U))} \|f_n - f\| + \big|e^{-sH_w} f(x) - e^{-sH_w} f(x_n)\big| \\
&\ \to 0, \text{ as } n \to \infty.
\end{aligned}$$

Finally, the asserted joint continuity follows from observing that for every $\epsilon > 0$ the map

$$(\epsilon, \infty) \times U \ni (t, x) \longmapsto e^{-tH_w} f(x) \in \mathbb{C}$$

is equal to the composition

$$(\epsilon, \infty) \times U \xrightarrow{(t,x)\mapsto\left(e^{-(t-\epsilon)H_w} f, x\right)} L^2(M) \times U \xrightarrow{(f,x)\mapsto e^{-\epsilon H_w} f(x)} \in \mathbb{C},$$

where the first map is norm continuous by the spectral calculus, and where the second map is continuous as explained above. This completes the proof. ■

12. Molecular Schrödinger operators

References

[1] Alonso, A. & Simon, B.: *The Birman-Krein-Vishik theory of selfadjoint extensions of semibounded operators.* J. Operator Theory 4 (1980), no. 2, 251–270.
[2] Azencott, R.: *Behavior of diffusion semi-groups at infinity.* Bull. Soc. Math. France 102 (1974), 193–240.
[3] Bei, F. & Güneysu, B.: *q-parabolicity of stratified pseudomanifolds and other singular spaces.* Ann. Global Anal. Geom. 51 (2017), no. 3, 267–286.
[4] Bianchi, D. & Setti, A.: *Laplacian cut-offs, fast diffusions on manifolds and other applications.* Preprint (2016). arXiv:1607.06008v1.
[5] Burago, D. & Burago, Y. & Ivanov, S.: *A course in metric geometry*, AMS (book).
[6] Davies, E.B.: *Heat kernels and spectral theory.* Cambridge Tracts in Mathematics, 92. Cambridge University Press, Cambridge, 1990.

[7] Elworthy, K.D.: *Geometric aspects of diffusions on manifolds.* Ecole d'EtÃ© de ProbabilitÃ©s de Saint-Flour XV-XVII, 1985-1987, 277–425.

[8] Grigor'yan, A.: *Heat kernel and analysis on manifolds.* AMS/IP Studies in Advanced Mathematics, 47. American Mathematical Society, Providence, RI; International Press, Boston, MA, 2009.

[9] Grigor'yan, A.: *Analytic and geometric background of recurrence and non-explosion of the Brownian motion on Riemannian manifolds.* Bulletin of Amer. Math. Soc. 36 (1999) 135–249.

[10] Güneysu, B. & Guidetti, D. & Pallara, D.: *L^1-elliptic regularity and $H{=}W$ on the whole L^p-scale on arbitrary manifolds.* Annales Academiae Scientiarum Fennicae, Mathematica (2017) Volumen 42, 497–521.

[11] Hackenbroch, W. & Thalmaier, A.: *Stochastische Analysis.* B.G. Teubner, Stuttgart, 1994.

[12] Hebey, E.: *Sobolev spaces on Riemannian manifolds.* Lecture Notes in Mathematics, 1635. Springer-Verlag, Berlin, 1996.

[13] Heinonen, J. & Koskela, P. & Shanmugalingam, N. & Tyson, J.T.: *Sobolev spaces on metric measure spaces. An approach based on upper gradients.* New Mathematical Monographs, 27. Cambridge University Press, Cambridge, 2015.

[14] Heinonen, J.: *Lectures on Lipschitz analysis.* http://www.math.jyu.fi/research/reports/rep100.pdf

[15] Hess, H. & Schrader, R. & Uhlenbrock, D.A.: *Kato's inequality and the spectral distribution of Laplacians on compact Riemannian manifolds.* J. Differential Geom. 15 (1980), no. 1, 27–37 (1981).

[16] Hess, H. & Schrader, R. & Uhlenbrock, D.A.: *Domination of semigroups and generalization of Kato's inequality.* Duke Math. J. 44 (1977), no. 4, 893–904.

[17] Hiai, F.: *Log-majorizations and norm inequalities for exponential operators.* Banach Cent. Publ. 38(1), 119–181 (1997).

[18] Hirsch, M.W.: *Differential topology.* Corrected reprint of the 1976 original. Graduate Texts in Mathematics, 33. Springer-Verlag, New York, 1994.

[19] Hinz, A.M. & Stolz, G.: *Polynomial boundedness of eigensolutions and the spectrum of Schrödinger operators.* Math. Ann. 294 (1992), no. 2, 195–211.

[20] Hörmander, L.: *The analysis of linear partial differential operators I.* Second edition. Grundlehren der Mathematischen Wissenschaften. Springer-Verlag, Berlin, 1990.

[21] Hunsicker, E. & Mazzeo, R.: *Harmonic forms on manifolds with edges*, Int. Math. Res. Not. 2005 (52) (2005) 3229–3272.

[22] Hsu, E.P.: *Stochastic analysis on manifolds.* Graduate Studies in Mathematics, 38. American Mathematical Society, Providence, RI, 2002.

[23] Kato, T.: *Perturbation theory for linear operators.* Reprint of the 1980 edition. Classics in Mathematics. Springer-Verlag, Berlin, 1995.

[24] Krein, M.: *The theory of self-adjoint extensions of semi-bounded Hermitian transformations and its applications.* I. Rec. Math. [Mat. Sbornik] N.S. 20(62), (1947). 431–495.

[25] Lee, J.M.: *Introduction to smooth manifolds. Graduate Texts in Mathematics, 218.* Graduate Texts in Mathematics, 218. Springer, New York, 2013.

[26] MÃ¼ller, O.: *A note on closed isometric embeddings.* J. Math.Anal. 349 (2009), 297–298.

[27] Nirenberg, L.: *Remarks on strongly elliptic partial differential equations.* Comm. Pure Appl. Math. 8 (1955), 649–675.

[28] Nicolaescu, L.I.: *Lectures on the geometry of manifolds.* Second edition. World Scientific Publishing Co. Pte. Ltd., Hackensack, NJ, 2007.

[29] Reed, M. & Simon, B.: *Methods of modern mathematical physics. I. Functional analysis.* Academic Press, New York-London, 1972.

[30] Reed, M. & Simon, B.: *Methods of modern mathematical physics. IV. Analysis of operators.* Academic Press, Inc., 1978.

[31] Saloff-Coste, L.: *Aspects of Sobolev-type inequalities.* London Mathematical Society Lecture Note Series, 289. Cambridge University Press, Cambridge, 2002.

[32] Schoen, R. & Yau, S.-T.: *Lectures on differential geometry.* Conference Proceedings and Lecture Notes in Geometry and Topology, I. International Press, Cambridge, MA, 1994.
[33] Spiegel, Daniel: *The Hopf-Rinow theorem.* Notes available online.
[34] Ikeda, N. & Watanabe, S.: *Stochastic Differential Equations and Diffusion Processes.* North Holland Publ. Co., 1981.
[35] Revuz, D. & Yor, M.: *Continuous martingales and Brownian motion.* Grundlehren der Mathematischen Wissenschaften, 293. Springer-Verlag, Berlin, 1991.
[36] Simon, B.: *Functional integration and quantum physics.* Academic Press. Inc., 1979.
[37] Sturm, K.-T.: *Heat kernel bounds on manifolds.* Math. Ann. 292 (1992), no. 1, 149–162.
[38] Varadhan, S.: *On the behavior of the fundamental solution of the heat equation with variable coefficients*, Comm. Pure Appl Math., 20 (1967), 431–455.
[39] Weidmann, J.: *Lineare Operatoren in Hilbertraeumen.* Mathematische Leitfaeden. B.G. Teubner, Stuttgart, 1976.
[40] Weidmann, J.: *Lineare Operatoren in Hilbertraeumen. Teil 1.* Grundlagen. Mathematische Leitfaeden. B.G. Teubner, Stuttgart, 2000.
[41] Yau, S.T.: *On the heat kernel of a complete Riemannian manifold.* J. Math. Pure Appl. (9) 57 (1978), no. 2, 191–201.

Batu Güneysu, Fakultät für Mathematik, Technische Universität Chemnitz, Germany
Email address: batu.gueneysu@math.tu-chemnitz.de