Heat kernels on Riemannian manifolds

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1. Introduction

Fourier in 1822 was the first to derive the heat equation in the following context: assume $M \subset \mathbb{R}^3$ is a sufficiently homogeneous body. Then the temperature function

$$u : (0, \infty) \times M \longrightarrow [0, \infty)$$

of M, that is, $u(t, x)$ is the temperature at the time t in $x \in M$, satisfies the heat equation

$$\partial_t u(t, x) = k\Delta_x u(t, x)$$

if M has no sources or sinks of heat. Above, $k > 0$ is a material constant (heat conductivity constant), and $\Delta = \sum_{j=1}^{m} \partial_j^2$ is the Laplace operator.

The heat equation was also the basis for modern probability theory: 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 he was sure that were not alive. His observations were that the trajectory X of each test particle was random independent 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. Then Brown observed that the expected displacement of the test particle was a decreasing function of its size and of viscosity of the medium, and 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

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

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 Gauss kernel

$$p : (0,\infty)\times\mathbb{R}^3\times\mathbb{R}^3 \longrightarrow [0,\infty), \quad p(t,x,y) := (4\pi t)^{3/2} e^{-\frac{|x-y|^2_{\mathbb{R}^3}}{4t}},$$

which is a solution of the heat equation in (t,x), one easily derives the fundamental relation

$$\int_\Omega |X^j_t - y^j|^2 dP \approx Dt, \tag{1}$$

for the average square displacment, which justifies all observations of Brown. The stochastic process underlying the random trajectory of a test particle as above is nowadays called a *Brownian motion.*

Einstein's conclusion was that the medium consists of very small particles (molecules), 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.

Let us now take a closer look at the properties of the m-dimensional Gauss kernel

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

In the sequel, we are going to consider $\mathbb{R}^m$ as a Riemannian manifold with its Euclidean metric $g_{ij}(x) = \delta_{ij}(x)$. Then Δ is the underlying Laplace-Beltrami operator, the Lebesgue measure dx becomes the Riemannian volume measure and the Euclidean distance $|x-y|$ the Riemannian distance. One can then prove the following facts for the Riemannian manifold $\mathbb{R}^m$:

i) $(t,x,y) \longmapsto p^{\mathbb{R}^m}(t,x,y)$ is jointly smooth and $(t,x) \mapsto p(t,x,y)$ satisfies

$$\partial_t u(t,x) = \Delta_x u(t,x), \quad \lim_{t\to 0+} u(t,\cdot) = \delta_y \quad \text{for all } y\in\mathbb{R}^m, \tag{2}$$

ii) one has

$$\int p(t,x,y)dy = 1 \quad \text{for all } t>0,\ x\in\mathbb{R}^m,$$

iii) one has $p(t,x,y) = p(t,y,x)$ for all $t > 0$, $x, y \in \mathbb{R}^m$,

iv) one has

$$p(t+s,x,y) = \int p(t,x,z)p(s,y,z)d^m z \quad t,s>0,\ x\in\mathbb{R}^m$$

v) one has

$$p > 0,$$

and p is the unique nonnegative function satisfying (2),

vi) there is exactly one self-adjoint realization $H \geq 0$ of $-\Delta$ in the Hilbert space $L^2(\mathbb{R}^m)$ and one has

$$e^{-tH} f(x) = \int p(t,x,y) f(y) dy \quad \text{for all } f \in L^2(\mathbb{R}^m),$$

where the heat semigroup on the left hand side is defined via the spectral theorem,

vii) if $m < 2$ we have

$$G(x,y) := \int_0^\infty p(t,x,y) dt = \infty \quad \text{for all } x,y \in \mathbb{R}^m,$$

while for $m \geq 3$ we have

$$G(x,y) < \infty \quad \text{for all } x,y \in \mathbb{R}^m \text{ with } x \neq y.$$

In this course we will attack the following problem: to what extend hold the above results Riemannian manifold? It is easy to convince onselve that some subtleties must appear: for example, even if we replace $\mathbb{R}^m$ above with an arbitrary bounded open subset U of $\mathbb{R}^m$, then there exist at least two nonnegative solutions to (2) in U and Δ has at least two self-adjoint realizations in $L^2(U)$: the Dirichlet realization and the Neumann realization, and the integral kernels of the corresponding heat semigroups both solve (2) in U.

Assume now (M,g) is an arbitrary Riemannian manifold, let Δ_g denote the induced Laplace-Beltrami operator, let μ_g denote the Riemannian volume measure, and $d_g(x,y)$ the Riemannian distance. The first question is: what is the analogue of the Gauss kernel and of H in this case? Firstly, we are going to show that Δ_g has a canonically given self-adjoint realization $H_g \geq 0$ in $L^2(M,g)$, its Friedrichs realization. Then one can define $p_g(t,x,y)$ as the integral kernel of the heat semigroup of H_g. It will turn out that without any further assumptions on the geometry,

- the map

$$p_g : (0,\infty) \times M \times M \longrightarrow [0,\infty)$$

is jointly smooth, and $(t,x) \mapsto p_g(t,x,y)$ satisfies

$$\partial_t u(t,x) = \Delta_{g,x} u(t,x), \quad \lim_{t \to 0+} u(t,\cdot) = \delta_y \quad \text{for all } y \in M, \tag{3}$$

which is why one calls p_g the *heat kernel* of (M,g),

- one has

$$\int p_g(t,x,y) d\mu_g(y) \leq 1 \quad \text{for all } t > 0,\ x \in M,$$

- one has the natural analogues of iii) and iv),
- and the analogue of vi) holds by definition.

Moreover, we are going to address the following facts:

- In general, H_g need not be the unique self-adjoint realization of $-\Delta_g$, but we are going to show that this is the case if (M, d_g) is complete.
- The property $\int p_g(t,x,y)d\mu_g(y) = 1$ turns out to be a property which is highly subtle for noncompact Riemannian manifolds and typically depends on the growth of the volume of metric balls. Riemannian manifolds having this property are called stochastically complete.
- While one always has $p_g \geq 0$, the strict positivity $p_g > 0$ turns out to be related with the connectedness of M.
- The property
$$G(x,y) = \int_0^\infty p_g(t,x,y)dt < \infty$$
for $x \neq y$ turns out to be subtle again: it implies the noncompactness of M and there are noncompact Riemannian manifolds of dimension ≥ 3 which need not satisfy the above finiteness, which is called *nonparabolicity*.
- Both, stochastic completeness and nonparabolity are linked with probability theory: on every Riemannian manifold one can define Brownian motion, and stochastic completeness means that this process cannot explode in a finite time, while nonparabolicity means that the process eventually leaves every relatively compact subset.
- the Gauss type behaviour of the heat kernel
$$C_1 t^{\dim(M)/2} e^{-\frac{d_g(x,y)^2}{C_2 t}} \leq p_g(t,x,y) \leq C_3 t^{\dim(M)/2} e^{-\frac{d_g(x,y)^2}{C_4 t}}$$
depends sensitively on the geometry of (M,g): in fact, it turns to be more natural in the above estimate to replace the factor $t^{\dim(M)/2}$ by the volume of a Riemannian ball centered in x with radius $\sqrt{t}$. These are the celebrated *Li-Yau* heat kernel estimates.

2. Some facts about linear operators

For the convenience of the reader, we collect some facts linear operators. For a detailed discussion of the below results, we refer the reader to [22, 15, **?**, 9].

We understand all our normed spaces to be over $\mathbb{C}$. We start by noting that in general, a linear operator T between Banach spaces $\mathscr{B}_1$ and $\mathscr{B}$ is only required to be defined on a subspace $\mathrm{Dom}(T) \subset \mathscr{B}_1$, called its domain of definition. Its range $\mathrm{Ran}(T) \subset \mathscr{B}$ is defined to be the linear space of all $f_2 \in \mathscr{B}$ 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. If $\mathrm{Dom}(T)$ is dense, then T can be uniquely extended to a bounded linear map $\mathscr{B}_1 \to \mathscr{B}$, which will be denoted with teh same symbol again. The linear space of bounded linear operators is denoted by $\mathscr{L}(\mathscr{B}_1, \mathscr{B})$ and becomesa Banach itself with the above operator norm. One sets

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

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

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

is closed.

We also record:

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

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

Let $\mathscr{H}$ be a separable 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*

$$T_f(h) = \langle f, h \rangle \,.$$

The map $f \mapsto T_f$ induces an antilinear 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 $\tilde{H}$, then the *adjoint* R^* of R is a linear operator from $\tilde{H}$ 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

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

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 is densely defined

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

for all $f_1, f_1 \in \mathrm{Dom}(S)$. Checking self-adjointness is a tricky business for unbounded operators.

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 2.4. *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 is in addition bounded as a linear operator from $\mathscr{H}$ to $\mathscr{H}$. If S is closed and $(S-z)^{-1}$ 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 [23]).

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 [22]), 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 2.5. 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:

Definition 2.6. 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 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 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 [23]), 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":

Theorem 2.7. *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*

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

One variant of the spectral theorem is:

Theorem 2.8. *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 2.7 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
$$\phi(S) := \phi(P_S).$$

Remark 2.9. 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 $f_1, f_2 \in \mathscr{H}$:

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

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 $\psi \in \mathscr{H}$ the path
$$[0, \infty) \ni t \longmapsto \psi(t) := e^{-tS}, \quad \psi \in \mathscr{H}$$
is the uniquely determined continuous path with $\psi(0) = \psi$ which is differentiable in $(0, \infty)$ and satisfies there the *abstract heat equation*
$$(d/dt)\psi(t) = -S\psi(t)$$
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 2.10. 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 there exists no $\epsilon > 0$ such that $|\psi - z| \geq \epsilon$ μ-a.e. and in the discrete spectrum if and only of

$$\mu\{|\psi - z|\} > 0.$$

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 $\phi(M_\psi) = M_{\phi\circ\psi}$.
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 $B = V^* A V$.

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 [9].

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[1] in its first slot, and linear in its second slot.

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 there exists a constant $C \geq 0$ such that

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

symbolically $Q \geq -C$. Again by complex polarization, every semibounded form is automatically symmetric.

Following Kato, given a sequence $(f_n) \subset \mathrm{Dom}(Q)$ and $f \in \mathrm{Dom}(Q)$ 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

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

[1]We warn the reader, however, that in [9] 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 [9] has to be applied to the complex conjugate form $Q(f_1, f_2)^*$.

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

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

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

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

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 $\overline{Q|_D} = Q$. Using the spectral calculus one defines:

Definition 2.11. 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 [15] for this exact formulation):

Theorem 2.12. *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 2.13. *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*
$$Q(f_1, f_3) = \langle f_2, f_3\rangle \quad \textit{for all } f_3 \in D,$$
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*
$$\begin{aligned}\min \sigma(S_Q) &= \inf\{Q(f,f) : f \in \mathrm{Dom}(Q),\ \|f\| = 1\}\\ &= \inf\{\langle S_Q f, f\rangle : f \in \mathrm{Dom}(S_Q),\ \|f\| = 1\}.\end{aligned}$$

Notation 2.14. 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 2.15. 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] [10].

Let us see how the Friedrichs construction can be used to define a self-adjoint realization of the Laplace-Beltrami 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 $C_c^\infty(U)$. For all $f_1, f_2 \in C_c^\infty(U)$ it follows from an integration by parts (Green's formula) that
$$\langle (-\Delta) f_1, f_2\rangle_U = \int_U (\nabla f_1, \nabla f_2) = \int_U \overline{f_2}(-\Delta) f_1 = \langle f_1, (-\Delta) f_2\rangle_U,$$
so $-\Delta$ is symmetric in $L^2(U)$, and in fact the second identity shows
$$\langle (-\Delta) f, f\rangle = \int_U |\nabla f|^2 \geq 0,$$

so $-\Delta \geq 0$ 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 case the reader is familiar with the Sobolev spaces $W^{k,p}(U)$ and $W_0^{k,p}(U)$: one has

$$\mathrm{Dom}(H_U) = \{f \in W_0^{1,2}(U) : \Delta f \in L^2(U)\}, \quad H_U f = -\Delta f,$$

where Δf is understood in the sense of distributions. We will come to a detailed explaination of these facts in the more general context of Riemannian manifolds later on.

3. Basic facts on differential operators on Riemann manifolds

Let M be a manifold[2] of dimension m and 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). We denote with $\Gamma_{C^\infty}(M, E)$ the smooth sections of $E \to N$, that is, the linear space (in fact C^∞ left module) of all smooth maps $\psi : M \to E$ with $\psi(x) \in E_x$ for all $x \in N$. Likewise, smooth compactly supported sections will be denoted with $\Gamma_{C_c^\infty}(M, E)$. In case $E = M \times \mathbb{C} \to M$ is the trivial vector bundle, then each fiber E_x is given by $\{x\} \times \mathbb{C}$ and we can identify $\Gamma_{C^\infty}(M, E)$ with $C^\infty(M)$.

A map

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

is called restrictable, if for all open $U \subset X$ 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[3] $e_1, \dots, e_{\ell_0} \in \Gamma_{C^\infty}(U, E)$, $f_1, \dots, f_{\ell_1} \in \Gamma_{C^\infty}(U, F)$, and any multi-index[4] $\alpha \in \mathbb{N}_k^m$, 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

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

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

---

[2]We understand all our manifolds to be smooth and without boundary.

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

[4]$\mathbb{N}_k^m$ 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 principal) symbol of P is the unique morphism

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

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 $\alpha_1 + \dots + \alpha_m = k$), one has

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

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

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 $x \in M$ zuwe 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 $M \times \mathbb{C} \to M$ is equipped with its canonic smooth metric which is induced by $(z, z') \mapsto \overline{z} z$, where $z, z' \in \mathbb{C}$. A Riemann metric on M is by definition a metric on $TM \to M$.

Proposition and definition 3.3. *For any Riemann 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, that is, one has $\mu_g(U) > 0$ for all open nonempty $U \subset M$.

Remark 3.4. 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 3.5. *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 of metrics (g, h_E) with*

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

(in particular, the above then holds for all pairs of metrics (g, h_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

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

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

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

in U, for all i, so $f_1 = f_2$ as $\sqrt{\det(g)} > 0$. ■

Now we can prove:

Proposition and definition 3.6. *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

$$P^{g,h_E,h_F}\sum_{j=1}^{\ell_1}\psi^{(i)}f_j := \frac{1}{\sqrt{\det(g)}}\sum_{i=1}^{\ell_0}\sum_{j=1}^{\ell_1}\sum_{\alpha\in\mathbb{N}_k^m}(-1)^{|\alpha|}\frac{\partial^{|\alpha|}\left(\overline{P_{\alpha ji}}\sqrt{\det(g)}\psi^{(j)}\right)}{\partial x^\alpha}e_i \quad \text{in } U \tag{8}$$

does the job. ■

There is a way to define the action of differential operators on locally integrable functions without using any distribution theory:

Proposition and definition 3.7. *Given P as above, $f\in\Gamma_{L^1_{\mathrm{loc}}}(X,E)$ and a subspace $A\subset\Gamma_{L^1_{\mathrm{loc}}}(X,F)$ 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*

$$\int_M h_E\left(P^{g,h_E,h_F}\psi,f\right)d\mu_g = \int_M h_F(\psi,h)\,d\mu_g \ \ \textit{for all } \psi\in\Gamma_{C^\infty_c}(M,F)\ . \tag{9}$$

Then h is uniquely determined and we set $Pf := h$. This property is equivalent to (9) 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 (9) holds for some triple (g,h_E,h_F) then it also holds for any other such triple. This is left as an exercise. ■

Lemma 3.8 (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 $f\in\Gamma_{L^q_{\mathrm{loc}}}(M,F)$ with $Pf\in\Gamma_{L^q_{\mathrm{loc}}}(M,F)$ one has $f\in\Gamma_{W^{k,q}_{\mathrm{loc}}}(M,F)$ if $q>1$ and $f\in\Gamma_{W^{k-1,1}_{\mathrm{loc}}}(M,F)$ if $q=1$.

Proof: The $q>1$ is a classical fact by Nirenberg [13] and can be found in many textbooks such as [14]. The $q=1$ case is nonstandard uses Besov spaces. Together with Guidetti and Pallara I have given a proof in [8]. ■

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

Proof: Step 1: $A := \Gamma_{L_c^q}(M, E)$ 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: $\Gamma_{C_c^\infty}(M, E)$ 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 $(\phi_n) \subset C_c^\infty(M)$ subordinate to (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

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

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

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

completing the proof. ■

4. The Friedrichs realizaiton 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, the symbol of Δ is given by g^{ij}, whose nondegeneracy implies that Δ is elliptic.

Lemma 4.2. *a) One has*

$$d(f_1 f_2) = f_1 df_2 + f_2 df_1, \tag{10}$$

$$d^\dagger(f\alpha) = f d^\dagger \alpha - (df, \alpha), \tag{11}$$

$$\Delta(f_1 f_2) = f_1 \Delta f_1 2 + f_2 \Delta f_1 + 2\Re(df_1, df_2), \tag{12}$$

$$\Delta(u \circ f) = (u'' \circ f) \cdot |df|^2 + (u' \circ f) \cdot \Delta f. \tag{13}$$

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 2.15), 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

$$W_0^{1,2}(M) := \quad \text{closure of } C_c^\infty(M) \text{ with respect to } \|\cdot\|_{W^{1,2}}.$$

Remark 4.3. If $M = \mathbb{R}^m$ (with its Euclidean metric) then one has $W_0^{1,2}(\mathbb{R}^m) = W^{1,2}(\mathbb{R}^m)$, while if M is a bounded open subset U of $\mathbb{R}^m$ then one has $W_0^{1,2}(U) \neq W^{1,2}(U)$. 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

$$\mathrm{Dom}(Q) = W_0^{1,2}(M), \quad Q(f_1, f_2) = \int (df_1, df_2) d\mu.$$

By Kato's theory (cf. Theorem 2.13) there exists a uniquely determined self-adjoint nonnegative operator H in $L^2(M)$ such that $\mathrm{Dom}(H) \subset \mathrm{Dom}(Q)$ and

$$\langle Hf_1, f_2 \rangle = Q(f_1, f_2) \text{ for all } f_1 \in \mathrm{Dom}(H),\ f_2 \in \mathrm{Dom}(Q).$$

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

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

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.

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

$$\overline{B(x,r)} = \{y : \varrho(x,y) \leq r\}. \tag{14}$$

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 $(\chi_n)\subset C^{\infty}_{\mathrm{c}}(M)$ 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* $\chi_n\mid_K = 1$,
- (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 $x^1,\dots,x^m$ 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

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

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

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

so

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

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

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

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

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

where $\gamma_{x,y}$ is the straight line from x to y.
We are going to show that on U the Euclidean ball in W around p of radious $r/3$ 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

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

and so

$$\ell(\gamma) \ge C^{-1}|x - y|. \tag{15}$$

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

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

Thus we have

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

for all γ's connecting x and y, so that taking infima we get

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

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 $\partial B_e(p, r)$, so that by taking infima we arrive at $\ell(\gamma) \ge C^{-1}r$, so $\varrho(x, p) \ge C^{-1}r > 0$. This completes the proof that ϱ is a distance.

The proof of (14) 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

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

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 $x \notin U$ then and 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 infima, $\varrho(y,p) \geq r$ and so $x \notin B(p,r)$. This completes the proof.
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 [12].
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 pick a compact $A_{\mathscr{O}} \subset M$ such that $\mathscr{O} \in A_{\mathscr{O}}$, 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

$$\sup_{x \in M} \left| d\chi_{n_{\mathscr{O},r}}(x) \right| \leq 1/(r+1). \tag{16}$$

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 (16) 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 Strichartz):

Theorem 5.3. *Assume M is complete. Then the symmetric nonnegative operator $-\Delta$ (defined on $C_c^\infty(M)$) 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 2.4, 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 4.2 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

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

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

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

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

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

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

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

we see

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

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 $f_1 \in W^{1,2}_0(M)$, $f_2 \in W^1(M)$, $\Delta f \in L^2(M)$. 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 $f_2 = P_t h$ for some $f \in L^2(M)$, $t > 0$, as we know that for all $t > 0$

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

by the spectral calculus.

A function $f : M \to \mathbb{R}$ on M is called *Lipschitz*, if there exists a constant C such that for all $x, y \in M$ one has

$$|f(x) - f(y)| \leq C \varrho(x, y). \tag{17}$$

Note in this context that if $U \subset M$ is open, then with an obvious notation one has

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

Lemma 6.2. *a) If $f : M \to \mathbb{R}$ is a Lipschitz function, then df exists as an element of $\Omega^1_{L^\infty}(M)$ and one has $\|df\|_\infty \leq C'$, where C' is the smallest C with (17). If $f : M \to \mathbb{R}$ is locally Lipschitz, that is, if for each compact $K \subset M$ there exists a $C = C_K$ with (17) for all $x, y \in K$, then df exists as an element of $\Omega^1_{L^\infty_{\mathrm{loc}}}(M)$.*
b) A C^1-function $f : M \to \mathbb{R}$ with $\|df\|_\infty$ is Lipschitz. In particular, C^1-functions are locally Lipschitz.

Proof: a) Exercise. The essential observation is that the result is actually local, but in $\mathbb{R}^m$ this is just the well-known Rademacher's theorem.
b) I will sketch a proof later on (cf. [7]). ■

Lemma 6.3. *Assume $f : M \to \mathbb{R}$ is a compactly supported Lipschitz function. Then one has $f \in W^{1,2}_0(M)$.*

Proof: Clearly we have that f is L^2 (continuous and compactly supported) and df is L^2 (bounded by the previous Lemma and compactly supported), so $f \in W^{1,2}(M)$. The stronger conclusion $f \in W^{1,2}_0(M)$ is seen as follows: if M is an open subset of the Euclidean $\mathbb{R}^m$, the statement follows from using Friedrichs mollifiers. The general case can be reduced to this case using a partition of unity which is associated to the a finite cover of the support of f, noting that locally g is equivalent to the Euclidean metric. ■

Lemma 6.4. *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: I will sketch a proof later on (cf. [7]). ■

Lemma 6.5. *Assume $f_1 : M \to \mathbb{R}$ is bounded and Lipschitz and $f_2 \in W^{1,2}_0(M)$. Then $f_1 f_2 \in W^{1,2}_0(M)$ and one has the product rule $d(f_1 f_2) = f_1 df_2 + f_2 df_1$.*

Proof: Exercise. ■

Lemma 6.6. *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 $f_1 f_2 \in W^{1,2}_0(M)$ and the product rule applies.*

Proof: Exercise. ■

Lemma 6.7. *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

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

one has $\psi \circ f \in W^{1,2}_{\mathrm{loc}}(M)$ *and*

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

Proof: a) This has been shown by Oliver in the lecture course.
b), c) I will sketch a proof later on (cf. [7]). ■

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 6.8. 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 the formula

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

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

$$e^{-tH}f(x) = \int p(t,x,y)f(y)d\mu(y). \tag{18}$$

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

$$\int p(t,x,y)^2 d\mu(y) < \infty, \tag{19}$$

$$p(t,y,x) = p(t,x,y), \tag{20}$$

$$p(t+s,x,y) = \int p(t,x,z)p(s,z,y)d\mu(z), \tag{21}$$

$$\int p(x,z)d\mu(z) \leq 1. \tag{22}$$

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

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

d) For all fixed $x \in X$, *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*

$$\lim_{t \to 0+} \int p(t,x,y)\phi(y)d\mu(y) = \phi(x).$$

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

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

by local elliptic regularity. By the spectral calculus and the local Sobolev embedding, 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 $t > 0$, $U \subset X$ open and relatively compact, the map

$$e^{-tH} : L^2(M) \longrightarrow C_b(U) \tag{23}$$

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, noting that the $L^2(M)$-convergence of a sequence implies the existence of a subsequence which converges μ-a.e.

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 $U \subset X$ 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

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

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

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

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

$$\{\Re > 0\} \ni z \longmapsto e^{-zH} f \in L^2(M) \tag{24}$$

is holomorphic. Note that, a priory, (24) 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

$$\frac{\partial}{\partial t} P_t f(x) = \Delta_x P_t f(x). \tag{25}$$

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 (24) 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* $x \in X$, 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 (24) 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 (25) 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

$$P_t f(x) = \langle p_{t,x}, f \rangle . \tag{26}$$

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"

$$p(t,x,y) := \left\langle p_{t/2,x}, p_{t/2,y} \right\rangle \tag{27}$$

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:

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

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 $f = p_{r,x}$,

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

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 (whose proof relies on Lemma 6.7 and Example 6.8) 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 taking $c \to 0$ we get $P_t(-f) \leq 0$, so $f \geq 0$ implies $P_t f \geq 0$. Thus writing

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

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) As by the fundamental lemma of distrbution theory we have $p_{t,x} = p(t,x,\cdot)$ μ-a.e., and $p_{t,x} \in L^2(M)$ it is clear that

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

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

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

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.

■

8. Strong parabolic maximum principle and its applications

From here on we will closely follows the presentation from Grigor'yan's book [7]. The following result (and all its consequences) relies heavily on our standing assumption that M is connected:

Theorem 8.1 (Strong parabolic minimum/maximum principle). *i) Assume $I \subset \mathbb{R}$ is an open interval and $0 \leq v \in C^2(I \times M)$ solves*

$$\partial_t v \geq \Delta v.$$

If there exists $(t',x') \in I \times M$ with $v(t',x') = 0$, then one has $v(t,x) = 0$ for all $x \in M$ and all $t \leq t'$.
ii) Assume $I \subset \mathbb{R}$ is an open interval and $0 \geq v \in C^2(I \times M)$ solves

$$\partial_t v \leq \Delta v.$$

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

Proof: The proof of i) has been given by Koen in the lecture course, and ii) follows from applying i) to $-v$. ■

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 (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 9.5 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 $0 \leq f_k \in W_0^{1,2}(M)$ with $f_k \to f$ as $k \to \infty$ in $W^{1,2}(M)$.*

Proof: The proof has been given by Oliver in the course. ■

Let $U \subset M$ be open and denote by $\tilde{f} : M \to \mathbb{C}$ the trivial extension by zero of a function $f : U \to \mathbb{C}$. Then we consider $L^2(U)$ as a closed subspace of $L^2(M)$ via the embedding $f \mapsto \tilde{f}$.

Lemma 9.3. *Let $U \subset M$ be open. Then for all $f \in W_0^{1,2}(U)$ one has $\tilde{f} \in W_0^{1,2}(M)$.*

Proof: The proof has been given by Oliver in the course. ■

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

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 one proves:

Theorem 9.4. *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: The proof has been given by Oliver in the course. ■

Corollary 9.5. *For all open relatively compact $U \subset M$ the operator H^U has a purely discrete spectrum.*

Proof: Combine Theorem 9.4 with Theorem 9.1. ■

10. Some informal comments on Brownian motion on Riemann manifolds

The aim of this sohort section is motivate the following definitions:

Definition 10.1. a) M is called *stochastically complete*, if for all $t > 0$, $x \in M$ one has

$$\int_M p(t,x,y) d\mu(y) = 1.$$

b) M is called *nonparabolic*, if for for all $x \neq y$ one has

$$\int_0^\infty p(t,x,y) d\mu(y) < \infty.$$

Remark 10.2. 1. In general geodesic completeness is unrelated with stochastic completeness, but there is the following state-of-the art criterium for stochastic completeness by Alexander Grigor'yan: assume M is geodesically complete, then M is stochastically complete if there exists x_0 with

$$\int_1^\infty \frac{rdr}{\log \mu(B(x_0, r))} = \infty.$$

So one has to control the volumes of balls exponentially from above. It is trivial from this result that compact M's (or more generally geodesically M's with finite volume) are stochastically complete.
2. If M is parabolic ('not nonparabolic'), then M is stochastically complete.
3. In general parabolicity is unrelated with stochastic completeness, but there is the following state-of-the art criterium for parabolicty by Alexander Grigor'yan: assume M is geodesically complete, then M is parabolic if there exists x_0 with

$$\int_1^\infty \frac{rdr}{\mu(B(x_0, r))} = \infty.$$

It is trivial from this result that compact M's (or more generally geodesically M's with finite volume) are parabolic.
4. The Euclidean $\mathbb{R}^m$ is stochastically complete for all m, and parabolic if and only if $m \leq 2$.

Let $\widetilde{\mu}$ denote the Borel measure on

$$\widetilde{M} := \begin{cases} M, \text{ if } M \text{ is compact} \\ \text{one point compactification } M \cup \{\infty_M\} \text{ of } M, \text{ if } M \text{ is noncompact,} \end{cases}$$

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

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

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

$$\int_{\widetilde{M}} \widetilde{p}(t, x, z) \widetilde{p}(s, y, z) d\widetilde{\mu}(z) = \widetilde{p}(s + t, x, y). \tag{28}$$

Furthermore, one has

$$\int_{\widetilde{M}} \widetilde{p}(t, x, y) d\widetilde{\mu}(y) = 1 \text{ for all } x \in \widetilde{M}, \tag{29}$$

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 (29) which motivates the above one-point machinery machinery.
Let the path space

$$\Omega_M := C([0,\infty),\tilde{M})$$

be equipped with the topology of locally uniform convergence and the induced Borel-sigma-algebra $\mathscr{F}^M$ and let

$$\zeta : \Omega_M \longrightarrow [0,\infty], \quad \zeta(\gamma) := \inf\{t \geq 0 : \ \gamma(t) = \infty_M\}$$

debote the *explosion time*. Note 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 M's are stochastically complete.

Proposition and definition 10.3. *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*

$$\mathbb{P}^{x_0}\left(\{\zeta = \infty\} \bigcup \Big\{\zeta < \infty \text{ and } \mathbb{X}_t = \infty_M \text{ for all } t \in [\zeta,\infty)\Big\}\right) = 1, \tag{30}$$

in other words, the point at infinity ∞_M *is a "trap" for* $\mathbb{P}^{x_0}$*-a.e. path.*[5]

It is possible to show that each of the measures $\mathbb{P}^{x_0}$ is concentrated on the set of paths that start in x_0, meaning that

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

as it should be.

Definition 10.4. Let $(\Omega,\mathscr{F},\mathbb{P})$ be a probability space, $x_0 \in M$, and let

$$X : [0,\infty) \times \Omega \longrightarrow \widetilde{M}, \quad (t,\omega) \longmapsto X_t(\omega)$$

be a continuous process. Then the tuple $(\Omega,\mathscr{F},\mathbb{P},X)$ is called a *Brownian motion on* M *with starting point* x_0, if the law of X 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 map

$$\Omega \longrightarrow \Omega_M, \ \omega \longmapsto \big(t \longmapsto X_t(\omega)\big) \tag{31}$$

is just $\mathbb{P}^{x_0}$.

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

In the above situation one again has

$$\mathbb{P}\{\omega : X_0(\omega) = x\} = 1,$$

which is a trivial consequence of

$$\mathbb{P}^{x_0}\{\gamma : \mathbb{X}_0(\gamma) = x_0\} = 1.$$

A canonical Brownian motion with starting point x_0 is given in terms of the Wiener measure by the datum

$$(\Omega, \mathscr{F}, \mathscr{F}_*, \mathbb{P}, X) := (\Omega_M, \mathscr{F}^M, \mathscr{F}^M_*, \mathbb{P}^{x_0}, \mathbb{X}), \tag{32}$$

where

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

denotes the coordinate process.

Remark 10.5. 1. It is straightforward to show that the following statements are equivalent:
i) M is stochastically complete,
ii) one has $P\{X_t \in M\} = 1$ for every Brownian motion X on M, and every $t > 0$, that is, every Brownian motion has an infinite lifetime,
iii) one has $P^x\{t < \zeta\} = 1$ for all $x \in M$, $t > 0$,
iv) one has $P^x\{\zeta = 0\} = 1$ for all $x \in M$.

2. With some more efforts oe can show that the following statements are equivalent:
i) M is nonparabolic,
ii) every Brownian motion X on M is transient, in the sense that for every precompact set $U \subset M$ one has

$$\mathbb{P}\{\text{there exists } s > 0 \text{ such that for all } t > s \text{ one has } X_t \notin U\} = 1,$$

that is, if and only if Brownian motions on M eventually leave each precompact set almost surely.

It follows easily from the definition of the Wiener measure that one has the following path integral formula:

$$P_t f(x) = e^{-tH} f(x) = \int_{\{\gamma : t < \zeta(\gamma)\}} f(\gamma(t)) dP^x(\gamma),$$

that is, one has to integrate over all paths that do not explode until t (in the stochastically complete case one has $1_{\{\gamma:t<\zeta(\gamma)\}} = 1$ P^x-almost surely!). More generally, if $V : M \to \mathbb{R}$ is a sufficiently nice potential, then one has the *Feynman-Kac path integral formula*:

$$P_t^V f(x) = e^{-t(H+V)} f(x) = \int_{\{\gamma : t < \zeta(\gamma)\}} e^{-\int_0^t V(\gamma(s))ds} f(\gamma(t)) dP^x(\gamma),$$

a central result in mathematical quantum mechanics.

11. Integrated maximum principle

Theorem 11.1 (Integrated Maximum Principe)**.** *Let $I \subset [0,\infty)$ be an interval and let $\zeta : I \times M \to \mathbb{R}$ be continuous such that*

i) *for all $t \in I$, the function $\zeta(t,\cdot)$ is locally Lipschitz,*
ii) *$\partial_t\zeta$ exists and is continuous on $I \times M$,*
- *one has*

$$\partial_t\zeta + \frac{1}{2}|d\zeta|^2 \leq 0.$$

Then with $\lambda_{\min}(M) := \inf\sigma(M)$, for all $f \in L^2(M)$ the function

$$I \ni t \longmapsto J(t) := \int (P_t f)^2(x) e^{\zeta(t,x)} d\mu(x) \in [0,\infty]$$

satisfies

$$J(t) \leq J(t_0) e^{-2\lambda_{\min}(M)(t-t_0)} \quad \text{for all } t, t_0 \in I \text{ with } t > t_0,$$

in particular, J is nonincreasing.

Remark 11.2. We make no statement here on the finiteness of $J(t)$!

Proof: Because of $(P_t f)^2 = (P_{t-t_0}P_{t_0}f)^2 \leq (P_{t-t_0}|P_{t_0}f|)^2$ WLOG (check this!) we can and we will assume $f \geq 0$. Then, in view of $P^U f \leq Pf$, it suffices to show that for all open relatively compact $U \subset M$ one has

$$J_U(t) := \int_U (P^U_t f)^2(x) e^{\zeta(t,x)} d\mu(x) \leq J^U(t_0) e^{-2\lambda_{\min}(U)(t-t_0)}. \tag{33}$$

Note that J_U is finite and continuous on I, for we have

$$J_U = \left\langle P^U f, e^{\zeta(\cdot,x)} P^U f \right\rangle_U.$$

Thus in order to show (33), it suffices to show that J_U is differentiable in $I \setminus \{0\}$ with

$$(d/dt) J_U(t) \leq -2\lambda_{\min}(U) J^U(t) \tag{34}$$

for all $t \in I \setminus \{0\}$. The functions $\zeta(t,\cdot)$ and $\partial_t\zeta(t,\cdot)$ are in $C_b(U)$, so that (exercise) $\partial_t\zeta$ is equal to the strong derivative $(d/dt)\zeta$. Likewise we have

$$(d/dt) e^{\zeta} = \partial_t e^{\zeta} = e^{\zeta}\partial_t\zeta. \tag{35}$$

On the other hand $P^U f$ is strongly differentiable as an $L^2(U)$-valued map by the spectral calculus with we record

$$(d/dt) P^U f = \Delta P^U f. \tag{36}$$

Using that e^{ζ} is strongly differentiable as an $C_b(U)$-valued map it is easily checked that $P^U f e^{\zeta}$ is a strongly differentiable $L^2(U)$-valued map and the product rule

$$(d/dt)(P^U f e^{\zeta}) = [(d/dt)P^U f] e^{\zeta} + [(d/dt)e^{\zeta}] P^U f \tag{37}$$

applied. Thus

$$J_U = \left\langle P^U f, e^{\zeta} P^U f \right\rangle_U$$

is differentiable with

$$(38)\qquad (d/dt)J_U = \left\langle (d/dt)P^U f, e^\zeta P^U f\right\rangle_U + \left\langle P^U f, (d/dt)[ue^\zeta]\right\rangle_U$$

$$(39)\qquad = 2\left\langle (d/dt)P^U f, e^\zeta P^U f\right\rangle_U + \left\langle (P^U f)^2, (d/dt)e^\zeta\right\rangle_U$$

$$(40)\qquad = 2\left\langle \Delta P^U f, e^\zeta P^U f\right\rangle_U + \left\langle (P^U f)^2, [\partial_t \zeta]e^\zeta\right\rangle_U.$$

By the Chain rule we have that $e^{\zeta(t,\cdot)}$ is locally Lipschitz on M, so this function is Lipschitz (and bounded) on U. As by the spectral calculus we have $P_t^U f \in W_0^{1,2}(U)$ it follows that $e^\zeta P_t^U f \in W_0^{1,2}(U)$ and we may integrate by parts

$$2\left\langle \Delta P^U f, e^\zeta P^U f\right\rangle_U = 2\int_U \Delta P^U f \cdot e^\zeta P^U f d\mu = -2\int_U (dP^U f, d(e^\zeta P^U f))d\mu.$$

In addition, $P_t^U f$ and $e^{\zeta(t,\cdot)}$ are locally Lipschitz in U so that using the product rule and the chain rule we get

$$d(e^\zeta P^U f) = P^U f \cdot de^\zeta + e^\zeta \cdot dP^U f = P^U f \cdot e^\zeta d\zeta + e^\zeta \cdot dP^U f$$

and so

$$2\left\langle \Delta P^U f, e^\zeta P^U f\right\rangle_U =$$
$$-2\int_U \Big(dP^U f, P^U f \cdot e^\zeta d\zeta\Big)d\mu - 2\int_U \Big(dP^U f, P^U f \cdot e^\zeta \cdot dP^U f\Big)d\mu.$$

Plugging this into (38) and using assumption ii) from the theorem we obtain

$$\begin{aligned}
&(d/dt)J_U = 2\left\langle \Delta P^U f, e^\zeta P^U f\right\rangle_U + \left\langle (P^U f)^2, (\partial_t\zeta)e^\zeta\right\rangle_U\\
&= -2\int_U e^\zeta P^U f\Big(dP^U f, d\zeta\Big)d\mu - 2\int_U e^\zeta P^U f\cdot\Big(dP^U f, dP^U f\Big) + \int_U (P^U f)^2\cdot(\partial_t\zeta)\cdot e^\zeta d\mu\\
&\le -2\int_U \left(e^\zeta P^U f\Big(dP^U f, d\zeta\Big) + \int_U e^\zeta P^U f\cdot\Big(dP^U f, dP^U f\Big) + \frac{1}{4}e^\zeta (P^U f)^2|d\zeta|^2\right)d\mu\\
&= -2\int_U \left|dP^U f + \frac{1}{2}P^U f d\zeta\right|^2 e^\zeta d\mu\\
&= -2\int_U \left|d(e^{\zeta/2}P^U f)\right|^2 d\mu \le -2\lambda_{\min}(U)\int_U |e^{\zeta/2}P^U f|^2 d\mu
\end{aligned}$$

where the last equality follows from

$$\Big(dP^U f + \frac{1}{2}P^U f d\zeta\Big)e^{\zeta/2} = d(e^{\zeta/2}P^U f)$$

and the last inequality from the variational principle (exercise)

$$\lambda_{\min}(U) = \inf_{\Psi\in W_0^{1,2}(U)}\left(\int_U |d\Psi|^2 d\mu\right)/\left(\int_U |\Psi|^2 d\mu\right),$$

since $e^{\zeta/2}P^U f \in W_0^{1,2}(U)$. Noting that

$$\int_U |e^{\zeta/2}P^U f|^2 d\mu = J_U,$$

this completes the proof. ■

12. L^2-mean-value-inquality (MVI)

Definition 12.1. Let $I \subset \mathbb{R}$ be an interval and $V \subset M$ be open. Then a C^2-function $u : I \times V \to \mathbb{R}$ is called a *subsolution of the heat equation*, if $\partial_t u \leq \Delta u$.

Theorem 12.2 (L^2-MVI)**.** *Assume $B(x,R) \subset M$ is relatively compact and that for some $a, n > 0$ one the following Faber-Krahn inequality:*

$$\lambda_{\min}(U) = \min \sigma(H^U) \geq a\mu(U)^{-2/n} \quad \textit{for all open } U \subset B(x,R).$$

Then there exists a constant C_n, which only depends on n, such that for all $T > 0$ and all subsolutions u of the heat equation in $\mathscr{C} := (0,T] \times B(x,R)$ one has

$$u_+^2(T,x) \leq \frac{C_n a^{-n/2}}{\min(\sqrt{T}), R)^{n+1}} \int u_+^2 d\nu,$$

where $d\mu := dt d\mu$ is the product of the Lebesgue measure on $\mathbb{R}$ and the Riemann volume measure on M.

The proof of the L^2-MVI requires two auxiliary results:

Lemma 12.3. *Let $V \subset M$ be open, $0 \leq T_0 < T$ and let η be a Lipschitz function on $\mathscr{C} := [T_0, T] \times V$ (considered as a Riemann manifold) such that for some compact $K \subset V$ one has* $\mathrm{supp}(\eta(t,\cdot)) \subset K$ *for all $t \in [T_0, T]$. Let u be a subsolition of the heat equation in $\mathscr{C}$ and set $v := (u - \theta)_+$ for some $\theta \geq 0$. Then one has*

$$\frac{1}{2}\left(\int_V v^2(T,\cdot)\eta^2(T,\cdot)d\mu - \int_V v^2(T_0,\cdot)\eta^2(T_0,\cdot)d\mu\right) + \int_{\mathscr{C}} |d(v\eta)|^2 d\nu$$

$$\leq \int_{\mathscr{C}} v^2(|d\eta|^2 + |\eta\partial_t\eta|)d\nu. \tag{41}$$

In particular, if $\eta(T_0,\cdot) = 0$, then the following two additional inequalities hold:

$$\int_V v^2(t,\cdot)\eta^2(t,\cdot)d\mu \leq 2\int_{\mathscr{C}} v^2(|d\eta|^2 + |\eta\partial_t\eta|)d\nu \quad \textit{for all } t \in [T_0, T], \tag{42}$$

and

$$\leq \int_{\mathscr{C}} v^2(|d\eta|^2 + |\eta\partial_t\eta|)d\nu \leq \int_{\mathscr{C}} v^2(|d\eta|^2 + |\eta\partial_t\eta|)d\nu. \tag{43}$$

Proof: Since $u(t,\cdot) \in C^2(V) \subset W^{1,2}_{\mathrm{loc}}(V)$ for all t, by Lemma 6.7 one has $v(t,\cdot) \in W^{1,2}_{\mathrm{loc}}(V)$ with

$$dv = 1_{\{u > \theta\}} du = 1_{\{v \neq 0\}} du, \tag{44}$$

so

$$(dv, du) = |dv|^2, \quad vdu = vdv. \tag{45}$$

Since $\eta(t,\cdot)$ is compactly supported and Lipschitz in V (and so its square, too) one has $v(t,\cdot)\eta(t,\cdot)^2 \in W_0^{1,2}(V)$ by Lemma 6.6, with

$$d(v\eta^2) = vd\eta^2 + \eta^2 dv = 2v\eta d\eta + \eta^2 dv, \tag{46}$$

thus

$$(du, d(v\eta^2)) = 2v\eta(dv, d\eta) + \eta^2|dv|^2. \tag{47}$$

If we multiply $\partial_t u \leq \Delta$ with $v\eta^2$ and perform $\int_{\mathscr{C}} \cdots d\nu$, we get

$$\begin{aligned}\int_{\mathscr{C}} (\partial_t u)v\eta^2 d\nu &\leq \int_{T_0}^T \int_V (\Delta u)v\eta^2 d\mu dt \\ &= -\int_{T_0}^T \int_V (du, d(n\eta^2))d\mu dt \\ &= -\int_{T_0}^T \int_V \Big(2v\eta(dv, d\eta) + \eta^2|dv|^2\Big)d\mu dt \\ &-\int_{T_0}^T \int_V \Big(|d(v\eta)|^2 - v^2|d\eta|^2\Big)d\mu dt,\end{aligned} \tag{48}$$

where have integrated by parts (Lemma 6.1; note that $v(t,\cdot)\eta(t,\cdot)^2 \in W_0^{1,2}(V')$ on some open relatively compact neighbourhood $V' \subset V$ of K and that $u(t,\cdot)$, $du(t,\cdot)$, $\Delta u(t,\cdot)$ are square integrable on V', $u(t,\cdot)$ is C^2 on V), and where we have used (47). Let us also record an application of Lemma 6.7 to the t-variable gives as above

$$v\partial_t u = v\partial_t v, \tag{49}$$

which shows the first identity in

$$\begin{aligned}\int_{T_0}^T (\partial_t u)v\eta^2 dt &= \frac{1}{2}\int_{T_0}^T (\partial_t v^2)\eta^2 dt \\ &= \frac{1}{2}\Big(v^2(T,\cdot)\eta^2(T,\cdot) - v^2(T_0,\cdot)\eta^2(T_0,\cdot)\Big) - \frac{1}{2}\int_{T_0}^T v^2\partial_t\eta^2 dt \\ &= \frac{1}{2}\Big(v^2(T,\cdot)\eta^2(T,\cdot) - v^2(T_0,\cdot)\eta^2(T_0,\cdot)\Big) - \frac{1}{2}\int_{T_0}^T v^2\eta\partial_t\eta dt,\end{aligned}$$

where we have integrated by parts several further times. If we perform $\int_V \cdots d\mu$ in the last identity and use (48), the proof is complete. ■

Lemma 12.4. *In the situation of the L^2-MVI consider*

$$\mathscr{C}_i := [T_i, T] \times B(x, R_i), \quad i = 0, 1,$$

where R_i, T_i are chosen with $0 < R_1 < R_0 \leq R$, $0 \leq T_0 < T_1 \leq T$. Chose $\theta_1 > \theta_0 \geq 0$ and set

$$J_i := \int_{\mathscr{C}_i} (u - \theta_j)^2 d\nu, \quad i = 0, 1.$$

Then for some constant c_n, which only depends on n, one has

$$J_1 \leq \frac{c_n J_0^{1+2/n}}{a\delta^{1+2/n}(\theta_1 - \theta_0)^{4/n}},$$

where

$$\delta := \min\big(T_1 - T_0, (R_0 - R_1)^2\big).$$

Proof: WLOG $\theta_0 = 0$, $\theta := \theta_1$. Define η by $\eta(t, y) := \phi(t)\psi(y)$, where

$$\phi(t) := \min\left(\frac{t - T_0}{T_1 - T_0}, 1\right),$$
$$\psi(y) := \min\left(\frac{(R_{1/4} - \varrho(x, y))_+}{R_{1/4} - R_{1/2}}, 1\right),$$

where $R_\lambda := \lambda R_1 + (1 - \lambda)R_0$, $\lambda \in [0, 1]$. Note that $R_\lambda \leq R_{\lambda'}$, iff $\lambda' \leq \lambda$. Note also that by construction $\eta(t, \cdot)$ is supported in the compact ball $K := \overline{B(x, R_{1/4})}$. Applying the second inequality from the previous lemma to $\mathscr{C}_0$, $v := u_+$, with $t \in [T_1, T] \subset [T_0, T]$ gives the bound

$$\int_{B(x,R_{1/2})} u_+^2(t, \cdot) d\mu \leq \int_{B(x,R_0)} u_+^2(t, \cdot) d\mu \leq 2 \int_{\mathscr{C}_0} u_+^2(|d\eta|^2 + |\eta\partial\eta|) d\nu,$$

where we have used that $\eta = 1$ in $[T_1, T] \times B(x, R_{1/2})$. Clearly we have

$$\eta \leq 1, \quad |d\eta|^2 \leq (R_{1/4} - R_{1/2})^{-2} = 16(R_0 - R_1)^{-2} \leq 16/\delta, \quad |\partial_t \eta| \leq (T_1 - T_0)^{-1} \leq 1/\delta,$$

and so

$$\int_{B(x,R_{1/2})} u_+^2(t, \cdot) d\mu \leq 34\delta^{-1} J_0.$$

Fix t as above and set

$$U_t := \{y \in B(x, R_{3/4}) : u(t, y) > \theta\},$$

so that by the latter inequality we get

$$\mu(\overline{U_t}) \leq \frac{1}{\theta^2} \int_{\overline{B(x,R_{3/4})}} u_+^2(t, \cdot) d\mu \leq \frac{1}{\theta^2} \int_{B(x,R_{1/2})} u_+^2(t, \cdot) \leq \frac{34 J_0}{\theta^2 \delta}. \tag{50}$$

Define now

$$\psi'(y) := \min\left(\frac{(R_{3/4} - d(x, y))_+}{R_{3/4} - R_1}, 1\right)$$

and $\eta'(t,y) := \phi(t)\eta'(y)$. Applying the third inequality of the previous lemma to $v' = (u-\theta)_+$ in $\mathscr{C}_0$ gives with a similar reasoning as above the inequality

$$\int_{\mathscr{C}_0} |d(v'\eta')|^2 d\nu \le \int_{\mathscr{C}_0} v'^2(|d\eta'|^2 + |\eta'\partial\eta'|) d\nu \le \frac{17}{\delta}\int_{\mathscr{C}_0} v'^2 d\nu \le \frac{17 J_0}{\delta}. \tag{51}$$

The function $\eta'(t,\cdot)v'(t,\cdot)$ is suppported in the compact set $\overline{U_t}$, thus an element of $W_0^{1,2}(V)$ for all open $V \subset M$ with $\overline{U_t} \subset V$. Choose such a V such that in addition $V \subset B(x,R_0)$ and[6]

$$\mu(V) \le 2\mu(\overline{U_t}) \le \frac{68 J_0}{\theta^2\delta},$$

where the second inequality follows from (50). Since $\eta'(t,\cdot)v'(t,\cdot) \in W_0^{1,2}(V)$ we can use the variational principle for V to conclude (using the support properties of $\eta'(t,\cdot)v'(t,\cdot)$)

$$\begin{aligned}
&\int_{B(x,R_0)} |d(\eta'(t,\cdot)v'(t,\cdot))|^2 d\mu \\
&= \int_V |d(\eta'(t,\cdot)v'(t,\cdot))|^2 d\mu \\
&\ge \lambda_{\min}(V)\int_V (\eta'(t,\cdot)v'(t,\cdot))^2 d\mu \\
&= \lambda_{\min}(V)\int_{B(x,R_0)} (\eta'(t,\cdot)v'(t,\cdot))^2 d\mu \\
&\ge a\mu(V)^{-2/n}\int_{B(x,R_0)} (\eta'(t,\cdot)v'(t,\cdot))^2 d\mu \\
&\ge a\left(\frac{\theta^2\delta}{68}\right)^{2/n} J_0^{-2/n}\int_{B(x,R_0)} (\eta'(t,\cdot)v'(t,\cdot))^2 d\mu,
\end{aligned}$$

where we have used the Faber-Krahn inequality (an assumption) and that $\eta' = 1$ in $[T_1,T]\times B(x,R_1)$. The lemma now immediately follows from integrating the latter inequality with respect to $\int_{T_1}^T \cdots dt$ and using (51). ■

Now we can give the

Proof of the L^2-MVI: Assume for the moment that $\theta \ge 0$ is arbitrary and define $\delta_k > 0$ by

$$\delta_k = \left(\frac{16^{2/n} C_n 16^{1-k/n} J_0^{2/n}}{a\theta^{4/n}}\right)^{n/(n+2)} =: \frac{C_n' 16^{-k/(n+2)} J_0^{2/(n+2)}}{a^{n/(n+1)}\theta^{4/(n+2}}$$

where C_n is as in the previous lemma and where

$$J_0 := \int_{\mathscr{C}} (u-\theta/2)_+^2 d\nu.$$

[6] In fact $\mu(V) \le 2\mu(\overline{U_t})$ is a little technical to prove, but replacing 2 with some $A = A_n$ follows straightforwardly from covering $B(x,R_0)$ with Euclidean balls and using that locally g is equivalent to the Euclidean metric.

Set

$$T_k := \sum_{i=0}^{k-1} \delta_i, \quad R_k := R - \sum_{i=0}^{k-1} \sqrt{\delta_i}.$$

Then there exists $C_n'' > 0$ such that (geometric series) if

$$\theta^2 := \frac{a^{-n/2}}{C_n'' \min(\sqrt{T}, R)^{n+2}}$$

then

$$T_k \leq \sum_{i=0}^{\infty} \delta_i \leq T/2, \quad R_k \geq R - \sum_{i=0}^{\infty} \sqrt{\delta_i} \leq R/2.$$

Define a sequence of cylinders by

$$\mathscr{C}_k := [T_k, T] \times B(x, R_k)$$

and further

$$\theta_k := (1 - 2^{-(k+1)})\theta, \quad J_k := \int_{\mathscr{C}_k} (u - \theta_k)_+^2 d\nu.$$

Then we have

$$\mathscr{C}_0 = \mathscr{C}, \quad [T/2, T] \times B(x, R/2) \subset \mathscr{C}_{k+1} \subset \mathscr{C}_k.$$

We claim that $J_k \to 0$ as $k \to \infty$, which would complete the proof, for one has

$$\int_{T/2}^{T} \int_{B(x,R/2)} (u - \theta)_+^2 d\nu \leq J_k \to 0,$$

so $u_+(T, x)^2 \leq \theta$, which is precisely the assertion of the L^2-MVI.
In order to show $J_k \to 0$, we apply the previous lemma to the pair $(\mathscr{C}_k, \mathscr{C}_{k+1})$, which using

$$\delta_k = (R_k - R_{k+1})^2 = (T_{k+1} - T_k) = \min((R_k - R_{k+1})^2, (T_{k+1} - T_k))$$

yields the inequality

$$J_{k+1} \leq \frac{C_n J_k^{1+2/n}}{a \delta_k^{1+2/n} (\theta_{k+1} - \theta_k)^{4/n}}.$$

Using this inequality and the defining formula for δ_k a simple induction on k shows

$$J_k \leq 16^{-k} J_0,$$

which completes the proof. ■

13. Equivalent characterizations of Li-Yau upper heat kernel bounds

Definition 13.1. Given $t, D > 0$, $x \in M$ define the weighted L^2-norm of the heat kernel by

$$E_D(t,x) := \int p(t,x,y)^2 e^{\frac{\varrho(x,y)^2}{Dt}} d\mu(y) \in [0,\infty)$$

Note that in $\mathbb{R}^m$ one has $E_D(t,x) = \infty$ for all t, x of $D \leq 2$.

Remark 13.2. Let $s > 0$ be arbitrary. As we have

$$E_D(t,x) = \int (P_{t-s}f)^2 e^{\zeta(t,\cdot)} d\mu,$$

for all $t > s$, where

$$f := p(s,x,\cdot), \quad \zeta(t,y) := \varrho(x,y)^2/(Dt),$$

it follows from the integrated maximum principle that $t \mapsto E_D(t,x)$ is nonincreasing on $(0,\infty)$, and

$$E_D(t,x) \leq E_D(t_0,x) e^{-2\lambda_{\min}(t-t_0)} \tag{52}$$

so long as $0 < t_0 \leq t$.

Theorem 13.3. *Let $B(x,r)$ be a relatively compact ball and the following Faber-Krahn inequality: there exist $a, n > 0$ such that for all open $U \subset B(x,r)$ one has*

$$\lambda_{\min}(U) \geq a\mu(U)^{-2/n}. \tag{53}$$

Then for all $t > 0$, $D > 2$ one has

$$E_D(t,x) \leq \frac{C_n (a\delta)^{-n/2}}{\min(t,r^2)^{n/2}} \quad \text{where } \delta := \min(D-2,1)$$

Remark 13.4. Using that on $\mathbb{R}^m$ the Faber-Krahn inequality holds on $B(x,\infty) = \mathbb{R}^m$ and that locally one has

$$Cg \leq g_{\mathrm{Eucl}} \leq (1/C)g,$$

one can easily show that for all $x \in M$ there exists $r > 0$ such that one has (53). Thus the above theorem shows that for all $t > 0$, $D > 2$, $x \in M$ one has $E_D(t,x)$, regardless of how bad the geometry of M is! This is a highly nontrivial fact.

We prepare the proof of Theorem 13.3 with

Lemma 13.5. *Let $B(x,r)$ be a relatively compact ball and the following Faber-Krahn inequality: there exist $a, n > 0$ such that for all open $U \subset B(x,r)$ one has*

$$\lambda_{\min}(U) \geq a\mu(U)^{-2/n}. \tag{54}$$

Set $\varrho(y) := (\varrho(x,y) - r)_+$, $y \in M$. Then for all $t > 0$ one has

$$\int p(t,x,y)^2 e^{\frac{\varrho(y)^2}{2t}} d\mu(y) \leq \frac{C_n a^{-n/2}}{\min(t,r^2)^{n/2}}$$

Proof: With the same argument as in Remark 13.2 one finds that the left hand side of the inequality is noncreasing in t, so WLOG we can assume $t \leq r^2$. For the moment let $0 \leq f \in L^2(M)$ be arbitrary and set $u := Pf$. The L^2-mean value inequality applied to the cylinder $[t/2, t] \times B(x, r)$ shows

$$u(t,x)^2 \leq \frac{C_n a^{-n/2}}{t^{1+2/n}} \int_0^t \int_{B(x,r)} u(s,y)^2 d\mu(y) ds.$$

Set $\zeta(s,y) := \varrho(y)^2(2(s-t))^{-1}$ and note $\mathrm{supp}(\zeta(s,\cdot)) \subset M \setminus B(x,r)$, so that the latter inequality is gives

$$u(t,x)^2 \leq \frac{C_n a^{-n/2}}{t^{1+2/n}} \int_0^t \int_{B(x,r)} u(s,y)^2 u^{\zeta(s,y)} d\mu(y) ds.$$

Again the integrated maximum principle implies that

$$J(s) := \int_0^t \int_{B(x,r)} u(s,y)^2 u^{\zeta(s,y)} d\mu(y) ds$$

is nonincreasing in $s \in [0, t)$ and so the latter inequality implies

$$\begin{aligned}
u(t,x)^2 &\leq \frac{C_n a^{-n/2}}{t^{1+2/n}} \int_0^{t/2} \int_{B(x,r)} u(s,y)^2 u^{\zeta(s,y)} d\mu(y) ds \\
&= \frac{C_n a^{-n/2}}{t^{1+2/n}} \int_0^{t/2} J(t/2) ds \\
&\leq \frac{C_n a^{-n/2}}{t^{1+2/n}} \int_0^{t/2} J(t/2) ds \\
&\leq \frac{C_n a^{-n/2}}{t^{2/n}} J(0) \\
&= C_n (at)^{-n/2} \int f^2 e^{-\varrho^2/(2t)} d\mu.
\end{aligned}$$

Pick ϕ smooth compactly supported with $0 \leq \phi \leq 1$ and applying the latter inequality with

$$f := p(t,x,\cdot) e^{\varrho^2/(2t)} \phi$$

to get

$$\begin{aligned}
\left(\int p(t,x,\cdot)^2 e^{\varrho^2/(2t)} \phi d\mu \right)^2 &\leq C_n (at)^{-n/2} \int p(t,x,\cdot)^2 e^{\varrho^2/(2t)} \phi^2 d\mu \\
&\leq C_n (at)^{-n/2} \int p(t,x,\cdot)^2 e^{\varrho^2/(2t)} \phi d\mu,
\end{aligned}$$

whish is equivalent to the assertion of the lemma. ■

Proof of Theorem 13.3: It suffices to prove the inequality for $D \leq 3$ and $t \leq r^2$ (as $E_D(t,x)$ is decreasing t and D).

We have $\sqrt{\delta t} \le r$. Thus Faber-Krahn holds in $B(x, \sqrt{\delta t})$ and applying the previous lemma on that ball we get

$$\int p(t,x,y)^2 e^{\frac{(\varrho(x,y)-\sqrt{t\delta})_+^2}{2t}} d\mu(y) \le \frac{C_n a^{-n/2}}{(\delta t)^{n/2}}$$

using

$$a^2/t_2 + b^2/t_1 \ge (a+b)^2/(t_1+t_2),$$

valid for all $a, b \in \mathbb{R}$, $t_1, t_1 > 0$, we get

$$\frac{(\varrho(x,y)-\sqrt{t\delta})_+^2}{2t} + \frac{\delta t}{2t} \ge \frac{\varrho(x,y)^2}{(2+\delta)t},$$

thus

$$\frac{(\varrho(x,y)-\sqrt{t\delta})_+^2}{2t} \ge \frac{\varrho(x,y)^2}{Dt} - 1,$$

which completes the proof. ■

The following lemma connects the weighted L^2-norm with Gaussian heat kernel upper bounds:

Lemma 13.6. *For all $D > 0$, $t \ge t_0 > 0$, $x, y \in M$ one has*

(55) $$p(t,x,y) \le \sqrt{E_D(t_0/2,x)E_D(t_0/2,y)}\, e^{-\varrho(x,y)^2/(2Dt)-\lambda_{\min}(M)(t-t_0)},$$

in particular,

(56) $$p(t,x,y) \le \sqrt{E_D(t/2,x)E_D(t/2,y)}\, e^{-\varrho(x,y)^2/(2Dt)}.$$

Proof: In view of (52) it suffices to prove (56). Set

$$a := \varrho(y,z), \quad b := \varrho(x,z), \quad c := \varrho(x,y).$$

Then $\exp((a^2+b^2-c^2/2)/(Dt)) \ge 1$ by the triangle inequality, and so

$$\begin{aligned} p(t,x,y) &= \int p(t/2,x,z)p(t/2,y,z)d\mu(z) \\ &\le \exp(-c^2/(2Dt)) \int p(t/2,x,\cdot)\exp(b^2/(Dt))p(t/2,y,\cdot)\exp(a^2/(Dt))d\mu(z) \end{aligned}$$

fro which the claim follows using Cauchy-Schwarz. ■

Theorem 13.7. *Assume $(B(x_i,r_i))_{i\in I}$ is a family of relatively compact balls such that there exists constant $n > 0$ and for each i a constant $a_i > 0$ with the following property: for each i and each open $U \subset B(x_i, r_i)$ one has the Faber-Krahn inequality*

$$\lambda_{\min}(U) \ge a_i \mu(U)^{-2/n}.$$

Then for all i, j, all $x \in B(x_i, r_i/2), y \in B(x_j, r_j/2)$, all $t \ge t_0 > 0$ one has

$$p(t,x,y) \le \frac{C_n(1+\varrho(x,y)^2/t)^{n/2} e^{-\varrho(x,y)^2/(4t)-\lambda_{\min}(t-t_0)}}{\big(a_i a_j \min(t_0, r_i^2)\min(t_0, r_j^2)\big)^{n/4}}.$$

Proof: We have $B(x,r_i/2)\subset B(x_i,r_i)$ so the Faber-Krahn inequality holds on $B(x,r_i/2)$ and Theorem 13.3 gives with

$$D := 2+(1+\varrho(x,y)^2/t)^{-1}$$

the bound

$$E_D(t,x)\leq \frac{C_n(a_i\delta)^{-n/2}}{\min(t,r_i^2)^{n/2}} \quad \text{where } \delta=\min(D-2,1)=(1+\varrho(x,y)^2/t)^{-1}.$$

Likewise we have

$$E_D(t,y)\leq \frac{C_n(a_j\delta)^{-n/2}}{\min(t,r_j^2)^{n/2}}.$$

and so the previous lemma gives

$$p(t,x,y)\leq \frac{C_n(1+\varrho(x,y)^2/t)^{n/2}e^{-\varrho(x,y)^2/(2Dt)-\lambda_{\min}(t-t_0)}}{\big(a_ia_j\min(t_0,r_i^2)\min(t_0,r_j^2)\big)^{n/4}}.$$

In view of

$$\frac{\varrho(x,y)^2}{4t}-\frac{\varrho(x,y)^2}{2Dt}=\frac{\delta\varrho(x,y)^2}{4Dt}<1,$$

we have

$$e^{-\varrho(x,y)^2/(2Dt)}=e^{-\varrho(x,y)^2/(2Dt)}e^{\frac{\varrho(x,y)^2}{4t}}e^{-\frac{\varrho(x,y)^2}{4t}}\leq ee^{-\frac{\varrho(x,y)^2}{4t}},$$

this completes the proof.

■

As a first application of the above estimate in combination with Remark 13.4 we obtain for all $x,y\in M$ the estimate

$$t\log p(t,x,y)\leq t\log(C(x)t^{-n/2})+t\log(1+\varrho(x,y)^2/2)^{n/2}-\varrho(x,y)^2/4,$$

and so

$$\limsup_{t\to 0+} 4t\log p(t,x,y)\leq -\varrho(x,y)^2,$$

which is one half of Varadhan's famous asymptotic formula [21]

$$\lim_{t\to 0+} 4t\log p(t,x,y)=-\varrho(x,y)^2,$$

The latter formula states that the heat kernel captures a Euclidean behaviour for small times, regardless of the geometry. A very noneuclidean behaviour may occur for large times, though.
Here comes the main result of this lecture course:

Theorem 13.8 (Grigor'yan 1994). *Assume M is geodesically complete. Then the following statements are equivalent:*
a) M satisfies a relative Faber-Krahn inequality, that is, there exist constants $b,n'>0$ such that for all $x\in M$, $r>0$ and all open relatively compact $U\subset B(x,r)$ one has

$$\lambda_{\min}(U)\geq \frac{b}{r^2}\left(\frac{\mu(x,r)}{\mu(U)}\right)^{2/n'} \tag{57}$$

b) M is volume doubling, that is, there exists a constant $C > 0$ such that for all $x \in M$, $r > 0$ one has

$$\mu(x, 2r) := \mu(B(x, 2r)) \le C\mu(x, r), \tag{58}$$

and *M satisfies the following Li-Yau upper heat kernel bound: there exists a constant $C' > 0$ such that for all $t > 0$, $x, y \in M$ one has*

$$p(t, x, y) \le C' \frac{(1 + \varrho(x, y)^2/t)^{n/2} e^{-\varrho(x,y)^2/(4t)}}{\sqrt{\mu(x, \sqrt{t})\mu(y, \sqrt{t})}}. \tag{59}$$

c) M is doubling and satisfies the following on-diagonal upper heat kernel bound: there exists a constant C"¿0 such that for all $t > 0, x \in M$ one has

$$p(t, x, x) \le \frac{C''}{\mu(x, \sqrt{t})}.$$

Proof: a) $\Rightarrow$ b): Let $x \in M$, $r > 0$ be arbitrary. Then for all open $U \subset B(x, r)$ we have

$$\lambda_{\min}(U) \ge a(x, r)\mu(U)^{-2/n'},$$

where

$$a(x, r) := br^{-2}\mu(x, r)^{2/n}.$$

Applying Theorem 13.7 to the family $B(x, \sqrt{t})$, $x \in M$, immediatly proves the heat kernel estimate. That relative Faber-Krahn implies doubling was an exercise.
b) $\Rightarrow$ c): trivial.
c) $\Rightarrow$ a): Let C be the doubling constant. Iterating the doubling inequality one gets that for all $0 < r \le R$, $x \in M$ one has

$$\mu(x, R)/\mu(x, r) \le C(R/r)^{n'}, \tag{60}$$

where $n' := \log_2(C)$. Indeed, $R \le 2^N r$, where N is the smallest natural number $\ge \log_2(R/r)$, and so $N \le \log_2(R/r) + 1$ and

$$\mu(x, R)/\mu(x, r) \le \mu(x, 2^N r)/\mu(x, r) \le C^N \le C^{1+\log_2(R/r)} = C(R/r)^{n'}.$$

Fix $x \in M$, $r > 0$. Then for all $t > 0$ one has

$$e^{-\lambda_{\min}(U)t} \le \mathrm{tr}(e^{-tH^U}) = \int_U p^U(t, y, y)d\mu(y) \le C'' \int_U \mu(y, \sqrt{t})^{-1}d\mu(y). \tag{61}$$

If $y \in U$, $t \le r^2$, then by (60)

$$\mu(x, r)/\mu(y, \sqrt{t}) \le (C(r/\sqrt{t})^{n'}\mu(y, 2r))/\mu(y, \sqrt{t}), \tag{62}$$

and so

$$e^{-\lambda_{\min}(U)t} \le C'' \int_U \mu(y, \sqrt{t})^{-1}d\mu(y) \le \frac{C''C\mu(U)}{\mu(x, r)} \left(\frac{r}{\sqrt{t}}\right)^{n'} \frac{C'''\mu(U)}{\mu(x, r)} \frac{r}{\sqrt{t}}^{n'}, \tag{63}$$

yielding

$$\lambda_{\min}(U) \geq -t^{-1} \log \left(\frac{C''' \mu(U)}{\mu(x,r)} \left(\frac{r}{\sqrt{t}} \right)^{n'} \right). \tag{64}$$

Case: $\mu(U) \leq (C'''e)^{-1}\mu(x,r)$. Define t by

$$(r/\sqrt{t})^{n'} = \frac{\mu(x,r))}{C'''e\mu(U)},$$

so

$$1/t = \frac{1}{r^2} \left(\frac{\mu(x,r))}{C'''e\mu(U)} \right)^{2/n'},$$

Then we have $t \leq r^2$ and so by (64),

$$\lambda_{\min}(U) \geq -t^{-1} \log \left(e^{-1} \right) = t^{-1} = \frac{1}{r^2} \left(\frac{\mu(x,r))}{C'''e\mu(U)} \right)^{2/n'}.$$

Proving relative Faber-Krahn in this case.
Case $\mu(U) > (C'''e)^{-1}\mu(x,r)$: using that balls are relatively compact, M is connected and noncompact one proves (exercise) that doubling implies reverse doubling: there exists n''', c (which only depend on the doubling constant C) such that for all $y \in M$, $0 < s \leq S$ one has

$$\frac{\mu(y,S)}{\mu(y,s)} \geq c(S/s)^{n'''}.$$

This reverse doubling implies that we can pick a constant $A > 1$, which only depends depends on n''', c, such that

$$\frac{\mu(x,Ar)}{\mu(x,r)} \geq C'''e.$$

Then we have $U \subset B(x,Ar)$ and $\mu(U) \leq (C'''e)^{-1}\mu(x,Ar)$ and the previous case applied to Ar implies the first inequality in

$$\lambda_{\min}(U) \geq \frac{1}{(Ar)^2} \left(\frac{\mu(x,Ar))}{C'''e\mu(U)} \right)^{2/n'} \geq \frac{1}{(Ar)^2} \left(\frac{\mu(x,r))}{C'''e\mu(U)} \right)^{2/n'},$$

completing the proof.

■

Remark 13.9. 1. The proof shows that the constants are related as follows:
a) implies b) with $n = n'$ and C', C depending only on n' and b.
b) implies c) with $C'' = C$.
c) implies a) with b depending only the doubling constant C and C'', and $n' = \log_2(C)$.
and b) implies a) with $n' = \log_2(C)$ with C chosen as in (58). Typically we will have $n = n' = m = \dim(M)$. Moreover, b only depends on C'

2. Using that for all $r, \epsilon > 0$ we can find a constant $C_{r,\epsilon} > 0$ such that for all $\zeta \geq 0$ one has

$$(1+\zeta)^r e^{-\zeta/4} \leq C_{r,\epsilon} e^{-\zeta/(4+\epsilon)}, \tag{65}$$

one immediately gets that b) is equivalent to the following condition: M is volume doubling and for all $\epsilon > 0$ there exists a constant $C_{\epsilon,n} > 0$ such that for all $t > 0$, $x, y \in M$ one has

$$p(t,x,y) \leq \frac{C_{\epsilon,n} e^{-\varrho(x,y)^2/((4+\epsilon)t)}}{\sqrt{\mu(x,\sqrt{t})\mu(y,\sqrt{t})}}.$$

3. As arguments from the proof entail, b) is also equivalent to the following condition: M is volume doubling and for all $\epsilon > 0$ there exists a constant $A_{\epsilon,n,C} > 0$, where C is the doubling constant, such that for all $t > 0$, $x, y \in M$ one has

$$p(t,x,y) \leq \frac{A_{\epsilon,n,C} e^{-\varrho(x,y)^2/((4+\epsilon)t)}}{\mu(x,\sqrt{t})}.$$

To see this, apply (60) to estimate

$$\mu(x,\sqrt{t})/\mu(y,\sqrt{t}) \leq \mu(y,\sqrt{t}+\varrho(x,y))/\mu(y,\sqrt{t}) \leq A_C(1+\varrho(x,y)^2/t)^{n''/2},$$

where $n'' = \log_2(C)$ and use again (65) with r depending on n and n''.

4. Note that the Theorem entails that certain heat kernel upper bounds (+ doubling) is stable under quasi-isometry[7]. This is very surprising, as the heat kernel depends on Δ which carries derivatives of the metric which can differ as dramatically as we wish for quasi-isometric metrics.

14. Riemann manifolds with nonnegative Ricci curvature

The aim of this section is to sketch a proof of the following result, whose doubling part is a consequence of a famous result by Bishop/Gromov and whose heat kernel part has been shown by Li/Yau:

Theorem 14.1. *Assume M is noncompact and geodesically complete with* $\mathrm{Ric} \geq 0$.
a) One has $\mu(x,2r) \leq 2^m \mu(x,r)$ for all $x \in M$, $r > 0$.
b) For all $\epsilon > 0$ there exists a constant $A_{\epsilon,m} > 0$, which only depends on m and ϵ, such that for all $t > 0$, $x, y \in M$ one has

$$p(t,x,y) \leq \frac{A_{\epsilon,n} e^{-\varrho(x,y)^2/((4+\epsilon)t)}}{\mu(x,\sqrt{t})}.$$

In principle, it is possible to show directly that M satisfies a relative Faber-Krahn inequality and appeal to part a) of the previous Theorem. Instead, I will sketch a proof of doubling and of the on-diagonal upper bound, so that the power of the previous theorem enfolds by producing an off-diagonal upper estimate for the heat kernel which contains a Gaussian damping factor.

[7] Two Riemann metrics g,h are called quasi-isometric, if $C_1 h \leq g \leq C_2 h$, which easily shows that the volume measures and the quadratic forms $\int |f|^2 d\mu$ are equivalent

Proof: I will only sketch a proof. Note that b) follows from the previous theorem and a) once we have shown

$$p(t,x,x) \leq C_m \mu(x,\sqrt{t})^{-1} \quad \text{for all } t>0,\, x\in M. \tag{66}$$

■

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