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Path Integrals on Manifolds with Boundary and their Asymptotic Expansions

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Abstract

It is "scientific folklore" coming from physical heuristics that solutions to the heat equation on a Riemannian manifold can be represented by a path integral. However, the problem with such path integrals is that they are notoriously ill-defined. One way to make them rigorous (which is often applied in physics) is finite-dimensional approximation, or time-slicing approximation: Given a fine partition of the time interval into small subintervals, one restricts the integration domain to paths that are geodesic on each subinterval of the partition. These finite-dimensional integrals are well-defined, and the (infinite-dimensional) path integral then is defined as the limit of these (suitably normalized) integrals, as the mesh of the partition tends to zero.
In this thesis, we show that indeed, solutions to the heat equation on a general compact Riemannian manifold with boundary are given by such time-slicing path integrals. Here we consider the heat equation for general Laplace type operators, acting on sections of a vector bundle. We also obtain similar results for the heat kernel, although in this case, one has to restrict to metrics satisfying a certain smoothness condition at the boundary.
One of the most important manipulations one would like to do with path integrals is taking their asymptotic expansions; in the case of the heat kernel, this is the short time asymptotic expansion. In order to use time-slicing approximation here, one needs the approximation to be uniform in the time parameter. We show that this is possible by giving strong error estimates.
Finally, we apply these results to obtain short time asymptotic expansions of the heat kernel also in degenerate cases (i.e. at the cut locus). Furthermore, our results allow to relate the asymptotic expansion of the heat kernel to a formal asymptotic expansion of the infinite-dimensional path integral, which gives relations between geometric quantities on the manifold and on the loop space. In particular, we show that the lowest order term in the asymptotic expansion of the heat kernel is essentially given by the Fredholm determinant of the Hessian of the energy functional. We also investigate how this relates to the zeta-regularized determinant of the Jacobi operator along minimizing geodesics.

Es ist "wissenschaftliche Folklore", abgeleitet von der physikalischen Anschauung, dass Lösungen der Wärmeleitungsgleichung auf einer riemannschen Mannigfaltigkeit als Pfadintegrale dargestellt werden können. Das Problem mit Pfadintegralen ist allerdings, dass schon deren Definition Mathematiker vor gewisse Probleme stellt. Eine Möglichkeit, Pfadintegrale rigoros zu definieren ist endlich-dimensionale Approximation, oder time-slicing-Approximation: Für eine gegebene Unterteilung des Zeitintervals in kleine Teilintervalle schränkt man den Integrationsbereich auf diejenigen Pfade ein, die auf jedem Teilintervall geodätisch sind. Diese endlichdimensionalen Integrale sind wohldefiniert, und man definiert das (unendlichdimensionale) Pfadintegral als den Limes dieser (passend normierten) Integrale, wenn die Feinheit der Unterteilung gegen Null geht.
In dieser Arbeit wird gezeigt, dass Lösungen der Wärmeleitungsgleichung auf einer allgemeinen riemannschen Mannigfaltigkeit tatsächlich durch eine solche endlichdimensionale Approximation gegeben sind. Hierbei betrachten wir die Wärmeleitungsgleichung für all-

gemeine Operatoren von Laplace-Typ, die auf Schnitten in Vektorbündeln wirken. Wir zeigen auch ähnliche Resultate für den Wärmekern, wobei wir uns allerdings auf Metriken einschränken müssen, die eine gewisse Glattheitsbedingung am Rand erfüllen.
Eine der wichtigsten Manipulationen, die man an Pfadintegralen vornehmen möchte, ist das Bilden ihrer asymptotischen Entwicklungen; in Falle des Wärmekerns ist dies die Kurzzeitasymptotik. Um die endlich-dimensionale Approximation hier nutzen zu können, ist es nötig, dass die Approximation uniform im Zeitparameter ist. Dies kann in der Tat erreicht werden; zu diesem Zweck geben wir starke Fehlerabschätzungen an.
Schließlich wenden wir diese Resultate an, um die Kurzzeitasymptotik des Wärmekerns (auch im degenerierten Fall, d.h. am Schittort) herzuleiten. Unsere Resultate machen es außerdem möglich, die asymptotische Entwicklung des Wärmekerns mit einer formalen asymptotischen Entwicklung der unendlichdimensionalen Pfadintegrale in Verbindung zu bringen. Auf diese Weise erhält man Beziehungen zwischen geometrischen Größen der zugrundeliegenden Mannigfaltigkeit und solchen des Pfadraumes. Insbesondere zeigen wir, dass der Term niedrigster Ordnung in der asymptotischen Entwicklung des Wärmekerns im Wesentlichen durch die Fredholm-Determinante der Hesseschen des Energie-Funktionals gegeben ist. Weiterhin untersuchen wir die Verbindung zur zeta-regularisierten Determinante des Jakobi-Operators entlang von minimierenden Geodätischen.

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Statement of Originality

This thesis contains no material which has been accepted for the award of any other degree or diploma at any other university or other tertiary institution and, to the best of my knowledge and belief, contains no material previously published or written by another person, except where due reference has been made in the text. I give consent to this copy of my thesis, when deposited in the University Library, being made available for loan and photocopying.

Potsdam, February 1, 2016
Matthias Ludewig

Für meine Eltern

Contents

Introduction

Consider a small particle moving on a manifold M according to Brownian motion. For example, this could be a pollen grain suspended in water, which undergoes random motion resulting from collisions with water molecules. Such a particle movement is governed by the heat equation [Ein05]: For example, the probability $\mathbb{P}_{x,A;t}$ that the particle is in some measurable set $A \subseteq M$ after time t if it started at a point $x \in M$ is given by $\mathbb{P}_{x,A;t} = (e^{-t\Delta}\chi_A)(x)$, where $e^{-t\Delta}$ is the heat semigroup on M and χ_A is the indicator function of the set A. On the other hand, physical heuristics state that the probability should be given by the path integral

$$\mathbb{P}_{x,A;t} = \frac{1}{Z}\int_{x\to A} \exp\left(-\frac{1}{4}\int_0^t \left|\dot{\gamma}(s)\right|^2 \mathrm{d}s\right)\mathcal{D}\gamma. \tag{I}$$

The domain of integration is here some space of continuous paths that travel from x to A in time t, $\mathcal{D}\gamma$ is a Lebesgue type volume measure on this path space and Z is a normalization constant (independent of A) that ensures $\mathbb{P}_{x,A;t} = 1$ in the case that $A = M$.
The reasoning behind this formula is that the particle has to take *some* path in order to move from x to A, so the probability is obtained by averaging over all such paths, weighted with their individual probability. To explain the integrand, notice that

$$E(\gamma) := \frac{1}{2}\int_0^t |\dot{\gamma}(s)|^2 \mathrm{d}s$$

is just the energy of the path (or rather classical action), so that the formula states that the particle is (exponentially) unlikely to take a path with large energy.
Of course, formula (I) does not make sense for a number of reasons: First it is unclear which space of paths to take (continuous paths? smooth paths? or something in between?), as it is well known that sample paths of Brownian paths are nowhere differentiable with probability one so that the energy is not defined. Either way, the space of paths would be infinite-dimensional and there are several non-existence theorems regarding Lebesgue type volume measures on infinite-dimensional spaces (see e.g. Thm. 17.2 in [Yam85]).

Despite these problems, there are several ways to make sense of the path integral (I): It is a classical observation that the expression

$$\mathrm{d}\mathbb{W} \overset{\text{formally}}{=} \frac{1}{Z}e^{-E(\gamma)/2}\mathcal{D}\gamma$$

can be rigorously defined as a measure $\mathbb{W}$ on path space, the *Wiener measure.* This connects path integration to the theory of stochastic processes. It allows to represent the solution to the heat equation with potential as a Wiener integral, which is the famous Feynman-Kac formula [Kac79].

In this thesis, we discuss another approach, the concept of *time-slicing approximation*, which was invented by Richard Feynman [Fey48] [FH65]. Here, the idea is to take a partition $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = t\}$ of the time interval and replace the infinite-dimensional space of paths by the space of paths which are a geodesic on each subinterval $[\tau_{j-1}, \tau_j]$. These spaces are finite-dimensional so that evaluating the integrals is unproblematic, and the value of the path integral is then defined as the limit of the values of these finite-dimensional integrals (suitably normalized) when the mesh $|\tau| = \max \Delta_j\tau$ goes to zero (here $\Delta_j\tau := \tau_j - \tau_{j-1}$).
This approach to define path integrals is often used in physics because of its explicit, hands down character and because it is easy to (at least formally) extend the formulas to "imaginary time" (i.e. replacing t by it), which is relevant in quantum mechanics (imaginary time was also used in Feynman's original treatment). However, a mathematical justification of this approach is not an easy matter in general: One first has to prove that the limit exists and secondly that it coincides with the heat equation result. While this is more or less trivial in $\mathbb{R}^n$, these results where only recently rigorously proved for Riemannian manifolds [AD99] [BP08].

In this thesis, we discuss two particular aspects of time-slicing approximation.

(1) We consider the case that the manifold M has a boundary. The observation is that in the case with boundary, one has to replace the spaces of piece-wise geodesics by spaces of piece-wise *reflected* geodesics, i.e. geodesics that reflect with the angle of reflection equal to the angle of incidence, when hitting the boundary. For the heat equation, we admit a certain class of boundary conditions (which we call *involutive boundary conditions*) that is particularly well-suited for path integration and includes standard Dirichlet and Neumann boundary conditions.

    This is only part of the story, however. While reflecting path spaces are suitable to approximate the heat operator, it turns out that there is an even better class of paths: Every Riemannian manifold with boundary has a natural orbifold structure (as we will explain), and it turns out that the right path spaces to integrate over are spaces of orbifold maps from intervals to our manifold with boundary, considered as an orbifold.

(2) Arguably one of the most important formal manipulations one would like to do with path integrals is forming their asymptotic expansions. This is of particular interest for the heat kernel: For the heat kernel p_t^Δ of the Laplace-Beltrami operator, one has the path integral formula

$$p_t^\Delta(x,y) \stackrel{\text{formally}}{=} (4\pi t)^{-n/2} \fint_{H_{xy}(M)} e^{-E(\gamma)/2t} \, \mathrm{d}^{H^1}\gamma,$$

where $H_{xy}(M)$ is the Hilbert manifold of finite-energy paths travelling from x to y in time one, equipped with its natural H^1 metric. Taking this formula seriously for the moment, one recognizes that the right hand side has the form of a Laplace integral: If there exists a unique minimizing geodesic γ_{xy} connecting x to y (i.e. the points are not in each other's cut locus), the function E has the unique non-degenerate minimum γ_{xy} with $E(\gamma_{xy}) = d(x,y)^2/2$ and the general theory of such integrals (see Chapter 3.1.1), formally applied to this infinite-dimensional situation, tells us that the integral has an asymptotic expansion of the form

$$(4\pi t)^{-n/2} \fint_{H_{xy}(M)} e^{-E(\gamma)/2t} \, \mathrm{d}^{H^1}\gamma \sim \frac{e^{-d(x,y)^2/4t}}{(4\pi t)^{n/2}} \sum_{j=0}^{\infty} t^j \frac{a_j}{\det\bigl(\nabla^2 E|_{\gamma_{xy}}\bigr)^{1/2}}, \tag{II}$$

where $\nabla^2 E|_{\gamma_{xy}}$ denotes the Hessian of the energy functional at the minimum, $a_0 = 1$ and the coefficients a_j, $j \geq 1$, depend on the jets of E at γ_{xy} and the geometry of $H_{xy}(M)$.
Now it is well known that the heat kernel $p_t^\Delta(x,y)$ has an asymptotic expansion for small t of *exactly the same form*,

$$p_t^\Delta(x,y) \sim \frac{e^{-d(x,y)^2/4t}}{(4\pi t)^{n/2}} \sum_{j=0}^{\infty} t^j \frac{\Phi_j(x,y)}{j!}.$$

Furthermore, it turns out that the Hessian of the energy indeed possesses a well-defined infinite-dimensional determinant on the Hilbert spaces $T_\gamma H_{xy}(M)$. Therefore, it is natural to ask whether the coefficients of the two asymptotic expansions in question − the asymptotic expansion of the heat kernel and the *formal* asymptotic expansion of the path integral − coincide, i.e. whether we have

$$\frac{a_j}{\det\bigl(\nabla^2 E|_{\gamma_{xy}}\bigr)^{1/2}} = \frac{\Phi_j(x,y)}{j!}.$$

In this thesis, we prove that this is true at least for the lowest order term, using time-slicing approximation of the heat kernel.

Of course, the theory of Brownian motion on manifolds is well understood and provides powerful tools for differential geometry and global analysis, so one could ask why one is interested in time-slicing approximation of path integrals in the first place. One answer we can give at this point is that while the asymptotic expansion of Wiener integrals is certainly well known (see e.g. [Aro88] or [Wat87]), it seems that the results obtained this way are less geometric, due to the fact that the domain of integration is not $H_{xy}(M)$ but the space of *all* continuous paths connecting x and y, and that the energy functional is "hidden inside the measure". Nevertheless, it would be interesting to see if asymptotic expansions of Wiener functionals can be cast in more geometric terms, involving the manifold $H_{xy}(M)$ (which is something like the "Cameron-Martin manifold" corresponding to the Wiener measure[1]).

[1] The Cameron-Martin space of a Gaussian measure on a Banach space E is a certain Hilbert space H which is continuously embedded into H, see [Gro70] for the notion of an abstract Wiener space. This notion, however, does not exist to the authors knowledge in the case that E is a *manifold* modelled on a Banach space.

Main Results

The following result was previously proved in [BP08]. Given a self-adjoint Laplace type operator $L = \nabla^*\nabla + V$, acting on sections u of a vector bundle $\mathcal{V}$ over a closed n-dimensional Riemannian manifold M (here, ∇ is a metric connection and V a symmetric endomorphism field), one has the formula

$$(e^{-tL}u)(x) = \lim_{|\tau|\to 0} (4\pi)^{-n/2} \fint_{H_{x;\tau}(M)} e^{-E(\gamma)/2}\, \mathcal{P}(\gamma)^{-1} u\big(\gamma(t)\big) \mathrm{d}^{\Sigma\text{-}H^1}\gamma, \tag{III}$$

where $H_{x;\tau}(M)$ is the space of continuous paths γ starting at x such that $\gamma|_{[\tau_{j-1},\tau_j]}$ is a geodesic for each j, the slash over the integral sign denotes division by $(4\pi)^{-\dim(H_{x;\tau}(M))/2}$, and $\mathcal{P}(\gamma) \in \mathrm{Hom}(\mathcal{V}_{\gamma(0)}, \mathcal{V}_{\gamma(t)})$ is a so-called *path-ordered exponential*, which is the solution of an ordinary differential equation along γ depending on the connection ∇ and the endomorphism field V. Here, the manifold $H_{x;\tau}(M)$ carries a certain discretized H^1 Sobolev metric and one integrates with respect to the Riemannian volume measure. In particular, this generalizes formula (I) from above, which is the special case $L = \Delta$ (so that $\mathcal{P}(\gamma) \equiv 1$), the Laplace-Beltrami operator, and $u = \chi_A$.
Formula (III) can be extended to the case that M is a compact manifold with smooth boundary, and L is endowed with what we call *involutive boundary conditions* in this thesis. Involutive boundary conditions arise as follows: Given a symmetric parallel endomorphism field $B \in \mathrm{End}(\mathcal{V}|_{\partial M})$ with $B^2 = \mathrm{id}$, this induces a splitting $\mathcal{V}|_{\partial M} = \mathcal{W}^+ \oplus \mathcal{W}^-$ into the plus and minus one eigenspaces of B. We then require Neumann boundary conditions on $\mathcal{W}^+$ and Dirichlet boundary conditions on $\mathcal{W}^-$. This includes the usual Dirichlet and Neumann boundary conditions as well as standard boundary conditions on vector fields and differential forms. One has the following result (see Thm. 1.3.14).

Theorem. *Let L be a self-adjoint Laplace type operator endowed with involutive boundary conditions B, acting on sections of a metric vector bundle $\mathcal{V}$ over a compact Riemannian manifold with boundary M. Then we have the following path integral formula*

$$(e^{-tL}u)(x) = \lim_{|\tau|\to 0} \fint_{H^{\mathrm{refl}}_{x;\tau}(M)} e^{-E(\gamma)/2}\, \mathcal{P}_B(\gamma)^{-1} u\big(\gamma(t)\big) \mathrm{d}^{\Sigma\text{-}H^1}\gamma$$

for the solution operator to the corresponding heat equation, where the limit goes over any sequence of partitions, the mesh of which tends to zero. Here, u is in any of the spaces $C^0(M, \mathcal{V})$ or $L^p(M, \mathcal{V})$, $1 \leq p < \infty$ (with convergence in the respective space) and the slash over the integral sign denotes divison by $(4\pi)^{\dim(H^{\mathrm{refl}}_{x;\tau}(M))/2}$.

In the theorem, $H^{\mathrm{refl}}_{x;\tau}(M)$ denotes the space of *reflected* piecewise geodesics, i.e. the space of continuous paths that are piecewise geodesics as long as they are in the interior of M and reflect with the angle of reflection equal to the angle of incidence when hitting the boundary. Furthermore, the path-ordered exponential $\mathcal{P}(\gamma)$ from (III) has to be replaced by a certain *B-path-ordered exponential* $\mathcal{P}_B(\gamma)$, which also depends on the boundary operator B.

Similar to the formulas above, we show (Thm. 2.2.7) that for the heat kernel p^L_t of the Laplace type operator L, one has

$$p^L_t(x, y) = \lim_{|\tau|\to 0} (4\pi t)^{-n/2} \fint_{H_{xy;\tau}(M)} e^{-E(\gamma)/2}\, \mathcal{P}(\gamma)^{-1} \mathrm{d}^{\Sigma\text{-}H^1}\gamma,$$

pointwise for each $x, y \in M$ and $t > 0$, where $H_{xy;\tau}(M)$ is the space of piece-wise geodesics connecting x to y in time t, which again carries a certain discretized version of the H^1 volume measure. Similar to the above, the slash over the integral sign in the formula denotes division by the number $(4\pi)^{\dim(H_{xy;\tau}(M))/2}$.
In this approximation however, one has no control over the uniformity of the approximation, which is needed to connect the asymptotic expansion of the heat kernel to the asymptotic expansion of the path integral. Therefore, we also prove the following result, which involves a precise error estimate (see Thm. 2.2.11).

Theorem. *Let L be a self-adjoint Laplace type operator, acting on sections of a metric vector bundle $\mathcal{V}$ over a closed n-dimensional Riemannian manifold M. Then for any $T > 0$ and any $\nu \in \mathbb{N}_0$, there exist constants $C, \delta > 0$ such that*

$$\left| p_t^L(x,y) - (4\pi t)^{-n/2} \fint_{H_{xy;\tau}(M)} e^{-E(\gamma)/2t} \Upsilon_{\tau,\nu}(t,\gamma)\, \mathrm{d}\gamma \right| \leq C t^{1+\nu} |\tau|^{\nu} p_t^{\Delta}(x,y)$$

for all $x, y \in M$, $t \leq T$ and partitions τ of the interval $[0,1]$ with $|\tau| \leq \delta$. Here the slash over the integral sign denotes divison by $(4\pi t)^{\dim(H_{xy;\tau}(M))/2}$.

In the theorem, the $\Upsilon_{\tau,\nu}$ are certain functions which are smooth in γ and depend polynomially on t. They depend on the geometry of M and the Laplace type operator and should be viewed to correct the error that one made by replacing $H_{xy}(M)$ by its finite-dimensional approximations. Notice in particular that the heat kernel of the Laplace-Beltrami operator $p_t^{\Delta}(x,y)$ is present on the right hand side. Since $p_t^L(x,y)$ decays exponentially in t away from the diagonal as $t \to 0$, this is a strong result, which allows to obtain precise statements on heat kernel asymptotics, even for distant points.

This allows to compare asymptotic expansions of the path integral with the asymptotic expansion of the heat kernel. We already mentioned above, that if x and y are close enough, then the path integral has a formal Laplace expansion of the form (II). More generally, if x and y are in each other's cut locus and the set $\Gamma_{xy}^{\min} \subset H_{xy}(M)$ of minimal geodesics connecting the two is a non-degenerate submanifold of dimension k, a generalized Laplace method asserts that

$$(4\pi t)^{-n/2} \fint_{H_{xy}(M)} e^{-E(\gamma)/2t}\, \mathrm{d}^{H^1}\gamma \;\sim\; \frac{e^{-d(x,y)^2/4t}}{(4\pi t)^{n/2+k/2}} \sum_{j=0}^{\infty} t^j \int_{\Gamma_{xy}^{\min}} \frac{a_j(\gamma)}{\det\big(\nabla^2 E|_{N_\gamma \Gamma_{xy}^{\min}}\big)^{1/2}}\, \mathrm{d}^{H^1}\gamma,$$

involving the determinant of the Hessian, restricted to the normal space of $\Gamma_{xy}^{\min}$. The result is now that this indeed describes the asymptotic behavior of the heat kernel (see Thm. 3.2.8).

Theorem (H^1 picture). *Let p_t^L be the heat kernel of a self-adjoint Laplace type operator L, acting on sections of a metric vector bundle $\mathcal{V}$ over a compact n-dimensional Riemannian manifold M. For $x, y \in M$, suppose that the set $\Gamma_{xy}^{\min}$ of minimal geodesics is a k-dimensional non-degenerate submanifold of $H_{xy}(M)$. Then we have*

$$p_t^L(x,y) \;\sim\; \frac{e^{-d(x,y)^2/4t}}{(4\pi t)^{n/2+k/2}} \int_{\Gamma_{xy}^{\min}} \frac{[\gamma\|_0^1]^{-1}}{\det\big(\nabla^2 E|_{N_\gamma \Gamma_{xy}^{\min}}\big)^{1/2}}\, \mathrm{d}^{H^1}\gamma,$$

where the determinant is an infinite-dimensional determinant on the Hilbert subspace $N_\gamma \Gamma_{xy}^{\min} \subseteq T_\gamma H_{xy}(M)$*,* $[\gamma\|_0^1]$ *denotes the parallel transport along* γ *and* $\Gamma_{xy}^{\min}$ *carries the* H^1 *metric* (1.2.5)*. Here the asymptotic relation means that the quotient of the two terms tends to one as* $t \to 0$*.*

In physics, one often uses zeta determinants instead of Hilbert space determinants to formally evaluate path integrals. This makes no reference to the H^1 regularity of paths, because the zeta determinant is defined for unbounded operators on L^2. It turns out that there is an L^2 version of the theorem above, involving the zeta determinant of the Jacobi operator (see Thm. 3.2.25).

Theorem (L^2 picture). *Let* p_t^L *be the heat kernel of a self-adjoint Laplace type operator* L*, acting on sections of a metric vector bundle* $\mathcal{V}$ *over a compact* n*-dimensional Riemannian manifold* M*. For* $x, y \in M$*, suppose that the set* $\Gamma_{xy}^{\min}$ *of minimal geodesics is a* k*-dimensional non-degenerate submanifold of* $H_{xy}(M)$*. Then we have*

$$p_t^L(x,y) \;\sim\; \frac{e^{-d(x,y)^2/4t}}{(4\pi t)^{n/2+k/2}} \int_{\Gamma_{xy}^{\min}} \frac{2^{n/2}[\gamma\|_0^1]^{-1}}{\det_\zeta'\big(-\nabla_s^2 + \mathcal{R}_\gamma\big)^{1/2}} \,\mathrm{d}^{L^2}\gamma,$$

involving the zeta determinant of the Jacobi operator

$$-\nabla_s^2 + \mathcal{R}_\gamma = -\nabla_s^2 + R(\dot\gamma(s), -)\dot\gamma(s).$$

Here $\Gamma_{xy}^{\min}$ *carries the* L^2 *metric 1.2.11.*

We see that there is an "H^1 picture" on such path integrals, where one chooses the path space such that the relevant determinant exists as an ordinary Hilbert space determinant (the H^1 space), and an "L^2 picture", where one has to regularize.

The proof of the approximation theorem for the heat kernel relies heavily on the near-diagonal short time asymptotics of the heat kernel. For manifolds with boundary, such heat-kernel asymptotics are much more complicated (see e.g. [Mel93, Chapter 7]). Therefore, we restrict to the following smoothness condition: Construct the double $\overline{M}$ of the manifold M, by glueing two copies of M together at the common boundary (this is then a closed manifold). The metric on M induces a natural $\mathbb{Z}_2$-invariant Riemannian metric on $\overline{M}$. The condition now is that this metric be smooth also at ∂M. In this case, the earlier results can be applied to the closed manifold $\overline{M}$.
In particular, we have $M = \overline{M}/\mathbb{Z}_2$, which gives M an orbifold structure in a natural way. We claim that the right thing to do is therefore to consider spaces of *orbifold paths*. Particularly interesting here is the approximation result for the heat trace. In the closed case, the heat trace can be formally expressed as an integral over the loop space of M; we show that in the boundary case, one has to integrate over the space of orbifold loops, i.e. the orbifold of maps from S^1 to the orbifold $M = \overline{M}/\mathbb{Z}_2$. One obtains that the trace $\operatorname{Tr} e^{-tL}$ can be approximated (up to any fixed order in t) by path integrals over finite dimensional approximations $L_\tau^{\mathrm{orb}}(M)$ of the orbifold loop space (see Thm. 2.2.13).

Theorem. *Let* L *be a self-adjoint Laplace type operator with involutive boundary conditions* B*, acting on sections of a metric vector bundle* $\mathcal{V}$ *over a compact Riemannian* *manifold with boundary M. Let e^{-tL} be the solution operator to the corresponding heat equation. Suppose that the smoothness Assumption 2.3.7 is satisfied. Then*

$$\operatorname{Tr} e^{-tL} = \lim_{|\tau|\to 0} \fint_{L_\tau^{\mathrm{orb}}(M)} e^{-E(\gamma)/2} \operatorname{tr} \mathcal{P}_B^{-1}(\gamma)\, \mathrm{d}^{\Sigma\text{-}H^1}\gamma.$$

for any $t > 0$, where the limit goes over any sequence of partitions, the mesh of which tends to zero. In the formula, the slash over the integral sign denotes division by $(4\pi)^{\dim(L_\tau(M))/2}$.

It turns out that the space of orbifold loops is *not* only the of loops in the manifold $\overline{M}$ modulo the $\mathbb{Z}_2$ action, but also contains paths that run from a point $x \in \overline{M}$ to the corresponding point $-x$ in the other half. Therefore, the space $L_\tau^{\mathrm{orb}}(M)$ decomposes into two components: The orbifold $L_\tau(M)/\mathbb{Z}_2$ of piecewise geodesic loops in $\overline{M}$ and the orbifold of paths in $\overline{M}$ that travel from points x to points $-x$. The set of constant loops $\Gamma_{\mathrm{c}} = E^{-1}(0)$ therefore also consists of two components: one isomorphic to M and one isomorphic to ∂M (as for a constant path γ with $\gamma(0) = x$ and $\gamma(1) = -x$, one necessarily has $x \in \partial M$, the fixed point set of the action). Since M is n-dimensional and ∂M is $(n-1)$-dimensional, we obtain from the Laplace method that the heat trace has an asymptotic expansion of the form

$$\operatorname{Tr} e^{-tL} \;\sim\; (4\pi t)^{-n/2} \int_M a_j(x)\,\mathrm{d}x + (4\pi t)^{-(n-1)/2} \int_{\partial M} b_j(x)\,\mathrm{d}x,$$

so one recovers the heat kernel asymptotics for a manifold with boundary in a natural way. Moreover, the coefficients a_j are given as the coefficients of a Laplace expansion on the finite-dimensional approximations of the loop space. It is an interesting task to express these as geometric quantities on the infinite-dimensional loop space.

Chapter 1

The Heat Operator as a Path Integral

In this chapter, we show how to approximate solutions of the heat equation corresponding to a Laplace type operator L on a compact manifold with boundary by finite-dimensional path integrals, i.e. we prove the formula

$$u(t,x) = \lim_{|\tau|\to 0} \fint_{H^{\mathrm{refl}}_{x;\tau}(M)} e^{-E(\gamma)/2} \mathcal{P}_B(\gamma) u_0\big(\gamma(t)\big)\, \mathrm{d}\gamma, \tag{1.0.1}$$

for solutions $u(t,x)$ to a vector-valued heat equation with initial condition u_0, where $H^{\mathrm{refl}}_{x;\tau}(M)$ are finite-dimensional path spaces of piece-wise reflecting geodesics (see Section 1.2.1 and Section 1.3.1) and $\mathcal{P}_B(\gamma)$ is the so-called path-ordered exponential determined by L and the boundary condition B (see Def. 1.3.10). Finally, the slash in the integral sign denotes division by $(4\pi)^{\dim(H^{\mathrm{refl}}_{x;\tau}(M))/2}$. Such a normalization constant will be present in all path integral formulas and is necessary in order that the mesh-limit is finite.

The chapter is organized as follows. In Section 1.1, we review the theory of Laplace type operators acting on sections of vector bundles over manifolds with boundary, and the corresponding heat equation. In particular, we introduce the class of boundary conditions we will consider. In Section 1.2, we first consider the case of a closed manifold, which gives us the opportunity to review the time-slicing approximation results that have been obtained so far. In Section 1.3, we then introduce the relevant path spaces and prove the formula (1.0.1).

1.1 The Heat Equation

In this section, we introduce the class of boundary conditions we will allow in this thesis, which we call *involutive boundary conditions*. To fix notation, we repeat standard material concerning Laplace type operators and the heat equation. More detailed expositions of these topics can be found in many places, e.g. [Gil95], [Roe98], [BGV04] or [Nik07].

In the next subsection, we introduce Brownian motion on closed Riemannian manifolds to discuss first path integral formulas. The material there is also very well known and may be found in [BP10], [Hsu02], [HT94], [Øks07], [Dri04], [Tay11] or [Eme89].

1.1.1 Laplace Type Operators

Let M be a Riemannian manifold of dimension n, possibly with boundary, and let $\mathcal{V}$ be a metric vector bundle over M, i.e. each fiber of $\mathcal{V}$ carries a positive definite symmetric bilinear form (or a Hermitean form if $\mathcal{V}$ is a complex bundle) that varies smoothly between the fibers. Smooth sections of $\mathcal{V}$ will be denoted by $C^\infty(M, \mathcal{V})$, while sections of L^2 regularity will be denoted by $L^2(M, \mathcal{V})$. The L^2 scalar product is defined by

$$(u, v)_{L^2} := \int_M \langle u(x), v(x)\rangle \, \mathrm{d}x,$$

where $\langle -,- \rangle$ denotes the fiber metric of $\mathcal{V}$ and we integrate with respect to the Riemannian volume measure.

If $\mathcal{W}$ is another metric vector bundle, a (linear) *differential operator* of order k turning sections of $\mathcal{V}$ into sections of $\mathcal{W}$ is a linear operator P from $C^\infty(M,\mathcal{V})$ to $C^\infty(M, \mathcal{W})$ that is given by

$$Pu(x) = \sum_{|\alpha|\leq k} P_\alpha(x) \frac{\partial^{|\alpha|}}{\partial x^\alpha} u(x)$$

in local charts, where $P_\alpha(x) \in \mathrm{Hom}(\mathcal{V}_x, \mathcal{W}_x)$. Because the manifold is Riemannian and the bundles carry a fiber metric, one can define the *formal adjoint* of such an operator P. This is the differential operator P^* that turns sections of $\mathcal{W}$ into sections of $\mathcal{V}$ such that

$$(Pu, v)_{L^2} = (u, P^* v)_{L^2}$$

for all $u \in C_c^\infty(M \setminus \partial M, \mathcal{V})$ and $v \in C_c^\infty(M \setminus \partial M, \mathcal{W})$, i.e. all compactly supported sections with support in the interior of M. One can show that this requirement indeed defines a unique differential operator P^* (compare Def. 2.6 in [BGV04]). We call the operator P *formally self-adjoint* if $P = P^*$. In terminology from functional analysis, this means in particular that P is symmetric as an unbounded operator on $L^2(M, \mathcal{V})$ with domain $C_c^\infty(M \setminus \partial M, \mathcal{V})$ (although on this domain, it will never be self-adjoint).

Definition 1.1.1 (Laplace Type Operators). [BGV04, Def. 2.2] A second-order differential operator L acting on sections of $\mathcal{V}$ is called *Laplace type operator*, if its principal symbol is given by the metric, that is, L has the form

$$L = -g^{ij}(x) \frac{\partial^2}{\partial x^i x^j} + \text{lower order terms}$$

in local coordinates, where g^{ij} is the inverse of the metric tensor in the coordinates.

Notice that we use the "geometric" convention for Laplace type operators that differs from the analytic convention by a sign.

Lemma 1.1.2. [BGV04, Prop. 2.5] *Let L be a formally self-adjoint Laplace type operator acting on sections of a vector bundle $\mathcal{V}$ over M. Then there exists a unique metric connection ∇ on $\mathcal{V}$ and a unique symmetric endomorphism field V of $\mathcal{V}$ such that*

$$L = \nabla^* \nabla + V.$$

We say that ∇ and V are the connection and endomorphism field determined by L.

Here, ∇^* is the formal adjoint of the operator ∇ that turns sections of $T^*M \otimes \mathcal{V}$ into sections of the bundle $\mathcal{V}$ (where $T^*M \otimes \mathcal{V}$ carries the tensor product metric).

Example 1.1.3. The following are standard examples for Laplace type operators.

(1) On functions (i.e. $\mathcal{V} = \underline{\mathbb{R}}$, the trivial real line bundle), we have the Laplace-Beltrami operator $\Delta = \delta d = -\operatorname{div}\operatorname{grad} = -\operatorname{tr}(\nabla^2)$, where ∇ is the Levi-Civita connection.

(2) On the bundle of differential forms $\mathcal{V} = \Lambda^\bullet T^*M$, one has the Hodge-Laplacian $L = \delta d + d\delta$. By the Weizenböck formula [BGV04, (3.16) on p. 130],

$$\delta d + d\delta = \nabla^*\nabla + \mathscr{R},$$

where ∇ is the Levi-Civita connection on forms and $\mathscr{R}$ is some endomorphism depending linearly on the curvature. On one-forms, $\mathscr{R} = \mathrm{Ric}^*$, the dual of the Ricci endomorphism on TM.

(3) If M is spin, one has the spinor bundle $\$M$, on which acts the *Dirac operator*, a first-order operator $D\!\!\!/$ with the property that $D\!\!\!/^2$ is a Laplace type operator. In this case,

$$D\!\!\!/^2 = \nabla^*\nabla + \frac{1}{4}\mathrm{scal},$$

by Lichnerowicz' formula [BGV04, Thm. 3.52]

1.1.2 Involutive Boundary Conditions and the Heat Equation

Let L be a formally self-adjoint Laplace type operator, acting on sections of a metric vector bundle $\mathcal{V}$ over a compact n-dimensional Riemannian manifold M, possibly with boundary. In this thesis, we are interested in the heat equation

$$(\partial_t + L)\, u(t,x) = 0 \tag{1.1.1}$$

for time-dependent sections of $\mathcal{V}$. In case that M has a boundary, one has to require boundary conditions to make the heat equation well-posed, where well-posed means that we have to find a subspace $\mathrm{dom}(L) \subset L^2(M,\mathcal{V})$ on which L generates a strongly continuous heat semigroup e^{-tL}. In particular, this will be the case if L is self-adjoint on $\mathrm{dom}(L)$ as an unbounded operator on $L^2(M,\mathcal{V})$. From the wide class of possible boundary conditions, we restrict ourselves to the class of boundary conditions, which behave particularly well when considering path integrals.

Definition 1.1.4 (Involutive Boundary Conditions). Given a formally self-adjoint Laplace type operator L, acting on sections of a metric vector bundle $\mathcal{V}$ over a Riemannian manifold with boundary M, a symmetric endomorphism field $B \in C^\infty(\partial M, \mathrm{End}(\mathcal{V}|_{\partial M}))$ is called an *involutive boundary operator for* L if $B^2 = \mathrm{id}$ and if B is parallel with respect to the connection determined by $L = \nabla^*\nabla + V$. To such a boundary operator B, there corresponds a splitting

$$\mathcal{V}|_{\partial M} = \mathcal{W}^+ \oplus \mathcal{W}^- \tag{1.1.2}$$

into the eigenspaces of the eigenvalues ± 1 (notice that only these two eigenvalues are possible since $B^2 = \mathrm{id}$). A section $u \in C^\infty(M, \mathcal{V})$ *satisfies the boundary condition* defined by B if

$$\nabla_{\mathbf{n}} u|_{\partial M} \in C^\infty(\partial M, \mathcal{W}^-), \qquad u|_{\partial M} \in C^\infty(\partial M, \mathcal{W}^+), \tag{1.1.3}$$

where $\mathbf{n} \in C^\infty(\partial M, N\partial M)$ denotes the interior normal vector to the boundary.

Notation 1.1.5. For a boundary operator B, let $C_B^\infty(M, \mathcal{V})$ be the space of smooth sections of $\mathcal{V}$ that satisfy the boundary condition and let $H_B^2(M, \mathcal{V}) := \overline{C_B^\infty(M, \mathcal{V})} \subseteq H^2(M, \mathcal{V})$ be its closure with respect to the H^2 norm.

The class of involutive boundary conditions is closely related to the class of *mixed boundary conditions*, as defined e.g. in [Gil04, Section 1.5.3]. However, mixed boundary conditions are slightly more general, therefore we stick to the term "involutive boundary condition" in this thesis (see e.g. Chapter II of [Gre71], Section 1.11.2 in [Gil95] or Sections 1.4-1.6 in [Gil04] for a much more general discussion).
Involutive boundary conditions ensure that the operator L as an unbounded operator on $L^2(M, \mathcal{V})$ is essentially self-adjoint on $C_B^\infty(M, \mathcal{V})$ and self-adjoint on $H_B^2(M, \mathcal{V})$. We say that L *is endowed with involutive boundary conditions* if L has the latter domain and B is an involutive boundary operator.
When L is endowed with an involutive boundary condition, it has discrete spectrum $\lambda_1 \leq \lambda_2 \leq \cdots \to \infty$, where the eigenvalues have finite multiplicity, and the corresponding eigenfunctions ϕ_j are contained in $C_B^\infty(M, \mathcal{V})$. In particular, L generates a strongly continuous semigroup e^{-tL}, defined by spectral calculus, with integral kernel

$$p_t^L(x, y) = \sum_{j=1}^\infty e^{-t\lambda_j} \phi_j(x) \otimes \phi_j(y)^*, \tag{1.1.4}$$

which can be shown to be smooth (using that the eigenvalues increase suffiently fast by Weyl's law) and which satisfies the boundary condition in each variable. For any initial condition $u_0 \in L^2(M, \mathcal{V})$, the function

$$u(t, x) := (e^{-tL} u_0)(x)$$

satisfies the heat equation (1.1.1) with initial condition $u(0, x) = u_0(x)$.

We now give a couple of examples for involutive boundary conditions.

Example 1.1.6 (Dirichlet and Neumann). For any Laplace type operator, there are the *Dirichlet* boundary conditions $u|_{\partial M} = 0$, associated to the boundary operator $B = -\mathrm{id}$, and the *Neumann* boundary conditions $\nabla_{\mathbf{n}} u|_{\partial M} = 0$ associated to the boundary operator $B = \mathrm{id}$. Here id denotes the identity endomorphism field of $\mathcal{V}|_{\partial M}$, which is parallel with respect to any connection on $\mathcal{V}$ (or more precisely: with respect to any connection on the bundle $\mathrm{End}(\mathcal{V})$ induced from a connection on $\mathcal{V}$). Both are therefore involutive boundary conditions.

Non-Example 1.1.7 (Robin Boundary Conditions). Given a metric connection ∇, the *generalized Neumann* boundary conditions or *Robin* boundary conditions

$$\nabla_{\mathbf{n}} u|_{\partial M} + A u|_{\partial M} = 0. \tag{1.1.5}$$

for an endomorphism field $A \in C^\infty(\partial M, \mathrm{End}(\mathcal{V}))$ are *not* involutive boundary conditions for operators of the form $L = \nabla^*\nabla + V$, unless $A \equiv 0$.

Example 1.1.8 (Boundary Conditions on Differential Forms). Let $\mathcal{V} = \Lambda^k T^*M$ be the bundle of k-forms. Any $\omega \in \Lambda^k T^*M$ can be decomposed at the boundary as

$$\omega = \omega_0 + dr \wedge \omega_1, \qquad \omega_0 \in \Lambda^k T^*\partial M, \;\; \omega_1 \in \Lambda^{k-1}T^*\partial M,$$

where $dr := \mathbf{n}^\flat$. Hence for the exterior products of the cotangent bundle, we have the orthogonal splitting

$$\Lambda^k T^*M|_{\partial M} \cong \Lambda^k T^*\partial M \oplus dr \wedge \Lambda^{k-1}T^*\partial M.$$

Defining B to be equal to 1 on one of these factors and equal to -1 on the other will induce involutive boundary conditions for Laplace type operators $L = \nabla^*\nabla + V$ on $\mathcal{V}$, where ∇ is any metric connection on $\mathcal{V}$. Specifically, setting

$$\mathcal{W}^+ := \Lambda^k T^*\partial M, \qquad \mathcal{W}^- := dr \wedge \Lambda^{k-1}T^*\partial M \tag{1.1.6}$$

gives the so-called *absolute boundary conditions.* Setting

$$\mathcal{W}^+ := dr \wedge \Lambda^{k-1}T^*\partial M, \qquad \mathcal{W}^- := \Lambda^k T^*\partial M \tag{1.1.7}$$

gives *relative boundary conditions.*

The examples show that the class of involutive boundary conditions includes most standard types of boundary conditions. Let us make a warning here that "involutive" is not standard terminology, but such a class of boundary conditions doesn't seem to have a name in the literature yet.

1.1.3 Brownian Motion and the Wiener Measure

Let M be a closed Riemannian manifold or $\mathbb{R}^n$.

Definition 1.1.9 (Stochastic Processes). An M-valued *stochastic process* is a family X_s, $s \in I$ of random variables with values in M, defined on a probability space (Ω, Σ, μ), where I is some open or closed, finite or infinite subinterval of $\mathbb{R}$.

Any M-valued stochastic process X_s, $s \in I$ induces a Borel probability measure $\mathbb{W}^X$ on M^I (carrying the product topology), namely

$$\mathbb{W}^X\big(A \in \mathscr{B}(M^I)\big) = \mu\big(\{\gamma \in M^I \mid X_\bullet(\gamma) \in A\}\big), \tag{1.1.8}$$

where $\mathscr{B}(M^I)$ denotes the Borel-sigma-algebra of M^I. This measure is called the *law* of the process X_s (Here, for a fixed $\gamma \in \Omega$, one can consider the function $s \mapsto X_s(\gamma)$, which is an element of M^I. Hence it makes sense to ask whether it is also in $A \subset M^I$). The notion of the law of a process gives rise to a natural equivalence relation on the class of M-valued stochastic processes:

Definition 1.1.10 (Versions). Two stochastic processes X_s, Y_s are said to be *versions* of each other, if their laws coincide.

Conversely, given a Borel probability measure $\mathbb{P}$ on M^I, one can define a stochastic process

$$X_s(\gamma) := \gamma(s) \tag{1.1.9}$$

on the probability space $(M^I, \mathscr{B}(M^I), \mathbb{P})$ (notice that the definition (1.1.9) is independent of the choice of $\mathbb{P}$). Clearly, the law of such a process X_s is just $\mathbb{P}$ again; furthermore, it is obvious that if we start with any process Y_s and then define X_s by (1.1.9), then X_s is a version of Y_s.

On M, there is a canonical stochastic process, called the *Brownian motion*. The following construction can be found in Section 11.1 of [Tay11]: Let $p_t^\Delta(x,y)$ be the heat kernel of the Laplace-Beltrami operator, as in (1.1.4). Then for any point $x \in M$, there is a stochastic process (X_s^x) on the interval $I = [0, \infty)$, the *Brownian motion* starting at x. It satisfies (using the convention $x_0 := x$)

$$\mathbb{E}\big[f(X^x_{\tau_1}, \dots, X^x_{\tau_M})\big] = \int_M \cdots \int_M f(x_1, \dots, x_N) \prod_{j=1}^N p^\Delta_{\tau_j - \tau_{j-1}}(x_{j-1}, x_j)\, \mathrm{d}x_1 \cdots \mathrm{d}x_N, \tag{1.1.10}$$

for any partition $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N\}$ and any measurable function f on $M \times \cdots \times M$, the N-fold product of M. In fact, it turns out that the process X_s^x is uniquely determined by this property, in the sense that any other process Y_s with the same property is a version of X_s^x. To see that the law of X_s^x is uniquely determined by the property (1.1.10), notice that the space $M^{[0,\infty)}$ is compact by Tychonoff's theorem, and by the Stone-Weierstraß theorem, functions of the form

$$F(\gamma) := f\big(\gamma(\tau_1), \dots, \gamma(\tau_N)\big)$$

for partitions τ and functions $f \in C(M \times \cdots \times M)$ are dense in $C(M^{[0,\infty)})$. Hence the right-hand side of (1.1.10) defines a continuous functional on $C(M^{[0,\infty)})$, which is the same as a measure on $M^{[0,\infty)}$ by the Markhov-Kakutani-Riesz representation theorem.

Using Kolmogoroff-Chentsov continuity theorem (see e.g. [Kal02, Thm. 3.23] or Thm. 2.17 in [BP11]), one can show that there is a continuous version of Brownian motion, i.e. a Brownian motion such that for each $\gamma \in \Omega$, the map $s \mapsto X_s^x(\gamma)$ is a continuous path in M (see e.g. [BP11, Thm. 2.5]). Therefore, we will henceforth only consider continuous versions of Brownian motion. Given a continuous version of Brownian motion defined on some probability space (Ω, Σ, μ), one can form the measure $X_*^x\mu$ on the space

$$C_x(M) := \big\{\gamma \in C([0,\infty), M) \mid \gamma(0) = x\big\}.$$

This turns out to be a Borel measure, when the latter is endowed with the compact-open topology, and any version produces the same measure.

Definition 1.1.11 (Wiener Measure). The law of Brownian m on $C_x(M)$ will be called the *Wiener measure* on M, denoted by $\mathbb{W}^x$.

Remark 1.1.12. Note that the definition given here differs from the stochastic literature, because there one usually uses the heat kernel of the operator $\frac{1}{2}\Delta$ instead of Δ.

1.1.4 Path-ordered Exponentials and the Feynman-Kac formula

Using the Wiener measure, it is easy to arrive at our first path integral formula,

$$e^{-tL}u(x) = \mathbb{E}\big[u(X_t^x)\big] = \int_{C_x(M)} u\big(\gamma(t)\big)\mathrm{d}\mathbb{W}^x(\gamma), \tag{1.1.11}$$

where X_s^x is the Brownian motion with drift Z starting at $x \in M$. Of course, this formula is tautological, having defined the Wiener measure the way we did above. If one adds a potential, however, one obtains a non-trivial result, namely the Feynman-Kac formula. To formulate this in generality, we need the following definition.

Definition 1.1.13 (Path-ordered Exponential). Let $\mathcal{V}$ be a vector bundle with connection ∇, and let $V \in C^\infty(M, \mathrm{End}(\mathcal{V}))$ be a smooth endomorphism field. For a piecewise smooth path $\gamma : [0,t] \longrightarrow M$, let $P(s) \in \mathrm{Hom}(\mathcal{V}_{\gamma(0)}, \mathcal{V}_{\gamma(s)})$ be the unique solution to the ordinary differential equation

$$\nabla_s P(s) = V\big(\gamma(s)\big)P(s), \qquad P(0) = \mathrm{id}. \tag{1.1.12}$$

The *path-ordered exponential* $\mathcal{P}(\gamma)$ is defined by $\mathcal{P}(\gamma) := P(t) \in \mathrm{Hom}(\mathcal{V}_{\gamma(0)}, \mathcal{V}_{\gamma(t)})$. If L is a self-adjoint Laplace type operator having the unique splitting $L = \nabla^*\nabla + V$ as in Lemma 1.1.2, we call $\mathcal{P}(\gamma) = \mathcal{P}^{\nabla,V}(\gamma)$ the path-ordered exponential *determined by* L.

For example, if $V \equiv 0$ along γ, we have $\mathcal{P}(\gamma) = [\gamma\|_0^t]$, the parallel transport map along γ with respect to the given connection ∇. In the scalar case, when $\nabla = d + i\omega$ for some one-form $\omega \in \Omega^1(M)$, the differential equation (1.1.12) can be solved explicitly,

$$\mathcal{P}(\gamma) = \exp\left(-i\int_0^t \omega\cdot\dot{\gamma}(s)\,\mathrm{d}s + \int_0^t V\big(\gamma(s)\big)\,\mathrm{d}s\right). \tag{1.1.13}$$

In the general vector-valued case, however, there is usually no closed-form solution for $\mathcal{P}(\gamma)$.

Remark 1.1.14 (Invertibility). $\mathcal{P}(\gamma)$ is always invertible, and $\mathcal{P}(\gamma)^{-1} = Q(t)$, where $Q(s) = P(s)^{-1} \in \mathrm{Hom}(\mathcal{V}_{\gamma(s)}, \mathcal{V}_{\gamma(0)})$ satisfies the differential equation

$$\nabla_s Q(s) = -Q(s)V\big(\gamma(s)\big), \qquad Q(0) = \mathrm{id}, \tag{1.1.14}$$

as is easy to verify by differentiation the product $\mathrm{id} = P(s)^{-1}P(s)$ and using uniqueness of solutions.

Remark 1.1.15 (Multiplicitivity). $\mathcal{P}(\gamma)$ is multiplicative, in the sense that if γ_1, γ_2 are paths parametrized by $[0,t_1]$ and $[0,t_2]$ respectively, such that $\gamma_1(t) = \gamma_2(0)$, then we have $\mathcal{P}(\gamma_2)\mathcal{P}(\gamma_1) = \mathcal{P}(\gamma_1 * \gamma_2)$, where

$$(\gamma_1 * \gamma_2)(s) := \begin{cases} \gamma_1(s) & \text{if } s \leq t_1 \\ \gamma_2(s - t_1) & \text{if } t_1 \leq s \leq t_1 + t_2 \end{cases} \tag{1.1.15}$$

denotes the concatenation. This follows because both $\mathcal{P}(\gamma_2)\mathcal{P}(\gamma_1)$ and $\mathcal{P}(\gamma_1 * \gamma_2)$ satisfy the same ordinary differential equation with the same initial condition.

In local coordinates, we have

$$\nabla_s P(s) = \frac{\mathrm{d}}{\mathrm{d}s} P(s) + \sum_{i=1}^{n} \dot{\gamma}^i(s) \big[\Gamma_i\big(\gamma(s)\big), P(s)\big] \overset{!}{=} V\big(\gamma(s)\big) P(s) \tag{1.1.16}$$

where $\Gamma_i = (\Gamma_{ij}^k)$ denotes the Christoffel symbols of the connection, written into a matrix. If the connection is flat, the Christoffel terms can be chosen to be zero using a suitable trivialization and the ODE (1.1.12) takes the form

$$\frac{\mathrm{d}}{\mathrm{d}s} P(s) = V\big(\gamma(s)\big) P(s),$$

which can be solved for any continuous path γ in M. If it is not flat, then one needs to require that γ is at least absolutely continuous in order that the differential equation (1.1.16) makes sense pointwise. In particular (since the set of absolutely continuous paths is a zero set with respect to the Wiener measure), the path-ordered exponential cannot be defined pointwise for the sample paths of Brownian motion. However, it is well known that $\mathcal{P}(\gamma)$ has a *stochastic extension* to a well-defined L^p function on path space − which we denote by $\widetilde{\mathcal{P}}(\gamma)$ − that is the solution of a stochastic differential equation. For example, it can be defined as the solution to the differential equation (1.1.12), when the latter is interpreted as a Stratonovich stochastic differential equation (see e.g. [GÏ0b, 2.17] or Chapter 8 in [Eme89]). This reduces to the usual parallel transport if the connection is flat. In the scalar case, where $\nabla = d + i\omega$ for a one-form $\omega \in \Omega^1(M)$ and $V \in C^\infty(M)$, the associated path-ordered integral is given by

$$\widetilde{\mathcal{P}}(\gamma) = \exp\left(-i \int_0^t \omega\big(\gamma(s)\big) \mathrm{d}\gamma(s) + \int_0^t V\big(\gamma(s)\big) \mathrm{d}s\right),$$

where the first term in the exponent denotes a Stratonovich integral (see e.g. [Eme89], Chapter VII for the definition of these).

Theorem 1.1.16 (Feynman-Kac). [BP11] *Let $L = \nabla^*\nabla + V$ be a Laplace type operator acting on sections of a vector bundle $\mathcal{V}$ over a closed Riemannian manifold M. Then*

$$e^{-tL} u(x) = \mathbb{E}\left[\widetilde{\mathcal{P}}(X_\bullet^x|_{[0,t]})^{-1} u(X_t^x)\right] = \int_{C_x(M)} \widetilde{\mathcal{P}}(\gamma|_{[0,t]})^{-1} u\big(\gamma(t)\big) \mathrm{d}\mathbb{W}^x(\gamma)$$

for all $u \in L^2(M, \mathcal{V})$.

This result is proved e.g. in [BP11, Thm. 6.2], [Øks07, Thm. 8.2.1] or [Tay11, Chapter 11, Prop. 2.1] in the scalar case and in [GÏ0b, Thm. 5.3], [GÏ0a] or [Hsu02, Thm. 7.2.1] in the vector-valued case. See also the original treatment by Kac, [Kac79].

1.2 The Case without Boundary

In this section, we review previous results regarding path integration in the case that M is closed. First we need to introduce the relevant path spaces.

1.2.1 Based Path Spaces and their Approximations

During the course of this thesis the *energy functional* will play an important role. For a path $\gamma : [0,t] \longrightarrow M$ (where M is a Riemannian manifold) it is defined by

$$E(\gamma) := \frac{1}{2}\int_0^t |\dot{\gamma}(s)|^2 \mathrm{d}s. \tag{1.2.1}$$

The paths for which E is finite are those that lie in the space $H^1([0,t],M)$, the space of paths that have Sobolev regularity H^1 in local coordinates. All elements of $H^1([0,t],M)$ turn out to be absolutely continuous.

Remark 1.2.1. From a physicist's point of view, the correct terminology would be that E is not the energy functional but rather the *action* functional. However, the term "energy functional" is traditional in differential geometry, in the context of studying geodesics.

Let M be a complete Riemannian manifold of dimension n. The space $H^1([0,t],M)$ has naturally the structure of an infinite-dimensional manifold modelled on Hilbert spaces; a natural model space is the Sobolev space $H^1([0,t],\mathbb{R}^n)$. The tangent space to $H^1([0,t],M)$ at a path γ can be canonically identified with the space of vector fields along γ, which have regularity H^1, that is, one has the natural isomorphism

$$T_\gamma H^1([0,t],M) \cong H^1([0,t],\gamma^*TM). \tag{1.2.2}$$

For details, see Section 2.3 in [Kli95].

Notation 1.2.2 (Based Path Spaces). For a point $x \in M$, we write

$$H_{x;t}(M) := \bigl\{\gamma \in H^1([0,t],M) \mid \gamma(0) = x\bigr\}$$

for the path space based at x. In the case $t = 1$, we also write $H_x(M) := H_{x;1}(M)$.

To see that $H_{x;t}(M)$ is a submanifold of $H^1([0,t],M)$, we can argue as follows. The manifold $H^1([0,t],M)$ comes with the endpoint evaluation map

$$\mathrm{ev}_{0,t} : H^1([0,t],M) \longrightarrow M \times M, \qquad \gamma \longmapsto \bigl(\gamma(0),\gamma(t)\bigr). \tag{1.2.3}$$

By Prop. 2.4.1 in [Kli95], this map is a submersion, hence pre-images of submanifolds are again submanifolds (this is also easy to verify directly). Now we have $H_{x;t}(M) = \mathrm{ev}_{0,t}^{-1}(\{x\} \times M)$, that is, $H_{x;t}(M)$ is the pre-image of the submanifold $\{x\} \times M \subset M \times M$ under the evaluation map, and therefore is a submanifold itself.

Remark 1.2.3. One can show that the evaluation map $\mathrm{ev}_{0,t}$ is in fact the projection of a (locally trivial) fiber bundle. This can be checked by hand or by using a theorem of Hermann [Her60], which states that a Riemannian submersion from a complete total space is always a fiber bundle (that $H^1([0,t],M)$ is complete with a suitable Riemannian metric is the statement of Thm. 2.4.7 in [Kli95]).

The spaces $H_{x;t}(M)$ have a natural global chart, the *anti-development map*

$$U : H_{x;t}(M) \longrightarrow H_{0;t}(T_xM), \qquad \gamma \longmapsto \Big[s \mapsto \int_0^t [\gamma\|_0^s]^{-1}\dot\gamma(s)\mathrm{d}s \Big], \tag{1.2.4}$$

where $H_{0;t}(T_xM)$ is the space of H^1 paths γ in T_xM with $\gamma(0) = 0$. Its inverse, the *rolling map*, rolls paths in T_xM onto M. The concept apparently goes back to Elie Cartan; A fun depiction of Cartan applying it to a manifold can be found in [Dri04, Figure 11].
We will not put a Riemannian metric on $H^1([0,t], M)$ itself; however, on $H_{x;t}(M)$ we will always consider the Riemannian metric

$$(X, Y)_{H^1} := \int_0^t \langle \nabla_s X(s), \nabla_s Y(s)\rangle \,\mathrm{d}s, \tag{1.2.5}$$

which turns out to be particularly well-suited for path space analysis. Any vector field X along γ with vanishing derivative must be parallel, hence zero since $X(0) = 0$. Therefore, this metric is non-degenerate on $H_{x;t}(M)$.

The idea of time-slicing approximation of path integrals is to replace the infinite-dimensional path spaces introduced above by finite-dimensional path spaces, which will be defined now. These will be certain submanifolds of the infinite-dimensional versions.

Notation 1.2.4 (Partitions). We denote by $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = t\}$ a partition of the interval $[0, t]$. By

$$\Delta_j\tau := \tau_j - \tau_{j-1}, \qquad \text{and} \qquad |\tau| = \max_{j=1,\dots,N} \Delta_j\tau \tag{1.2.6}$$

we denote the *increment* and the *mesh*, respectively. Throughout this thesis, we will usually write N for the length of the partition, which may depend on the partition, $N = N(\tau)$. We suppress this dependence for the sake of notational simplicity.

Notation 1.2.5 (Finite-dimensional Approximations). For a partition $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = t\}$ of the interval $[0, t]$, we write

$$H_{x;\tau}(M) := \big\{\gamma \in H_{x;t}(M) \mid \gamma|_{[\tau_{j-1},\tau_j]} \text{ is a geodesic for each } j = 1, \dots, N\big\}.$$

This is a finite-dimensional submanifold of $H_{x;t}(M)$, because anti-development map defined in (1.2.4) sends them to the subspace of polygon paths in T_xM that start at zero. To see this, notice that for $s \in (\tau_{j-1}, \tau_j)$,

$$\frac{\mathrm{d}^2}{\mathrm{d}s^2}U(\gamma)(s) = \frac{\mathrm{d}}{\mathrm{d}s}[\gamma\|_0^s]^{-1}\dot\gamma(s) = [\gamma\|_0^s]^{-1}\nabla_s\dot\gamma(s) = 0,$$

because $\gamma|_{(\tau_{j-1},\tau_j)}$ is a geodesic. Hence $U(\gamma)(s)$ is a straight line in T_xM on the interval $[\tau_{j-1}, \tau_j]$.
The tangent space at $\gamma \in H_{x;\tau}(M)$ is the space of piece-wise Jacobi fields along γ, i.e. the space of continuous vector fields X such that

$$\nabla_s^2 X(t) = R\big(\dot\gamma(s), X(s)\big)\dot\gamma(s) \tag{1.2.7}$$

holds on the intervals (τ_{j-1}, τ_j), R being the Riemannian curvature tensor of M (see Prop. 4.4 in [AD99]).

Remark 1.2.6 (Approximation Property). The finite-dimensional approximations exhaust $H_{x;t}(M)$ in the sense that the union of $H_{x;\tau}(M)$ over all partitions τ of $[0,t]$ is dense in $H_{x;t}(M)$. This can be seen by showing that the spaces $H_{x;\tau}(T_xM)$ are dense in $H_{x;t}(T_xM)$ just as in Step 1 of the proof of Lemma 3.2.10 and then using the development map U^{-1}.

For any partition τ, the spaces $H_{x;\tau}(M)$ carry the induced submanifold metric (1.2.5). However, it seems that the discretized H^1 metric

$$(X,Y)_{\Sigma\text{-}H^1} := \sum_{j=1}^{N} \big\langle \nabla_s X(\tau_{j-1}+), \nabla_s Y(\tau_{j-1}+)\big\rangle \Delta_j\tau \tag{1.2.8}$$

is more natural to consider on the spaces $H_{x;\tau}(M)$, as it gives cleaner formulas for approximation. Here $\nabla_s X(\tau_{j-1}+)$ denotes the right-sided derivative of X.

1.2.2 Path Integral Formulas for the Heat Operator

In this section, we give an overview over previous results regarding the approximation of heat operators e^{-tL} by integrals over the finite-dimensional path spaces $H_{x,\tau}(M)$, for partitions τ of the interval $[0,t]$. Here L is a self-adjoint Laplace type operator, acting on sections of a metric vector bundle $\mathcal{V}$ over M, where we assume M to be a *closed* Riemannian manifold of dimension n. The case that M has a boundary will be considered in the next section.
Such an approximation is usually called *time-slicing approximation* in the physics literature, because the time interval is sliced up into small bits by the partition. In the mathematical literature, the term *finite-dimensional approximation* seems to be more common, which refers to the fact that the (non-existent) integral over the infinite-dimensional Hilbert manifold $H_x(M)$ is approximated by an integral over the finite-dimensional manifolds $H_{x;\tau}(M)$ (in fact, they have dimension nN).

The following theorem was proved by [BP10], and previously (in the case that $L = \Delta$, the Laplace-Beltrami operator) in [AD99].

Theorem 1.2.7 (The Heat Operator as a Path Integral). *Let L be a self-adjoint Laplace type operator, acting on sections of a metric vector bundle $\mathcal{V}$ over a compact Riemannian manifold. Let $\mathcal{P}(\gamma)$ be the path-ordered exponential determined by L as in Def. 1.1.13. Then for any $u \in C^0(M,\mathcal{V})$, we have*

$$e^{-tL}u(x) = \lim_{|\tau|\to 0} \fint_{H_{x;\tau}(M)} e^{-E(\gamma)/2}\mathcal{P}(\gamma)^{-1} u\big(\gamma(t)\big)\,\mathrm{d}^{\Sigma\text{-}H^1}\gamma,$$

uniformly in x, where the limit goes over any sequence of partitions the mesh of which goes to zero. Here $H_{x;\tau}(M)$ carries the discrete H^1 metric introduced in (1.2.8) *and he slash over the integral sign denotes divison by* $(4\pi)^{\dim(H_{x;\tau}(M))/2}$.

We will see later that this result is also true for $u \in L^p(M,\mathcal{V})$, $1 \le p < \infty$ (where the convergence holds in the respective space).

One can show (see [AD99, Thm. 4.8]) that the anti-development map $U : H_{x;\tau}(M) \longrightarrow H_{0;\tau}(T_xM)$ is measure preserving if $H_{x;\tau}(M)$ carries the discrete H^1 metric. Furthermore, one has $E(\gamma) = \frac{1}{2}\|U(\gamma)\|^2_{\Sigma\text{-}H^1}$ so that for any integrable function F on $H_{x;\tau}(M)$,

$$(4\pi)^{-nN/2}\int_{H_{x;\tau}(M)} e^{-E(\gamma)/2}F(\gamma)\mathrm{d}^{\Sigma\text{-}H^1}\gamma = (4\pi)^{-nN/2}\int_{H_{0;\tau}(T_xM)} e^{-\|X\|^2/4}F\big(U^{-1}(X)\big)\mathrm{d}^{\Sigma\text{-}H^1}X,$$

is a standard Gaussian integral over the vector space $H_{0;\tau}(T_xM)$. Note now that the normalization constant was chosen such that the integral on the right hand side evaluates to one in the case $u \equiv 1$.

Example 1.2.8 (Quantizing Hamiltonian Functions). In the classical mechanics of point particles, one considers Hamiltonian functions on phase space, which are smooth functions on the cotangent bundle of a Riemannian manifold M (we assume it to be compact here). A typical electromagnetic Hamiltonian function is of the form

$$h(x,p) = |p - \omega(x)|^2 + V(x), \qquad x \in M, \ \ p \in T_x^*M \tag{1.2.9}$$

where $\omega \in \Omega^1(M)$ is a given one-form and $V \in C^\infty(M)$ is a potential. The corresponding quantum mechanical Hamiltonian is the Laplace type operator

$$H = \nabla^*\nabla + V$$

where $\nabla = d + i\omega$ is the connection determined by ω. The corresponding time evolution operator is e^{itH}, which we cannot deal with; however, the "Euclidean" solution operator e^{-tH} *can* be represented by a path integral as follows. It involves the Lagrange function ℓ associated to the Hamiltonian function h in a natural way. In our example, the Lagrangian is the smooth function

$$\ell(x,v) = \frac{1}{4}|v|^2 + \omega(x)\cdot v - V(x), \qquad x \in M, \ \ v \in T_xM$$

on the tangent bundle of M. Because the term $\mathcal{P}(\gamma)^{-1}$ can be computed explicitly for our particular Laplace type operator, the Hamiltonian operator H, we have

$$e^{-E(\gamma)/2}\mathcal{P}(\gamma)^{-1} = \exp\left(\int_0^t\Big(-\frac{1}{4}\big|\dot\gamma(s)\big|^2 + i\omega\big(\gamma(s)\big)\dot\gamma(s) - V\big(\gamma(s)\big)\Big)\mathrm{d}s\right),$$

see (1.1.13) and (1.2.1). We obtain the path integral formula

$$e^{-tL}u(x) = \lim_{|\tau|\to 0}\fint_{H_{x;\tau}(M)}\exp\left(\int_0^t \ell\big(\gamma(s), i\dot\gamma(s)\big)\mathrm{d}s\right)u\big(\gamma(t)\big)\mathrm{d}^{\Sigma\text{-}H^1}\gamma,$$

where we extended ℓ to a fiber-wise polynomial on $TM \otimes \mathbb{C}$. Notice the imaginary unit in the Lagrangian; it is due to the fact that we substituted $t \mapsto -it$ in order to be able to use our results.

Thm. 1.2.7 is *not* true as written if one uses the submanifold metric on $H_{x;\tau}(M)$ instead of the discrete H^1 metric. If one uses this metric instead, one needs a certain correction term in the integrand, which depends on the curvature of the manifold in a complicated

way, as proved in [Lim07] (curiously, in the reference, the restriction $0 \leq K < 3/17n$ on the sectional curvature K is made).
Also L^2 metrics have been considered on the spaces $H_{x;\tau}(M)$. In this case, one obtains the result

$$e^{-tL}u(x) = \lim_{|\tau|\to 0} \frac{1}{Z_\tau} \int_{H_{x;\tau}(M)} e^{-E(\gamma)/2+\alpha\int_0^t \mathrm{scal}(\gamma(s))\mathrm{d}s} \mathcal{P}(\gamma)^{-1} u\big(\gamma(t)\big)\mathrm{d}\gamma,$$

where the constant Z_τ is a different normalization constant (which in this case depends on the partition itself, not only on the dimension of the path space) and α is a certain number. We have $\alpha = 1/3$ in the case that one takes the discrete L^2 metric

$$(X,Y)_{\Sigma\text{-}L^2} := \sum_{j=1}^N \langle X(\tau_j), Y(\tau_j)\rangle\, \Delta_j\tau \tag{1.2.10}$$

(see [BP08] or [AD99]) and $\alpha = (2+\sqrt{3})/10\sqrt{3}$ in the case that one takes the continuous L^2 metric

$$(X,Y)_{L^2} := \int_0^t \langle X(s), Y(s)\rangle\, \mathrm{d}s \tag{1.2.11}$$

(see [Lae13]; in the latter reference, it is assumed that the sectional curvature is non-negative).

Remark 1.2.9 (Discrete Brownian Motion). Consider a particle a starting at x with a random initial impulse, which travels along a geodesic until it collides with another particle. Suppose these collisions happen at positions $x_j \in M$ and times τ_j, and suppose that they inflict a new impulse on a, which is determined by drawing a random vector in $T_{x_j}M$ according to the n-dimensional normal distribution with variance $2/\Delta_j\tau$. This means that the mean distance travelled by the particle a in the time interval $[\tau_{j-1}, \tau_j]$ is proportional to $\sqrt{\Delta_j\tau}$, which is plausible from physical arguments (compare [Ein05, Section 4]). The space of possible paths for a, given fixed collision times τ_j, is then the path space $H_{x;\tau}(M)$. The probability measure induced on $H_{x;\tau}(M)$ by the above process is then exactly the measure $(4\pi)^{-nN/2}e^{-E(\gamma)/2}\mathrm{d}^{\Sigma\text{-}H^1}\gamma$, where $\mathrm{d}^{\Sigma\text{-}H^1}\gamma$ denotes the Riemannian volume on $H_{x;\tau}(M)$ induced by the discrete H^1-metric. From this point of view, the discrete H^1 metric may indeed be the most natural metric to consider on the finite-dimensional path spaces.

1.3 The Case with Boundary

If the manifold has a boundary, the key question to derive path integral formulas is to ask what happens to paths when they hit the boundary of the manifold. The answer to this is that they should reflect with the angle of reflection equal to the angle of incidence. We will now consider the space of such paths and discuss how the boundary condition enters the game. In Section 1.3.3, we will then state and prove a time-slicing approximation result for solutions of the heat equation on manifolds with boundary, which generalizes Thm. 1.2.7.

1.3.1 Reflected Geodesics and the Broken Billiard Flow

Let M be a compact n-dimensional Riemannian manifold with boundary. Denote by $\mathbf{n} \in C^\infty(\partial M, N\partial M)$ the interior unit normal field. We say that a vector $v \in TM|_{\partial M}$ *points inward* if $\langle v, \mathbf{n}\rangle > 0$ and we say that it *points outward* if $\langle v, \mathbf{n}\rangle < 0$. If v points neither outward nor inward, then clearly $v \in T\partial M$.

Notation 1.3.1 (Reflection at the Boundary). Set

$$Rv := v - 2\langle v, \mathbf{n}\rangle \mathbf{n}, \qquad v \in TM|_{\partial M} \tag{1.3.1}$$

for the reflection at $T\partial M$. We have $R \in C^\infty(\partial M, \mathrm{End}(TM|_{\partial M}))$.

Definition 1.3.2 (Reflected Geodesics). A *reflected geodesic* is a continuous map $\gamma : [a, b] \longrightarrow M$ such that

(i) γ hits the boundary only at finitely many times $a \leq \sigma_1 < \sigma_2 < \dots < \sigma_k \leq b$, $k \in \mathbb{N}_0$;

(ii) on each of the intervals (a, σ_1), (σ_1, σ_2), $\dots$, (σ_{k-1}, σ_k), (σ_k, b), γ is a geodesic;

(iii) $\dot\gamma(\sigma_j\pm) \notin T\partial M$, where $\dot\gamma(\sigma_j\pm)$ denotes the right-/left-sided derivative, i.e. γ always hits the boundary transversally;

(iv) we have $\dot\gamma(\sigma_j-) = R\dot\gamma(\sigma_j+)$ for each $j = 1, \dots, k$, that is, γ reflects with the angle of reflection equal to the angle of incidence. (If $\sigma_1 = a$ or $\sigma_k = b$, this condition is empty for $j = 1$ respectively $j = k$.)

The requirement (iii) excludes geodesics that "scratch along the boundary", the so-called grazing rays, which can appear e.g. when M is the exterior of a ball in $\mathbb{R}^n$.

Notation 1.3.3. For $v \in TM$, let $T(v)$ be the supremum over all times $t > 0$ such that a reflected geodesic $\gamma_v : [0, t] \longrightarrow M$ exists with $\dot\gamma_v(0+) = v$ or, if $v \in TM|_{\partial M}$ is pointing outward, with $\dot\gamma_v(0+) = Rv$). Denote

$$\Omega_t := \big\{ v \mid T(v) > t \big\}$$

for the set of vectors v such that there exists a reflected geodesic with initial condition v (respectively Rv) up to a time larger than t.

Obviously, we have $T(v) = -\infty$ for $v \in T\partial M$ and $T(v) > 0$ otherwise. Hence $\Omega_0 = TM \setminus T\partial M$. Since restrictions of reflected geodesics are reflected geodesics, we have furthermore $\Omega_t \supseteq \Omega_{t'}$ for $t \leq t'$.

Remark 1.3.4. We generally do *not* have the equality $\Omega_t = TM \setminus T\partial M$ here, as two things could go wrong:

(a) We may have $\lim_{s\to t_0} \dot\gamma_v(s) \in T\partial M$.

(b) There may be infinitely many reflections in finite time, i.e. reflection times $\sigma_1 < \sigma_2 < \dots$ converging to a time $t_0 < \infty$ as $j \to \infty$.

In both cases, one cannot continue γ_v beyond the time t_0 (at least not as a reflected geodesic). In case (a), the "physically reasonable" outcome would be that γ_v "glides along the boundary" for $t > T$, but this would mean that γ_v is a geodesic in ∂M, not in M ($\nabla_s\dot\gamma(s)$ would be proportional to $-\mathbf{n}$).
If M is convex (i.e. the second fundamental form of the boundary points outward everywhere), then (a) cannot happen. Also (b) cannot happen in the case that ∂M is smooth (which is always assumed here) and convex, at least if M is a subset of $\mathbb{R}^2$, but there is an example of a convex $M \subset \mathbb{R}^2$ with only C^2 boundary, where (b) can occur [Hal77]. However, to the author's knowledge, there is no (non-convex) example of a manifold M with *smooth* boundary in literature, where (b) happens. The author does not know if (b) can happen at all.

Lemma 1.3.5. *For each $t \geq 0$, the set Ω_t is an open set of full measure in TM and for each $x \in M$, the set $\Omega_{t,x} := \Omega_t \cap T_xM$ is an open set of of full measure in T_xM.*

Proof. That the sets $\Omega_{t,x}$ and Ω_t have full measure is a result from the theory of dynamical systems and ergodic theory, see for example Chapter 6 of [KFS82]. Furthermore, that the sets $\Omega_{t,x}$ and Ω_t are open is due to the fact that solutions of ordinary differential equations depend continuously on the initial data. More precisely, one can show by induction on the number of reflections that for each $v \in \Omega_t$, there exists a small neighborhood of v such that for each w in that neighborhood, there exists a reflected geodesic γ_w up to time larger than t, and the value $\dot\gamma_w(t)$ depends continuously on w in this neighborhood. $\square$

Definition 1.3.6 (Broken Billiard Flow). The *broken billiard flow* is the measurable map $\Theta : \mathbb{R} \times TM \longrightarrow TM$ defined as follows. Set $\Theta_0(v) := v$. For $t > 0$ and $v \in \Omega_t$, we set

$$\Theta_t(v) = \dot\gamma_v(t)$$

where $\gamma_v : [0, t] \longrightarrow M$ is the maximal reflected geodesic with $\dot\gamma_v(0+) = v$, respectively $\dot\gamma_v(0+) = Rv$ if $v \in TM|_{\partial M}$ is outward directed. For $v \notin \Omega_t$, set $\Theta_t(v) = v$. For negative times, $t < 0$, set $\Theta_t(v) := -\Theta_{-t}(-v)$.

Remark 1.3.7. If $\partial M = \emptyset$, this is just the usual geodesic flow on the tangent bundle.

Remark 1.3.8. The broken billiard flow is often considered on the unit sphere bundle SM instead of on TM. Because we have

$$\Theta_t(v) = |v|\Theta_{t|v|}(v/|v|), \tag{1.3.2}$$

both flows can be obtained from one another.

Because $TM \setminus \Omega_t$ is a zero set, for each $t \in \mathbb{R}$, the broken billiard map Θ_t is almost invertible, in the sense that $\Theta_t \circ \Theta_{-t} = \mathrm{id}$ except for a zero set. Furthermore, it is well known [KFS82, Lemma 4] that Θ_t preserves the volume of TM, just as the geodesic flow does on a complete Riemannian manifold without boundary.

1.3.2 Reflected Path Spaces

Notation 1.3.9. For a partition $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = t\}$ of the interval $[0,t]$ and $x \in M \setminus \partial M$, write

$$H^{\mathrm{refl}}_{x;\tau}(M) := \big\{\gamma \in C^0([0,t], M \mid \gamma|_{[\tau_{j-1},\tau_j]} \text{ is a reflected geodesic and } \gamma(\tau_j) \notin \partial M \text{ for } 1 \leq j \leq N-1\big\},$$

for the space of piece-wise reflected geodesics. For $x \in \partial M$, set

$$H^{\mathrm{refl}}_{x;\tau}(M) := \big\{\gamma \in C^0([0,t], M \mid \gamma|_{[\tau_{j-1},\tau_j]} \text{ is a reflected geodesic and } \gamma(\tau_j) \notin \partial M \text{ for } 1 \leq j \leq N-1\big\}$$

We always use the multiplicative representation $\mathbb{Z}_2 = \{+1, -1\}$.

If $x \notin \partial M$, then $H^{\mathrm{refl}}_{x;\tau}(M)$ is just the space of reflected geodesics. If $x \in \partial M$, the elements of $H^{\mathrm{refl}}_{x;\tau}(M)$ carry the additional information of an element $\epsilon \in \mathbb{Z}_2$. Heuristically, this element encodes whether or not the path reflects at time zero, i.e. whether it starts inward or it start outward and reflects immediately. This number ϵ will be called the *sign* of the path.
We will often just write γ instead of (γ, ϵ) for elements of $H^{\mathrm{refl}}_{x;\tau}(M)$, $x \in \partial M$ (especially when integrating over this space) and consider γ as an ordinary path "with decoration". However, the additional information on the sign has to be kept in mind.

Definition 1.3.10 (*B*-path-ordered Exponential). If $L = \nabla^*\nabla + V$ is a self-adjoint Laplace type operator with involutive boundary condition B, this determines a *B-path-ordered exponential* $\mathcal{P}_B(\gamma)$ along paths $\gamma \in H^{\mathrm{refl}}_{x;\tau}(M)$, for any partition τ of the interval $[0,t]$. Let $\sigma_1 < \cdots < \sigma_k$ be the times in $(0,t)$ such that $\gamma(\sigma_j) \in \partial M$ (i.e. $\gamma(s) \notin \partial M$ for $s \neq 0$, $s \neq \sigma_j$, $j = 1, \dots, k$). Set

$$\mathcal{P}_B(\gamma) := \mathcal{P}(\gamma|_{[\sigma_k,t]})\, B\, \mathcal{P}(\gamma|_{[\sigma_{k-1},\sigma_k]})\, B \cdots B\, \mathcal{P}(\gamma|_{[\sigma_1,\sigma_2]})\, B\, \mathcal{P}(\gamma|_{[0,\sigma_1]}) A, \tag{1.3.3}$$

where $A := \mathrm{id}$ if $x \notin \partial M$ or if $x \in \partial M$ and the sign of γ is $+1$, and $A := B$ if $x \in \partial M$ and the sign of γ is -1. That is, we take the usual path-ordered exponential (see Def. 1.1.13), but whenever the path γ hits the boundary, we use the boundary involution B before continuing to solve the differential equation (1.1.12). In particular, if $V = 0$, we obtain the *B-parallel transport* $[\gamma\|_0^t]_B$.

Remark 1.3.11 (Multiplicativity). For paths γ_1, γ_2 with $\gamma_1(t_1) = \gamma_2(0)$, we have

$$\mathcal{P}_B(\gamma_2)\mathcal{P}_B(\gamma_1) = \mathcal{P}_B(\gamma_1 * \gamma_2)$$

if $\gamma_1(t_1) \notin \partial M$, similar to the multiplicative property for the usual path-ordered exponential, see Remark 1.1.15.

The B-path-ordered exponential can be used to obtain a manifold structure on $H^{\mathrm{refl}}_{x;\tau}(M)$. Notice that on the vector bundle $\mathcal{V} := TM$, there is a natural boundary operator, namely $B := R$, the reflection at $T\partial M$. We define the *reflected anti-development map*

$$U_R(\gamma)(s) := \int_0^s [\gamma\|_0^u]_R^{-1}\dot\gamma(u)\mathrm{d}u.$$

Then U_R maps $H^{\mathrm{refl}}_{x;\tau}(M)$ to $H_{0;\tau}(T_xM)$, the space of piece-wise polygon paths starting at zero in T_xM. To verify this, we need to show that $U_R(\gamma)$ is a straight line on each of the intervals $[\tau_{j-1}, \tau_j]$, $j = 1, \dots, N$. This is clear for all times s where $\gamma(s) \notin \partial M$ (by the same argument as for U). If now $\gamma(s) \in \partial M$, then

$$\frac{\mathrm{d}}{\mathrm{d}s} U_R(\gamma)(s-) = [\gamma\|_0^{s-}]_R^{-1}\dot{\gamma}(s-) = (R[\gamma\|_0^{s+}]_R)^{-1}R\dot{\gamma}(s+) = \frac{\mathrm{d}}{\mathrm{d}s} U_R(\gamma)(s+),$$

because the two reflections cancel each other. Hence γ does not have a kink at s and is therefore a straight line near s. That U_R is injective is clear for $x \notin \partial M$. On the other hand, if $x \in \partial M$, then each piece-wise reflected geodesic γ starting at x appears twice, once with negative sign and one with positive sign. But by definition of the reflected anti-development, we have $U_R(\gamma, +1)(s) = RU_R(\gamma, -1)(s)$. This shows that U_R is injective. Because of Lemma 1.3.5, the image $U_R(H^{\mathrm{refl}}_{x;\tau}(M)) \subseteq H_{0,\tau}(T_xM)$ is an open and dense set of full measure, so that one obtains a manifold structure on $H^{\mathrm{refl}}_{x;\tau}(M)$ by using U_R as global chart.

Remark 1.3.12. If $\partial M = \emptyset$, then $\Omega_t = TM$ for all t, and we have $H^{\mathrm{refl}}_{x;\tau}(M) = H_{x;\tau}(M)$.

Notice that for two partitions τ and τ' of intervals $[0, t]$ and $[0, t']$, respectively, if $\gamma \in H^{\mathrm{refl}}_{x;\tau}(M)$ and $\gamma' \in H^{\mathrm{refl}}_{\gamma(t);\tau'}(M)$, then the concatenation $\gamma * \gamma'$ (as defined in (1.1.15)) is contained in $H^{\mathrm{refl}}_{x;\tau*\tau'}(M)$. This fact is used in the following Lemma.

Lemma 1.3.13 (A Co-Area Formula). *Let $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = t\}$ and $\tau' = \{0 = \tau'_0 < \tau'_1 < \cdots < \tau'_{N'} = t'\}$ be partitions of the interval $[0, t]$ and $[0, t']$. Then for any integrable function F on $H^{\mathrm{refl}}_{x;\tau*\tau'}(M)$, we have the co-area formula*

$$\int_{H^{\mathrm{refl}}_{x;\tau*\tau'}(M)} F(\gamma)\, \mathrm{d}^{\Sigma\text{-}H^1}\gamma = \int_{H^{\mathrm{refl}}_{x;\tau}(M)} \int_{H^{\mathrm{refl}}_{\gamma(t);\tau'}(M)} F(\gamma * \gamma')\, \mathrm{d}^{\Sigma\text{-}H^1}\gamma'\, \mathrm{d}^{\Sigma\text{-}H^1}\gamma,$$

where each of the spaces carries the discrete H^1-metric.

Proof. Consider the restriction maps

$$\mathrm{res} : H^{\mathrm{refl}}_{x;\tau*\tau'}(M) \longrightarrow H^{\mathrm{refl}}_{x;\tau}(M), \qquad \gamma \longmapsto \gamma|_{[0,t]}$$

We show that res is a Riemannian submersion, i.e. that for any $\gamma * \gamma' \in H^{\mathrm{refl}}_{x;\tau*\tau'}(M)$, the linear map

$$d\mathrm{res}|_{\gamma*\gamma'} : T_{\gamma*\gamma'}H^{\mathrm{refl}}_{x;\tau*\tau'}(M) \longrightarrow T_\gamma H^{\mathrm{refl}}_{x;\tau}(M)$$

is an isometry when restricted to the orthogonal complement of its kernel. The kernel of $d\mathrm{res}|_{\gamma*\gamma'}$ is the set of Jacobi fields that are constant up to time t. Therefore, looking at the formula (1.2.8) for the metric, the orthogonal complement of the kernel is the set of Jacobi fields X such that

$$\nabla_s X\big((\tau * \tau')_{j-1}+\big) = 0, \qquad j = N+1, \dots, N+N'.$$

Therefore, if X is such a vector field in the orthogonal complement, then

$$\|X\|^2_{\Sigma\text{-}H^1} = \sum_{j=1}^{N+N'} \big|\nabla_s X\big((\tau * \tau')_{j-1}+\big)\big|^2 \Delta_j\tau = \sum_{j=1}^{N} \big|\nabla_s X\big(\tau_{j-1}+\big)\big|^2 \Delta_j\tau = \big\|X|_{[0,t]}\big\|^2_{\Sigma\text{-}H^1}$$

so that because $d\mathrm{res}\, X = X|_{[0,t]}$, $d\mathrm{res}$ is indeed an isometry when restricted to this subspace. From the co-area formula, we obtain

$$\int_{H^{\mathrm{refl}}_{x;\tau*\tau'}(M)} F(\gamma)\, \mathrm{d}^{\Sigma\text{-}H^1}\gamma = \int_{H^{\mathrm{refl}}_{x;\tau}(M)} \int_{\mathrm{res}^{-1}(\gamma)} F(\eta)\, \mathrm{d}^{\Sigma\text{-}H^1}\eta\, \mathrm{d}^{\Sigma\text{-}H^1}\gamma,$$

so the proof is finished if we show that the map

$$\mathrm{ext}_\gamma : H_{\gamma(t);\tau'}(M) \longrightarrow \mathrm{res}^{-1}(\gamma), \qquad \gamma' \mapsto \gamma * \gamma'$$

is an isometry. So let $X \in T_{\gamma'} H_{\gamma(t);\tau'}(M)$. Then

$$\big(d\mathrm{ext}_\gamma|_{\gamma'} X\big)(s) = \begin{cases} 0 & 0 \leq s \leq t \\ X(s-t) & t < s \leq t + t' \end{cases}$$

which implies $\|d\mathrm{ext}_\gamma|_{\gamma'} X\|_{\Sigma\text{-}H^1} = \|X\|_{\Sigma\text{-}H^1}$. Thus ext_γ is indeed an isometry for every γ and the lemma follows. □

1.3.3 Reflecting Path Integrals

We can now give a path integral formula for the heat operator in the case that M is a compact manifold with boundary.

Theorem 1.3.14 (The Heat Operator as a Reflecting Path Integral). *Let L be a self-adjoint Laplace type operator, acting on sections of a metric vector bundle $\mathcal{V}$ over a compact Riemannian manifold M with boundary, endowed with involutive boundary conditions B. Let $\mathcal{P}_B(\gamma)$ denote the B-path-ordered exponential, induced by L as in Def. 1.3.10. For a partition $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = t\}$, define*

$$P_\tau u(x) := \fint_{H^{\mathrm{refl}}_{x;\tau}(M)} e^{-E(\gamma)/2} \mathcal{P}_B(\gamma)^{-1} u\big(\gamma(t)\big)\, \mathrm{d}^{\Sigma\text{-}H^1}\gamma, \tag{1.3.4}$$

where the slash over the integral sign denotes divison by $(4\pi)^{\dim(H_{x;\tau}(M))/2}$. Then

$$e^{-tL} u = \lim_{|\tau|\to 0} P_\tau u, \tag{1.3.5}$$

where the limit goes over any sequence of partitions the mesh of which tends to zero and the section u is in any of the spaces $C^0(M, \mathcal{V})$ or $L^p(M, \mathcal{V})$, $1 \leq p < \infty$ (with convergence in the respective space).

Remark 1.3.15. Of course, the definition (1.3.4) makes sense pointwise only for $u \in C^0(M, \mathcal{V})$. However, we will show that each operator P_τ is a bounded operator on $L^p(M, \mathcal{V})$, $1 \leq p < \infty$, which extends uniquely to a bounded operator on $L^p(M, \mathcal{V})$ (also denoted by P_τ), because $C^0(M, \mathcal{V})$ is dense in $L^p(M, \mathcal{V})$. For a general $u \in L^p(M, \mathcal{V})$, $P_\tau u$ is defined by formula (1.3.4) almost everywhere.

Example 1.3.16 (The Laplace-Beltrami Operator). If we have $L = \Delta$, the Laplace-Beltrami operator with Dirichlet boundary conditions (i.e. $B \equiv -1$), then we have $\mathcal{P}_B(\gamma) = (-1)^{\mathrm{refl}(\gamma)}$, where $\mathrm{refl}(\gamma)$ denotes the number of reflections, i.e. the number of times $0 \leq s \leq t$ such that $\gamma(s) \in \partial M$. In this case, we therefore have

$$e^{-tL}u(x) = \lim_{|\tau|\to 0} \fint_{H^{\mathrm{refl}}_{x;\tau}(M)} e^{-E(\gamma)/2}\, u\big(\gamma(t)\big)\, (-1)^{\mathrm{refl}(\gamma)}\, \mathrm{d}^{\Sigma\text{-}H^1}\gamma.$$

If we consider, the Neumann boundary conditions, then $B = 1$ and $\mathcal{P}_B(\gamma) \equiv 1$, so the factor $(-1)^{\mathrm{refl}(\gamma)}$ has to be replaced by one.

The proof of Thm. 1.3.14 is based on the following result, which is due to Chernoff [Che86]. In the following form, the it can be found in [SvWW07, Prop. 1] and [BP08, Thm. 2.8], where it was already used to approximate the heat semigroup on closed manifolds.

Proposition 1.3.17 (Chernoff). *Let $(P_t)_{t\geq 0}$ be a family of bounded linear operators on a Banach space E and assume that P_t is a* proper family, *i.e.*

(i) $\|P_t\| = 1 + O(t)$ *as* $t \to 0$;

(ii) P_t *is strongly continuous with* $P_0 = \mathrm{id}$;

(iii) P_t *has an infinitesimal generator, meaning that there exists a (possibly unbounded) closed operator L on E with dense domain* $\mathrm{dom}(L)$ *that generates a strongly continuous semigroup e^{-tL} and such that*

$$\frac{1}{t}\big(P_t u - u\big) \longrightarrow -Lu$$

as $t \to 0$ for all $u \in E$ of the form $u = e^{-\varepsilon L}v$ with $\varepsilon > 0$ and $v \in \mathrm{dom}(L)$.

Then we have

$$\lim_{|\tau|\to 0} P_{\Delta_1 \tau} \cdots P_{\Delta_N \tau} u = e^{-tL}u,$$

for any $u \in E$, where the limit goes over any sequence of partitions τ of the interval $[0,t]$ the mesh of which tends to zero.

We will subsequently prove the following result:

Proposition 1.3.18. *Set for $t > 0$ and $u \in C^0(M, \mathcal{V})$*

$$P_t u := P_{\{0<t\}} u,$$

where $\{0 < t\}$ is the trivial partition of the interval $[0,t]$ and the right hand side was defined in (1.3.4). *Furthermore, set $P_0 u := u$. Then P_t is a proper family on $C^0(M, \mathcal{V})$ with infinitesimal generator L. Furthermore, P_t extends uniquely to a proper family $L^p(M, \mathcal{V})$, $1 \leq p < \infty$ with L as infinitesimal generator.*

Using this proposition, we can prove the path integral formula above.

Proof (of Thm. 1.3.14). By Prop. 1.3.17, we have

$$\lim_{|\tau|\to 0} P_{\Delta_1\tau}\cdots P_{\Delta_N\tau}u = e^{-tL}u,$$

where P_t is the proper family from Prop. 1.3.18. We now show by induction on the length N of the partition that

$$P_{\Delta_1\tau}\cdots P_{\Delta_N\tau}u = P_\tau u \tag{1.3.6}$$

for any partition τ and any $u \in L^1(M, \mathcal{V})$, where P_τ is defined as in (1.3.4). This is clear for $N = 1$. Suppose that the result is also true for some $N \geq 1$. If then $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = t\}$ is some partition of length N and $\tau' = \{0 = \tau_0' < \tau_1' < \cdots < \tau_{N'}'\}$ is a partition of length $N' \leq N$ (e.g. $N' = 1$), then for $x \in M \setminus \partial M$,

$$\begin{aligned}
P_\tau P_{\tau'}u(x) &= (4\pi)^{-n(N+N')/2}\int_{H_{x;\tau}(M)}\int_{H_{\gamma(t);\tau'}(M)} e^{-E(\gamma)/2-E(\gamma')/2}\mathcal{P}_B(\gamma)^{-1}\mathcal{P}_B(\gamma')^{-1}u\big(\gamma'(t')\big)\mathrm{d}\gamma'\mathrm{d}\gamma\\
&= (4\pi)^{-n(N+N')/2}\int_{H_{x;\tau}(M)}\int_{H_{\gamma(t);\tau'}(M)} e^{-E(\gamma*\gamma')/2}\mathcal{P}_B(\gamma*\gamma')^{-1}u\big((\gamma*\gamma')(t+t')\big)\mathrm{d}\gamma'\mathrm{d}\gamma\\
&= \fint_{H_{x;\tau*\tau'}(M)} e^{-E(\gamma)/2}\mathcal{P}_B(\gamma)^{-1}u\big(\gamma(t+t')\big)\mathrm{d}\gamma = P_{\tau*\tau'}u(x),
\end{aligned}$$

where we always integrate with the respect to the discrete H^1 volume. Here we used the multiplicativity of $\mathcal{P}_B(\gamma)$ (see Remark 1.3.11) and additivity $E(\gamma)+E(\gamma') = E(\gamma*\gamma')$ of the energy, as well as the co-area formula from Lemma 1.3.13. A similar calculation can be made in the case $x \in \partial M$.
This shows that if (1.3.6) holds for partitions τ of length N, then it also holds for partitions τ of length less or equal than $2N$. In total, (1.3.6) holds for all partitions. ☐

The remainder of this section is dedicated to giving a proof of Prop. 1.3.18. This is split up into several lemmas. We generally assume that we are in the setup of Thm. 1.3.14, i.e. L is a self-adjoint Laplace type operator with involutive boundary conditions B, acting on sections of a metric vector bundle $\mathcal{V}$ over a compact Riemannian manifold M with boundary. By Lemma 1.1.2, we have $L = \nabla^*\nabla + V$ for a unique metric connection ∇ on $\mathcal{V}$ and a symmetric endomorphism field $V \in C^\infty(M, \mathrm{End}(\mathcal{V}))$.

Lemma 1.3.19. *Let α be a bound on the pointwise operator norm of V. Then for the path-ordered integral $\mathcal{P}_B(\gamma)$ determined by L, we have*

$$|\mathcal{P}_B(\gamma)^{-1}| \leq e^{(b-a)\alpha}$$

where $\gamma : [a,b] \longrightarrow M$ is any absolutely continuous path and $|-|$ denotes the pointwise operator norm.

Proof. Suppose first that $\gamma(s) \in M \setminus \partial M$ for $s \in (0,t)$. Let $Q(s)$ be the solution to the ordinary differential equation (1.1.14). Then

$$\begin{aligned}
2|Q(s)|\frac{\mathrm{d}}{\mathrm{d}s}|Q(s)| = \frac{\mathrm{d}}{\mathrm{d}s}|Q(s)|^2 &= 2\langle Q(s), \nabla_s Q(s)\rangle = -2\big\langle Q(s), V\big(\gamma(s)\big)Q(s)\big\rangle\\
&\leq 2|Q(s)|\big|V\big(\gamma(s)\big)Q(s)\big| \leq 2\alpha|Q(s)|^2,
\end{aligned}$$

hence

$$\frac{\mathrm{d}}{\mathrm{d}s}|Q(s)| \leq \alpha |Q(s)|.$$

From Gronwall's lemma [Die69, 10.5.1.3], we obtain therefore $|\mathcal{P}_B(\gamma)^{-1}| = |Q(t)| \leq e^{t\alpha}$. Now if $\sigma_1 < \cdots < \sigma_k$ are the times in (a,b) that γ hits the boundary, we have

$$\begin{aligned}|\mathcal{P}_B(\gamma)^{-1}| &\leq \big|\mathcal{P}_B\big(\gamma|_{[a,\sigma_1]}\big)^{-1}\big|\big|\mathcal{P}_B\big(\gamma|_{[\sigma_1,\sigma_2]}\big)^{-1}\big|\cdots\big|\mathcal{P}_B\big(\gamma|_{[\sigma_{k-1},\sigma_k]}\big)^{-1}\big|\big|\mathcal{P}_B\big(\gamma|_{[\sigma_k,b]}\big)^{-1}\big| \\ &\leq e^{(\sigma_1-a)\alpha+(\sigma_2-\sigma_1)\alpha+\cdots+(\sigma_k-\sigma_{k-1})\alpha+(b-\sigma_k)\alpha} = e^{(b-a)\alpha},\end{aligned}$$

where we used that B is a self-adjoint involution, hence an isometry. □

Throughout the proof, we use the following notation.

Notation 1.3.20. Let $x \in M$, $t > 0$ and $v \in \Omega_{t,x} \subseteq T_xM$.

(a) If $x \in M \setminus \partial M$, denote by $\gamma_v \in H^{\mathrm{refl}}_{x;\{0<t\}}(M)$ the unique reflected geodesic with $\dot\gamma_v(0) = v$ of length t.

(b) If $x \in \partial M$, and $v \in T_x^{>0}M = \{v \mid \langle v, \mathbf{n}\rangle > 0\}$ is inward directed, denote by $\boldsymbol{\gamma}_v := (\gamma_v, +1) \in H^{\mathrm{refl}}_{x;\{0<t\}}(M)$ the unique reflected geodesic with $\dot\gamma_v(0) = v$ and positive sign.

(c) If $x \in \partial M$, and $v \in T_x^{<0}M = \{v \mid \langle v, \mathbf{n}\rangle < 0\}$ is outward directed, denote by $\boldsymbol{\gamma}_v := (\gamma_v, -1) \in H^{\mathrm{refl}}_{x;\{0<t\}}(M)$ the unique reflected geodesic with $\dot\gamma_v(0) = Rv$ and negative sign.

We defined the smooth structure on $H^{\mathrm{refl}}_{x;\{0<t\}}(M)$ in such a way that the map

$$\Phi : T_xM \supseteq \Omega_{t,x} \longrightarrow H^{\mathrm{refl}}_{x;\{0<t\}}(M), \qquad v \longmapsto \gamma_v$$

is a diffeomorphism for any $x \in M$. The differential $d\Phi|_v$ assigns to a vector $w \in T_xM$ the Jacobi field X_w along γ_v with $X_w(0) = 0$ and $\nabla_s X_w(0+) = w$. Therefore

$$\big(d\Phi|_v w_1, d\Phi|_v w_2\big)_{\Sigma\text{-}H^1} = \langle X_{w_1}(0+), X_{w_2}(0+)\rangle\, t = t\,\langle w_1, w_2\rangle$$

so that Φ is a conformal mapping with

$$\big|\det\big(d\Phi|_v\big)\big| = t^{-n/2}. \tag{1.3.7}$$

Because $|\dot\gamma_v(s)| \equiv |v|$ for all s as γ_v is a piecewise geodesic and R is an isometry, we obtain

$$E(\gamma_v) = \frac{1}{2}\int_0^t |\dot\gamma_v(s)|^2 \mathrm{d}s = \frac{t|v|^2}{2}.$$

Therefore, the transformation formula on the map Φ yields (using that $\Omega_{t,x}$ has full measure in T_xM by Lemma 1.3.5) that

$$P_t u(x) = \int_{T_xM} \varphi_t(v)\, \mathcal{P}(\gamma_v)^{-1} u\big(\gamma_v(t)\big)\mathrm{d}v \tag{1.3.8}$$

where we set $\varphi_t(v) := t^{n/2}(4\pi)^{-n/2}e^{-t|v|^2/4}$. The function φ_t is a simple Gaussian function, where the pre-factor just ensures that it integrates to one over T_xM.

Lemma 1.3.21. *Let α be a bound on the pointwise operator norm of V. Then for all $u \in C^0(M, \mathcal{V})$ and for any $1 \leq p \leq \infty$, $t \geq 0$, we have*

$$\|P_t u\|_{L^p} \leq e^{\alpha t} \|u\|_{L^p}$$

where P_t is the family of Prop 1.3.18.

Because $C^0(M, \mathcal{V})$ is dense in $L^p(M, \mathcal{V})$ if $p < \infty$, Lemma 1.3.21 implies that P_t extends uniquely to a family of bounded operators on $L^p(M, \mathcal{V})$ satisfying the same norm bound for such p. In particular, P_t satisfies property (i) of Prop. 1.3.17 on each of the spaces $L^p(M, \mathcal{V})$, $1 \leq p < \infty$.
In the proof and later, we denote by

$$\pi : TM \longrightarrow M$$

the canonical projection.

Proof. From (1.3.8) follows the estimate

$$\|P_t u\|_\infty \leq \sup_{x \in M} \int_{T_xM} \varphi_t(v) \left|\mathcal{P}_B(\gamma_v)^{-1}\right| \left|u\big(\gamma_v(t)\big)\right| \mathrm{d}v \leq e^{t\alpha} \|u\|_\infty,$$

where we used that $|\mathcal{P}_B(\gamma_v)^{-1}| \leq e^{t\alpha}$ for all v by Lemma 1.3.19, and the fact that the function $\varphi_t(v)$ integrates to one over T_xM. Hence the operator family $(P_t)_{t \geq 0}$ is uniformly bounded near zero on $C^0(M, \mathcal{V})$.
For $1 \leq p < \infty$, we can use Jensen's inequality on the probability measure $\varphi_v(v)\,\mathrm{d}v$ to obtain

$$\|P_t u\|_{L^p}^p \leq \int_{TM} \varphi_t(v) |\mathcal{P}_B(\gamma_v)^{-1}|^p |u\big(\gamma_v(t)\big)|^p \mathrm{d}v \leq e^{tp\alpha} \int_{TM} \varphi_t(v) \big|\pi^* u\big(\Theta_t(v)\big)\big|^p \mathrm{d}v$$

using the definition of the broken billiard flow. Now remember that the broken billiard flow preserves the measure on TM, as well as the norm of vectors, $|\Theta_t(v)| = |v|$, which implies $\varphi_t(v) = \varphi_t(\Theta_s(v))$ for all s. Hence transforming $v \mapsto \Theta_{-t}(v)$ gives

$$\begin{aligned} \int_{TM} \varphi_t(v) \big|\pi^* u\big(\Theta_t(v)\big)\big|^p \mathrm{d}v &= \int_{TM} \varphi_t\big(\Theta_{-t}(v)\big) \big|\pi^* u(v)\big|^p \mathrm{d}v = \int_{TM} \varphi_t(v) \big|\pi^* u(v)\big|^p \mathrm{d}v \\ &= \int_M \big|u(x)\big|^p \int_{T_xM} \varphi_t(v) \mathrm{d}v \, \mathrm{d}x = \|u\|_{L^p}^p. \end{aligned} \tag{1.3.9}$$

This shows the norm bound in the case $p < \infty$. ☐

Lemma 1.3.22. *If $u \in C^0(M, \mathcal{V})$, then also $P_t u \in C^0(M, \mathcal{V})$, for all $t \geq 0$.*

Proof. Choose a local trivialization $\psi : U \times \mathbb{R}^n \longrightarrow TM|_U$ over an open set $U \subseteq M$ that is an isometry in each fiber. Then since $\varphi(v) = \varphi(\psi_x v)$ for each $v \in \mathbb{R}^n$ and each $x \in U$,

$$P_t u(x) = \int_{\mathbb{R}^n} \varphi_t(v) \mathcal{P}_B(\gamma_{\psi_x v})^{-1} u\big(\gamma_{\psi_x v}(t)\big) \mathrm{d}v.$$

If x_j is a sequence in U converging to $x \in U$ as $j \to \infty$, then $\psi_{x_j} v$ converges to $\psi_x v$ in the topology of TM. Therefore, by the Lebesgue's theorem of dominated convergence, it suffices to show that the function

$$f(t, v) := \mathcal{P}_B(\gamma_v)^{-1} u\big(\gamma_v(t)\big)$$

is uniformly bounded and continuous in v at almost all $v \in TM$. The function $u(\gamma_v(t))$ is continuous, since u is continuous and $\gamma_v(t)$ depends continuously on $v \in \Omega_{t,x}$ (because the solutions of ordinary differential equations depend continuously on the initial data). For the same reason, $\mathcal{P}_B(\gamma_v)$ is continuous near all $v \in \Omega_{t,x}$ such that either $\pi(v) \notin \partial M$ or $v \in T_x^{>0} M = \{v \mid \langle v, \mathbf{n} \rangle > 0\}$ for $x \in \partial M$.
It remains to check the case that $v \in T_x^{<0} M = \{v \mid \langle v, \mathbf{n} \rangle < 0\}$ for $x \in \partial M$. To this end, let $v \in TM|_{\partial M}$ be outward directed and let $v_j \in TM$ be a sequence of vectors that converges to v. Let $0 \leq \sigma_{1,j} < \cdots < \sigma_{k,j} < t$ be the times when γ_{v_j} hits the boundary (the number k of hits stabilizes for j large enough). Then

$$\begin{aligned}\mathcal{P}_B(\gamma_{v_j})_B^{-1} = \mathcal{P}(\gamma_{v_j}|_{[0,\sigma_{1,j}]})^{-1} B \mathcal{P}(\gamma_{v_j}|_{[\sigma_{1,j},\sigma_{2,j}]})^{-1} B \cdots& \\ \cdots B \mathcal{P}(\gamma_{v_j}|_{[\sigma_{k-1,j},\sigma_{k,j}]})^{-1} B \mathcal{P}(\gamma_{v_j}|_{[\sigma_{k,j},t]})^{-1}&\end{aligned}$$

and if $0 = \sigma_1 < \cdots < \sigma_k < t$ are the times when γ_v hits the boundary, we have

$$\mathcal{P}_B(\gamma_v)_B^{-1} = B\mathcal{P}(\gamma_v|_{[\sigma_1,\sigma_2]})^{-1} B \cdots B \mathcal{P}(\gamma_v|_{[\sigma_{k-1},\sigma_k]})^{-1} B \mathcal{P}(\gamma_v|_{[\sigma_k,t]})^{-1}$$

Because $\sigma_{i,j} \to \sigma_i$ as $j \to \infty$ (in particular $\sigma_{1,j} \to 0$), $\mathcal{P}(\gamma_{v_j}|_{[0,\sigma_{1,j}]})^{-1}$ converges to the identity in this limit and hence $\mathcal{P}_B(\gamma_{v_j})^{-1}$ converges to $\mathcal{P}_B(\gamma_v)^{-1}$. □

Lemma 1.3.22 together with Lemma 1.3.21 shows that P_t preserves the space $C^0(M, \mathcal{V})$ and that the family $(P_t)_{t \geq 0}$ satisfies property (i) of Prop. 1.3.17 on this space.

From now on, we assume that we have $V = 0$, that is $L = \nabla^* \nabla$ in the decomposition from Lemma 1.1.2. Then $\mathcal{P}_B(\gamma) = [\gamma\|_0^t]_B$, the B-parallel transport, so that (1.3.8) reads

$$P_t u(x) = \int_{T_x M} \varphi_t(v) [\gamma_v\|_0^t]_B^{-1} \pi^* u\big(\Theta_t(v)\big) \mathrm{d}v, \tag{1.3.10}$$

using the definition of the broken billiard flow. Now substituting $v \mapsto v t^{-1/2}$, we obtain

$$P_t u(x) = \int_{T_x M} \varphi(v) [\gamma_v\|_0^{t^{1/2}}]_B^{-1} \pi^* u\big(\Theta_{t^{1/2}}(v)\big) \mathrm{d}v,$$

where we set $\varphi(v) := \varphi_1(v)$ and used that $\Theta_t(sv) = s\Theta_{ts}(v)$ (which follows from (1.3.2)) and the fact that $\pi^* u(t^{-1/2}\Theta_{t^{1/2}}(v)) = \pi^* u(\Theta_{t^{1/2}}(v))$. This suggests defining

$$Q_t u(x) := P_{t^2} u(x) = \int_{T_x M} \varphi(v) [\gamma_v\|_0^t]_B^{-1} \pi^* u\big(\Theta_t(v)\big) \mathrm{d}v \tag{1.3.11}$$

for $u \in C^0(M, \mathcal{V})$. Because Q_t is just a rescaling of P_t, Q_t, $t \geq 0$ extends to a uniformly bounded family of operators just as P_t. Notice that Q_t is actually well defined for all $t \in \mathbb{R}$ with $Q_0 = \mathrm{id}$.

Lemma 1.3.23. *In the case $V = 0$, the operator family $(Q_t)_{t\in\mathbb{R}}$ (and hence also $(P_t)_{t\geq 0}$), is strongly continuous on $L^p(M, \mathcal{V})$ for any $1 \leq p < \infty$.*

Proof. We first show that for each $u \in C^0(M, \mathcal{V})$ and any $x \in M$, the function $t \mapsto Q_t u(x)$ is continuous. For $u \in C^0(M, \mathcal{V})$, consider the function

$$f(t, v) := [\gamma_v\|_0^t]_B^{-1}\pi^* u\big(\Theta_t(v)\big) = [\gamma_v\|_0^t]_B^{-1} u\big(\gamma_v(t)\big).$$

for $t \in \mathbb{R}$, $v \in T_xM$. If for a given $t_0 \in \mathbb{R}$, we have $\gamma_v(t) \notin \partial M$ (which is the case for almost all v), then $f(t, v)$ is clearly continuous in t. Therefore $\varphi(v)f(t, v) \to \varphi(v)f(t_0, v)$ as $t \to t_0$ for almost all $v \in T_xM$. Since $\varphi(v)f(t, v) \leq \|u\|_\infty \varphi(v)$, we also found a dominating integrable function, hence

$$Q_t u(x) = \int_{T_xM} \varphi(v)f(t, v)\mathrm{d}v \longrightarrow \int_{T_xM} \varphi(v)f(t_0, v)\mathrm{d}v = Q_{t_0}u(x)$$

as $t \to t_0$, by the dominated convergence theorem. Furthermore, since $u \in C^0(M, \mathcal{V})$, $Q_t u$ is uniformly bounded for t in compact subsets of $\mathbb{R}$, by Lemma 1.3.21, and we have $Q_t u \to Q_{t_0} u$ pointwise almost everywhere as $t \to t_0$, hence also $Q_t u \to Q_{t_0} u$ in L^p, again by the dominated convergence theorem.
For a general $u \in L^p(M, \mathcal{V})$, choose a family of continuous sections $u_k \in C^0(M, \mathcal{V})$ such that $u_k \to u$ in L^p. Then

$$\|Q_t u - Q_{t_0} u\|_{L^p} \leq \|Q_t(u - u_k)\|_{L^p} + \|Q_{t_0}(u_k - u)\|_{L^p} + \|Q_t u_k - Q_{t_0} u_k\|_{L^p}.$$

By the uniform boundedness of the family $(Q_t)_{t\in\mathbb{R}}$, one can now choose first k large enough to make the first two terms as small as one likes and then t close enough to t_0 to make the third term arbitrarily small. This shows that $Q_t u \to Q_{t_0} u$ as $t \to t_0$ in the general case, hence $(Q_t)_{r\in\mathbb{R}}$ is strongly continuous on $L^p(M, \mathcal{V})$, for all $1 \leq p < \infty$. □

Lemma 1.3.24. *In the case $V = 0$, the operator family $(Q_t)_{t\in\mathbb{R}}$ (and hence also $(P_t)_{t\geq 0}$), is strongly continuous on $C^0(M, \mathcal{V})$.*

Proof. Fix $t \in \mathbb{R}$. For any $x \in M$, $s \in \mathbb{R}$ and $u \in C^0(M, \mathcal{V})$, we have

$$\big|Q_t u(x) - Q_s u(x)\big| \leq \int_{T_xM} \varphi(v)\big|[\gamma_v\|_0^t]_B^{-1} u\big(\gamma_v(t)\big) - [\gamma_v\|_0^s]_B^{-1} u\big(\gamma_v(s)\big)\big|\mathrm{d}v.$$

Let $\varepsilon > 0$ and choose $R > 0$ so large that

$$2\|u\|_\infty \int_{B_R(0)^c} \varphi(v)\mathrm{d}v \leq \frac{\varepsilon}{2}.$$

Now because $u \in C^0(M, \mathcal{V})$ and M is compact, u is uniformly continuous. Therefore, there exists $\delta > 0$ such that

$$\big|[\gamma_v\|_0^t]_B^{-1} u\big(\gamma_v(t)\big) - [\gamma_v\|_0^s]_B^{-1} u\big(\gamma_v(s)\big)\big| \leq \frac{\varepsilon}{2}\left(\int_{B_R(0)} \varphi(v)\mathrm{d}v\right)^{-1}$$

for all $v \in TM$ with $|v| \leq R$ and all s with $|t-s| \leq \delta$. Because

$$\big|[\gamma_v\|_0^t]_B^{-1} u\big(\gamma_v(t)\big) - [\gamma_v\|_0^s]_B^{-1} u\big(\gamma_v(s)\big)\big| \leq 2\|u\|_\infty$$

as $[\gamma_v\|_0^t]_B^{-1}$ is a fiberwise isometry, we obtain in total that

$$\begin{aligned}
&\big|Q_t u(x) - Q_s u(x)\big| \\
&\leq \int_{B_R(0)} \varphi(v)\big|[\gamma_v\|_0^t]_B^{-1} u\big(\gamma_v(t)\big) - [\gamma_v\|_0^s]_B^{-1} u\big(\gamma_v(s)\big)\big| \mathrm{d}v + 2\|u\|_\infty \int_{B_R(0)^c} \varphi(v) \\
&\leq \frac{\varepsilon}{2} + \frac{\varepsilon}{2} \leq \varepsilon.
\end{aligned}$$

for all $x \in M$, whenever $|t-s| \leq \delta$. The lemma follows. □

Lemma 1.3.25. *Let $u \in C^2_B(M, \mathcal{V})$, meaning that u is a C^2 section of $\mathcal{V}$ satisfying the involutive boundary condition given by B. Then for each $x \in M$, the function $t \mapsto Q_t u(x)$ is C^2 and we have*

$$\begin{aligned}
Q_t' u(x) &= \int_{T_xM} \varphi(v)[\gamma_v\|_0^t]_B^{-1} \nabla_{\Theta_t(v)} u\big(\gamma_v(t)\big)\, \mathrm{d}v, \\
Q_t'' u(x) &= \int_{T_xM} \varphi(v)[\gamma_v\|_0^t]_B^{-1} \nabla^2 u|_{\gamma_v(t)}\big[\Theta_t(v), \Theta_t(v)\big]\, \mathrm{d}v.
\end{aligned}$$

Proof. Set as before

$$f(t,v) := [\gamma_v\|_0^t]_B^{-1} \pi^* u\big(\Theta_t(v)\big).$$

We first show that given $v \in T_xM$, $f(t,v)$ is $C^{1,1}$ on the interval $[0, T(v))$, where $T(v)$ is the maximal life-time of the reflected geodesic γ_v with $\dot\gamma_v(0+) = v$ (respectively $\dot\gamma_v(0+) = Rv$ if $v \in TM|_{\partial M}$ and v is outward directed). Let $0 \leq \sigma_1 < \sigma_2 < \cdots < T(v)$ be the times in this interval where γ_v hits the boundary (these are finitely many if $T(v)$ is finite, but may be infinitely many otherwise). Then clearly, $f(t,v)$ is C^2 on $[0, T(v)) \setminus \{\sigma_1, \sigma_2, \dots\}$ with

$$\begin{aligned}
\frac{\partial f}{\partial t}(t,v) &= [\gamma_v\|_0^t]_B^{-1} \nabla_{\Theta_t(v)} u\big(\gamma_v(t)\big), \\
\frac{\partial^2 f}{\partial t^2}(t,v) &= [\gamma_v\|_0^t]_B^{-1} \nabla^2 u|_{\gamma_v(t)}\big[\Theta_t(v), \Theta_t(v)\big].
\end{aligned}$$

Here we used that $\nabla_t \Theta_t(v) = 0$, which follows from the fact that $\Theta_t(v)$ is the velocity vector field of a geodesic. We need to check continuity of the derivatives at the times σ_j. Decompose $\dot\gamma_v(\sigma_j+) = w' + w_0\mathbf{n}$ with $w' \in T_{\gamma(\sigma_j)}\partial M$ and $w_0 \in \mathbb{R}$, so that $\dot\gamma_v(\sigma_j-) = w' - w_0\mathbf{n}$. Then because u satisfies the boundary condition, we have $u|_{\partial M} \in C^\infty(\partial M, \mathcal{W}^+)$ and $\nabla_{\mathbf{n}} u|_{\partial M} \in C^\infty(\partial M, \mathcal{W}^-)$, hence

$$Bu\big(\gamma_v(\sigma_j)\big) = u\big(\gamma_v(\sigma_j)\big), \qquad B\nabla_{\mathbf{n}} u\big(\gamma_v(\sigma_j)\big) = -\nabla_{\mathbf{n}} u\big(\gamma_v(\sigma_j)\big),$$

and

$$\begin{aligned}
B\nabla_{\dot\gamma_v(\sigma_j+)} u\big(\gamma_v(\sigma_j)\big) &= B\nabla_{w'} u\big(\gamma_v(\sigma_j)\big) + w_0 B\nabla_{\mathbf{n}} u\big(\gamma_v(\sigma_j)\big) \\
&= \nabla_{w'} u\big(\gamma_v(\sigma_j)\big) - w_0 \nabla_{\mathbf{n}} u\big(\gamma_v(\sigma_j)\big) \\
&= \nabla_{\dot\gamma_v(\sigma_j-)} u\big(\gamma_v(\sigma_j)\big).
\end{aligned} \tag{1.3.12}$$

For the second equality, notice that if $\eta : (-\varepsilon, \varepsilon) \longrightarrow \partial M$ with $\dot{\eta}(0) = w'$, then

$$\nabla_{w'} u\big(\gamma_v(\sigma_j)\big) = \nabla_s\big|_{s=0}\big\{u\big(\eta(s)\big)\big\} \in \mathcal{W}^+,$$

since $u(\eta(s)) \in \mathcal{W}^+$ for each s and the splitting is parallel by assumption. Hence indeed $B\nabla_{w'} u\big(\gamma_v(\sigma_j)\big) = \nabla_{w'} u\big(\gamma_v(\sigma_j)\big)$. Now by (1.3.12) and the definition of $[\gamma_v\|_0^{\sigma_j+}]_B^{-1}$, we have

$$\begin{aligned} \frac{\partial f}{\partial t}(\sigma_j+, v) &= [\gamma_v\|_0^{\sigma_j+}]_B^{-1} \nabla_{\dot{\gamma}_v(\sigma_j+)} u\big(\gamma_v(\sigma_j)\big) \\ &= [\gamma_v\|_0^{\sigma_j+}]_B^{-1} B \nabla_{\dot{\gamma}_v(\sigma_j-)} u\big(\gamma_v(\sigma_j)\big) \\ &= [\gamma_v\|_0^{\sigma_j-}]_B^{-1} \nabla_{\dot{\gamma}_v(\sigma_j+)} u\big(\gamma_v(\sigma_j)\big) = \frac{\partial f}{\partial t}(\sigma_j-, v) \end{aligned}$$

so that the derivative is indeed continuous.
To check that the derivative of f is Lipschitz, notice that

$$\left|\frac{\partial^2 f}{\partial t^2}(t, v)\right| \leq \|\nabla^2 u\|_\infty |v|^2 =: \ell(v)$$

so that $\frac{\partial f}{\partial t}(t, v)$ is uniformly Lipschitz with Lipschitz constant $\ell(v)$. Now because the function $\varphi(v) f(t, v)$ is C^1 in t for almost all v, with integrable derivative, we may differentiate under the integral sign to obtain

$$Q' u(x) = \int_{T_x M} \varphi(v)\, \frac{\partial f}{\partial t}(t, v)\, \mathrm{d}v = \int_{T_x M} \varphi(v) [\gamma_v\|_0^t]_B^{-1} \nabla_{\Theta_t(v)} u\big(\gamma_v(t)\big)\, \mathrm{d}v.$$

For the second derivative, note that we have

$$\lim_{\varepsilon \to 0} \frac{1}{\varepsilon}\left(\frac{\partial f}{\partial t}(t+\varepsilon, v) - \frac{\partial f}{\partial t}(t, v)\right) = \frac{\partial^2 f}{\partial t^2}(t, v)$$

for almost all v (since for fixed t, $\gamma_v(t) \notin \partial M$ for almost all v) and

$$\left|\frac{1}{\varepsilon}\left(\frac{\partial f}{\partial t}(t+\varepsilon, v) - \frac{\partial f}{\partial t}(t, v)\right)\right| \leq \ell(v)$$

by the considerations before. Hence $\varphi(v)\ell(v)$ is an integrable dominating function for the difference quotient, and

$$\begin{aligned} Q_t'' u(x) &= \lim_{\varepsilon \to 0} \int_{T_x M} \varphi(v) \frac{1}{\varepsilon}\left(\frac{\partial f}{\partial t}(t+\varepsilon, v) - \frac{\partial f}{\partial t}(t, v)\right) \mathrm{d}v \\ &= \int_{T_x M} \varphi(v) \lim_{\varepsilon \to 0} \frac{1}{\varepsilon}\left(\frac{\partial f}{\partial t}(t+\varepsilon, v) - \frac{\partial f}{\partial t}(t, v)\right) \mathrm{d}v \\ &= \int_{T_x M} \varphi(v) \frac{\partial^2 f}{\partial t^2}(t, v) \mathrm{d}v, \end{aligned}$$

where the exchange of integration and taking the limit is justified by the dominated convergence theorem. Continuity of $Q_t'' u(x)$ in t can be shown just as in the proof of Lemma 1.3.23. □

Proof (of Prop. 1.3.18). The proof consists of two steps.
Step 1. Assume that $V=0$ so that $P_t = Q_{t^{1/2}}$, with Q_t given by (1.3.11). In this case we already know from the Lemmas 1.3.21 and 1.3.23, respectively Lemma 1.3.24 that P_t satisfies properties (i)-(ii) of Prop. 1.3.17 on each of the spaces $L^p(M,\mathcal{V})$ with $1 \leq p < \infty$ and $C^0(M,\mathcal{V})$, so it remains to verify property (iii). To this end, for $u \in C^2_B(M,\mathcal{V})$, notice that

$$Q_0' u(x) = \int_{T_xM} \varphi(v) \nabla_v u(x) \mathrm{d}v = 0,$$

since the integrand is an odd function. Therefore, pointwise Taylor expansion yields

$$Q_t u(x) = u(x) + \int_0^t (t-s) Q_s'' u(x) \mathrm{d}s = u(x) + t^2 \int_0^1 (1-s) Q_{ts}'' u(x) \mathrm{d}s. \tag{1.3.13}$$

The Taylor expansion is justified since $t \mapsto Q_t u(x)$ is C^2 for all $x \in M$, by Lemma 1.3.25. Formula (1.3.13) implies that for each $x \in M$, we have

$$\frac{1}{t}\big(P_t u(x) - u(x)\big) = \int_0^1 (1-s) Q''_{t^{1/2}s} u(x) \mathrm{d}s, \tag{1.3.14}$$

so that limit evaluates to

$$\lim_{t\to 0} \frac{1}{t}\big(P_t u(x) - u(x)\big) = \int_0^1 (1-s) Q_0'' u(x) \mathrm{d}s = \frac{1}{2} Q_0'' u(x),$$

as $t \mapsto Q_t'' u(x)$ is continuous. Here we have

$$Q_0'' u(x) = \int_{T_xM} \varphi(v) \nabla^2 u|_x[v,v] \mathrm{d}v = 2\,\mathrm{tr}\, \nabla^2 u|_x = -2Lu(x),$$

where the second equality is an elementary result for Gaussian integrals. Hence for any $x \in M$.

$$\lim_{t\to 0} \frac{1}{t}\big(P_t u(x) - u(x)\big) = -Lu(x).$$

Furthermore, one shows similarly to the proof of Lemma 1.3.24 that the convergence here is even uniformly in x, so that this convergence is true in the spaces $C^0(M,\mathcal{V})$ and $L^p(M,\mathcal{V})$. By parabolic regularity up to the boundary (which follows e.g. from Thm. 2.1.1 (iii) below), we have $e^{-tL}v \in C^\infty_B(M,\mathcal{V})$ for each $v \in L^p(M,\mathcal{V})$, so it indeed satisfies to check this limit for $u \in C^2_B(M,\mathcal{V})$. This proves property (iii) in the case that $V=0$.
Step 2. For the case that $V \neq 0$, we use the Taylor expansion

$$\mathcal{P}(\gamma)_B^{-1} = [\gamma\|_0^t]_B^{-1} - \int_0^t \mathcal{P}_B(\gamma|_{[0,s]})^{-1} V\big(\gamma(s)\big) [\gamma\|_s^t]_B^{-1} \mathrm{d}s.$$

Let P_t be defined as in the proposition for the operator $L = \nabla^*\nabla + V$ and write $\widetilde{P}_t$ for the operator family corresponding to the operator $\widetilde{L} := \nabla^*\nabla$. Then by (1.3.8), we have for $u \in C^0(M,\mathcal{V})$

$$P_t u(x) = \widetilde{P}_t u(x) - \int_0^t \int_{T_xM} \varphi_t(v) \mathcal{P}_B\big(\gamma_v|_{[0,s]}\big)^{-1} V\big(\gamma_v(s)\big) [\gamma_v\|_s^t]_B^{-1} u\big(\gamma_v(t)\big)\, \mathrm{d}v\, \mathrm{d}s.$$

Setting $\alpha := \|V\|_\infty$, Jensen's inequality and Lemma 1.3.19 imply

$$\begin{aligned}\|P_t u - \widetilde{P}_t u\|_{L^p}^p &= t^p \int_M \left| \frac{1}{t} \int_0^t \int_{T_xM} \varphi_t(v) \mathcal{P}_B\big(\gamma_v|_{[0,s]}\big)^{-1} V\big(\gamma_v(s)\big) [\gamma_v\|_s^t]_B^{-1} u\big(\gamma_v(t)\big) \mathrm{d}v \, \mathrm{d}s \right|^p \mathrm{d}x \\ &\leq t^{p-1} \int_0^t \alpha e^{\alpha s} \int_{TM} \varphi_t(v) \big|u\big(\gamma_v(t)\big)\big|^p \mathrm{d}v \, \mathrm{d}s = \|u\|_{L^p}^p t^{p-1} (e^{\alpha t} - 1)\end{aligned}$$

where in the last step, we used the calculation (1.3.9). This shows that $P_t - \widetilde{P}_t$ converges to zero in norm as $t \to 0$, hence P_t is strongly continuous at zero on L^p (since $\widetilde{P}_t$ is, by Lemma 1.3.23). For the C^0 case, we similarly find $\|P_t u - \widetilde{P}_t u\|_{C^0} \leq \alpha t e^{\alpha t} \|u\|_{C^0}$, so P_t is also strongly continuous at zero on C^0 (by virtue of Lemma 1.3.24). Strong continuity near $t_0 \neq 0$ can be shown similar as before, by using the fact that the integrand

$$\int_0^t \varphi_t(v) \mathcal{P}_B\big(\gamma_v|_{[0,s]}\big)^{-1} V\big(\gamma_v(s)\big) [\gamma_v\|_s^t]_B^{-1} u\big(\gamma_v(t)\big) \, \mathrm{d}v$$

depends continuously on t near $t_0 \neq 0$ for almost all $v \in T_xM$ and has a dominating integrable function.

It remains to check that P_t has the correct infinitesimal generator. From the Taylor expansion above follows that

$$\begin{aligned}\frac{1}{t}\big(P_t u(x) - u(x)\big) &= \frac{1}{t}\big(\widetilde{P}_t u(x) - u(x)\big) \\ &\qquad - \frac{1}{t} \int_0^t \int_{T_xM} \varphi_t(v) \mathcal{P}_B\big(\gamma_v|_{[0,s]}\big)^{-1} V\big(\gamma_v(s)\big) [\gamma_v\|_s^t]_B^{-1} u\big(\gamma_v(t)\big) \, \mathrm{d}v \, \mathrm{d}s\end{aligned}$$

The first term converges to $-\widetilde{L}u(x) = -\nabla^*\nabla u(x)$ uniformly by Step 1, while the second term converges uniformly to $-Vu(x)$, which can be shown similar to the proof of Lemma 1.3.24. This finishes the proof in the general case. □

Chapter 2

The Heat Kernel as a Path Integral

This chapter is dedicated to representing the heat kernel of a Laplace type operator as a path integral. In order to do this, we need to study of the heat kernel and its short time asymptotics, which will be discussed in the first Section 2.1. In this section, we also introduce convolution approximation of the heat kernel, which will be the key to derive the path integral formulas from Section 2.2.
If M has a boundary, it is essential to find the right path spaces to obtain path integral formulas. It turns out that the right step is to consider M as an orbifold. This will be explained in Section 2.3.

2.1 The Heat Kernel and its Asymptotic Expansion

This section is the analytical core of the chapter. We first repeat some general facts regarding the heat kernel and its short time asymptotic expansion (Subsections 2.1.1 and 2.1.2). Related to this, we introduce the Brownian bridge, a stochastic process associated to the heat kernel just as the Brownian motion is associated to the heat operator. Finally in Subsection 2.1.4, we show how to approximate the heat kernel by certain convolutions of other kernels, which will be the main result enabling us to obtain path integral formulas.

2.1.1 The Heat Kernel of a Riemannian Manifold

Let M be a compact n-dimensional Riemannian manifold, possibly with boundary and let L be a self-adjoint Laplace type operator with involutive boundary conditions, acting on sections of a metric vector bundle $\mathcal{V}$ over M. As noted before, the heat semigroup e^{-tL} is smoothing for $t > 0$ and therefore given by a smooth integral kernel,

$$(e^{-tL}u)(x) = \int_M p_t^L(x,y)u(y)\mathrm{d}y.$$

This follows from a smooth version of the Schwartz kernel theorem (see Prop. 2.14 in [BGV04]). $p_t^L(x,y)$ is called the *heat kernel*. It is a time-dependent smooth section of the bundle $\mathcal{V} \boxtimes \mathcal{V}^*$ over $M \times M$, the fiber of which at a point $(x,y) \in M \times M$ is $\mathcal{V}_x \otimes \mathcal{V}_y^* \cong \mathrm{Hom}(\mathcal{V}_y, \mathcal{V}_x)$. In terms of the spectral decomposition (λ_k, ϕ_k) of L, it is given by the formula (1.1.4) above.

There are a few cases where $p_t^L(x,y)$ can be given explicitly. For example on $\mathbb{R}^n$, the heat kernel of the Laplace-Beltrami operator is given by

$$\mathrm{e}_t(x,y) = (4\pi t)^{-n/2} \exp\left(-\frac{1}{4t} d(x,y)^2\right), \tag{2.1.1}$$

where $d(x,y) = |x-y|$ is the Euclidean distance. There are also formulas for the heat kernel on hyperbolic space [GN98] or spheres [FJW85], albeit the latter formula is already much less explicit. Notice that the function (2.1.1) makes sense on any complete Riemannian manifold M, if one takes for $d(x,y)$ the Riemannian distance in M. $\mathrm{e}_t(x,y)$ is then a smooth function on the set

$$M \bowtie M := \big\{(x,y) \in M \times M \;\mid\; \text{there exists a unique minimizing geodesic connecting } x \text{ and } y\big\} \tag{2.1.2}$$

of points that do not lie in the mutual cut locus. $\mathrm{e}_t(x,y)$ will be called the *Euclidean heat kernel* and will play an important role when it comes to approximating general heat kernels.

The heat kernel has the following properties (see e.g. [BGV04, Chapter 2]).

Theorem 2.1.1 (On the Heat Kernel). *Let $p_t^L(x,y)$ be the heat kernel of a self-adjoint Laplace type operator L endowed with involutive boundary conditions, acting on sections of a vector bundle $\mathcal{V}$ of a compact Riemannian manifold with boundary M. Then the following is true.*

(i) $\lim_{t\to 0} \int_M p_t^L(x,y)u(y)\mathrm{d}y = u(x)$ *uniformly in x for all $u \in C^0(M,\mathcal{V})$;*

(ii) $p_t^L(x,y)$ *satisfies the heat equation in any of the two variables when the other is fixed;*

(iii) $p_t^L(x,y)$ *satisfies the boundary condition with respect to both variables;*

(iv) we have $\int_M p_t^L(x,z)p_s^L(z,y)\mathrm{d}z = p_{t+s}^L(x,y)$.

Furthermore, if $q_t(x,y)$ is any time-dependent section of $\mathcal{V} \boxtimes \mathcal{V}^*$ which is C^1 in the t variable and C^2 in the x and y variables and satisfies (i) $-$ (iii) above, then $q_t(x,y) = p_t^L(x,y)$.

2.1.2 Near-Diagonal Asymptotics of the Heat Kernel

Let M be a *closed* Riemannian manifold of dimension n and let L be a self-adjoint Laplace-type operator, acting on sections of a metric vector bundle $\mathcal{V}$ over M. Let $p_t^L(x,y)$ be the corresponding heat kernel. It is a well-known fact that the heat kernel $p_t^L(x,y)$ has a short time asymptotic expansion of the form

$$p_t^L(x,y) \;\sim\; \mathrm{e}_t(x,y) \sum_{j=0}^{\infty} t^j \frac{\Phi_j(x,y)}{j!}, \tag{2.1.3}$$

where $\mathrm{e}_t(x,y)$ is the Euclidean heat kernel introduced in (2.1.1). One way to make the asymptotic relation (2.1.3) precise is as follows: There exist smooth sections $\Phi_j(x,y)$ of the bundle $\mathcal{V} \boxtimes \mathcal{V}^*$ defined on $M \bowtie M$ such that for any $\nu > n/2$, $T > 0$ and for any compact subset $K \subset M \bowtie M$, there exists $C > 0$ such that

$$\left| p_t^L(x,y) - \mathrm{e}_t(x,y) \sum_{j=0}^{\nu} t^j \frac{\Phi_j(x,y)}{j!} \right| \leq C t^{\nu+1-n/2} \tag{2.1.4}$$

whenever $(x,y) \in K$ and $0 < t \leq T$. This result is proved in [BGV04, Thm. 2.30], [BGM71, III.E], [Ros97, Prop. 3.23], [Roe98, Thm. 7.15] and many more.
The coefficients $\Phi_j(x,y)$ are uniquely determined as solutions to the *recursive transport equations* [BGV04, Thm. 2.26]

$$(\nabla_{\mathcal{R}} + G - n/2 + j)\Phi_j = -jL\Phi_{j-1} \tag{2.1.5}$$

with respect to the x variable, subject to the initial condition $\Phi_0(x,x) = \mathrm{id}$. Here ∇ is the connection determined by L as in Lemma 1.1.2 and

$$\mathcal{R}(x,y) = \frac{1}{2}\operatorname{grad}_x d(x,y)^2, \qquad G(x,y) = -\frac{\Delta_x d(x,y)^2}{4}. \tag{2.1.6}$$

One can show that these equations possess unique solutions Φ_j, given the initial condition.

Remark 2.1.2 (The Jacobian of the Exponential Map). An important object related to the heat kernel coefficients is the Jacobian of the exponential map

$$J(x,y) := \big|\det\big(d\exp_x|_{\dot\gamma_{xy}(0)}\big)\big|, \tag{2.1.7}$$

where γ_{xy} is the unique minimizing geodesic travelling from x to y in time one. J is well-defined and smooth on all of $M \bowtie M$. $J(x,y)$ has the Taylor expansion

$$J(x,y) = 1 - \frac{1}{6}\mathrm{ric}\big(\dot\gamma_{xy}(0), \dot\gamma_{xy}(0)\big) + O\big(d(x,y)^3\big) \tag{2.1.8}$$

near the diagonal in $M \times M$, where γ_{xy} denotes the shortest geodesic connecting x to y in time one (see the proof of Lemma 4.7 in [BP08]). This function will play an important role in the course of this thesis; in particular, it will turn out that J has a representation in terms of the energy functional on the space of paths between x and y (see Corollary 3.2.11). On manifolds of constant sectional curvature κ (where $\mathrm{ric} = \kappa(n-1)g$), one has in the case that $\kappa > 0$

$$J(x,y) = \left(\frac{\sin\big(\sqrt{\kappa}\, d(x,y)\big)}{\sqrt{\kappa}\, d(x,y)}\right)^{n-1}, \tag{2.1.9}$$

see [Hsu02, Example 5.1.2]. In the case that $\kappa < 0$, sin has to be replaced by sinh.

Example 2.1.3 (The first two Coefficients). The first heat kernel coefficient can be expressed in terms of the function $J(x,y)$ by

$$\Phi_0(x,y) = J(x,y)^{-1/2}[\gamma_{xy}\|_0^1]^{-1}, \tag{2.1.10}$$

where $[\gamma_{xy}\|_0^1]$ denotes the parallel transport along γ_{xy}. For the second coefficient, there is no such expression off the diagonal, but it can be explicitly computed on the diagonal, namely we have

$$\Phi_1(x,x) = \left(\frac{1}{6}\mathrm{scal}(x) - V(x)\right)[\gamma_{xy}\|_0^t]^{-1}, \tag{2.1.11}$$

where scal denotes the scalar curvature and V denotes the potential determined by the Laplace type operator L in the respresentation $L = \nabla^*\nabla + V$ from Lemma 1.1.2 (see equation (16) in [BP08]).

Remark 2.1.4. There are several equivalent ways to write down the transport equations (2.1.5), which result in slightly different coefficients. The coefficients Ψ_j from [BGV04, Thm. 2.26] are related to ours by $\Phi_j(x,y) = j!J(x,y)^{-1/2}\Psi_j(x,y)$, where J is the Jacobian of the exponential map and the Ψ_j satisfy

$$(\nabla_{\mathcal{R}} + j)\Psi_j = -J^{1/2}L\big\{J^{-1/2}\Psi_{j-1}\big\}$$

with the convention $\Psi_{-1} = 0$. In [Roe98, (7.17)] and [Cha84, p. 149], the equations are

$$(\nabla_{\mathcal{R}} + G - n/2 + j)\widetilde{\Phi}_j = -L\widetilde{\Phi}_{j-1},$$

and the resulting coefficients $\widetilde{\Phi}_j$ compare to our coefficients by $\Phi_j(x,y) = j!\widetilde{\Phi}_j(x,y)$.

The statement (2.1.4) is sufficient to show results related to the heat kernel along the diagonal, such as Weyl asymptotics, the local Atiyah-Singer index theorem and many more. For our purposes, this is not enough, however, because we need more information about the *off-diagonal* behavior of the heat kernel. In fact, the following much stronger result is true; a proof is given in Appendix A.

Theorem 2.1.5 (Strong Heat Kernel Asymptotics). *Let $p_t^L(x,y)$ by the heat kernel of a Laplace type operator L, acting on sections of a metric vector bundle $\mathcal{V}$ over a closed Riemannian manifold M. Let K be a compact subset of $M \bowtie M$ and fix $T > 0$ and $\nu, m, l \in \mathbb{N}_0$. Then there exists a constant $C > 0$ such that*

$$\left|\nabla_x^l\nabla_y^m\left\{\frac{p_t^L(x,y)}{\mathrm{e}_t(x,y)} - \sum_{j=0}^{\nu} t^j\frac{\Phi_j(x,y)}{j!}\right\}\right| \leq Ct^{\nu+1} \tag{2.1.12}$$

for all $(x,y) \in K$ and $0 < t \leq T$.

This implies that for any ν, we have

$$\lim_{t\to 0} t^{-\nu}\left(\frac{p_t^L(x,y)}{\mathrm{e}_t(x,y)} - \sum_{j=0}^{\nu} t^j\frac{\Phi_j(x,y)}{j!}\right) = 0$$

in the topological vector space $C^\infty(M \bowtie M, \mathcal{V} \boxtimes \mathcal{V}^*)$ (with its Fréchet topology). Hence we have the complete asymptotic expansion

$$\frac{p_t^L(x,y)}{\mathrm{e}_t(x,y)} \sim \sum_{j=0}^{\infty} t^j\frac{\Phi_j(x,y)}{j!} \tag{2.1.13}$$

in $C^\infty(M \bowtie M, \mathcal{V} \boxtimes \mathcal{V}^*)$.
Thm. 2.1.5 directly implies the result (2.1.4), by setting $m = l = 0$ and multiplying by $\mathrm{e}_t(x, y)$; in fact, this way one obtains the following much stronger result.

Corollary 2.1.6. *Under the assumptions of Thm. 2.1.5, for any $T > 0$, any $\nu, m, l \in \mathbb{N}_0$ and any compact subset K of $M \bowtie M$, there exists a constant $C > 0$ such that*

$$\left|\nabla_x^l \nabla_y^m \Bigl\{p_t^L(x, y) - \mathrm{e}_t(x, y) \sum_{j=0}^{\nu} t^j \frac{\Phi_j(x, y)}{j!}\Bigr\}\right| \leq C\mathrm{e}_t(x, y)\, t^{\nu+1} \left(\frac{d(x, y)}{t}\right)^{l+m},$$

whenever $0 < t \leq T$ and $(x, y) \in K$.

Proof. This follows directly from Thm. 2.1.5 by pulling out the $\mathrm{e}_t(x, y)$ term and calculating its derivatives. □

Remark 2.1.7. The statement of Thm. 2.1.5 is indeed much stronger than (2.1.4). Dividing (2.1.4) by $\mathrm{e}_t(x, y)$, one can only conclude that the remainder is of the order $O(t^{N+1}e^{d(x,y)^2/4t})$, which increases exponentially away from the diagonal as $t \downarrow 0$.

The strong heat kernel asymptotics seem to be somewhat folklore; similar results go back to Molchanov [Mol75], Azencott [Aze84], Watanabe [Wat87] and Ben Arous [Aro88], all relying on techniques from stochastic analysis. All these references, however, prove results that are slightly weaker than Thm. 2.1.5. In Appendix A, we give a complete proof, following a proof of Kannai [Kan77] for the scalar case, using purely analytical methods.

We will also need the following Gaussian estimate from below on the heat kernel of the Laplace-Beltrami operator p_t^Δ.

Theorem 2.1.8 (Gaussian lower Bound). *For any $T > 0$, there exist a constant $\gamma_1, \gamma_2 > 0$ such that*

$$\mathrm{e}_t(x, y) \leq e^{\gamma_1 t + \gamma_2 d(x,y)^2} p_t^\Delta(x, y)$$

for all $x, y \in M$, whenever $0 < t \leq T$. Here p_t^Δ is the heat kernel of the Laplace-Beltrami operator.

Proof. For $x, y \in M$ with $d(x, y) < R$ (where $R > 0$ is any number smaller than the injectivity radius), this follows from the heat kernel asymptotics, Corollary 2.1.6. Namely, the zeroth heat kernel coefficient is given by $\Phi_0(x, y) = J(x, y)^{-1/2}$ (see (2.1.10)), where $J(x, y)$ is the Jacobian of the exponential map. From its Taylor expansion (2.1.8), we can conclude

$$J(x, y)^{-1/2} \leq e^{\gamma_2 d(x,y)^2},$$

so that the result follows for near points x, y. For general points x, y, the result follows if we can find a constant $C > 0$ such that

$$\mathrm{e}_t(x, y) \leq C p_t^\Delta(x, y)$$

for all $x, y \in M$. Such a constant is well known to exist (see e.g. Corollary 5.3.5 in [Hsu02]). □

2.1.3 Brownian Bridge

Just as the Brownian motion is naturally associated to the solution operator of the Laplace-Beltrami operator, the stochastic process that belongs to the heat kernel $p_t^\Delta(x, y)$ is the Brownian bridge, a process that travels from the point x to the y in a fixed time t. For more details on the Brownian bridge, see e.g. [Hsu90] or [Hsu02, Section 5.4].
Again, let M be a closed Riemannian manifold or $\mathbb{R}^n$. Given two points $x, y \in M$ and a time $t > 0$, we can consider the conditioned process $X_s^{xy;t}$ defined on the interval $I = [0, t]$. It can be defined to be the unique process satisfying

$$\mathbb{E}\big[f(X_{\tau_1}^{xy;t}, \dots, X_{\tau_{N-1}}^{xy;t})\big] = \int\limits_M \cdots \int\limits_M f(x_1, \dots, x_{N-1}) \frac{\prod_{j=1}^N p_{\tau_j - \tau_{j-1}}^\Delta(x_{j-1}, x_j)}{p_t^\Delta(x, y)} \, \mathrm{d}x_1 \cdots \mathrm{d}x_{N-1} \tag{2.1.14}$$

for all measurable functions f on $M \times \cdots \times M$ ($N-1$ factors) and partitions τ of the interval $[0, t]$ [Hsu02, Section 5.4] (in the above formula, we used the convention $x_0 = x$, $x_N = y$). This implies that it has the inhomogeneous transition density

$$q_{s_0, s_1}(z_0, z_1) := \frac{p_{s_1 - s_0}^\Delta(z_0, z_1) p_{t - s_1}^\Delta(z_1, y)}{p_{t - s_0}^\Delta(z_0, y)}, \qquad 0 < s_0 < s_1 < t.$$

Indeed, if in formula (1.1.10), one replaces the kernels $p_{\tau_j - \tau_{j-1}}(x_{j-1}, x_j)$ by $q_{\tau_{j-1}, \tau_j}(x_{j-1}, x_j)$, one obtains (2.1.14). Similar to the above, its law then descends to a Borel measure $\mathbb{W}^{xy;t}$ on the space

$$C_{xy;t}(M) := \big\{\gamma \in C([0, t], M) \mid \gamma(0) = x, \gamma(t) = y\big\}.$$

Definition 2.1.9 (Brownian Bridge). The process $X_s^{xy;t}$ is called *Brownian Bridge*. The corresponding law $\mathbb{W}^{xy;t}$, which is a probability measure on $C_{xy;t}(M)$, is called *Brownian bridge measure* or *conditional Wiener measure*.

Remark 2.1.10. In the construction of Brownian motion from Section 1.1.3, one can replace the heat kernel p_t^Δ of the operator Δ by the transition density of the operator $\Delta + \partial_Z$, where Z is some (possibly time-dependent) vector field on M. Brownian bridge can be understood in this manner. Namely, one can show (see Thm. 5.4.4 in [Hsu02]) that the Brownian bridge $X_s^{xy;t}$ is in fact just a Brownian *motion* starting at x with time-dependent drift

$$Z(s, z) := \operatorname{grad}_z \log p_{t-s}(z, y)$$

and that the kernel $q_{s_0, s_1}(z_0, z_1)$ is exactly the transition density corresponding to this situation. As can be seen from Thm. 2.1.5, the drift becomes singular as s approaches t, which explains the finite life-time of the process.

For the Brownian Bridge, the Feynman-Kac formula takes the form

$$p_t^L(x, y) = p_t^\Delta(x, y) \mathbb{E}\Big[\widetilde{\mathcal{P}}(X_\bullet^{xy;t})^{-1}\Big] \tag{2.1.15}$$

using the stochastic parallel transport (see Section 1.1.3). This result can be obtained from the usual Feynman-Kac formula (Thm. 1.1.16) by the "co-area formula" for the Wiener measure, see e.g. Lemma 2.24 in [BP11].

2.1.4 Convolution Approximation of the Heat Kernel

This section is the analytical core of the thesis. We first prove a general result which allows to compare certain integral kernels. Throughout this section, let M be a closed Riemannian manifold of dimension n and let $\mathcal{V}$ be a metric vector bundle over M. We define the convolution of integral kernels as follows.

Notation 2.1.11. Let $k, \ell \in L^\infty(M \times M, \mathcal{V} \boxtimes \mathcal{V}^*)$ be two bounded kernels. We define their *convolution* by

$$(k * \ell)(x, y) := \int_M k(x, z)\ell(z, y)\mathrm{d}z$$

Then $k * \ell \in L^\infty(M \times M, \mathcal{V} \boxtimes \mathcal{V}^*)$ is again a kernel.

Using this, we can formulate the following theorem.

Theorem 2.1.12 (Convolution Approximation). *Let k_t, $\ell_t \in L^\infty(M \times M, \mathcal{V} \boxtimes \mathcal{V}^*)$ be two time-dependent kernels. Let $T, R > 0$ be constants. Suppose that for all $0 < t \leq T$ and all $x, y \in M$, we have*

$$|\ell_t(x, y)|, |k_t(x, y)| \leq e^{\gamma_1 t + \gamma_2 d(x,y)^2} p_t^\Delta(x, y) \tag{2.1.16}$$

for constants $\gamma_1, \gamma_2 > 0$ and suppose furthermore that for all $0 < t \leq T$ and all $x, y \in M$ with $d(x, y) < R$, we have

$$|k_t(x, y) - \ell_t(x, y)| \leq c \sum_{j=1}^{m} t^{\alpha_j} d(x, y)^{\beta_j} p_t^\Delta(x, y) \tag{2.1.17}$$

for constants $c, \nu, \alpha_1, \dots, \alpha_m, \beta_1, \dots, \beta_m \geq 0$ such that $\alpha_i + \beta_i/2 \geq 1 + \nu$ for each i. Then there exist constants $C, \delta > 0$ such that for each partition $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = t\}$ of intervals $[0, t]$ with $0 < t \leq T$ and $|\tau| \leq \delta t$, we have

$$\left| k_{\Delta_1 \tau} * \cdots * k_{\Delta_N \tau} - \ell_{\Delta_1 \tau} * \cdots * \ell_{\Delta_N \tau} \right| \leq C t^{1-\beta/2} |\tau|^\nu p_t^\Delta$$

uniformly on $M \times M$. Here, $\beta := \max_{1 \leq i \leq m} \beta_i$ and p_t^Δ denotes the heat kernel of the Laplace-Beltrami operator on M.

Remark 2.1.13. In particular, if one of the kernels (say, ℓ_t) satisfies the Markhov property $\ell_t * \ell_s = \ell_{t+s}$, then $\ell_{\Delta_1 \tau} * \cdots * \ell_{\Delta_N \tau} = \ell_t$ so that from Thm. 2.1.12 follows

$$\lim_{|\tau| \to 0} k_{\Delta_1 \tau} * \cdots * k_{\Delta_N \tau} = \ell_t, \tag{2.1.18}$$

where the limit goes over any sequence of partitions such that $|\tau| \to 0$. However, the statement of the theorem is much stronger in the sense that one simultaneously keeps track of the error of this approximation.

Remark 2.1.14. Thm. 2.1.12 is related to a result by Bär (Prop. 1 in [Bär12]), where two kernels k_t and ℓ_t are called *heat-related* if they satisfy an estimate similar to (2.1.17). The condition of Bär is weaker than the condition here (i.e. two kernels satisfying (2.1.17) are automatically heat-related, but not vice versa), and therefore, Bär's result is applicable to more general pairs of kernels. However, it turns out that all kernels relevant for our purposes also satisfy the stronger assumptions of Thm. 2.1.12 above, which makes it possible to obtain a stronger result as well (the statement of Prop. 1 in [Bär12] is that the limit (2.1.18) holds, but does not contain an error estimate).

For the proof of Thm. 2.1.12, we need the following lemma, or rather a corollary of it, which roughly says that it is exponentially unlikely for a Brownian Bridge path to move far in short times.

Lemma 2.1.15. *Set for $R > 0$ and $0 \leq s_0 \leq s_1 \leq t$*

$$A^R_{s_0,s_1;t} := \bigl\{\gamma \in C([0,t], M) \mid d\bigl(\gamma(s_0), \gamma(s_1)\bigr) > R\bigr\}. \tag{2.1.19}$$

Then for any $0 < \varepsilon < 1$ and $T > 0$, there exist constants $C, \delta > 0$ such that for all $x, y \in M$, we have

$$\mathbb{W}^{xy;t}\bigl(A^R_{s_0,s_1;t}\bigr) < Ce^{-(1-\varepsilon)\frac{R^2}{4(s_1-s_0)}}$$

whenever $0 \leq s_0 < s_1 \leq t \leq T$ and $s_1 - s_0 \leq t\delta$. Here, $\mathbb{W}^{xy;t}$ is the Wiener measure associated to the Brownian bridge on M.

Proof. Set

$$\chi(r) = \begin{cases} 0 & r < R \\ 1 & r \geq R \end{cases}$$

and let p^Δ_t be the heat kernel of the Laplace-Beltrami operator. By Thm. 2.1.8 and Corollary 15.15 in [Gri09], there exist constants $C_1, C_2 > 0$ such that for all $0 < t \leq T$ and all $x, y \in M$, we have

$$C_1 t^{-n/2} e^{-\frac{d(x,y)^2}{4t}} \leq p^\Delta_t(x,y) \leq C_2 t^{-n} e^{-\frac{d(x,y)^2}{4t}}. \tag{2.1.20}$$

Using this, we obtain

$$\begin{aligned}\mathbb{W}^{xy;t}(A^R_{s_0,s_1;t}) &= \frac{1}{p^\Delta_t(x,y)} \int_M \int_M p^\Delta_{s_0}(x,z_0) p^\Delta_{s_1-s_0}(z_0,z_1) p^\Delta_{t-s_1}(z_1,y) \chi\bigl(d(z_0,z_1)\bigr) \mathrm{d}z_0 \mathrm{d}z_1 \\ &\leq \frac{C_2(s_1-s_0)^{-n}}{p^\Delta_t(x,y)} \int_M \int_M e^{-\frac{d(z_0,z_1)^2}{4(s_1-s_0)}} p^\Delta_{s_0}(x,z_0) p^\Delta_{t-s_1}(z_1,y) \chi\bigl(d(z_0,z_1)\bigr) \mathrm{d}z_0 \mathrm{d}z_1.\end{aligned}$$

Now set for any ε' with $0 < \varepsilon' < \varepsilon$

$$\delta := \varepsilon' \frac{R^2}{\mathrm{diam}(M)^2}. \tag{2.1.21}$$

Then on the set where $\chi(d(z_0,z_1)) \neq 0$, i.e. $d(z_0,z_1) \geq R$, we have whenever $s_1 - s_0 \leq t\delta$ the estimate

$$\begin{aligned}\frac{d(z_0,z_1)^2}{4(s_1-s_0)} - \frac{d(x,y)^2}{4t} &\geq \frac{R^2}{4(s_1-s_0)} - \frac{d(x,y)^2\delta}{4(s_1-s_0)} = \frac{R^2}{4(s_1-s_0)} - \varepsilon' \frac{R^2 d(x,y)^2}{4(s_1-s_0)\mathrm{diam}(M)^2} \\ &\geq \bigl(1-\varepsilon'\bigr)\frac{R^2}{4(s_1-s_0)}.\end{aligned}$$

Hence under this restriction on $s_1 - s_0$ and using that the function $p_t^\Delta(x, -)$ integrates to one for each $x \in M$, as well as (2.1.20), we have for each $0 < t \leq T$ that

$$\begin{aligned}\mathbb{W}^{xy;t}(A^R_{s_0,s_1;t}) &\leq \frac{C_2(s_1-s_0)^{-n}}{p_t^\Delta(x,y)} e^{-(1-\varepsilon')\frac{R^2}{4(s_1-s_0)} - \frac{d(x,y)^2}{4t}} \int_M \int_M p^\Delta_{s_0}(x,z_0) p^\Delta_{t-s_1}(z_1,y) \mathrm{d}z_0 \mathrm{d}z_1 \\ &\leq C_2(s_1-s_0)^{-n} e^{-(1-\varepsilon')\frac{R^2}{4(s_1-s_0)}} T^{n/2} \frac{t^{-n/2} e^{-\frac{d(x,y)^2}{4t}}}{p_t^\Delta(x,y)} \\ &\leq C_3(s_1-s_0)^{-n} e^{-(1-\varepsilon')\frac{R^2}{4(s_1-s_0)}} < C_4 e^{-(1-\varepsilon)\frac{R^2}{4(s_1-s_0)}},\end{aligned}$$

if the constants C_3, C_4 are chosen appropriately. □

The following result is a consequence of Lemma 2.1.15 and states that it is also exponentially unlikely for a path to travel a large distance on some subinterval of a given partition.

Corollary 2.1.16. *Fix $R > 0$. Given $t > 0$ and a partition $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = t\}$ of the interval $[0, t]$, set*

$$B^R_\tau = \bigl\{\gamma \in C_{xy;t}(M) \mid \forall j = 1, \dots, N : d\bigl(\gamma(\tau_{j-1}), \gamma(\tau_j)\bigr) \leq R\bigr\}.$$

Then for any $T > 0$ and any $0 < \varepsilon < 1$, there exist constants $C, \delta > 0$ such that

$$\mathbb{W}^{xy;t}\bigl(\{\gamma \notin B^R_\tau\}\bigr) < Ce^{-(1-\varepsilon)\frac{R^2}{4|\tau|}}$$

for all $x, y \in M$ and all partitions τ of intervals $[0, t]$ with $0 < t \leq T$ and $|\tau| \leq t\delta$. Here, $\mathbb{W}^{xy;t}$ denotes any Brownian bridge measure with drift on M.

Proof. From Lemma 2.1.15 above follows that there exist constants $C_1, \delta, \varepsilon' > 0$ such that

$$\mathbb{W}^{xy;t}(A^R_{s_0,s_1;t}) < C_1 e^{-(1-\varepsilon')\frac{R^2}{4(s_1-s_0)}}$$

whenever $0 \leq s_0 < s_1 \leq t \leq T$ and $s_1 - s_0 \leq t\delta$. Now notice that the complement of the set B^R_τ is exactly the union of the sets $A^R_{\tau_{j-1},\tau_j;t}$, because if a path is not in B^R_τ, it must travel a distance greater than R in at least one of the subintervals $[\tau_{j-1}, \tau_j]$. Hence

$$\mathbb{W}^{xy;t}\bigl(\{\gamma \notin B_{\delta,\tau}\}\bigr) = \mathbb{W}^{xy;t}\left(\bigcup_{j=1}^N A^R_{\tau_{j-1},\tau_j;t}\right) \leq \sum_{j=1}^N \mathbb{W}^{xy;t}\left(A^R_{\tau_{j-1},\tau_j;t}\right) < \sum_{j=1}^N C_1 e^{-(1-\varepsilon')\frac{R^2}{4\Delta_j\tau}}.$$

Now choose $0 < \varepsilon < \varepsilon'$ and C_2 so large that $C_1 e^{-(1-\varepsilon')R^2/4s} < C_2 s e^{-(1-\varepsilon)R^2/4s}$ for all $0 < s \leq \delta T$. Then

$$\sum_{j=1}^N C_1 e^{-(1-\varepsilon)\frac{R^2}{4\Delta_j\tau}} \leq C_2 \sum_{j=1}^N \Delta_j e^{-(1-\varepsilon')\frac{R^2}{4\Delta_j\tau}} \leq C_2 T e^{-(1-\varepsilon)\frac{R^2}{4|\tau|}},$$

whenever $|\tau| \leq \delta t \leq \delta T$, where in the last step, we used Hölder's inequality. □

For the proof, we also need two other estimates, Lemma B.2.1 and Lemma B.2.6, which were divested to the appendix. However, going through the proof of Thm. 2.1.12 shows that these latter results are not needed in the particular case that $\gamma_2 = \beta_1 = \cdots = \beta_m = 0$. This "baby version" of Thm. 2.1.12 is enough to prove most of the thesis; the full version of Thm. 2.1.12 is needed only for Thm. 2.2.7. In particular, Chapter 3.1 is independent from the results of Appendix B.

Proof (of Thm. 2.1.12). Throughout the proof, write $\Delta_j := \Delta_j\tau$ for abbreviation.
Step 1. We first show that we may assume without loss of generality that (2.1.17) holds everywhere on M and not only on the set of those points $x, y \in M$ with $d(x,y) < R$. Namely, set

$$\chi(x,y) := \begin{cases} 1 & \text{if } d(x,y) < R \\ 0 & \text{otherwise.} \end{cases}$$

Then the kernels χk_t and $\chi \ell_t$ satisfy (2.1.16) and (2.1.17) for all $x, y \in M$ and we have

$$\begin{aligned} \big|k_{\Delta_1\tau} * \cdots * k_{\Delta_N\tau} - \ell_{\Delta_1\tau} * \cdots * \ell_{\Delta_N\tau}\big| \leq & \big|k_{\Delta_1\tau} * \cdots * k_{\Delta_N\tau} - \chi k_{\Delta_1\tau} * \cdots * \chi k_{\Delta_N\tau}\big| \\ & + \big|\chi k_{\Delta_1\tau} * \cdots * \chi k_{\Delta_N\tau} - \chi \ell_{\Delta_1\tau} * \cdots * \chi \ell_{\Delta_N\tau}\big| \\ & + \big|\chi \ell_{\Delta_1\tau} * \cdots * \chi \ell_{\Delta_N\tau} - \ell_{\Delta_1\tau} * \cdots * \ell_{\Delta_N\tau}\big|. \end{aligned}$$

Now for the first term on the right hand side, we have using (2.1.16)

$$\begin{aligned} &\big|\big(k_{\Delta_1\tau} * \cdots * k_{\Delta_N\tau}\big)(x,y) - \big(\chi k_{\Delta_1\tau} * \cdots * \chi k_{\Delta_N\tau}\big)(x,y)\big| \\ &\leq \int_M \cdots \int_M \left(1 - \prod_{j=1}^N \chi(x_{j-1}, x_j)\right) \prod_{j=1}^N \big|k_{\Delta_j}(x_{j-1}, x_j)\big| \, \mathrm{d}x_1 \cdots \mathrm{d}x_{N-1} \\ &\leq \int_M \cdots \int_M \left(1 - \prod_{j=1}^N \chi(x_{j-1}, x_j)\right) \prod_{j=1}^N e^{\gamma_1 \Delta_j + \gamma_2 d(x_{j-1}, x_j)^2} p^\Delta_{\Delta_j}(x_{j-1}, x_j) \, \mathrm{d}x_1 \cdots \mathrm{d}x_{N-1}. \end{aligned}$$

Using the definition of the Brownian bridge, this equals

$$\begin{aligned} & e^{t\gamma_1} p^\Delta_t(x,y) \mathbb{E}\left[\left(1 - \prod_{j=1}^N \chi(X^{xy;t}_{\tau_{j-1}}, X^{xy;t}_{\tau_j})\right) \exp\left(\gamma_2 \sum_{j=1}^N d\big(X^{xy;t}_{\tau_{j-1}}, X^{xy;t}_{\tau_j}\big)^2\right)\right] \\ &\quad \leq C_0 p^\Delta_t(x,y) \mathbb{E}\left[\left(1 - \prod_{j=1}^N \chi(X^{xy;t}_{\tau_{j-1}}, X^{xy;t}_{\tau_j})\right)^2\right]^{1/2} \mathbb{E}\left[\exp\left(2\gamma_2 \sum_{j=1}^N d\big(X^{xy;t}_{\tau_{j-1}}, X^{xy;t}_{\tau_j}\big)^2\right)\right]^{1/2}, \end{aligned}$$

where we used Hölder's inequality and set $C_0 := e^{T\gamma_1}$. The second expectation value can be estimated by a universal constant using Lemma B.2.6. Regarding the first expectation value, notice that the product over the $\chi(X^{xy;t}_{\tau_{j-1}}, X^{xy;t}_{\tau_j})$ is equal to one if $d(X^{xy;t}_{\tau_{j-1}}, X^{xy;t}_{\tau_j}) < R$ for all j and zero otherwise. Hence we have

$$\mathbb{E}\left[\left(1 - \prod_{j=1}^N \chi(X^{xy;t}_{\tau_{j-1}}, X^{xy;t}_{\tau_j})^2\right)^2\right] = \mathbb{W}^{xy;t}\big(\{\gamma \notin B^R_\tau\}\big) < C_1 e^{-\varepsilon/|\tau|}$$

for some $C_1 > 0$ independent of x, y and $t \leq T$, where B_τ^R is defined in Corollary 2.1.16 and the estimate is precisely the statement of that corollary. In total,

$$\big|\big(k_{\Delta_1\tau} * \cdots * k_{\Delta_N\tau}\big)(x,y) - \big(\chi k_{\Delta_1\tau} * \cdots * \chi k_{\Delta_N\tau}\big)(x,y)\big| \leq C_2 e^{-\varepsilon/|\tau|} p_t^\Delta(x,y)$$

for some consant $C_2 > 0$. The difference $|\chi\ell_{\Delta_1\tau} * \cdots * \chi\ell_{\Delta_N\tau} - \ell_{\Delta_1\tau} * \cdots * \ell_{\Delta_N\tau}|$ can be estimated exactly the same way. Finally, notice that for any $\nu \geq 1$, we have

$$e^{-\varepsilon/|\tau|} \leq C_3|\tau|^{\nu+1} \leq C_3 t|\tau|^\nu \leq C_3 T^{\beta/2} t^{1-\beta/2}|\tau|^\nu$$

for some constant $C_3 > 0$ whenever $|\tau| \leq t \leq T$. This shows that the statement of the theorem holds for k_t and ℓ_t if it holds for χk_t and $\chi\ell_t$; hence we may assume that (2.1.17) holds for all $(x,y) \in M \times M$.

Step 2. Following Step 1, assume without loss of generality that (2.1.17) holds for all $(x,y) \in M \times M$. With the telescoping sum identity

$$a_1 \cdots a_N - b_1 \cdots b_N = \sum_{j=1}^N a_1 \cdots a_{j-1}(a_j - b_j) b_{j+1} \cdots b_N, \tag{2.1.22}$$

we obtain

$$\begin{aligned}
\big|k_{\Delta_1} * \cdots * k_{\Delta_N} - \ell_{\Delta_1} * \cdots * \ell_{\Delta_N}\big| &\leq \sum_{j=1}^N \big|k_{\Delta_1}\big| * \cdots * \big|k_{\Delta_{j-1}}\big| * \big|k_{\Delta_j} - \ell_{\Delta_j}\big| * \big|\ell_{\Delta_{j+1}}\big| * \cdots * \big|\ell_{\Delta_N}\big| \\
\leq \sum_{j=1}^N (e^{\gamma_1\Delta_1 + \gamma_2 d^2} p_{\Delta_1}^\Delta) * \cdots * (e^{\gamma_1\Delta_{j-1}+\gamma_2 d^2} p_{\Delta_{j-1}}^\Delta) * \left(c\sum_{i=1}^m \Delta_j^{\alpha_i} d^{\beta_i} p_{\Delta_j}^\Delta\right) * \\
* (e^{\gamma_1\Delta_{j+1}+\gamma_2 d^2} p_{\Delta_{j+1}}^\Delta) * \cdots * (e^{\gamma_1\Delta_N + \gamma_N d^2} p_{\Delta_N}^\Delta)
\end{aligned}$$

using (2.1.16) respectively (2.1.17) for each factor. The latter term may be expressed in terms of the Brownian bridge; namely, at $(x,y) \in M \times M$, it equals

$$\begin{aligned}
&c e^{\gamma_1 t} p_t^\Delta(x,y) \sum_{j=1}^N \sum_{i=1}^m \Delta_j^{\alpha_i} \mathbb{E}\left[d(X_{\tau_{j-1}}^{xy;t}, X_{\tau_j}^{xy;t})^{\beta_i} \exp\left(\gamma_2 \sum_{k\neq j} d(X_{\tau_{k-1}}^{xy;t}, X_{\tau_k}^{xy;t})^2\right)\right] \\
&\leq c e^{\gamma_1 t} p_t^\Delta(x,y) \sum_{j=1}^N \sum_{i=1}^m \Delta_j^{\alpha_i} \mathbb{E}\left[d(X_{\tau_{j-1}}^{xy;t}, X_{\tau_j}^{xy;t})^{2\beta_i}\right]^{1/2} \mathbb{E}\left[\exp\left(2\gamma_2 \sum_{k=1}^N d(X_{\tau_{k-1}}^{xy;t}, X_{\tau_k}^{xy;t})^2\right)\right]^{1/2} \\
&\leq C_4 e^{\gamma_1 t} p_t^\Delta(x,y) \sum_{j=1}^N \sum_{i=1}^m \Delta_j^{\alpha_i} \left(\frac{\Delta_j}{t}\right)^{\beta_i/2}
\end{aligned}$$

using first the Cauchy-Schwarz inequality and then Lemma B.2.1 and Lemma B.2.6. In total,

$$\big|k_{\Delta_1} * \cdots * k_{\Delta_N} - \ell_{\Delta_1} * \cdots * \ell_{\Delta_N}\big| \leq C_4 p_t^\Delta \sum_{i=1}^m t^{-\beta_i/2} \sum_{j=1}^N \Delta_j^{\alpha_i+\beta_i/2} \leq C_5 p_t^\Delta \sum_{i=1}^m t^{1-\beta_i/2}|\tau|^\nu.$$

Here in the last step, we used

$$\sum_{j=1}^{N} \Delta_j^{\alpha_i+\beta_i/2} = \sum_{j=1}^{N} \Delta_j \Delta_j^{\alpha_i+\beta_i/2-1} \leq |\tau|^{\alpha_i+\beta_i/2-1} \sum_{j=1}^{N} \Delta_j = |\tau|^{\alpha_i+\beta_i/2-1} t \leq C_6 t |\tau|^{\nu}$$

since $\nu \leq \alpha_i + \beta_i/2 - 1$. The theorem follows. □

If we set $\ell_t = p_t^L$ in Thm. 2.1.12, where p_t^L is the heat kernel of a self-adjoint Laplace type operator, we can use the Markhov property to obtain

$$\ell_{\Delta_1\tau} * \cdots * \ell_{\Delta_N\tau} = p^L_{\Delta_1\tau} * \cdots * p^L_{\Delta_N\tau} = p_t^L.$$

This way, one obtains an approximation of the heat kernel p_t^L by a convolution product $k_{\Delta_1\tau} * \cdots * k_{\Delta_N\tau}$. For example, one can take for k_t the *approximate heat kernel* e_t^ν, defined for $\nu \in \mathbb{N}_0$ by

$$\mathrm{e}_t^\nu(x,y) := \chi\big(d(x,y)\big)\mathrm{e}_t(x,y) \sum_{j=0}^{\nu} t^j \frac{\Phi_j(x,y)}{j!}. \tag{2.1.23}$$

Here, χ is a smooth cutoff function, satisfying $\chi(r) = 1$ for $r \leq R/2$ and $\chi(r) = 0$ for $r \geq R$, where R satisfies $0 < R < \mathrm{inj}(M)$. Then e_t^ν is a smooth time-dependent kernel. Using Thm. 2.1.12 for this kernel gives the following result.

Corollary 2.1.17 (Heat Kernel as a Convolution I). *Let L be a self-adjoint Laplace type operator, acting on sections of a metric vector bundle $\mathcal{V}$ over a closed Riemannian manifold M and let p_t^L be the associated heat kernel. Then for each $\nu \in \mathbb{N}_0$ and each $T > 0$, there exist constants $C, \delta > 0$ such that*

$$\big|p_t^L - \mathrm{e}^\nu_{\Delta_1\tau} * \cdots * \mathrm{e}^\nu_{\Delta_N\tau}\big| \leq C\,t\,|\tau|^\nu p_t^\Delta$$

uniformly on $M \times M$ for each partition τ of the interval $[0,t]$ such that $|\tau| \leq \delta t$ and each $0 < t \leq T$. Here, p_t^Δ is the heat kernel of the Laplace-Beltrami operator on M.

Proof. The estimate (2.1.16) for p_t^L is just the Hess-Schrader-Uhlenbrock estimate

$$|p_t^L(x,y)| \leq e^{t\gamma} p_t^\Delta(x,y)$$

(see [HSU80]) and for e_t^ν, the estimate $|\mathrm{e}_t^\nu| \leq e^{t\gamma_1 + d^2\gamma_2} p_t^\Delta$ is automatic using the Gaussian lower bound in Thm. 2.1.8. To verify (2.1.17), notice that by Corollary 2.1.6 and Thm. 2.1.8, we have

$$\big|p_t^L(x,y) - \mathrm{e}_t^\nu(x,y)\big| \leq c_1 t^{\nu+1}\mathrm{e}_t(x,y) \leq c_2 t^{\nu+1} p_t^\Delta(x,y), \tag{2.1.24}$$

uniformly for (x,y) in compact subsets of $M \bowtie M$ and $0 < t \leq T$. Hence we can apply Thm. 2.1.12 with $m = 1$, $\alpha_1 = \nu + 1$ and $\beta_1 = 0$. □

Remark 2.1.18. In contrast to the near-diagonal short time estimates from Thm. 2.1.5, Corollary 2.1.17 shows how one can approximate heat kernels p_t^L arbitrarily well uniformly on all of $M \times M$, not only on $M \bowtie M$.

Remark 2.1.19 (The geometric Meaning of $\boldsymbol{\delta}$). The proof of Lemma 2.1.15 shows that in Corollary 2.1.17, one can take any δ satisfying

$$0 < \delta < \left(\frac{\mathrm{inj}(M)}{\mathrm{diam}(M)}\right)^2.$$

Then if τ is a partition of $[0,t]$ satisfying $|\tau| \leq \delta t$, the approximation result of Corollary 2.1.17 applies. In particular, the number N of subintervals that the interval $[0,t]$ is divided into by a sufficiently fine partition τ needs to satisfy $N \geq 1/\delta$. For example, for $M = S^n$, where $\mathrm{inj}(M) = \mathrm{diam}(M)$, it suffices to choose $\delta < 1$, so that one can get away with $N = 2$, i.e. it suffices to subdivide the time interval into two pieces.

Corollary 2.1.17 above shows how the heat kernel p_t^L can be approximated by the convolution product $\mathrm{e}^\nu_{\Delta_1\tau} * \cdots * \mathrm{e}^\nu_{\Delta_N\tau}$ of approximate heat kernels e_t^ν. The approximate heat kernels are built of the Euclidean heat kernel $\mathrm{e}_t(x,y)$ and the heat kernel coefficients $\Phi_j(x,y)$ as correction terms, which are solutions to certain differential equations. While one can theoretically compute these at the diagonal $x = y$ (which gets immensely complicated for large j), it is usually not possible to give explicit formulas for Φ_j away from the diagonal, even for Φ_1. Therefore, it may be desirable to obtain an approximation result depending in an explicit way on quantities such as curvature as well as the connection and the potential determined by the decomposition $L = \nabla^*\nabla + V$ from Lemma 1.1.2. This can be done, but one has to pay the price of loosing higher order uniformity in t, which will be a problem when we are going to take asymptotic expansions in Chapter 3.1.

Corollary 2.1.20 (Heat Kernel as a Convolution II). *Let M and let L be a self-adjoint Laplace type operator, acting on sections of a metric vector bundle $\mathcal{V}$ over M. Let p_t^L be the heat kernel of L and define the kernel e_t^L by*

$$\mathrm{e}_t^L(x,y) := \mathrm{e}_t(x,y)\exp\left(\frac{t}{6}\mathrm{scal}(x) + \frac{1}{12}\mathrm{ric}\big(\dot\gamma_{xy}(0), \dot\gamma_{xy}(0)\big)\right)\mathcal{P}(\gamma_{xy;t})^{-1}$$

for $(x,y) \in M \bowtie M$, where $\gamma_{xy;t}$ is the unique minimizing geodesic connecting x to y in time t, $\gamma_{xy} := \gamma_{xy;1}$ and $\mathcal{P}(\gamma)$ is the path-ordered exponential determined by L (see Def. 1.1.13). Then for each $T > 0$, there exist constants $C, \delta > 0$ such that

$$\left|p_t^L(x,y) - \big(\mathrm{e}^L_{\Delta_1\tau} * \cdots * \mathrm{e}^L_{\Delta_N\tau}\big)(x,y)\right| \leq C\left(\frac{|\tau|}{t}\right)^{1/2} p_t^\Delta(x,y)$$

for all $x, y \in M$, for each partition τ of the interval $[0,t]$ such that $|\tau| \leq \delta t$ and each $0 < t \leq T$.

Remark 2.1.21. The formula for $\mathrm{e}_t^L(x,y)$ is only defined for $(x,y) \in M \bowtie M$. Because the complement $M \times M \setminus M \bowtie M$ is a set of measure zero, e_t^L extends to a well-defined L^∞ function on all of $M \times M$, which is not continuous in general.

Proof. Again, this is an application of Thm. 2.1.12. The estimates (2.1.16) can be shown as in the proof above, so we only need to verify (2.1.17). By Corollary 2.1.6, for $T > 0$ and $0 < R < \mathrm{inj}(M)$ given, we have

$$p_t^L(x,y) = \mathrm{e}_t(x,y)\Big(\Phi_0(x,y) + t\Phi_1(x,y) + O(t^2)\Big)$$

for all $(x,y) \in M \times M$ with $d(x,y) \leq R < \mathrm{inj}(M)$ and $t \leq T$, where the remainder is uniform over this set of points. Here Φ_0 and Φ_1 are the zeroth and first heat kernel coefficients of the heat kernel p_t^L. Using (2.1.10) and the Taylor expansion (2.1.8), we obtain

$$\Phi_0(x,y) = 1 + \frac{1}{12}\mathrm{ric}\big(\dot\gamma_{xy}(0), \dot\gamma_{xy}(0)\big) + O\big(d(x,y)^3\big)$$

while from (2.1.11), we have

$$\Phi_1(x,y) = \left(\frac{1}{6}\mathrm{scal}(x) - V(x)\right)[\gamma_{xy}\|_0^1]^{-1}.$$

Put together, we have

$$\frac{p_t^L(x,y)}{\mathrm{e}_t(x,y)} = \left(\mathrm{id} + \frac{t}{6}\mathrm{scal}(x) + \frac{1}{12}\mathrm{ric}\big(\dot\gamma_{xy}(0), \dot\gamma_{xy}(0)\big) - t\,V(x)\right)[\gamma_{xy}\|_0^1]^{-1} \\ + O\big(d(x,y)^3 + td(x,y) + t^2\big),$$

where the remainder is uniform over the set of points $(x,y) \in M \times M$ with $d(x,y) \leq R$. Because

$$\mathcal{P}(\gamma_{xy;t})^{-1} = \big(\mathrm{id} - tV(x)\big)[\gamma_{xy}\|_0^1]^{-1} + O(t^2),$$

the function $\mathrm{e}_t^L(x,y)/\mathrm{e}_t(x,y)$ has exactly the same expansion for small t and $d(x,y)$. Hence

$$\big|p_t^L(x,y) - \mathrm{e}_t^L(x,y)\big| \leq C\mathrm{e}_t(x,y)\big(d(x,y)^3 + td(x,y) + t^2\big).$$

From Corollary 2.1.6 follows that we may replace $\mathrm{e}_t(x,y)$ by $p_t^\Delta(x,y)$, so (2.1.17) follows. Setting

$$\begin{aligned} \alpha_1 &= 0, & \alpha_2 &= 1, & \alpha_3 &= 2, \\ \beta_1 &= 3, & \beta_2 &= 1, & \beta_3 &= 0, \end{aligned} \tag{2.1.25}$$

the result follows from Thm. 2.1.12 with $m = 3$, $\nu = 1/2$. □

Remark 2.1.22. In a similar fashion, one can show that for any $\Lambda \in \mathbb{R}$, the same result holds when the kernel $\mathrm{e}_t^L(x,y)$ is replaced by the kernel

$$\mathrm{e}_t^{L,\Lambda}(x,y) := \mathrm{e}_t(x,y)\exp\left(\frac{t}{6}\mathrm{scal}(x) + \frac{1-2\Lambda}{12}\mathrm{ric}\big(\dot\gamma_{xy}(0), \dot\gamma_{xy}(0)\big)\right)\mathcal{P}(\gamma_{xy;t})^{-1}J(x,y)^{-\Lambda},$$

where $J(x,y)$ is the Jacobian of the exponential map (2.1.7). We will later use this result with $\Lambda = 1$. Compare this to Remark 4.8 and Thm. 5.2 in [BP08].

The result of Corollary 2.1.20 is nice because it gives a heat kernel approximation involving only quantities which are explicitly given in terms of curvature of the underlying manifold. For example, on a manifold of constant sectional curvature κ, one has $\mathrm{ric} = \kappa(n-1)g$ and $\mathrm{scal} = n(n-1)\kappa$, hence for $L = \Delta$, the Laplace-Beltrami operator on such a space, we obtain

$$\mathrm{e}_t^\Delta(x,y) = (4\pi t)^{-n/2}\exp\left(-\frac{d(x,y)^2}{4t} + \frac{\kappa\, n(n-1)}{6}t + \frac{\kappa(n-1)}{12}d(x,y)^2\right)$$

so that the heat kernel can be approximated arbitrarily well using repeated convolutions of this kernel.

2.2 The Heat Kernel as a Path Integral

In this section, we give path integral formulas for the heat kernel. In Subsection 2.2.1, we first introduce the relevant path spaces, which will be the path spaces with two fixed endpoints. Afterwards, in Subsection 2.2.3, we show how to represent the heat kernel of general self-adjoint Laplace type operators using time-slicing approximation of the heat kernel. We also give a path integral formula for the trace of the heat operator, which will be an integral over certain loop spaces.

2.2.1 Pinned Path Spaces and their Approximations

In this section, let M be an n-dimensional complete Riemannian manifold. To approximate the heat kernel of M by a path integral, we need path spaces with two fixed endpoints.

Notation 2.2.1 (Pinned Path Spaces). We write

$$H_{xy;t}(M) := \bigl\{\gamma \in H^1([0,t], M) \mid \gamma(0) = x, \gamma(t) = y\bigr\}$$

for the pinned path space with endpoints x and y. In the case $t = 1$, we also write $H_{xy}(M) := H_{xy;1}(M)$.

Remember from Section 1.2.1 that the space $H^1([0,t], M)$ of finite energy paths comes with an evaluation map

$$\mathrm{ev}_{0,t} : H^1([0,t], M) \longrightarrow M \times M, \qquad \gamma \longmapsto \bigl(\gamma(0), \gamma(t)\bigr),$$

which is a submersion. This shows that the spaces $H_{xy;t}(M)$ are submanifolds of the manifold $H^1([0,t], M)$, because they can be written as the pre-image of the submanifolds $\{(x,y)\} \subset M \times M$ under the evaluation map, $H_{xy;t}(M) = \mathrm{ev}_{0,t}^{-1}(\{(x,y)\})$.
$H_{xy;t}(M)$ is also a submanifold of $H_{x;t}(M)$ and as such inherits a Riemannian metric by restricting to it the H^1 metric (1.2.5).

Finite-dimensional approximation of the spaces $H_{xy;t}(M)$ is not quite as straight forward as in the case of one fixed endpoint. In particular, it is not clear if for a partition τ and given points $x, y \in M$, the set of paths $\gamma \in H_{x;\tau}(M)$ with $\gamma(t) = y$ is a submanifold of $H_{xy;t}(M)$, as it is not clear if the endpoint evaluation map is still a submersion when restricted to the submanifold $H_{x;\tau}(M)$. Therefore, we make the following definition.

Notation 2.2.2 (Finite-dimensional Approximations). For a partition $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = t\}$ of the interval $[0,t]$, we set

$$H_{xy;\tau}(M) := \bigl\{\gamma \in H_{xy;t}(M) \mid \gamma|_{[\tau_{j-1},\tau_j]} \text{ is unique minimizing for each } j\bigr\}$$

by which we mean that for each $\gamma \in H_{xy;\tau}(M)$ and each $j = 1, \dots, N$, $\gamma|_{[\tau_{j-1},\tau_j]}$ is a minimizing geodesic between its endpoints with $(\gamma(\tau_{j-1}), \gamma(\tau_j)) \in M \bowtie M$.

$H_{xy;\tau}(M)$ is a submanifold of $H_{xy;t}(M)$, because near points $\gamma \in H_{xy;\tau}(M)$, it is the transversal intersection of the submanifolds $H_{xy;t}(M)$ and $H_{x;\tau}(M)$ of $H_{x;t}(M)$: For a given vector field $X \in T_\gamma H_{x;t}(M)$, let $Y \in T_\gamma H_{x;\tau}(M)$ be a piece-wise Jacobi field with $Y(t) = X(t)$ (such a vector field Y exists because along unique minimizing geodesics, boundary value problems for Jacobi fields have a solution). Now $X - Y \in T_\gamma H_{xy;t}(M)$ and $X = (X-Y) + Y$, hence the intersection is transversal.
Also notice that the τ-evaluation map

$$\mathrm{ev}_\tau : H_{xy;\tau}(M) \longrightarrow \underbrace{M \times \cdots \times M}_{N-1 \text{ times}}, \qquad \gamma \mapsto \big(\gamma(\tau_1), \dots, \gamma(\tau_{N-1})\big) \tag{2.2.1}$$

is a smooth embedding with image $M \bowtie \cdots \bowtie M$, i.e. the set of tuples $(x_1, \dots, x_{N-1})$ such that $(x_{j-1}, x_j) \in M \bowtie M$ for each $j = 1, \dots, N$ (where we set $x_0 := x, x_N := y$). Therefore we have the diffeomorphism

$$H_{xy;\tau}(M) \approx M \bowtie \cdots \bowtie M.$$

Remark 2.2.3 (Approximation Property). It seems likely that if one takes the union of the spaces $H_{xy;\tau}(M)$ over all partitions τ of $[0,t]$, the result will be dense in $H_{xy;t}(M)$, but apparently, there is no easy argument for this (notice that the argument given in Remark 1.2.6 for the spaces with one fixed endpoint does not work in this case). We will not need such a result. However, later we will prove an "infinitesimal version" of this statement, Lemma 3.2.10 below.

The tangent space of $H_{xy;\tau}(M)$ at a path γ is the space of piece-wise Jacobi fields X with $X(0) = X(t) = 0$. Of course, $H_{xy;\tau}(M)$ inherits a Riemannian metric, namely the submanifold metric, from $H_{xy;t}(M)$. In the case of the spaces $H_{x;\tau}(M)$, it turned out that the discretized metric (1.2.8) yielded the simplest path integral formulas and in that sense that metric was more suitable for the finite-dimensional path spaces. The situation is similar for the spaces $H_{xy;\tau}(M)$, but it is not completely straight forward what the discrete analog of the metric (1.2.8) should be. Of course, one could just restrict the discrete metric (1.2.8) to the subspace $H_{xy;\tau}(M)$, but this will not give good path integral formulas formulas; also the metric obtained this way does not seem natural since it does not respect the inherent symmetry (i.e. the flip map $H_{xy;\tau}(M) \longrightarrow H_{yx;\tilde{\tau}}(M)$ sending γ to the path $s \mapsto \gamma(t-s)$ is not an isometry).
In fact, we will not define a discretized metric on $H_{xy;\tau}(M)$, but a good discretized *volume measure*. To this end, consider the endpoint evaluation map

$$\mathrm{ev}_t : H_{x;t}(M) \longrightarrow M, \qquad \gamma \longmapsto \gamma(t).$$

The fibers of this map are exactly the spaces $H_{xy;t}(M)$, while at a path $\gamma \in H_{x;t}(M)$ with $\gamma(t) = y$ the normal space to $H_{xy;t}(M)$ is the space of affine-linear vector fields,

$$N_\gamma H_{xy;t}(M) = \big\{X \in T_\gamma H_{x;t}(M) \mid X(s) = s[\gamma\|_0^s]X_0, X_0 \in T_x M\big\},$$

as is easy to verify. For $X, Y \in N_\gamma H_{xy;t}(M)$, we therefore have

$$\langle \mathrm{dev}_t|_\gamma X, \mathrm{dev}_t|_\gamma Y\rangle = \langle X(t), Y(t)\rangle = t(X,Y)_{H^1}, \tag{2.2.2}$$

so that ev_t is a Riemannian submersion up to a conformal factor. Formally using the co-area formula, this would mean that integrals over $H_{x;t}(M)$ can be written as a double integral over M and $H_{xy;t}(M)$ in a particularly simple form (which doesn't make sense because the integrands are infinite-dimensional). For the finite-dimensional path spaces however, this can be turned into a sensible condition for a measure on $H_{xy;\tau}(M)$, namely we require that

$$\int_{H_{x;\tau}(M)} f\big(\gamma(\tau_1),\dots,\gamma(\tau_N)\big)\,\mathrm{d}\gamma = t^{-n/2}\int_M \int_{H_{xy;\tau}(M)} f\big(\gamma(\tau_1),\dots,\gamma(\tau_N)\big)\,\mathrm{d}\gamma\,\mathrm{d}y \qquad (2.2.3)$$

for all $f \in C^0(M^{N+1})$ such that $f(x_1,\dots,x_N) = 0$ whenever $(x_{j-1},x_j) \notin M \bowtie M$ for some j (where $x_0 = x$). Here the additional factor of $t^{-n/2}$ is motivated by the co-area formula: It is the determinant of $d\mathrm{ev}_t|_\gamma$, restricted to the orthonal complement of its kernel, the normal space.
To make explicit what (2.2.3) means, we use the following Lemma.

Lemma 2.2.4. *Denote by $\widetilde{H}_{x;\tau}(M) \subseteq H_{x;\tau}(M)$ the open subset of paths γ where each segment $\gamma|_{[\tau_{j-1},\tau_j]}$ is minimizing with $(\gamma(\tau_{j-1}),\gamma(\tau_j)) \in M \bowtie M$. Then for all integrable functions $f \in C^0(M^{N+1})$, we have (setting $x_0 := x$) that*

$$\int_{\widetilde{H}_{x;\tau}(M)} f\big(\gamma(\tau_1),\dots,\gamma(\tau_N)\big)\mathrm{d}\gamma = \int_{M^N} f(x_1,\dots,x_N)\left(\prod_{j=1}^N J(x_{j-1},x_j)(\Delta_j\tau)^{n/2}\right)^{-1}\mathrm{d}x,$$

where J is the Jacobian of the exponential map, see Remark 2.1.2.

Proof. We calculate the Jacobian determinant of the evaluation map

$$\mathrm{ev}_\tau : \widetilde{H}_{x;\tau}(M) \longrightarrow M^N, \qquad \gamma \longmapsto \big(\gamma(\tau_1),\dots,\gamma(\tau_N)\big).$$

For any $\gamma \in \widetilde{H}_{x;\tau}(M)$, we have an isomorphism

$$\phi_\gamma : T_\gamma\widetilde{H}_{x;\tau}(M) \longrightarrow \bigoplus_{j=1}^N T_{\gamma(\tau_{j-1})}M, \qquad X \longmapsto \big(\nabla_s X(\tau_0+),\dots,\nabla_s X(\tau_{N-1}+)\big).$$

If $e_1(s),\dots,e_n(s)$ is a parallel orthonormal basis along γ, then the vectors $e_i(\tau_{j-1})$, $i = 1,\dots,n$, $j = 1,\dots,N$ form an orthonormal basis of the latter space, while the piecewise Jacobi fields $E_{ij} := \phi_\gamma^{-1}(0,\dots,0,e_i(\tau_{j-1}),0,\dots,0)$ satisfy

$$\nabla_s E_{ij}(\tau_{k-1}+) = \begin{cases} e_i(\tau_{j-1}) & \text{if } k = j \\ 0 & \text{otherwise.}\end{cases}$$

Hence, with a view on the definition of the discrete H^1 metric, we find

$$(E_{ij},E_{kl})_{\Sigma\text{-}H^1} = \sum_{m=1}^N \big\langle \nabla_s E_{ij}(\tau_{m-1}+), \nabla_s E_{kl}(\tau_{m-1}+)\big\rangle \Delta_m\tau = \delta_{ik}\delta_{jl}\Delta_j\tau$$

so that these vectors form an orthogonal basis (not normalized) of $T_\gamma \widetilde{H}_{x;\tau}(M)$ and

$$|\det(\phi_\gamma)| = \det\Big((E_{ij}, E_{kl})_{\Sigma\text{-}H^1}\Big)^{-1/2}_{\substack{1\le i,k\le n\\ 1\le j,l\le N-1}} = \prod_{j=1}^N (\Delta_j\tau)^{-n/2}. \tag{2.2.4}$$

We obtain a linear map

$$\mathrm{dev}_\tau|_\gamma \circ \phi_\gamma^{-1} : \bigoplus_{j=1}^N T_{\gamma(\tau_{j-1})}M \longrightarrow \bigoplus_{j=1}^N T_{\gamma(\tau_j)}M,$$

which is given with respect to these direct sum decompositions by the lower triangular matrix

$$\mathrm{dev}_\tau|_\gamma \circ \phi_\gamma^{-1} = \begin{pmatrix} \Delta_1\tau\, d\exp_{x_0}|_{v_0} & 0 & \cdots & 0 \\ * & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ * & \dots & * & \Delta_N\tau\, d\exp_{x_{N-1}}|_{v_{N-1}} \end{pmatrix},$$

where we set $x_j = \gamma(\tau_j)$, $v_j = \dot\gamma(\tau_j+)$. Therefore

$$\det\big(\mathrm{dev}_\tau|_\gamma\big) = \det\big(\mathrm{dev}_\tau|_\gamma \circ \phi_\gamma^{-1}\big)\det(\phi_\gamma) = \prod_{j=1}^N J(x_{j-1}, x_j)(\Delta_j\tau)^{n/2}.$$

The result follows from the transformation formula. □

This lemma motivates to define the *discretized volume* $\mathrm{d}^{\Sigma\text{-}H^1}\gamma$ on $H_{xy;\tau}(M)$ by setting

$$\begin{aligned} &\int_{H_{xy;\tau}(M)} f\big(\gamma(\tau_1), \dots, \gamma(\tau_{N-1})\big)\mathrm{d}^{\Sigma\text{-}H^1}\gamma \\ &\qquad := t^{n/2}\int_{M^{N-1}} f(x_1, \dots, x_{N-1})\left(\prod_{j=1}^N J(x_{j-1}, x_j)(\Delta_j\tau)^{n/2}\right)^{-1} \mathrm{d}x_1\cdots \mathrm{d}x_{N-1} \end{aligned} \tag{2.2.5}$$

for measurable functions f on M^{N-1} (where as usual we set $x_0 := x$, $x_N := y$). By Lemma 2.2.4, this measure satisfies the co-area formula (2.2.3). We do not know if this measure is the Riemannian volume measure to some natural Riemannian metric, nor if one should expect it to be.

2.2.2 The Loop Space and its Approximations

As before, let M be an n-dimensional complete Riemannian manifold. The trace of the heat operator can be represented by a path integral over the loop space.

Notation 2.2.5 (Loop Space). The infinite-dimensional H^1 loop space of M is the Hilbert manifold

$$L_t(M) := H^1(S^1_t, M),$$

where $S^1_t := \mathbb{R}/t\mathbb{Z}$ is the circle of length t. We will write $L(M) := L_1(M)$.

We will not put a Riemannian metric on $L_t(M)$ as it is not clear which one could be the most natural one; we just remark that the usual H^1 metric (1.2.5) may be degenerate, depending on the Riemannian metric on M.

Notation 2.2.6 (Finite-Dimensional Approximation). For a partition $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = t\}$ of the interval $[0,t]$, we write

$$L_\tau(M) := \big\{\gamma \in L_t(M) \mid \gamma|_{[\tau_{j-1},\tau_j]} \text{ is a unique minimizing geodesic}\big\}$$

for the finite-dimensional approximation of the loop space.

Similar to before, one can show that this is a submanifold of $L_t(M)$. On $L_\tau(M)$, we define the discretized volume $\mathrm{d}^{\Sigma\text{-}H^1}\gamma$ by

$$\begin{aligned}\int_{L_\tau(M)} & f\big(\gamma(\tau_1),\dots,\gamma(\tau_N)\big)\mathrm{d}^{\Sigma\text{-}H^1}\gamma \\ &:= \int_{M^N} f(x_1,\dots,x_N)\left(\prod_{j=1}^N J(x_{j-1},x_j)(\Delta_j\tau)^{n/2}\right)^{-1}\mathrm{d}x_1\cdots\mathrm{d}x_N\end{aligned} \tag{2.2.6}$$

using the convention $x_0 :\equiv x_N$. Using this volume, we have the co-area formula

$$\int_{L_\tau(M)} F(\gamma)\,\mathrm{d}^{\Sigma\text{-}H^1}\gamma = t^{-n/2}\int_M\int_{H_{xx;\tau}(M)} F(\gamma)\,\mathrm{d}^{\Sigma\text{-}H^1}\gamma\mathrm{d}x \tag{2.2.7}$$

for measurable functions F on $L_\tau(M)$.

2.2.3 Path Integral Formulas for the Heat Kernel

We are ready to formulate the following result.

Theorem 2.2.7 (Heat Kernel as a Path Integral I). *Let p_t^L be the heat kernel of a self-adjoint Laplace type operator L, acting on sections of a metric vector bundle $\mathcal{V}$ over a compact n-dimensional Riemannian manifold M. Let $\mathcal{P}(\gamma)$ be the path-ordered exponential determined by L as in Def. 1.1.13. Then for each $x,y\in M$ and any $t>0$, we have*

$$p_t^L(x,y) = \lim_{|\tau|\to 0}(4\pi t)^{-n/2}\,⨍_{H_{xy;\tau}(M)} e^{-E(\gamma)/2}\,\mathcal{P}(\gamma)^{-1}\,\mathrm{d}^{\Sigma\text{-}H^1}\gamma,$$

where the limit goes over any sequence of partitions τ of the interval $[0,t]$ the mesh of which tend to zero. Here the slash in the integral sign denotes division by $(4\pi)^{\dim(H_{xy;\tau}(M))/2}$.

Remark 2.2.8. One can also show that

$$p_t^L(x,y) = \lim_{|\tau|\to 0}\frac{1}{Z_\tau}\int_{H_{xy;\tau}(M)} e^{-E(\gamma)/2}\,\exp\left(\frac{1}{3}\int_0^t \mathrm{scal}\big(\gamma(s)\big)\mathrm{d}s\right)\mathcal{P}(\gamma)^{-1}\,\mathrm{d}^{\Sigma\text{-}L^2}\gamma,$$

where the normalization constant is $Z_\tau := (4\pi)^{nN/2}(\Delta_N\tau)^{-n/2}\prod_{j=1}^N(\Delta_j\tau)^n$ and $H_{xy;\tau}(M)$ carries the discrete L^2 metric (1.2.10). This latter result is contained in [Bär12], Thm. 1. Compare also [BP08, Thm. 6.1].

Lemma 2.2.9. *For any* $\gamma \in H_{xy;\tau}(M)$*, we have*

$$E(\gamma) = \sum_{j=1}^{N} \frac{d\big(\gamma(\tau_{j-1}), \gamma(\tau_j)\big)^2}{2\Delta_j\tau}, \tag{2.2.8}$$

where $E(\gamma)$ *denotes the energy functional defined in* (1.2.1)*.*

Proof. By definition, each segment $\gamma|_{[\tau_{j-1},\tau_j]}$ is the unique shortest geodesic connecting $\gamma(\tau_{j-1})$ and $\gamma(\tau_j)$ in time $\Delta_j\tau$. Therefore, its speed is equal to $\frac{1}{\Delta_j\tau}d(\gamma(\tau_{j-1}), \gamma(\tau_j))$. Hence

$$2E(\gamma) = \sum_{j=1}^{N} \int_{\tau_{j-1}}^{\tau_j} |\dot\gamma(s)|^2 \mathrm{d}s = \sum_{j=1}^{N} \int_{\tau_{j-1}}^{\tau_j} \frac{d\big(\gamma(\tau_{j-1}), \gamma(\tau_j)\big)^2}{(\Delta_j\tau)^2} \mathrm{d}s = \sum_{j=1}^{N} \frac{d\big(\gamma(\tau_{j-1}), \gamma(\tau_j)\big)^2}{\Delta_j\tau}. \qquad \square$$

Proof (of Thm. 2.2.7). The proof will consist of two steps. In the first step, we write the path integral over $H_{xy;\tau}(M)$ as an integral over M^{N-1} to connect it to the results from Section 2.1.4. This is very elementary. The second step then relies on additional tools from stochastic analysis that are contained in Appendix B.1.
Step 1. By Lemma 2.2.9 and by definition of the discrete volume on $H_{xy;\tau}(M)$ (see (2.2.5)), we have

$$\begin{aligned}&\int_{H_{xy;\tau}(M)} e^{-E(\gamma)/2}\,\mathcal{P}(\gamma)^{-1}\,\mathrm{d}^{\Sigma\text{-}H^1}\gamma \\ &\qquad = t^{n/2} \int_{M^{N-1}} \exp\left(-\sum_{j=1}^{N} \frac{d(x_{j-1}, x_j)^2}{4\Delta_j\tau}\right) \mathcal{P}(\gamma_{\mathbf{x}})^{-1} \left(\prod_{j=1}^{N} J(x_{j-1}, x_j)(\Delta_j\tau)^{n/2}\right)^{-1} \mathrm{d}\mathbf{x},\end{aligned}$$

where we set $x_0 := x$, $x_N := y$ and for $\mathbf{x} = (x_1, \dots, x_{N-1}) \in M^{N-1}$ we wrote $\gamma_{\mathbf{x}}$ for the path in $H_{xy;\tau}(M)$ with $\gamma_{\mathbf{x}}(\tau_j) = x_j$. This is well-defined for all $\mathbf{x}M \bowtie \cdots \bowtie M$, which is a set of full measure. If $\gamma_i : [0, t_i] \to M$, $i = 1, 2$ are paths with $\gamma_2(0) = \gamma_1(t_1)$, then path ordered exponential satisfies $\mathcal{P}(\gamma_1 * \gamma_2) = \mathcal{P}(\gamma_2)\mathcal{P}(\gamma_1)$, where $\gamma_1 * \gamma_2$ denotes the concatenation of the paths (see Remark 1.1.15). Therefore

$$\mathcal{P}(\gamma_{\mathbf{x}})^{-1} = \prod_{j=1}^{N} \mathcal{P}(\gamma_{x_{j-1}x_j;\Delta_j\tau})^{-1} = \mathcal{P}(\gamma_{x_0x_1;\Delta_1\tau})^{-1} \cdots \mathcal{P}(\gamma_{x_{N-1}x_N;\Delta_N\tau})^{-1},$$

where $\gamma_{x_{j-1}x_j;\Delta_j\tau}$ denotes the unique geodesic connecting x_{j-1} to x_j in time $\Delta_j\tau$. We hence find

$$(4\pi t)^{-n/2} \fint_{H_{xy;\tau}(M)} e^{-E(\gamma)/2}\,\mathcal{P}(\gamma)^{-1}\,\mathrm{d}^{\Sigma\text{-}H^1}\gamma = \int_{M^{N-1}} \prod_{j=1}^{N} \widetilde{\mathrm{e}}_{\Delta_j\tau}(x_{j-1}, x_j)\,\mathrm{d}\mathbf{x},$$

where $\widetilde{\mathrm{e}}_t$ is the kernel

$$\widetilde{\mathrm{e}}_t(x, y) = \mathrm{e}_t(x, y) J(x, y)^{-1} \mathcal{P}(\gamma_{xy;t})^{-1}$$

Comparing with the kernel $\mathrm{e}_t^{L,\Lambda}(x, y)$ from Remark 2.1.22 for $\Lambda = 1$, we have

$$\widetilde{\mathrm{e}}_t(x, y) = \mathrm{e}_t^{L,1}(x, y) \exp\left(\frac{1}{12}\mathrm{ric}\big(\dot\gamma_{xy}(0), \dot\gamma_{xy}(0)\big) - \frac{t}{6}\mathrm{scal}(x)\right)$$

so that

$$(4\pi t)^{-n/2} \fint_{H_{xy;\tau}(M)} e^{-E(\gamma)/2}\,\mathcal{P}(\gamma)^{-1}\,\mathrm{d}^{\Sigma\text{-}H^1}\gamma$$
$$= \int_{M^{N-1}} \exp\left(\sum_{j=1}^N \left(\frac{1}{12}\mathrm{ric}\big(\Delta_j\gamma_{\mathbf{x}}, \Delta_j\gamma_{\mathbf{x}}\big) - \frac{1}{6}\mathrm{scal}(x_{j-1})\Delta_j\tau\right)\right) \prod_{j=1}^N \mathrm{e}^{L,1}_{\Delta_j\tau}(x_{j-1}, x_j)\,\mathrm{d}\mathbf{x},$$

where we set $\Delta_j\gamma_{\mathbf{x}} = \dot\gamma_{\mathbf{x}}(\tau_{j-1}+)\Delta_j\tau = \dot\gamma_{x_{j-1},x_j}(0)$. By Thm. 2.1.20 (or rather by Remark 2.1.22), the convolution product $e^{L,1}_{\Delta_1\tau} * \cdots * e^{L,1}_{\Delta_N\tau}$ converges to p_t^L uniformly on M as $|\tau| \to 0$. Therefore, it is left to show that we may replace the term

$$\exp\left(\sum_{j=1}^N \left(\frac{1}{12}\mathrm{ric}\big(\Delta_j\gamma_{\mathbf{x}}, \Delta_j\gamma_{\mathbf{x}}\big) - \frac{1}{6}\mathrm{scal}(x_{j-1})\Delta_j\tau\right)\right), \tag{2.2.9}$$

by one in this limit. This is the content of the next step.

Step 2. For a partition τ of the interval $[0,t]$ and $\gamma \in C_{xy;t}(M)$, let $\gamma^\tau \in H_{xy;\tau}(M)$ be the *best piecewise geodesic approximation* of γ, i.e. the piecewise geodesic path with $\gamma^\tau(\tau_j) = \gamma(\tau_j)$. This is well defined for $\mathbb{W}^{xy;t}$-almost all paths γ, since the set of paths such that $(\gamma(\tau_{j-1}), \gamma(\tau_j)) \notin M \bowtie M$ for some j is a zero set. Now for $\gamma \in C_{xy;t}(M)$, we have

$$S_\tau(\gamma) := \exp\left(\frac{1}{6}\sum_{j=1}^N \mathrm{scal}\big(\gamma(\tau_{j-1})\big)\Delta_j\tau\right) \longrightarrow \exp\left(\frac{1}{6}\int_0^t \mathrm{scal}\big(\gamma(s)\big)\mathrm{d}s\right) := S(\gamma)$$

in $L^p(\mathbb{W}^{xy;t})$ for any $1 \le p < \infty$ as $|\tau| \to 0$, by Lemma B.1.4. Now readers familiar with stochastic analysis will notice that the function S is exactly the exponential of the *quadratic variation* of the Brownian motion (see Def. B.1.1) and the Brownian bridge, while the functions

$$R_\tau(\gamma) := \exp\left(\frac{1}{12}\sum_{j=1}^N \mathrm{ric}\big(\Delta_j\gamma^\tau, \Delta_j\gamma^\tau\big)\right)$$

are exponentials of the *approximations* of the quadratic variation, which converge to the quadratic variation in probability (see Prop. 3.23 and Prop. 5.18 in [Eme89]). This is the short explanation why we indeed may replace the term $R_\tau S_\tau^{-1} = (2.2.9)$ by 1. To make this argument rigorous is a technical matter, which is the content of the remainder of the proof.

By (2.1.15), we have the Feynman-Kac formula for the heat kernel

$$p_t^L(x,y) = p_t^\Delta(x,y)\int_{C_{xy;t}(M)} \widetilde{\mathcal{P}}(\gamma)^{-1}\,\mathrm{d}\mathbb{W}^{xy;t}(\gamma) \tag{2.2.10}$$

where $\widetilde{\mathcal{P}}(\gamma)$ is the stochastic parallel transport. The stochastic parallel transport $\widetilde{\mathcal{P}}(\gamma)$ can be approximated by the path-ordered exponentials $\mathcal{P}(\gamma^\tau)$,

$$\lim_{|\tau|\to 0} \mathcal{P}(\gamma^\tau)^{-1} = \widetilde{\mathcal{P}}(\gamma)^{-1}. \tag{2.2.11}$$

This result is the content of Prop. 8.15 in [Eme89], and the precise statement is that the convergence (2.2.11) is in measure, with respect to the Brownian bridge measure $\mathbb{W}^{xy;t}$. (This may also serve as a definition of $\widetilde{\mathcal{P}}(\gamma)^{-1}$ as a measurable function on $C_{xy;t}(M)$.) However, in our case, the convergence (2.2.11) is even better: Because the connection ∇ determined by the self-adjoint operator L is metric, the family $\mathcal{P}(\gamma^\tau)^{-1}$ is pointwise uniformly bounded, by Lemma 1.3.19. This implies that the limit (2.2.11) even holds in $L^p(\mathbb{W}^{xy;t})$ for any $1 \leq p < \infty$. In particular, the stochastic parallel transport is a well-defined L^p-function. The convergence (2.2.11) can also be seen using the approximation result Thm. 4.14 in [AD99] on (1.1.16) in local charts.
By Step 1, we want to estimate the difference

$$\begin{aligned}
&\left| p_t^L(x,y) - (4\pi t)^{-n/2} \fint_{H_{xy;\tau}(M)} e^{-E(\gamma)/2}\mathcal{P}(\gamma)^{-1}\mathrm{d}^{\Sigma\text{-}H^1}\gamma \right| \\
&\qquad = \left| p_t^\Delta(x,y)\mathbb{E}\left[\widetilde{\mathcal{P}}(X_\cdot^{xy;t})^{-1}\right] - \int_{M^{N-1}} \left(\prod_{j=1}^N \mathrm{e}_{\Delta_j\tau}^{L,1}(x_{j-1},x_j)\right) R_\tau(\gamma_{\mathbf{x}})S_\tau(\gamma_{\mathbf{x}})^{-1}\mathrm{d}\mathbf{x}\right| \\
&\qquad \leq (1) + (2)
\end{aligned}$$

where

$$(1) = p_t^\Delta(x,y)\left|\mathbb{E}\left[\widetilde{\mathcal{P}}(X_\cdot^{xy;t})^{-1} - \mathcal{P}\big([X_\cdot^{xy;t}]^\tau\big)^{-1}R_\tau(X_\cdot^{xy;t})S_\tau(X_\cdot^{xy;t})^{-1}\right]\right|.$$

and with a constant $C_0 > 0$ such that $\mathcal{P}(\gamma) \leq C_1$ for all $\gamma \in H_{xy;t}(M)$ (which exists by Lemma 1.3.19),

$$\begin{aligned}
(2) &= \int_{M^{N-1}} \left| \mathcal{P}(\gamma_{\mathbf{x}})^{-1}\prod_{j=1}^N p_{\Delta_j\tau}^\Delta(x_{j-1},x_j) - \prod_{j=1}^N \mathrm{e}_{\Delta_j\tau}^{L,1}(x_{j-1},x_j)\right| R_\tau(\gamma_{\mathbf{x}})S_\tau(\gamma_{\mathbf{x}})^{-1}\mathrm{d}\mathbf{x} \\
&\leq C_0 \int_{M^{N-1}} \left| \prod_{j=1}^N p_{\Delta_j\tau}^\Delta(x_{j-1},x_j) - \prod_{j=1}^N \mathrm{e}_{\Delta_j\tau}^{\Delta,1}(x_{j-1},x_j)\right| R_\tau(\gamma_{\mathbf{x}})S_\tau(\gamma_{\mathbf{x}})^{-1}\mathrm{d}\mathbf{x},
\end{aligned}$$

In this estimate, $\mathrm{e}_t^{\Delta,\Lambda}(x,y) = \mathrm{e}_t^{L,\Lambda}(x,y)\mathcal{P}(\gamma_{xy;t})$ is the kernel from Corollary 2.1.20 for the Laplace-Beltrami operator Δ on M and we inserted the term

$$\begin{aligned}
&\int_{M^{N-1}} \mathcal{P}(\gamma_{\mathbf{x}})^{-1}R_\tau(\gamma_{\mathbf{x}})S_\tau(\gamma_{\mathbf{x}})^{-1}\prod_{j=1}^N p_{\Delta_j\tau}^\Delta(x_{j-1},x_j)\mathrm{d}\mathbf{x} \\
&\qquad\qquad = p_t^\Delta(x,y)\mathbb{E}\left[\mathcal{P}\big([X_\cdot^{xy;t}]^\tau\big)^{-1}R_\tau(X_\cdot^{xy;t})S_\tau(X_\cdot^{xy;t})^{-1}\mathrm{d}\right]
\end{aligned}$$

to use the triangle inequality. For the term (1), we have

$$\begin{aligned}
(1) \leq p_t^\Delta(x,y)&\left|\mathbb{E}\left[\widetilde{\mathcal{P}}(X_\cdot^{xy;t})^{-1} - \mathcal{P}\big([X_\cdot^{xy;t}]^\tau\big)^{-1}\right]\right| \\
&+ p_t^\Delta(x,y)\left|\mathbb{E}\left[\mathcal{P}\big([X_\cdot^{xy;t}]^\tau\big)^{-1}\Big(1 - R_\tau(X_\cdot^{xy;t})S_\tau(X_\cdot^{xy;t})^{-1}\Big)\right]\right|.
\end{aligned}$$

The first summand converges to zero as $|\tau| \to 0$ because of (2.2.11) and the second summand converges to zero by Lemma B.1.3 and Lemma B.1.4, so it remains to show that the term (2) converges to zero as well.

After choosing some $R > 0$ with $R < \mathrm{inj}(M)$, a similar calculation as in the proof of Thm. 2.1.12 shows that there exists a constant $C_1 > 0$ independent of τ such that

$$\left|\prod_{j=1}^{N} \mathrm{e}^{\Delta,1}_{\Delta_j\tau}(x_{j-1},x_j) - \prod_{j=1}^{N} p^{\Delta}_{\Delta_j\tau}(x_{j-1},x_j)\right| \leq C_1 \left(\sum_{j=1}^{N}\sum_{i=1}^{3}(\Delta_j\tau)^{\alpha_i} d(x_{j-1},x_j)^{\beta_i}\right)\prod_{j=1}^{N} p^{\Delta}_{\Delta_j\tau}(x_{j-1},x_j)$$

for all $(x_1,\dots,x_{N-1}) \in M^{N-1}$ such that $d(x_{j-1},x_j) \leq R$ for all $j = 1,\dots,N$, and where a_i, β_i, $i = 1,2,3$ are as in (2.1.25) (i.e. $\alpha_i + \beta_i/2 \geq 3/2$). On the complement, i.e. on the set of those tuples $(x_1,\dots,x_{N-1}) \in M^{N-1}$ where $d(x_{j-1},x_j) > R$ for some j, we have

$$\left|\prod_{j=1}^{N} \mathrm{e}^{\Delta,1}_{\Delta_j\tau}(x_{j-1},x_j) - \prod_{j=1}^{N} p^{\Delta}_{\Delta_j\tau}(x_{j-1},x_j)\right| \leq 2e^{ta_1}\prod_{j=1}^{N} e^{a_2 d(x_{j-1},x_j)^2} p^{\Delta}_{\Delta_j\tau}(x_{j-1},x_j),$$

employing Thm. 2.1.8. Let χ_τ be the indicator function of the set $B^R_\tau \subset C_{xy;t}(M)$ appearing in Corollary 2.1.16, i.e. $\chi_\tau(\gamma) = 1$ if $d(\gamma(\tau_{j-1}),\gamma(\tau_j)) \leq R$ for all $j = 1,\dots,N$ and $\chi_\tau(\gamma) = 0$ otherwise. Furthermore, we have

$$R_\tau(\gamma)S_\tau(\gamma)^{-1} \leq \exp\left(a_3 t + a_4 \sum_{k=1}^{N} d\big(\gamma(\tau_{k-1}),\gamma(\tau_k)\big)^2\right),$$

where a_3 is a bound on the scalar curvature and a_4 a bound on the Ricci curvature. Putting all these estimates together, we obtain $(2) \leq (2a) + (2b)$, where

$$(2a) = C_2 p^{\Delta}_t(x,y)\sum_{j=1}^{N}\sum_{i=1}^{3}(\Delta_i\tau)^{\alpha_i}\mathbb{E}\left[\chi_\tau\big(X^{xy;t}_{\cdot}\big) d\big(X^{xy;t}_{\tau_{j-1}}, X^{xy;t}_{\tau_j}\big)^{\beta_i}\exp\left(a_4\sum_{k=1}^{N} d(X^{xy;t}_{\tau_{k-1}}, X^{xy;t}_{\tau_k})^2\right)\right],$$

and

$$(2b) = C_3 p^{\Delta}_t(x,y)\mathbb{E}\left[\big(1-\chi_\tau(X^{xy;t}_{\cdot})\big)\exp\left((a_2+a_4)\sum_{j=1}^{N} d(X^{xy;t}_{\tau_{j-1}}, X^{xy;t}_{\tau_j})^2\right)\right].$$

All constants are independent of the partition τ. Using Lemma B.2.1 and Lemma B.2.6 together with the Hölder inequality, we obtain

$$(2a) \leq C_4 p^{\Delta}_t(x,y)\sum_{k=1}^{N}\sum_{i=1}^{3} t^{-\beta_i/2}(\Delta_k\tau)^{\alpha_i+\beta_i/2} \leq C_5 p^{\Delta}_t(x,y)\left(\frac{|\tau|}{t}\right)^{1/2}.$$

Similarly, Corollary 2.1.16 combined with Lemma B.2.6 and the Hölder inequality gives

$$(2b) \leq C_6 p^{\Delta}_t(x,y)e^{-\varepsilon/|\tau|} \tag{2.2.12}$$

for some $\varepsilon > 0$. This shows that $(2) \to 0$ as $|\tau| \to 0$ and finishes the proof. □

Already from Step 1 of the above proof, we obtain the following corollary.

Corollary 2.2.10 (A uniform Approximation). *Let p_t^L be the heat kernel of a self-adjoint Laplace type operator L, acting on sections of a metric vector bundle $\mathcal{V}$ over a compact n-dimensional Riemannian manifold M. Let $\mathcal{P}(\gamma)$ be the path-ordered exponential determined by L as in Def. 1.1.13. For a partition $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = t\}$ of some interval $[0,t]$, define the kernel $E_\tau^L(x,y)$ equal to*

$$(4\pi t)^{-n/2} \fint_{H_{xy;\tau}(M)} e^{-E(\gamma)/2} \exp\left(\sum_{j=1}^N \left(\frac{1}{6}\mathrm{scal}\big(\gamma(\tau_j)\big)\Delta_j\tau - \frac{1}{12}\mathrm{ric}\big(\Delta_j\gamma, \Delta_j\gamma\big)\right)\right) \mathcal{P}(\gamma)^{-1} \mathrm{d}^{\Sigma\text{-}H^1}\gamma,$$

where $\Delta_j\gamma := \dot\gamma(\tau_{j-1}+)\Delta_j\tau$ and the slash over the integral sign denotes division by $(4\pi)^{\dim(H_{xy;\tau}(M))/2}$. Then for any $T > 0$ there exist constants $\delta, C > 0$ such that

$$\big|p_t^L(x,y) - E_\tau^L(x,y)\big| \leq C\left(\frac{|\tau|}{t}\right)^{1/2} p_t^\Delta(x,y)$$

for all $x, y \in M$ and all partitions τ of intervals $[0,t]$ with $t \leq T$ such that $|\tau| \leq \delta t$.

This result is stronger than Thm. 2.2.7 in the sense that one has a precise error estimate, but weaker in the sense that the integrand is more complicated.

While the formula in Thm. 2.2.7 is quite simple and explicit, the drawback is that we have no control over the uniformity of the approximation in t. This is problematic when calculating asymptotic expansions of the path integrals in Chapter 3.1. Using the kernel from Corollary 2.1.17, we will now derive time-slicing approximations of the heat kernel which are uniformly in t, at the price of a more complicated integrand.

Since we will be taking asymptotic expansions, it will be convenient to have an integration domain independent of t. Therefore, we will formulate the result involving only the path spaces $H_{xy;\tau}(M)$ associated to partitions τ of the interval $[0,1]$. This can be arranged by substitution: Let τ be a partition of the interval $[0,t]$ and let $\widetilde\tau$ be the corresponding partition of the interval $[0,1]$ (meaning that $\tau_j = t\widetilde\tau_j$ for every j). Similarly, if $\gamma \in H_{xy;\tau}(M)$, denote by $\widetilde\gamma \in H_{xy;\widetilde\tau}(M)$ the path defined by $\widetilde\gamma(s) := \gamma(st)$. Then we have

$$E(\widetilde\gamma) = \frac{1}{2}\int_0^1 \big|\dot\gamma(st)\big|^2 \mathrm{d}s = \frac{t}{2}\int_0^t \big|\dot\gamma(s)\big|^2 t^2 \mathrm{d}s = tE(\gamma), \tag{2.2.13}$$

so $e^{-E(\gamma)/2}$ becomes $e^{-E(\widetilde\gamma)/2t}$ in the path integral formulas. Similarly, the integrals now have to be normalized through dividing by $(4\pi t)^{\dim(H_{xy;\tau}(M))/2}$ instead of $(4\pi)^{\dim(H_{xy;\tau}(M))/2}$

Theorem 2.2.11 (Heat Kernel as a Path Integral II). *Let p_t^L be the heat kernel of a self-adjoint Laplace type operator L, acting on sections of a metric vector bundle $\mathcal{V}$ over a compact n-dimensional Riemannian manifold M. Then for each $T > 0$ and each $\nu \in \mathbb{N}_0$, there exist constants $C, \delta > 0$ such that*

$$\left| p_t^L(x,y) - (4\pi t)^{-n/2} \fint_{H_{xy;\tau}(M)} e^{-E(\gamma)/2t}\, \Upsilon_{\tau,\nu}(t,\gamma)\, \mathrm{d}\gamma \right| \leq C t^{1+\nu} |\tau|^\nu p_t^\Delta(x,y)$$

for all $x, y \in M$, $0 < t \leq T$ and all partitions τ of the interval $[0,1]$ with $|\tau| \leq \delta$. Here the slash over the integral sign denotes divison by $(4\pi t)^{\dim(H_{xy;\tau}(M))/2}$ and $\Upsilon_{\tau,\nu}(t,\gamma)$ are certain $\mathrm{Hom}(\mathcal{V}_y, \mathcal{V}_x)$*-valued functions on $H_{xy;\tau}(M)$ which are smooth and compactly supported in γ and depend polynomially on t.*

More specifically, the functions $\Upsilon_{\tau,\nu}$ from Thm. 2.2.11 are given by the complicated expression

$$\Upsilon_{\tau,\nu}(t,\gamma) := \big|\det\big(d\mathrm{ev}_\tau|_\gamma\big)\big| \prod_{j=1}^{N} \chi\big(d(\gamma(\tau_{j-1}),\gamma(\tau_j))\big) \sum_{i=0}^{\nu} t^i (\Delta_j\tau)^{i-n/2} \frac{\Phi_i\big(\gamma(\tau_{j-1}),\gamma(\tau_j)\big)}{i!} \tag{2.2.14}$$

involving the heat kernel coefficients Φ_j of p_t^L and a cutoff function χ with $\chi(r) = 1$ if $r \leq R/2$ and $\chi(r) = 0$ if $r \geq R$, where $0 < R < \mathrm{inj}(M)$. Furthermore, $|\det(d\mathrm{ev}_\tau|_\gamma)|$ is the Jacobian determinant of τ-evaluation map

$$\mathrm{ev}_\tau : H_{xy;\tau}(M) \longrightarrow M^{N-1}, \quad \gamma \longmapsto \big(\gamma(\tau_1), \dots, \gamma(\tau_{N-1})\big). \tag{2.2.15}$$

The determinant depends on the chosen metric (or volume measure) on $H_{xy;\tau}(M)$, and in fact, Thm. 2.2.11 holds for any volume on $H_{xy;\tau}(M)$; the difference then lies in this determinant, which is explicitly computable only in special cases.

Example 2.2.12 (Jacobian of $\boldsymbol{\tau}$-evaluation Map). For some metrics or volumes on $H_{xy;\tau}(M)$ (τ being a partition of the interval $[0,1]$), the Jacobian determinant $|\det(d\mathrm{ev}_\tau|_\gamma)|$ is computable explicitly. For a curve $\gamma \in H_{xy;\tau}(M)$, let $e_1(s), \dots, e_n(s)$, $s \in [0,1]$, be a parallel orthonormal frame along γ. Then the vectors

$$\big(0, \dots, e_i(\tau_j), \dots, 0\big) \in \bigoplus_{j=1}^{N-1} T_{\gamma(\tau_j)}M, \qquad 1 \leq i \leq n, \quad 1 \leq j \leq N-1$$

form an orthonormal basis of $T_{\mathrm{ev}_\tau(\gamma)}M^{N-1}$. Let $E_{ij} \in T_\gamma H_{xy;\tau}(M)$ be the pre-images of these vectors under the differential of the evaluation map.

1. With respect to the discrete L^2 metric (1.2.10), we have

$$\big(E_{ij}, E_{kl}\big)_{\Sigma\text{-}L^2} = \delta_{ik}\delta_{jl}\Delta_j\tau. \tag{2.2.16}$$

   Hence if $H_{xy;\tau}(M)$ carries the discrete L^2 metric, the Jacobian determinant is constant,

$$\big|\det\big(d\mathrm{ev}_\tau|_\gamma\big)\big| = \det\Big(\big(E_{ki}, E_{lj}\big)_{\Sigma\text{-}L^2}\Big)^{-1/2}_{\substack{1\leq k,l\leq n\\ 1\leq i,j\leq N-1}} \equiv \prod\nolimits_{j=1}^{N-1} (\Delta_j\tau)^{-n/2}. \tag{2.2.17}$$

   Note the slight asymmetry here with respect to time inversion, which comes from the same asymmetry of the discrete L^2 metric.

2. Directly from the definition of the discrete H^1 volume measure (2.2.5) on $H_{xy;\tau}(M)$, one obtains that in this case,

$$\big|\det\big(d\mathrm{ev}_\tau|_\gamma\big)\big| = \prod_{j=1}^{N} J\big(\gamma(\tau_{j-1}), \gamma(\tau_j)\big)(\Delta_j\tau)^{n/2},$$

   where $J(x,y)$ is the Jacobian of the exponential map, see (2.1.7).

In Lemma 3.2.9, we calculate $|\det(dev_\tau|_\gamma)|$ with respect to the continuous H^1 metric (1.2.5); however, we only consider the case that γ is a minimal geodesic connecting x to y, and furthermore calculate only the limit of the determinants as $|\tau| \to 0$. This already turns out to be quite involved.

Proof (of Thm. 2.2.11). Let $T > 0$ and $\nu \in \mathbb{N}_0$. For a partition τ of the interval $[0, t]$, let $\widetilde{\tau} = \tau/t = \{0 = \widetilde{\tau}_0 < \widetilde{\tau}_1 < \cdots < \widetilde{\tau}_N = 1\}$ be the associated partition of the interval $[0, 1]$, i.e. $\widetilde{\tau}_j = \tau_j/t$. By Corollary 2.1.17, we have

$$\big|p_t(x, y) - E_\tau^\nu(x, y)\big| \leq Ct|\tau|^\nu p_t^\Delta(x, y) = Ct^{1+\nu}|\widetilde{\tau}|^\nu p_t^\Delta(x, y),$$

where $E_\tau^\nu(x, y)$ is the convolution product

$$E_\tau^\nu(x, y) = \big(\mathrm{e}_{\Delta_1\tau}^\nu * \cdots * \mathrm{e}_{\Delta_N\tau}^\nu\big)(x, y) = \big(\mathrm{e}_{t\Delta_1\widetilde{\tau}}^\nu * \cdots * \mathrm{e}_{t\Delta_N\widetilde{\tau}}^\nu\big)(x, y)$$

involving the approximate heat kernel

$$\mathrm{e}_t^\nu(x, y) = \mathrm{e}_t(x, y)\chi\big(d(x, y)\big) \sum_{i=0}^{\nu} t^i \frac{\Phi_i(x, y)}{i!} =: \mathrm{e}_t(x, y)\Phi(t; x, y).$$

The convolution can be written as an integral over M^{N-1}. The set $M \bowtie \cdots \bowtie M \subset M^{N-1}$ of points $(x_1, \ldots, x_{N-1})$ such that $(x_{j-1}, x_j) \in M \bowtie M$ for each $j = 1, \ldots, N$ (where $x_0 := x$, $x_N := y$) is an open set of full measure in M^{N-1}. Hence we may restrict the integration to this subset. Furthermore, the τ-evaluation map ev_τ is a diffeomorphism between $H_{xy;\tau}(M)$ and $M \bowtie \cdots \bowtie M$. Using the transformation formula on this diffeomorphism yields

$$E_\tau^\nu(x, y) = (4\pi)^{-nN/2} \int_{H_{xy;\tau}(M)} e^{-E(\gamma)/2} \left(\prod_{j=1}^{N} \frac{\Phi\big(\Delta_j\tau; \gamma(\tau_{j-1}), \gamma(\tau_j)\big)}{(\Delta_j\tau)^{n/2}}\right) \big|\det\big(\mathrm{dev}_\tau|_\gamma\big)\big| \mathrm{d}\gamma.$$

Now consider the *rescaling map*

$$S_t : H_{xy;\tau}(M) \longrightarrow H_{xy;\widetilde{\tau}}(M), \qquad \gamma \longmapsto \widetilde{\gamma} = \Big[s \mapsto \gamma(st)\Big].$$

We have $\mathrm{ev}_\tau = \mathrm{ev}_{\widetilde{\tau}} \circ S_t$, $\Delta_j\tau = t\Delta_j\widetilde{\tau}$ and

$$\Phi\big(\Delta_j\tau; \gamma(\tau_{j-1}), \gamma(\tau_j)\big) = \Phi\big(t\Delta_j\widetilde{\tau}; \widetilde{\gamma}(\widetilde{\tau}_{j-1}), \widetilde{\gamma}(\widetilde{\tau}_j)\big) \tag{2.2.18}$$

for each $j = 1, \ldots, N$ so that, again with the transformation formula,

$$E_\tau^\nu(x, y) = (4\pi t)^{-nN/2} \int_{H_{xy;\widetilde{\tau}}(M)} e^{-E(\widetilde{\gamma})/2t} \left(\prod_{j=1}^{N} \frac{\Phi\big(t\Delta_j\widetilde{\tau}; \widetilde{\gamma}(\widetilde{\tau}_{j-1}), \widetilde{\gamma}(\widetilde{\tau}_j)\big)}{(\Delta_j\widetilde{\tau})^{n/2}}\right) \big|\det\big(\mathrm{dev}_{\widetilde{\tau}}|_{\widetilde{\gamma}}\big)\big| \mathrm{d}\widetilde{\gamma},$$

where we used (2.2.13) above. This finishes the proof. □

2.2.4 Path Integral Formulas for the Heat Trace

For the heat trace, Thm. 2.2.7 yields the following result.

Theorem 2.2.13 (Heat Trace as a Path Integral I). *Let L be a self-adjoint Laplace type operator, acting on sections of a metric vector bundle $\mathcal{V}$ over a closed Riemannian manifold M. Let $\mathcal{P}(\gamma)$ be the path ordered exponential determined by L as in Def. 1.1.13. Then for each $t > 0$, we have*

$$\operatorname{Tr} e^{-tL} = \lim_{|\tau|\to 0} ⨍_{L_\tau(M)} e^{-E(\gamma)/2} \operatorname{tr} \mathcal{P}(\gamma)^{-1} \, \mathrm{d}^{\Sigma\text{-}H^1}\gamma,$$

where the limit goes over any sequence of partitions τ of the interval $[0, t]$ the mesh of which tend to zero and the slash in the integral sign denotes division by $(4\pi)^{\dim(L_\tau(M))/2}$.

Remark 2.2.14. In the case that $L = \nabla^*\nabla$ for a metric connection ∇, i.e. $V = 0$, we have $\operatorname{tr} \mathcal{P}(\gamma)^{-1} = \operatorname{tr}[\gamma\|_0^t]^{-1} = \operatorname{tr} \operatorname{hol}(\gamma)$, the trace of the *holonomy* of the loop γ.

Proof. It is well known that the trace of a trace-class operator is given by integrating its kernel over the diagonal in $M \times M$,

$$\operatorname{Tr} e^{-tL} = \int_M \operatorname{tr} p_t^L(x, x)\mathrm{d}x. \tag{2.2.19}$$

Let n be the dimension of M. Then the dimension of $H_{xx;\tau}(M)$ is $n(N-1)$. From Thm. 2.2.7 and the co-area formula (2.2.7) for the discrete H^1 volume, we therefore obtain

$$\begin{aligned}
\operatorname{Tr} e^{-tL} &= \int_M \lim_{|\tau|\to 0} (4\pi t)^{-n/2} ⨍_{H_{xx;\tau}(M)} e^{-E(\gamma)/2} \operatorname{tr} \mathcal{P}(\gamma)^{-1} \mathrm{d}\gamma \, \mathrm{d}^{\Sigma\text{-}H^1} x \\
&= \lim_{|\tau|\to 0} (4\pi)^{-nN/2} t^{-n/2} \int_M \int_{H_{xx;\tau}(M)} e^{-E(\gamma)/2} \operatorname{tr} \mathcal{P}(\gamma)^{-1} \mathrm{d}\gamma^{\Sigma\text{-}H^1} \mathrm{d}x \\
&= \lim_{|\tau|\to 0} (4\pi)^{-nN/2} \int_{L_\tau(M)} e^{-E(\gamma)/2} \operatorname{tr} \mathcal{P}(\gamma)^{-1} \mathrm{d}\gamma^{\Sigma\text{-}H^1} \mathrm{d}x
\end{aligned}$$

This finishes the proof (because $\dim(L_\tau(M)) = nN/2$), if we justify the exchange of integration and taking the limit $|\tau| \to 0$. This follows if we show that the integrand

$$\operatorname{tr} E_\tau^L(x, x) = \int_{H_{xx;\tau}(M)} e^{-E(\gamma)/2} \operatorname{tr} \mathcal{P}(\gamma)^{-1} \mathrm{d}^{\Sigma\text{-}H^1}\gamma.$$

is uniformly bounded. By the calculations from the proof of Thm. 2.2.7, we have

$$\begin{aligned}
E_\tau^L(x, x) &= \int_{M^{N-1}} \prod_{j=1}^N \mathrm{e}_{\Delta_j\tau}(x_{j-1}, x_j) \mathcal{P}(\gamma_{x_{j-1}x_j;t})^{-1} J(x_{j-1}, x_j)^{-1} \mathrm{d}x_1 \cdots \mathrm{d}x_{N-1} \\
&\leq \int_{M^{N-1}} \prod_{j=1}^N p^\Delta_{\Delta_j\tau}(x_{j-1}, x_j) e^{a_1\Delta_j\tau + a_2 d(x_{j-1}, x_j)^2} \cdots \mathrm{d}x_{N-1} \\
&= e^{a_1 t} p_t^\Delta(x, x) \mathbb{E}\left[\exp\left(a_2 \sum_{j=1}^N d\big(X^{xx;t}_{\tau_{j-1}}, X^{xx;t}_{\tau_j}\big)^2\right)\right] \leq C e^{a_1 t} t^{-n/2}
\end{aligned}$$

for some constants a_1, a_2, where we set $x_0 := x_N := x$ and again used several estimates that we applied earlier in this thesis already, namely Thm. 2.1.8 and the Taylor expansion (2.1.8) in the first step, as well as the estimate on $\mathcal{P}(\gamma)$ (Lemma 1.3.19), Lemma. B.2.6 and Thm. 2.1.5 in the third step. This provides a uniform bound and the compactness of the integration domain implies that we may exchange integration and taking the limit. □

Again, we cannot replace the limit $t \to 0$ with the limit $|\tau| \to 0$, which is a considerable limitation when taking asymptotic expansions. The following result is the analog of Thm. 2.2.11; again, we obtain a precise remainder estimate at the cost of a more complicated integrand.

Theorem 2.2.15 (Heat Trace as a Path Integral II). *Let L be a self-adjoint Laplace type operator, acting on sections of a metric vector bundle $\mathcal{V}$ over a closed Riemannian manifold M of dimension n. Then for each $T > 0$, $\nu \in \mathbb{N}_0$, there exist constants $C, \delta > 0$ such that*

$$\left| \operatorname{Tr} e^{-tL} - \fint_{L_\tau(M)} e^{-E(\gamma)/2t} \operatorname{tr} \Upsilon^\circ_{\tau,\nu}(t,\gamma)\, \mathrm{d}\gamma \right| \leq C t^{1+\nu-n/2} |\tau|^\nu$$

for all $0 < t \leq T$ and all partitions τ of the interval $[0,1]$ with $|\tau| \leq \delta$. Here the slash over the integral sign denotes divison by $(4\pi t)^{\dim(L_\tau(M))/2}$ and $\Upsilon^\circ_{\tau,\nu}$ is given by the same formula as $\Upsilon_{\tau,\nu}$ in Thm. 2.2.11 above, but taking the Jacobian determinant of the τ-evaluation map

$$\mathrm{ev}^\circ_\tau : L_\tau(M) \longrightarrow M^N, \qquad \gamma \longmapsto \big(\gamma(\tau_0), \gamma(\tau_1), \dots, \gamma(\tau_{N-1})\big) \tag{2.2.20}$$

instead of $|\det d(\mathrm{ev}_\tau|_\gamma)|$.

Proof. Let n be the dimension of M so that $\dim(H_{xy;\tau}(M)) = n(N-1)$ for all $x, y \in M$. Let $T > 0$, $\nu \in \mathbb{N}_0$ and let τ be a partition of the interval $[0,1]$. Using (2.2.19) above, we obtain from Thm. 2.2.11 that

$$\left| \operatorname{Tr} e^{-tL} - (4\pi t)^{-nN/2} \int_M \int_{H_{xx;\tau}(M)} e^{-E(\gamma)/2t} \operatorname{tr} \Upsilon_{\tau,\nu}(t,\gamma)\, \mathrm{d}\gamma \mathrm{d}x \right| \leq C_0 t^{1+\nu} |\tau|^\nu \int_M p_t^\Delta(x,x) \mathrm{d}x,$$

The estimate $p_t^\Delta(x,x) \leq C_1 t^{-n/2}$, which follows from Thm. 2.1.5, then implies that the right hand side can be estimated from above by $C_2 t^{1+\nu-n/2}|\tau|^\nu$ for some constant C_2. Now by the co-area formula,

$$\begin{aligned}\int_M \int_{H_{xx;\tau}(M)} & e^{-E(\gamma)/2t} \operatorname{tr} \Upsilon_{\tau,\nu}(t,\gamma)\, \mathrm{d}\gamma\, \mathrm{d}x \\ &= \int_{L_\tau(M)} e^{-E(\gamma)/2t} \operatorname{tr} \Upsilon_{\tau,\nu}(t,\gamma) \left|\det\big(d\mathrm{ev}_0|_{N_\gamma H_{\gamma(0),\gamma(0);\tau}(M)}\big)\right| \mathrm{d}\gamma,\end{aligned}$$

where $\mathrm{ev}_0 : L_\tau(M) \longrightarrow M$, $\gamma \mapsto \gamma(0) = \gamma(1)$ is the evaluation map. Hence it remains to show that for each $\gamma \in H_{xx;\tau}(M)$, we have $\Upsilon^\circ_{\tau,\nu}(\gamma) = \Upsilon_{\tau,\nu}(\gamma) |\det\big(d\mathrm{ev}_0|_{N_\gamma H_{xx;\tau}(M)}\big)|$, or equivalently

$$\left|\det\big(d\mathrm{ev}^\circ_\tau|_\gamma\big)\right| = \left|\det\big(d\mathrm{ev}_t|_{N_\gamma H_{xx;\tau}(M)}\big)\right| \left|\det\big(d\mathrm{ev}_\tau|_\gamma\big)\right|,$$

where $\mathrm{ev}_\tau : H_{xx;\tau}(M) \to M^{N-1}$ is the evaluation map defined in (2.2.15). However, with respect to the orthogonal splittings $T_\gamma L_\tau(M) = T_\gamma H_{xx;\tau}(M) \oplus N_\gamma H_{xx;\tau}(M)$ and $T_{\mathrm{ev}^\circ_\tau(\gamma)} M^N = T_{\gamma(0)} M \oplus T_{\mathrm{ev}_\tau(\gamma)} M^{N-1}$, we have

$$\mathrm{dev}^\circ_\tau|_\gamma = \begin{pmatrix} \mathrm{dev}_0|_{N_\gamma H_{xx;\tau}(M)} & 0 \\ 0 & \mathrm{dev}_\tau|_\gamma \end{pmatrix},$$

whence the result follows. □

2.3 The Case of a Manifold with Boundary

When trying to define the infinite-dimensional versions of the spaces of reflected geodesics, i.e. spaces of "reflecting paths of finite energy", one encounters considerable problems. To illustrate these, consider the half space $M := \{(x, y) \in \mathbb{R}^2 \mid x \geq 0\}$ and let $\gamma = (\gamma_1, \gamma_2) \in H^1([0, t], \mathbb{R}^2)$. Setting

$$\widetilde{\gamma}(s) := \begin{cases} \big(\gamma_1(s), \gamma_2(s)\big) & \text{if } \gamma_1(s) \geq 0 \\ \big(-\gamma_1(s), \gamma_2(s)\big) & \text{if } \gamma_1(s) < 0, \end{cases}$$

we associate a path $\widetilde{\gamma}$ in M to each path γ in $\mathbb{R}^2$. However, this mapping is not injective: For example, the path

$$\widetilde{\gamma}(s) = \begin{cases} \big(1 - s, 0\big) & \text{if } s \leq 1 \\ \big(s - 1, 0\big) & \text{if } s \geq 1. \end{cases} \tag{2.3.1}$$

defined on $[0, 2]$ has the pre-images $\widetilde{\gamma}$ and $\gamma(s) := (1 - s, 0)$. Heuristically, if one notices a particle in M that moving along the trajectory $\widetilde{\gamma}$ as in (2.3.1), one might ask whether the particle reflects at the boundary at time 1, or if it changes direction for some other reason (e.g. due to collisions with other molecules). Put differently: If the boundary wasn't there, would the particle have continued as a straight line or would it have taken the reverse gear anyway?
This issue is not relevant for the path integrals over the finite-dimensional spaces $H^{\mathrm{refl}}_{x;\tau}(M)$ because they can only change directions at the times τ_j, and the set of paths γ with $\gamma(\tau_j)$ form a zero set. In the infinite-dimensional setup, however, there are no nodes, so every instance that an absolutely continuous path γ hits the boundary is potentially problematic. Of course, an "integral" over such a set of paths is not defined anyway, but one also runs into trouble even defining a good manifold structure on this set of paths.

A solution to these problems is to consider the Riemannian manifold with boundary M as an *orbifold*. Remember, one class of orbifolds M arises as the quotient of a manifold $\overline{M}$ by the action of a finite group (called good orbifolds), and it is exactly this kind of orbifolds that we need. Namely, given a Riemannian manifold M with boundary, we can define the *double of* M as the topological space

$$\overline{M} := M \coprod\nolimits_{\partial M} M,$$

that is, two copies of M glued together at the boundary. $\overline{M}$ comes with a natural $\mathbb{Z}_2$-action that exchanges the two halves, with the quotient $\overline{M}/\mathbb{Z}_2$ homeomorphic to M, so that this

construction gives M the structure of an orbifold in a natural way. This construction is also intimately related to involutive boundary conditions, as we will explain in the next section.
Now taking the view that a manifold with boundary is nothing but a certain kind of orbifold, it seems natural that the appropriate path spaces should be spaces of *orbifold maps* from the orbifold $[0, t]$ (which is a manifold with boundary, hence an orbifold as argued above − see also Example 2.3.4) into the orbifold M. Essentially, what orbifold paths do is remembering the additional information discussed earlier, namely whether a path hitting the boundary reflects there or not. The spaces of such maps carry again the structure of an orbifold. These spaces indeed turn out to be a good notion of path spaces for path integrals on manifolds with boundary.

To obtain path integral formulas for the heat kernel, we need a certain restriction on the metric of the manifold M, namely that the $\mathbb{Z}_2$-invariant extension to the double $\overline{M}$ is smooth (similar assumptions need to be made on the scalar product of the vector bundle and the Laplacian L, for details see Assumption 2.3.7 below). In particular, this is fulfilled if M has a metric collar decomposition near the boundary.

This section is organized as follows. First, in Subsection 2.3.1, we give a more detailed construction of the orbifold structure on a Riemannian manifold with boundary and explain the relation between equivariant vector bundles on the double and involutive boundary conditions. Then, in Subsection 2.3.2, we introduce the relevant path spaces as well as their finite-dimensional approximations. Finally, in Subsection 2.3.3, we give path integral formulas for the heat kernel and the heat trace on manifolds with boundary, using the orbifold path spaces introduced before.

2.3.1 The Double of a Manifold with Boundary

We now give a more detailed construction of the double of a manifold with boundary. During the course of this thesis, we always take the multiplicative representation $\mathbb{Z}_2 := \{+1, -1\}$. Elements of $\mathbb{Z}_2$ will usually be denoted by ϵ.

Construction 2.3.1 (The Double of a Manifold with Boundary). For a compact M Riemannian manifold with boundary M, set

$$\overline{M} = (M \times \mathbb{Z}_2)/\sim,$$

where $(x, \epsilon) \sim (x', \epsilon')$ if either $(x, \epsilon) = (x', \epsilon')$ or if $x = x'$ and both lie in ∂M. The equivalence classes of (x, ϵ) will be denoted by square brackets, $[x, \epsilon]$. We identify M with the points $[x, 1] \in \overline{M}$. A $\mathbb{Z}_2$-action on $\overline{M}$ is defined by $\epsilon' \cdot [x, \epsilon] := [x, \epsilon'\epsilon]$. This action fixes exactly the boundary $\partial M \subset \overline{M}$ and we have

$$M \cup (-M) = \overline{M} \qquad \text{and} \qquad M \cap (-M) = \partial M.$$

At first, $\overline{M}$ is only a topological space with a continuous $\mathbb{Z}_2$-action. However, there is a natural smooth structure on $\overline{M}$ such that the $\mathbb{Z}_2$-action is smooth and isometric (with respect to the − possibly non-smooth − induced Riemannian metric on $\overline{M}$). It is defined as follows: Near points $x = [x, \epsilon] \in \overline{M}$ with $x \notin \partial M$, the map $[x, \epsilon] \mapsto x$ is a homeomorphism, so near x, a smooth structure on $\overline{M}$ is induced by the one of M, by requiring that this projection map be smooth. To define a smooth structure near points $[x, \epsilon]$ with $x \in \partial M$, define the map

$$\phi_M : \partial M \times [0, R) \longrightarrow M, \qquad (x, r) \longmapsto \exp_x(r\mathbf{n}),$$

where $\mathbf{n}$ is the unit normal to ∂M pointing into $M \subset \overline{M}$. ϕ is an open embedding for $R > 0$ small enough. Now define

$$\overline{\phi}_M : \partial M \times (-R, R) \longrightarrow \overline{M}, \qquad (x, r) \mapsto \big[\phi_M(x, |r|), \mathrm{sign}(r)\big].$$

Then $\overline{\phi}_M$ is a homeomorphism onto its image, which contains all points $x \in \partial M \subset \overline{M}$. This defines a smooth structure on a neighborhood of $\partial M \subset \overline{M}$, by requiring that $\overline{\phi}_M$ be a diffeomorphism. Hence $\overline{M}$ is a closed manifold.
Because the quotient $\overline{M}/\mathbb{Z}_2$ is homeomorphic to M via the projection map, this induces an orbifold structure on M.

Remark 2.3.2 (Functoriality). If $f : M \longrightarrow N$ is a local isometry of compact manifolds with boundary (which by definition sends ∂M to ∂N), then

$$\overline{f} : \overline{M} \longrightarrow \overline{N}, \qquad [x, \epsilon] \longmapsto [f(x), \epsilon]$$

is clearly an equivariant map from $\overline{M}$ to $\overline{N}$. It is smooth because for r small enough,

$$\begin{aligned}(\overline{\phi}_N^{-1} \circ \overline{f} \circ \overline{\phi}_M)(x, r) &= \overline{\phi}_N^{-1}\big(\big[f\big(\exp_x^M(|r|\mathbf{n})\big), \mathrm{sign}(r)\big]\big) = \overline{\phi}_N^{-1}\big(\big[\exp_{f(x)}^N\big(df_x(|r|\mathbf{n})\big), \mathrm{sign}(r)\big]\big)\\ &= \overline{\phi}_N^{-1}\big(\big[\exp_{f(x)}^N(|r|\mathbf{n}), \mathrm{sign}(r)\big]\big) = (f(x), r),\end{aligned}$$

where in the second step, we used that f is a local isometry. One can easily check that we obtain a functor from the category of compact Riemannian manifolds with boundary (with local isometries as morphisms) to the category of (closed) $\mathbb{Z}_2$-manifolds with equivariant maps. From the latter category, there is a faithful (but not full) functor to the category of orbifolds, so in total, one obtains a functor from the category of Riemannian manifolds with boundary to the category of orbifolds.
Notice however the following subtlety in this construction: *The above construction does not give a functor from the category of manifolds with boundary (without Riemannian metric, where the morphisms are local diffeomorphisms preserving the boundary) to the category of* $\mathbb{Z}_2$*-manifolds*, because there are issues with a smooth structure. For example, the homeomorphism of $M := [0, \infty) \times \mathbb{R}$ sending (x, y) to $(x, y + ax)$, $a \in \mathbb{R}$ is an automorphism of manifolds with boundary, but for $a \neq 0$, there is no smooth extension of it as an equivariant smooth automorphism of $\overline{M}$, no matter how the smooth structure is chosen on $\overline{M}$.

Remark 2.3.3 (The Metric on the Double). A compact Riemannian manifold with boundary M induces an equivariant metric $\overline{g}$ on the double $\overline{M}$. However, this metric need not be smooth: With respect to the chart $\overline{\phi}_M$ described above, it has the Taylor expansion near the boundary

$$\overline{g}(x, r) = dr^2 + g_0(x) + |r|g_1(x) + O(r^2), \qquad x \in \partial M, r \in (-R, R),$$

where g_0 and g_1 are smooth metrics on ∂M. Hence $\overline{g}$ will generally be only Lipschitz continuous.

Example 2.3.4 (The Interval). The double of an interval $[a, b]$ is equivariantly diffeomorphic to $S^1 \subset \mathbb{C}$, with the $\mathbb{Z}_2$-action coming from complex conjugation. In particular, $[a, b]$ carries the structure of an orbifold in a natural way.

Construction 2.3.5 (Equivariant Bundles on the Double). Let $\mathcal{V}$ be a vector bundle over M, and let $B \in C^\infty(\partial M, \mathrm{End}(\mathcal{V}|_{\partial M}))$ be a symmetric endomorphism field with $B^2 = \mathrm{id}$. The pair $(\mathcal{V}, B)$ gives rise to an equivariant bundle $\overline{\mathcal{V}}$ on the double $\overline{M}$. It is defined by setting

$$\overline{\mathcal{V}} := \mathcal{V} \times \mathbb{Z}_2 / \sim$$

for the total space, where $(v, \epsilon) \sim (Bv, -\epsilon)$ if v lies over a point in the boundary. That is, one takes two copies of the total space $\mathcal{V}$ and glue them together at the boundary using the involution B. The fibers of $\overline{\mathcal{V}}$ at points $\epsilon x \in \overline{M}$ with $x \in M$ are

$$\overline{\mathcal{V}}_{\epsilon x} := \{[v, \epsilon] \mid v \in \mathcal{V}_x\} \cong \mathcal{V}_x.$$

The bundle $\mathcal{V}$ has a $\mathbb{Z}_2$-equivariant structure, i.e. a group homomorphism

$$\rho : \mathbb{Z}_2 \longrightarrow \mathrm{Aut}(\overline{\mathcal{V}})$$

that projects down to the $\mathbb{Z}_2$-action on $\overline{M}$. Namely, we can set for $x \in \overline{M}$

$$\rho(\epsilon) : \overline{\mathcal{V}}_x \longrightarrow \overline{\mathcal{V}}_{\epsilon x}, \qquad [v, \epsilon'] \longmapsto [v, \epsilon\epsilon'].$$

Note that if $x \in \partial M$, then $\rho(-1)[v, \epsilon] = [v, -\epsilon] = [Bv, \epsilon]$, so $\rho(-1)|_{\partial M} = B$ under the identification $\overline{\mathcal{V}}|_M \cong \mathcal{V}$.
Orbifold vector bundles over M are precisely given by equivariant vector bundles over $\overline{M}$ [Rua00]. Hence a vector bundle $\mathcal{V}$ over M together with an endomorphism field B as above defines an orbifold vector bundle over M considered as an orbifold.
If furthermore $\mathcal{V}$ is a metric vector bundle and L is a formally self-adjoint Laplace type operator such that B is an involutive boundary condition for L, then by equivariant extension, we obtain an equivariant Laplace type operator $\overline{L}$ acting on sections of $\overline{\mathcal{V}}$.

Conversely, if $\overline{\mathcal{V}}$ is a $\mathbb{Z}_2$-equivariant metric vector bundle over $\overline{M}$ (i.e. an orbifold vector bundle over the orbifold M), and $\overline{L}$ is a formally self-adjoint, equivariant Laplace type operator acting on sections of $\overline{\mathcal{V}}$, then $\mathcal{V} := \overline{\mathcal{V}}|_M$ is a metric vector bundle over M and the operator $L := \overline{L}|_M$ is a formally self-adjoint Laplace type operator. with involutive boundary condition $B := \rho(-1)|_{\partial M} \in C^\infty(\partial M, \mathcal{V}|_{\partial M})$.

Example 2.3.6. We review the examples given in Section 1.1.2 in this setup.

(a) If $\overline{\mathcal{V}} = \underline{\mathbb{R}}$ or $\underline{\mathbb{C}}$ a trivial line bundle, there are basically two reasonable ways to turn $\overline{\mathcal{V}}$ into an equivariant bundle: We can set $\rho(-1) = -1$ or $\rho(-1) = 1$. The first case induces Dirichlet boundary conditions, while the other choice induces Neumann boundary conditions on functions on M.

(b) The bundle $\overline{\mathcal{V}} = \Lambda^k T^* \overline{M}$ can be turned into an equivariant bundle by setting $\rho(-1) = \alpha^*$, the pullback along the "flip map" $\alpha : \overline{M} \to \overline{M}$, $x \mapsto -x$. Because this sends dr to $-dr$, this induces absolute boundary conditions on sections of $\Lambda^k T^* \partial M$ over M. Taking $\rho(-1) = -\alpha^*$ instead induces relative boundary conditions.

From now on, we make the following assumption, which allows us to obtain path integral formulas for the heat kernel on compact manifolds with boundary.

Assumption 2.3.7 (Smoothness). The induced invariant metrics on $\overline{M}$ and $\overline{\mathcal{V}}$ are smooth, as well as the coefficients of the operator $\overline{L}$.

Of course Assumption 2.3.7 is very strong. In particular, it implies that ∂M is a totally geodesic submanifold of M, i.e. the second fundamental form of the boundary vanishes identically. This follows from the fact that ∂M is the fixed point set of the flip map $\alpha : \overline{M} \to \overline{M}$, $x \mapsto -x$, which is an isometry (and smooth by our assumption). Assumption 2.3.7 is satisfied for example if M is a metric collar near the boundary.
In particular, Assumption 2.3.7 implies that $\overline{M}$ is a closed Riemannian manifold with a smooth Riemannian metric, so that all results from the closed case apply.

Example 2.3.8 (Hemisphere). An example for a manifold satisfying Assumption 2.3.7 is

$$M = \{v = (v_1, \ldots, v_{n+1}) \in S^n \subset \mathbb{R}^{n+1} \mid v_{n+1} \geq 0\},$$

the northern hemisphere of S^n, so that $\partial M \approx S^{n-1}$ is the equator and $\overline{M} = S^n$. Here the $\mathbb{Z}_2$ action on $\overline{M}$ is given by $\epsilon \cdot (v_1, \ldots, v_n, v_{n+1}) = (v_1, \ldots, v_n, \epsilon v_{n+1})$ for $\epsilon = \pm 1 \in \mathbb{Z}_2$.

2.3.2 Orbifold Path Spaces

Having noticed above that a Riemannian manifold M with boundary naturally carries an orbifold structure, induced by the $\mathbb{Z}_2$-manifold $\overline{M}$, the natural consequence is that the space of paths in M should have the structure of an (infinite-dimensional) orbifold as well. However, maps between orbifolds are a complicated matter and it took mathematicians quite a while to realize what the correct notion of maps should be. Namely, it turns out that given two orbifolds $N = \overline{N}/H$ and $M = \overline{M}/G$, the set of (let's say continuous) orbifold maps should in general *not* be equal to the set of equivariant maps (f, φ) from $\overline{N}$ to $\overline{M}$, i.e. smooth maps $f : \overline{N} \longrightarrow \overline{M}$ with $f(h \cdot x) = \varphi(h) \cdot f(x)$. Although each equivariant map induces an orbifold map, there may be *more* orbifold maps than those that come from equivariant maps (see [Che06, p. 5f]). This effect does not occur when we consider the maps from an interval $[0, t]$ into an orbifold M (this is related to the fact that $[0, t]$ is contractible), but it will occur when we consider maps from S^1 into an orbifold, i.e. when we consider the loop space of an orbifold (see Remarks (1) and (2) on p. 9 in [Che06] and our definition of the space of orbifold loops below).
We will not further elaborate on the theory of orbifolds and their maps here, instead we will make *ad hoc* definitions, which is enough for our purposes. For details, we refer to the literature: A good introduction to orbifolds and maps between them is given in [MP97] and [ALR07]. In [Che06], mapping spaces of orbifolds are constructed as infinite-dimensional orbifolds. See also [CR02], [Rua00] or [Poh10].

Remark 2.3.9. As discussed in Example 2.3.4, closed intervals are manifolds with boundary and therefore can be considered as orbifolds as in Section 2.3.1. Therefore, maps from an interval into an orbifold can be treated without needing the concept of an orbifold with boundary.

To start with, let us define the orbifold path space $H^{1,\mathrm{orb}}([0,t],M)$, which is the orbifold quotient of the (infinite-dimensional) manifold

$$\overline{H^{1,\mathrm{orb}}([0,t],M)} := H^1([0,t],\overline{M}),$$

by its $\mathbb{Z}_2$-action, which is given by post-composition. That is, we set

$$H^{1,\mathrm{orb}}([0,t],M) := \overline{H^{1,\mathrm{orb}}([0,t],M)}/\mathbb{Z}_2$$

which then naturally carries the structure of an (infinite-dimensional) orbifold.
To find the appropriate notion of orbifold path spaces with one fixed endpoint, notice that in the case that M is closed, the space $H_{x;t}(M)$ can be defined as the pullback

$$\begin{tikzcd} H_{xy;t}(M) \arrow[r, dotted] \arrow[d, dotted] & H^1([0,t],M) \arrow[d, "\mathrm{ev}_{0,t}"] \\ \bullet \arrow[r, "(x,y)"'] & M \times M \end{tikzcd} , \tag{2.3.2}$$

where $\mathrm{ev}_{0,t}$ is the evaluation sending γ to $(\gamma(0),\gamma(t))$, $\bullet$ denotes the one-point manifold and (x,y) denotes the map that sends the one point to $(x,y) \in M \times M$. Mirroring this construction, we define the space $H^{\mathrm{orb}}_{xy;t}(M)$ as the pullback

$$\begin{tikzcd} H^{\mathrm{orb}}_{xy;t}(M) \arrow[r, dotted] \arrow[d, dotted] & H^{1,\mathrm{orb}}([0,t],M) \arrow[d, "\mathrm{ev}_{0,t}"] \\ \bullet \arrow[r, "(x,y)"'] & M \times M \end{tikzcd} \tag{2.3.3}$$

in the category of orbifolds.
To explicitly calculate pullbacks of orbifolds, the easiest way it is probably to associate to each orbifold a representing Lie groupoid (see Def. 1.47 in [ALR07]) and then calculate the pullback of Lie groupoids (see e.g. Def. 1.41 in [ALR07]). This must be done as a homotopy-pullback, i.e. a pullback in a 2-category (since Lie groupoids form a 2-category). However, we do not need that the orbifold path spaces defined are actually given as certain pullbacks, so we will not further delve into these details; instead we will present the outcome and use the following *ad hoc* definition for the space $H^{\mathrm{orb}}_{xy;t}(M)$ in this thesis. We just claim that this is indeed a representative of the pullback in (2.3.3).

Notation 2.3.10 (Pinned Orbifold Paths). The pullback $H^{\mathrm{orb}}_{xy;t}(M)$ can be explicitly described as the quotient of the manifold

$$\overline{H^{\mathrm{orb}}_{xy;t}(M)} := \coprod_{\epsilon_1,\epsilon_2\in\mathbb{Z}_2} H_{\epsilon_1 x,\epsilon_2 y;t}(\overline{M}) \times \{(\epsilon_1,\epsilon_2)\}$$

by the diagonal $\mathbb{Z}_2$-action, i.e.

$$H^{\mathrm{orb}}_{xy;t}(M) = \overline{H^{\mathrm{orb}}_{xy;t}(M)}/\mathbb{Z}_2$$

with the induced orbifold structure.

Notice that this action is free so that $H^{\mathrm{orb}}_{xy;t}(M)$ is actually a manifold.
The elements of $H^{\mathrm{orb}}_{xy;t}(M)$ are equivalence classes $[\gamma, \epsilon_1, \epsilon_2]$ containing the to representatives $(\gamma, \epsilon_1, \epsilon_2)$ and $(-\gamma, -\epsilon_1, -\epsilon_2)$. We will often abuse notation and write just γ instead of $[\gamma, \epsilon_1, \epsilon_2]$ for elements of $H^{\mathrm{orb}}_{xy;t}(M)$ (in particular when integrating over these spaces, where γ is used as an integration variable). Of course, when doing so, one has to keep this inaccuracy in mind and remember that such an element γ also contains information on the signs ϵ_1 and ϵ_2 (which can be recovered from the path though, if x respectively y is in $M \setminus \partial M$), and that the path γ can also be replaced by $-\gamma$. However since the map $x \mapsto -x$ is an isometry, the energy of such an element is well defined (because $E(\gamma) = E(-\gamma)$).

Moreover, we define the *orbifold loop space* $L_t^{\mathrm{orb}}(M)$ as the pullback

$$\begin{tikzcd} L_t^{\mathrm{orb}}(M) \arrow[r, dotted] \arrow[d, dotted] & H^{1,\mathrm{orb}}([0,t], M) \arrow[d, "\mathrm{ev}_{0,t}"] \\ M \arrow[r, "\Delta"'] & M \times M, \end{tikzcd}$$

where $\Delta : M \longrightarrow M \times M$, $x \mapsto (x, x)$ is the inclusion as the diagonal (induced by the diagonal map $\overline{\Delta} : \overline{M} \longrightarrow \overline{M} \times \overline{M}$). In this case, the pullback is *not* a manifold, but a proper orbifold.

Notation 2.3.11 (The Orbifold Loop Space). The orbifold loop space $L_t^{\mathrm{orb}}(M)$ consists of two components,

$$L_t^{\mathrm{orb}}(M) = L_t^{\mathrm{orb},+}(M) \coprod L_t^{\mathrm{orb},-}(M),$$

which we call *positive* and *negative* component. The positive component is given as the orbifold quotient of the manifold

$$\overline{L_t^{\mathrm{orb},+}(M)} := L_t(\overline{M}) \times \{+1\} = H^1(S^1_t, \overline{M}) \times \{+1\}$$

by the $\mathbb{Z}_2$-action given by $\epsilon \cdot (\gamma, 1) = (\epsilon \circ \gamma, 1)$ (where $S^1_t = \mathbb{R}/t\mathbb{Z}$ is the circle of length t). This is nothing but the $\mathbb{Z}_2$-manifold of equivariant maps from S^1_t to $\overline{M}$. The negative component is the orbifold quotient of the manifold

$$\overline{L_t^{\mathrm{orb},-}(M)} = \bigcup_{x \in \overline{M}} H_{x,-x;t}(\overline{M}) \times \{-1\}$$

by the $\mathbb{Z}_2$-action given by $\epsilon \cdot (\gamma, -1) = (\epsilon \circ \gamma, -1)$. Hence orbifold loops in M are not only loops in $\overline{M}$ (i.e. paths with $\gamma(t) = \gamma(0)$), but also paths that return to *minus* the starting point (i.e. $\gamma(t) = -\gamma(0)$).

Put together, $L_t^{\mathrm{orb}}(M)$ is the orbifold quotient of the manifold

$$\overline{L_t^{\mathrm{orb}}(M)} = \coprod_{\epsilon \in \mathbb{Z}_2} \bigcup_{x \in M} H_{x,\epsilon x;t}(\overline{M}) \times \{\epsilon\}$$

by the $\mathbb{Z}_2$-action given by $\epsilon' \cdot (\gamma, \epsilon) = (\epsilon' \gamma, \epsilon)$ (note that this is *not* the diagonal $\mathbb{Z}_2$-action). Here the information about the $\epsilon \in \mathbb{Z}_2$ indicates whether the path γ lies in the positive or

negative component of M. This is clear for the path γ with $\gamma(0) \notin \partial M$, but paths γ with $\gamma(0) \in \partial M$ appear twice in $L_t^{\mathrm{orb}}(M)$, because then both $\gamma(0) = \gamma(t)$ and $\gamma(0) = -\gamma(t)$. These paths can only be distinguished by the element $\epsilon \in \mathbb{Z}_2$.
$L_t^{\mathrm{orb}}(M)$ is not a manifold (unless $\partial M = \emptyset$), since any $\gamma \in L_t^{\mathrm{orb}}(M)$ that lies completely in ∂M is a fixed point of the $\mathbb{Z}_2$ action.

To define the finite-dimensional approximations of the spaces defined above in (2) and (3), we suppose that the smoothness Assumption 2.3.7 is satisfied. In this case, the definition is straight forward:

Notation 2.3.12 (Finite-dimensional Approximations). For a partition $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = t\}$ of an interval $[0, t]$, we define $H_{xy;\tau}^{\mathrm{orb}}(M)$ by the orbifold quotient of

$$\overline{H_{xy;\tau}^{\mathrm{orb}}(M)} := \coprod_{\epsilon_1,\epsilon_2 \in \mathbb{Z}_2} H_{\epsilon_1 x, \epsilon_2 y;\tau}(\overline{M}) \times \{(\epsilon_1, \epsilon_2)\}$$

by the diagonal $\mathbb{Z}_2$-action. We write $L_\tau^{\mathrm{orb}}(M)$ be the orbifold quotient of

$$\overline{L_\tau^{\mathrm{orb}}(M)} := \coprod_{\epsilon \in \mathbb{Z}_2} \bigcup_{x \in \overline{M}} H_{x,\epsilon x;\tau}(\overline{M}) \times \{\epsilon\}$$

by the post-composition $\mathbb{Z}_2$-action (which is *not* the diagonal $\mathbb{Z}_2$-action). Here the spaces $H_{z_0,z_1;\tau}(\overline{M})$ are defined using the definition from Section 2.2.1 for the closed Riemannian manifold $\overline{M}$.

The orbifold path spaces $H_{xy;\tau}^{\mathrm{orb}}(M)$ can be endowed with the same Riemannian metrics as before, in the obvious way, which turns them into Riemannian manifolds. The corresponding integral is then defined by

$$\int_{H_{xy;\tau}^{\mathrm{orb}}(M)} F(\gamma)\,\mathrm{d}\gamma = \frac{1}{2} \sum_{\epsilon_1,\epsilon_2 \in \mathbb{Z}_2} \int_{H_{\epsilon_1 x, \epsilon_2 x;\tau}(\overline{M})} F([\gamma, \epsilon_1, \epsilon_2])\,\mathrm{d}\gamma, \tag{2.3.4}$$

compare Remark 2.3.13 below. On $L_\tau^{\mathrm{orb}}(M)$, one defines measures by defining invariant measures on $\overline{L_\tau^{\mathrm{orb}}(M)}$ and pushing them down with the reflection map. For example the discrete H^1 volume will be defined analogously to (2.2.6) by the formula

$$\begin{aligned} &\int_{L_\tau^{\mathrm{orb}}(M)} f\big(\gamma(\tau_1), \dots, \gamma(\tau_N), \epsilon\big)\,\mathrm{d}^{\Sigma\text{-}H^1}\gamma \\ &\qquad = \frac{1}{2} \sum_{\epsilon \in \mathbb{Z}_2} \int_{\overline{M}^N} f(x_1, \dots, x_N, \epsilon) \left(\prod_{j=1}^N J(x_{j-1}, x_j)(\Delta_j \tau)^{n/2} \right)^{-1} \mathrm{d}x_1 \cdots \mathrm{d}x_N \end{aligned} \tag{2.3.5}$$

for integrable functions f on $\overline{M}^N \times \mathbb{Z}_2$, where we set $x_0 := \epsilon x_N$ in the summand with index ϵ.

Remark 2.3.13 (Integration over Orbifolds). In general, the integral over a Riemannian orbifold Σ of the form $\Sigma := \overline{\Sigma}/G$ is defined as

$$\int_\Sigma f(x)\,\mathrm{d}x = \frac{1}{|G|} \int_{\overline{\Sigma}} f(x)\,\mathrm{d}x.$$

In the case that Σ is a manifold (as above, when $\Sigma = H_{xy;\tau}^{\mathrm{orb}}(M)$ and $G = \mathbb{Z}_2$, $|G| = 2$), this reduces to the usual integral over the Riemannian volume density.

Notice that there is a well-defined map

$$\alpha : H^{\mathrm{orb}}_{xx;\tau}(M) \longrightarrow L^{\mathrm{orb}}_{\tau}(M), \qquad [\gamma, \epsilon_1, \epsilon_2] \longmapsto [\gamma, \epsilon_1\epsilon_2]. \tag{2.3.6}$$

This allows us to formulate a co-area formula. Namely, similar to before (see (2.2.7)), the discrete H^1 volume measures are manufactured in such a way that we have

$$\int_{L^{\mathrm{orb}}_{\tau}(M)} F(\gamma)\, \mathrm{d}^{\Sigma\text{-}H^1}\gamma = t^{-n/2} \int_M \int_{H^{\mathrm{orb}}_{xx;\tau}(M)} \alpha^* F(\gamma)\, \mathrm{d}^{\Sigma\text{-}H^1}\gamma\, \mathrm{d}x \tag{2.3.7}$$

for integrable functions F on $L^{\mathrm{orb}}_{\tau}(M)$. To verify (2.3.7), write $F(\gamma) = F([\gamma, \epsilon]) = f(\gamma(\tau_1), \dots, \gamma(\tau_N), \epsilon)$ for an integrable function f on $\overline{M}^N \times \mathbb{Z}_2$ and calculate

$$\begin{aligned}
&\int_M \int_{H^{\mathrm{orb}}_{xx;\tau}(M)} \alpha^* F(\gamma)\, \mathrm{d}^{\Sigma\text{-}H^1}\gamma\, \mathrm{d}x \\
&\qquad = \frac{1}{2} \sum_{\epsilon_1, \epsilon_2 \in \mathbb{Z}_2} \int_M \int_{H_{\epsilon_1 x, \epsilon_2 x;\tau}(\overline{M})} F\big([\gamma, \epsilon_1\epsilon_2]\big)\, \mathrm{d}^{\Sigma\text{-}H^1}\gamma\, \mathrm{d}x \\
&\qquad = \frac{1}{2} \sum_{\epsilon \in \mathbb{Z}_2} \int_{\overline{M}} \int_{H_{x,\epsilon x;\tau}(\overline{M})} F\big([\gamma, \epsilon]\big)\, \mathrm{d}^{\Sigma\text{-}H^1}\gamma\, \mathrm{d}x \\
&\qquad = t^{n/2} \sum_{\epsilon \in \mathbb{Z}_2} \int_{\overline{M}^N} f(x_1, \dots, x_N, \epsilon]) \left(\prod_{j=1}^{N} J(x_{j-1}, x_j)(\Delta_j\tau)^{n/2}\right)^{-1} \mathrm{d}x_1 \cdots \mathrm{d}x_N \\
&\qquad = t^{n/2} \int_{L^{\mathrm{orb}}_{\tau}(M)} F(\gamma)\, \mathrm{d}^{\Sigma\text{-}H^1}\gamma,
\end{aligned}$$

using Remark 2.3.13, the definition (2.2.5) of the discrete H^1 volume on $H_{xy;\tau}(\overline{M})$ as well as (2.3.5).

2.3.3 Orbifold Path Integrals

Again, we are in the setting that L is a self-adjoint Laplace type operator with involutive boundary condition B, that acts on sections of a metric vector bundle $\mathcal{V}$ over an n-dimensional Riemannian manifold M. From the constructions in Section 2.3.1, we obtain an equivariant metric vector bundle $\overline{\mathcal{V}}$ on the double $\overline{M}$, and an equivariant self-adjoint Laplace type operator $\overline{L}$. We always assume that Assumption 2.3.7 is satisfied, hence this is a Laplace type operator with smooth coefficients on the compact manifold $\overline{M}$.
For the spaces $H^{\mathrm{orb}}_{xy;\tau}(M)$ and $L^{\mathrm{orb}}_{\tau}(M)$, there are B-path ordered exponentials as well.

Definition 2.3.14 (B-path-ordered exponential). On the orbifold path spaces, we define the B-path-ordered exponential as follows.

(1) For $\gamma = [\gamma, \epsilon_1, \epsilon_2] \in H^{\mathrm{orb}}_{xy;t}(M)$, define

$$\mathcal{P}_B(\gamma) := \mathcal{P}_B([\gamma, \epsilon_1, \epsilon_2]) = \rho(\epsilon_2)\overline{\mathcal{P}}(\gamma)\rho(\epsilon_1) \in \mathrm{Hom}(\mathcal{V}_x, \mathcal{V}_y).$$

(2) For $\gamma = [\gamma, \epsilon] \in L_t^{\mathrm{orb}}(M)$, set

$$\mathcal{P}_B(\gamma) := \mathcal{P}_B([\gamma, \epsilon]) = \rho(\epsilon'\epsilon)\overline{\mathcal{P}}(\gamma)\rho(\epsilon') \in \mathrm{End}(\mathcal{V}_{\gamma(0)}),$$

where $\epsilon' = 1$ if $\gamma(0) \in M$ and $\epsilon' = -1$ otherwise.

In the above formulas, $\overline{\mathcal{P}}(\gamma)$ is the path-ordered exponential along paths in $\overline{M}$ associated to $\overline{L}$ and $\rho : \mathbb{Z}_2 \to \mathrm{Aut}(\overline{\mathcal{V}})$ is the representation that makes $\overline{\mathcal{V}}$ an equivariant bundle.

Remark 2.3.15 (Well-Definedness). Let us make some explanations regarding the definition of the B-path-ordered exponential above. We need to check that for $\gamma \in H_{xy;t}^{\mathrm{orb}}$, $\mathcal{P}_B(\gamma)$ is independent of the choice of representative $(\gamma, \epsilon_1, \epsilon_2)$ or $(-\gamma, -\epsilon_1, -\epsilon_2)$. Because $\overline{L}$ and hence the connection $\overline{\nabla}$ and the potential $\overline{V}$ determined by L are equivariant, so is the path-ordered exponential, i.e.

$$\overline{\mathcal{P}}(-\gamma) = \rho(-1)\overline{\mathcal{P}}(\gamma)\rho(-1).$$

Hence

$$\rho(-\epsilon_2)\overline{\mathcal{P}}(-\gamma)\rho(-\epsilon_1) = \rho(-\epsilon_2)\rho(-1)\overline{\mathcal{P}}(\gamma)\rho(-1)\rho(-\epsilon_1) = \rho(\epsilon_2)\overline{\mathcal{P}}(\gamma)\rho(\epsilon_1).$$

Therefore, $\mathcal{P}_B(\gamma)$ does not depend on the representative and descends to a well-defined function on $H_{xy;\tau}^{\mathrm{orb}}(M)$.
Similarly, one shows that for $\gamma \in L_\tau^{\mathrm{orb}}(M)$, $\mathcal{P}_B(\gamma)$ as defined in formula (2) is independent of the representative.

Remark 2.3.16 (Compatibility). Notice that the definitions (1) and (2) behave well together in the sense that for any element $[\gamma, \epsilon_1, \epsilon_2] \in H_{xx;t}^{\mathrm{orb}}(M)$, we have

$$\mathcal{P}_B^{H_{xx;t}(M)}([\gamma, \epsilon_1, \epsilon_2]) = \mathcal{P}_B^{L_t(M)}([\gamma, \epsilon_1\epsilon_2]) = (\alpha^*\mathcal{P}_B^{L_t(M)})([\gamma, \epsilon_1, \epsilon_2]),$$

where α is the map from $H_{xx;\tau}^{\mathrm{orb}}(M)$ to $L_\tau^{\mathrm{orb}}(M)$ defined above in (2.3.6). Therefore, no confusion can arise from denoting these different maps with the same letter.

With this definition, we have the following result.

Theorem 2.3.17 (The Heat Kernel as an Orbifold Path Integral I). *Let L be a self-adjoint Laplace type operator with involutive boundary condition B, acting on sections of a metric vector bundle $\mathcal{V}$ over a compact n-dimensional Riemannian manifold with boundary M. Suppose that the smoothness Assumption 2.3.7 is satisfied and let $\mathcal{P}_B(\gamma)$ be the B-path-ordered exponential determined by L as in Def. 2.3.14 (1). Then*

$$p_t^L(x, y) = \lim_{|\tau|\to 0} (4\pi t)^{-n/2} \fint_{H_{xy;\tau}^{\mathrm{orb}}(M)} e^{-E(\gamma)/2}\, \mathcal{P}_B(\gamma)^{-1}\, \mathrm{d}^{\Sigma\text{-}H^1}\gamma$$

for any $x, y \in M$ and $t > 0$. Here the slash in the integral sign denotes division by $(4\pi)^{\dim(H_{xy;\tau}^{\mathrm{orb}}(M))/2}$.

We need the following Lemma.

Lemma 2.3.18. *Under Assumption 2.3.7, the heat kernel p_t^L of L is given by*

$$p_t^L(x,y) = p_t^{\overline{L}}(x,y) + p_t^{\overline{L}}(x,-y)\rho(-1) = p_t^{\overline{L}}(x,y) + \rho(-1)p_t^{\overline{L}}(-x,y), \tag{2.3.8}$$

where $p_t^{\overline{L}}$ is the heat kernel of $\overline{L}$.

Remark 2.3.19. Note that because $\overline{L}$ is equivariant, its heat kernel $p^{\overline{L}}$ satisfies the equivariance condition

$$p_t^{\overline{L}}(x,y) = \rho(-1)p_t^{\overline{L}}(-x,-y)\rho(-1). \tag{2.3.9}$$

This shows that indeed the two terms on the right hand side of (2.3.8) agree.

Proof. For $u \in L^2(M,\mathcal{V})$, set

$$P_t u(x) := \int_M \big(p_t^{\overline{L}}(x,y) + \rho(-1)p_t^{\overline{L}}(-x,y)\big)u(y)\mathrm{d}y, \qquad x \in M.$$

Clearly, P_t is a bounded operator on $L^2(M,\mathcal{V})$. For $u \in L^2(M,\mathcal{V})$, denote by

$$\overline{u}(x) := \begin{cases} u(x) & \text{if } x \in M \\ \rho(-1)u(-x) & \text{if } x \notin M. \end{cases}$$

the section in $L^2(\overline{M},\overline{\mathcal{V}})$ obtained from u by equivariant extension. Then

$$\begin{aligned} P_t u(x) &= \int_M \big(p_t^{\overline{L}}(x,y) + \rho(-1)p_t^{\overline{L}}(-x,y)\big)u(y)\mathrm{d}y \\ &= \int_M p_t^{\overline{L}}(x,y)u(y)\mathrm{d}y + \int_{-M} \rho(-1)p_t^{\overline{L}}(-x,-y)u(-y)\mathrm{d}y \\ &= \int_M p_t^{\overline{L}}(x,y)\overline{u}(y)\mathrm{d}y + \int_{-M} \underbrace{\rho(-1)p_t^{\overline{L}}(-x,-y)\rho(-1)}_{=p_t^{\overline{L}}(x,y)}\overline{u}(y)\mathrm{d}y \\ &= \int_{\overline{M}} p_t^{\overline{L}}(x,y)\overline{u}(y)\mathrm{d}y = e^{-t\overline{L}}\overline{u}(x) \end{aligned}$$

so that $P_t u = (e^{-t\overline{L}}\overline{u})|_M$. Hence for any $u \in L^2(M,\mathcal{V})$, $P_t u$ is smooth for $t > 0$ and satisfies the heat equation,

$$(\partial_t + L)P_t u = \big((\partial_t + \overline{L})e^{-t\overline{L}}\overline{u}\big)|_M = 0. \tag{2.3.10}$$

(Notice here that L and $\overline{L}$ are local operators, which agree on smooth functions on M.) Furthermore, this shows that

$$\lim_{t\to 0} P_t u = \lim_{t\to 0}(e^{-t\overline{L}}\overline{u})|_M = \overline{u}|_M = u \tag{2.3.11}$$

for all $u \in L^2(M,\mathcal{V})$.

We show that $P_t u$ also satisfies the boundary condition defined by B (see Def. 1.1.4) for every $u \in L^2(M, \mathcal{V})$ and $t > 0$: For $x \in \partial M$, i.e. $x = -x$, we have

$$P_t u(x) = \big(1 + \rho(-1)\big) \int_M p_t^{\overline{L}}(x, y) u(y) \mathrm{d}y = \big(1 + B\big) \int_M p_t^{\overline{L}}(x, y) u(y) \mathrm{d}y,$$

which is in $\mathcal{W}_x^+$, the $+1$-eigenspace of B_x. Furthermore, if $\gamma(s) = \exp_x(s\mathbf{n})$ is the geodesic starting at x normal to the boundary, we have $-\gamma(s) = \gamma(-s)$, hence

$$\begin{aligned}
\nabla_{\mathbf{n}} P_t u(x) &= \nabla_s|_{s=0} \Big\{ \int_M \Big(p_t^{\overline{L}}\big(\gamma(s), y\big) + \rho(-1) p_t^{\overline{L}}\big(\gamma(-s), y\big) \Big) u(y) \mathrm{d}y \Big\} \\
&= \int_M \Big(\nabla_s|_{s=0} p_t^{\overline{L}}\big(\gamma(s), y\big) + \rho(-1) \nabla_s|_{s=0} p_t^{\overline{L}}\big(\gamma(-s), y\big) \Big) u(y) \mathrm{d}y \Big\} \\
&= (\mathrm{id} - B) \int_M \nabla_{\mathbf{n}} p_t^{\overline{L}}(x, y) u(y) \mathrm{d}y,
\end{aligned}$$

which is an element of $\mathcal{W}_x^-$, the -1-eigenspace of B_x. Hence $P_t u$ satisfies the boundary condition for any $u \in L^2(M, \mathcal{V})$.
Now for any $u \in L^2(M, \mathcal{V})$ and $t > 0$, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}s} \big\{ e^{-(t-s)L} P_s u \big\} = L e^{-(t-s)L} P_s u - e^{-(t-s)L} L P_s u = e^{-(t-s)L} (L P_s u - L P_s u) = 0.$$

Here in the first step, we used (2.3.10) and the second step is justified because $P_s u$ is in the domain of the operator L, since we verified above that $P_s u$ satisfies the boundary condition (this uses the fact that $L e^{-tL} v = e^{-tL} L v$ for sections v, provided that v is in the domain of L). Hence the function $e^{-(t-s)L} P_s u$ is constant in s on the interval $(0, t)$. Thus for any $t > 0$ and $u \in L^2(M, \mathcal{V})$,

$$P_t u = \lim_{s \nearrow t} e^{-(t-s)L} P_s u = \lim_{s \searrow 0} e^{-(t-s)L} P_s u = e^{-tL} u,$$

where we used (2.3.11). This shows that the operator families P_t and e^{-tL} coincide. Therefore, their kernels do as well. □

Proof (of Thm. 2.3.17). Let $\overline{\mathcal{P}}(\gamma)$ is the path-ordered exponential associated to the operator $\overline{L}$ on $\overline{M}$. By Lemma 2.3.18 and Thm. 2.2.7, we have

$$\begin{aligned}
p_t^L(x, y) &= \sum_{\epsilon \in \mathbb{Z}_2} p_t^{\overline{L}}(x, \epsilon y) \rho(\epsilon) = \frac{1}{2} \sum_{\epsilon_1} \sum_{\epsilon \in \mathbb{Z}_2} \rho(\epsilon_1) p_t^{\overline{L}}(\epsilon_1 x, \epsilon_1 \epsilon y) \rho(\epsilon) \rho(\epsilon_1) \\
&= \frac{1}{2} \sum_{\epsilon_1, \epsilon_2 \in \mathbb{Z}_2} \rho(\epsilon_1) p_t^{\overline{L}}(\epsilon_1 x, \epsilon_2 y) \rho(\epsilon_2) \\
&= \lim_{|\tau| \to 0} (4\pi t)^{-n/2} \frac{1}{2} \sum_{\epsilon_1, \epsilon_2 \in \mathbb{Z}_2} \fint_{H_{\epsilon_1 x, \epsilon_2 y; \tau}(\overline{M})} e^{-E(\gamma)/2} \rho(\epsilon_1) \overline{\mathcal{P}}(\gamma)^{-1} \rho(\epsilon_2) \mathrm{d}^{\Sigma\text{-}H^1} \gamma \\
&= \lim_{|\tau| \to 0} (4\pi t)^{-n/2} \fint_{H_{xy;\tau}^{\mathrm{orb}}(M)} e^{-E(\gamma)/2} \mathcal{P}_B(\gamma)^{-1} \mathrm{d}^{\Sigma\text{-}H^1} \gamma,
\end{aligned}$$

where we used the equivariance (2.3.9) of $p_t^{\overline{L}}$ and the definition (2.3.4) of the measure on $H_{xy;\tau}^{\mathrm{orb}}(M)$, □

The heat trace can be approximated by finite-dimensional integrals over the orbifold loop spaces $L_\tau^{\mathrm{orb}}(M)$.

Theorem 2.3.20 (The Heat Trace as an Orbifold Path Integral I). *Let M be a compact Riemannian manifold with boundary and let L be a self-adjoint Laplace type operator with involutive boundary condition B, acting on sections of a metric vector bundle $\mathcal{V}$ over M. Suppose that the smoothness Assumption 2.3.7 is satisfied and let $\mathcal{P}_B(\gamma)$ be the B-path-ordered integral determined by L as in Def. 2.3.14 (2). Then*

$$\operatorname{Tr} e^{-tL} = \lim_{|\tau|\to 0} \fint_{L_\tau^{\mathrm{orb}}(M)} e^{-E(\gamma)/2} \operatorname{tr} \mathcal{P}_B(\gamma)^{-1} \, \mathrm{d}^{\Sigma\text{-}H^1}\gamma.$$

for any $t > 0$, where the limit goes over any sequence of partitions τ the mesh of which tends to zero, and the slash over the integral sign denotes division by $(4\pi)^{\dim(L_\tau^{\mathrm{orb}}(M))/2}$.

Proof. If $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = t\}$ is a partition of the interval $[0, t]$, notice that the dimension of $L_\tau^{\mathrm{orb}}(M)$ is nN, while the dimension of $H_{xy;\tau}^{\mathrm{orb}}(M)$ is $n(N-1)$. By Lemma 2.3.18 and Thm. 2.3.17, we have

$$\begin{aligned}
\operatorname{Tr} e^{-tL} &= \int_M \operatorname{tr} p_t^L(x,x)\mathrm{d}x \\
&= \int_M \lim_{|\tau|\to 0} (4\pi t)^{-n/2} (4\pi)^{-n(N-1)/2} \int_{H_{xx;\tau}^{\mathrm{orb}}(M)} e^{-E(\gamma)/2} \operatorname{tr} \mathcal{P}_B(\gamma)^{-1} \, \mathrm{d}^{\Sigma\text{-}H^1}\gamma \mathrm{d}x \\
&= \lim_{|\tau|\to 0} (4\pi)^{-nN/2} t^{-n/2} \int_M \int_{H_{xx;\tau}^{\mathrm{orb}}(M)} e^{-E(\gamma)/2} \operatorname{tr} \mathcal{P}_B(\gamma)^{-1} \, \mathrm{d}^{\Sigma\text{-}H^1}\gamma \mathrm{d}x
\end{aligned}$$

where the exchange of integration and the limit $|\tau| \to 0$ is justified by showing that the integrand is uniformly bounded, just as in the proof of Thm. 2.2.13. The result now follows from the co-area formula (2.3.7), using Remark 2.3.16. $\square$

Just as before, the heat kernel can be approximated by finite-dimensional integrals over orbifold path spaces uniformly in t, by taking a more complicated integrand.

Theorem 2.3.21 (Heat Kernel as an Orbifold Path Integral II). *Let L be a self-adjoint Laplace type operator with involutive boundary condition B, acting on sections of a metric vector bundle $\mathcal{V}$ over a compact n-dimensional Riemannian manifold with boundary M. Suppose that the smoothness Assumption 2.3.7 is satisfied. Then for any $\nu \in \mathbb{N}_0$ and $T > 0$, there exist constants $C, \delta > 0$ such that*

$$\left| p_t^L(x,y) - (4\pi t)^{-n/2} \fint_{H_{xy;\tau}^{\mathrm{orb}}(M)} e^{-E(\gamma)/2t} \, \Upsilon_{\tau,\nu}^{\mathrm{orb}}(t,\gamma) \, \mathrm{d}\gamma \right| \leq C t^{\nu+1} |\tau|^\nu p_t^\Delta(x,y)$$

for all $x, y \in M$, all $0 < t \leq T$ and partitions τ of an interval $[0,1]$ with $|\tau| \leq \delta$. Here, p_t^Δ denotes the heat kernel of the Laplace-Beltrami operator on M with Neumann boundary conditions and

$$\Upsilon_{\tau,\nu}^{\mathrm{orb}}(t,\gamma) = \Upsilon_{\tau,\nu}^{\mathrm{orb}}(t,[\gamma,\epsilon_1,\epsilon_2]) := \rho(\epsilon_1)\overline{\Upsilon}_{\tau,\nu}(t,\gamma)\rho(\epsilon_2), \tag{2.3.12}$$

involves the integrand $\overline{\Upsilon}_{\tau,\nu}(t,\gamma)$ from Thm. 2.2.11 for the operator $\overline{L}$ on $\overline{M}$. The slash over the integral sign denotes division by $(4\pi t)^{\dim(H_{xy;\tau}(M))/2}$.

Remark 2.3.22 ($\Upsilon^{\mathrm{orb}}_{\tau,\nu}$ is well defined). We need to check that the value of $\overline{\Upsilon}_{\tau,\nu}(t,\gamma) \in \mathrm{Hom}(\mathcal{V}_y, \mathcal{V}_x)$ does not depend on the choice of a representative of the element $\gamma \in H^{\mathrm{orb}}_{xy;\tau}(M)$. Because $\overline{L}$ is equivariant, so are the heat kernel $\overline{p}^L_t$ and its coefficients $\overline{\Phi}_j$, meaning that

$$\overline{\Phi}_j(x,y) = \rho(-1)\overline{\Phi}_j(-x,-y)\rho(-1). \tag{2.3.13}$$

Because $\overline{\Upsilon}_{\tau,\nu}$ is built out of the heat kernel coefficients (see (2.2.14)), we similarly obtain

$$\overline{\Upsilon}_{\tau,\nu}(t,-\gamma) = \rho(-1)\overline{\Upsilon}_{\tau,\nu}(t,\gamma)\rho(-1). \tag{2.3.14}$$

Hence if $(-\gamma, -\epsilon_1, -\epsilon_2)$ is the other representative of γ, we get

$$\rho(-\epsilon_1)\overline{\Upsilon}_{\tau,\nu}(t,-\gamma)\rho(-\epsilon_2) = \rho(-\epsilon_1)\rho(-1)\overline{\Upsilon}_{\tau,\nu}(t,\gamma)\rho(-1)\rho(-\epsilon_2) = \rho(\epsilon_1)\overline{\Upsilon}_{\tau,\nu}(t,\gamma)\rho(\epsilon_2).$$

This shows that $\Upsilon^{\mathrm{orb}}_{\tau,\nu}$ is a well-defined $\mathrm{Hom}(\mathcal{V}_y, \mathcal{V}_x)$-valued function on $\mathbb{R} \times H^{\mathrm{orb}}_{xy;\tau}(M)$.

Proof. By Thm. 2.2.11, the heat kernel $p^{\overline{L}}_t(x,y)$ of the $\overline{L}$ on $\overline{M}$ can be approximated by the finite-dimensional path integrals

$$\overline{J}_{\tau,\nu}(x,y;t) := (4\pi t)^{-n/2} \fint_{H_{xy;\tau}(\overline{M})} e^{-E(\gamma)/2t}\, \overline{\Upsilon}_{\tau,\nu}(t,\gamma)\, \mathrm{d}\gamma \tag{2.3.15}$$

in the sense that for all $T > 0$ and all $x, y \in \overline{M}$,

$$\big|p^{\overline{L}}_t(x,y) - \overline{J}_{\tau,\nu}(x,y;t)\big| \leq Ct^{\nu+1}|\tau|^\nu p^\Delta_t(x,y)$$

whenever $|\tau|$ is small enough and $0 < t \leq T$. Set

$$J_{\tau,\nu}(x,y;t) := \sum_{\epsilon\in\mathbb{Z}_2} \rho(\epsilon)\overline{J}_{\tau,\nu}(\epsilon x, y; t).$$

Then by Lemma 2.3.18, we have

$$\big|p^L_t(x,y) - J_{\tau,\nu}(x,y;t)\big| \leq \sum_{\epsilon\in\mathbb{Z}_2} \big|\rho(\epsilon)\big(p^{\overline{L}}_t(\epsilon x,y) - \overline{I}_{\tau,\nu}(\epsilon x,y;t)\big)\big| \leq Ct^{\nu+1}|\tau|^\nu \underbrace{\sum_{\epsilon\in\mathbb{Z}_2} p^{\overline{\Delta}}_t(\epsilon x,y)}_{=p^\Delta_t(x,y)}.$$

Now

$$\begin{aligned}
\sum_{\epsilon\in\mathbb{Z}_2} \rho(\epsilon)\overline{I}_{\tau,\nu}(\epsilon x,y;t) &= \sum_{\epsilon\in\mathbb{Z}_2} (4\pi t)^{-n/2} \fint_{H_{\epsilon x,y;\tau}(\overline{M})} e^{-E(\gamma)/2t}\, \rho(\epsilon)\overline{\Upsilon}_{\tau,\nu}(t,\gamma)\, \mathrm{d}\gamma \\
&= \frac{1}{2}(4\pi t)^{-n/2} \sum_{\epsilon_1,\epsilon_2\in\mathbb{Z}_2} \fint_{H_{\epsilon_1 x,\epsilon_2 y;\tau}(\overline{M})} e^{-E(\gamma)/2t}\, \rho(\epsilon_1)\overline{\Upsilon}_{\tau,\nu}(t,\gamma)\rho(\epsilon_2)\, \mathrm{d}\gamma \\
&= (4\pi t)^{-n/2} \fint_{H^{\mathrm{orb}}_{xy;\tau}(M)} e^{-E(\gamma)/2t}\, \Upsilon^{\mathrm{orb}}_{\tau,\nu}(t,\gamma)\, \mathrm{d}\gamma,
\end{aligned}$$

which finishes the proof. Here we used the equivariance (2.3.14) of $\overline{\Upsilon}_{\tau,\nu}$ and the definition (2.3.4) of the measure on $H^{\mathrm{orb}}_{xy;\tau}(M)$. □

Similarly, the heat trace can by approximated by finite-dimensional orbifold path integrals uniformly in t.

Theorem 2.3.23 (The Heat Trace as an orbifold Path Integral II). *Let L be a self-adjoint Laplace type operator with involutive boundary condition B, acting on sections of a metric vector bundle $\mathcal{V}$ over a compact manifold with boundary M. Suppose that the smoothness Assumption 2.3.7 is satisfied. Then for each $\nu \in \mathbb{N}_0$ and $T > 0$, there exist constants $C, \delta > 0$ such that*

$$\Big|\mathrm{Tr}\, e^{-tL} - \fint_{L_\tau^{\mathrm{orb}}(M)} e^{-E(\gamma)/2t}\, \mathrm{tr}\, \Upsilon^{\circ,\mathrm{orb}}_{\tau,\nu}(t,\gamma)\, \mathrm{d}\gamma\Big| \leq C t^{\nu+1-n/2}|\tau|^{\nu}$$

for each $0 < t \leq T$ and each partition τ of the interval $[0,1]$ with $|\tau| \leq \delta$. Here we have

$$\Upsilon^{\circ,\mathrm{orb}}_{\tau,\nu}(t,\gamma) := \Upsilon^{\circ,\mathrm{orb}}_{\tau,\nu}(t,[\gamma,\epsilon]) := \overline{\Upsilon}^{\circ}_{\tau,\nu}(t,\gamma)\rho(\epsilon),$$

involving the integrand $\overline{\Upsilon}^{\circ}_{\tau,\nu}$ which comes from applying Thm. 2.2.15 to $\overline{M}$. The slash over the integral sign denotes division by $(4\pi t)^{\dim(L_\tau(M))}$.

Remark 2.3.24. Because the flip is an isometry and by the equivariance (2.3.13) of the heat kernel coefficients, we have $\overline{\Upsilon}^{\circ}_{\tau,\nu}(t,\gamma) = \overline{\Upsilon}^{\circ}_{\tau,\nu}(t,-\gamma)$. Therefore, $\Upsilon^{\circ,\mathrm{orb}}_{\tau,\nu}(t,\gamma)$ is well-defined.

Remark 2.3.25. The precise form of the integrand is irrelevant for our purposes; we only take from it that it is a smooth, compactly supported function on $L_\tau^{\mathrm{orb}}(M)$, which depends polynomially on t.

Proof. From Lemma 2.3.18 and (2.2.19) follows (with a view on Remark 2.3.13) that

$$\mathrm{Tr}\, e^{-tL} = \frac{1}{2}\int_{\overline{M}} \mathrm{tr}\, p_t^{\overline{L}}(x,x)\mathrm{d}x + \frac{1}{2}\int_{\overline{M}} \mathrm{tr}\left\{p_t^{\overline{L}}(x,-x)\rho(-1)\right\}\mathrm{d}x$$

The first term is just one half of the trace of $e^{-t\overline{L}}$, which by Thm. 2.2.15 can be approximated by the finite-dimensional path integral

$$\overline{I}_{\tau,\nu}(t) := \fint_{L_\tau(\overline{M})} e^{-E(\gamma)/2t}\mathrm{tr}\, \overline{\Upsilon}^{\circ}_{\tau,\nu}(t,\gamma)\mathrm{d}\gamma$$

that is,

$$\left|e^{-t\overline{L}} - \overline{I}_{\tau,\nu}(t)\right| \leq C_1 t^{\nu+1-n/2}|\tau|^{\nu} \tag{2.3.16}$$

for all partitions τ of $[0,1]$ fine enough and all $0 < t \leq T$. Write

$$I^{\mathrm{orb},+}_{\nu,\tau}(t) = \fint_{L_\tau^{\mathrm{orb},+}(M)} e^{-E(\gamma)/2t}\mathrm{tr}\, \Upsilon^{\circ,\mathrm{orb}}_{\tau,\nu}(t,\gamma)\mathrm{d}\gamma = \frac{1}{2}\overline{I}_{\tau,\nu}(t)$$

By Thm. 2.2.11, the second part may be approximated by

$$I^{\mathrm{orb},-}_{\tau,\nu}(t) = \frac{1}{2}\int_{\overline{M}} \mathrm{tr}\big\{\overline{J}_{\tau,\nu}(x,-x;t)\rho(-1)\big\}\, \mathrm{d}x = \frac{1}{2}\fint_{\overline{L_\tau^{\mathrm{orb},-}(M)}} e^{-E(\gamma)/2t}\, \mathrm{tr}\, \Upsilon^{\circ,\mathrm{orb}}_{\tau,\nu}(\gamma)\mathrm{d}\gamma,$$

with $J_{\tau,\nu}(x,y;t)$ as in (2.3.15) and where the second equality is justified by a similar calculation as in the proof of Thm. 2.2.15. Now

$$I^{\mathrm{orb},+}_{\tau,\nu}(t) + I^{\mathrm{orb},-}_{\tau,\nu}(t) = \fint_{L^{\mathrm{orb}}_{\tau}(M)} e^{-E(\gamma)/2t}\,\mathrm{tr}\,\Upsilon^{\circ,\mathrm{orb}}_{\tau,\nu}(t,\gamma)\,\mathrm{d}\gamma =: I^{\mathrm{orb}}_{\tau,\nu}(t)$$

so that

$$\left|\mathrm{Tr}\,e^{-tL} - I^{\mathrm{orb}}_{\tau,\nu}(t)\right| \leq \frac{1}{2}\left|e^{-t\overline{L}} - \overline{I}_{\tau,\nu}(t)\right| + \left|\frac{1}{2}\int_{\overline{M}} \mathrm{tr}\left\{p_t^{\overline{L}}(x,-x)\rho(-1)\right\}\mathrm{d}x - I^{-}_{\tau,\nu}(t)\right|.$$

The first term is estimated by (2.3.16) while for the second, we have

$$\begin{aligned}
&\left|\frac{1}{2}\int_{\overline{M}} \mathrm{tr}\left\{p_t^{\overline{L}}(x,-x)\rho(-1)\right\}\mathrm{d}x - I^{-}_{\tau,\nu}(t)\right| \\
&\qquad\qquad \leq \int_{\overline{M}} \left|\mathrm{tr}\left\{p_t^{\overline{L}}(x,-x)\rho(-1) - \overline{J}_{\tau,\nu}(x,-x;t)\rho(-1)\right\}\right|\mathrm{d}x \\
&\qquad\qquad \leq C_2 t^{\nu+1}|\tau|^{\nu}\int_{\overline{M}} p_t^{\overline{\Delta}}(x,-x)\mathrm{d}x \leq C_3 t^{\nu+1-n/2}|\tau|^{\nu}
\end{aligned}$$

by Thm. 2.2.11 and Thm. 2.1.5. The result follows. $\square$

Chapter 3

Asymptotic Expansions of Path Integrals

This section is dedicated to investigating short time asymptotic expansions of the path integral formulas for the heat kernel.

In Section 2.2, we learned that the heat kernel can be approximated by the integrals

$$J_{\tau,\nu}(x,y;t) := (4\pi t)^{-nN/2} \int_{H_{xy;\tau}(M)} e^{-E(\gamma)/2t}\, \Upsilon_{\tau,\nu}(t,\gamma)\, \mathrm{d}\gamma$$

appearing in Thm. 2.2.11. These integrals have the form of a Laplace integral, and Laplace's method assigns to these integrals an asymptotic expansion (see Thm. 3.1.2 below). Using that the finite-dimensional path integrals from Thm. 2.2.11 approximate the heat kernel $p_t^L(x,y)$ up to any desired order in t (if ν is chosen large enough), we can use Laplace's method to obtain short time asymptotic expansions of the heat kernel (Thm. 3.1.12).

Of course, if $(x,y) \in M \bowtie M$, then this just gives the result of Thm. 2.1.5. But we can also obtain short time asymptotics in cases where x and y lie in each others cut locus. This is the point of Section 3.1.

In Section 3.2, we give an explicit formula for the lowest order term of the heat kernel expansion in terms of infinite-dimensional quantities on the H^1 path spaces.

3.1 Laplace's Method and Heat Asymptotics

We first give a review of Laplace's method (Section 3.1.1). In Section 3.1.2, this will be used to derive asymptotic expansions for the heat kernel $p_t^L(x,y)$ that also work in cases where x and y lie in each others cut locus. Finally (in Section 3.1.4), we will derive asymptotic expansions of the heat trace.

Of course, we also discuss the situation that M is a manifold with boundary (under the Assumption (2.3.7)), in which case we are dealing with orbifold path integrals.

3.1.1 Laplace's method

Laplace's method is a way to calculate asymptotic expansions as $t \to 0$ from above for integrals of the form

$$I(t,a) := (4\pi t)^{-\dim(\Omega)/2} \int_\Omega e^{-\phi(x)/2t} a(t,x)\,\mathrm{d}x. \tag{3.1.1}$$

Here, $t > 0$, Ω is a Riemannian manifold, $\phi \in C^\infty(\Omega)$ and $a(t,x)$ is smooth and compactly supported with respect to the x variable and depends smoothly on t.

Definition 3.1.1 (Non-degenerate Submanifolds). Suppose that $\phi(x) \geq \lambda$ and that the subset $\Gamma := \phi^{-1}(\lambda)$ is a submanifold of Ω. We say that Γ is a *non-degenerate submanifold* (with respect to ϕ), if for each $x \in \Gamma$, we have $\nabla^2\phi|_{N_x\Gamma} > 0$, i.e. the restriction of the Hessian of ϕ to the normal bundle of Γ is positive definite.

Later, we will have $\Omega = H_{xy;\tau}(M)$ for a partition τ fine enough and $\phi(\gamma) = E(\gamma) - d(x,y)^2/2$ so that we have $\Gamma = \phi^{-1}(0) = \Gamma_{xy}^{\min}$, the set of minimal geodesics connecting x and y.

Theorem 3.1.2 (Laplace Expansion). *Assume that ϕ is non-negative and that $\Gamma := \phi^{-1}(0)$ is a k-dimensional non-degenerate submanifold of Ω. Then $I(t,a)$ has a complete asymptotic expansion as t goes to zero from above. More explicitly, there exists a second order differential operator P such that we have*

$$I(t,a) \sim (4\pi t)^{-k/2} \sum_{j=0}^\infty t^j \sum_{i=0}^j \frac{1}{i!(j-i)!} \int_\Gamma \frac{P^{j-i}a^{(i)}(0,x)}{\det\big(\nabla^2\phi|_{N_x\Gamma}\big)^{1/2}}\,\mathrm{d}x \tag{3.1.2}$$

where $a^{(i)}(0,x)$ denotes the i-th derivative of a with respect to t at $t=0$. In particular, if a does not depend on t, this simplifies to

$$I(t,a) \sim (4\pi t)^{-k/2} \sum_{j=0}^\infty t^j \int_\Gamma \frac{P^j a(x)}{j!\det\big(\nabla^2\phi|_{N_x\Gamma}\big)^{1/2}}\,\mathrm{d}x. \tag{3.1.3}$$

Remark 3.1.3. The asymptotic relation in (3.1.3) means that for all $\nu \in \mathbb{N}_0$ and all $T > 0$, there exists a constant $C > 0$ such that

$$\left| I(t,a) - (4\pi t)^{-k/2} \sum_{j=0}^\nu t^j \int_\Gamma \frac{P^j a(x)}{j!\det\big(\nabla^2\phi|_{N_x\Gamma}\big)^{1/2}}\,\mathrm{d}x \right| \leq C t^{\nu+1-k/2}$$

whenever $0 < t \leq T$, and analogous for (3.1.2).

Remark 3.1.4. The Laplace expansion of an integral of the form $I(t,a)$ is closely related to the *method of stationary phase*, which calculates asymptotic expansions of the integral $t \mapsto I(it,a)$. Laplace's method is easier in the sense that here, only critical points which are minima contribute to the asymptotic expansion, while for integrals with imaginary exponent, all critical points contribute. Compare e.g. [Arn73] or [Dui96, Section 1.2].

In the remainder of this section, we give a proof of this result. While the method of stationary phase is treated in various places in the literature, there seems to be no good reference for the result of Thm. 3.1.2 available in quite the generality that we need.

Lemma 3.1.5. *Under the assumptions of Thm. 3.1.2, suppose that $a(t,x) = 0$ for all x in a neighborhood of Γ and all $0 \leq t \leq \delta$, for some $\delta > 0$. Then there exist constants $T, C, \varepsilon > 0$ such that for all $t \leq T$, we have $I(t,a) \leq Ce^{-\varepsilon/t}$.*

Proof. Let $N := \dim(\Omega)$. Set

$$A := \text{closure of} \bigcup_{0 \leq t \leq \delta} \operatorname{supp} a(t,-) \tag{3.1.4}$$

(which is compact) and set

$$\varepsilon' := \min_{x \in A} \phi(x).$$

Notice that $\varepsilon' > 0$ because $A \cap \Gamma = \emptyset$. Therefore,

$$I(t,a) \leq (4\pi t)^{-N/2} e^{-\varepsilon'/2t} \int_\Omega a(t,x) \mathrm{d}x \leq (4\pi t)^{-N/2} e^{-\varepsilon'/2t} \|a(t,-)\|_{L^1} \leq Ce^{-\varepsilon/t},$$

if we choose $0 < \varepsilon < \varepsilon'$ and $C > 0$ appropriately. □

Proof (of Thm. 3.1.2). Let $N := \dim(\Omega)$ and let A as in (3.1.4). Since A is compact, we may without loss of generality assume that also Ω and hence Γ is compact. Otherwise embed some open neighborhood of A isometrically into a compact manifold Ω', transplant ϕ and a there and replace Ω by Ω' in the definition of $I(t,a)$. This does not alter the value of $I(t,a)$.

Let $N\Gamma \subseteq T\Omega$ be the normal bundle of Γ. Then there is an open neighborhood V of the zero section in $N\Gamma$ and an open neighborhood U of Γ in Ω together with a diffeomorphism $\kappa : V \longrightarrow U$ such that

$$\big(\phi \circ \kappa\big)(x,v) = \nabla^2\phi|_x[v,v], \qquad (x,v) \in V.$$

This can be proved using the implicit function theorem, compare e.g. Lemma 1.2.2 in [Dui96]. Clearly, we have $d\kappa|_{(x,0)} = \mathrm{id}_x$.

W.l.o.g., we assume that $A \subset U$. Namely otherwise, we can choose a cutoff function $\chi \in C_c^\infty(U)$ that is equal to one on a neighborhood of Γ and split $I(t,a) = I(t,\chi a) + I(t,(1-\chi)a)$, where the second summand does not contribute to the asymptotic expansion because of Lemma 3.1.5.

We now may use the transformation formula to obtain

$$\begin{aligned} I(t,a) &= (4\pi t)^{-N/2} \int_U e^{-\phi(x)/2t} a(t,x)\, \mathrm{d}x \\ &= (4\pi t)^{-N/2} \int_\Gamma \int_{V_x} e^{-\langle v, Q(x)v\rangle/4t} a\big(t,\kappa(x,v)\big) \big|\det\big(d\kappa|_{(x,v)}\big)\big| \mathrm{d}v\mathrm{d}x, \end{aligned} \tag{3.1.5}$$

where we wrote $Q(x) := \nabla^2\phi|_{N_x\Gamma}$ and $V_x := V \cap N_x\Gamma$. It is well known that for any $(N-k)$-dimensional Euclidean vector space W, any positive definite endomorphism Q of

W and any continuous function $f = f(t, x)$ on $\mathbb{R} \times W$ which is bounded in the x variable and depends smoothly on t, one has

$$\lim_{t \to 0} (4\pi t)^{-(N-k)/2} \int_W e^{-\langle v, Qv \rangle / 4t} f(t, v) \mathrm{d}v = \det(Q)^{-1/2} f(0, 0).$$

Furthermore, for all t, we have

$$\left| (4\pi t)^{-(N-k)/2} \int_W e^{-\langle v, Qv \rangle / 4t} f(t, v) \mathrm{d}v \right| \leq \| f(t, -) \|_\infty.$$

Therefore since Γ is compact, we may exchange integration over Γ and the limit $t \to 0$ in (3.1.5) to conclude

$$\lim_{t \to 0} (4\pi t)^{k/2} I(t, a) = \int_\Gamma \frac{a\big(0, \kappa(x, 0)\big)}{\det\big(Q(x)\big)^{1/2}} \big|\det\big(d\kappa|_{(x,0)}\big)\big| \mathrm{d}x = \int_\Gamma \frac{a(0, x)}{\det\big(\nabla^2 \phi|_{N_x \Gamma}\big)^{1/2}} \mathrm{d}x \quad (3.1.6)$$

Now on the vector spaces $N_x\Gamma$, define the Q-Laplacian Δ_Q by the formula

$$\Delta_Q f(v) = -\left\langle Q(x)^{-1}, D^2 f|_v \right\rangle.$$

This patches together to a smooth differential operator on $N\Gamma$ satisfying

$$\Big(\frac{\partial}{\partial t} + \Delta_Q\Big) \big\{ (4\pi t)^{-(N-k)/2} e^{-\langle v, Q(x) v \rangle / 4t} \big\} = 0.$$

Therefore, integrating by parts, we obtain

$$\begin{aligned} &\frac{\partial}{\partial t} \big\{ (4\pi t)^{k/2} I\big(t, a\big) \big\} - (4\pi t)^{k/2} I\big(t, \frac{\partial}{\partial t} a\big) \\ &\qquad = -(4\pi t)^{-(N-k)/2} \int_\Gamma \int_{V_x} e^{-\langle v, Q(x) v \rangle / 4t} \Delta_Q \Big\{ a\big(t, \kappa(x, v)\big) \big|\det\big(d\kappa|_{(x,v)}\big)\big| \Big\} \mathrm{d}v \mathrm{d}x \\ &\qquad = (4\pi t)^{-(N-k)/2} \int_U e^{-\phi(x)/2t} P a(t, x) \mathrm{d}x = (4\pi t)^{k/2} I(t, Pa), \end{aligned}$$

where for $f \in C^\infty(U)$, we set

$$(Pf)(y) = -\Delta_Q \big\{ f(v) \big|\det\big(d\kappa|_{(x,v)}\big)\big| \big\} \big|_{(x,v) = \kappa^{-1}(y)} \big|\det\big(d\kappa^{-1}|_y\big)\big|,$$

so that P is some second-order differential operator. Let $J(t, a) := (4\pi t)^{k/2} I(t, a)$. Then by Taylor's formula and the Leibniz rule, for all $\varepsilon > 0$ and $\nu \in \mathbb{N}$,

$$\begin{aligned} J(t, a) &= \sum_{j=0}^{\nu} \frac{1}{j!} \frac{\partial^j}{\partial \varepsilon^j} \big\{ J(\varepsilon, a) \big\} (t - \varepsilon)^j + \int_\varepsilon^t \frac{(t - s)^\nu}{\nu!} \frac{\partial^{\nu+1}}{\partial s^{\nu+1}} \big\{ J(s, a) \big\} \mathrm{d}s \\ &= \sum_{j=0}^{\nu} \frac{1}{j!} \sum_{i=0}^{j} \binom{j}{i} J\big(\varepsilon, P^{j-i} a^{(i)}\big) (t - \varepsilon)^j + R^\nu(\varepsilon, t), \end{aligned}$$

where

$$R^\nu(\varepsilon, t) = \sum_{i=0}^{\nu+1} \binom{\nu+1}{i} \int_\varepsilon^t \frac{(t-s)^\nu}{\nu!} J\big(s, P^{\nu+1-i} a^{(i)}\big) \mathrm{d}s. \tag{3.1.7}$$

Because of (3.1.6), we may take the limit $\varepsilon \to 0$ to obtain

$$\lim_{\varepsilon \to 0} J(\varepsilon, P^{j-i} a^{(i)}) = \int_\Gamma \frac{P^{j-i} a^{(i)}(0,x)}{\det\big(\nabla^2 \phi|_{N_x\Gamma}\big)^{1/2}} \mathrm{d}x.$$

Therefore,

$$J(t,a) = \sum_{j=0}^{\nu} t^j \sum_{i=0}^{j} \frac{1}{(j-i)!i!} \int_\Gamma \frac{P^{j-i} a^{(i)}(0,x)}{\det\big(\nabla^2 \phi|_{N_x\Gamma}\big)^{1/2}} \mathrm{d}x + R^\nu(\epsilon, t),$$

for any $\nu \in \mathbb{N}_0$, where the remainder term is of order $t^{\nu+1}$. Multiplying with $(4\pi t)^{-k/2}$, we obtain (3.1.3). □

Remark 3.1.6. Of course, if the zero set of ϕ is the disjoint union

$$\phi^{-1}(0) = \Gamma_1 \coprod \cdots \coprod \Gamma_m$$

of non-degenerate submanifolds Γ_i of Ω, possibly of different dimensions, then $I(t,a)$ has an asymptotic expansion consisting of the sum of individual asymptotic expansions, which can be calculated just as in Thm. 3.1.2.

3.1.2 Heat Kernel Asymptotics

Let L be a self-adjoint Laplace type operator, acting on sections of a metric vector bundle $\mathcal{V}$ over an n-dimensional compact Riemannian manifold M. In this section, we use Laplace's method on the path integral approximations of the heat kernel. As seen in Thm. 2.2.11, we can approximate the heat kernel by the integrals

$$J_{\tau,\nu}(x,y;t) := (4\pi t)^{-nN/2} \int_{H_{xy;\tau}(M)} e^{-E(\gamma)/2t}\, \Upsilon_{\tau,\nu}(t,\gamma)\, \mathrm{d}\gamma, \tag{3.1.8}$$

where $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = 1\}$ is a partition of the interval $[0,1]$ and $\Upsilon_{\tau,\nu}(t,\gamma)$ is given by the complicated expression (2.2.14). For the purposes of this section, the particular formula for $\Upsilon_{\tau,\nu}$ is not relevant; we only need to know that $\Upsilon_{\tau,\nu}$ is a compactly supported smooth function on $H_{xy;\tau}(M)$ which depends polynomially on the t variable (that $\Upsilon_{\tau,\nu}$ is compactly supported comes from the cutoff function in the approximate heat kernel).

The integral (3.1.8) is not yet in the form (3.1.1) that we can deal with using Thm. 3.1.2: The pre-factor does not fit (since $H_{xy;\tau}(M)$ has dimension $n(N-1)$) and the minimum of the energy on $H_{xy;\tau}(M)$ is not zero in general, so that the zero set would be empty. This will be fixed now.

Notation 3.1.7. For $x, y \in M$, denote by $\Gamma_{xy}^{\min} \subset H_{xy}(M)$ the set of minimal geodesics connecting x and y in time one.

Remark 3.1.8. The set $\Gamma_{xy}^{\min}$ is always compact, by Prop. 2.4.11 in [Kli95].

Lemma 3.1.9 (The Hessian of the Energy). *On every space $H_{xy;\tau}(M)$ with τ fine enough as well as on $H_{xy}(M)$, we have $E(\gamma) \geq d(x,y)^2/2$ and*

$$\Gamma_{xy}^{\min} = \{\gamma \mid E(\gamma) = d(x,y)^2/2\}. \tag{3.1.9}$$

For any $\gamma \in \Gamma_{xy}^{\min}$, we have

$$\nabla^2 E|_\gamma[X,Y] = \int_0^1 \langle \nabla_s X(s), \nabla_s Y(s)\rangle \mathrm{d}s + \int_0^1 \langle R(\dot\gamma(s), X(s))\dot\gamma(s), Y(s)\rangle \,\mathrm{d}s, \tag{3.1.10}$$

for all $X, Y \in T_\gamma H_{xy}(M)$.

Remark 3.1.10. The result does not depend on the metric and connection used on $H_{xy;\tau}(M)$ or $H_{xy}(M)$, because if $\gamma \in \Gamma_{xy}^{\min}$, it is necessarily a critical point, and at critical points, the Hessian is independent of the metric used.

Proof. For any $\gamma \in H_{xy}(M)$, we have by the Cauchy-Schwarz-Inequality

$$\mathrm{length}(\gamma) = \int_0^1 |\dot\gamma(s)|\mathrm{d}s \leq 1 \cdot \left(\int_0^1 |\dot\gamma(s)|^2 \mathrm{d}s\right)^{1/2} \leq \sqrt{2E(\gamma)},$$

with equality if and only if the function 1 and $|\dot\gamma(s)|$ are linearly dependent, i.e. $|\dot\gamma(s)|$ is constant. Because $d(x,y)$ is by definition the infimum of the length, we obtain $E(\gamma) \geq d(x,y)^2/2$, and if γ is minimizing geodesic, then $|\dot\gamma(s)|$ is constant, hence $E(\gamma) = d(x,y)^2/2$. Conversely, it is well-known that minimizer of the energy are exactly minimizing geodesics. The statement about the Hessian is a standard result in Riemannian geometry, see e.g. [Mil63, Section 13]. □

Therefore, we set for $\gamma \in H_{xy}(M)$

$$\phi(\gamma) := E(\gamma) - \frac{d(x,y)^2}{2}.$$

This is then a non-negative function, which takes the value zero exactly on the set $\Gamma_{xy}^{\min}$ of minimal geodesics connecting x to y. Now

$$\frac{J_{\tau,\nu}(x,y;t)}{\mathrm{e}_t(x,y)} = (4\pi t)^{-n(N-1)/2} \int_{H_{xy;\tau}(M)} e^{-\phi(\gamma)/2t}\, \Upsilon_{\tau,\nu}(t,\gamma)\,\mathrm{d}\gamma$$

has the form of a Laplace integral, as considered in Subsection 3.1.1: The dimension of $H_{xy;\tau}(M)$ is exactly $n(N-1)$.
Suppose that $\Gamma_{xy}^{\min}$ is a k-dimensional non-degenerate submanifold of $H_{xy}(M)$. Clearly, $\Gamma_{xy}^{\min}$ is then also a non-degenerate submanifold of $H_{xy;\tau}(M)$, provided the partition τ is so fine that $(\gamma(\tau_{j-1}), \gamma(\tau_j)) \in M \bowtie M$ for each j and each $\gamma \in \Gamma_{xy}^{\min}$ (this is clearly satisfied

if $|\tau| < \mathrm{inj}(M)/\mathrm{diam}(M)$). Then from Thm. 3.1.2, we obtain that for such partitions, we have a complete asymptotic expansion

$$\frac{J_{\tau,\nu}(t,x,y)}{\mathrm{e}_t(x,y)} \sim (4\pi t)^{-k/2} \sum_{j=0}^{\infty} t^j \frac{\Phi_{\tau,\nu,j}(x,y)}{j!}, \tag{3.1.11}$$

where $\Phi_{\nu,\tau,j}(x,y)$ is given by the integral

$$\Phi_{\tau,\nu,j}(x,y) := \sum_{i=0}^{j} \binom{j}{i} \int_{\Gamma_{xy}^{\min}} \frac{P_\tau^{j-i} \Upsilon_{\tau,\nu}^{(i)}(0,\gamma)}{\det_\tau\big(\nabla^2 E|_{N_\gamma \Gamma_{xy}^{\min}}\big)^{1/2}} \,\mathrm{d}\gamma \tag{3.1.12}$$

over the set of minimal geodesics $\Gamma_{xy}^{\min}$ (where we integrate with respect to the Riemannian volume induced to it from $H_{xy;\tau}(M)$). Here P_τ is a certain second order differential operator defined on a neighborhood of $\Gamma_{xy}^{\min}$ in $H_{xy;\tau}(M)$, $\Upsilon_{\tau,\nu}^{(i)}$ denotes the i-th time derivative of $\Upsilon_{\nu,\tau}$ and $\det_\tau(\nabla^2 E|_{N_\gamma \Gamma_{xy}^{\min}})$ denotes the determinant of the Hessian of the energy at γ restricted to the normal space $N_\gamma \Gamma_{xy}^{\min}$ of $T_\gamma \Gamma_{xy}^{\min}$ in $T_\gamma H_{xy;\tau}(M)$.

Remark 3.1.11. Notice that for each $\gamma \in H_{xy;\tau}(M)$, $\Upsilon_{\nu,\tau}(t,\gamma)$ is an element of the fixed finite-dimensional vector space $\mathrm{Hom}(\mathcal{V}_y, \mathcal{V}_x)$. Therefore Laplace's method applies without changes to this case (let's say, by choosing a basis and applying Thm. 3.1.2 entrywise).

With these observations, we prove the following result.

Theorem 3.1.12 (The Heat Kernel Expansion). *Let L be a self-adjoint Laplace type operator, acting on sections of a metric vector bundle $\mathcal{V}$ over a closed Riemannian manifold M of dimension n. For $x, y \in M$, suppose that $\Gamma_{xy}^{\min}$ is a non-degenerate k-dimensional submanifold of $H_{xy}(M)$ (with respect to the energy functional on $H_{xy}(M)$. Then the heat kernel has a complete asymptotic expansion of the form*

$$\frac{p_t^L(x,y)}{\mathrm{e}_t(x,y)} \sim (4\pi t)^{-k/2} \sum_{j=0}^{\infty} t^j \frac{\Phi_j(x,y)}{j!} \tag{3.1.13}$$

for homomorphisms $\Phi_j(x,y) \in \mathrm{Hom}(\mathcal{V}_y, \mathcal{V}_x)$.

Remark 3.1.13. If $\Gamma_{xy}^{\min}$ is the disjoint union of submanifolds Γ_i, $i = 1, \dots, m$ of dimensions k_i, then of course the theorem generalizes in the obvious way; one obtains in this case, that the heat kernel has a complete asymptotic expansion of the form

$$\frac{p_t^L(x,y)}{\mathrm{e}_t(x,y)} \sim \sum_{i=1}^{m} (4\pi t)^{-k_i/2} \sum_{j=0}^{\infty} t^j \frac{\Phi_j^i(x,y)}{j!},$$

where each $\Phi_j^i(x,y)$ is given by an integral over the set Γ_i.

Remark 3.1.14 (Degenerate Cases). In the case that $\Gamma_{xy}^{\min}$ is a degenerate submanifold, one can also obtain an asymptotic expansion in good cases, which depends on the type of degeneracy of the energy functional (the corresponding Laplace's method is discussed in [Arn73]). This is discussed in Molchanov [Mol75]. See also [BBN12].

Proof (of Thm. 3.1.12). By Thm. 2.2.11, for each $T > 0$ and each $\nu \in \mathbb{N}_0$, there exist constants $C_1, \delta > 0$ such that

$$\left|\frac{p_t^L(x,y)}{\mathrm{e}_t(x,y)} - \frac{J_{\tau,\nu}(x,y;t)}{\mathrm{e}_t(x,y)}\right| \leq C_1 t^{1+\nu}|\tau|^\nu \frac{p_t^\Delta(x,y)}{\mathrm{e}_t(x,y)}, \tag{3.1.14}$$

for any partition τ of the interval $[0,1]$ with $|\tau| \leq \delta$. From the Gaussian estimate from above (see (2.1.20)) follows $p_t^\Delta(x,y) \leq C_2 t^{-n/2}\mathrm{e}_t(x,y)$. Therefore (3.1.14) yields

$$\left|\frac{p_t^L(x,y)}{\mathrm{e}_t(x,y)} - \frac{J_{\tau,\nu}(x,y;t)}{\mathrm{e}_t(x,y)}\right| \leq C_3 t^{1+\nu-n/2}|\tau|^\nu. \tag{3.1.15}$$

Using (3.1.15) for the Laplace-Beltrami operator on M and some $\nu \geq n/2 - k/2 - 1$ and $|\tau| \leq \delta$, we get

$$\begin{aligned}\frac{p_t^\Delta(x,y)}{\mathrm{e}_t(x,y)} \leq \left|\frac{p_t^\Delta(x,y)}{\mathrm{e}_t(x,y)} - \frac{J_{\tau,\nu}^\Delta(x,y;t)}{\mathrm{e}_t(x,y)}\right| + \left|\frac{J_{\tau,\nu}^\Delta(x,y;t)}{\mathrm{e}_t(x,y)}\right| &\leq C_4 t^{1+\nu-n/2}|\tau|^\nu + C_5 t^{-k/2}\\ &\leq (C_4\delta^\nu + C_5)t^{-k/2} =: C_6 t^{-k/2}.\end{aligned}$$

using (3.1.11). Therefore, (3.1.14) improves to

$$\left|\frac{p_t^L(x,y)}{\mathrm{e}_t(x,y)} - \frac{J_{\tau,\nu}(x,y;t)}{\mathrm{e}_t(x,y)}\right| \leq C_1 t^{1+\nu}|\tau|^\nu \frac{p_t^\Delta(x,y)}{\mathrm{e}_t(x,y)} \leq C_1 C_6 t^{1+\nu-k/2}.$$

From this follows that the heat kernel has an asymptotic expansion up to the order t^ν, the coefficients of which must coincide with the asymptotic expansion (3.1.11) of $J_{\tau,\nu}(x,y;t)$ up to that order. Because asymptotic expansions are unique, this also shows that the coefficients $\Phi_{\tau,\nu,j}(x,y)$ from (3.1.11) must stabilize for ν large enough and τ fine enough. More precisely, if $j \leq \nu, \nu'$ and $|\tau|, |\tau'| \leq \delta$, we have $\Phi_{\tau,\nu,j}(x,y) = \Phi_{\tau',\nu',j}(x,y)$. Therefore

$$\Phi_j(x,y) := \Phi_{\tau,\nu,j}(x,y) \tag{3.1.16}$$

for any choice of $\nu \geq j$ and $|\tau| \leq \delta$ is well defined.
Because ν was arbitrary, we obtain that $p_t^L(x,y)/\mathrm{e}_t(x,y)$ has a complete asymptotic expansion of the form (2.1.3), with the coefficients $\Phi_j(x,y)$ given by the formula (3.1.16) for ν large enough and $|\tau|$ small enough. □

From the proof, we obtain the following corollary.

Corollary 3.1.15. *Under the assumptions of Thm. 3.1.12, for ν large enough and $|\tau|$ small enough, the coefficients $\Phi_{\nu,\tau,j}(x,y)$ in* (3.1.12) *stabilize. More precisely, there exists $\delta > 0$ such that*

$$\Phi_{\nu,\tau,j}(x,y) = \Phi_j(x,y)$$

whenever $|\tau| \leq \delta$ and $j \leq \nu$. If $(x,y) \in M \bowtie M$, the $\Phi_j(x,y)$ are exactly the coefficients appearing in Thm. 2.1.5.

Remark 3.1.16. Of course, if $(x,y) \in M \bowtie M$, uniqueness of asymptotic expansions implies that the $\Phi_j(x,y)$ given in the above theorem are precisely the heat kernel coefficients from Thm. 2.1.5.

3.1.3 Heat Kernel Asymptotics on a Manifold with Boundary

In the case that the smoothness Assumption 2.3.7 is satisfied, similar results hold if M is a compact Riemannian manifold with boundary and the Laplace type operator L is endowed with involutive boundary conditions. As before, let $\overline{M}$ be the double of M, and we denote by overlines all objects associated to the manifold $\overline{M}$.
Remember that by Thm. 2.3.21, the heat kernel $p_t^L(x, y)$ can be approximated by the finite-dimensional path integrals

$$J_{\tau,\nu}^{\mathrm{orb}}(x, y; t) := (4\pi t)^{-nN/2} \int_{H_{xy;\tau}^{\mathrm{orb}}(M)} e^{-E(\gamma)/2t}\, \Upsilon_{\tau,\nu}^{\mathrm{orb}}(t, \gamma)\, \mathrm{d}\gamma.$$

Let $\Gamma_{xy}^{\min,\mathrm{orb}} \subset H_{xy}^{\mathrm{orb}}(M)$ denote the space of paths of minimal energy connecting x to y. Assume again that $\Gamma_{xy}^{\min,\mathrm{orb}}$ is a k-dimensional non-degenerate submanifold of the manifold $H_{xy}^{\mathrm{orb}}(M)$. From Laplace's method (Thm. 3.1.2) follows then that $J_{\tau,\nu}(x, y; t)$ has an asymptotic expansion of the form

$$\frac{J_{\tau,\nu}^{\mathrm{orb}}(x, y; t)}{\mathrm{e}_t(x, y)} \sim (4\pi t)^{-k/2} \sum_{j=0}^{\infty} t^j \frac{\Phi_{\tau,\nu,j}(x, y)}{j!}, \tag{3.1.17}$$

where

$$\Phi_{\tau,\nu,j}(x, y) := \sum_{i=0}^{j} \binom{j}{i} \int_{\Gamma_{xy}^{\min,\mathrm{orb}}} \frac{P_\tau^{j-i} \Upsilon_{\tau,\nu}^{\mathrm{orb}\,(i)}(0, \gamma)}{\det_\tau\bigl(\nabla^2 E|_{N_\gamma \Gamma_{xy}^{\min,\mathrm{orb}}}\bigr)^{1/2}}\, \mathrm{d}\gamma \tag{3.1.18}$$

with some second-order operator P_τ defined in the vicinity of $\Gamma_{xy}^{\min,\mathrm{orb}}$ inside $H_{xy;\tau}^{\mathrm{orb}}(M)$. The following result on the asymptotic expansion of the heat kernel is proved just as Thm. 3.1.12.

Theorem 3.1.17 (The Heat Kernel Expansion, Boundary Case). *Let L be a self-adjoint Laplace type operator with involutive boundary condition B, acting on sections of a metric vector bundle $\mathcal{V}$ over a compact n-dimensional Riemannian manifold with boundary M. Suppose that the smoothness Assumption 2.3.7 is satisfied. For $x, y \in M$, suppose furthermore that the set $\Gamma_{xy}^{\min,\mathrm{orb}}$ is a non-degenerate k-dimensional submanifold of $H_{xy}^{\mathrm{orb}}(M)$ (with respect to the energy functional). Then the heat kernel p_t^L of L has a complete asymptotic expansion of the form*

$$\frac{p_t^L(x, y)}{\mathrm{e}_t(x, y)} \sim (4\pi t)^{-k/2} \sum_{j=0}^{\infty} t^j \frac{\Phi_j(x, y)}{j!},$$

for homomorphisms $\Phi_j(x, y) \in \mathrm{Hom}(\mathcal{V}_y, \mathcal{V}_x)$.

Remark 3.1.18. Similar to before, the coefficients $\Phi_{\tau,\nu,j}(x, y)$ from (3.1.17) stabilize for ν large enough and $|\tau|$ small enough and are equal to the coefficients $\Phi_j(x, y)$ from Thm. 3.1.17; more precisely, there exists $\delta > 0$ such that

$$\Phi_j(x, y) = \Phi_{\tau,\nu,j}(x, y)$$

for any $|\tau| \leq \delta$ and $\nu \geq j$.

The goal of the rest of this subsection is to compare the coefficients $\Phi_j(x,y)$ associated to the heat kernel of the operator L on the manifold with boundary M by Thm. 3.1.17 with the coefficients $\overline{\Phi}_j(x,y)$ obtained by applying Thm. 3.1.12 to the heat kernel of the operator $\overline{L}$ on the closed manifold $\overline{M}$.
We need the following preliminary observations.

Lemma 3.1.19. *Any element $\gamma = [\gamma, \epsilon_1, \epsilon_2] \in \Gamma_{xy}^{\text{min,orb}}$ has a representative $(\gamma, \epsilon_1, \epsilon_2)$ such that γ runs completely inside M, i.e. shortest geodesics do not cross the boundary.*

Proof. Let $[\gamma, \epsilon_1, \epsilon_2] \in \Gamma_{xy}^{\text{min,orb}}$ by represented by the geodesic γ in $\overline{M}$. Let $\widetilde{\gamma}$ be the path in M running from x to y obtained from γ by post-composing with the projection map from $\overline{M}$ to M, i.e.

$$\widetilde{\gamma}(s) := \begin{cases} \gamma(s) & \text{if } \gamma(s) \in M \\ -\gamma(s) & \text{if } \gamma(s) \in -M. \end{cases} \tag{3.1.19}$$

Then $\widetilde{\gamma} \in H_{xy}(\overline{M})$ has the same energy as γ. Because by assumption, γ is energy-minimizing among all paths in $H_{xy}^{\text{orb}}(M)$ (i.e. among all finite-energy paths in $\overline{M}$ that run between $\epsilon_1 x$ and $\epsilon_2 y$, $\epsilon_1, \epsilon_2 \in \mathbb{Z}_2$), so is $\widetilde{\gamma}$. In particular, $\widetilde{\gamma}$ is a minimum of the energy functional on $H_{xy}(\overline{M})$ and therefore a geodesic between x and y.
We now show that $\widetilde{\gamma}$ does not hit the boundary at any $s \in (0,t)$ unless both $x, y \in \partial M$. To this end, suppose that $\widetilde{\gamma}(s) \in \partial M$ (hence also $\gamma(s) \in \partial M$). Then because $\widetilde{\gamma}$ is the reflection of the geodesic γ, we necessarily have $\dot{\widetilde{\gamma}}(s) \in T_{\widetilde{\gamma}(s)}\partial M$, because otherwise $\widetilde{\gamma}$ would have a kink at the time s, contradicting the fact that $\widetilde{\gamma}$ is a geodesic.
Because ∂M is the fixed point set of the isometry $x \mapsto -x$ of $\overline{M}$, it is a totally geodesic submanifold. Hence because $\dot{\widetilde{\gamma}}(s) \in T_{\widetilde{\gamma}(s)}\partial M$, $\widetilde{\gamma}$ runs inside ∂M for all times. This implies $x, y \in \partial M$.
We have shown that either at most one of x, y is in ∂M, in which case $\gamma(s) \in M \setminus \partial M$ for all $s \in (0,1)$; or both $x, y \in \partial M$, in which case γ runs completely in ∂M. ☐

Lemma 3.1.20. *For $x, y \in M$, suppose that $\Gamma_{xy}^{\text{min,orb}}$ is a k-dimensional submanifold of $H_{xy}^{\text{orb}}(M)$ and let $\overline{\Gamma}_{xy}^{\text{min}}$ the set of minimizing geodesics in $\overline{M}$ between x and y. If at least one of x, y is contained in ∂M, set $G := \mathbb{Z}_2$. Otherwise, set $G = \{1\}$. Then the map*

$$\varphi : \Gamma_{xy}^{\text{min,orb}} \longrightarrow \overline{\Gamma}_{xy}^{\text{min}} \times G, \qquad [\gamma, \epsilon_1, \epsilon_2] \longmapsto (\widetilde{\gamma}, \epsilon_1\epsilon_2)$$

is an isometry of Riemannian manifolds, if both are endowed with the H^1 metric induced from $H_{xy}(\overline{M})$. Here for $\gamma \in H_{xy}(\overline{M})$, $\widetilde{\gamma}$ is defined as in (3.1.19)

Proof. We first check that φ is well defined. Any element in $H_{xy}^{\text{orb}}(M)$ has exactly two representatives, $(\gamma, \epsilon_1, \epsilon_2)$ and $(-\gamma, -\epsilon_1, -\epsilon_2)$. Because of Lemma 3.1.19, γ must run either completely in M or completely in $-M$, so either γ is a geodesic from x to y or from $-x$ to $-y$. Therefore, $\widetilde{\gamma} \in \overline{\Gamma}_{xy}^{\text{min}}$. Furthermore, if neither x nor y lies in ∂M, then ϵ_1, ϵ_2 must have the same sign because of Lemma 3.1.19, so that in this case indeed $\epsilon_1\epsilon_2 = 1$. Furthermore,

$$\big(\widetilde{-\gamma}, (-\epsilon_1)(-\epsilon_2)\big) = (\widetilde{\gamma}, \epsilon_1\epsilon_2),$$

which shows independence of the choice of representative.

To see that φ is injective, suppose that $\varphi([\gamma, \epsilon_1, \epsilon_2]) = \varphi([\gamma', \epsilon_1', \epsilon_2'])$. Then $\widetilde{\gamma} = \widetilde{\gamma}'$ and $\epsilon_1\epsilon_2 = \epsilon_1'\epsilon_2'$. By Lemma 3.1.19, we may assume that the representatives are chosen in such a way that γ and γ' run completely in M, so that $\widetilde{\gamma} = \widetilde{\gamma}'$ implies $\gamma = \gamma'$. If $x \notin \partial M$, then $\epsilon_1 = \epsilon_1' = 1$, so $\epsilon_1\epsilon_2 = \epsilon_1'\epsilon_2'$ implies $\epsilon_2 = \epsilon_2'$. Similarly, if $y \notin \partial M$, then $\epsilon_2 = \epsilon_2' = 1$ and therefore $\epsilon_1 = \epsilon_1'$. Finally, if both $x, y \in \partial M$, then γ runs completely in ∂M (because the boundary is totally geodesic), hence $\gamma = -\gamma$. Thus, $\epsilon_1 \cdot (\gamma, \epsilon_1, \epsilon_2) = (\gamma, 1, \epsilon_1\epsilon_2)$ is a representative of $[\gamma, \epsilon_1, \epsilon_2]$ and $\epsilon_1' \cdot (\gamma', \epsilon_1', \epsilon_2') = (\gamma', 1, \epsilon_1'\epsilon_2')$ is a representative of $[\gamma', \epsilon_1', \epsilon_2']$. On the other hand, we have $(\gamma', 1, \epsilon_1'\epsilon_2') = (\gamma, 1, \epsilon_1\epsilon_2)$. We obtain $[\gamma, \epsilon_1, \epsilon_2] = [\gamma', \epsilon_1', \epsilon_2']$, hence φ is injective.
To see that φ is surjective, let $(\gamma, \epsilon) \in \overline{\Gamma}_{xy}^{\min} \times G$. If $x \in \partial M$, then $[\gamma, \epsilon, 1] \in \Gamma_{xy}^{\min,\mathrm{orb}}$ is a pre-image of (γ, ϵ) under φ. If $y \in \partial M$, then $[\gamma, 1, \epsilon]$ is a pre-image of (γ, ϵ) under φ. If neither x nor y is in ∂M, then necessarily $\epsilon = 1$ and $[\gamma, 1, 1]$ is a pre-image of (γ, ϵ) under φ.
That φ is an isometry follows directly from the way the metrics are defined. □

This allows us to conclude the following result.

Proposition 3.1.21 (Heat Kernel Coefficients near the Boundary). *For the coefficients from Thm. 3.1.17 we have*

$$\Phi_j(x,y) = \begin{cases} \overline{\Phi}_j(x,y) & x, y \in M \setminus \partial M \\ (\mathrm{id} + B)\overline{\Phi}_j(x,y) & x \ \in \partial M \\ \overline{\Phi}_j(x,y)(\mathrm{id} + B) & y \in \partial M. \end{cases}$$

Here the $\overline{\Phi}_j(x,y)$ are the heat kernel coefficients associated to the heat kernel of the operator $\overline{L}$ on $\overline{M}$ by Thm. 3.1.12. In particular, for x, y in the interior, $\Phi_j(x,y)$ does not depend on the boundary condition.

Remark 3.1.22 (Principle of not feeling the Boundary). In particular, in the interior of M, the heat kernel coefficients of L are the same as the heat kernel coefficients of $\overline{L}$. This is related to the "principle of not feeling the boundary", compare [Hsu95].

Proof (of Prop. 3.1.21). Using Lemma 3.1.20, we may write $\Phi_j(x,y)$ from (3.1.18) as an integral over $\overline{\Gamma}_{xy}^{\min}$, respectively $\overline{\Gamma}_{xy}^{\min} \times \mathbb{Z}_2$. If $x, y \in M \setminus \partial M$, we obtain using (3.1.18), the definition of $\Upsilon_{\tau,\nu}^{\mathrm{orb}}$ (2.3.12)

$$\Phi_j(x,y) = \sum_{i=0}^{j} \binom{j}{i} \int_{\overline{\Gamma}_{xy}^{\min}} \frac{P_\tau^{j-i}\overline{\Upsilon}_{\tau,\nu}^{(i)}(0,\gamma)}{\det_\tau\big(\nabla^2 E|_{N_\gamma \overline{\Gamma}_{xy}^{\min}}\big)^{1/2}} \, \mathrm{d}\gamma = \overline{\Phi}_j(x,y),$$

If $x \in \partial M$ and $y \notin \partial M$, we get

$$\begin{aligned} \Phi_j(x,y) &= \sum_{\epsilon \in \mathbb{Z}_2} \sum_{i=0}^{j} \binom{j}{i} \int_{\overline{\Gamma}_{xy}^{\min}} \frac{\rho(\epsilon) P_\tau^{j-i}\overline{\Upsilon}_{\tau,\nu}^{(i)}(0,\gamma)}{\det_\tau\big(\nabla^2 E|_{N_\gamma \overline{\Gamma}_{xy}^{\min}}\big)^{1/2}} \, \mathrm{d}\gamma \\ &= \sum_{\epsilon \in \mathbb{Z}_2} \rho(\epsilon)\overline{\Phi}_j(x,y) = (\mathrm{id} + B)\overline{\Phi}_j(x,y) \end{aligned}$$

and similarly, if $y \in \partial M$ but $x \notin \partial M$, we obtain $\Phi_j(x,y) = \overline{\Phi}_j(x,y)(\mathrm{id}+B)$. Finally, if both $x, y \in \partial M$, we obtain

$$\begin{aligned}\Phi_j(x,y) &= \frac{1}{2}\sum_{\epsilon_1,\epsilon_2\in\mathbb{Z}_2}\sum_{i=0}^{j}\binom{j}{i}\int_{\overline{\Gamma}_{xy}^{\min}}\frac{\rho(\epsilon_1)P_\tau^{j-i}\overline{\Upsilon}^{(i)}_{\tau,\nu}(0,\gamma)\rho(\epsilon_2)}{\det_\tau\big(\nabla^2 E|_{N_\gamma\overline{\Gamma}_{xy}^{\min}}\big)^{1/2}}\,\mathrm{d}\gamma\\ &= \frac{1}{2}\sum_{\epsilon_1,\epsilon_2\in\mathbb{Z}_2}\rho(\epsilon_1)\overline{\Phi}_j(x,y)\rho(\epsilon_2) = (\mathrm{id}+B)\overline{\Phi}_j(x,y) = \overline{\Phi}_j(x,y)(\mathrm{id}+B),\end{aligned}$$

using the equivariance of $\overline{\Phi}_j(x,y)$, see (2.3.13). □

Example 3.1.23 (The Laplace-Beltrami Operator). In particular, for the Laplace-Beltrami operator, one has

$$\Phi_j(x,y) = \begin{cases}\overline{\Phi}_j(x,y) & x,y\in M\setminus\partial M\\ 2\overline{\Phi}_j(x,y) & x \text{ or } y\in\partial M,\ \text{Neumann boundary conditions}\\ 0 & x \text{ or } y\in\partial M,\ \text{Dirichlet boundary conditions},\end{cases}$$

because we have $B \equiv \pm 1$. Here $\overline{\Phi}_j(x,y)$ are the heat kernel coefficients to the Laplace-Beltrami operator of $\overline{M}$.

Remember that we had to restrict to metrics on M such that the induced metric on the double $\overline{M}$ is smooth. If one drops this assumption, matters get more complicated. Hsu [Hsu89] proves that in the special case where M is the exterior of a convex body in $\mathbb{R}^n$ and $x, y \in \partial M$ are such that there is a unique shortest path $\gamma_{xy} \in H_{xy}(M)$ along which x and y are non-conjugate, the Neumann heat kernel of M satisfies the asymptotic relation

$$\begin{aligned}p_t^\Delta(x,y) \sim (4\pi t)^{-n/2}\sqrt{8\pi}\left(\frac{N(0)N(1)}{2t}\right)^{1/6} & J(x,y)^{-1/2}\big|\phi_1(0)\big|^2\\ &\exp\left(-\frac{1}{4t}d(x,y)^2 - \mu_1\frac{d(x,y)^{2/3}}{t^{1/3}}\int_0^1 N(s)^{2/3}\mathrm{d}s\right),\end{aligned} \tag{3.1.20}$$

where $N(s) := \mathrm{II}\big(\dot\gamma_{xy}(s),\dot\gamma_{xy}(s)\big)$ is the normal curvature along γ_{xy} (involving the second fundamental form II of the boundary) and (ϕ_1, μ_1) is the first normalized eigenpair of the eigenvalue problem

$$\phi''(x) - |x|\phi(x) + \mu\phi(x) = 0.$$

in $L^2(\mathbb{R})$. The asymptotic relation (3.1.20) is meant in the sense that the quotient of the two sides tends to one as $t \to 0$. It is not clear to the author how the $t^{-1/3}$ term in the exponent could be derived as a Laplace expansion on a path space.

3.1.4 Asymptotics of the Heat Trace

Let M be a closed Riemannian manifold of dimension n and let L be a self-adjoint Laplace type operator, acting on sections of a metric vector bundle $\mathcal{V}$ over M. Consider for partitions $\tau = \{\tau_0 < \tau_1 < \cdots < \tau_N = 1\}$ of the interval $[0,1]$ the integral

$$I_{\tau,\nu}(t) := (4\pi t)^{-nN/2}\int_{L_\tau(M)} e^{-E(\gamma)/2t}\,\mathrm{tr}\Upsilon^\circ_{\tau,\nu}(t,\gamma)\,\mathrm{d}\gamma$$

discussed in Thm. 2.2.15. Remember from the mentioned theorem that $I_{\tau,\nu}(t)$ approximates the heat trace $\operatorname{Tr} e^{-tL}$. Again, for a qualitative investigation of the asymptotic properties of the integral $I_{\tau,\nu}(t)$, the specific formula for $\Upsilon^{\circ}_{\tau,\nu}$ is not important; we only need that it is a compactly supported smooth function on $L_\tau(M)$ which depends polynomially on t.

Lemma 3.1.24. *The set*

$$\Gamma_{\mathrm{c}} := E(0)^{-1} \subset L(M)$$

of constant loops is a non-degenerate submanifold of the loop space $L(M)$ and as well of $L_\tau(M)$ for any partition τ of the interval $[0,1]$. It is diffeomorphic to M.

Proof. Clearly, a loop γ with zero energy must have vanishing derivative and hence be constant. Therefore, the evaluation map is a diffeomorphism from Γ_{c} to M. By Lemma 3.1.9, the Hessian of the energy at a constant loop γ is given by

$$\nabla^2 E|_\gamma[X,Y] = \int_{S^1} \big\langle \nabla_s X(s), \nabla_s Y(s)\big\rangle \mathrm{d}s.$$

The tangent space $T_\gamma\Gamma_{\mathrm{c}}$ is the space of parallel vector fields along γ. Now if for some $X \in T_\gamma L(M)$, we have $\nabla^2 E|_\gamma[X,Y] = 0$ for each $Y \in T_\gamma L(M)$, then X is a weak solution of $-\nabla_s^2 X = 0$, hence smooth and (because of the boundary conditions) parallel. This implies $X \in T_\gamma\Gamma_{\mathrm{c}}$. Because $\nabla^2 E|_\gamma$ is positive definite, the same result is true for the subspace $L_\tau(M)$. $\square$

Therefore, we can apply Thm. 3.1.2 on the integral $I_{\tau,\nu}(t)$ which gives that it has an asymptotic expansion

$$I_{\tau,\nu}(t) \;\sim\; (4\pi t)^{-n/2} \sum_{j=0}^{\infty} t^j a_{\tau,\nu,j}, \tag{3.1.21}$$

where

$$a_{\tau,\nu,j} := \sum_{i=0}^{j} \frac{1}{i!(j-i)!} \int_{\Gamma_{\mathrm{c}}} \frac{P_\tau^{j-i} {\Upsilon^{\circ}_{\nu,\tau}}^{(i)}(0,\gamma)}{\det_\tau\big(\nabla^2 E|_{N_\gamma\Gamma_{\mathrm{c}}}\big)^{1/2}} \mathrm{d}\gamma, \tag{3.1.22}$$

with a certain second-order differential operator P_τ defined on a neighborhood of Γ_{c} in $L_\tau(M)$, ${\Upsilon^{\circ}_{\tau,\nu}}^{(i)}$ denotes the i-th derivative of $\Upsilon^{\circ}_{\tau,\nu}$ with respect to t and $\det_\tau$ denotes the determinant on the normal space of Γ_{c} in $L_\tau(M)$.

Theorem 3.1.25 (Asymptotics of the Heat Trace). *Let L be a self-adjoint Laplace type operator, acting on sections of a metric vector bundle over a closed n-dimensional Riemannian manifold M. Then the heat trace has a complete asymptotic expansion,*

$$\operatorname{Tr} e^{-tL} \;\sim\; (4\pi t)^{-n/2} \sum_{j=0}^{\infty} t^j a_j,$$

for certain coefficients a_j. Furthermore, there exists a constant $\delta > 0$ such that these coefficients a_j are given by

$$a_j := a_{\tau,\nu,j} \tag{3.1.23}$$

with $a_{\tau,\nu,j}$ as in (3.1.22), *whenever ν and τ satisfy $\nu \geq j$ and $|\tau| \leq \delta$.*

Corollary 3.1.26. *By uniqueness of asymptotic expansions, the coefficients $a_{j,\tau,\nu}$ stabilize, i.e. we have $a_{j,\tau',\nu'} = a_{j,\tau,\nu}$ whenever $j \leq \nu, \nu'$ and $|\tau|, |\tau'| \leq \delta$.*

Proof. As seen before, the integrals $I_{\tau,\nu}(t)$ have a complete asymptotic expansion, given in (3.1.21). By Thm. 2.2.15, for any $\nu \in \mathbb{N}_0$ and $T > 0$, there exists constants $C, \delta > 0$ such that

$$\left|\mathrm{Tr}\, e^{-tL} - I_{\tau,\nu}(t)\right| \leq C t^{1+\nu-n/2} |\tau|^{\nu},$$

whenever $0 < t \leq T$ and $|\tau| \leq \delta$. If we apply this $|\tau| \leq \delta$ and $\nu \in \mathbb{N}_0$ fixed, this implies that $\mathrm{Tr}\, e^{-tL}$ must have an asymptotic expansion up to the order $\nu - n/2$, the coefficients of which coincide with those of the asymptotic expansion of $I_{\tau,\nu}(t)$ up to this order. Because ν is arbitrary, $\mathrm{Tr}\, e^{-tL}$ must have a complete asymptotic expansion. By uniqueness of asymptotic expansions, the coefficients coincide with $a_{j,\tau,\nu}$ as long as $j \leq \nu$ and $|\tau| \leq \delta$.□

Of course, it is a well-known result that the heat trace has an asymptotic expansion of the form given above (see [BGM71], [Gil95], [BGV04], [Gre71] and many more). However, the theorem above tells us more, namely that these coefficients are given as certain expressions on the finite-dimensional approximations of the loop space.

Example 3.1.27. It is well known [Gil04, Thm. 3.41] that the first two terms in the asymptotic expansion of $\mathrm{Tr}\, e^{-tL}$ are

$$a_0 = m \,\mathrm{vol}(M), \qquad a_1 = \frac{1}{6} \int_M \big(6 \,\mathrm{tr}\, V + m \,\mathrm{scal}\big), \tag{3.1.24}$$

where m is the fiber-dimension of the bundle $\mathcal{V}$ and V is the potential determined by the decomposition $L = \nabla^* \nabla + V$ as in Lemma 1.1.2.

A particular case is when $L = D^2$ for a Dirac operator D on a graded Clifford bundle. In this case, it is well known that the *supertrace* $\mathrm{Str}\, e^{-tD^2}$ is in fact independent of t and equal to the index of D (with respect to the grading). Therefore (if one replaces the trace by a supertrace in the above arguments), the above considerations yield that the index of D is zero in the case that $n = \dim(M)$ is odd and $\mathrm{ind}(D) = a_{n/2}$, in the case that n is even. Therefore we obtain the following corollary.

Corollary 3.1.28. *Let D be a self-adjoint Dirac type operator on a graded Clifford bundle $\mathcal{V}$ over a closed Riemannian manifold M. Suppose that the dimension n of M is even. Then the graded index of D is given by*

$$\mathrm{ind}(D) = \sum_{i=0}^{n/2} \frac{1}{i!(n/2-i)!} \int_{\Gamma_c} \frac{\mathrm{tr}\, P_\tau^{n/2-i} {\Upsilon^\circ_{\tau,\nu}}^{(i)}(0,\gamma)}{\det_\tau\big(\nabla^2 E|_{N_\gamma \Gamma_c}\big)^{1/2}} \mathrm{d}\gamma,$$

for any $\nu \geq n/2$ and any partition τ of the interval $[0,1]$ with $|\tau|$ small enough, where $\Upsilon^\circ_{\tau,\nu}$ is the loop space integrand associated to the associated Laplace type operator D^2 by Thm. 2.3.23.

It seems intriguing to compare this with results such as [BE15], where in a setting of super geometry, the index is represented as an integral over a (super) space of constant loops.

3.1.5 The Heat Trace on a Manifold with Boundary

Let now L be a self-adjoint Laplace type operator endowed with involutive boundary conditions, acting on sections of a metric vector bundle $\mathcal{V}$ over a compact n-dimensional Riemannian manifold with boundary M. Suppose that the smoothness Assumption 2.3.7 is satisfied. Then the trace of its solution operator e^{-tL} can be approximated by the integrals

$$I^{\mathrm{orb}}_{\tau,\nu}(t) := (4\pi t)^{-nN/2} \int_{L^{\mathrm{orb}}_\tau(M)} e^{-E(\gamma)/2t}\, \mathrm{tr}\Upsilon^{\circ,\mathrm{orb}}_{\tau,\nu}(t,\gamma)\,\mathrm{d}\gamma$$

over the finite-dimensional orbifold loop spaces $L^{\mathrm{orb}}_\tau(M)$, see Thm. 2.3.23. Evaluating the integral $I^{\mathrm{orb}}_{\tau,\nu}(t)$ with Laplace's method is not completely straight forward as $L^{\mathrm{orb}}_\tau(M)$ is a proper orbifold. However, by definition of the integral over Riemannian orbifolds (see Remark 2.3.13), we may replace the integral over $L^{\mathrm{orb}}_\tau(M)$ by an integral over $\overline{L^{\mathrm{orb}}_\tau(M)}$, which is a manifold. Remember furthermore that $\overline{L^{\mathrm{orb}}_\tau(M)}$ separates into two components: A positive and a negative component, so that the path integral splits as

$$I^{\mathrm{orb}}_{\tau,\nu}(t) = (4\pi t)^{-nN/2} \frac{1}{2} \sum_{\epsilon\in\mathbb{Z}_2} \int_{\overline{L^{\mathrm{orb},\epsilon}_\tau(M)}} e^{-E(\gamma)/2t}\, \mathrm{tr}\bigl\{\overline{\Upsilon}^{\circ}_{\tau,\nu}(t,\gamma)\rho(\epsilon)\bigr\}\,\mathrm{d}\gamma,$$

using the definition of $\Upsilon^{\circ,\mathrm{orb}}_{\tau,\nu}(t,\gamma)$ on $L^{\mathrm{orb}}_\tau(M)$.

Of course, the energy is again non-negative. We need to understand the structure of the set $\overline{\Gamma^{\mathrm{orb}}_{\mathrm{c}}} := E^{-1}(0) \subseteq \overline{L^{\mathrm{orb}}_\tau(M)}$. Similar to the proof of Lemma 3.1.24, one shows that this is a non-degenerate submanifold of $\overline{L^{\mathrm{orb}}(M)}$ and of $\overline{L^{\mathrm{orb}}_\tau(M)}$, for every partition τ of $[0,1]$. Set

$$\overline{\Gamma^{\mathrm{orb},\pm}_{\mathrm{c}}} := E^{-1}(0) \cap \overline{L^{\mathrm{orb},\pm}_\tau(M)}$$

for the critical sets contained in the positive, respectively negative component of $\overline{L^{\mathrm{orb}}_\tau(M)}$. The orbifold quotients $\Gamma^{\mathrm{orb},\pm}_{\mathrm{c}}$ are then suborbifolds of $L^{\mathrm{orb},\pm}_\tau(M)$. Clearly, we just have $\overline{\Gamma^{\mathrm{orb},+}_{\mathrm{c}}} = \overline{\Gamma}_c$, the set of constant loops in $\overline{M}$ (which is diffeomorphic to $\overline{M}$), while $\overline{\Gamma_{\mathrm{c}}}^{\mathrm{orb},-}$ is diffeomorphic to ∂M: For a constant loop, $\gamma \in \overline{\Gamma_{\mathrm{c}}}^{\mathrm{orb},-}$ means that $\gamma = -\gamma$, which means that γ must lie in the boundary.

Remark 3.1.29. Of course, loops that lie in ${\Gamma_{\mathrm{c}}}^{\mathrm{orb},-}$ also have a copy lying in ${\Gamma_{\mathrm{c}}}^{\mathrm{orb},+}$, but they differ by a sign, so ${\Gamma_{\mathrm{c}}}^{\mathrm{orb},-}$ is not a subset of ${\Gamma_{\mathrm{c}}}^{\mathrm{orb},+}$.

By the above considerations, the Laplace expansion of $I^{\mathrm{orb}}_{\tau,\nu}(t)$ is the sum of two asymptotic expansions; one over the positive part and one over the negative part. Because the positive part of the critical set has dimension n, we obtain from Thm. 3.1.2

$$(4\pi t)^{-nN/2} \int_{L^{\mathrm{orb},+}_\tau(M)} e^{-E(\gamma)/2t}\, \mathrm{tr}\Upsilon^{\circ,\mathrm{orb}}_{\tau,\nu}(t,\gamma)\,\mathrm{d}\gamma \;\sim\; (4\pi t)^{-n/2} \sum_{j=0}^{\infty} t^j a_j$$

with

$$a_j = \frac{1}{2} \sum_{i=0}^{j} \frac{1}{i!(j-i)!} \int_{\overline{\Gamma}_{\mathrm{c}}} \frac{\mathrm{tr}\, P_\tau^{j-i} {\overline{\Upsilon}^{\circ}_{\tau,\nu}}^{(i)}(0,\gamma)}{\det_\tau\bigl(\nabla^2 E|_{N_\gamma \overline{\Gamma}_{\mathrm{c}}}\bigr)^{1/2}} \mathrm{d}\gamma = \frac{1}{2}\overline{a}_j, \tag{3.1.25}$$

where $\overline{a}_j$ is the j-th coefficient in the asymptotic expansion of $\operatorname{Tr} e^{-t\overline{L}}$. For the negative part, notice that $\overline{\Gamma_{\mathrm{c}}^{\mathrm{orb},-}} \approx \partial M$ has dimension $(n-1)$ so that

$$(4\pi t)^{-nN/2} \int_{L_\tau^{\mathrm{orb},-} M)} e^{-E(\gamma)/2t} \operatorname{tr} \Upsilon_{\tau,\nu}^{\circ,\mathrm{orb}}(t,\gamma)\, \mathrm{d}\gamma \;\sim\; (4\pi t)^{-(n-1)/2} \sum_{j=0}^{\infty} t^j b_j$$

with

$$b_j = \frac{1}{2} \sum_{i=0}^{j} (-1)^{j-i} \binom{j}{i} \int_{\overline{\Gamma_{\mathrm{c}}^{\mathrm{orb},-}}} \frac{\operatorname{tr}\bigl\{ P_\tau^{j-i} \overline{\Upsilon}_{\tau,\nu}^{\circ\,(i)}(0,\gamma)\rho(-1) \bigr\}}{\det_\tau \bigl(\nabla^2 E|_{N_\gamma \overline{\Gamma_{\mathrm{c}}^{\mathrm{orb},-}}} \bigr)^{1/2}} \mathrm{d}\gamma. \tag{3.1.26}$$

We obtain the following result.

Theorem 3.1.30 (Asymptotics of the Heat Trace, Boundary Case). *Let L be a self-adjoint Laplace type operator endowed with involutive boundary conditions B, acting on sections of a metric vector bundle $\mathcal{V}$ over a compact n-dimensional Riemannian manifold with boundary. Suppose that the smoothness Assumption 2.3.7 is satisfied. Then the trace of the solution operator e^{-tL} to the heat equation has a complete asymptotic expansion as $t \searrow 0$, of the form*

$$\operatorname{Tr} e^{-tL} \;\sim\; (4\pi t)^{-n/2} \sum_{j=0}^{\infty} t^j a_j + (4\pi t)^{-(n-1)/2} \sum_{j=0}^{\infty} t^j b_j,$$

where the coefficients a_j and b_j are given above. Moreover, if we change the boundary operator from B to $-B$, this amounts to replacing b_j by $-b_j$, while the coefficients a_j remain the same.

Proof. The proof that $\operatorname{Tr} e^{-tL}$ has this asymptotic expansion is analogous to the proof of Thm. 3.1.25. The addendum is proved by noticing that under the change of B into $-B$, the equivariant structure ρ of the bundle $\overline{\mathcal{V}}$ over $\overline{M}$ is changed, namely, $\rho(-1)$ is replaced by $-\rho(-1)$. Therefore, the b_j change into $-b_j$, as seen from formula (3.1.26).
To see that the coefficients a_j do not depend on B, notice that the map

$$\varphi : \overline{\mathcal{V}}_B \longrightarrow \overline{\mathcal{V}}_{-B}, \qquad [v,\epsilon] \longmapsto [\epsilon v, \epsilon]$$

is a well-defined isometry of vector bundles, where $\overline{\mathcal{V}}_B$ denotes the vector bundle constructed with the help of the boundary condition B as in Construction 2.3.5 and $\overline{\mathcal{V}}_{-B}$ denotes the bundle constructed this way using $-B$ instead (don't get confused, however: the map φ above is just an isometry of vector bundles, not of *equivariant* vector bundles). This induces an isometry of the spaces $L^2(\overline{M},\overline{\mathcal{V}}_B)$ and $L^2(\overline{M},\overline{\mathcal{V}}_{-B})$ that takes the respective heat operators to each other. Hence they have the same trace and the same coefficients $\overline{a}_j$ as in Thm. 3.1.25. The result follows now because by (3.1.25), the a_j are just one half of the coefficients $\overline{a}_j$. □

Remark 3.1.31. As seen by Example 1.1.6 respectively Example 1.1.8, the change of B into $-B$ could be the swap from Dirichlet to Neumann boundary conditions, or from absolute to relative boundary conditions on forms.

Of course, again, it is well known that the heat trace has an asymptotic expansion involving half integer powers of t, but the theorem above illustrates where these terms come from: They are the contributions from the suborbifold $\Gamma_c^{\mathrm{orb},-} \approx \partial M$ of the energy, when employing the Laplace method on the loop space.

Example 3.1.32. In the case of Neumann boundary conditions, i.e. $B \equiv \mathrm{id}$, the first two boundary coefficients in the asymptotic expansion of e^{-tL} are given by [Gil04, Thm. 3.5.1]

$$b_0^+ = \frac{1}{4} m \operatorname{vol}(\partial M), \qquad b_1^+ = \frac{1}{384} \int_{\partial M} \Big(96 \operatorname{tr} V + m \big(16 \operatorname{scal} - 8 \operatorname{tr} \langle R(-, \mathbf{n})\mathbf{n}, -\rangle \big) \Big),$$

where m is the fiber-dimension of $\mathcal{V}$ and V is the potential determined by the decomposition $L = \nabla^*\nabla + V$ from Lemma 1.1.2. The coefficients b_0^-, b_1^- corresponding to Dirichlet boundary conditions are given by $b_0^- = -b_0^+$, $b_1^- = -b_1^+$, according to Thm. 3.1.30.
The term $\langle R(-, \mathbf{n})\mathbf{n}, -\rangle$ is zero in the case that M has a metric collar decomposition at the boundary, but not for general metrics satisfying the Smoothness Assumption 2.3.7: For example, if M is a hemisphere of S^n as in Example 2.3.8, we have $\operatorname{tr} \langle R(-, \mathbf{n})\mathbf{n}, -\rangle = n-1$.

If one drops the smoothness Assumption 2.3.7, then the heat trace asymptotics become more complicated, and the symmetry of the boundary coefficients with respect to the change of B into $-B$ disappears. Let us write $a_j = \widetilde{a}_j + a_j^{\mathrm{II}}$ and $b_j = \widetilde{b}_j + b_j^{\mathrm{II}}$, where $\widetilde{a}_j$ and $\widetilde{b}_j$ are given by the same expressions as before (see Examples 3.1.27 and 3.1.32). One always has $\widetilde{a}_0^{\mathrm{II}} = 0$, $\widetilde{b}_0^{\mathrm{II}} = 0$. In the Neumann case, we furthermore have

$$\begin{aligned} a_1^{\mathrm{II},+} &= \frac{m}{3} \int_{\partial M} \operatorname{tr} \mathrm{II} \\ b_1^{\mathrm{II},+} &= \frac{m}{384} \int_{\partial M} \big(13 (\operatorname{tr} \mathrm{II})^2 + 2 |\mathrm{II}|^2 \big), \end{aligned}$$

where m is the fiber dimension of $\mathcal{V}$ and II is the second fundamental form of the boundary (see Thm. 3.5.1 in [Gil04]). In the Dirichlet case, one has $a_1^{\mathrm{II},-} = a_1^{\mathrm{II},+}$ and

$$b_1^{\mathrm{II},-} = \frac{m}{384} \int_{\partial M} \big(7 (\operatorname{tr} \mathrm{II})^2 - 10 |\mathrm{II}|^2 \big),$$

which illustrates that there is no symmetry in these contributions from the second fundamental form [Gil04, Thm. 3.4.1].

3.2 The lowest Order Term

This section is dedicated to giving a formula for the first order term in the asymptotic heat kernel expansion Thm. 3.1.12 in terms of geometric quantities on the path spaces $H_{xy}(M)$.
To motivate this, let L be a self-adjoint Laplace type operator, acting on sections of a metric vector bundle $\mathcal{V}$ over a closed Riemannian manifold M. For simplicity, assume for the moment that $L = \nabla^*\nabla$ for a metric connection ∇, i.e. the potential term from the

decomposition of Lemma 1.1.2 is zero. Then for the heat kernel of L, we have the formal path integral formula

$$p_t^L(x,y) \overset{\text{formally}}{=} (4\pi t)^{-n/2} \fint_{H_{xy}(M)} e^{-E(\gamma)/2t} \, [\gamma\|_0^1]^{-1} \, \mathrm{d}^{H^1}\gamma, \tag{3.2.1}$$

where the slash over the integral sign denotes the (formal) division by $(4\pi t)^{\dim(H_{xy}(M))/2}$. This "formula" can be justified by looking at Thm. 2.2.7 or the Feynman-Kac formula Thm. 1.1.16 (in either case, we rescaled the paths to be defined on the interval $[0,1]$).
Pretending for the moment that the formal expression on the right hand side of (3.2.1) makes sense, we see that after dividing by the Euclidean heat kernel $\mathrm{e}_t(x,y)$, it has the form of a Laplace integral, as discussed in Section 3.1.1: The function $\phi(\gamma) := E(\gamma) - d(x,y)^2/2$ is non-negative on $H_{xy}(M)$ and takes the value zero exactly on the set $\Gamma_{xy}^{\min}$ of minimal geodesics connecting x and y (see Lemma 3.1.9). In the case that $\Gamma_{xy}^{\min}$ is a non-degenerate k-dimensional submanifold of $H_{xy}(M)$, we can apply Thm. 3.1.2 (only formally, of course, since the "integration domain" is infinite-dimensional) to obtain a formal Laplace expansion of the path integral (3.2.1). The lowest order term of this expansion is

$$\phi_0(x,y) = \int_{\Gamma_{xy}^{\min}} \frac{[\gamma\|_0^1]^{-1}}{\det\bigl(\nabla^2 E|_{N_\gamma \Gamma_{xy}^{\min}}\bigr)^{1/2}} \, \mathrm{d}^{H^1}\gamma$$

and it turns out that this is a well-defined quantity: The Hessian of the energy, as given in Lemma 3.1.9, is determinant-class on each of the Hilbert spaces $T_\gamma H_{xy}(M)$ when these carry the H^1 metric (1.2.5), and therefore has a well-defined (non-zero) Fredholm-determinant when restricted to the orthogonal complement of its kernel. We will discuss this in Subsection 3.2.1.
The question now is whether the coefficient $\phi_0(x,y)$ coming from the formal asymptotic expansion of the right hand side of (3.2.1) coincides with the lowest order term $\Phi_0(x,y)$ coming from the honest asymptotic expansion of the heat kernel in Thm. 3.1.12. The answer turns out to be "yes", and we will prove it in Subsection 3.2.2.
There is also another way to assign a determinant to an operator on an infinite-dimensional space than the Fredholm determinant, namely the zeta determinant. In Subsection 3.2.3 below, we will connect the heat kernel asymptotics of $p_t^L(x,y)$ with the zeta determinant of the Jacobi operator along geodesics connecting x and y. This "L^2 version" makes no reference to the H^1 metric. Alongside this, we will prove an interesting result regarding zeta determinants, the Gelfand-Yaglom theorem.

3.2.1 Sobolev Spaces along Paths and the Hessian of the Energy

For $a, b \in \mathbb{R}$, $a < b$, consider the closed interval $I := [a,b]$. Let M be a Riemannian manifold of dimension n. For a smooth path γ in M parametrized by I, consider the operator $P := -\nabla_s^2$ on $L^2(I, \gamma^*TM)$ with Dirichlet boundary conditions. By the considerations from Section 1.1.2, it is essentially self-adjoint on the domain $C_0^\infty(I, \gamma^*TM)$ (the space of smooth sections u of γ^*TM with $u(a) = u(b) = 0$) and self-adjoint on the Sobolev space $H_0^2(I, \gamma^*TM)$. Its eigenvalues can be explicitly computed: For a parallel orthonormal frame $e_1(s), \dots, e_n(s)$ of TM along γ, the sections E_{ik}, $i = 1, \dots, n$, $k = 1, 2, \dots$, given by

$$E_{ik}(a+s) := \sqrt{\frac{2}{b-a}} \sin\left(\frac{\pi k s}{b-a}\right) e_i(a+s), \qquad 0 \le s \le b-a \tag{3.2.2}$$

form an orthonormal basis of $L^2(I, \gamma^*TM)$ (the completeness can be easily checked using the Stone-Weierstraß theorem for locally compact spaces [dB59]). Obviously, the corresponding eigenvalues to E_{ik} are the numbers

$$\lambda_k := \frac{\pi^2 k^2}{(b-a)^2}, \tag{3.2.3}$$

each eigenvalue having multiplicity n.
Since the operator P is positive and self-adjoint, we can form the powers P^m for $m \in \mathbb{R}$ and define the Sobolev spaces

$$H_0^m(I, \gamma^*TM) := P^{-m/2} L^2(I, \gamma^*TM) \subset H^m(I, \gamma^*TM)$$

with the Sobolev norm

$$\|X\|_{H^m} := \|P^{m/2} X\|_{L^2}, \tag{3.2.4}$$

which is non-degenerate because P has a trivial kernel. By definition, this norm turns the map $P^{m/2} : H_0^l(I, \gamma^*TM) \longrightarrow H_0^{l-m}(I, \gamma^*TM)$ into an isometry, for any $m, l \in \mathbb{R}$.
Notice that for smooth $X \in H_0^1(I, \gamma^*TM)$, we have

$$(P^{1/2}X, P^{1/2}X)_{L^2} = (PX, X)_{L^2} = -(\nabla_s^2 X, X)_{L^2} = (\nabla_s X, \nabla_s X)_{L^2} = \|X\|_{H^1}^2$$

so that for $m = 1$, the norm defined in (3.2.4) coincides with the H^1 norm defined before in (1.2.5) and there is no ambiguity in the notation. In particular, in the case that $I = [0, t]$, we have

$$H_0^1(I, \gamma^*TM) = T_\gamma H_{xy;t}(M),$$

similar to (1.2.2), where $x := \gamma(0)$, $y := \gamma(y)$. Of course, orthonormal bases on the spaces $H_0^m(I, \gamma^*TM)$ can be obtained by rescaling the L^2 orthonormal basis (3.2.2) appropriately. In particular, the basis

$$F_{ik}(a+s) := \frac{\sqrt{2(b-a)}}{\pi k} \sin\left(\frac{\pi k s}{b-a}\right) e_i(a+s), \qquad 0 \le s \le b-a, \tag{3.2.5}$$

$i = 1, \dots, n$, $k = 1, 2, \dots$, is an orthonormal basis of $H_0^1(I, \gamma^*TM)$.
For later use, we need the following two lemmas.

Lemma 3.2.1. *For any $m \in \mathbb{R}$, the inclusion of $H_0^{m+1}(I, \gamma^*TM)$ into $H_0^m(I, \gamma^*TM)$ is a Hilbert-Schmidt operator. Furthermore, the inclusion operator from $H_0^{m+2}(I, \gamma^*TM)$ into $H_0^m(I, \gamma^*TM)$ is nuclear, and P^{-1} is trace-class when considered as a bounded operator on $H_0^m(I, \gamma^*TM)$.*

Proof. Denote the inclusion operator from H_0^{m+1} into H_0^m by J_m. In the case $m = 1$, we have using the orthonormal basis (3.2.5) of $H_0^1(I, \gamma^*TM)$ that

$$\|J_0\|_2^2 = \sum_{i=1}^n \sum_{k=1}^\infty \|J_0 F_{ik}\|_{L^2}^2 = \sum_{i=1}^n \sum_{k=1}^\infty \|F_{ik}\|_{L^2}^2 = n \sum_{k=1}^\infty \frac{(b-a)^2}{\pi^2 k^2} = (b-a)^2 \frac{n}{6},$$

where we used that $\sum_{k=1}^{\infty} 1/k^2 = \pi^2/6$ [Eul40]. For $m \neq 1$, we have $J_m = P^{-m/2} J_0 P^{m/2}$, so that J_m is also Hilbert-Schmidt by the ideal property of Hilbert-Schmidt operators. The inclusion of $H_0^{m+2}(I, \gamma^*TM)$ into $H_0^m(I, \gamma^*TM)$ is equal to $J_m J_{m+1}$ and the composition of two Hilbert-Schmidt operators is trace-class, so the second statement follows. Finally, we can write

$$\big[P^{-1} : H_0^m \to H_0^m\big] = J_m\, J_{m+1}\, \big[P^{-1} : H_0^m \to H_0^{m+2}\big],$$

which finishes the proof, because nuclear operators form an ideal. □

Lemma 3.2.2. *For any $l, m \in \mathbb{R}$ with $l \leq m$, we have*

$$\|P^{(l-m)/2} X\|_{H^m} = \|X\|_{H^l} \leq \left(\frac{b-a}{\pi}\right)^{m-l} \|X\|_{H^m}.$$

Proof. Using the basis E_{ik} from (3.2.2) to the eigenvalues λ_k, decompose a given vector field $X \in H_0^m([a,b], \gamma^*TM)$ as $X = \sum_{i=1}^n \sum_{k=1}^\infty X_{ik} E_{ik}$. Then for any $l \leq m$, we have

$$\|X\|_{H^m}^2 = \sum_{i=1}^n \sum_{k=1}^\infty \lambda_k^m |X_{ik}|^2 \geq \lambda_1^{m-l} \sum_{i=1}^n \sum_{k=1}^\infty \lambda_k^l |X_{ik}|^2 = \left(\frac{\pi^2}{(b-a)^2}\right)^{m-l} \|X\|_{H^l}^2,$$

using the explicit value for λ_1 as in (3.2.3). This is the statement. □

Let us now discuss the determinant of the Hessian of the energy. If T is a bounded linear operator on a separable Hilbert space $\mathcal{H}$, then its determinant can be defined if it has the form $T = \mathrm{id} + W$ with a trace-class operator W. We will call such operators *determinant-class* and their *(Fredholm) determinant* can be defined by

$$\det(T) := \prod_{j=1}^{\infty} (1 + \lambda_j), \tag{3.2.6}$$

where λ_j are the eigenvalues of W, repeated with algebraic multiplicity. Because as a trace-class operator, W is compact, its non-zero spectrum consists only of eigenvalues of finite algebraic multiplicity (see e.g. Thm. 7.1 in [Con94]) and the trace-class condition means just that $\sum_{j=1}^\infty |\lambda_j| < \infty$, which by definition means that the product converges absolutely [FB05, Def. IV.1.4]. In particular, $\det(T) = 0$ if and only if $\lambda_j = -1$ for some j. There are many other ways to define the determinant of T, see [Sim77]. For us, the following equivalent way to calculate a determinant will be useful.

Proposition 3.2.3. *Let $\mathcal{H}$ be a separable Hilbert space and let $T := \mathrm{id} + W$ be a bounded operator on T with W trace-class. Let $V_1 \subseteq V_2 \subseteq \dots$ be a nested sequence of finite-dimensional subspaces such that their union is dense in $\mathcal{H}$. Then we have*

$$\det(T) = \lim_{k\to\infty} \det\big(T|_{V_k}\big).$$

Remark 3.2.4. In particular, if $e_1, e_2, \ldots$ is an orthonormal basis of $\mathcal{H}$, then setting V_k to be the span of $e_1, \ldots, e_k$ yields that

$$\det(T) = \lim_{k\to\infty} \det\bigl(\langle e_i, Te_j\rangle\bigr)_{1\le i,j\le k},$$

where the latter is an ordinary determinant of matrices.

Proof. Let π_k be the orthogonal projection on V_k. Because $\mathrm{id} + \pi_k W \pi_k$ has the block diagonal form

$$\mathrm{id} + \pi_k W \pi_k = \begin{pmatrix} T|_{V_k} & 0 \\ 0 & \mathrm{id} \end{pmatrix}$$

with respect to the orthogonal splitting $\mathcal{H} = V_k \oplus V_k^\perp$, we have

$$\det\bigl(T|_{V_k}\bigr) = \det\bigl(\mathrm{id} + \pi_k W \pi_k\bigr),$$

where the right hand side denotes the Fredholm determinant on $\mathcal{H}$. Let n_k be the dimension of V_k and let $e_1, e_2, \ldots$ be an orthonormal basis of $\mathcal{H}$ such that $e_1, \ldots, e_{n_k}$ is an orthonormal basis of V_k. Using this orthonormal basis, we have

$$\operatorname{tr} W_k = \sum_{j=1}^{\infty} \langle e_j, \pi_k W \pi_k e_j\rangle = \sum_{j=1}^{n_k} \langle e_j, W e_j\rangle \longrightarrow \sum_{j=1}^{\infty} \langle e_j, W e_j\rangle = \operatorname{tr} W. \tag{3.2.7}$$

For the Hilbert-Schmidt norm, we find

$$\|W_k - W\|_2^2 = \sum_{ij=1}^{\infty} \langle e_i, (\pi_k W \pi_k - W) e_j\rangle^2 = \sum_{\{i,j \,|\, i>n_k \text{ or } j>n_k\}} \langle e_i, W e_j\rangle^2,$$

which converges to zero since W is Hilbert-Schmidt (this follows e.g. from the dominated convergence theorem). Thus $W_k \to W$ in the Hilbert-Schmidt norm.
The 2-regularized determinant of a determinant-class operator $\mathrm{id} + V$ is defined by

$$\det\nolimits_2(\mathrm{id} + V) = \det(\mathrm{id} + V) e^{-\operatorname{tr} V},$$

see Section 6 in [Sim77]. Because $\det_2$ is continuous in the topology induced by Hilbert-Schmidt norm (Thm. 6.5 in [Sim77]) and because of (3.2.7), we have

$$\lim_{k\to\infty} \det(\mathrm{id} + W_k) = \lim_{k\to\infty} \det\nolimits_2(\mathrm{id} + W_k) e^{\operatorname{tr} W_k} = \det\nolimits_2(\mathrm{id} + W) e^{\operatorname{tr} W} = \det(\mathrm{id} + W).$$

This finishes the proof. $\square$

For $s \in I$, define

$$\mathcal{R}_\gamma(s) v := R\bigl(\dot\gamma(s), v\bigr)\dot\gamma(s), \qquad v \in T_{\gamma(s)} M, \tag{3.2.8}$$

where R is the Riemann curvature tensor of M. Because of the symmetries of R, $\mathcal{R}_\gamma$ is a symmetric endomorphism field of the bundle $\gamma^* TM$ over I. Since $\mathcal{R}_\gamma$ is smooth and uniformly bounded on I, we can form the operator $P + \mathcal{R}_\gamma$, which is then self-adjoint on the same domain as P, and possesses the same mapping properties as P.

From now on, suppose that γ is a geodesic. Then by Lemma 3.1.9, the Hessian $\nabla^2 E|_\gamma$ is given by

$$\nabla^2 E|_\gamma[X,Y] = (\nabla_s X, \nabla_s Y)_{L^2} + (\mathcal{R}_\gamma X, Y)_{L^2} = \big((P+\mathcal{R}_\gamma)X, Y\big)_{L^2} \tag{3.2.9}$$

for $X, Y \in H_0^1(I, \gamma^*TM)$. Hence on $H_0^1(I,\gamma^*TM) \subset L^2(I,\gamma^*TM)$, the Hessian is given by the operator $P + \mathcal{R}_\gamma$. Of course, this is far from being determinant-class, since it is even unbounded. But by (3.2.9), we also have

$$\nabla^2 E|_\gamma[X,Y] = (X,Y)_{H^1} + (P^{-1}\mathcal{R}_\gamma X, Y)_{H^1} = \big(X, P^{-1}(P+\mathcal{R}_\gamma)Y\big)_{H^1}, \tag{3.2.10}$$

so on the space $H_0^1(I,\gamma^*TM)$, the bilinear form $\nabla^2 E|_\gamma$ is given by the operator $\mathrm{id}+P^{-1}\mathcal{R}_\gamma$. Now, indeed, $P^{-1}\mathcal{R}_\gamma$ is trace-class on $H_0^1(I,\gamma^*TM)$, by Lemma 3.2.1. In fact, we can even calculate its value in terms of a curvature integral, as the following proposition shows.

Proposition 3.2.5 (The Hessian of the Energy). *Let γ be a geodesic between points $x, y \in M$, parametrized $[0,t]$ and consider $\nabla^2 E|_\gamma$ as an operator on $T_\gamma H_{xy;t}(M)$, by dualizing with the H^1 metric. Then $\nabla^2 E|_\gamma - \mathrm{id}$ is trace-class with*

$$\mathrm{Tr}\big(\nabla^2 E|_\gamma - \mathrm{id}\big) = -\frac{1}{t}\int_0^t \mathrm{ric}\big(\dot\gamma(s),\dot\gamma(s)\big)\, s(t-s)\,\mathrm{d}s,$$

where ric *denotes the Ricci tensor of M.*

Remark 3.2.6. This implies that $\nabla^2 E|_\gamma$ is determinant-class as a bilinear form on the Hilbert space $H_0^1([0,t],\gamma^*TM)$. Furthermore, it is easy to see from the above considerations, that $\nabla^2 E|_\gamma$ is determinant-class on $H_0^m([0,t],\gamma^*TM)$ if and *only if* $m=1$.

Proof. By (3.2.10), we have using the orthonormal basis F_{ik} from (3.2.5) that

$$\begin{aligned}\mathrm{Tr}\big(\nabla^2 E|_\gamma - \mathrm{id}\big) &= \sum_{i=1}^n\sum_{k=1}^\infty \big(P^{-1}\mathcal{R}_\gamma F_{ik}, F_{ik}\big)_{H^1} = \sum_{i=1}^n\sum_{k=1}^\infty \big(\mathcal{R}_\gamma F_{ik}, F_{ik}\big)_{L^2}\\ &= \int_0^t \underbrace{\left(\sum_{j=1}^n \langle R(\dot\gamma(s), e_i(s))\dot\gamma(s), e_i(s)\rangle\right)}_{=-\mathrm{ric}\left(\dot\gamma(s),\dot\gamma(s)\right)}\left(\sum_{k=1}^\infty \frac{2t}{\pi^2k^2}\sin\left(\frac{\pi s k}{t}\right)^2\right)\mathrm{d}s.\end{aligned}$$

Now because of $2\sin(z)^2 = 1-\cos(2z)$, we have

$$\sum_{k=1}^\infty \frac{2t}{\pi^2k^2}\sin\left(\frac{\pi sk}{t}\right)^2 = \frac{t}{\pi^2}\sum_{k=1}^\infty\frac{1}{k^2} - t\sum_{k=1}^\infty \frac{1}{\pi^2k^2}\cos\left(\frac{2\pi sk}{t}\right) = \frac{1}{t}s(t-s),$$

where we used the Fourier transform identity of the second Bernoulli polynomial [Sch13],

$$\sum_{k=1}^\infty \frac{1}{\pi^2k^2}\cos(2\pi kz) = z^2 - z + \frac{1}{6}. \qquad \square$$

Example 3.2.7 (Constant Curvature Manifolds). Set $[a,b] = [0,1]$. We calculate $\det(\nabla^2 E|_\gamma)$ in the case that γ is a unique minimizing geodesic between points x, y on a Riemannian manifold M of constant sectional curvature κ. In this special case, the Jacobi eigenvalue equation along a geodesic γ is (see e.g. [Cha84, p. 63])

$$\big(P + \mathcal{R}_\gamma(s)\big)X(s) = -\nabla_s^2 X(s) - \kappa|\dot\gamma(s)|^2 X(s) + \kappa\,\langle X(s), \dot\gamma(s)\rangle\,\dot\gamma(s) = \lambda X(s).$$

Because γ is a geodesic, the eigenspaces separate into spaces of vector fields that are either parallel to $\dot\gamma$ or orthogonal to $\dot\gamma$. Write $r := |\dot\gamma(s)| = d(x,y)$ (which is independent of s because γ is a geodesic). Set $e_1(s) := \dot\gamma(s)/r$ and let $e_2(s), \dots, e_n(s)$ be a parallel orthonormal basis of the orthogonal complement of $\dot\gamma$ along γ.
If we use the frame $e_1(s), \dots, e_n(s)$ to define the orthonormal basis F_{ik} as in (3.2.5), then this is an orthonormal basis of eigenvectors of $P + \mathcal{R}_\gamma$ on the space $H_0^1([0,1], \gamma^*TM)$: The F_{1k} are eigenvectors to the eigenvalues $\lambda_k = \pi^2 k^2$ (so these have multiplicity one each), while the F_{ik}, $i = 2, \dots, n$, are eigenvectors to the eigenvalues $\mu_k = \pi^2 k^2 - \kappa r^2$ (each of these has multiplicity $n-1$). The eigenvalues for the operator $\mathrm{id} + P^{-1}\mathcal{R}_\gamma$ are then

$$\widetilde{\lambda}_k = \frac{\lambda_k}{\pi^2 k^2} = 1, \qquad \widetilde{\mu}_k = \frac{\mu_k}{\pi^2 k^2} = 1 - \frac{\kappa r^2}{\pi^2 k^2}. \tag{3.2.11}$$

(If $\kappa > 0$, this reflects that in order to have no zero eigenvalues, we need to have $r^2\kappa < \pi^2$.) We obtain by (3.2.6) and (3.2.10)

$$\det\big(\nabla^2 E|_\gamma\big) = \det\big(\mathrm{id} + P^{-1}\mathcal{R}_\gamma\big) = \prod_{k=1}^\infty \left(1 - \frac{\kappa r^2}{\pi^2 k^2}\right)^{n-1} = \left(\frac{\sin(\sqrt{\kappa} r)}{\sqrt{\kappa} r}\right)^{n-1}$$

by the product formula for the sine [FB05, p. 220] (if κ is negative, then sin becomes sinh). Note that these results coincide with the explicit formulas for the Jacobian of the exponential map $J(x,y)$ on manifolds with constant curvature, compare Remark 2.1.2. This is no coincidence, as we will see in Corollary 3.2.11 below.

3.2.2 The lowest Order Term as a Fredholm Determinant

We start with the main result of this section.

Theorem 3.2.8 (Lowest Order Term, H^1 picture). *Let L be a self-adjoint Laplace type operator, acting on sections of a metric vector bundle $\mathcal{V}$ over a compact Riemannian manifold M of dimension n. For $x, y \in M$, suppose that the set $\Gamma_{xy}^{\min}$ of minimal geodesics connecting x and y is a k-dimensional non-degenerate submanifold of $H_{xy}(M)$. Then for the lowest order coefficient $\Phi_0(x,y)$ from Thm. 3.1.12, we have*

$$\Phi_0(x,y) = \lim_{t\to 0} (4\pi t)^{k/2} \frac{p_t^L(x,y)}{\mathrm{e}_t(x,y)} = \int_{\Gamma_{xy}^{\min}} \frac{[\gamma\|_0^1]^{-1}}{\det\big(\nabla^2 E|_{N_\gamma \Gamma_{xy}^{\min}}\big)^{1/2}}\, \mathrm{d}^{H^1}\gamma,$$

where $[\gamma\|_0^1]$ denotes the parallel transport along γ with respect to the connection determined by the decomposition $L = \nabla^*\nabla + V$ as in Lemma 1.1.2, and the determinant is the Fredholm determinant of the bilinear form $\nabla^2 E$ on the Hilbert subspace $N_\gamma \Gamma_{xy}^{\min} \subseteq T_\gamma H_{xy}(M)$. Here the Hilbert manifold $H_{xy}(M)$ is endowed with the H^1 metric (1.2.5) and $\Gamma_{xy}^{\min}$ carries the induced submanifold metric.

For the proof, we need the following two lemmas, the (somewhat involved) proof of which will be given at the end of this section.

Lemma 3.2.9. *Let M be a compact Riemannian manifold and $x, y \in M$. Then for every $C > 0$, there exist constants $\alpha > 0$ and $N_0 \in \mathbb{N}$ such that the following holds: For any geodesic $\gamma \in \Gamma_{xy}^{\min}$ in M, we have*

$$e^{-\alpha|\tau|^{-3}} \leq \left|\det\bigl(\mathrm{dev}_\tau|_\gamma\bigr)\right| \prod_{j=1}^{N} (\Delta_j \tau)^{-n/2} \leq e^{\alpha|\tau|^{-3}}$$

for any partition $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = 1\}$ of the interval $[0,1]$ with $N \geq N_0$ and $|\tau| \leq C/N$.

Lemma 3.2.10. *Let S be a set of partitions of the interval $[0,1]$ such that for any $\varepsilon > 0$, there exists $\tau \in S$ with $|\tau| < \varepsilon$. Then for any $\gamma \in \Gamma_{xy}^{\min}$, the union of the spaces $T_\gamma H_{xy;\tau}(M)$, $\tau \in S$ is dense in $T_\gamma H_{xy}(M) = H_0^1([0,1], \gamma^* TM)$.*

Proof (of Thm. 3.2.8). By Thm. 3.1.12, we have

$$\lim_{t \to 0} (4\pi t)^{k/2} \frac{p_t^L(x,y)}{\mathrm{e}_t(x,y)} = \Phi_0(x,y)$$

for the coefficient $\Phi_0(x,y)$, which is given for arbitrary $\nu \geq 0$ and partitions τ fine enough by the integral

$$\Phi_0(x,y) = \int_{\Gamma_{xy}^{\min}} \frac{\Upsilon_{\tau,\nu}(0,\gamma)}{\det_\tau\bigl(\nabla^2 E|_{N_\gamma \Gamma_{xy}^{\min}}\bigr)^{1/2}} \mathrm{d}\gamma, \tag{3.2.12}$$

compare (3.1.12). The result now follows by taking the limit over a suitable sequence of partitions. By formula (2.2.14) for $\Upsilon_{\tau,\nu}$, we have

$$\Upsilon_{\tau,\nu}(0,\gamma) = \left(\left|\det\bigl(\mathrm{dev}_\tau|\gamma\bigr)\right| \prod_{j=1}^{N} (\Delta_j \tau)^{-n/2} \right) \left(\prod_{j=1}^{N} \Phi_0\bigl(\gamma(\tau_{j-1}), \gamma(\tau_j)\bigr) \right)$$

independent of ν, provided the partition τ is so fine that $\chi(\gamma(\tau_{j-1}), \gamma(\tau_j)) = 1$ for each j, where χ is the cutoff function appearing in the formula. Remember from (2.1.10) that for $(z_0, z_1) \in M \bowtie M$, the coefficient Φ_0 is given by $\Phi_0(z_0,z_1) = J(z_0,z_1)^{-1/2}[\gamma_{z_0 z_1}\|_0^1]^{-1}$, where $J(z_0,z_1)$ is the Jacobian of the exponential map (see Remark 2.1.2) and $\gamma_{z_0 z_1}$ is the shortest geodesic connecting z_0 to z_1 in time one. From the Taylor expansion (2.1.8) of the function J, we obtain that there exists a constant $\alpha > 0$ such that

$$e^{-\alpha|t-s|^2} \leq J\bigl(\gamma(s), \gamma(t)\bigr)^{-1/2} \leq e^{\alpha|t-s|^2}$$

for all $0 \leq s, t \leq 1$ and all $\gamma \in \Gamma_{xy}^{\min}$ and consequently

$$e^{-\alpha|\tau|} \leq e^{-\alpha \sum_{j=1}^{N} (\Delta_j \tau)^2} \leq \prod_{j=1}^{N} J\bigl(\gamma(\tau_{j-1}), \gamma(\tau_j)\bigr)^{-1/2} \leq e^{\alpha \sum_{j=1}^{N} (\Delta_j \tau)^2} \leq e^{\alpha|\tau|}. \tag{3.2.13}$$

Hence by Lemma 3.2.9, we have for any γ that

$$\lim_{|\tau|\to 0} \Upsilon_{\tau,\nu}(0,\gamma) = [\gamma\|_0^1]^{-1},$$

where for a fixed $C > 0$, the limit goes over any sequence of partitions $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = 1\}$ with $|\tau| \to 0$, where each such τ additionally satisfies $|\tau| \leq C/N$.
By Lemma 3.2.10, if (τ^k), $k \in \mathbb{N}$ is any sequence of partitions the mesh of which tends to zero, then the union of the spaces $T_\gamma H_{xy;\tau^k}(M)$, $k \in \mathbb{N}$, is dense in $T_\gamma H_{xy}(M)$ for every $\gamma \in \Gamma_{xy}^{\min}$. Furthermore, also the union of the spaces $N_\gamma \Gamma_{xy}^{\min} \cap T_\gamma H_{xy;\tau^k}(M)$ is dense in $N_\gamma\Gamma_{xy}^{\min}$. For let $X \in N_\gamma\Gamma_{xy}^{\min}$. Then there exists a sequence $X_k \in T_\gamma H_{xy;\tau^k}(M)$ with $\|X - X_k\|_{H^1} \to 0$ by Lemma 3.2.10. But if $Y_k \in T_\gamma \Gamma_{xy}^{\min}$ is the part of X_k tangent to $\Gamma_{xy}^{\min}$, we have

$$\|X - X_k\|_{H^1}^2 = \big\|X - (X_k - Y_k)\big\|_{H^1}^2 + \|Y_k\|_{H^k}^2,$$

so that $X_k - Y_k$ is an approximating sequence of X in $N_\gamma\Gamma_{xy}^{\min} \cap T_\gamma H_{xy;\tau^k}(M)$. By Prop. 3.2.3, we therefore have

$$\lim_{|\tau|\to 0} \det{}_\tau\big(\nabla^2 E|_{N_\gamma\Gamma_{xy}^{\min}}\big) = \lim_{|\tau|\to 0} \det\big(\nabla^2 E|_{N_\gamma\Gamma_{xy}^{\min}\cap T_\gamma H_{xy;\tau}(M)}\big) = \det\big(\nabla^2 E|_{N_\gamma\Gamma_{xy}^{\min}}\big)$$

if the limit goes over any *nested* sequence of partitions τ the mesh of which tends to zero (since then the corresponding sequence of spaces $N_\gamma\Gamma_{xy}^{\min} \cap T_\gamma H_{xy;\tau}(M)$ is nested, too).
We obtain that if for a fixed $C > 0$, we take the limit over some nested sequence of partitions τ with $|\tau| \to 0$ that additionally satisfies $|\tau| \leq C/N$, then the integrand in (3.2.12) converges to the integrand from the theorem pointwise.
To justify the exchange of integration and taking the limit, we give a uniform bound. The term $\Upsilon_{\tau,\nu}(0,\gamma)$ is uniformly bounded by (3.2.13) and Lemma 3.2.9. Because of (3.2.10), we have

$$\det{}_\tau\big(\nabla^2 E|_{N_\gamma\Gamma_{xy}^{\min}}\big) = \det\big(\nabla^2 E|_{N_\gamma\Gamma_{xy}^{\min}\cap H_{xy;\tau}(M)}\big) = \det\big((\mathrm{id} + \pi_\tau P^{-1}\mathcal{R}_\gamma\pi_\tau)|_{N_\gamma\Gamma_{xy}^{\min}}\big),$$

where π_τ is the orthogonal projection of $H_{xy}(M)$ onto $H_{xy;\tau}(M)$. Because of the standard determinant estimate for Fredholm determinants (see [Sim77, Thm. 3.2])

$$e^{-\|T\|_1} \leq \det(\mathrm{id} + T) \leq e^{\|T\|_1}, \tag{3.2.14}$$

which holds for all trace-class operators T, we have

$$\det{}_\tau\big(\nabla^2 E|_{N_\gamma\Gamma_{xy}^{\min}}\big)^{-1/2} \leq e^{\|\pi_\tau P^{-1}\mathcal{R}_\gamma\pi_\tau\|_1/2}.$$

But

$$\|\pi_\tau P^{-1}\mathcal{R}_\gamma\pi_\tau\|_1 \leq \|\pi_\tau\|\|P^{-1}\mathcal{R}_\gamma\|_1\|\pi_\tau\| \leq \|P^{-1}\|_1\|\mathcal{R}_\gamma\|,$$

which is finite by Lemma 3.2.1 and bounded uniformly over $\gamma \in \Gamma_{xy}^{\min}$ since $\Gamma_{xy}^{\min}$ is compact. The proof now follows from Lebesgue's theorem of dominated convergence. □

Restricting to the case $(x,y) \in M \bowtie M$ gives the following corollary.

Corollary 3.2.11 (The Jacobian of the Exponential Map). *Let M be a complete Riemannian manifold. Let $(x,y) \in M \bowtie M$ and let γ_{xy} be the unique minimizing geodesic connecting x to y in time one. Then we have*

$$\det\big(\nabla^2 E|_{\gamma_{xy}}\big) = J(x,y),$$

where $J(x,y)$ is the Jacobian determinant of the exponential map, as in Remark 2.1.2. Here, $H_{xy}(M)$ carries the H^1 metric (1.2.5).

Proof. Of course, this is a local result, so in the case that M is non-compact, we can take some patch of M containing γ_{xy} and embed it isometrically into some compact Riemannian manifold M' in such a way that γ_{xy} is still a minimizing geodesic, without changing $J(x,y)$ or the determinant of the Hessian of the energy. This shows that we may assume that M is compact so that the above results apply.
Taking the heat kernel of the Laplace-Beltrami operator in Thm. 3.2.8 and restricting to the case $(x,y) \in M \bowtie M$ (which implies $\Gamma_{xy}^{\min} = \{\gamma_{xy}\}$ and $k = \dim(\Gamma_{xy}^{\min}) = 0$), we have

$$\Phi_0(x,y) = \lim_{t\to 0} \frac{p_t^{\Delta}(x,y)}{\mathrm{e}_t(x,y)} = \det\big(\nabla^2 E|_{\gamma_{xy}}\big)^{-1/2}.$$

By (2.1.10), we have $\Phi_0(x,y) = J(x,y)^{-1/2}$ so the result follows. □

Another way to formulate Thm. 3.2.8 is that if $\Gamma_{xy}^{\min}$ is a non-degenerate submanifold of dimension k, we have

$$p_t^L(x,y) \;\sim\; (4\pi t)^{-n/2-k/2} \int_{\Gamma_{xy}^{\min}} e^{-E(\gamma)/2t} \frac{[\gamma\|_0^1]^{-1}}{\det\big(\nabla^2 E|_{N_\gamma \Gamma_{xy}^{\min}}\big)^{1/2}}\,\mathrm{d}^{H^1}\gamma, \tag{3.2.15}$$

where the asymptotic relation means that the quotient of the two sides converges to one as $t \to 0$. This involves the space of minimal geodesics parametrized by the interval $[0,1]$. One can also formulate this result using the space $\Gamma_{xy;t}^{\min}$ of minimal geodesics between x and y parametrized by $[0,t]$.

Corollary 3.2.12. *Under the assumptions of Thm. 3.2.8, we have*

$$p_t^L(x,y) \;\sim\; (4\pi t)^{-n/2} \int_{\Gamma_{xy;t}^{\min}} e^{-E(\gamma)/2} \frac{[\gamma\|_0^t]^{-1}}{\det\big(\nabla^2 E|_{N_\gamma \Gamma_{xy;t}^{\min}}\big)^{1/2}}\,\mathrm{d}^{\widetilde{H}^1}\gamma.$$

Here, $\Gamma_{xy;t}^{\min}$ denotes the space of minimizing geodesics parametrized by $[0,t]$ connecting x to y, carrying the rescaled H^1 metric

$$(X,Y)_{\widetilde{H}^1} := \frac{1}{4\pi}\int_0^t \langle \nabla_s X(s), \nabla_s Y(s)\rangle\,\mathrm{d}s. \tag{3.2.16}$$

The asymptotic relation above means that the quotient of the two sides converges to one as $t \to 0$.

Remark 3.2.13. Notice that the formula of Corollary 3.2.12 is independent of the dimension k. Therefore, the above formula is also true if $\Gamma_{xy;t}^{\min}$ is a disjoint union of non-degenerate submanifolds of various dimensions. However, only the component of $\Gamma_{xy}^{\min}$ of the highest dimension will contribute in the limit, because the integrals over the other components are of lower order in t.

Proof. Consider the rescaling map

$$S_t : H_{xy;t}(M) \longrightarrow H_{xy}(M), \qquad \gamma \longmapsto \widetilde{\gamma} := \Big[s \mapsto \gamma(st)\Big]. \tag{3.2.17}$$

For $X \in T_\gamma H_{xy;t}(M)$, we have $dS_t|_\gamma X = \widetilde{X}$, where $\widetilde{X}(s) = X(st)$. Therefore,

$$\begin{aligned}\big(dS_t|_\gamma X, dS_t|_\gamma Y\big)_{H^1} &= \int_0^1 \Big\langle \nabla_s \widetilde{X}(s), \nabla_s \widetilde{Y}(s)\Big\rangle \,\mathrm{d}s = t^2 \int_0^1 \langle \nabla_s X(st), \nabla_s Y(st)\rangle \,\mathrm{d}s\\ &= t \int_0^t \langle \nabla_s X(s), \nabla_s Y(s)\rangle \,\mathrm{d}s = 4\pi t \big(X, Y\big)_{\widetilde{H}^1}\end{aligned}$$

so that S_t is a conformal mapping with conformal factor $4\pi t$. S_t restricts to a map $S_t : \Gamma_{xy;t}^{\min} \longrightarrow \Gamma_{xy}^{\min}$ and by the above calculation, we find in the case that $\Gamma_{xy}^{\min}$ is a k-dimensional submanifold of $H_{xy}(M)$ that

$$\det(dS_t) = \det\big((dS_t)^* dS_t\big)^{1/2} \equiv (4\pi t)^{k/2},$$

Hence

$$\Phi_0(x, y) = \int_{\Gamma_{xy}^{\min}} \frac{[\widetilde{\gamma}\|_0^1]^{-1}}{\det\big(\nabla^2 E|_{N_{\widetilde{\gamma}}\Gamma_{xy}^{\min}}\big)^{1/2}} \mathrm{d}\widetilde{\gamma} = (4\pi t)^{k/2} \int_{\Gamma_{xy;t}^{\min}} \frac{[\gamma\|_0^t]^{-1}}{\det\big(\nabla^2 E|_{N_{\widetilde{\gamma}}\Gamma_{xy}^{\min}}\big)^{1/2}} \mathrm{d}\gamma. \tag{3.2.18}$$

To see that the determinant is independent of t, i.e.

$$\det(\nabla^2 E|_{N_{\widetilde{\gamma}}\Gamma_{xy}^{\min}}) = \det(\nabla^2 E|_{N_\gamma \Gamma_{xy;t}^{\min}})$$

for any $t > 0$, note that if $E_1, E_2, \dots$ is an orthonormal basis of $N_\gamma \Gamma_{xy;t}^{\min}$, then the vector fields $\widetilde{E}_j(s) := \sqrt{t} E_j(s/t)$ form an orthonormal basis of $N_{\widetilde{\gamma}}\Gamma_{xy}^{\min}$. Now

$$\begin{aligned}\nabla^2 E|_\gamma[E_i, E_j] &= \int_0^t \Big(\langle \nabla_s E_i(s), \nabla_s E_j(s)\rangle + \big\langle R\big(\dot\gamma(s), E_i(s)\big)\dot\gamma(s), E_j(s)\big\rangle\Big)\mathrm{d}s\\ &= \frac{1}{t}\int_0^t \Big(\Big\langle \nabla_s \widetilde{E}_i(s/t), \nabla_s \widetilde{E}_j(s/t)\Big\rangle + \Big\langle R\big(\dot{\widetilde{\gamma}}(s/t), \widetilde{E}_i(s/t)\big)\dot{\widetilde{\gamma}}(s/t), \widetilde{E}_j(s/t)\Big\rangle\Big)\,\mathrm{d}s\\ &= \nabla^2 E|_{\widetilde{\gamma}}\big[\widetilde{E}_i, \widetilde{E}_j\big].\end{aligned}$$

From this follows using Prop. 3.2.3 (or rather Remark 3.2.4) that

$$\begin{aligned}\det\big(\nabla^2 E|_{N_{\widetilde{\gamma}}\Gamma_{xy}^{\min}}\big) &= \lim_{N\to\infty} \det\Big(\nabla^2 E|_{\widetilde{\gamma}}\big[\widetilde{E}_i, \widetilde{E}_j\big]\Big)_{1\le i,j\le N}\\ &= \lim_{N\to\infty} \det\Big(\nabla^2 E|_\gamma\big[E_i, E_j\big]\Big)_{1\le i,j\le N} = \det\big(\nabla^2 E|_{N_\gamma\Gamma_{xy;t}^{\min}}\big)\end{aligned}$$

whence the result. $\square$

Example 3.2.14 (The first Coefficient on Spheres). On an n-dimensional sphere of radius $R = 1/\sqrt{\kappa}$, the determinant of the Hessian of the energy, respectively the Jacobian of the exponential map, is given by (2.1.9) in the case that x and y are not antipodal points, which gives an explicit formula for $\Phi_0(x, y)$ because of (2.1.10). We now use Thm. 3.2.8 to calculate $\Phi_0(x, y)$ for the Laplace-Beltrami operator on S^n_R in the case that x and y are antipodal points.
Without loss of generality, we assume that $x = (R, 0, \ldots, 0)$ and $y = (-R, 0, \ldots, 0)$ are the north and south pole. In this case, the set $\Gamma^{\min}_{xy}$ is diffeomorphic to S^{n-1}_R, the $n-1$-dimensional sphere of radius R, via the diffeomorphism

$$\rho : S^{n-1}_R \longrightarrow \Gamma^{\min}_{xy} \qquad \theta \longmapsto \left[s \mapsto \begin{pmatrix} R\cos(\pi s) \\ \theta \sin(\pi s)\end{pmatrix}\right].$$

For $v \in T_\theta S^{n-1}_R$, we have

$$d\rho|_\theta v =: X_v = \left[s \mapsto \begin{pmatrix} 0 \\ v\sin(\pi s)\end{pmatrix}\right].$$

Since $v \in T_\theta S^{n-1}_R$, we have $\langle v, \theta\rangle = 0$, hence $\left\langle \dot{X}_v(s), \rho(\theta)(s)\right\rangle = 0$ so that

$$\nabla_s X_v(s) = \dot{X}_v(s) - \kappa \left\langle \dot{X}_v(s), \rho(\theta)(s)\right\rangle \rho(\theta)(s) = -\pi \begin{pmatrix} 0 \\ v\sin(\pi s)\end{pmatrix},$$

by the explicit formula for the Levi-Civita connection on the round sphere. Therefore, if $e_1, \ldots, e_{n-1}$ is an orthonormal basis of $T_\theta S^{n-1}_R$, the Jacobian determinant of ρ is given by

$$\begin{aligned}\left|\det\big(d\rho|_\theta\big)\right| &= \det\Big(\big(X_{e_i}, X_{e_j}\big)_{H^1}\Big)^{1/2}_{1\leq i,j\leq n-1} = \det\left(\pi^2\langle e_i, e_j\rangle \int_0^1 \cos(\pi s)^2 \mathrm{d}s\right)^{1/2}_{1\leq i,j\leq n-1} \\ &= \pi^{n-1}2^{(1-n)/2},\end{aligned}$$

which is constant. To calculate the determinant of the Hessian of the energy, remember that the eigenvalues are given by (3.2.11). In our case, $r = R\pi$ and $\kappa = 1/R^2$ so $\widetilde{\mu}_1 = 0$, which has to be left out to calculate the Hessian on the normal space to $\Gamma^{\min}_{xy}$. We obtain

$$\det\big(\nabla^2 E|_{N_\gamma \Gamma^{\min}_{xy}}\big) = \prod_{k=2}^\infty \widetilde{\mu}_k^{n-1} = \prod_{k=2}^\infty \left(1 - \frac{\kappa r^2}{\pi^2 k^2}\right)^{n-1} = \prod_{k=2}^\infty \left(1 - \frac{1}{k^2}\right)^{n-1} = 2^{1-n},$$

because the product "telescopes", that is

$$\prod_{k=2}^\infty \left(1 - \frac{1}{k^2}\right) = \lim_{N\to\infty}\left(\prod_{k=2}^N \frac{k-1}{k}\right)\left(\prod_{k=2}^N \frac{k+1}{k}\right) = \lim_{N\to\infty} \frac{1}{N}\frac{N+1}{2} = \frac{1}{2}.$$

Therefore, by Thm. 3.2.8, we have

$$\begin{aligned}\Phi_0(x, y) &= \int_{\Gamma^{\min}_{xy}} 2^{(n-1)/2}\mathrm{d}^{H^1}\gamma = 2^{(n-1)/2}\int_{S^{n-1}_R} \det\big(d\rho|_\theta\big)\mathrm{d}\theta \\ &= \pi^{n-1}R^{n-1}\mathrm{vol}(S^{n-1}) = 2\frac{\pi^{3n/2-1}R^{n-1}}{\Gamma(n/2)}.\end{aligned}$$

This result can also be found in [Hsu02, Example 5.3.3].

Remark 3.2.15. Using Prop. 3.1.21, these results can be extended to the case that M has a boundary, in the case that the smoothness Assumption 2.3.7 is satisfied.

To finish the section, it is left to prove the Lemmas 3.2.9 and 3.2.10.

Proof (of Lemma 3.2.9). Identify the tangent spaces $T_{\gamma(s)}M$ with $T_{\gamma(0)}M$ using parallel transport along γ. Let $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = 1\}$, $N \geq 2$, be a partition of the interval $[0,1]$ and write for abbreviation $\Delta_j := \Delta_j\tau = \tau_j - \tau_{j-1}$.
Step 1. Define the subspace $W_\tau \subset T_\gamma H_{xy}(M) = H_0^1([0,1], \gamma^*TM)$ by

$$W_\tau := \big\{X \in T_\gamma H_{xy}(M) \mid X \text{ smooth on } (\tau_{j-1}, \tau_j) \text{ with } \nabla_s^2 X(s) = 0\big\}. \tag{3.2.19}$$

This means that elements $X \in W_\tau$ are piecewise linear, i.e. they have the form

$$X(\tau_{j-1} + s) = \left(1 - \frac{s}{\Delta_j}\right) v_{j-1} + \frac{s}{\Delta_j} v_j, \qquad v_j := X(\tau_j), \quad 0 \leq s \leq \Delta_j. \tag{3.2.20}$$

Define

$$\Psi_\tau : \bigoplus_{j=1}^N T_{\gamma(\tau_j)}M \longrightarrow W_\tau, \qquad (v_1, \dots, v_{N-1}) \longmapsto X_v,$$

where X_v is the unique element in W_τ with $X_v(\tau_j) = v_j$ (where we set $v_0 = v_N = 0$). Then by the explicit form (3.2.20) of $X_v = \Psi_\tau(v_1, \dots, v_{N-1})$, $X_w = \Psi_\tau(w_1, \dots, w_{N-1})$, we have (using the convention $v_0 = v_N = w_0 = w_N = 0$)

$$\begin{aligned}
\big(X_v, X_w\big)_{H^1} &= \sum_{j=1}^N \int_{\tau_{j-1}}^{\tau_j} \left\langle \frac{1}{\Delta_j}(v_j - v_{j-1}), \frac{1}{\Delta_j}(w_j - w_{j-1}) \right\rangle \mathrm{d}s \\
&= \sum_{j=1}^N \frac{1}{\Delta_j} \big(\langle v_j, w_j\rangle + \langle v_{j-1}, w_{j-1}\rangle - \langle v_j, w_{j-1}\rangle - \langle v_{j-1}, w_j\rangle\big) \\
&= \left\langle \begin{pmatrix} v_1 \\ \vdots \\ v_{N-1} \end{pmatrix}, D_\tau \begin{pmatrix} w_1 \\ \vdots \\ w_{N-1} \end{pmatrix} \right\rangle
\end{aligned}$$

where D_τ is the $n(N-1) \times n(N-1)$ matrix

$$D_\tau := \begin{pmatrix} \left(\frac{1}{\Delta_1} + \frac{1}{\Delta_2}\right)\mathrm{id} & -\frac{1}{\Delta_2}\mathrm{id} & & \\ -\frac{1}{\Delta_2}\mathrm{id} & \left(\frac{1}{\Delta_2} + \frac{1}{\Delta_3}\right)\mathrm{id} & \ddots & \\ & \ddots & \ddots & -\frac{1}{\Delta_{N-1}}\mathrm{id} \\ & & -\frac{1}{\Delta_{N-1}}\mathrm{id} & \left(\frac{1}{\Delta_{N-1}} + \frac{1}{\Delta_N}\right)\mathrm{id} \end{pmatrix}.$$

Per induction, one shows that $\det(D_\tau) = \prod_{j=1}^N \Delta_j^{-n}$. As a subspace of $H_0^1([0,1], \gamma^*TM)$, W_τ carries the induced H^1 scalar product. With respect to this scalar product, we obtain that

$$|\det(\Psi_\tau)| = \det(\Psi_\tau^*\Psi_\tau)^{1/2} = \det(D_\tau)^{1/2} = \prod_{j=1}^N \Delta_j^{-n/2}. \tag{3.2.21}$$

Step 2. Define the operator

$$K_\tau : W_\tau \longrightarrow T_\gamma H_{xy}(M), \qquad X \longmapsto K_\tau X, \tag{3.2.22}$$

where $Y := K_\tau X$ is the unique solution of

$$\begin{cases} -\nabla_s^2 Y(s) + \mathcal{R}_\gamma(s) Y(s) = -\mathcal{R}_\gamma(s) X(s) & \text{for} \quad s \neq \tau_j \\ Y(\tau_j) = 0 & \text{for} \quad j = 1, \dots, N, \end{cases}$$

with $\mathcal{R}_\gamma$ the curvature endomorphism along γ considered in Section 3.2.1. This problem indeed has a unique solution, because $Y = K_\tau X$ is just patched together from the unique solutions of Dirichlet problems on each subinterval $[\tau_{j-1}, \tau_j]$. Namely, the self-adjoint operator $-\nabla_s^2 + \mathcal{R}_\gamma$ with Dirichlet boundary conditions is invertible on each of the subintervals $[\tau_{j-1}, \tau_j]$, because it has trivial kernel: Elements in the kernel are Jacobi fields with vanishing endpoints. A non-zero element in the kernel would therefore imply that $\gamma(\tau_{j-1})$ and $\gamma(\tau_j)$ are conjugate, which cannot happen for $N \geq 2$ as γ is a minimizing geodesic. Because the right hand side is smooth on these subintervals, Y is as well. For $X \in W_\tau$, set $\widetilde{X} := X + K_\tau X := X + Y$. Then $\widetilde{X} \in T_\gamma H_{xy;\tau}(M)$, because for $s \neq \tau_j$, we have

$$\nabla_s^2 \widetilde{X} = \underbrace{\nabla_s^2 X(s)}_{=0} + \nabla_s^2 Y(s) = \mathcal{R}_\gamma(s) Y(s) + \mathcal{R}_\gamma(s) X(s) = \mathcal{R}_\gamma(s) \widetilde{X}(s).$$

Thus $\widetilde{X}$ is a piecewise Jacobi field, i.e. an element of $T_\gamma H_{xy;\tau}(M)$. Notice that

$$\mathrm{id} + K_\tau : W_\tau \longrightarrow T_\gamma H_{xy;\tau}(M)$$

is an isomorphism of vector spaces, because the dimensions coincide and it is injective: If $X = -K_\tau X$, for $X \in W_\tau$, then in particular $X(\tau_j) = -(K_\tau X)(\tau_j) = 0$ for all j, hence $X = 0$. Furthermore, for vectors $v_j \in T_{\gamma(\tau_j)} M$, $X := (\mathrm{id} + K_\tau)\Psi_\tau(v_1, \dots, v_{N-1})$ is the piece-wise Jacobi field with $X(\tau_j) = v_j$. Therefore,

$$\big(d\mathrm{ev}_\tau|_\gamma\big)^{-1} = (\mathrm{id} + K_\tau)\Psi_\tau. \tag{3.2.23}$$

Extend K_τ to a bounded linear operator on $T_\gamma H_{xy}(M)$ through extension by zero on the orthogonal complement $W_\tau^\perp$. Denote by i_τ, p_τ and ι_τ, π_τ the inclusions and orthogonal projections corresponding to the subspaces W_τ respectively $T_\gamma H_{xy;\tau}(M)$ of $T_\gamma H_{xy}(M)$. Using (3.2.23) and (3.2.21), we obtain

$$\big|\det\big(d\mathrm{ev}_\tau|_\gamma\big)\big| \prod_{j=1}^N \Delta_j^{-n/2} = \big|\det\big(\pi_\tau(\mathrm{id} + K_\tau) i_\tau\big)\big|^{-1} \frac{\prod_{j=1}^N \Delta_j^{-n/2}}{\big|\det(\Psi_\tau)\big|} = \big|\det\big(\pi_\tau(\mathrm{id} + K_\tau) i_\tau\big)\big|^{-1}$$

Furthermore,

$$\begin{aligned} \big|\det\big(\pi_\tau(\mathrm{id} + K_\tau) i_\tau\big)\big| &= \det\big(p_\tau(\mathrm{id} + K_\tau)^* \iota_\tau \pi_\tau (\mathrm{id} + K_\tau) i_\tau\big)^{1/2} \\ &= \det\big(p_\tau(\mathrm{id} + K_\tau)^* (\mathrm{id} + K_\tau) i_\tau\big)^{1/2}, \end{aligned}$$

where in the last step we used that the image of $\mathrm{id} + K_\tau$ is contained in $T_\gamma H_{xy;\tau}(M)$ so that the projection and inclusion in the middle can be left out. For $X_1, X_2 \in W_\tau$, let $Y_1 := K_\tau X_1$, $Y_2 := K_\tau X_2$ and calculate

$$(X_1, K_\tau X_2)_{H^1} = (X_1, Y_2)_{H^1} = \sum_{j=1}^{N} \int_{\tau_{j-1}}^{\tau_j} \langle \nabla_s X_1(s), \nabla_s Y_2(s) \rangle \, \mathrm{d}s = 0,$$

which follows from integration by parts since $\nabla_s^2 X_1 = 0$ for $s \in [\tau_{j-1}, \tau_j]$ and $Y_2(\tau_j) = Y_2(\tau_{j-1}) = 0$ for all $j = 1, \dots, N$. This shows $K_\tau X \subset W_\tau^\perp$. Put together, we get for $X_1, X_2 \in W_\tau$ that

$$\begin{aligned}\big(X_1, (\mathrm{id}{+}K_\tau)^*(\mathrm{id} + K_\tau)X_2\big)_{H^1} &= (X_1, X_2)_{H^1} + \underbrace{(X_1, K_\tau X_2)_{H^1}}_{=0} + \underbrace{(K_\tau X_1, X_2)_{H^1}}_{=0} + (K_\tau X_1, K_\tau X_2)_{H^1} \\ &= \big(X_1, (\mathrm{id} + K_\tau^* K_\tau)X_2\big)_{H^1},\end{aligned}$$

i.e. $p_\tau(\mathrm{id} + K_\tau)^*(\mathrm{id} + K_\tau)i_\tau = p_\tau(\mathrm{id} + K_\tau^* K_\tau)i_\tau$, and

$$\det\big(p_\tau(\mathrm{id}{+}K_\tau)^*(\mathrm{id}{+}K_\tau)i_\tau\big)^{1/2} = \det\big(p_\tau(\mathrm{id}{+}K_\tau^*K_\tau)i_\tau\big)^{1/2} = \det\big(\mathrm{id}{+}K_\tau^*K_\tau\big)^{1/2}, \quad (3.2.24)$$

where the last determinant is a Fredholm determinant and the last step uses that $\mathrm{id}{+}K_\tau^* K_\tau$ has block diagonal form with respect to the decomposition $T_\gamma H_{xy}(M) = W_\tau \oplus W_\tau^\perp$. Therefore, with a view on the standard determinant estimate (3.2.14), we are led to estimate $\|K_\tau^* K_\tau\|_1 = \mathrm{tr}(K_\tau^* K_\tau) = \|K_\tau\|_2^2$, the Hilbert-Schmidt norm of K_τ.

Step 3. We need some preliminary considerations. Let $[a, b]$ be any subinterval of $[0, 1]$ and write P for the operator $-\nabla_s^2$ on $L^2([a, b], \gamma^* TM)$ with Dirichlet boundary conditions, as in Section 3.2.1. Suppose that $[a, b] \subsetneq [0, 1]$. Then $P + \mathcal{R}_\gamma$ is an isomorphism from $H_0^m([a, b], \gamma^* TM)$ to $H_0^{m-2}([a, b], \gamma^* TM)$ for each $m \in \mathbb{R}$ (remember that γ is a minimizing geodesic, hence $\gamma|_{[a,b]}$ is unique minimizing, so there are no non-trivial Jacobi fields with vanishing endpoints along $\gamma|_{[a,b]}$, i.e. the kernel of $P + \mathcal{R}_\gamma$ is trivial). We now show that

$$\big\|(P + \mathcal{R}_\gamma)^{-1} X\big\|_{H^1} \leq \frac{(b - a)^2}{\pi^2 - \|\mathcal{R}_\gamma\|(b - a)^2} \|X\|_{H^1}, \qquad (3.2.25)$$

for each $X \in H^1([a, b], \gamma^* TM)$ and any $\gamma \in \Gamma_{xy}^{\min}$, where $\|\mathcal{R}_\gamma\|$ is the operator norm of the operator $X \mapsto \mathcal{R}_\gamma X$ on $H_0^1([0, 1], \gamma^* TM)$. First we have using Lemma 3.2.2 above that

$$\|P^{-1}\mathcal{R}_\gamma X\|_{H^1} \leq \frac{(b - a)^2}{\pi^2} \|\mathcal{R}_\gamma X\|_{H^1} \leq \frac{(b - a)^2}{\pi^2} \|\mathcal{R}_\gamma\| \|X\|_{H^1},$$

since the operator norm of $\mathcal{R}_\gamma$ on $[a, b]$ is less or equal to the operator norm of $\mathcal{R}_\gamma$ on the interval $[0, 1]$. We find for all $X \in H_0^1([a, b], \gamma^* TM)$ that

$$\big\|(\mathrm{id} + P^{-1}\mathcal{R}_\gamma)X\big\|_{H^1} \geq \|X\|_{H^1} - \|P^{-1}\mathcal{R}_\gamma X\|_{H^1} \geq \left(1 - \|\mathcal{R}_\gamma\| \frac{(b - a)^2}{\pi^2}\right) \|X\|_{H^1}^2.$$

Because $\mathrm{id} + P^{-1}\mathcal{R}_\gamma$ is self-adjoint on $H_0^1([a, b], \gamma^* TM)$ as is easy to verify, we obtain for its smallest eigenvalue

$$\mu_{\min} = \inf_{X \neq 0} \frac{\|(\mathrm{id} + P^{-1}\mathcal{R}_\gamma)X\|_{H^1}}{\|X\|_{H^1}} \geq \left(1 - \|\mathcal{R}_\gamma\| \frac{(b - a)^2}{\pi^2}\right).$$

The spectral radius of the inverse $(\mathrm{id} + P^{-1}\mathcal{R}_\gamma)^{-1}$ is equal to $1/\mu_{\min}$. Since $\mathrm{id} + P^{-1}\mathcal{R}_\gamma$ is self-adjoint on $H_0^1([a,b], \gamma^*TM)$ and so is its inverse, the spectral radius equals the operator norm, whence

$$\big\|(\mathrm{id} + P^{-1}\mathcal{R}_\gamma)^{-1}X\big\|_{H^1} \leq \frac{1}{\mu_{\min}}\|X\|_{L^2} \leq \frac{\pi^2}{\pi^2 - \|\mathcal{R}_\gamma\|(b-a)^2}\|X\|_{H^1}$$

Finally, using Lemma 3.2.2 again, we get

$$\begin{aligned}\big\|(P+\mathcal{R}_\gamma)^{-1}X\big\|_{H^1} &= \big\|P^{-1}(\mathrm{id} + P^{-1}\mathcal{R}_\gamma)^{-1}X\big\|_{H^1} \\ &\leq \frac{(b-a)^2}{\pi^2}\big\|(\mathrm{id} + P^{-1}\mathcal{R}_\gamma)^{-1}X\big\|_{H^1} \\ &\leq \frac{(b-a)^2}{\pi^2 - \|\mathcal{R}_\gamma\|(b-a)^2}\|X\|_{H^1},\end{aligned}$$

which is the claim.
Step 4. We finally derive a bound on $\|K_\tau\|_2^2$. For any vector $X \in T_\gamma H_{xy;\tau}(M)$ and any $j = 1, \dots, N$, we have $K_\tau X|_{[\tau_{j-1},\tau_j]} = -(P+\mathcal{R}_\gamma)^{-1}\mathcal{R}_\gamma X|_{[\tau_{j-1},\tau_j]}$, where $(P+\mathcal{R}_\gamma)^{-1}$ is the operator discussed in Step 3 on the interval $[a,b] := [\tau_{j-1}, \tau_j]$.
Let $E_1, E_2, \dots, E_{n(N-1)}$ be an orthonormal basis of W_τ. Using the estimate (3.2.25) from Step 3 on the operator norm of $(P+\mathcal{R}_\gamma)^{-1}$ on $H^1([\tau_{j-1},\tau_j], \gamma^*TM)$, we obtain

$$\begin{aligned}\|K_\tau\|_2^2 &= \sum_{i=1}^{n(N-1)} \|K_\tau E_i\|_{H^1}^2 = \sum_{i=1}^{n(N-1)}\sum_{j=1}^{N}\big\|K_\tau E_i|_{[\tau_{j-1},\tau_j]}\big\|_{H^1}^2 \\ &= \sum_{i=1}^{n(N-1)}\sum_{j=1}^{N}\big\|-(P+\mathcal{R}_\gamma)^{-1}\mathcal{R}_\gamma E_i|_{[\tau_{j-1},\tau_j]}\big\|_{H^1}^2 \\ &\leq \sum_{i=1}^{n(N-1)}\sum_{j=1}^{N}\left(\frac{\Delta_j^2}{\pi^2 - \|\mathcal{R}_\gamma\|\Delta_j^2}\right)^2\big\|\mathcal{R}_\gamma E_i|_{[\tau_{j-1},\tau_j]}\big\|_{H^1}^2 \\ &\leq \sum_{i=1}^{n(N-1)}\left(\frac{|\tau|^2}{\pi^2 - \|\mathcal{R}_\gamma\||\tau|^2}\right)^2\big\|\mathcal{R}_\gamma E_i\big\|_{H^1}^2 \leq n(N-1)\left(\frac{\|\mathcal{R}_\gamma\||\tau|^2}{\pi^2 - \|\mathcal{R}_\gamma\||\tau|^2}\right)^2\end{aligned}$$

We now suppose that $|\tau| \leq C/N$ for some $C > 0$. Suppose additionally the partition τ be so fine that $|\tau| \leq \pi/\sqrt{2\|\mathcal{R}_\gamma\|}$, or equivalently $\pi^2 - \|\mathcal{R}_\gamma\||\tau|^2 \geq \pi^2/2$. By the assumption $|\tau| \leq C/N$, this is the case in particular if $N \geq N_0 := \lceil C\sqrt{2\|\mathcal{R}_\gamma\|}/\pi\rceil$. For such τ, we have

$$\frac{\|\mathcal{R}_\gamma\||\tau|^2}{\pi^2 - \|\mathcal{R}_\gamma\||\tau|} \leq \frac{2\|\mathcal{R}_\gamma\||\tau|^2}{\pi^2} \leq \frac{2\|\mathcal{R}_\gamma\|C^2}{\pi^2 N^2} = \frac{N_0^2}{N^2}$$

and

$$\|K_\tau\|_2^2 \leq n(N-1)\left(\frac{N_0^2}{N^2}\right)^2 \leq nN_0^2\frac{1}{N^3}.$$

With a view on (3.2.24), this concludes the proof using (3.2.14), because the operator norm $\|\mathcal{R}_\gamma\|$ is uniformly bounded for $\gamma \in \Gamma_{xy}^{\min}$. □

Remark 3.2.16. Notice that if M is flat, we have $W_\tau = H_{xy;\tau}(M)$ and the operator K_τ of the above proof is zero. Hence in the flat case, we have

$$\big|\det\big(\mathrm{dev}_\tau|_\gamma\big)\big| \prod_{j=1}^{N} (\Delta_j \tau)^{-n/2} \equiv 1,$$

for each partition $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = 1\}$ of the interval $[0,1]$.

Proof (of Lemma 3.2.10). The proof is divided into two steps.
Step 1. We first show that the union of the spaces W_τ for $\tau \in S$ is dense in the space $H_0^1([0,1],\gamma^*TM)$, where W_τ is the space defined in (3.2.19). Namely, we claim that given a partition $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N\}$, a vector field $X \in H_0^1([0,1],\gamma^*TM)$ is in the orthogonal complement of W_τ if only if $X(\tau_j) = 0$ for all $j = 1,\dots,N-1$. Indeed, for a given $v \in T_{\gamma(\tau_j)}M$, define $Y \in W_\tau$ by

$$Y(s) = \begin{cases} s(1-\tau_j)v & s \le \tau_j \\ (1-s)\tau_j v & s \ge \tau_j, \end{cases}$$

where we identified the spaces $T_{\gamma(s)}M$ by parallel transport along γ. Then integrating by parts and using that $\nabla_s^2 X \equiv 0$ on (τ_{j-1},τ_j) yields

$$(X,Y)_{H^1} = \sum_{j=1}^{N} \int_{\tau_{j-1}}^{\tau_j} \langle \nabla_s X(s), \nabla_s Y(s)\rangle \,\mathrm{d}s = \sum_{j=1}^{N-1} \langle X(\tau_j), Y(\tau_j-) - Y(\tau_j+)\rangle = \langle X(\tau_j), v\rangle \,.$$

This proves the claim, since this scalar product is zero for all v chosen this way if and only if $X(\tau_j) = 0$ for all j.
Now suppose that $X \in H_{xy;\tau}(M)$ is in the orthogonal complement of W_τ for all $\tau \in S$. Then by the observation before, we obtain that necessarily $X(s) = 0$ for all $s \in [0,1]$ for which there exists a partition $\tau \in S$ with $s \in \tau$. Because of the condition on the set S, the set of such s in dense in $[0,1]$, so from continuity follows $X \equiv 0$. Therefore the union of all W_τ, $\tau \in S$ must be a dense subset.
Step 2. Suppose that $W_\tau \neq H_{xy;\tau}(M)$, i.e. $\mathcal{R}_\gamma \neq 0$ (otherwise, we are already done with the proof). Let $Y \in W_\tau$. Then if K_τ is the operator defined in (3.2.22), then $Y + K_\tau Y \in T_\gamma H_{xy;\tau}(M)$, as seen in Step 2 of the proof of Lemma 3.2.9 above. By (3.2.25), we have

$$\begin{aligned} \|K_\tau Y\|_{H^1}^2 &= \sum_{j=1}^{N} \big\| -(P+\mathcal{R}_\gamma)^{-1}\mathcal{R}_\gamma Y|_{\tau_{j-1},\tau_j}\big\|_{H^1}^2 \le \sum_{j=1}^{N} \left(\frac{\Delta_j^2}{\pi^2 - \|\mathcal{R}_\gamma\|\Delta_j^2}\right)^2 \|\mathcal{R}_\gamma Y|_{\tau_{j-1},\tau_j}\|_{H^1}^2 \\ &\le |\tau|^4 \frac{4}{\pi^4}\|\mathcal{R}_\gamma Y\|_{H^1}^2 \le |\tau|^4 \frac{4}{\pi^4}\|\mathcal{R}_\gamma\|^2 \|Y\|_{H^1}^2 \end{aligned}$$

whenever $\pi^2 - \|\mathcal{R}_\gamma\||\tau|^2 \le \pi^2/2$, or equivalently $|\tau| \le \pi/\sqrt{2\|\mathcal{R}_\gamma\|}$ (here $\|\mathcal{R}_\gamma\|$ is the operator norm of the operator $X \mapsto \mathcal{R}_\gamma X$ on $H_0^1([0,1],\gamma^*TM)$. We conclude that the operator norm of the operators K_τ for $|\tau|$ small enough satisfies the bound $\|K_\tau\| \le C|\tau|^2$ with a constant $C > 0$ independent of τ. Hence

$$\begin{aligned} \big\|X - (Y + K_\tau Y)\big\|_{H^1} &\le \|X - Y\|_{H^1} + \|K_\tau Y\|_{H^1} \le \|X - Y\|_{H^1} + \|K_\tau\|\|Y\|_{H^1} \\ &\le \|X - Y\|_{H^1} + C|\tau|^2\big(\|X - Y\|_{H^1} + \|X\|_{H^1}\big). \end{aligned}$$

Now given $\varepsilon > 0$, choose $\delta > 0$ such that

$$\delta^2 < \min\left\{\frac{\varepsilon}{C\big(\varepsilon + 2\|X\|_{H^1}\big)}, \frac{\pi^2}{2\|\mathcal{R}_\gamma\|}\right\}$$

and let $S' \subset S$ be the set containing all partitions $\tau \in S$ with $|\tau| \leq \delta$. Then S' still has the property from the lemma, so by Step 1, for some $\tau \in S'$, we find $Y \in W_\tau$ such that $\|X - Y\|_{H^1} < \varepsilon/2$. Then by the choice of δ, if $|\tau| \leq \delta$, we have $\big\|X - (Y + K_\tau Y)\big\|_{H^1} \leq \varepsilon$. Because ε was arbitrary and $Y + K_\tau Y \in H_{xy;\tau}(M)$, $\tau \in S$, this shows that the union of all $H_{xy;\tau}(M)$, $\tau \in S$ is dense in $H_0^1([0,1], \gamma^*TM)$. □

3.2.3 Zeta Determinants and the Gelfand-Yaglom Theorem

In the section above, we saw that in the case that the set $\Gamma_{xy}^{\min}$ of minimizing geodesics between the points x, y is a non-degenerate submanifold of $H_{xy}(M)$ (with respect to the energy functional), we have

$$(4\pi t)^{-n/2} \fint_{H_{xy}(M)} e^{-E(\gamma)/2t}[\gamma\|_0^1]^{-1}\mathrm{d}^{H^1}\gamma \overset{\text{formally}}{\sim} (4\pi t)^{-n/2-k/2}\int_{\Gamma_{xy}^{\min}} \frac{e^{-E(\gamma)/2t}[\gamma\|_0^1]^{-1}}{\det\big(\nabla^2 E|_{N_\gamma\Gamma_{xy}^{\min}}\big)^{1/2}}\,\mathrm{d}^{H^1}\gamma,$$

which is exactly the result expected when taking a formal Laplace expansion of the Laplace integral, as in Thm. 3.1.2 (more precisely: we saw that the heat kernel, which is formally represented by the path integral on the left hand side, actually behaves asymptotically as shown on the right hand side).
The expression on the right hand side above depends on the choice of a Riemannian metric on the manifold $H_{xy}(M)$ in two ways: First, because we integrate over the submanifold $\Gamma_{xy}^{\min}$ using the Riemannian volume density of the induced metric. Secondly, because we take the determinant of the bilinear form $\nabla^2 E|_{N_\gamma\Gamma_{xy}^{\min}}$ using the metric on $N_\gamma\Gamma_{xy}^{\min}$ (because to calculate the determinant of a bilinear form, we need a metric). In both cases, the H^1 metric (1.2.5) turned out to be the correct choice.

However, there is yet another possible choice for the determinant of an operator on an infinite-dimensional space: the zeta determinant, which is defined for a certain class of unbounded operators on a Hilbert space. This approach is often used in physics to assign finite values to otherwise ill-defined path integrals, see e.g. [Haw77] or [Wit99]. Because we have $\nabla^2 E|_\gamma[X, Y] = ((-\nabla_s^2 + \mathcal{R}_\gamma)X, Y)_{L^2}$ (see (3.2.9)), one could get the idea to replace the determinant of $\nabla^2 E|_\gamma$ by the zeta determinant of the Jacobi-operator $-\nabla_s^2 + \mathcal{R}_\gamma$.
This determinant does not depend on the choice of a Sobolev metric on the path spaces. Instead, it only depends on the eigenvalues of $-\nabla_s^2 + \mathcal{R}_\gamma$, considered as an unbounded operator on the Hilbert space $L^2([0,1], \gamma^*TM)$. Since the H^1 metric on $H_{xy}(M)$ does no longer play a role then, it seems that one should also equip $\Gamma_{xy}^{\min}$ with another metric when performing the integral. Here the L^2 metric comes into play.

It is a "well-known fact" in physics that zeta determinants only give the value of path integrals "up to an arbitrary multiplicative constant", by which is usually meant that one can only calculate the *quotient* of two path integrals, which is then given by the quotient of the respective zeta determinants. In this section, we will indeed see that in some sense, the quotient of the zeta-regularization of the path integral for the heat kernel on a Riemannian manifold by the same path integral for flat space is indeed given by the quotient of the respective zeta determinants.

For an elliptic positive self-adjoint pseudo-differential operator P of order $d > 0$, acting on an m-dimensional compact manifold Σ, the *zeta function* ζ_P is defined by

$$\zeta_P(z) := \sum_{\lambda \neq 0} \lambda^{-z}, \tag{3.2.26}$$

where the sum runs over all non-zero eigenvalues λ of P. Here, Σ may have a boundary, in which case we assume that P is endowed with appropriate boundary conditions. This sum converges for $\mathrm{Re}(z) > m/d$; however, one can check that ζ_P possesses a meromorphic extension to all of $\mathbb{C}$ and that zero is not a pole [Gil95, Section 1.12]. Therefore, one can define the *zeta-regularized determinant*

$$\det\nolimits_\zeta(P) := e^{-\zeta_P'(0)}.$$

If P actually has zero modes that were left of in the sum (3.2.26), it is conventional to write $\det'_\zeta(P)$ instead. The definition is motivated by the fact that if one (formally!) plugs the series (3.2.26) into the right hand side of this definition (which is not possible since one cannot evaluate it at zero), one obtains

$$e^{-\zeta_P'(0)} \overset{\text{formally}}{=} \prod_{\lambda \neq 0} \lambda,$$

the product of the non-zero eigenvalues, which of course diverges; the zeta determinant "magically" assigns a finite value to this product.

Example 3.2.17 (Dirichlet-Laplacian along a Geodesic). Let γ be a smooth path in an n-dimensional Riemannian manifold M parametrized by $[0, t]$. Already in Section 3.2.1, we found the eigenvalues of the operator $P = -\nabla_s^2$ with Dirichlet boundary conditions on the space $L^2([0,t], \gamma^*TM)$ to be the numbers $\lambda_k = \pi^2 k^2/t^2$, each of multiplicity n. Hence for $\mathrm{Re}\, z > 1/2$, we have

$$\zeta_P(z) = n \sum_{k=1}^{\infty} \left(\frac{\pi^2 k^2}{t^2}\right)^{-z} = n \frac{t^{2z}}{\pi^{2z}} \sum_{k=1}^{\infty} k^{-2z} = n \frac{t^{2z}}{\pi^{2z}} \zeta(2z),$$

where ζ without subscript denotes the usual Riemann zeta function. Therefore,

$$\zeta_P'(0) = 2n\big(\log(t) - \log(\pi)\big)\zeta(0) + 2n\zeta'(0) = -n\log(2t)$$

as it is well known that $\zeta(0) = -1/2$ and $\zeta'(0) = -\log(2\pi)/2$ [Son94]. We obtain

$$\det\nolimits_\zeta(-\nabla_s^2) = e^{-\zeta_P'(0)} = (2t)^n \tag{3.2.27}$$

for the zeta determinant.

More generally, the zeta determinant can be defined for a wide class of (necessarily unbounded) closed operators with discrete spectrum on an abstract Hilbert space H, called *zeta-admissible* (for the definition, see [Sco02, Section 2]). That an operator is zeta-admissible essentially means that it has a well-defined zeta function which does not have a pole at zero. We will not need the exact definition here (which is somewhat involved); we will only need that Laplace type operators P on intervals with Dirichlet boundary conditions are zeta-admissible, as well as their positive powers. Such operators P are well-known to be zeta-admissible; this can be shown e.g. using the heat trace expansion Thm. 3.1.30 as in [Gil95, Section 10]. For the operators P^m, $m > 0$, one immediately sees that $\zeta_{P^s}(z) = \zeta_P(mz)$, hence $\det_\zeta(P^m) = \det_\zeta(P)^m$.
The following result then generates many more examples.

Proposition 3.2.18 (Multiplicativity). [Sco02, Thm. 2.18] *Let $\mathcal{H}$ be a Hilbert space, let P be a closed and invertible operator on $\mathcal{H}$ with positive spectrum and let $T := \mathrm{id} + W$ with W trace-class on $\mathcal{H}$. If P is zeta-admissible, then so are PT and TP and we have*

$$\det_\zeta(PT) = \det_\zeta(TP) = \det_\zeta(P)\det(T),$$

where $\det(T)$ *denotes the usual Fredholm determinant.*

Remark 3.2.19. We generally have $\det_\zeta(AB) \neq \det_\zeta(A)\det_\zeta(B)$. Instead, the above product rule holds.

Corollary 3.2.20 (Zeta Relativity). *Let P_1, P_2 be positive self-adjoint Laplace type operators with Dirichlet boundary conditions on the interval $[0,t]$, acting on the bundle γ^*TM, where γ is a smooth path in some Riemannian manifold M. Suppose that the difference $P_1 - P_2$ is of order zero and that P_1 and P_2 have trivial kernels. Then $P_1^{-1}P_2$ is well defined and determinant-class on $L^2([0,t],\gamma^*TM)$ and we have*

$$\det(P_1^{-1}P_2) = \frac{\det_\zeta(P_2)}{\det_\zeta(P_1)},$$

where the left hand side is the usual Fredholm determinant.

Proof. Because P_1 has trivial kernel, its inverse P_1^{-1} is well defined by spectral calculus, and $P_1^{-1} : L^2([0,t],\gamma^*TM) \longrightarrow H_0^2([0,t],\gamma^*TM)$ is a bounded operator. By Lemma 3.2.1, the inclusion $H_0^2([0,t],\gamma^*TM) \longrightarrow L^2([0,t],\gamma^*TM)$ is nuclear; hence the operator $P_1^{-1} : L^2([0,t],\gamma^*TM) \longrightarrow L^2([0,t],\gamma^*TM)$ is trace-class, because it can be written as the composition of a bounded operator and a nuclear operator.
Write $P_2 = P_1 + V$ for an endomorphism field $V \in C^\infty([0,t],\gamma^*TM)$. Then

$$P_1^{-1}P_2 = P_1^{-1}(P_1 + V) = \mathrm{id} + P_1^{-1}V$$

is determinant-class, because $P_1^{-1}V$ is trace-class. We can now apply Prop. 3.2.18 on the Hilbert space $L^2([0,t],\mathbb{R}^n)$ with $P = P_1$ and $T = P_1^{-1}P_2$ to obtain the required determinant identity. □

Similarly, the following is true.

Proposition 3.2.21. *Let M be a Riemannian manifold and let $(x,y) \in M \bowtie M$. Then we have*

$$\det\bigl(\nabla^2 E|_{\gamma_{xy;t}}\bigr) = \frac{\det_\zeta(-\nabla_s^2 + \mathcal{R}_{\gamma_{xy;t}})}{\det_\zeta(-\nabla_s^2)},$$

where $\gamma_{xy;t}$ is the unique minimizing geodesic travelling from x to y in time t and $-\nabla_s^2 + \mathcal{R}_{\gamma_{xy;t}}$ is the Jacobi operator *as in Section 3.2.1. Both operators on the right hand side carry Dirichlet boundary conditions.*

Combining this with Corollary 3.2.11 and Example 3.2.17, we may express the Jacobian of the exponential map as the zeta determinant of the Jacobi operator.

Corollary 3.2.22. *Let M be a Riemannian manifold and $(x,y) \in M \bowtie M$. Then for any $t > 0$,*

$$J(x,y) = (2t)^{-n} \det_\zeta(-\nabla_s^2 + \mathcal{R}_{\gamma_{xy;t}}),$$

where $\gamma_{xy;t}$ is the shortest geodesic connecting x to y in time t and $-\nabla_s^2 + \mathcal{R}_\gamma$ is the Jacobi operator with Dirichlet boundary conditions on $L^2([0,t], \gamma^*TM)$. Here $J(x,y)$ denotes the Jacobian of the exponential map, as in Remark 2.1.2.

Proof (of Prop. 3.2.21). Write $P := -\nabla_s^2$ and $\gamma := \gamma_{xy;t}$ for abbreviation. By (3.2.10), we have

$$\nabla^2 E|_\gamma[X,Y] = \bigl(X, P^{-1}(P + \mathcal{R}_\gamma)Y\bigr)_{H^1}.$$

Set $T := P^{-1}(P + \mathcal{R}_\gamma)$. Because $P^{-1/2} : L^2([0,t], \gamma^*TM) \longrightarrow H_0^1([0,t], \gamma^*TM)$ is an isometry, we have

$$\det\bigl(\nabla^2 E|_\gamma\bigr) = \det{}^{H^1}\bigl(T\bigr) = \det{}^{L^2}\bigl(P^{1/2} T P^{-1/2}\bigr) = \det{}^{L^2}\bigl(P^{-1/2}(P + \mathcal{R}_\gamma)P^{-1/2}\bigr).$$

The operator $P^{-1/2}(P + \mathcal{R}_\gamma)P^{-1/2}$ is indeed determinant-class, since

$$P^{-1/2}(P + \mathcal{R}_\gamma)P^{-1/2} = \mathrm{id} + P^{-1/2}\mathcal{R}_\gamma P^{-1/2} =: \mathrm{id} + \widetilde{W},$$

where $\widetilde{W}$ is the composition of two Hilbert-Schmidt operators and a bounded operator, hence trace-class. Set $W := P^{-1}\mathcal{R}_\gamma$. Then by Prop. 3.2.18,

$$\begin{aligned}\det{}^{L^2}\bigl(\mathrm{id} + \widetilde{W}\bigr) \det_\zeta\bigl(P^{1/2}\bigr) &= \det_\zeta\bigl((\mathrm{id} + \widetilde{W})P^{1/2}\bigr) = \det_\zeta\bigl(P^{1/2}(\mathrm{id} + W)\bigr)\\ &= \det_\zeta\bigl(P^{1/2}\bigr) \det{}^{L^2}\bigl(\mathrm{id} + W\bigr),\end{aligned}$$

since $P^{1/2}$ is zeta-admissible. This shows that the L^2-determinant of $\mathrm{id} + \widetilde{W}$ is equal to the L^2-determinant of $\mathrm{id} + W = P^{-1}(P + \mathcal{R}_\gamma)$ (the latter now being an operator on $L^2([0,t], \gamma^*TM)$!). The result now follows from Corollary 3.2.20. □

The quotient of two zeta determinants of one-dimensional operators can be calculated using the Gel'fand-Yaglom theorem below.

Theorem 3.2.23 (Gel'fand-Yaglom). *Let $V_i \in C^\infty([0,t], \mathbb{R}^{n\times n})$, $i = 1, 2$ be functions with values in symmetric matrices and consider the differential operators*

$$P_i := -\frac{\mathrm{d}^2}{\mathrm{d}s^2} + V_i.$$

Assume that all eigenvalues of P_1 and P_2 are positive. Then we have

$$\frac{\det_\zeta(P_2)}{\det_\zeta(P_1)} = \frac{\det\big(J_2(t)\big)}{\det\big(J_1(t)\big)},$$

where the $J_i(s)$ are the unique matrix-valued solutions of

$$J_i''(s) = V_i(s)J_i(s), \qquad J_i(0) = 0, \quad J_i'(0) = \mathrm{id}.$$

It seems that the name of the theorem stems from an older result by Gel'fand and Yaglom [GY60], who express the expectation value of certain Wiener functionals as the solution to an ordinary differential equation, but without mentioning zeta determinants. A rigorous proof of Thm. 3.2.23 can be found in [Kir10] or [KM03] for the scalar case (i.e. $m = 1$), using contour integrals. As demonstrated below, Thm. 3.2.23 combined with Prop. 3.2.21 enables a different proof of the identity

$$\det\big(\nabla^2 E|_{\gamma_{xy}}\big) = J(x, y)$$

that gets away without having to calculate the messy term $\Upsilon_{\tau,\nu}(0,\gamma)$. However, this works only in the non-degenerate case. Furthermore, it turns out that the results obtained with our methods (Corollary 3.2.11 and 3.2.21) suffice to prove Thm. 3.2.23.

Proof (of Corollary 3.2.11, using Thm. 3.2.23). The vector bundle $\gamma_{xy}^* TM$ over $[0, 1]$ has a canonical trivialization using parallel transport along γ_{xy}, so that Thm. 3.2.23 is applicable. In this local trivialization, set $V_1(s) \equiv 0$ and $V_2(s) = \mathcal{R}_{\gamma_{xy}}(s)$, the Jacobi endomorphism (3.2.8) along γ_{xy}. Then use Thm. 3.2.23 with $P_1 = -\nabla_s^2$ and $P_2 = -\nabla_s^2 + \mathcal{R}_{\gamma_{xy}}$, the Jacobi operator. Clearly, P_1 has only positive eigenvalues, and since $(x, y) \in M \bowtie M$, P_2 has only positive eigenvalues as well (compare Thm. 15.1 in [Mil63]).
Now $J_1(s) = s\,\mathrm{id}$ so that $\det(J_1(1)) = 1$. On the other hand, in the trivialization, the columns $v_i(s)$ of $J_2(s)$ are Jacobi fields along γ_{xy} with initial conditions $v_i(0) = 0$, $v_i'(0) = e_i$ (with $e_1, \dots, e_n$ the standard basis in $\mathbb{R}^n$). It is a well-known fact from Riemannian geometry that

$$v_i(s) = s\, d\exp_x|_{s\dot\gamma_{xy}(0)} e_i, \qquad i = 1, \dots, n,$$

see Corollary 1.12.5 in [Kli95] or Thm. II.7.1 in [Cha06]. We obtain $\det(J_2(1)) = J(x, y)$, the Jacobian determinant of the exponential map. Therefore,

$$\det\big(\nabla^2 E|_{\gamma_{xy}}\big) = \frac{\det_\zeta(-\nabla_s^2 + \mathcal{R}_{\gamma_{xy}})}{\det_\zeta(-\nabla_s^2)} = \frac{\det\big(J_2(1)\big)}{\det\big(J_1(1)\big)} = \frac{J(x, y)}{1},$$

where we first used Prop. 3.2.21 and then Thm. 3.2.23. $\square$

Proof (of Thm. 3.2.23). Since we only calculate the ratio, we may assume $V_1 \equiv 0$. Now given a smooth function $V := V_2$ with values in symmetric $(n \times n)$-matrices, define on $M = \mathbb{R} \times \mathbb{R}^n$ (equipped with coordinates $s, x^1, \ldots, x^n$) a Riemannian metric as follows. Choose neighborhoods U and V of $[0,t] \times \{0\}$ in M such that $\overline{U} \subset V$. On U set

$$g_{ss}(s,x) = 1 + V_{ij}(s)x^i x^j, \qquad g_{sj}(s,x) = 0, \qquad g_{ij}(s,x) = \delta_{ij},$$

where $1 \leq i,j \leq n$ and $V_{ij}(s)$ are the entries of $V(s)$; on the complement on V, set $g_{ss} = 1$, $g_{sj} = 0$, $g_{ij} = \delta_{ij}$; on $V \setminus U$, choose a smooth interpolation between the two metrics. One can choose the open sets and the interpolation in such a way that the resulting metric is non-degenerate; then M becomes a complete Riemannian manifold.
The curve $\gamma(s) := (s, 0, \ldots, 0)$ is a geodesic from $x := (0, \ldots, 0)$ to $y := (t, 0, \ldots, 0)$, because all Christoffel symbols vanish at points in $[0,t] \times \{0\}$, as is easy to calculate. It is the unique shortest geodesic between x and y if and only if the Jacobi operator $-\nabla_s^2 + \mathcal{R}_\gamma$ on $[0,t]$ has only positive eigenvalues (see [Mil63, Thm 15.1]), which we assume from now on. On the other hand, one can easily compute that the Jacobi endomorphism (3.2.8) is explicitly given by

$$\mathcal{R}_\gamma(s) = \begin{pmatrix} 1 & 0 \\ 0 & V(s) \end{pmatrix}, \tag{3.2.28}$$

so that the differential of the exponential map is given by

$$d\exp_x|_{s\dot{\gamma}(0)} = \frac{1}{s}\begin{pmatrix} 1 & 0 \\ 0 & J_2(s) \end{pmatrix},$$

where $J_2(s)$ is the unique matrix solution of

$$J_2{}''(s) = V(s)J_2(s), \qquad\qquad J_2(0) = 0, \quad J_2'(0) = \mathrm{id}.$$

The shortest geodesic travelling from x to y in time one, on the other hand, is given by $\gamma_{xy}(s) = \gamma_{xy;t}(st)$. Hence

$$J(x,y) = \det\bigl(d\exp_x|_{\dot{\gamma}_{xy}(0)}\bigr) = \det\bigl(d\exp_x|_{t\dot{\gamma}_{xy;t}(0)}\bigr) = \frac{\det\bigl(J_2(t)\bigr)}{t^{n+1}} = \frac{\det\bigl(J_2(t)\bigr)}{\det\bigl(J_1(t)\bigr)},$$

where $J_1 = t\,\mathrm{id}$ is the matrix solution of the equation $J_1''(t) = 0$ with initial conditions $J_1(0) = 0$, $J_1'(0) = \mathrm{id}$. By Prop. 3.2.21 and Corollary 3.2.11, we therefore have

$$\frac{\det_\zeta(-\nabla_s^2 + \mathcal{R}_{\gamma_{xy;t}})}{\det_\zeta(-\nabla_s^2)} = \det\bigl(\nabla^2 E|_{\gamma_{xy;t}}\bigr) = \det\bigl(\nabla^2 E|_{\gamma_{xy}}\bigr) = J(x,y) = \frac{\det\bigl(J_2(t)\bigr)}{\det\bigl(J_1(t)\bigr)},$$

where we also used that $\det(\nabla^2 E|_\gamma)$ does not depend on t, as seen in the proof of Corollary 3.2.12. Finally, because of (3.2.28), the bundle separates into the direction tangent to $\dot{\gamma}_{xy;t}$ and the orthogonal directions, so we obtain

$$\frac{\det\bigl(J_2(t)\bigr)}{\det\bigl(J_1(t)\bigr)} = \frac{\det_\zeta(-\nabla_s^2 + \mathcal{R}_{\gamma_{xy;t}})}{\det_\zeta(-\nabla_s^2)} = \frac{\det_\zeta(P_2)\det_\zeta(-\partial_s^2)}{\det_\zeta(P_1)\det_\zeta(-\partial_s^2)} = \frac{\det_\zeta(P_2)}{\det_\zeta(P_1)}.$$

This finishes the proof of Thm. 3.2.23. $\square$

Remark 3.2.24. Of course, in the formulation of Thm. 3.2.23, one could use the Fredholm determinant of $P_1^{-1}P_2$ instead of the quotient of the zeta determinants. This way, one would get away without having to use Prop. 3.2.21. That is, Thm. 3.2.23 can also be written as a theorem about usual Fredholm determinants.

Finally, we formulate the lowest order asymptotics of the heat kernel of a Laplace type operator L using the zeta determinant of the Jacobi operator.

Theorem 3.2.25 (Lowest Order Term, L^2 picture). *Let L be a self-adjoint Laplace type operator, acting on sections of a metric vector bundle $\mathcal{V}$ over a closed n-dimensional Riemannian manifold M. For $x, y \in M$, suppose the set $\Gamma_{xy}^{\min}$ is a k-dimensional non-degenerate submanifold of $H_{xy}(M)$ (with respect to the energy functional). Then the lowest order term of the heat kernel expansion of Thm. 3.1.12 is given by*

$$\Phi_0(x,y) = \lim_{t\to 0}(4\pi t)^{k/2}\frac{p_t^L(x,y)}{\mathrm{e}_t(x,y)} = 2^{n/2}\int_{\Gamma_{xy}^{\min}}\frac{[\gamma\|_0^1]^{-1}}{\det_\zeta'(-\nabla_s^2+\mathcal{R}_\gamma)^{1/2}}d^{L^2}\gamma,$$

where $[\gamma\|_0^1]$ denotes the parallel transport along γ with respect to the connection ∇ determined by L as in Lemma 1.1.2 and we integrate with respect to the Riemannian volume measure corresponding to the L^2 metric (1.2.11) *on $\Gamma_{xy}^{\min}$.*

Remark 3.2.26. Put into the form analogous to (3.2.15), Thm. 3.2.25 gives that

$$p_t^L(x,y) \;\sim\; (4\pi t)^{-n/2-k/2}\int_{\Gamma_{xy}^{\min}} e^{-E(\gamma)/2t}\frac{2^{n/2}[\gamma\|_0^1]^{-1}}{\det_\zeta'(-\nabla_s^2+\mathcal{R}_\gamma)^{1/2}}d^{L^2}\gamma, \tag{3.2.29}$$

meaning that the quotient of the two sides converges to one as $t \to 0$.

Because $2^{n/2} = \det_\zeta(-\nabla_s^2)$ by Example 3.2.17, we obtain in the particular case $(x, y) \in M \bowtie M$ and $L = \Delta$ that

$$\frac{p_t^\Delta(x,y)}{\mathrm{e}_t(x,y)} \sim \frac{\det_\zeta'(-\nabla_s^2+\mathcal{R}_\gamma)^{-1/2}}{\det_\zeta(-\nabla_s^2)^{-1/2}}.$$

Replacing the expressions on the left hand side formally by the corresponding path integrals, we obtain that in the small-time limit, the quotient of the curved path integral and the "Euclidean" path integral is equal to the quotients of the corresponding zeta determinants.

Proof. By Thm. **??**, we have

$$\lim_{t\to 0}\,(4\pi t)^{k/2}\,\frac{p_t^L(x,y)}{\mathrm{e}_t(x,y)} = \int_{\Gamma_{xy}^{\min}}\frac{[\gamma\|_0^1]^{-1}}{\det\big(\nabla^2 E|_{N_\gamma\Gamma_{xy}^{\min}}\big)^{1/2}}\mathrm{d}^{H^1}\gamma,$$

when $\Gamma_{xy}^{\min}$ is endowed with the H^1 metric (1.2.5). By the transformation formula, we have

$$\lim_{t\to 0}\,(4\pi t)^{k/2}\,\frac{p_t^L(x,y)}{\mathrm{e}_t(x,y)} = \int_{\Gamma_{xy}^{\min}}\frac{[\gamma\|_0^1]^{-1}}{\det\big(\nabla^2 E|_{N_\gamma\Gamma_{xy}^{\min}}\big)^{1/2}\det\big(d\mathrm{id}|_\gamma\big)}\mathrm{d}^{L^2}\gamma, \tag{3.2.30}$$

where $\det(d\mathrm{id}|_\gamma)$ denotes the determinant of the identity map from $\Gamma_{xy}^{\min}$ with the H^1 metric to the same space with the L^2 metric. Fix $\gamma \in \Gamma_{xy}^{\min}$ and let $f_1, \dots, f_k$ be an H^1-orthonormal basis of $T_\gamma \Gamma_{xy}^{\min} \cong \ker(P + \mathcal{R}_\gamma)$. Then

$$\det\bigl(d\mathrm{id}|_\gamma\bigr) = \det\Bigl((f_i, f_j)_{L^2}\Bigr)_{1\leq i,j\leq k}^{1/2}. \tag{3.2.31}$$

Notice that $f_1, \dots, f_k$ are smooth by elliptic regularity. Let $f_{k+1}, f_{k+2}, \dots$ be a smooth H^1-orthonormal basis of $N_\gamma \Gamma_{xy}^{\min}$. By Thm. **??** (respectively Remark 3.2.4) and (3.2.9), we have

$$\det\bigl(\nabla^2 E|_{N_\gamma \Gamma_{xy}^{\min}}\bigr) = \lim_{N\to\infty} \det\Bigl(\bigl(f_i, (P + \mathcal{R}_\gamma) f_j\bigr)_{L^2}\Bigr)_{k+1\leq i,j\leq N}. \tag{3.2.32}$$

Let Π be the H^1-orthogonal projection in $H_0^1([0,1], \gamma^*TM)$ onto $\ker(P + \mathcal{R}_\gamma)$. Because Π has finite rank, it is bounded with respect to the L^2 norm and therefore extends uniquely to a bounded operator on $L^2([0,1], \gamma^*TM)$, which is still a projection onto $\ker(P+\mathcal{R}_\gamma)$ (since it is idempotent), but not necessary an orthogonal projection. Set $Q := P + \mathcal{R}_\gamma + \Pi$. Then Q is zeta-admissible by Prop. 3.2.18 because it can be written in the form $Q = P(\mathrm{id} + W)$ with $W = P^{-1}(\mathcal{R}_\gamma + \Pi)$, which is trace-class by Lemma 3.2.1. Hence Q is zeta-admissible. With respect to the orthogonal basis $f_1, f_2, \dots$ of the space $H_0^1([0,1], \gamma^*TM)$ used above, we have

$$(f_i, Q f_j)_{L^2} = \begin{cases} (f_i, f_j)_{L^2} & \text{if } 1 \leq i,j \leq k \\ \bigl(f_i, (P + \mathcal{R}_\gamma) f_j\bigr)_{L^2} & \text{if } i,j > k \\ 0 & \text{if } 1 \leq i \leq k \text{ and } j > k. \end{cases}$$

To see that third case, if $1 \leq i \leq k$ and $j > k$, calculate

$$(f_i, Q f_j)_{L^2} = \bigl(f_i, (P + \mathcal{R}_\gamma) f_j\bigr)_{L^2} + (f_i, \Pi f_j)_{L^2} = \bigl((P + \mathcal{R}_\gamma) f_i, f_j\bigr)_{L^2} = 0.$$

Hence the infinite matrix with entries $(f_i, Q f_j)_{L^2}$ is block triangular with respect to the orthogonal splitting of $H_0^1([0,1], \gamma^*TM)$ into $\ker(P + \mathcal{R}_\gamma)$ and its orthogonal complement, and we have

$$\det\Bigl((f_i, Q f_j)_{L^2}\Bigr)_{1\leq i,j\leq N} = \det\Bigl((f_i, f_j)_{L^2}\Bigr)_{1\leq i,j\leq k} \det\Bigl(\bigl(f_i, (P + \mathcal{R}_\gamma) f_j\bigr)_{L^2}\Bigr)_{k+1\leq i,j\leq N}.$$

for all $N > k$. Plugging in (3.2.31) and (3.2.32), we then obtain

$$\begin{aligned} \det\bigl(\nabla^2 E|_{N_\gamma \Gamma_{xy}^{\min}}\bigr)^{1/2} \det\bigl(d\mathrm{id}|_\gamma\bigr) &= \lim_{N\to\infty} \det\Bigl((f_i, Q f_j)_{L^2}\Bigr)_{1\leq i,j\leq N}^{1/2} \\ &= \lim_{N\to\infty} \det\Bigl((f_i, P^{-1} Q f_j)_{H^1}\Bigr)_{1\leq i,j\leq N}^{1/2} \\ &= \det{}^{H^1}(P^{-1}Q)^{1/2}. \end{aligned}$$

Because $P^{-1/2} : L^2([0,1], \gamma^*TM) \longrightarrow H_0^1([0,1], \gamma^*TM)$ is an isometry, we obtain

$$\det{}^{H^1}(P^{-1}Q) = \det{}^{L^2}(P^{-1/2} Q P^{-1/2}).$$

Again, we have by Prop. 3.2.18,

$$\det{}^{L^2}(P^{-1/2}QP^{-1/2})\,\det_\zeta(P^{1/2}) = \det_\zeta(P^{-1/2}Q) = \det_\zeta(P^{1/2})\,\det{}^{L^2}(P^{-1}Q)$$

so that $\det^{L^2}(P^{-1/2}QP^{-1/2}) = \det^{L^2}(P^{-1}Q)$.

Let now $\widetilde{\Pi}$ be the L^2-orthogonal projection in $L^2([0,t],\gamma^*TM)$ onto $\ker(P+\mathcal{R}_\gamma)$ and set $\widetilde{Q} := P+\mathcal{R}_\gamma+\widetilde{\Pi}$. We claim that $\det_\zeta(\widetilde{Q}) = \det_\zeta(Q)$. To see this, notice first that

$$P+\mathcal{R}_\gamma+\widetilde{\Pi} = (P+\mathcal{R}_\gamma+\Pi)(\mathrm{id}+W),$$

where $W = (P+\mathcal{R}_\gamma+\Pi)^{-1}(\widetilde{\Pi}-\Pi)$, which is trace-class. Now with respect to the orthogonal splitting of $L^2([0,1],\gamma^*TM)$ into $\ker(P+\mathcal{R}_\gamma)$ and its orthogonal complement, the operators in question are given by

$$\Pi \mathrel{\widehat{=}} \begin{pmatrix}\mathrm{id} & * \\ 0 & 0\end{pmatrix} \qquad \widetilde{\Pi} \mathrel{\widehat{=}} \begin{pmatrix}\mathrm{id} & 0 \\ 0 & 0\end{pmatrix} \qquad P+\mathcal{R}_\gamma+\Pi \mathrel{\widehat{=}} \begin{pmatrix}\mathrm{id} & * \\ 0 & P+\mathcal{R}_\gamma\end{pmatrix}.$$

Therefore W is upper triangular with respect to the splitting, hence quasi-nilpotent so that $\det(\mathrm{id}+W)=1$. Thus by Prop. 3.2.18, we have

$$\det_\zeta(\widetilde{Q}) = \det_\zeta(Q)\det(\mathrm{id}+W) = \det_\zeta(Q).$$

Clearly, the spectrum of $\widetilde{Q}$ is the same as the spectrum of $P+\mathcal{R}_\gamma$ except that the k-fold eigenvalue zero is replaced by k times the eigenvalue one. Hence $\zeta_{\widetilde{Q}}(z) = \zeta_{P+\mathcal{R}_\gamma}(z)+k$ and $\det_\zeta(\widetilde{Q}) = \det'_\zeta(P+\mathcal{R}_\gamma)$. By Prop. 3.2.18 and Example 3.2.17, we therefore have

$$\det\bigl(\nabla^2 E|_{N_\gamma\Gamma_{xy}^{\min}}\bigr)^{1/2}\det(d\mathrm{id}) = \det{}^{L^2}\bigl(P^{-1}\widetilde{Q}\bigr)^{1/2} = \frac{\det_\zeta(\widetilde{Q})^{1/2}}{\det_\zeta(P)^{1/2}} = \frac{\det'_\zeta(-\nabla_s^2+\mathcal{R}_\gamma)^{1/2}}{\det'_\zeta(-\nabla_s^2)^{1/2}}.$$

Plugging this into (3.2.30) gives the result. $\square$

Appendix A

A Proof of the Strong Heat Kernel Asymptotics

In this section, we give a proof of Thm. 2.1.5, following the method of Kannai [Kan77]. The proof is based on the fact that the solution operator e^{-tL} of the heat equation is related to the solution operator $W_t := \cos(t\sqrt{L})$ of the wave equation by the so-called *transmutation formula*

$$e^{-tL}u(x) = (4\pi t)^{-1/2} \int_{-\infty}^{\infty} e^{-s^2/4t} W_s u(x) \, \mathrm{d}s \tag{A.0.1}$$

so that the short time asymptotics of the heat kernel follow from the asymptotic expansion of the wave kernel. A particularly interesting feature of this approach is that the asymptotics

$$\log p_t^{\Delta}(x,y) \sim -\frac{d(x,y)^2}{4t},$$

for x, y close follow from (A.0.1) using the fact that the wave equation (as opposed to the heat equation) has finite propagation speed.

A.1 The Wave Equation

Let M be a closed Riemannian manifold of dimension n and let L be a Laplace type operator, acting on sections of a metric vector bundle $\mathcal{V}$ (here we do not need L to be self-adjoint). For the proof of Thm. 2.1.5, we need some facts concerning the wave equation

$$(\partial_{tt} + L)u_t = 0, \tag{A.1.1}$$

which we collect now. It has the two independent solution operators W_t and G_t, which map sections $u \in C^\infty(M, \mathcal{V})$ to solutions u_t of the wave equation, with the initial conditions

$$u_0 = u, \quad \partial_t u_0 = 0 \qquad \text{and} \qquad u_0 = 0, \quad \partial_t u_0 = u,$$

respectively. If L is self-adjoint, it is possible to define $W_t := \cos(t\sqrt{L})$ and $G_t := \sin(t\sqrt{L})/\sqrt{L}$ by usual functional calculus, but the above definition works in any case (for the solution theory to the Cauchy problem of the wave equation, see e.g. Section 3.2 of [BGP07]). G_t is related to W_t by $W_t = G_t'$ and is given as the difference

$$G_t = G_t^+ - G_t^-,$$

where G_t^+ and G_t^- are the advanced and retarded Green's operators for the wave operator $\Box := \partial_{tt} + L$, (see Section 3.4 in [BGP07]).
To describe the asymptotic expansion of $G(t,x,y)$, we introduce the *Riesz distributions* $R(\alpha;t,x,y)$. For $\mathrm{Re}(\alpha) > n+1$, set

$$R(\alpha;t,x,y) := C(\alpha)\,\mathrm{sign}(t)\,\big(t^2 - d(x,y)^2\big)_+^{\frac{\alpha-n-1}{2}}, \qquad C(\alpha) := \frac{2^{1-\alpha}\pi^{\frac{1-n}{2}}}{\Gamma\left(\frac{\alpha}{2}\right)\Gamma\left(\frac{\alpha-n+1}{2}\right)},$$

where $(t^2 - d(x,y)^2)_+$ denotes the positive part, i.e. it is zero whenever $|t| \leq d(x,y)$ (The constant $C(\alpha)$ here equals the constant $C(\alpha, n+1)$ in Def. 1.2.1 of [BGP07] because our spacetime $\mathbb{R}\times M$ is $n+1$-dimensional. The distributions $R(\alpha)$ discussed here are related to the distributions $R_\pm(\alpha)$ in Section 1.4 of [BGP07] by $R(\alpha) = R_+(\alpha) - R_-(\alpha)$). For $\mathrm{Re}\,\alpha > n+1$, the $R(\alpha;t,x,y)$ are then continuous functions on $\mathbb{R}\times M \bowtie M$ and one can show that they define a holomorphic family of distributions on $\{\mathrm{Re}(\alpha) > n+1\}$ that has a holomorphic extension to all of $\mathbb{C}$ [BGP07, Lemma 1.2.2 (4)]. This defines $R(\alpha;t,x,y) \in \mathscr{D}'(\mathbb{R}\times M \bowtie M)$ for all $\alpha \in \mathbb{C}$.
Now on $M \bowtie M$, the distribution $G(t,x,y)$ has the asymptotic expansion [BGP07, Ch. 2]

$$G(t,x,y) \;\sim\; \sum_{j=0}^{\infty} \Phi_j(x,y) R(2+2j;t,x,y), \tag{A.1.2}$$

where the $\Phi_j(x,y) \in C^\infty(M \bowtie M, \mathcal{V}\boxtimes\mathcal{V}^*)$ are exactly the same coefficients that appear in the asymptotic heat kernel expansion (It is easy to work out that in the present setting, the coefficients Φ_j must be t-independent and that the transport equation (2.3) in [BGP07] reduces to our equation (2.1.5)). The asymptotic expansion (A.1.2) is meant in the sense that the difference

$$\delta^\nu(t,x,y) := G(t,x,y) - \sum_{j=0}^{\nu} \Phi_j(x,y) R(2+2j;t,x,y) \tag{A.1.3}$$

can be made arbitrarily smooth by increasing the number ν of correction terms; in fact, $\delta^\nu \in C^k(\mathbb{R}\times M \bowtie M, \mathcal{V}\boxtimes\mathcal{V}^*)$ whenever $\nu \geq (n+1)/2 + k$ [BGP07, Prop. 2.5.1]. Furthermore, the fact that the wave equation has finite propagation speed (i.e. $G(t,x,y) \equiv 0$ on the region where $|t| < d(x,y)$) implies that when ν is so large that δ^ν is C^k, one has the estimate

$$\Big|\nabla_x^l \nabla_y^m \delta^\nu(t,x,y)\Big| \leq C\big(t^2 - d(x,y)^2\big)_+^{(k-l-m)/2} \tag{A.1.4}$$

uniformly over compact subsets of $M \bowtie M$ and $t \leq T$, whenever $k \geq l+m$ (compare [BGP07, Thm. 2.5.2]).

A.2 The Proof

We first show that the transmutation formula given above is indeed valid.

Lemma A.2.1. *Let L be a Laplace type operator, acting on sections of a vector bundle $\mathcal{V}$ over a compact Riemannian manifold M. Then the solution operator to the heat equation is related to the solution operator of the wave equation by formula* (A.0.1)*.*

Proof. By the energy estimate for the wave equation [BTW15, Thm. 8], for all $m \in \mathbb{N}$, there exists a constant $\alpha \in \mathbb{R}$ such that

$$\|W_s u\|_{H^m} \leq \|u\|_{H^m} e^{\alpha|s|}, \qquad \|G_s u\|_{H^m} \leq \|u\|_{H^m} e^{\alpha|s|} \tag{A.2.1}$$

for all $s \in \mathbb{R}$ and $u \in C^\infty(M, \mathcal{V})$. Therefore, for any $u \in L^2(M, \mathcal{V})$ and $t > 0$, the Hilbert-space-valued integral

$$P_t u := (4\pi t)^{-1/2} \int_{-\infty}^{\infty} e^{-s^2/4t}\, W_s u \,\mathrm{d}s \tag{A.2.2}$$

is absolutely convergent and defines a bounded operator P_t on $L^2(M, \mathcal{V})$ with

$$\|P_t u\|_{L^2}^2 \leq (4\pi t)^{-1/2} \int_{-\infty}^{\infty} e^{-s^2/4t}\, \|W_s u\|_{L^2}^2 \,\mathrm{d}s \leq \|u\|_{L^2}^2 (4\pi t)^{-1/2} \int_{-\infty}^{\infty} e^{-s^2/4t + 2\alpha|s|} \,\mathrm{d}s$$

using Jensen's inequality and (A.2.1). Hence P_t is uniformly bounded for t near zero. Set furthermore $P_0 u := u$. We show that P_t is a strongly continuous semigroup of operators on $L^2(M, \mathcal{V})$: The semigroup property $P_t P_s = P_{t+s}$ follows from the standard convolution identity for the one-dimensional Gauss kernel.
To show strong continuity at zero, suppose first that $u \in C^\infty(M, \mathcal{V})$. It is well known [BGP07, Prop. 3.2.5] that in this case, for any $x \in M$, the map $s \mapsto W_s u(x)$ is a smooth $\mathcal{V}_x$-valued map. Using the Sobolev embedding theorem [Ada03, Thm. 4.12.I.A], one obtains from (A.2.1) that there exist constants $C_1, C_2, \alpha > 0$ such that

$$\big|W_s u(x)\big| \leq C_1 \|W_s u\|_{H^m} \leq C_2 \|u\|_{H^m} e^{\alpha|s|}. \tag{A.2.3}$$

whenever $m > n/2$. Therefore the integral (A.2.2) is pointwise absolutely convergent, and one has pointwise $P_t u(x) \to W_0 u(x) = u(x)$ as $t \to 0$, because the Gaussian $(4\pi t)^{-1/2} e^{-s^2/4t}$ converges to the delta distribution in this limit. We also obtain

$$|P_t u(x)| \leq C_2 \|u\|_{H^m} (4\pi t)^{-1/2} \int_{-\infty}^{\infty} e^{-s^2/4t + \alpha|s|} \,\mathrm{d}s,$$

which shows that for $T > 0$, there exists a constant $C_3 > 0$ such that $\|P_t u\|_\infty \leq C_3$ for all $0 \leq t \leq T$. From the dominated convergence theorem, we obtain $P_t u \longrightarrow u$ in L^2 as $t \to 0$, for all $u \in C^\infty(M, \mathcal{V})$. By the uniform boundedness of the operator family P_t near zero, this implies that also $P_t u \to u$ in L^2 as $t \to 0$ for arbitrary $u \in L^2(M, \mathcal{V})$ (by the same argument as in the proof of Lemma 1.3.23).
It remains to show that the infinitesimal generator of P_t is the Laplace type operator L; then $P_t = e^{-tL}$, because any two operator families with the same infinitesimal generator coincide.

Because the Gaussian function appearing in (A.0.1) solves the one-dimensional heat equation,

$$\frac{\partial}{\partial t}\big\{(4\pi t)^{-1/2}e^{-s^2/4t}\big\} = \frac{\partial^2}{\partial s^2}\big\{(4\pi t)^{-1/2}e^{-s^2/4t}\big\},$$

one has in the case that u is smooth

$$\begin{aligned}\frac{\partial}{\partial t}P_t u(x) &= (4\pi t)^{-1/2}\int_{-\infty}^{\infty}\frac{\partial^2}{\partial s^2}e^{-s^2/4t}\,W_s u(x)\,\mathrm{d}s = (4\pi t)^{-1/2}\int_{-\infty}^{\infty}e^{-s^2/4t}\,\frac{\partial^2}{\partial s^2}W_s u(x)\,\mathrm{d}s\\ &= -(4\pi t)^{-1/2}\int_{-\infty}^{\infty}e^{-s^2/4t}\,LW_s u(x)\,\mathrm{d}s = -LP_t u(x).\end{aligned}$$

Here the integration by parts is justified by the pointwise energy estimate (A.2.3). This shows that the infinitesimal generator of P_t is some closure of the operator L with domain $C^\infty(M,\mathcal{V})$. However, it is well known that L has a unique closure on this domain (see e.g. Section 1.3 in [Gil95] or Section 10.4.1 in [Nik07]), namely the infinitesimal generator of the semigroup e^{-tL}. This shows $P_t = e^{-tL}$. □

From (A.0.1) follows the identity

$$\begin{aligned}p_t^L(x,y) &= (4\pi t)^{-1/2}\int_{-\infty}^{\infty}e^{-s^2/4t}\,\frac{\partial G}{\partial s}(s,x,y)\,\mathrm{d}s\\ &= (4\pi t)^{-1/2}\int_{-\infty}^{\infty}e^{-s^2/4t}\,G(s,x,y)\,\frac{s}{2t}\,\mathrm{d}s\end{aligned}\tag{A.2.4}$$

of kernels where $G(t,x,y)\in\mathscr{D}'(\mathbb{R}\times M\times M,\mathcal{V}\boxtimes\mathcal{V}^*)$ denotes the Schwartz kernel of G_t and the identity is to be interpreted in the distributional sense (for the second equality, we integrated by parts, which is again justified by the energy estimate (A.2.1)).

Lemma A.2.2. *For all $j\in\mathbb{N}_0$, $t>0$ and all $(x,y)\in M\bowtie M$, we have*

$$\frac{1}{2t(4\pi t)^{1/2}}\int_{-\infty}^{\infty}e^{-s^2/4t}R(2+2j;s,x,y)\,s\,\mathrm{d}s = \mathrm{e}_t(x,y)\frac{t^j}{j!},\tag{A.2.5}$$

where $\mathrm{e}_t(x,y)$ is the Euclidean heat kernel, defined in (2.1.1)*. In particular, the distributional integral on the left hand side actually yields a smooth function.*

Proof. For $\mathrm{Re}(\alpha)>n+1$, consider the absolutely convergent integral

$$\begin{aligned}\frac{1}{2t(4\pi t)^{1/2}}\int_{-\infty}^{\infty}e^{-s^2/4t}R(\alpha;s,x,y)\,s\,\mathrm{d}s &= \frac{C(\alpha)}{2t(4\pi t)^{1/2}}\int_{-\infty}^{\infty}e^{-s^2/4t}\big(s^2-d(x,y)^2\big)_+^{\frac{\alpha-n-1}{2}}|s|\,\mathrm{d}s\\ &= \frac{C(\alpha)}{t(4\pi t)^{1/2}}\int_{0}^{\infty}e^{-s^2/4t}\big(s^2-d(x,y)^2\big)_+^{\frac{\alpha-n-1}{2}}s\,\mathrm{d}s\\ &= \frac{C(\alpha)}{t(4\pi t)^{1/2}}\int_{d(x,y)}^{\infty}e^{-s^2/4t}\big(s^2-d(x,y)^2\big)^{\frac{\alpha-n-1}{2}}s\,\mathrm{d}s\end{aligned}$$

Performing the substitution $u^2=s^2-d(x,y)^2$ which transforms the interval $(d(x,y),\infty)$ into the interval $(0,\infty)$, we have $s\mathrm{d}s=u\mathrm{d}u$. Therefore, we obtain

$$\int_{d(x,y)}^{\infty}e^{-s^2/4t}\big(s^2-d(x,y)^2\big)^{\frac{\alpha-n-1}{2}}s\,\mathrm{d}s = e^{-\frac{d(x,y)^2}{4t}}\int_0^\infty e^{-u^2/4t}u^{\alpha-n}\,\mathrm{d}u.$$

Now, substituting $u^2/4t = r$, the integral can be brought into the form of a gamma-integral, giving

$$\int_0^\infty e^{-u^2/4t} u^{\alpha-n}\,\mathrm{d}u = t^{1/2}(4t)^{\frac{\alpha-n}{2}} \int_0^\infty e^{-r} r^{\frac{\alpha-n-1}{2}}\,\mathrm{d}r = t^{1/2}(4t)^{\frac{\alpha-n}{2}}\Gamma\left(\frac{\alpha-n+1}{2}\right).$$

Put together, we arrive at

$$\begin{aligned}\frac{1}{2t(4\pi t)^{1/2}}\int_{-\infty}^\infty e^{-s^2/4t} R(\alpha; s, x, y)\, s\,\mathrm{d}s &= e^{-\frac{d(x,y)^2}{4t}} \frac{C(\alpha)}{t\sqrt{4\pi t}} t^{1/2}(4t)^{\frac{\alpha-n}{2}}\Gamma\left(\frac{\alpha-n+1}{2}\right)\\ &= \mathrm{e}_t(x,y)\frac{t^{\frac{\alpha-2}{2}}}{\Gamma(\alpha/2)}.\end{aligned} \tag{A.2.6}$$

Until now, we have restricted ourselves to the case $\operatorname{Re}\alpha > n+1$. However, for both sides of the last equation, if we pair them with a test function $\varphi \in \mathscr{D}(M \bowtie M)$, the result will be an entire holomorphic function in α. Because they coincide for $\operatorname{Re}\alpha > n+1$, they must therefore coincide everywhere, by the identity theorem for holomorphic functions. The statement of the Lemma is the particular result for $\alpha = 2+2j$, $j \in \mathbb{N}_0$. $\square$

Proof (of Thm. 2.1.5). By (A.2.4) and (A.1.3), we have for any $\nu \in \mathbb{N}$ that

$$p_t^L(x,y) = \sum_{j=0}^{\nu} \frac{\Phi_j(x,y)}{2t\sqrt{4\pi t}} \int_{-\infty}^\infty e^{-\frac{s^2}{4t}} R(2+2j; s, x, y)\, s\,\mathrm{d}s + \frac{1}{2t\sqrt{4\pi t}}\int_{-\infty}^\infty e^{-\frac{s^2}{4t}}\delta^\nu(s,x,y)\, s\,\mathrm{d}s,$$

where $\delta^\nu(t,x,y)$ is in C^k whenever $\nu \geq (n+1)/2 + k$. The first term evaluates using Lemma A.2.2 to

$$\sum_{j=0}^{\nu} \frac{\Phi_j(x,y)}{2t\sqrt{4\pi t}} \int_{-\infty}^\infty e^{-\frac{s^2}{4t}} R(2+2j; s, x, y)\, s\,\mathrm{d}s = \mathrm{e}_t(x,y)\sum_{j=0}^{\nu} t^j \frac{\Phi_j(x,y)}{j!}.$$

It remains to estimate the error term. Because $G_t = -G_{-t}$ and the Riesz distributions are odd in t, the remainder term $\delta^\nu(t,x,y)$ is an odd function in the t variable. We conclude

$$r^\nu(t,x,y) := \frac{1}{2t\sqrt{4\pi t}}\int_{-\infty}^\infty e^{-\frac{s^2}{4t}}\delta^\nu(s,x,y)\, s\,\mathrm{d}s = \frac{1}{t\sqrt{4\pi t}}\int_{d(x,y)}^\infty e^{-\frac{s^2}{4t}}\delta^\nu(s,x,y)\, s\,\mathrm{d}s,$$

as $\delta^\nu(s,x,y) = 0$ if $s < d(x,y)$, because of (A.1.4). Substituting $s = \sqrt{u^2 + d(x,y)^2}$ as before, one obtains

$$r^\nu(t,x,y) = \frac{e^{-\frac{d(x,y)^2}{4t}}}{t(4\pi t)^{1/2}}\int_0^\infty e^{-\frac{u^2}{4t}}\delta^\nu\big(\sqrt{u^2+d(x,y)^2}, x, y\big)\, u\,\mathrm{d}u.$$

Set $\widetilde{\delta}^\nu(u,x,y) := \delta_\nu(\sqrt{u^2+d(x,y)^2}, x, y)$. Then for any $l, m \in \mathbb{N}_0$, we obtain

$$\nabla_x^l \nabla_y^m \left\{\frac{r^\nu(t,x,y)}{\mathrm{e}_t(x,y)}\right\} = (4\pi t)^{(n-1)/2}\frac{1}{t}\int_0^\infty e^{-\frac{u^2}{4t}}\nabla_x^l\nabla_y^m\widetilde{\delta}^\nu(u,x,y) u\,\mathrm{d}u.$$

If ν is so large that δ^ν is C^{k+l+m} for $k, l, m \in \mathbb{N}_0$, then from (A.1.4) follows the estimate

$$\left|\nabla_x^l \nabla_y^m \widetilde{\delta}^\nu(u, x, y)\right| \leq C|u|^{k-l-m}, \tag{A.2.7}$$

which is uniform over (x, y) in compact subsets of $M \bowtie M$ and $u \leq T$. In this case,

$$\left|\nabla_x^l \nabla_y^m \left\{\frac{r^\nu(t, x, y)}{\mathrm{e}_t(x, y)}\right\}\right| \leq C(4\pi t)^{(n-1)/2} \frac{1}{t} \int_0^\infty e^{-\frac{u^2}{4t}} u^k \mathrm{d}u \leq C_2 t^{n/2+k/2-1}$$

We obtain that for any $\nu \in \mathbb{N}_0$, one can find $\widetilde{\nu}$ large enough so that

$$\left|\nabla_x^l \nabla_y^m \left\{\frac{p_t^L(x, y)}{\mathrm{e}_t(x, y)} - \sum_{j=0}^{\widetilde{\nu}} t^j \frac{\Phi_j(x, y)}{j!}\right\}\right| \leq C_3 t^{\nu+1},$$

where the estimate is uniform for (x, y) in a compact subset of $M \bowtie M$ and $t \leq T$. However, the calculation

$$\begin{aligned} &\left|\nabla_x^l \nabla_y^m \left\{\frac{p_t^L(x, y)}{\mathrm{e}_t(x, y)} - \sum_{j=0}^{\nu} t^j \frac{\Phi_j(x, y)}{j!}\right\}\right| \\ &\qquad \leq \left|\nabla_x^l \nabla_y^m \left\{\frac{p_t^L(x, y)}{\mathrm{e}_t(x, y)} - \sum_{j=0}^{\nu} t^j \frac{\Phi_j(x, y)}{j!}\right\}\right| + \left|\sum_{j=\nu+1}^{\widetilde{\nu}} t^j \frac{\nabla_x^l \nabla_y^m \Phi_j(x, y)}{j!}\right| \leq C_4 t^{\nu+1} \end{aligned}$$

shows that in fact $\widetilde{\nu} = \nu$ suffices. $\square$

Appendix B

Some Results from Stochastic Analysis

In this section, we prove some measure-theoretic preliminaries needed for the proof of Thm. 2.1.12 and Thm. 2.2.7, which are related to the quadratic variation of the Brownian bridge and the moments of the functions $d(X_{s_0}^{xy;t}, X_{s_1}^{xy;t})$, where $X_s^{xy;t}$ is the Brownian bridge.

B.1 Approximation of the Quadratic Variation

Throughout, let M be a compact Riemannian manifold or $\mathbb{R}^n$.

Definition B.1.1 (Quadratic Variation). If β is a symmetric section of the bundle $T^*M \odot T^*M$, i.e. we are given a symmetric bilinear form on each fiber, we can define the *β-quadratic variation* of a continuous path $\gamma : [a, b] \longrightarrow M$ as the limit

$$[\gamma]_\beta := \lim_{|\tau|\to 0} \sum_{j=1}^{N} \beta\big(\Delta_j\gamma, \Delta_j\gamma\big),$$

if it exists, where the limit goes over any sequence of partitions $\tau = \{a = \tau_0 < \tau_1 < \cdots < \tau_N = b\}$ of $[a, b]$ the mesh of which tends to zero (we require that the limit exists for any such sequence and all limits coincide). Here we wrote $\Delta_j\gamma := \exp^{-1}_{\gamma(\tau_{j-1})}(\gamma(\tau_j))$ for the shortest tangent vector in $T_{\gamma(\tau_{j-1})}M$ that gets mapped to $\gamma(\tau_j)$ under the exponential map (this is well defined for a generic partition).

Remark B.1.2. If $\gamma \in H_{xy;\tau}(M)$, we have

$$\Delta_j\gamma = \exp^{-1}_{\gamma(\tau_{j-1})}(\gamma(\tau_j)) = \dot\gamma(\tau_{j-1}+)\Delta_j\tau, \tag{B.1.1}$$

which is the definition of $\Delta_j\gamma$ from Corollary 2.2.10.

Notice that this limit is zero if the path γ is absolutely continuous. The paths of the Brownian motion and the Brownian bridge, however, are very irregular: We have

$$\lim_{|\tau|\to 0} \sum_{j=1}^{N} \beta(\Delta_j X, \Delta_j X) = 2\int_0^t \operatorname{tr}\beta(X_s)\,\mathrm{d}s, \tag{B.1.2}$$

where the limit is taken in probability, see Prop. 3.23 and Prop. 5.18 in [Eme89] (the difference of a factor 2 in comparison to the literature comes from our "analytic" convention of Brownian motion, i.e. that we constructed it using the heat kernel of Δ instead of $\frac{1}{2}\Delta$). Here, X_s is either a Brownian motion or Brownian bridge; the quadratic variation is the same because drift terms do not alter the quadratic variation (compare Remark 2.1.10). In measure-theoretic terms, this means that we have

$$\lim_{|\tau|\to 0} \sum_{j=1}^{N} \beta\big(\Delta_j\gamma, \Delta_j\gamma\big) = 2\int_0^t \operatorname{tr} \beta\big(\gamma(s)\big)\, \mathrm{d}s, \tag{B.1.3}$$

where the limit is taken in measure on $C_x(M)$ or $C_{xy;t}(M)$ (with respect to the measure $\mathbb{W}^x$ respectively $\mathbb{W}^{xy;t}$).

Lemma B.1.3. *Let $\beta \in C^\infty(M, T^*M \odot T^*M)$. Then we have*

$$\lim_{|\tau|\to 0} \exp\left(\sum_{j=1}^{N} \beta\big(\Delta_j\gamma, \Delta_j\gamma\big)\right) = \exp\left(2\int_0^t \operatorname{tr} \beta\big(\gamma(s)\big)\, \mathrm{d}s\right)$$

in the weak topology of $L^p(C_{xy;t}(M); \mathbb{W}^{xy;t})$, for any $1 < p < \infty$. Here the limit runs over any sequence of partitions of the interval $[0,t]$, the mesh of which tends to zero.

Proof. Set for $\gamma \in C_{xy;t}(M)$

$$F_\tau(\gamma) := \sum_{j=1}^{N} \beta\big(\Delta_j\gamma, \Delta_j\gamma\big), \qquad F(\gamma) := 2\int_0^t \operatorname{tr} \beta\big(\gamma(s)\big)\, \mathrm{d}s$$

Step 1. By (B.1.3), we have

$$\lim_{|\tau|\to 0} F_\tau = F$$

in measure with respect to $\mathbb{W}^{xy;t}$. Remember that convergence in measure means that for each $\varepsilon > 0$, we have

$$\lim_{|\tau|\to 0} \mathbb{W}^{xy;t}\big(\{\gamma \,|\, |F_\tau(\gamma) - F(\gamma)| \geq \varepsilon\}\big) = 0$$

so that be continuity of the exponential function, we directly obtain that also

$$\lim_{|\tau|\to 0} e^{F_\tau} = e^F$$

in measure with respect to $\mathbb{W}^{xy;t}$.
Step 2. Let a by a global bound on β so that

$$\beta(\Delta_j\gamma, \Delta_j\gamma) \leq a|\Delta_j\gamma|^2 = a\, d\big(\gamma(\tau_{j-1}), \gamma(\tau_j)\big)^2.$$

By Lemma B.2.6, for any $1 \leq p < \infty$, there exists a constant $C > 0$ such that

$$\big\|e^{F_\tau}\big\|_{L^p} \leq \left(\int_{C_{xy;t}(M)} \exp\left(ap\sum_{j=1}^{N} d\big(\gamma(\tau_{j-1}), \gamma(\tau_j)\big)^2\right) \mathrm{d}\mathbb{W}^{xy;t}(\gamma)\right)^{1/p} \leq C \tag{B.1.4}$$

for all partitions $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = t\}$ of the interval $[0,t]$. In other words, the family (e^{F_τ}) is uniformly bounded in L^p. If $1 < p < \infty$, since L^p is the dual space of L^q, where $q = p/(p-1)$, we obtain from the Banach-Alaoglu theorem [Con94, Thm. 3.1] that the family (e^{F_τ}) is pre-compact with respect to the weak topology, i.e. any subsequence of e^{F_τ} has a weakly convergent subsequence. Suppose that we know that the only accumulation point of (e^{F_τ}) is e^F (this will be shown in Step 3), then we can conclude that $(e^{F_{\tau^k}})$ converges to e^F for any sequence of partitions $(\tau^k)_{k\in\mathbb{N}}$, the mesh of which goes to zero. Namely, suppose the converse, i.e. there exists a function $G \in L^q$ and an $\varepsilon > 0$ such that

$$\left|\int_{C_{xy;t}(M)} G\big(e^{F_{\tau^k}} - e^F\big)\right| \geq \varepsilon \tag{B.1.5}$$

for infinitely many indices $k_1, k_2, \ldots$ This leads to a contradiction: The sequence $(e^{F_{\tau^{k_j}}})_{j\in\mathbb{N}}$ must have a weakly convergent subsequence (by pre-compactness), the limit of which must be e^F, because e^F was assumed to be the only accumulation point; hence we can have (B.1.5) for only finitely many j.

Step 3. It remains to show that the family (e^{F_τ}) has the unique accumulation point e^F, i.e. that whenever a subsequence $(e^{F_{\tau^k}})$ converges weakly to some $G \in L^p$, then $G = e^F$. So suppose that $(e^{F_{\tau^k}})$ converges to G in the weak topology for some sequence of partitions $(\tau^k)_{k\in\mathbb{N}}$ with $|\tau^k| \to 0$ as $k \to \infty$. On the other hand, we know that $e^{F_{\tau^k}} \to e^F$ in measure, and it is well known [Els11, VI 4.9 b)] that this implies the existence of a subsequence (again denoted by $(e^{F_{\tau^k}})$) converging to e^F almost everywhere. We now conclude $e^F = G$ as follows.

Set $\Omega := C_{xy;t}(M)$. By Egoroff's Theorem [Els11, VI 3.5], for any $\delta > 0$, there exists a set $S \subseteq \Omega$ with $\mathbb{W}^{xy;t}(S) \leq \delta$ such that $e^{F_{\tau^k}}$ converges to e^F uniformly on $\Omega \setminus S$. Now for any $H \in L^q$, we have

$$\left|\int_\Omega H(e^F - G)\right| \leq \left|\int_\Omega H(e^F - e^{F_{\tau^k}})\right| + \left|\int_\Omega H(G - e^{F_{\tau^k}})\right|$$

and

$$\begin{aligned}\left|\int_\Omega H(e^F - e^{F_{\tau^k}})\right| &\leq \left|\int_{\Omega\setminus S} H(e^F - e^{F_{\tau^k}})\right| + \left|\int_S H(e^F - e^{F_{\tau^k}})\right| \\ &\leq \|H\|_{L^1}\big\|(e^F - e^{F_{\tau^k}})|_{\Omega\setminus S}\big\|_\infty + \|e^F - e^{F_{\tau^k}}\|_{L^p}\|H|_S\|_{L^q}.\end{aligned}$$

For a given $\varepsilon > 0$, using the uniform boundedness of the family $(e^{F_{\tau^k}})$ in L^p, we can choose δ (hence S) so small that

$$\|e^F - e^{F_{\tau^k}}\|_{L^p}\big\|H|_S\big\|_{L^q} \leq C\big\|H|_S\big\|_{L^q} \leq \frac{\varepsilon}{3},$$

and then n so large that

$$\|H\|_{L^1}\big\|(e^F - e^{F_{\tau^k}})|_{\Omega\setminus S}\big\|_\infty \leq \frac{\varepsilon}{3} \quad \text{and} \quad \left|\int_\Omega H(G - e^{F_{\tau^k}})\right| \leq \frac{\varepsilon}{3},$$

where in the last step, we used that $e^{F_{\tau^k}} \to G$ weakly. We have shown that for an $H \in L^q$ and any $\varepsilon > 0$, we have

$$\left| \int_\Omega H(e^F - G) \right| \leq \|H\|_{L^1} \big\| (e^f - e^{F_{\tau^k}})|_{\Omega \setminus S} \big\|_\infty + \|e^F - e^{F_{\tau^k}}\|_{L^p} \|H|_S\|_{L^q} + \left| \int_\Omega H(G - e^{F_{\tau^k}}) \right|$$
$$\leq \frac{\varepsilon}{3} + \frac{\varepsilon}{3} + \frac{\varepsilon}{3} \leq \varepsilon.$$

Therefore $G = e^F$. This finishes the proof. □

Lemma B.1.4. *Let $f \in C^\infty(M)$. Define*

$$F_\tau(\gamma) := \exp\left(\int_0^t f\big(\gamma^\tau(s)\big) \mathrm{d}s \right), \qquad F(\gamma) := \exp\left(\int_0^t f\big(\gamma(s)\big) \mathrm{d}s \right). \tag{B.1.6}$$

Then we have $F_\tau \longrightarrow F$ in $L^p(C_{xy;t}(M); \mathbb{W}^{xy;t})$ for any $1 \leq p < \infty$. Here for a partition τ of the interval $[0,t]$ and $\gamma \in C_{xy;t}(M)$, $\gamma^\tau \in H_{xy;\tau}(M)$ denotes the "best polygon approximation" of γ, i.e. the piecewise geodesic path with $\gamma^\tau(\tau_j) = \gamma(\tau_j)$. This is well defined for $\mathbb{W}^{xy;t}$-almost all paths γ, since the set of paths such that $(\gamma(\tau_{j-1}), \gamma(\tau_j)) \notin M \bowtie M$ for some j is a zero set.

Proof. Clearly, the functions F_τ are uniformly bounded. To see that $F_\tau \to F$ pointwise $\mathbb{W}^{xy;t}$-almost everywhere, notice that by the mean value theorem for integrals,

$$\int_0^t f\big(\gamma(s)\big) \mathrm{d}s = \sum_{j=1}^N \int_{\tau_{j-1}}^{\tau_j} f\big(\gamma(s)\big) \mathrm{d}s = \sum_{j=1}^N f\big(\gamma(s_j^\tau)\big) \Delta_j \tau$$

for numbers $s_1^\tau, \dots, s_N^\tau$. Similarly,

$$\int_0^t f\big(\gamma^\tau(s)\big) \mathrm{d}s = \sum_{j=1}^N f\big(\gamma^\tau(r_j^\tau)\big) \Delta_j \tau$$

for numbers $r_1^\tau, \dots, r_N^\tau$. Hence for all paths γ that are α-Hölder continuous for some $\alpha > 0$, we have

$$\left| \int_0^t f\big(\gamma(s)\big) \mathrm{d}s - \int_0^t f\big(\gamma^\tau(s)\big) \mathrm{d}s \right| \leq \sum_{j=1}^N \big| f\big(\gamma(s_j^\tau)\big) - f\big(\gamma^\tau(r_j^\tau)\big) \big| \Delta_j \tau$$
$$\leq \sum_{j=1}^N \Big(\big| f\big(\gamma(s_j^\tau)\big) - f\big(\gamma(\tau_j)\big) \big| + \big| f\big(\gamma^\tau(\tau_j)\big) - f\big(\gamma^\tau(r_j^\tau)\big) \big| \Big) \Delta_j \tau$$
$$\leq C_1 \sum_{j=1}^N \Big(d\big(\gamma(s_j^\tau), \gamma(\tau_j)\big) + d\big(\gamma^\tau(\tau_j), \gamma^\tau(r_j^\tau)\big) \Big) \Delta_j \tau$$
$$\leq C_2 \sum_{j=1}^N \big(|s_j^\tau - \tau_j|^\alpha + (\Delta_j \tau)^\alpha \big) \Delta_j \tau \leq C_3 \sum_{j=1}^N (\Delta_j \tau)^{1+\alpha} \leq C_3 |\tau|^\alpha,$$

since f is Lipschitz continuous, $|s_j^\tau - \tau_j| \leq \Delta_j \tau$ and

$$d\big(\gamma^\tau(\tau_j), \gamma^\tau(r_j^\tau)\big) = d\big(\gamma^\tau(\tau_{j-1}), \gamma^\tau(\tau_j)\big) = d\big(\gamma(\tau_{j-1}), \gamma(\tau_j)\big) \leq C_4(\Delta_j \tau)^\alpha,$$

where C_4 is the Hölder constant of γ. Because the set of α-Hölder continuous paths with $0 < \alpha < 1/2$ is a set of full $\mathbb{W}^{xy;t}$ measure in $C_{xy;t}(M)$ [BP11, Corollary 3.7], we indeed obtain $F_\tau \longrightarrow F$ pointwise almost-everywhere and then also in L^p for $1 \leq p < \infty$. The result now follows from Lebesgue's theorem of dominated convergence. $\square$

B.2 Moments of the Distance Function

Throughout, let M be a compact Riemannian manifold. This section is dedicated to the proof of the following estimate on the expectation value of the moments of the Riemannian distance travelled by the Brownian bridge in M, which will be needed in Section 2.1.4. Another related result, Lemma B.2.6 below, will also be proved in a similar fashion.

Lemma B.2.1 (Moment Estimate). *Let M be a compact Riemannian manifold. For each $T > 0$, there exists a constant $C > 0$ such that for each $k \in \mathbb{N}$, we have*

$$\mathbb{E}\Big[d\big(X_{s_0}^{xy;t}, X_{s_1}^{xy;t}\big)^k\Big] \leq C^k \frac{\Gamma\left(\frac{n}{2} + \frac{k}{2}\right)}{\Gamma\left(\frac{n}{2}\right)} \left(\frac{s_1 - s_0}{t}\right)^{k/2} \tag{B.2.1}$$

for all $x, y \in M \times M$ and $0 \leq s_0 \leq s_1 \leq t \leq T$.

Similar results can be found in Hsu's book [Hsu02, Section 5.4]. However, we need the slightly stronger results above, which are not proved in the reference. We do not know other references having the estimates needed for this presentation.

The proof of the results of this section relies on some techniques from the theory of stochastic processes. For points $x, y \in M$ and $t > 0$, set $\rho(z) := d(x, z)$ and let

$$r_s = r_s^{xy;t} := \rho(X_s^{xy;t}), \qquad s \leq t \tag{B.2.2}$$

be the radial process of the Brownian bridge, which measures the distance from the starting point. Let

$$Z(s, z) := \operatorname{grad}_z \log p_{t-s}(z, y)$$

be the time-dependent drift term of the Brownian bridge (see Remark 2.1.10). The process r_s then satisfies the equation

$$r_s = B_s + \int_0^s \Big(\Delta\rho(X_u^{xy;t}) + d\rho \cdot Z(u, X_u^{xy;t})\Big) \mathrm{d}u - L_s, \tag{B.2.3}$$

where B_s is a Brownian motion in $\mathbb{R}$ (with $B_0 = 0$) and L_s is a non-decreasing process which increases only when $X_s^{xy;t}$ is in the cut locus of x. For times s before $X_s^{xy;t}$ hits the cut-locus, this follows directly from the Ito formula, using that Brownian bridge is a Brownian motion with drift $Z(s, x)$ (Remark 2.1.10). The general proof of (B.2.3) can be found in [Hsu02], Thm. 3.5.1 or in [HT94], Satz 7.247 and 7.254 (the proof in the

literature is for the Brownian motion only, but the Brownian bridge case can be proved similarly. The difference of the factor 1/2 compared to formula (3.5.1) in [Hsu02] is due to the different convention for Brownian motion).
Using comparison theorems for the Laplacian of the distance function (see e.g. Thm. 3.4.2 in [Hsu02] or Thm. 1 in [MMU14]), we can compare this to the similar result on a hyperbolic space, which can be explicitly computed. More precisely, fix a number $\kappa \geq 0$ until the end of this section such that the Ricci curvature of M is bounded below by $-\kappa$ times the metric. Then we have

$$\Delta\rho(y) \leq \sqrt{\kappa}(n-1)\coth\bigl(\sqrt{\kappa}\,\rho(y)\bigr)$$

for any point $y \neq x$ which is not in the cut locus of x. Hence by definition of r_s, we have

$$\Delta\rho(X_s^{xy;t}) \leq \sqrt{\kappa}(n-1)\coth\bigl(\sqrt{\kappa}\,r_s\bigr). \tag{B.2.4}$$

Plugging this into (B.2.3) and then estimating the drift term with the Cauchy-Schwarz inequality yields

$$r_s \leq B_s + \sqrt{\kappa}(n-1)\int_0^s \coth\bigl(\sqrt{\kappa}\,r_u\bigr)\,\mathrm{d}u + \int_0^s \|Z(u,-)\|_\infty \mathrm{d}u, \tag{B.2.5}$$

where $\|Z(u,-)\|_\infty$ denotes the sup norm of the vector field $Z(u,-)$. Here we used that L_s is non-decreasing and $|d\rho| \equiv 1$. Using the elementary inequality

$$\coth(r) = 1 + 2\frac{1}{e^{2r}-1} \leq 1 + \frac{1}{r},$$

valid for $r > 0$, we furthermore obtain from (B.2.5) that

$$r_s \leq B_s + (n-1)\int_0^s \frac{1}{r_u}\,\mathrm{d}u + \int_0^s \|Z(u,-)\|_\infty \mathrm{d}u + \sqrt{\kappa}(n-1)s. \tag{B.2.6}$$

Remark B.2.2. The radial process r_s^κ corresponding to Brownian motion in the n-dimensional hyperbolic space of curvature $-\kappa$ satisfies

$$r_s^\kappa = B_s + \sqrt{\kappa}(n-1)\int_0^s \coth\bigl(\sqrt{\kappa}\,r_u^\kappa\bigr)\,\mathrm{d}u.$$

Hence (B.2.5) estimates the radial process in M from above by the radial process in a hyperbolic space with a certain drift. Letting κ tend to zero, the above equation becomes the first part of inequality (B.2.6). Hence the latter inequality is related to the radial process in $\mathbb{R}^n$, which we will use below.

The well-known gradient estimate on the heat kernel (see [Hsu99], [ST97] or Thm. 5.5.3 in [Hsu02])

$$\bigl|\mathrm{grad}_z \log p_{t-s}(z,y)\bigr| \leq C_1\left(\frac{d(z,y)^2}{t-s} + \frac{1}{\sqrt{t-s}}\right)$$

valid for all $z, y \in M$ and all $0 \leq s < t \leq T$ shows that

$$\int_0^s \|Z(u,-)\|_\infty \mathrm{d}u \leq C_1 \mathrm{diam}(M)^2\bigl(\log(t) - \log(t-s)\bigr) + 2C_1\bigl(\sqrt{t} - \sqrt{t-s}\bigr).$$

This explodes for $s \to t$, but is bounded on the interval $[0, t/2]$: Looking at the Taylor expansion of each individual term, we obtain that for any $T > 0$, there exists a constant $\zeta = \zeta(T) > 0$ such that whenever $t \leq T$,

$$\int_0^s \|Z(u, -)\|_\infty \mathrm{d}u + \sqrt{\kappa}(n-1)s \leq \frac{\zeta s}{t} \quad \text{for all} \quad s \leq t/2.$$

Let us emphasize that this constant depends on the manifold and the time bound T, but neither on the times s and t nor the end points x and y in M of the Brownian bridge. This implies that

$$r_s^{xy;t} \leq B_s + (n-1) \int_0^s \frac{1}{r_u^{xy;t}} \, \mathrm{d}u + \frac{\zeta s}{t} \tag{B.2.7}$$

for all s with $s \leq t$, if $t \leq T$. Namely, for $s \in [0, t/2]$, we can plug the above estimate into (B.2.6), while for $s \in [t/2, t]$, we can use that we always have $r_s \leq \mathrm{diam}(M)$ (so that we possibly increase ζ to $2\mathrm{diam}(M)$). The following lemma relates the radial processes $r_s^{xy;t}$ in M to the radial process in $\mathbb{R}^n$.

Lemma B.2.3. *For any $T > 0$, there exists a constant $\zeta \in \mathbb{R}$ such that*

$$r_s^{xy;t} \leq |B_s^n| + \frac{\zeta s}{t}$$

for all $x, y \in M$, whenever $0 \leq s \leq t \leq T$. Here $r_s^{xy;t}$ is the radial process defined by (B.2.3) *and B_s^n is a standard Brownian motion in $\mathbb{R}^n$.*

Remark B.2.4. Notice that throughout this thesis, standard Brownian motions have variance 2 instead of one, because we use Δ instead of $\frac{1}{2}\Delta$ for their infinitesimal generator.

The proof of Lemma B.2.3 will use the following comparison result from stochastic analysis, which can be found e.g. in [DW98, Thm. 3.1] in a much more general form than stated below.

Lemma B.2.5. *Suppose that the real-valued stochastic processes r_s and ℓ_s satisfy*

$$\begin{aligned} r_s &\leq B_s + \int_0^s f(u, r_u)\mathrm{d}u, \\ \ell_s &\geq B_s + \int_0^s f(u, \ell_u)\mathrm{d}u \end{aligned}$$

for all $s \leq t$, where B_s is a one-dimensional Brownian motion f is a function on $\mathbb{R}^+ \times \mathbb{R}$, measurable with respect to the second variable. Then we have $r_s \leq \ell_s$ almost surely for all $0 \leq s \leq t$.

Proof (of Lemma B.2.3). Consider the stochastic differential equation

$$\beta_s = B_s + (n-1) \int_0^s \frac{1}{\beta_u} \, \mathrm{d}u.$$

This equation is well known (see e.g. Ex. 8.4.1 of [Øks07]). It has a unique positive solution, the so-called Bessel process, which is exactly the radial process to Brownian

motion starting at zero in $\mathbb{R}^n$. If now U_s is a Brownian motion on $S^{n-1} \subset \mathbb{R}^n$ with U_0 being the uniform distribution on S^{n-1}, then one can check that $B_s^n := \beta_s U_s$ is a Brownian motion in $\mathbb{R}^n$ with $\beta_s = |B_s^n|$.
Now the process $\ell_s := \beta_s + \zeta s/t$ satisfies

$$\ell_s = B_s + (n-1)\int_0^s \frac{1}{\ell_u - \zeta u/t}\,\mathrm{d}u + \frac{\zeta s}{t} \geq B_s + (n-1)\int_0^s \frac{1}{\ell_u}\,\mathrm{d}u + \frac{\zeta s}{t}$$

where the estimate is justified since $\ell_s - \zeta s/t = \beta_s \geq 0$. This proves the lemma with a view on (B.2.7) by setting $r_s = r_s^{xy;t}$ in Lemma B.2.5. □

We are now in the position to prove Lemma B.2.1.

Proof (of Lemma B.2.1). We may assume $s_0 \leq t/2$ since otherwise, we can reverse the time: The process $X_{t-s}^{yx;t}$ coincides in law with $X_s^{xy;t}$, so that

$$\mathbb{E}\Big[d\big(X_{s_0}^{xy;t}, X_{s_1}^{xy;t}\big)^k\Big] = \mathbb{E}\Big[d\big(X_{t-s_1}^{yx;t}, X_{t-s_0}^{yx;t}\big)^k\Big],$$

compare [Hsu02, Prop. 5.4.3]. Now after reversing time the new s_0 equals $t - s_1$, which is smaller than $t/2$ if the previous s_0 was larger than $t/2$.
We therefore assume that $s_0 \leq t/2$. By definition of the Brownian bridge (2.1.14), we have

$$p_t^{\Delta}(x,y)\mathbb{E}\Big[d\big(X_{s_0}^{xy;t}, X_{s_1}^{xy;t}\big)^k\Big] = \int_M p_{s_0}^{\Delta}(x,z)p_{t-s_0}^{\Delta}(z,y)\mathbb{E}\Big[d\big(z, X_{s_1-s_0}^{zy;t-s_0}\big)^k\Big]\,\mathrm{d}z. \qquad \text{(B.2.8)}$$

Because of Lemma B.2.3, we find

$$d(z, X_s^{zy;s_1-s_0}) = r_{s_1-s_0}^{zy;t-s_0} \leq |B_{s_1-s_0}^n| + \frac{\zeta(s_1-s_0)}{t-s_0} \leq |B_{s_1-s_0}^n| + 2\frac{\zeta(s_1-s_0)}{t}$$

whenever $s_1 - s_0 \leq t - s_0 \leq T$. Set $\alpha = 2\zeta/t$ and $s := s_1 - s_0$. We compute

$$\begin{aligned}
\mathbb{E}\Big[\big(|B_s^n| + \alpha s\big)^k\Big] &= \sum_{j=0}^k \binom{k}{j}\big(\alpha s\big)^j \mathbb{E}\big[|B_s^n|^{k-j}\big] \\
&= \sum_{j=0}^k \binom{k}{j}\big(\alpha s\big)^j \int_{\mathbb{R}^n} \mathrm{e}_s(0,x)|x|^{k-j}\,\mathrm{d}x \\
&= \sum_{j=0}^k \binom{k}{j}\big(\alpha s\big)^j (4\pi s)^{k/2-j/2}\frac{\Gamma\left(\frac{n}{2}+\frac{k}{2}-\frac{j}{2}\right)}{\Gamma\left(\frac{n}{2}\right)} \\
&\leq \frac{\Gamma\left(\frac{n}{2}+\frac{k}{2}\right)}{\Gamma\left(\frac{n}{2}\right)} \sum_{j=0}^k \binom{k}{j}\big(\alpha s\big)^j (4\pi s)^{k/2-j/2} \\
&= \frac{\Gamma\left(\frac{n}{2}+\frac{k}{2}\right)}{\Gamma\left(\frac{n}{2}\right)}\big(\sqrt{4\pi s} + \alpha s\big)^k.
\end{aligned}$$

Hence

$$\mathbb{E}\Big[d(z, X^{zy;t-s_0}_{s_1-s_0})^k\Big] \leq \frac{\Gamma\left(\frac{n}{2}+\frac{k}{2}\right)}{\Gamma\left(\frac{n}{2}\right)}\left(\sqrt{4\pi(s_1-s_0)} + 2\zeta\frac{(s_1-s_0)}{t}\right)^k.$$

Finally,

$$\sqrt{4\pi(s_1-s_0)} + 2\zeta\frac{(s_1-s_0)}{t} = \left(\sqrt{4\pi t} + 2\zeta\sqrt{\frac{s_1-s_0}{t}}\right)\sqrt{\frac{s_1-s_0}{t}},$$

so we can set $C := \big(\sqrt{4\pi T} + 2\zeta\big)$. As this estimate does not depend on z, this shows the proposition together with (B.2.8). $\square$

The final result of this appendix will be the following estimate, which says that the approximate quadratic variations of the Brownian Bridge are uniformly bounded in expectation value.

Lemma B.2.6 (Exponential Estimate). *Let $T > 0$ and $\gamma \geq 0$. Then there exists a constant $C > 0$ such that*

$$\mathbb{E}\left[\exp\left(\gamma\sum_{j=1}^N d\big(X^{xy;t}_{\tau_{j-1}}, X^{xy;t}_{\tau_j}\big)^2\right)\right] \leq C$$

for all $x, y \in M$ and for all partitions $\tau = \{0 = \tau_0 < \tau_1 < \cdots < \tau_N = t\}$ of intervals $[0,t]$ with $t \leq T$.

Proof. The proof consists of three steps.
Step 1. We first show that there exist constants $\lambda, \varepsilon > 0$ (depending only on γ, T and the manifold) such that

$$\mathbb{E}\left[\exp\left(\gamma\, d\big(z, X^{zy;t}_s\big)^2\right)\right] \leq e^{\lambda s/t} \tag{B.2.9}$$

$z, y \in M$, all $s \leq \varepsilon$ and $s \leq t \leq T$. To this end, let again $r^{zy;t}_s := d\big(z, X^{zy;t}_s\big)$. By Lemma B.2.3, we have $r^{zy;t}_s \leq |B^n_s| + \zeta s/t$ for an n-dimensional Brownian motion starting at zero in $\mathbb{R}^n$, where ζ is independent of t, z and y. Abbreviate $\alpha := \zeta/t$. By the standard inequality $2|B^n_s| \leq 1 + |B^n_s|^2$, we have

$$(r^{zy;t}_s)^2 \leq \big(|B^n_s| + \alpha s\big)^2 = |B^n_s|^2 + 2\alpha s|B^n_s| + \alpha^2 s^2 \leq (1+\alpha s)|B^n_s|^2 + \alpha s + \alpha^2 s^2.$$

Therefore

$$\mathbb{E}\left[\exp\left(\gamma\, d\big(z, X^{zy;t}_s\big)^2\right)\right] \leq \mathbb{E}\left[\exp\left(\gamma\left(|B^n_s| + \alpha s\right)^2\right)\right] \leq e^{\gamma(\alpha s + \alpha^2 s^2)}\mathbb{E}\left[e^{\gamma(1+\alpha s)|B^n_s|^2}\right],$$

where the second factor evaluates explicitly to

$$\mathbb{E}\left[e^{\gamma(1+\alpha s)|B^n_s|^2}\right] = (4\pi s)^{-n/2}\int_{\mathbb{R}^n} e^{-|v|^2/4s} e^{\gamma(1+\alpha s)|v|^2}\mathrm{d}v \;\; = \left(\frac{1}{1 - 4s\gamma(1+\alpha s)}\right)^{n/2}$$

whenever $s \leq 1/(4\gamma(1+\alpha s))$ (otherwise, the integral diverges). Remembering that $\alpha = \zeta/t$, calculate

$$\frac{1}{4\gamma(1+\alpha s)} = \frac{t}{4\gamma t + \zeta s} \geq \frac{t}{4\gamma t + \zeta t} = \frac{1}{4\gamma + \zeta} =: 2\varepsilon. \tag{B.2.10}$$

Hence if $s \le \varepsilon$, we have

$$\mathbb{E}\left[\exp\left(\gamma\, d\big(z, X_s^{zy;t}\big)^2\right)\right] \le e^{\gamma(\alpha s+\alpha^2 s^2)} \left(\frac{1}{1-4s\gamma(1+\alpha s)}\right)^{n/2}.$$

Furthermore, if $s \le \varepsilon$, then $4s\gamma(1+\alpha s) \le 1/2$ by (B.2.10), so that we can use the estimate $\frac{1}{1-q} \le 1+2q$ valid for all $q \in [0, 1/2]$ to obtain

$$\frac{1}{1-4s\gamma(1+\alpha s)} \le 1+8s\gamma(1+\alpha s) \le 1+8s\gamma(1+\zeta) \le 1+8T\gamma(1+\zeta)\frac{s}{t} \le e^{8T\gamma(1+\zeta)s/t}$$

if also $t \le T$ (which is always assumed). Therefore

$$\left(\frac{1}{1-4s\gamma(1+\alpha s)}\right)^{n/2} \le e^{4nT\gamma(1+\zeta)s/t}.$$

Furthermore

$$\alpha s+\alpha^2 s^2 = \frac{\zeta s}{t} + \frac{\zeta^2 s^2}{t^2} \le (\zeta+\zeta^2)\frac{s}{t}, \qquad \text{hence} \qquad e^{\gamma(\alpha s+\alpha^2 s^2)} \le e^{\gamma(\zeta+\zeta^2)s/t},$$

so that (B.2.9) follows from the calculations above by setting $\lambda := \gamma(\zeta+\zeta^2)+4nT\gamma(1+\zeta)$.
Step 2. Next we show that the lemma is true for all partitions $|\tau|$ such that $|\tau| \le \varepsilon$, where $\varepsilon > 0$ is the constant given in (B.2.10). Namely, setting $x_0 := x$, $x_N := y$, we have for any $1 \le k \le N$

$$\begin{aligned}
p_t^\Delta(x,y)&\mathbb{E}\left[\exp\left(\gamma \sum_{j=1}^k d\big(X_{\tau_{j-1}}^{xy;t}, X_{\tau_j}^{xy;t}\big)^2\right)\right] \\
&= \int_M \cdots \int_M \left(\prod_{j=1}^k p_{\Delta_j\tau}^\Delta(x_{j-1},x_j)\exp\Big(\gamma\, d(x_{j-1},x_j)^2\Big)\right) p_{t-\tau_k}^\Delta(x_k,y)\,\mathrm{d}x_1\cdots \mathrm{d}x_{k-1} \\
&= \int_M \cdots \int_M \left(\prod_{j=1}^{k-1} p_{\Delta_j\tau}^\Delta(x_{j-1},x_j)\exp\Big(\gamma\, d(x_{j-1},x_j)^2\Big)\right) \cdot \\
&\qquad\qquad \cdot p_{t-\tau_{k-1}}^\Delta(x_{k-1},y)\mathbb{E}\left[\exp\left(\gamma\, d\big(x_{k-1}, X_{\Delta_k\tau}^{x_{k-1}y;t-\tau_{k-1}}\big)^2\right)\right]\mathrm{d}x_1\cdots\mathrm{d}x_{k-1},
\end{aligned}$$

that is

$$\begin{aligned}
\mathbb{E}&\left[\exp\left(\gamma \sum_{j=1}^k d\big(X_{\tau_{j-1}}^{xy;t}, X_{\tau_j}^{xy;t}\big)^2\right)\right] \\
&= \mathbb{E}\left[\exp\left(\gamma \sum_{j=1}^{k-1} d\big(X_{\tau_{j-1}}^{xy;t}, X_{\tau_j}^{xy;t}\big)^2\right)\mathbb{E}\left[\exp\left(\gamma\, d\big(X_{\tau_{k-1}}^{xy;t}, X_{\Delta_k\tau}^{X_{\tau_{k-1}}^{xy;t},y;t-\tau_{k-1}}\big)^2\right)\right]\right].
\end{aligned}$$

Assume that k is so small that $t-\tau_k \ge t/3$. Then if we assume that $\Delta_k\tau \le \varepsilon$, the last expectation value can be estimated by (B.2.9). Namely

$$\mathbb{E}\left[\exp\left(\gamma\, d\big(z, X_{\Delta_k\tau}^{zy;t-\tau_{k-1}}\big)^2\right)\right] \le e^{\lambda\Delta_k\tau/(t-\tau_{k-1})} \le e^{3\lambda\Delta_k\tau/t}.$$

for any $z \in M$. Therefore, under the assumption $|\tau| \le \varepsilon$, we have inductively

$$\mathbb{E}\left[\exp\left(\gamma\sum_{j=1}^{k} d\big(X^{xy;t}_{\tau_{j-1}}, X^{xy;t}_{\tau_j}\big)^2\right)\right] \le e^{3\lambda\Delta_k\tau/t}\mathbb{E}\left[\exp\left(\gamma\sum_{j=1}^{k-1} d\big(X^{xy;t}_{\tau_{j-1}}, X^{xy;t}_{\tau_j}\big)^2\right)\right]$$
$$\le \cdots \le e^{3\lambda\sum_{j=1}^{k}\Delta_j\tau/t} = e^{3\lambda\tau_k/t}.$$

Now choose $1 \le k \le N$ such that both $\tau_k \ge t/3$ and $t - \tau_k \ge t/3$, i.e. $\tau_k \in [t/3, 2t/3]$. Then by the Cauchy-Schwarz inequality,

$$\mathbb{E}\left[\exp\left(\gamma\sum_{j=1}^{N} d\big(X^{xy;t}_{\tau_{j-1}}, X^{xy;t}_{\tau_j}\big)^2\right)\right]$$
$$\le \mathbb{E}\left[\exp\left(2\gamma\sum_{j=1}^{k} d\big(X^{xy;t}_{\tau_{j-1}}, X^{xy;t}_{\tau_j}\big)^2\right)\right]^{1/2}\mathbb{E}\left[\exp\left(2\gamma\sum_{j=k+1}^{N} d\big(X^{xy;t}_{\tau_{j-1}}, X^{xy;t}_{\tau_j}\big)^2\right)\right]^{1/2}$$
$$\le e^{3\lambda\tau_k/2t}e^{3\lambda(t-\tau_k)/2t} = e^{3\lambda/2},$$

where to estimate the second factor, we reversed time and used the assumption $\tau_k \ge t/3$ (note that also, we used the constant λ from (B.2.9) corresponding to the exponent 2γ instead of γ). This proves the lemma for all partitions τ of intervals $[0, t]$ with $t \le T$ such that $|\tau| \le \varepsilon$ with ε given by (B.2.10).

Step 3. We now generalize to arbitrary partitions. For a given partition τ, let $m(\tau)$ denote the number of indices j such that $\Delta_j\tau \ge \varepsilon$. We now use induction on $m(\tau)$. For $m(\tau) = 0$, the estimate was shown above with the constant $C_0 := e^{3\lambda/2}$. Suppose that the estimate is true with a constant C_i for all partitions τ with $m(\tau) \le i$, $i \ge 0$. We now show that in this case, the estimate is also true for all partitions τ with $m(\tau) \le i + 1$, with a constant $C_{i+1} \ge C_i$.

To this end, let τ be a partition with $m(\tau) = i + 1$ and let k be the first index with $\Delta_k\tau \ge \varepsilon$. Write $\widetilde{\tau} := \{0 = \tau_0 < \tau_1 < \cdots < \tau_{k-1}\}$ and define the partition σ of the interval $[0, t - \tau_k]$ by

$$\sigma := \{\sigma_0 := 0 < \sigma_1 := \tau_{k+1} - \tau_k < \cdots < \sigma_{N-k} := \tau_N - \tau_k\}$$

Then $\widetilde{\tau}$ is a partition of the interval $[0, \tau_{k-1}]$, σ is a partition of the interval $[0, t - \tau_k]$ and we have $m(\widetilde{\tau}) = 0$, $m(\sigma) = i$. Therefore, if the estimate is true with a constant $C_i > 0$ for all partitions τ' with $m(\tau') \le i$, then it is in particular true for $\widetilde{\tau}$ and σ. We get

$$p^{\Delta}_t(x, y)\mathbb{E}\left[\exp\left(\gamma\sum_{j=1}^{N} d\big(X^{xy;t}_{\tau_{j-1}}, X^{xy;t}_{\tau_j}\big)^2\right)\right] =$$
$$= \int_M\int_M \mathbb{E}\left[\exp\left(\gamma\sum_{j=1}^{k-1} d\big(X^{xz_0;t}_{\widetilde{\tau}_{j-1}}, X^{xz_0;t}_{\widetilde{\tau}_j}\big)^2\right)\right]\mathbb{E}\left[\exp\left(\gamma\sum_{j=1}^{N-k} d\big(X^{z_1y;t-\tau_k}_{\sigma_{j-1}}, X^{z_1y;t-\tau_k}_{\sigma_j}\big)^2\right)\right]$$
$$\cdot\, e^{\gamma\, d(z_0,z_1)^2}p^{\Delta}_{\tau_{k-1}}(x, z_0)p^{\Delta}_{\Delta_k\tau}(z_0, z_1)p^{\Delta}_{t-\tau_k}(z_1, y)\,\mathrm{d}z_0\mathrm{d}z_1$$
$$\le C_0C_i\int_M\int_M e^{\gamma\, d(z_0,z_1)^2}p^{\Delta}_{\tau_{k-1}}(x, z_0)p^{\Delta}_{\Delta_k\tau}(z_0, z_1)p^{\Delta}_{t-\tau_k}(z_1, y)\,\mathrm{d}z_0\mathrm{d}z_1$$
$$\le C_0C_i\, e^{\gamma\mathrm{diam}(M)^2}\int_M\int_M p^{\Delta}_{\tau_{k-1}}(x, z_0)p^{\Delta}_{\Delta_k\tau}(z_0, z_1)p^{\Delta}_{t-\tau_k}(z_1, y)\,\mathrm{d}z_0\mathrm{d}z_1$$
$$= C_0C_i\, e^{\gamma\mathrm{diam}(M)^2}p^{\Delta}_t(x, y)$$

so that the lemma also holds for all partitions τ such that $m(\tau) \leq i+1$, with the constant $C_{i+1} := C_0 C_i e^{\gamma \operatorname{diam}(M)^2}$. Since for all partitions τ of intervals $[0,t]$ with $t \leq T$, we have $m(\tau) \leq \lfloor T/\varepsilon \rfloor$, the constant $C_{\lfloor T/\varepsilon \rfloor}$ gives a bound for all such partitions, with no further restrictions. $\square$

Remark B.2.7. It is a fun fact, related to the above proof, that for a standard Brownian motion B_s^n in $\mathbb{R}^n$, the random variable $e^{|B_s|^2}$ is in L^1 (or equivalently, has a finite expectation value) if and only if $s < 1/4$. In particular, the lemma is true in $\mathbb{R}^n$ only if one restricts to partitions τ with $|\tau| < 1/4$. On a compact interval however, this expectation value is always finite.

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