



Strong short-time asymptotics and convolution approximation of the heat kernel

Matthias Ludewig¹

Received: 6 March 2018 / Accepted: 15 September 2018 / Published online: 22 September 2018
© The Author(s) 2018

Abstract

We give a short proof of a strong version of the short-time asymptotic expansion of heat kernels associated with Laplace-type operators acting on sections of vector bundles over compact Riemannian manifolds, including exponential decay of the difference of the approximate heat kernel and the true heat kernel. We use this to show that repeated convolution of the approximate heat kernels can be used to approximate the heat kernel on all of M , which is related to expressing the heat kernel as a path integral. This scheme is then applied to obtain a short-time asymptotic expansion of the heat kernel at the cut locus.

Keywords Heat kernel · Laplace operator · Manifold · Asymptotic expansion · Heat equation · Wave equation · Transmutation formula

1 Introduction and main results

Let M be a compact Riemannian manifold of dimension n and let L be a Laplace-type operator, acting on sections of a vector bundle \mathcal{V} over M . For $t > 0$, the heat kernel p_t^L of L is a smooth section of the bundle $\mathcal{V} \boxtimes \mathcal{V}^*$ over $M \times M$ (the vector bundle with fiber $\text{Hom}(V_y, V_x)$ over the point $(x, y) \in M \times M$). It is well known that for $x, y \in M$ close, the heat kernel has an asymptotic expansion of the form

$$p_t^L(x, y) \sim e_t(x, y) \sum_{j=0}^{\infty} t^j \frac{\Phi_j(x, y)}{j!}, \quad (1.1)$$

where

$$e_t(x, y) = \frac{e^{-d(x,y)^2/4t}}{(4\pi t)^{n/2}} \quad (1.2)$$

is the Euclidean heat kernel. (The name comes from the fact that $e_t(x, y)$ is the heat kernel in case that $M = \mathbb{R}^n$ and $L = \Delta$, the usual Laplace operator.) In (1.1), the “correction terms” $\Phi_j(x, y)$ are certain smooth sections of the bundle $\mathcal{V} \boxtimes \mathcal{V}^*$ over $M \times M$, where

✉ Matthias Ludewig
matthias_ludewig@gmx.de

¹ Max-Planck Institute for Mathematics, Vivatgasse 7, 53119 Bonn, Germany

$M \bowtie M = M \times M \setminus \{\text{cut points}\}$ is the set of points $(x, y) \in M \times M$ such that there is a unique minimizing geodesic connecting x and y (compare, e.g., [7, Section 2.5]). In this paper, we will prove that the asymptotic relation (1.1) can be made precise as follows.

Theorem 1.1 (Strong heat kernel asymptotics) *Let L be a Laplace-type operator, acting on sections of a vector bundle \mathcal{V} over a compact Riemannian manifold M . Then for any compact subset K of $M \bowtie M$, any $T > 0$ and any numbers $\nu, k, l, m \in \mathbb{N}_0$, there exists a constant $C > 0$ such that*

$$\left| \frac{\partial^k}{\partial t^k} \nabla_x^l \nabla_y^m \left\{ \frac{p_t^L(x, y)}{e_t(x, y)} - \sum_{j=0}^{\nu} t^j \frac{\Phi_j(x, y)}{j!} \right\} \right| \leq Ct^{\nu+1-k} \tag{1.3}$$

for all $(x, y) \in K$, whenever $0 < t \leq T$. Here $\Phi_j(x, y)$ are the heat kernel coefficients as discussed above.

In the theorem, ∇_x and ∇_y denote the covariant derivative with respect to the x (respectively y) variable, where we use any metric connection on the bundle \mathcal{V} (changing the connection only alters the constant C on the right-hand side).

Corollary 1.2 *We have the complete asymptotic expansion*

$$\frac{p_t^L(x, y)}{e_t(x, y)} \sim \sum_{j=0}^{\infty} t^j \frac{\Phi_j(x, y)}{j!}$$

in the sense of topological vector spaces, in the Fréchet topology of $C^\infty(M \bowtie M, \mathcal{V} \boxtimes \mathcal{V})$.

Usually, the asymptotic relation (1.1) is interpreted to say that for any $\nu \in \mathbb{N}_0$,

$$\left| p_t^L(x, y) - e_t(x, y) \sum_{j=0}^{\nu} t^j \frac{\Phi_j(x, y)}{j!} \right| \leq Ct^{\nu+1} \tag{1.4}$$

uniformly for (x, y) over compact subsets of $M \bowtie M$. This statement is much weaker than Thm. 1.1 (even in the case that $k = l = m = 0$), since the latter implies that the right-hand side of (1.4) can be replaced by $Ct^{\nu+1}e_t(x, y)$, which decays exponentially when $d(x, y) > 0$. Proofs for the weaker statement can be found in various places in the literature (see [7, Thm. 2.30], [30, Thm. 7.15], [31, 3.2], [5, III.E] just to name a few¹). The stronger result of Thm. 1.1 seems to be somewhat folklore, but to the author’s knowledge, no easily accessible proof exists in the literature outside either the theory of pseudo-differential operators, where one usually proves more general statements using a somewhat huge machinery (see, e.g., [17,24]), or the realm of stochastic analysis (e.g., [2,3,26]).

To illustrate the power of these results, we note that an easy corollary is the following result on the symmetry of heat kernel coefficients (compare Corollary 3.3), which is not at all obvious from the defining equations of the Φ_j and was previously proved using substantially more involved arguments (see Remark 3.4).

Theorem 1.3 *The heat kernel coefficients satisfy the symmetry relation*

$$\Phi_j(x, y) = (\Phi_j^*(y, x))^*,$$

where Φ_j^* are the heat kernel coefficients for the heat kernel p_t^* of the formally adjoint operator L^* and $(\Phi_j^*(y, x))^*$ denotes the fiberwise metric adjoint of $\Phi_j^*(y, x)$.

¹ Moreover, Chavel [10, p. 154] claims to prove a version of the strong statement, but his proof is based on the wrong Lemma 1 on p. 152, which is incorrectly cited from [5].

The first goal of this paper is to give an easy proof of Thm. 1.1 using the so-called *transmutation formula*, which relates the heat equation to the wave equation, and the Hadamard expansion of the wave kernel. This approach goes back to an older paper of Kannai [22], who proves a variant of Thm. 1.1 in the scalar case (compare also [34]).

Thm. 1.1 can be generalized to general complete manifolds. However, this is a somewhat intricate matter, as general Laplace-type operators need not have closed extensions generating operator semigroups. For formally self-adjoint Laplace-type operators L , we prove that they have at most one such self-adjoint extension and that if they do, a version of Thm. 1.1 holds for the corresponding heat kernel.

The asymptotic expansion (1.1) suggests to define *approximate heat kernels* $e_t^v(x, y)$ by

$$e_t^v(x, y) := \chi(d(x, y)) e_t(x, y) \sum_{j=0}^v t^j \frac{\Phi_j(x, y)}{j!}, \tag{1.5}$$

where $\chi : [0, \infty) \rightarrow [0, 1]$ is a smooth function with $\chi(r) = 1$ near zero and support contained in $[0, \text{inj}(M))$ (with $\text{inj}(M)$ denoting the injectivity radius of M). If for general smooth kernels $k, \ell \in C^\infty(M \times M, \mathcal{V} \boxtimes \mathcal{V}^*)$, we define their convolution $k * \ell$ by

$$(k * \ell)(x, y) := \int_M k(x, z)\ell(z, y)dz,$$

it turns out that the heat kernel $p_t^L(x, y)$ can be approximated by repeated convolutions of the kernel $e_t^v(x, y)$. More precisely, we have the following result.

Theorem 1.4 (Approximation by convolution) *Let L be a formally self-adjoint Laplace-type operator, acting on sections of a metric vector bundle \mathcal{V} over a compact Riemannian manifold M . Then for any $\delta > 0$ with*

$$\delta < \left(\frac{\text{inj}(M)}{\text{diam}(M)} \right)^2, \tag{1.6}$$

any $v \in \mathbb{N}_0$ and each $T > 0$, there exists a constant $C > 0$ such that

$$\left| p_t^L(x, y) - (e_{\Delta_1\tau}^v * \dots * e_{\Delta_N\tau}^v)(x, y) \right| \leq C p_t^\Delta(x, y) |\tau|^v t \tag{1.7}$$

for all $x, y \in M$ and for any partition $\tau = \{0 = \tau_0 < \tau_1 < \dots < \tau_N = t \leq T\}$ of an interval $[0, t]$ with $|\tau| \leq \delta t$, where p_t^Δ is the heat kernel of the Laplace–Beltrami operator on M . Here we used the notations $\Delta_j\tau := \tau_j - \tau_{j-1}$ and $|\tau| := \max_{1 \leq j \leq N} \Delta_j\tau$ for the increment, respectively the mesh of a partition τ .

This approximation result can be used in different regimes: If one fixes $t > 0$, one can make the C^k difference in between p_t^L and $e_{\Delta_1\tau}^v * \dots * e_{\Delta_N\tau}^v$ smaller than any given $\varepsilon > 0$, by choosing a partition τ fine enough. On the other hand, by choosing v large enough, this error can be made uniform in t .

The estimate from Thm. 1.4 is an *a posteriori* estimate, in the sense that the error depends on $p_t^\Delta(x, y)$, which itself is the (a priori unknown) solution to a differential equation. One can obtain an a priori estimate by using the Gaussian estimate from above [20, Thm. 5.3.4], $p_t^\Delta(x, y) \leq Ct^{-n/2+1/2}e_t(x, y)$, which holds on compact Riemannian manifolds: One gets that one can replace the result of Thm. 1.4 by the estimate

$$\left| p_t^L(x, y) - (e_{\Delta_1\tau}^v * \dots * e_{\Delta_N\tau}^v)(x, y) \right| \leq C e_t(x, y) |\tau|^v t^{3/2+v-n/2}. \tag{1.8}$$

This is a weaker statement, however, since, for example, if $(x, y) \in M \bowtie M$, one even has $p_t^\Delta(x, y) \leq C e_t(x, y)$ for all $0 < t \leq T$, so in this case, the additional factor of $t^{-n/2}$ can be dropped on the right-hand side of (1.8) (with the constant being uniform over compact subsets of $M \bowtie M$ in this case).

Similar approximation schemes and their relation to finite-dimensional approximation of path integrals have also been considered by Fine and Sawin, who use these to give a “path integral proof” of the Atiyah–Singer index theorem, see [14–16].

In this paper, we use Thm. 1.1 to analyze the short-time asymptotics of the heat kernel at the cut locus. We show that if the set of minimizing geodesics between x and y is a disjoint union of k submanifolds of the space of finite energy paths connecting x and y , having dimensions d_1, \dots, d_k (see Def. 5.1), then under a natural non-degeneracy condition, the heat kernel has an asymptotic expansion of the form

$$\frac{p_t^L(x, y)}{e_t(x, y)} \sim \sum_{l=1}^k (4\pi t)^{-d_l/2} \sum_{j=0}^\infty t^j \frac{\Phi_{j,l}(x, y)}{j!},$$

as $t \rightarrow 0$. In order to derive this result, we show that the convolution product $e_{\Delta_1 \tau}^\nu * \dots * e_{\Delta_N \tau}^\nu$ can be written as an integral over a certain space of piecewise geodesics paths, which can then be evaluated with Laplace’s method. See, e.g., [21,26,29], we obtain similar results using methods from stochastic analysis.

This paper is organized as follows. First we summarize some facts about the solution theory of the wave equation and introduce the transformation formula, which relates it to the heat equation. Here we also highlight some conditions for the Laplace-type operator that suffice to have the transmutation formula valid on complete manifolds and we use the formula to prove some results on essential self-adjointness. Subsequently, in Sect. 3, we introduce the Hadamard expansion of the solution operator to the heat equation and combine it with the transmutation formula to prove Thm. 1.1. We also briefly demonstrate how the well-known Gaussian estimates from above and below are derived using this technique. In the next section, we give a proof of Theorem. 1.4. In a final section, we reformulate this convolution product as a path integral, which is then analyzed to obtain an asymptotic expansion of the heat kernel $p_t^L(x, y)$ also in the case that x and y lie in each other’s cut locus. In “Appendix,” we prove a general version of Laplace’s method, which is needed in our considerations.

2 The wave equation and the transmutation formula

Let M be a complete Riemannian manifold of dimension n and let \mathcal{V} be a metric vector bundle over M . A Laplace-type operator L on \mathcal{V} is a second-order differential operator acting on sections of \mathcal{V} , which in local coordinates is given by

$$L = -\text{id}_{\mathcal{V}} g^{ij} \frac{\partial^2}{\partial x^i \partial x^j} + \text{lower-order terms},$$

where $\text{id}_{\mathcal{V}}$ is the identity endomorphism on the vector bundle \mathcal{V} and (g^{ij}) is the inverse matrix of the matrix (g_{ij}) describing the metric in the local coordinates. Any such operator can be written as $L = \nabla^* \nabla + V$ for a unique metric connection ∇ and a self-adjoint endomorphism field V [7, Section 2.1]. For example, if L is acting on functions (i.e., sections of the trivial line bundle), we could have $L = \Delta + v$ with Δ the Laplace–Beltrami operator and v some potential function. Considered as an unbounded operator on $L^2(M, \mathcal{V})$, a natural domain for L is the space $\mathcal{D}(M, \mathcal{V}) := C_c^\infty(M, \mathcal{V})$, the space of smooth, compactly supported sections

of the bundle \mathcal{V} (which, when necessary, is endowed with the usual test function topology). We say that L is formally self-adjoint if it is symmetric on this domain.

Given such a Laplace-type operator L , one can consider the *wave equation*

$$(\partial_{tt} + L)u_t = 0. \tag{2.1}$$

A fundamental feature of the wave equation is the *energy estimate*, which states that for any compact set $K \subseteq M$, any $m \in \mathbb{R}$ and any $T > 0$, there exists a constant $\alpha \in \mathbb{R}$ such that for all smooth solutions u of the wave equation with $\text{supp } u_0 \subseteq K$, one has

$$\|u_t\|_{H^m}^2 + \|u'_t\|_{H^{m-1}}^2 \leq e^{\alpha(t-s)} (\|u_s\|_{H^m}^2 + \|u'_s\|_{H^{m-1}}^2) \tag{2.2}$$

whenever $-T \leq s \leq t \leq T$ (see, e.g., [9, Thm. 8]).

From the theory of wave equations follows that there is a family of solution operators $G_t : \mathcal{D}(M, \mathcal{V}) \rightarrow \mathcal{D}(M, \mathcal{V})$ such that for $\psi \in \mathcal{D}(M, \mathcal{V})$, $u_t := G_t\psi$ solves the wave equation (2.1) with initial conditions $u_0 = 0, u'_0 = \psi$. We also have its derivative G'_s , which has the property that $u_t := G'_t\psi$ solves the wave equation with initial condition $u_0 = \psi, u'_0 = 0$ (see, e.g., Corollary 14 in [9]).

Instead of the wave equation, we can also consider the *heat equation*

$$(\partial_t + L)u_t = 0. \tag{2.3}$$

Here we only need to specify an initial condition ψ at time zero to have a unique (bounded) solution. This leads to a solution operator e^{-tL} , mapping the initial condition ψ to the solution u_t . The heat equation is related to the wave equation as follows.

Theorem 2.1 (Transmutation formula) *Let M be a complete Riemannian manifold and let L be a Laplace-type operator, acting on sections of a metric vector bundle \mathcal{V} over M . Suppose that the wave operators G_t and G'_t defined on $\mathcal{D}(M, \mathcal{V})$ extend to strongly continuous families of operators on $L^2(M, \mathcal{V})$ satisfying the norm bound*

$$\|G_t\|, \|G'_t\| \leq Ce^{\alpha|t|} \tag{2.4}$$

for some $C > 0, \alpha \in \mathbb{R}$. Then setting

$$e^{-tL}u = \int_{-\infty}^{\infty} \gamma_t(s)G'_s u \, ds, \quad \text{with} \quad \gamma_t(s) := (4\pi t)^{-1/2}e^{-s^2/4t} \tag{2.5}$$

for $u \in L^2(M, \mathcal{V})$ defines a strongly continuous semigroup of operators, the infinitesimal generator of which is an extension of L with $\text{dom}(L) = \mathcal{D}(M, \mathcal{V})$.

Remark 2.2 Of course, the continuous extensions of G_t respectively G'_t , if they exist, are unique, since $\mathcal{D}(M, \mathcal{V})$ is dense in $L^2(M, \mathcal{V})$.

Remark 2.3 The same result is true when $L^2(M, \mathcal{V})$ is replaced by any Banach space E of distributions containing $\mathcal{D}(M, \mathcal{V})$ as a dense subset and such that the inclusion of E into $\mathcal{D}'(M, \mathcal{V})$ is continuous.

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

$$P_t u := \int_{-\infty}^{\infty} \gamma_t(s)G'_s u \, ds.$$

By the norm bound on G'_t , the integral on the right-hand (2.5) converges absolutely for each $t > 0$, and P_t is a locally uniformly bounded family of operators. We now verify that P_t is a strongly continuous semigroup. First, because γ_t integrates to one over the line, we have

$$\|P_t u - u\|_{L^2} = \left\| \int_{-\infty}^{\infty} \gamma_t(s)(G'_s u - u) ds \right\|_{L^2} \leq \int_{-\infty}^{\infty} \gamma_t(s) \|G'_s u - u\|_{L^2} ds.$$

for all $u \in L^2(M, \mathcal{V})$. Because G'_s is strongly continuous by assumption and $G'_0 u = u$, the function $\|G'_s u - u\|_{L^2}$ is continuous in s and vanishes at zero. Now $\|P_t u - u\|_{L^2} \rightarrow 0$ follows from the well-known fact that $\gamma_t \rightarrow \delta_0$ as $t \rightarrow 0$.

To verify the semigroup property, we use that for any $s, t \in \mathbb{R}$ and $\psi \in \mathcal{D}(M, \mathcal{V})$, we have the “trigonometric formula”

$$G'_s G'_t \psi = G'_{s+t} \psi - G_s G_t L \psi,$$

which can easily be verified by fixing s and noticing that both sides satisfy the wave equation with respect to the variable t and with the same initial conditions. The energy estimate (2.2) implies then that their difference must be zero. Now

$$\begin{aligned} (\varphi, P_s P_t \psi)_{L^2} &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \gamma_t(u) \gamma_s(v) (\varphi, G'_u G'_v \psi)_{L^2} dv du \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \gamma_t(u) \gamma_s(v) ((\varphi, G'_{u+v} \psi)_{L^2} - (\varphi, G_u G_v L \psi)_{L^2}) dv du, \end{aligned}$$

where the integral over each individual term is absolutely convergent by the bound (2.4) on G_u and G'_u . Because G_u is an odd function of u , the term involving $G_u G_v L \psi$ integrates to zero. Therefore,

$$\begin{aligned} (\varphi, P_s P_t \psi)_{L^2} &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \gamma_t(u) \gamma_s(v) (\varphi, G'_{u+v} \psi)_{L^2} dv du \\ &= \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} \gamma_t(r - v) \gamma_s(v) dv \right) (\varphi, G'_r \psi)_{L^2} dr \\ &= \int_{-\infty}^{\infty} \gamma_{s+t}(r) (\varphi, G'_r \psi)_{L^2} dr = (\varphi, P_{t+s} \psi)_{L^2}. \end{aligned}$$

Hence, $P_s P_t = P_{t+s}$ on the dense subset $\mathcal{D}(M, \mathcal{V}) \subset L^2(M, \mathcal{V})$ and by boundedness also on all of $L^2(M, \mathcal{V})$. This shows that P_t is a strongly continuous semigroup of operators.

To see what the infinitesimal generator of P_t is, notice that for $\psi \in \mathcal{D}(M, \mathcal{V})$, the estimates on G_t and G'_t justify the calculation

$$\begin{aligned} P'_t \psi &= \int_{-\infty}^{\infty} \gamma'_t(s) G'_s \psi ds = \int_{-\infty}^{\infty} \frac{\partial^2}{\partial s^2} \gamma_t(s) G'_s \psi ds \\ &= \int_{-\infty}^{\infty} \frac{\partial}{\partial s} \gamma_t(s) G_s L \psi ds = - \int_{-\infty}^{\infty} \gamma_t(s) G'_s L \psi ds = -L P_t \psi. \end{aligned}$$

This shows that the infinitesimal generator \bar{L} (which is always closed for a strongly continuous semigroup) is an extension of the operator L with $\text{dom}(L) = \mathcal{D}(M, \mathcal{V})$. □

In particular, the result is applicable to the compact setting:

Lemma 2.4 *For any Laplace-type operator acting on sections of a metric vector bundle over a compact Riemannian manifold, the assumptions of Thm. 2.1 are satisfied.*

Proof The bound (2.4) follows directly from the energy estimate (2.2) in this case, since one can take $K = M$ and it is also clear that one can take the same α for each T . \square

Furthermore, it is well known that on a compact manifold, any Laplace-type operator L has a unique closed extension that is the generator of a strongly continuous semigroup (this follows, e.g., from Lemma 2.16 in [7]).

A consequence of Thm. 2.1 is the following.

Theorem 2.5 *Let L be a formally self-adjoint Laplace-type operator, acting on sections of a metric vector bundle over a complete Riemannian manifold. Considered as an unbounded symmetric operator with domain $\mathcal{D}(M, \mathcal{V})$, L admits at most one self-adjoint extension \bar{L} that generates a strongly continuous semigroup of operators. If there is such an extension, then the assumptions of Thm. 2.1 are satisfied.*

Proof Let \bar{L} be a self-adjoint extension of L that generates a strongly continuous semigroup of operators. By the Hille–Yosida theorem, there exists $\omega \in \mathbb{R}$ such that the spectrum of \bar{L} is contained in $[\omega, \infty)$, and $e^{-t\bar{L}}$ is given in terms of spectral calculus via the absolutely convergent integral

$$(u, e^{-t\bar{L}}v)_{L^2} = \int_{-\infty}^{\infty} e^{-t\lambda} d(u, E_\lambda v)_{L^2},$$

for $u, v \in L^2(M, \mathcal{V})$, where E_λ is the spectral measure associated with \bar{L} . Consider the entire function

$$g_s(\lambda) := \sum_{k=0}^{\infty} \frac{s^{2k+1}\lambda^k}{(2k+1)!}$$

For $\lambda > 0$, we have $g_s(\lambda) = \sin(s\sqrt{\lambda})/\sqrt{\lambda}$ and $g_s(-\lambda) = \sinh(s\sqrt{\lambda})/\sqrt{\lambda}$, while $g'_s(\lambda) = \cos(s\sqrt{\lambda})$ and $g'_s(-\lambda) = \cosh(s\sqrt{\lambda})$. Hence, we obtain that

$$\|g_s|_{[\omega, \infty)}\|_{\infty} \leq e^{s\omega}, \quad \|g'_s|_{[\omega, \infty)}\|_{\infty} \leq e^{s\omega}.$$

By standard properties of the functional calculus, one obtains the estimates $\|g_s(\bar{L})\| \leq e^{s\omega}$, $\|g'_s(\bar{L})\| \leq e^{s\omega}$ on the operator norms.

We now claim that the wave operator G_s on $\mathcal{D}(M, \mathcal{V})$ is given by $G_s = g_s(\bar{L})|_{\mathcal{D}(M, \mathcal{V})}$. To see this, notice that for any $\psi \in \mathcal{D}(M, \mathcal{V})$, $g_s(\bar{L})\psi$ satisfies the wave equation (2.1) with initial conditions $g_0(\bar{L})\psi = 0$, $g'_0(\bar{L})\psi = \psi$. Hence, $u_s := G_s\psi - g_s(\bar{L})\psi$ satisfies the wave equation with initial conditions $u_0 = 0$, $u'_0 = 0$, which implies $u_s \equiv 0$ by the energy estimate (2.2). The same argument shows that $G'_s = g'_s(\bar{L})|_{\mathcal{D}(M, \mathcal{V})}$.

By the above, G_s and G'_s satisfy the norm bound (2.4). To see that G_s and G'_s are strongly continuous, we argue as follows: By Lebesgue’s theorem of dominated convergence, one obtains that for all $u, v \in L^2(M, \mathcal{V})$, one has $(u, G_s v)_{L^2} \rightarrow (u, G_t v)_{L^2}$ as $s \rightarrow t$, i.e., $G_s v \rightarrow G_t v$ weakly. Similarly, $\|(G_s v)_{L^2} = (v, G_s^2 v)_{L^2} \rightarrow (v, G_t^2 v)_{L^2} = \|G_t v\|_{L^2}$. Now it is well known that in Hilbert spaces, weak convergence plus convergence of norms implies convergence in norm, so we obtain $G_s v \rightarrow G_t v$ in $L^2(M, \mathcal{V})$. This shows that G_s is strongly continuous and the argument for G'_s is the same.

Now by Thm. 2.1, there is some extension \bar{L}_2 of L with domain containing $\mathcal{D}(M, \mathcal{V})$ that generates a strongly continuous semigroup of operators given by the transmutation formula (2.5). However, by Fubini’s theorem,

$$\int_{-\infty}^{\infty} \gamma_t(s)(u, G'_s v)_{L^2} ds = \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} \gamma_t(s)g_s(\lambda) ds \right) d(u, E_\lambda v)_{L^2},$$

where the interior integral is easily found to equal $e^{-t\lambda}$, e.g., by expanding $g_s(\lambda)$ into its power series and using standard formulas for the moments of a one-dimensional Gaussian measure (see, e.g., Lemma 2.12 in [7]). Therefore, the semigroup generated by \bar{L}_2 equals the semigroup generated by \bar{L} .

These arguments show that self-adjoint extension of L generating a strongly continuous semigroup of operators, this semigroup is given by the transmutation formula (3.1). However, this formula does not depend on the self-adjoint extension (because the operator G_s doesn't), so any two strongly continuous operator semigroups generated by self-adjoint extensions of L must coincide. But this implies that also the self-adjoint extensions coincide, because the infinitesimal generator of an operator semigroup is unique. \square

Example 2.6 For example, if $L = \nabla^* \nabla + V$ for some connection ∇ on \mathcal{V} and a symmetric endomorphism field V that is bounded from below (meaning that there exists $\omega \in \mathbb{R}$ such that $\langle w, Vw \rangle > \omega$ for all $w \in \mathcal{V}$), then L has a self-adjoint extension that generates a strongly continuous semigroup. Namely, because for $u \in L^2(M, \mathcal{V})$,

$$(u, Lu)_{L^2} = \|\nabla u\|_{L^2}^2 + (u, Vu)_{L^2} \geq \omega \|u\|_{L^2}^2,$$

the operator L is semi-bounded and it is well known that it has a self-adjoint extension, called Friedrich extension (see, e.g., [35, VII.2.11]), which satisfies the same bound and therefore generates an operator semigroup by functional calculus. We obtain that in this setting, the Friedrichs extension is the only self-adjoint extension that is the generator of a strongly continuous semigroup.

In particular, this applies to $\Delta = d^*d$, the Laplace–Beltrami operator acting on functions.

Example 2.7 The Hodge Laplacian $L = (d + d^*)^2$ on differential forms is a positive operator and hence has a self-adjoint extension generating a strongly continuous semigroup by the same argument. By Thm. 2.5, this is the only self-adjoint extension generating a strongly continuous semigroup of operators. In fact, it is the only self-adjoint extension, by Thm. 2.4 in [33]. For the same reason, for any self-adjoint Dirac-type operator D , the corresponding Laplacian D^2 has a unique self-adjoint extension generating a strongly continuous semigroup of operators. Also in this case, it is known that D and D^2 are even essentially self-adjoint (i.e., they have unique self-adjoint extensions), compare [36].

Example 2.8 In contrast, there are formally self-adjoint Laplace-type operators that do not admit any self-adjoint extension. For example, the operator $L = -\Delta - x^4$ on $M = \mathbb{R}$ does not admit a self-adjoint extension (see Ex. 3 on p. 86 in [8]). There are also essentially self-adjoint Laplace-type operators which do not generate a strongly continuous family of operators, see, e.g., [32].

Remark 2.9 Our observations show that matters can be quite subtle on general complete manifolds: A formally self-adjoint Laplace-type operator need not have a self-adjoint extension, nor need it be unique. Furthermore, not all self-adjoint extensions generate a strongly continuous semigroup of operators. (They do if and only if the spectrum is bounded from below.) However, there is at most one self-adjoint extension that generates a strongly continuous semigroup of operators. We do not know of an example of a formally self-adjoint Laplace-type operator that admits two different self-adjoint extensions, one of which generates a strongly continuous semigroup and the other doesn't. (By Thm. 2.5, not both of them can generate a strongly continuous semigroup of operators.)

3 Heat kernel asymptotics

In this section, we prove the following more general version of Thm. 1.1.

Theorem 3.1 (Strong heat kernel asymptotics) *Let L be a Laplace-type operator, acting on sections of a vector bundle \mathcal{V} over a complete Riemannian manifold M . Suppose that the assumptions of Thm. 2.1 are satisfied (e.g., when M is compact or L is formally self-adjoint and semi-bounded). Then for any compact subset K of $M \bowtie M$, any $T > 0$ and any numbers $\nu, k, l, m \in \mathbb{N}_0$, there exists a constant $C > 0$ such that*

$$\left| \frac{\partial^k}{\partial t^k} \nabla_x^l \nabla_y^m \left\{ \frac{p_t^L(x, y)}{e_t(x, y)} - \sum_{j=0}^{\nu} t^j \frac{\Phi_j(x, y)}{j!} \right\} \right| \leq C t^{\nu+1-k}$$

for all $(x, y) \in K$, whenever $0 < t \leq T$. Here $\Phi_j(x, y)$ are certain smooth sections of the bundle $\mathcal{V} \boxtimes \mathcal{V}^*$ over $M \bowtie M$.

The proof will use the transmutation formula (3.1), which in terms of integral kernels translates into

$$p_t^L(x, y) := \int_{-\infty}^{\infty} \gamma_t(s) G'(s, x, y) ds, \tag{3.1}$$

where $G'(s, x, y)$ is the Schwartz kernel of the operator G_s . This integral is meant as a distributional integral, i.e., for test functions $\varphi \in \mathcal{D}(M, \mathcal{V}^*)$, $\psi \in \mathcal{D}(M, \mathcal{V})$, we set

$$p_t^L[\varphi \otimes \psi] := \int_{-\infty}^{\infty} \gamma_t(s) G'_s[\varphi \otimes \psi] ds \tag{3.2}$$

Let us verify that this indeed defines a distribution on $M \times M$ for each $t > 0$, provided that the assumptions of Thm. 2.1 hold. Namely, by the estimate on G'_s , we have

$$|G'_s[\varphi \otimes \psi]| = |(\varphi, G_s \psi)_{L^2}| \leq C e^{\alpha|s|} \|\varphi\|_{L^2} \|\psi\|_{L^2}, \tag{3.3}$$

which shows that the integral (3.1) is absolutely convergent. We furthermore have

$$|p_t^L[\varphi \otimes \psi]| \leq \left(C \int_{-\infty}^{\infty} \gamma_t(s) e^{\alpha|s|} ds \right) \|\varphi\|_{L^2} \|\psi\|_{L^2}$$

for all $\varphi \in \mathcal{D}(M, \mathcal{V}^*)$, $\psi \in \mathcal{D}(M, \mathcal{V})$, which shows that p_t^L is indeed a well-defined distribution.

The wave kernel $G(t, x, y)$ has an asymptotic expansion, the Hadamard expansion, which describes its singularity structure. To state the result, we introduce the *Riesz distributions* $R(\alpha; t, x, y) \in \mathcal{D}(M \bowtie M)$. Namely, for $\text{Re}(\alpha) > n + 1$, we set

$$R(\alpha; t, x, y) := C(\alpha) \text{sign}(t) (t^2 - d(x, y)^2)_+^{\frac{\alpha-n-1}{2}}, \quad C(\alpha) := \frac{2^{1-\alpha} \pi^{\frac{1-n}{2}}}{\Gamma(\frac{\alpha}{2}) \Gamma(\frac{\alpha-n+1}{2})},$$

where $(t^2 - d(x, y)^2)_+$ denotes the positive part. Hence, $R(\alpha; t, x, y)$ 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 [6] because our space time $\mathbb{R} \times M$ is $n + 1$ -dimensional. The distributions $R(\alpha)$ discussed here are related to the distributions $R_{\pm}(\alpha)$ in Section 1.4 of [6] by $R(\alpha) = R_+(\alpha) - R_-(\alpha)$). For $\text{Re}(\alpha) > n + 1$, 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 $\{\text{Re}(\alpha) > n + 1\}$ that

has a holomorphic extension to all of \mathbb{C} [6, Lemma 1.2.2 (4)]. This defines $R(\alpha; t, x, y) \in \mathcal{D}'(\mathbb{R} \times M \times M)$ for all $\alpha \in \mathbb{C}$.

Now on $M \times M$, the distribution $G(t, x, y)$ has the asymptotic expansion [6, Ch. 2]

$$G(t, x, y) \sim \sum_{j=0}^{\infty} \Phi_j(x, y)R(2 + 2j; t, x, y), \tag{3.4}$$

where the $\Phi_j(x, y) \in C^\infty(M \times M, \mathcal{V} \boxtimes \mathcal{V}^*)$ are coefficients determined by certain transport equations. The asymptotic expansion (3.4) is meant in the sense that the difference

$$\delta^\nu(t, x, y) := G(t, x, y) - \sum_{j=0}^{\nu} \Phi_j(x, y)R(2 + 2j; t, x, y) \tag{3.5}$$

can be made arbitrarily smooth by increasing the number ν of correction terms; in fact, $\delta^\nu \in C^k(\mathbb{R} \times M \times M, \mathcal{V} \boxtimes \mathcal{V}^*)$ whenever $\nu \geq (n + 1)/2 + k$ [6, 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

$$\left| \frac{\partial^j}{\partial t^j} \nabla_x^l \nabla_y^m \delta^\nu(t, x, y) \right| \leq C(t^2 - d(x, y)^2)_+^{(k-j-l-m)/2} \tag{3.6}$$

uniformly over compact subsets of $M \times M$ and $t \leq T$, whenever $k \geq l + m$ (compare [6, Thm. 2.5.2]).

Lemma 3.2 *For all $j \in \mathbb{N}_0$, $t > 0$ and all $(x, y) \in M \times M$, we have*

$$\frac{1}{2t} \int_{-\infty}^{\infty} \gamma_t(s)R(2 + 2j; s, x, y) s \, ds = e_t(x, y) \frac{t^j}{j!}, \tag{3.7}$$

where $e_t(x, y)$ is the Euclidean heat kernel, defined in (1.2). In particular, the distributional integral on the left-hand side actually yields a smooth function.

Proof For $\text{Re}(\alpha) > n + 1$, consider the absolutely convergent integral

$$\begin{aligned} \frac{1}{2t} \int_{-\infty}^{\infty} \gamma_t(s)R(\alpha; s, x, y) s \, ds &= \frac{C(\alpha)}{2t} \int_{-\infty}^{\infty} \gamma_t(s)(s^2 - d(x, y)^2)_+^{\frac{\alpha-n-1}{2}} |s| \, ds \\ &= \frac{C(\alpha)}{t} \int_0^{\infty} \gamma_t(s)(s^2 - d(x, y)^2)_+^{\frac{\alpha-n-1}{2}} s \, ds \\ &= \frac{C(\alpha)}{t} \int_{d(x,y)}^{\infty} \gamma_t(s)(s^2 - d(x, y)^2)^{\frac{\alpha-n-1}{2}} s \, ds \end{aligned}$$

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 $s ds = u du$. Therefore, we obtain

$$\int_{d(x,y)}^{\infty} \gamma_t(s)(s^2 - d(x, y)^2)^{\frac{\alpha-n-1}{2}} s \, ds = \gamma_t(d(x, y)) \int_0^{\infty} e^{-u^2/4t} u^{\alpha-n} \, du.$$

Now, substituting $u^2/4t = r$, the integral can be brought into the form of a gamma-integral, giving

$$\int_0^{\infty} e^{-u^2/4t} u^{\alpha-n} \, du = t^{1/2} (4t)^{\frac{\alpha-n}{2}} \int_0^{\infty} e^{-r} r^{\frac{\alpha-n-1}{2}} \, dr = t^{1/2} (4t)^{\frac{\alpha-n}{2}} \Gamma\left(\frac{\alpha - n + 1}{2}\right).$$

Put together, we arrive at

$$\begin{aligned} \frac{1}{2t} \int_{-\infty}^{\infty} \gamma_t(s) R(\alpha; s, x, y) s \, ds &= \gamma_t(d(x, y)) \frac{C(\alpha)}{t} t^{1/2} (4t)^{\frac{\alpha-n}{2}} \Gamma\left(\frac{\alpha-n+1}{2}\right) \\ &= e_t(x, y) \frac{t^{\frac{\alpha-2}{2}}}{\Gamma(\alpha/2)}. \end{aligned} \tag{3.8}$$

Until now, we have restricted ourselves to the case $\text{Re } \alpha > n + 1$. However, for both sides of the last equation, if we pair them with a test function $\varphi \in \mathcal{D}(M \times M)$, the result will be an entire holomorphic function in α . Because they coincide for $\text{Re } \alpha > n + 1$, they must coincide everywhere, by the identity theorem for holomorphic functions.

The statement of the lemma is the particular result for $\alpha = 2 + 2j, j \in \mathbb{N}_0$. □

Proof (of Thm. 3.1) Integrating by parts in (3.1), which is justified by the estimate (2.4), we obtain

$$\begin{aligned} p_t^L(x, y) &= \int_{-\infty}^{\infty} \gamma_t(s) G'(s, x, y) \, ds \\ &= \int_{-\infty}^{\infty} \gamma_t(s) G(s, x, y) \frac{s}{2t} \, ds \end{aligned} \tag{3.9}$$

where the identity is to be interpreted in the distributional sense. Now for any $\nu \in \mathbb{N}$, we have

$$p_t^L(x, y) = \sum_{j=0}^{\nu} \frac{\Phi_j(x, y)}{2t} \int_{-\infty}^{\infty} \gamma_t(s) R(2 + 2j; s, x, y) s \, ds + \frac{1}{2t} \int_{-\infty}^{\infty} \gamma_t(s) \delta^\nu(s, x, y) s \, ds,$$

where $\delta^\nu(t, x, y)$ is in C^k whenever $\nu \geq (n+1)/2+k$. By Lemma 3.2, the first term evaluates to

$$\sum_{j=0}^{\nu} \frac{\Phi_j(x, y)}{2t} \int_{-\infty}^{\infty} \gamma_t(s) R(2 + 2j; s, x, y) s \, ds = e_t(x, y) \sum_{j=0}^{\nu} t^j \frac{\Phi_j(x, y)}{j!}.$$

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

$$r^\nu(t, x, y) := \frac{1}{2t} \int_{-\infty}^{\infty} \gamma_t(s) \delta^\nu(s, x, y) s \, ds = \frac{1}{t} \int_{d(x,y)}^{\infty} \gamma_t(s) \delta^\nu(s, x, y) s \, ds,$$

as $\delta^\nu(s, x, y) = 0$ if $s < d(x, y)$, because of (3.6). Substituting $s = \sqrt{u^2 + d(x, y)^2}$ as before, one obtains

$$r^\nu(t, x, y) = \frac{\gamma_t(d(x, y))}{t} \int_0^{\infty} e^{-\frac{u^2}{4t}} \delta^\nu(\sqrt{u^2 + d(x, y)^2}, x, y) u \, du.$$

Setting $\tilde{\delta}^\nu(u, x, y) := \delta_\nu(\sqrt{u^2 + d(x, y)^2}, x, y)$ one has that $\tilde{\delta}^\nu$ is C^k whenever δ^ν is C^k , and from (3.6) follows the estimate

$$\left| \frac{\partial^i}{\partial u^i} \nabla_x^l \nabla_y^m \tilde{\delta}^\nu(u, x, y) \right| \leq C u^{k-i-l-m}. \tag{3.10}$$

which is valid whenever $k \geq i + l + m$ and uniform over x, y in compact subsets of $M \times M$ and $u \leq T$. Now the function $e^{-u^2/4t}$ satisfies

$$-\frac{2t}{u} \frac{\partial}{\partial u} e^{-u^2/4t} = e^{-u^2/4t},$$

hence for any $r, l, m \in \mathbb{N}_0$, one obtains

$$\nabla_x^l \nabla_y^m \left\{ \frac{r^\nu(t, x, y)}{e_t(x, y)} \right\} = \frac{(2t)^r}{t} \int_0^\infty \gamma_t(u) \frac{\partial}{\partial u} \left(\frac{1}{u} \frac{\partial}{\partial u} \right)^{r-1} \nabla_x^l \nabla_y^m \delta^\nu(u, x, y) du.$$

if ν is large enough, depending on l and m . The estimate (3.10) shows that these manipulations make sense when ν is large enough, i.e., in this case, the integral is absolutely convergent and uniformly bounded independent of t . Therefore, for any ν , one can find $\tilde{\nu} \geq \nu$ large enough so that

$$\left| \frac{\partial^i}{\partial t^i} \nabla_x^l \nabla_y^m \left\{ \frac{p_t^L(x, y)}{e_t(x, y)} - \sum_{j=0}^{\tilde{\nu}} t^j \frac{\Phi_j(x, y)}{j!} \right\} \right| \leq C t^{\nu+1-i},$$

where the estimate is uniform for (x, y) in compact subsets of $M \bowtie M$ and $t \leq T$. However, the calculation

$$\begin{aligned} & \left| \frac{\partial^i}{\partial t^i} \nabla_x^l \nabla_y^m \left\{ \frac{p_t(x, y)}{e_t(x, y)} - \sum_{j=0}^{\nu} t^j \frac{\Phi_j(x, y)}{j!} \right\} \right| \\ & \leq \left| \frac{\partial^i}{\partial t^i} \nabla_x^l \nabla_y^m \left\{ \frac{p_t(x, y)}{e_t(x, y)} - \sum_{j=0}^{\tilde{\nu}} t^j \frac{\Phi_j(x, y)}{j!} \right\} \right| + \left| \frac{\partial^i}{\partial t^i} \sum_{j=\nu+i}^{\nu} t^j \frac{\nabla_x^l \nabla_y^m \Phi_j(x, y)}{j!} \right| \\ & \leq C' t^{\nu+1-i} \end{aligned}$$

shows that in fact $\tilde{\nu} = \nu$ suffices. □

Corollary 3.3 *The heat kernel coefficients satisfy the symmetry relation*

$$\Phi_j(x, y) = (\Phi_j^*(y, x))^*,$$

where Φ_j^* are the heat kernel coefficients for the heat kernel p_t^* of the formally adjoint operator L^* and $(\Phi_j^*(y, x))^*$ denotes the fiberwise metric adjoint of $\Phi_j^*(y, x)$.

Proof By Theorem 1.1, this follows from the fact that the heat kernel itself satisfies the same symmetry relation by Prop. 2.17 (2) in [7]. Note that this argument does not work if one only knows (1.4). □

Remark 3.4 Corollary 3.3 is not at all obvious from the defining transport equations for the Φ_j . The result was previously proved in the scalar case by Moretti [27,28] for the heat equation and the Hadamard coefficients by approximating the given metric by real analytic metrics. However, for the heat kernel coefficients, this comes out directly from Thm. 1.1.

In the remainder of this section, we demonstrate how to obtain Gaussian estimates on p_t^L using our techniques.

Theorem 3.5 (Gaussian upper bound) *Let L be a formally self-adjoint Laplace-type operator acting on sections of a vector bundle \mathcal{V} over a compact manifold M and let p_t be its heat kernel. Then for any $T > 0$, there exists a constant $C > 0$ such that*

$$\left| \frac{\partial^j}{\partial t^j} \nabla_x^m \nabla_y^l p_t(x, y) \right| \leq C t^{-(n+2j+m+l+1)} e^{-\frac{d(x,y)^2}{4t}}$$

for all $x, y \in M$, whenever $t \leq T$.

Remark 3.6 In fact, the upper bound can be improved to have a pre-factor of $t^{-n+1/2}$ instead of t^{-n-1} in the case $j = m = l = 0$ [20, Thm. 5.3.4]. This result is then sharp, as seen, e.g., by the example of two antipodal points of a sphere [20, Example 5.3.3]. Of course, if $(x, y) \in M \bowtie M$, then the correct exponent is $t^{-n/2}$ near (x, y) , by Thm. 1.1.

Proof (sketch) The Schwartz kernel $G'(t, x, y)$ of G'_t as a distribution on $\mathbb{R} \times M \times M$ has order at most $n + 1$, i.e., it is a sum of $(n + 1)$ -st distributional derivatives of continuous functions. This follows from the asymptotic expansion (3.4) and the fact that the Riesz distribution $R(2 + 2j)$ has distributional order at most $n + 1 - 2j$ for $0 \leq 2j < n + 1$ and is continuous if $2j \geq n + 1$ [6, Section 1.2]. The wavefront set of $G'(t, x, y)$ is contained in the characteristics of the wave operator $\partial_{tt} + L$, (i.e., the “light cone”) which are transversal to the submanifolds $\mathbb{R} \times \{(x, y)\} \subset \mathbb{R} \times M \times M$. Therefore, one can restrict G' to these submanifolds, so that for $(x, y) \in M \times M$ fixed, $G'(t, x, y)$ is a distribution on \mathbb{R} of order at most $n + 1$ in the variable t . Similarly, $\frac{\partial^j}{\partial t^j} \nabla_x^k \nabla_y^l G'(t, x, y)$ is a distribution of order at most $k := n + 1 + m + l + j$ on \mathbb{R} . This means that

$$\frac{\partial^j}{\partial t^j} \nabla_x^m \nabla_y^l G'(t, x, y) = \frac{\partial^k}{\partial t^k} f(t, x, y) \tag{3.11}$$

in the sense of distributions for some L^1 function $f(s, x, y)$. Using the transmutation formula (3.1) and integration by parts, we obtain

$$\nabla_x^m \nabla_y^l p_t(x, y) = (-1)^k \int_{-\infty}^{\infty} \frac{\partial^k}{\partial s^k} \gamma_t(s) f(s, x, y) ds,$$

which gives a pre-factor of order $-k$ in t . Here, the integration by parts is justified by standard energy estimates. Differentiating j times by t gives another pre-factor of order $-2j$ in t .

The result now follows from the fact that $G'(s, x, y)$ and hence also $f(s, x, y)$ is equal to zero for $|s| < d(x, y)$, by finite propagation speed of the wave equation. \square

Remark 3.7 If n is even, $R(2 + 2j)$ is in fact of order $n - 2j$. This improves the estimate of Thm. 3.5 to a pre-factor of $t^{-(n+2j+m+l)}$ on the right-hand side in even dimensions.

Theorem 3.8 (Gaussian lower bound) *Let M be a compact Riemannian manifold and let L be a scalar Laplace-type operator L , i.e., a Laplace-type operator acting on functions on M . Then for any $T > 0$, there exists a constant $C > 0$ such that*

$$e_t(x, y) \leq C p_t^L(x, y)$$

for all $x, y \in M$, whenever $t \leq T$.

Proof (sketch) For some $\nu \geq 1$, let $e_t^\nu(x, y)$ be the approximate heat kernel of L defined in (1.5). Because of Thm. 1.1, there exists $C > 0$ such that for any $N \in \mathbb{N}$, we have

$$\underbrace{(e_{t/N}^\nu * \dots * e_{t/N}^\nu)}_{N \text{ times}}(x, y) \leq (C p_{t/N}^L * \dots * C p_{t/N}^L)(x, y) = C^N p_t^L(x, y)$$

On the other hand, by Lemma 5.7², the convolution product $e_{t/N}^\nu * \dots * e_{t/N}^\nu$ can be written as an integral over the manifold $H_{xy;\tau}(M)$ of piecewise geodesics (introduced in Sect. 5),

² In order to not raise the impression that our arguments are circular, we emphasize here that Lemma 5.7 used here does not depend on Thm. 3.8 or any material in between; it is a purely elementary calculation.

where $\tau := \{0 < \frac{1}{N} < \frac{2}{N} < \dots < \frac{N-1}{N} < 1\}$ denotes the equidistant partition of the interval $[0, 1]$. More specifically,

$$(e_{t/N} * \dots * e_{t/N}^v)(x, y) = (4\pi t)^{-nN/2} \int_{H_{xy;\tau}(M)} e^{-E(\gamma)/2t} \Upsilon_{\tau,v}(t, \gamma) d\gamma,$$

where E is the energy functional (5.1) and $\Upsilon_{\tau,v}(t, \gamma)$ is some smooth function on $H_{xy;\tau}(M)$, depending polynomially on t . An investigation of the integral using Laplace’s method (see “Appendix 1”) shows that for N large,

$$\frac{(e_{t/N} * \dots * e_{t/N}^v)(x, y)}{e_t(x, y)} \geq \varepsilon,$$

where $\varepsilon > 0$ is independent of x and y , where one uses that $\Upsilon_{\tau,v}(0, \gamma) > 0$ for all minimal geodesics γ connecting x and y , if N is large enough. □

Remark 3.9 There is a rich literature containing Gaussian bounds for the Laplace–Beltrami operator. In the stochastic literature, two-sided estimates can be found, e.g., in [26], [20, Thm. 5.3.4] and [4]. Using analytic methods, the Gaussian estimate from above is derived, e.g., in [12], [18, Thm. 15.14] and [11].

4 Convolution approximation

In this section, we prove Thm. 1.4. Throughout, M is a compact Riemannian manifold and L is a Laplace-type operator, acting on sections of a metric vector bundle \mathcal{V} over M .

The proof relies the following lemma.

Lemma 4.1 *For any $0 < \varepsilon < 1$ and all $R, T > 0$, there exist constants $C, \delta > 0$ such that for all $x, y \in M$, we have*

$$\int_{d(z_0, z_1) \geq R} p_{s_0}^\Delta(x, z_0) p_{s_1-s_0}^\Delta(z_0, z_1) p_{t-s_1}^\Delta(z_1, y) d(z_0, z_1) < C e^{-(1-\varepsilon)\frac{R^2}{4(s_1-s_0)}} p_t^\Delta(x, y)$$

whenever $0 \leq s_0 < s_1 \leq t \leq T$ and $s_1 - s_0 \leq t\delta$. Here p_t^Δ denotes the heat kernel of the Laplace–Beltrami operator on M .

Proof Set

$$I := \frac{1}{p_t^\Delta(x, y)} \int_{d(z_0, z_1) \geq R} p_{s_0}^\Delta(x, z_0) p_{s_1-s_0}^\Delta(z_0, z_1) p_{t-s_1}^\Delta(z_1, y) d(z_0, z_1)$$

and put

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

By Thms. 3.5 and 3.8, there exist constants $C_1, C_2 > 0$ such that for all $0 < t \leq T$ and all $x, y \in M$, we have

$$C_1 t^{-n/2} e^{-\frac{d(x,y)^2}{4t}} \leq p_t^\Delta(x, y) \leq C_2 t^{-n-1} e^{-\frac{d(x,y)^2}{4t}}. \tag{4.1}$$

Using this, we obtain

$$I \leq \frac{C_2(s_1 - s_0)^{-n-1}}{p_t^\Delta(x, y)} \int_M \int_M e^{-\frac{d(z_0, z_1)^2}{4(s_1 - s_0)}} p_{s_0}^\Delta(x, z_0) p_{t-s_1}^\Delta(z_1, y) \varphi(d(z_0, z_1)) dz_0 dz_1.$$

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

$$\delta := \varepsilon' \frac{R^2}{\text{diam}(M)^2}. \tag{4.2}$$

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

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

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 (4.1), we have for each $0 < t \leq T$ that

$$\begin{aligned} I &\leq \frac{C_2(s_1 - s_0)^{-n-1}}{p_t^\Delta(x, y)} e^{-(1-\varepsilon')\frac{R^2}{4(s_1-s_0)} - \frac{d(x,y)^2}{4t}} \int_M \int_M p_{s_0}^\Delta(x, z_0) p_{t-s_1}^\Delta(z_1, y) dz_0 dz_1 \\ &\leq C_2(s_1 - s_0)^{-n-1} e^{-(1-\varepsilon')\frac{R^2}{4(s_1-s_0)}} T^{n/2} \frac{t^{-n/2} e^{-\frac{d(x,y)^2}{4t}}}{p_t^\Delta(x, y)} \\ &\leq C_3(s_1 - s_0)^{-n-1} e^{-(1-\varepsilon')\frac{R^2}{4(s_1-s_0)}} < C_4 e^{-(1-\varepsilon)\frac{R^2}{4(s_1-s_0)}}, \end{aligned}$$

if the constants C_3, C_4 are chosen appropriately. □

Remark 4.2 The proof above shows that one can choose δ as in Thm. 1.4 in order that the statement of Lemma 4.1 holds.

We can now prove Thm. 1.4.

Proof (of Thm. 1.4) Throughout the proof, write $\Delta_j := \Delta_j \tau$ for abbreviation. By the Markov property of the heat kernel, we have $p_t^L = p_s^L * p_{t-s}^L$ for all $0 < s < t$. We obtain that

$$p_t^L - e_{\Delta_1}^v * \dots * e_{\Delta_N}^v = \sum_{j=1}^N p_{\tau_{j-1}}^L * \dots * p_{\Delta_{j-1}}^L * (p_{\Delta_j}^L - e_{\Delta_j}^v) * e_{\Delta_{j+1}}^v * \dots * e_{\Delta_N}^v,$$

since the sum on the right-hand side telescopes. By the Hess–Schrader–Uhlenbrock estimate [19], we have $|p_t^L| \leq e^{\alpha t} p_t^\Delta$ for some constant $\alpha \in \mathbb{R}$, where p_t^Δ denotes the heat kernel of the Laplace–Beltrami operator (here we use self-adjointness of the operator L). Similarly,

$$\begin{aligned} |e_t^v(x, y)| &\leq |p_t^L(x, y)| + |e_t^v(x, y) - \chi(d(x, y)) p_t^L(x, y)| \leq e^{\alpha t} p_t^\Delta(x, y) + C t^{\nu+1} e_t(x, y) \\ &\leq e^{\alpha' t} p_t^\Delta(x, y) \end{aligned}$$

for some $\alpha' > 0$, where we used Thm. 1.1 and the Gaussian estimate from below, Thm. 3.8. Here, χ is a smooth function with $\chi(r) = 1$ near zero and support contained in $[0, \text{inj}(M))$,

with $\text{inj}(M)$ the injectivity radius. Therefore,

$$\begin{aligned} |p_t^L - e_{\Delta_1}^v * \dots * e_{\Delta_N}^v| &\leq \sum_{j=1}^N |p_{\tau_{j-1}}^L| * |p_{\Delta_j}^L - e_{\Delta_j}^v| * |e_{\Delta_{j+1}}^v| * \dots * |e_{\Delta_N}^v| \\ &\leq \sum_{j=1}^N e^{\tau_j - 1\alpha} p_{\tau_{j-1}}^\Delta * |p_{\Delta_j}^L - e_{\Delta_j}^v| * e^{\alpha\Delta_{j+1}} p_{\Delta_{j+1}}^\Delta * \dots * e^{\alpha\Delta_N} p_{\Delta_N}^\Delta \\ &\leq e^{\alpha t} \sum_{j=1}^N p_{\tau_{j-1}}^\Delta * |p_{\Delta_j}^L - e_{\Delta_j}^v| * p_{t-\tau_j}^\Delta. \end{aligned}$$

Now, by Thm. 1.1 and the Gaussian estimate from below,

$$\begin{aligned} |p_t^L(x, y) - e_t^v(x, y)| &\leq \left| (1 - \chi(d(x, y))) p_t^L(x, y) \right| + \left| \chi(d(x, y)) \left(p_t^L(x, y) - e_t(x, y) \sum_{j=0}^v t^j \frac{\Phi_j(x, y)}{j!} \right) \right| \\ &\leq e^{t\alpha} (1 - \chi(d(x, y))) p_t^\Delta(x, y) + C_1 t^{v+1} p_t^\Delta(x, y) \end{aligned}$$

Therefore,

$$\begin{aligned} |p_t^L(x, y) - (e_{\Delta_1}^v * \dots * e_{\Delta_N}^v)(x, y)| &\leq \underbrace{e^{\alpha t} \sum_{j=1}^N C_1 \Delta_j^{v+1} p_t^\Delta(x, y)}_{(1)} + \underbrace{e^{\alpha t} \sum_{j=1}^N \int_{d(z_0, z_1) \geq R} p_{\tau_{j-1}}^\Delta(x, z_0) p_{\Delta_j}^\Delta(z_0, z_1) p_{t-\tau_j}(z_1, y) d(z_0, z_1)}_{(2)}, \end{aligned}$$

where R is such that $\chi(r) = 1$ for $0 \leq r \leq R$. The first term can be estimated by

$$(1) \leq C_1 |\tau|^v \sum_{j=1}^N \Delta_j p_t^\Delta(x, y) = C_1 t |\tau|^v p_t^\Delta(x, y).$$

By Lemma 4.1, whenever $|\tau| \leq \delta t$, the second term can be estimated by

$$(2) \leq C_2 \sum_{j=1}^N e^{-\epsilon/\Delta_j} p_t^\Delta(x, y) \leq C_3 e^{-\epsilon'/|\tau|} p_t^\Delta(x, y) \leq C_4 t |\tau|^v p_t^\Delta(x, y),$$

with $\epsilon, \epsilon' > 0$. This finishes the proof. □

5 Heat kernel asymptotics at the cut locus

In this section, we use the convolution approximation from Thm. 1.4 to obtain short-time asymptotic expansions of the heat kernel also in the case that $x, y \in M$ lie in each other’s cut locus. As we will see, the form of such an asymptotic expansion depends on the behavior of the energy functional near its critical points on the space of paths between x and y .

For an absolutely continuous path $\gamma : [0, 1] \rightarrow M$, consider the *energy functional*

$$E(\gamma) = \frac{1}{2} \int_0^1 |\dot{\gamma}(s)|^2 ds. \tag{5.1}$$

Set

$$H_{xy}(M) := \{\gamma \mid \gamma \text{ is absolutely continuous with } E(\gamma) < \infty\}.$$

This is an infinite-dimensional manifold modeled on the Hilbert space $H^1([0, 1], \mathbb{R}^n)$. For details on the manifold structure on $H_{xy}(M)$, see, e.g., Section 2.3 in [23].

Let $\Gamma_{xy}^{\min} \subset H_{xy}(M)$ denote the set of length minimizing geodesics between the points $x, y \in M$. It is well known that for each $\gamma \in \Gamma_{xy}^{\min}$, we have $E(\gamma) = d(x, y)^2/2$, and conversely, the set Γ_{xy}^{\min} is exactly the set of global minima of E on $H_{xy}(M)$. Moreover, Γ_{xy}^{\min} is compact in $H_{xy}(M)$ [23, Prop. 2.4.11].

Definition 5.1 Let $x, y \in M$. We say that Γ_{xy}^{\min} is a *non-degenerate submanifold*, if it is a submanifold of $H_{xy}(M)$, and if furthermore for each $\gamma \in \Gamma_{xy}^{\min}$, the Hessian of E is non-degenerate when restricted to a complementary subspace to the tangent space $T_\gamma \Gamma_{xy}^{\min}$.

This is just the well-known Morse–Bott condition on the energy function near the submanifold Γ_{xy}^{\min} .

Theorem 5.2 (Short-time asymptotics, cut locus) *Let M be a compact manifold and let L be a self-adjoint Laplace-type operator, acting on sections of a metric vector bundle \mathcal{V} over M . For $x, y \in M$, assume that the set Γ_{xy}^{\min} is a disjoint union of k non-degenerate submanifolds of dimensions d_1, \dots, d_k . Then the heat kernel has the complete asymptotic expansion*

$$\frac{P_t^L(x, y)}{e_t(x, y)} \sim \sum_{l=1}^k (4\pi t)^{-d_l/2} \sum_{j=0}^{\infty} t^j \frac{\Phi_{j,l}(x, y)}{j!}$$

as $t \rightarrow 0$.

Remark 5.3 In particular, if $(x, y) \in M \bowtie M$ so that $\Gamma_{xy}^{\min} = \{\gamma\}$ with γ the unique minimizing geodesic between x and y , then we recover the asymptotic expansion from before, Thm. 1.1.

Remark 5.4 The Hessian of the energy at an element $\gamma \in \Gamma_{xy}^{\min}$ can be explicitly calculated and is closely related to the Jacobi equation, see, e.g., [25, Section 13].

Remark 5.5 Thm. 5.2 can be generalized to the case that Γ_{xy}^{\min} is a *degenerate* submanifold of $H_{xy}(M)$. In this case, the explicit form of the asymptotic expansion depends on the type of degeneracy of E . In general, it can become quite complicated; for example it may contain logarithmic terms. For a discussion of this, see [26, pp. 20–24].

Example 5.6 A prototypical example where Γ_{xy}^{\min} is a non-degenerate submanifold of dimension greater than zero is when x and y are antipodal points on a sphere. In this case, $\dim \Gamma_{xy}^{\min} = n - 1$. For an explicit calculation of $\Phi_0(x, y)$ in this case, see [20, Example 5.3.3].

The convolution approximation from Thm. 1.4 is connected to the energy functional as follows. For $x, y \in M$ fixed, set

$$M^{(N-1)} := \{(x_1, \dots, x_{N-1}) \in M^{N-1} \mid (x_{j-1}, x_j) \in M \bowtie M \text{ for } j = 1, \dots, N\},$$

with the convention $x_0 := x, x_N := y$. For any partition $\tau = \{0 = \tau_0 < \tau_1 < \dots < \tau_N = 1\}$ of the interval $[0, 1]$, the manifold $M^{(N-1)}$ is diffeomorphic to the finite-dimensional submanifold

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

of $H_{xy}(M)$. (By the condition that the paths γ by unique minimizing, we want to express that we require $(\gamma(\tau_{j-1}), \gamma(\tau_j)) \in M \bowtie M$.) Namely, the evaluation map

$$ev_\tau : H_{xy;\tau}(M) \longrightarrow M^{(N-1)}, \quad \gamma \longmapsto (\gamma(\tau_1), \dots, \gamma(\tau_{N-1}))$$

is a diffeomorphism between the two. For our purpose, it doesn't matter which Riemannian metric (or volume) we put on $H_{xy;\tau}(M)$; for simplicity we take the one that makes ev_τ an isometry.

Lemma 5.7 *The heat convolution product from Thm. 1.4 can be written as an integral over $H_{xy;\tau}(M)$. More specifically, for a partition $\tau = \{0 = \tau_0 < \tau_1 < \dots < \tau_N = t\}$, denote by $\tilde{\tau}$ the corresponding partition of the interval $[0, 1]$, given by $\tilde{\tau}_j = \tau_j/t$. Then we have*

$$(e_{\Delta_1\tau}^v * \dots * e_{\Delta_N\tau}^v)(x, y) = (4\pi t)^{-nN/2} \int_{H_{xy;\tilde{\tau}}(M)} e^{-E(\gamma)/2t} \Upsilon^{\tilde{\tau},v}(t, \gamma) d\gamma, \quad (5.2)$$

where the integrand $\Upsilon_{\tilde{\tau},v}(t, \gamma)$ is a certain smooth and compactly supported function on $H_{xy;\tau}(M)$ with values in $\text{Hom}(\mathcal{V}_y, \mathcal{V}_x)$ that depends polynomially on t .

Proof Notice that for the path $\gamma \in H_{xy;\tau}(M)$ with $\gamma(\tau_j) = x_j$, we have

$$E(\gamma) = \frac{1}{2} \sum_{j=1}^N \frac{d(x_{j-1}, x_j)^2}{\Delta_j\tau}.$$

Now because the approximate heat kernel e_t^v is supported in $M \bowtie M$ (by choice of the cutoff function present in its definition), the convolution $e_{\Delta_1\tau}^v * \dots * e_{\Delta_N\tau}^v$ can be written as an integral over $M^{(N-1)}$,

$$\begin{aligned} &(e_{\Delta_1\tau}^v * \dots * e_{\Delta_N\tau}^v)(x, y) \\ &= \int_{M^{(N-1)}} \exp\left(-\frac{1}{4t} \sum_{j=1}^N d(x_{j-1}, x_j)^2\right) \cdot \\ &\quad \cdot \prod_{j=1}^N \left[\frac{\chi(d(x_{j-1}, x_j))}{(4\pi \Delta_j\tau)^{n/2}} \sum_{i=1}^v (\Delta_j\tau)^j \frac{\Phi_i(x_{j-1}, x_j)}{i!} \right] dx_1 \dots dx_{N-1}. \end{aligned}$$

We obtain formula (5.2), where

$$\Upsilon^{\tilde{\tau},v}(t, \gamma) = \prod_{j=1}^N \left[(\Delta_j\tilde{\tau})^{-n/2} \chi(d(\gamma(\tilde{\tau}_{j-1}), \gamma(\tilde{\tau}_j))) \sum_{i=1}^v (t \Delta_j\tilde{\tau})^j \frac{\Phi_i(\gamma(\tilde{\tau}_{j-1}), \gamma(\tilde{\tau}_j))}{i!} \right]. \quad (5.3)$$

This finishes the proof. □

The explicit formula for $\Upsilon^{\tilde{\tau},v}$ is entirely unimportant for our purposes; we only take from it that $\Upsilon^{\tilde{\tau},v}$ is a smooth, compactly supported function on $H_{xy;\tau}(M)$ that depends polynomially on t .

Below, we will always write τ instead of $\tilde{\tau}$ for a partition of the interval $[0, 1]$.

Proof (of Thm. 5.2) We will use Laplace's method on the path integral (5.2). In order to do this, we have to bring it into the form of Thm. A.1 first, which is achieved by dividing by

$e_t(x, y)$ and setting $\phi(\gamma) := E(\gamma) - d(x, y)/2$. Then by Lemma 5.7, we obtain

$$\frac{(e_{i\Delta_1\tau}^v * \dots * e_{i\Delta_N\tau}^v)(x, y)}{e_t(x, y)} = (4\pi t)^{-n(N-1)/2} \int_{H_{xy;\tau}(M)} e^{-\phi(\gamma)/2t} \Upsilon^{\tau,v}(t, \gamma) d\gamma,$$

which has the form (A.1) since $\dim(H_{xy;\tau}(M)) = n(N - 1)$.

It is clear that whenever the partition $\tau = \{0 = \tau_0 < \tau_1 < \dots < \tau_N = 1\}$ is fine enough, we have $\Gamma_{xy}^{\min} \subset H_{xy;\tau}(M)$. By assumption, Γ_{xy}^{\min} is the direct sum of non-degenerate submanifolds $\Gamma_1, \dots, \Gamma_k$ of dimension d_1, \dots, d_k . Therefore, by Thm. A.1 we obtain the asymptotic expansion

$$\frac{(e_{i\Delta_1\tau}^v * \dots * e_{i\Delta_N\tau}^v)(x, y)}{e_t(x, y)} \sim \sum_{l=1}^k (4\pi t)^{-d_l/2} \sum_{j=0}^{\infty} t^j \frac{\Phi_{j,l}^{\tau,v}(x, y)}{j!}, \tag{5.4}$$

where

$$\Phi_{j,l}^{\tau,v}(x, y) = \sum_{i=0}^j \frac{1}{i!(j-i)!} \int_{\Gamma_l} \frac{P^{j-i} \Upsilon^{\tau,v(i)}(0, \gamma)}{\det(\nabla^2 E|_{N_\gamma \Gamma_l})^{1/2}} d\gamma \tag{5.5}$$

for some second-order differential operator P on $H_{xy;\tau}(M)$. Here, $\det(\nabla^2 E|_{N_\gamma \Gamma_l})^{1/2}$ denotes the determinant of $\nabla^2 E|_\gamma$, restricted to the normal space $N_\gamma \Gamma_l$ of $T_\gamma \Gamma_l$ in $T_\gamma H_{xy;\tau}(M)$. In particular, if we set $d := \max_{1 \leq l \leq k} d_l$, there exists a constant $C_0 > 0$ such that

$$\left| \frac{(e_{i\Delta_1\tau}^v * \dots * e_{i\Delta_N\tau}^v)(x, y)}{e_t(x, y)} \right| \leq C_0 t^{-d/2} \tag{5.6}$$

for all $0 < t \leq T$.

By Thm. 1.4, for each $T > 0$ and each $v \in \mathbb{N}_0$, there exist constants $C_1, \delta > 0$ such that

$$\left| \frac{p_t^L(x, y)}{e_t(x, y)} - \frac{(e_{i\Delta_1\tau}^v * \dots * e_{i\Delta_N\tau}^v)(x, y)}{e_t(x, y)} \right| \leq C_1 t^{1+v} |\tau|^v \frac{p_t^\Delta(x, y)}{e_t(x, y)}, \tag{5.7}$$

for any partition τ of the interval $[0, 1]$ with $|\tau| \leq \delta$. By the Gaussian estimate from above (Thm. 3.5) follows $p_t^\Delta(x, y) \leq C_2 t^{-n/2-1} e_t(x, y)$. Therefore, (5.7) yields

$$\left| \frac{p_t^L(x, y)}{e_t(x, y)} - \frac{(e_{i\Delta_1\tau}^v * \dots * e_{i\Delta_N\tau}^v)(x, y)}{e_t(x, y)} \right| \leq C_3 t^{v-n/2} |\tau|^v. \tag{5.8}$$

Using (5.8) and (5.6) for $L = \Delta$, the Laplace–Beltrami operator on M , some $v \geq n/2 - k/2 - 1$ and $|\tau| \leq \delta$, we get

$$\begin{aligned} \frac{p_t^\Delta(x, y)}{e_t(x, y)} &\leq \left| \frac{p_t^\Delta(x, y)}{e_t(x, y)} - \frac{(e_{i\Delta_1\tau}^v * \dots * e_{i\Delta_N\tau}^v)(x, y)}{e_t(x, y)} \right| + \left| \frac{(e_{i\Delta_1\tau}^v * \dots * e_{i\Delta_N\tau}^v)(x, y)}{e_t(x, y)} \right| \\ &\leq C_4 t^{v-n/2} |\tau|^v + C_5 t^{-d/2} \leq (C_4 \delta^v + C_5) t^{-d/2} =: C_6 t^{-d/2}. \end{aligned}$$

Therefore, (5.7) improves to

$$\left| \frac{p_t^L(x, y)}{e_t(x, y)} - \frac{(e_{i\Delta_1\tau}^v * \dots * e_{i\Delta_N\tau}^v)(x, y)}{e_t(x, y)} \right| \leq C_1 t^{1+v} |\tau|^v \cdot C_6 t^{-d/2} \leq C_7 t^{1+v-d/2}$$

From this follows that the heat kernel has an asymptotic expansion up to the order $t^{v-d/2}$, the coefficients of which must coincide with the asymptotic expansion (5.4) of $e_{i\Delta_1\tau}^v * \dots *$

$e_{t\Delta_N\tau}^\nu$ up to that order. Because asymptotic expansions are unique, this also shows that the coefficients $\Phi_{j,l}^{\tau,\nu}(x, y)$ from (5.4) must stabilize for ν large enough and τ fine enough. More precisely, if $j \leq \nu, \nu'$ and $|\tau|, |\tau'| \leq \delta$, we have

$$\Phi_{j,l}^{\tau,\nu}(x, y) = \Phi_{j,l}^{\tau',\nu'}(x, y).$$

Therefore,

$$\Phi_{j,l}(x, y) := \Phi_{j,l}^{\tau,\nu}(x, y)$$

for any choice of $\nu \geq j$ and $|\tau| \leq \delta$ is well defined.

Because ν was arbitrary, we obtain that $p_t^L(x, y)/e_t(x, y)$ has a complete asymptotic expansion of the claimed form, with the coefficients $\Phi_{j,l}(x, y)$ given by the formula (5.5) for ν large enough and $|\tau|$ small enough. □

Acknowledgements Open access funding provided by Max Planck Society. I would like to thank Christian Bär, Rafe Mazzeo, Franziska Beitz, Florian Hanisch and Ahmad Afuni for helpful discussions. Furthermore, I am indebted to Potsdam Graduate School, The Fulbright Program, SFB 647 and the Max-Planck-Institute for Mathematics in Bonn for financial support.

Open Access This article is distributed under the terms of the Creative Commons Attribution 4.0 International License (<http://creativecommons.org/licenses/by/4.0/>), which permits unrestricted use, distribution, and reproduction in any medium, provided you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons license, and indicate if changes were made.

A Laplace’s method

Laplace’s method is a way to calculate asymptotic expansions as $t \rightarrow 0$ from above for integrals of the form

$$I(t, a) := (4\pi t)^{-\dim(\Omega)/2} \int_{\Omega} e^{-\phi(x)/2t} a(t, x) dx. \tag{A.1}$$

Here, $t > 0, \Omega$ is a Riemannian manifold, $\phi \in C^\infty(\Omega)$ is a nonnegative function and $a(t, x)$ is smooth and compactly supported with respect to the x variable and depends smoothly on t . The following result is very well known; however, it seems that it is nowhere to be found in quite the form needed, so for convenience of the reader, we give a proof in this “Appendix”.

Theorem A.1 (Laplace expansion)

Assume that ϕ is nonnegative and that $\Gamma := \phi^{-1}(0)$ is a disjoint union of submanifolds $\Gamma_1, \dots, \Gamma_k$ of dimensions d_1, \dots, d_k . Suppose that for each $l = 1, \dots, k$, and each $x \in \Gamma_l$, the Hessian $\nabla^2\phi|_x$ is non-degenerate when restricted to the normal space $N_x\Gamma_l$ in $T_x\Omega$. 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

$$I(t, a) \sim \sum_{l=1}^k (4\pi t)^{-d_l/2} \sum_{j=0}^{\infty} t^j \sum_{i=0}^j \frac{1}{i!(j-i)!} \int_{\Gamma_l} \frac{P^{j-i} a^{(i)}(0, x)}{\det(\nabla^2\phi|_{N_x\Gamma_l})^{1/2}} dx \tag{A.2}$$

where $a^{(i)}(0, x)$ denotes the i th derivative of a with respect to t at $t = 0$.

Remark A.2 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 simpler 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., [1] or [13, Section 1.2].

Lemma A.3 *Under the assumptions of Thm. A.1, 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

$$A := \text{closure of } \bigcup_{0 \leq t \leq \delta} \text{supp } a(t, -) \tag{A.3}$$

(which is compact) and set

$$\varepsilon' := \min_{x \in A} \phi(x).$$

Notice that $\varepsilon' > 0$ because $A \cap \Gamma = \emptyset$. Therefore,

$$I(t, a) \leq (4\pi t)^{-N/2} e^{-\varepsilon'/2t} \int_{\Omega} a(t, x) dx \leq (4\pi t)^{-N/2} e^{-\varepsilon'/2t} \|a(t, -)\|_{L^1} \leq Ce^{-\varepsilon/t},$$

if we choose $0 < \varepsilon < \varepsilon'$ and $C > 0$ appropriately. □

Proof (of Thm. A.1) We may write the integral over Ω as a sum of integrals over open subsets $\Omega_1, \dots, \Omega_k$ such that the union of the Ω_l is dense in Ω , and such that $\Gamma_l \subset \Omega_l$ for each $l = 1, \dots, k$. The asymptotic expansion of the integral over Ω will then be the sum of the asymptotic expansions of the integrals over the manifolds Ω_l . Therefore, we may assume that $k = 1$, i.e., Γ is a non-degenerate submanifold of dimension d .

Let $N := \dim(\Omega)$ and let A as in (A.3). 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 $\kappa : V \rightarrow U$ such that

$$(\phi \circ \kappa)(x, v) = \nabla^2 \phi|_x[v, v], \quad (x, v) \in V.$$

This can be proved using the implicit function theorem, compare, e.g., Lemma 1.2.2 in [13]. Clearly, we have $d\kappa|_{(x,0)} = \text{id}_x$.

Furthermore, we may 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 A.3.

We now may use the transformation formula to obtain

$$\begin{aligned} I(t, a) &= (4\pi t)^{-N/2} \int_U e^{-\phi(x)/2t} a(t, x) dx \\ &= (4\pi t)^{-N/2} \int_{\Gamma} \int_{V_x} e^{-(v, Q(x)v)/4t} a(t, \kappa(x, v)) |\det(d\kappa|_{(x,v)})| dv dx, \end{aligned} \tag{A.4}$$

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 $(N - d)$ -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

$$\lim_{t \rightarrow 0} (4\pi t)^{-(N-d)/2} \int_W e^{-\langle v, Qv \rangle / 4t} f(t, v) dv = \det(Q)^{-1/2} f(0, 0).$$

Furthermore, for all t , we have

$$\left| (4\pi t)^{-(N-d)/2} \int_W e^{-\langle v, Qv \rangle / 4t} f(t, v) dv \right| \leq \|f(t, -)\|_\infty.$$

Therefore, since Γ is compact, we may exchange integration over Γ and the limit $t \rightarrow 0$ in (A.4) to conclude

$$\lim_{t \rightarrow 0} (4\pi t)^{d/2} I(t, a) = \int_\Gamma \frac{a(0, \kappa(x, 0))}{\det(Q(x))^{1/2}} |\det(d\kappa|_{(x,0)})| dx = \int_\Gamma \frac{a(0, x)}{\det(\nabla^2 \phi|_{N_x \Gamma})^{1/2}} dx \tag{A.5}$$

Now on the vector spaces $N_x \Gamma$, define the Q -Laplacian Δ_Q by the formula

$$\Delta_Q f(v) = -\langle Q(x)^{-1}, D^2 f|_v \rangle.$$

This patches together to a smooth differential operator on $N\Gamma$ satisfying

$$\left(\frac{\partial}{\partial t} + \Delta_Q \right) \{ (4\pi t)^{-(N-d)/2} e^{-\langle v, Q(x)v \rangle / 4t} \} = 0.$$

Therefore, integrating by parts, we obtain

$$\begin{aligned} & \frac{\partial}{\partial t} \{ (4\pi t)^{d/2} I(t, a) \} - (4\pi t)^{d/2} I(t, \dot{a}) \\ &= -(4\pi t)^{-(N-d)/2} \int_\Gamma \int_{V_x} e^{-\langle v, Q(x)v \rangle / 4t} \Delta_Q \{ a(t, \kappa(x, v)) |\det(d\kappa|_{(x,v)})| \} dv dx \\ &= (4\pi t)^{-(N-d)/2} \int_U e^{-\phi(x)/2t} P a(t, x) dx = (4\pi t)^{d/2} I(t, Pa), \end{aligned}$$

where for $f \in C^\infty(U)$, we set

$$(Pf)(y) = -\Delta_Q \{ f(v) |\det(d\kappa|_{(x,v)})| \} |_{(x,v)=\kappa^{-1}(y)} |\det(d\kappa^{-1}|_y)|,$$

so that P is some second-order differential operator. Let $J(t, a) := (4\pi t)^{d/2} I(t, a)$. Then by Taylor’s formula and the Leibnitz rule, for all $\varepsilon > 0$ and $v \in \mathbb{N}$,

$$\begin{aligned} J(t, a) &= \sum_{j=0}^v \frac{1}{j!} \frac{\partial^j}{\partial \varepsilon^j} \{ J(\varepsilon, a) \} (t - \varepsilon)^j + \int_\varepsilon^t \frac{(t-s)^v}{v!} \frac{\partial^{v+1}}{\partial s^{v+1}} \{ J(s, a) \} ds \\ &= \sum_{j=0}^v \frac{1}{j!} \sum_{i=0}^j \binom{j}{i} J(\varepsilon, P^{j-i} a^{(i)}) (t - \varepsilon)^j + R^v(\varepsilon, t), \end{aligned}$$

where

$$R^v(\varepsilon, t) = \sum_{i=0}^{v+1} \binom{v+1}{i} \int_\varepsilon^t \frac{(t-s)^v}{v!} J(s, P^{v+1-i} a^{(i)}) ds. \tag{A.6}$$

Because of (A.5), we may take the limit $\varepsilon \rightarrow 0$ to obtain

$$\lim_{\varepsilon \rightarrow 0} J(\varepsilon, P^{j-i} a^{(i)}) = \int_{\Gamma} \frac{P^{j-i} a^{(i)}(0, x)}{\det(\nabla^2 \phi|_{N_x \Gamma})^{1/2}} dx.$$

Therefore,

$$J(t, a) = \sum_{j=0}^{\nu} t^j \sum_{i=0}^j \frac{1}{(j-i)! i!} \int_{\Gamma} \frac{P^{j-i} a^{(i)}(0, x)}{\det(\nabla^2 \phi|_{N_x \Gamma})^{1/2}} dx + R^{\nu}(0, t),$$

for any $\nu \in \mathbb{N}_0$, where the remainder term is of order $t^{\nu+1}$. This finishes the proof. \square

References

1. Arnol'd, V.I.: Remarks on the method of stationary phase and on the Coxeter numbers. *Uspehi Mat. Nauk* **28**(5), 17–44 (1973)
2. Azencott, R.: Densité des diffusions en temps petit: développements asymptotiques. In: Azéma, J., Yor, M. (eds.) *Séminaire de Probabilités XVIII 1982/83. Lecture Notes in Mathematics*, vol. 1059, pp. 402–498. Springer, Berlin, Heidelberg (1984)
3. Ben rous, G.: Developpement asymptotique du noyau de la chaleur hypoelliptique hors du cut-locus. *Ann. Sci. École Norm. Sup. (4)* **21**(3), 307–331 (1988)
4. Barilari, D., Boscain, U., Neel, R.W.: Small-time heat kernel asymptotics at the sub-Riemannian cut locus. *J. Differ. Geom.* **92**(3), 373–416 (2012)
5. Berger, M., Gauduchon, P., Mazet, E.: *Le spectre d'une variété riemannienne*, vol. 194. Springer, Berlin (1971)
6. Bär, C., Ginoux, N., Pfäffle, F.: *Wave Equations on Lorentzian Manifolds and Quantization*. European Mathematical Society (EMS), Zürich, ESI Lectures in Mathematics and Physics (2007)
7. Berline, N., Getzler, E., Vergne, M.: *Heat Kernels and Dirac Operators*. Grundlehren Text Editions. Springer, Berlin (2004). Corrected reprint of the 1992 original
8. Berezin, F.A., Shubin, M.A.: *The Schrödinger equation*, volume 66 of *Mathematics and its Applications (Soviet Series)*. Kluwer Academic Publishers Group, Dordrecht (1991). Translated from the 1983 Russian edition by Yu. Rajabov, D. A. Leites and N. A. Sakharova and revised by Shubin, With contributions by G. L. Litvinov and Leites
9. Bär, C., Wafo, R.T.: Initial value problems for wave equations on manifolds. *Math. Phys. Anal. Geom.* **18**(1), 7–29 (2015)
10. Chavel, I.: *Eigenvalues in Riemannian Geometry*, volume 115 of *Pure and Applied Mathematics*. Academic Press, Inc., Orlando (1984). Including a chapter by Burton Randol, With an appendix by Jozef Dodziuk
11. Coulhon, T., Sikora, A.: Gaussian heat kernel upper bounds via the Phragmén–Lindelöf theorem. *Proc. Lond. Math. Soc. (3)* **96**(2), 507–544 (2008)
12. Davies, E.B., Pang, M.M.H.: Sharp heat kernel bounds for some Laplace operators. *Quart. J. Math. Oxford Ser. (2)* **40**(159), 281–290 (1989)
13. Duistermaat, J.J.: *Fourier Integral Operators*. Modern Birkhäuser Classics. Birkhäuser/Springer, New York (2011). Reprint of the 1996 edition [MR1362544], based on the original lecture notes published in 1973 [MR0451313]
14. Fine, D.S., Sawin, S.F.: A rigorous path integral for supersymmetric quantum mechanics and the heat kernel. *Commun. Math. Phys.* **284**(1), 79–91 (2008)
15. Fine, D.S., Sawin, S.: Short-time asymptotics of a rigorous path integral for $N = 1$ supersymmetric quantum mechanics on a Riemannian manifold. *J. Math. Phys.* **55**(6), 062104 (2014)
16. Fine, D.S., Sawin, S.: Path integrals, supersymmetric quantum mechanics, and the Atiyah–Singer index theorem for twisted Dirac. *J. Math. Phys.* **58**(1), 012102 (2017)
17. Greiner, P.: An asymptotic expansion for the heat equation. In: *Global Analysis (Proceedings of Symposia in Pure Mathematics)*, vol. XVI, Berkeley, CA, 1968), pp. 133–135. American Mathematical Society, Providence (1970)
18. Grigor'yan, A.: *Heat Kernel and Analysis on Manifolds*, volume 47 of *AMS/IP Studies in Advanced Mathematics*. American Mathematical Society, Providence; International Press, Boston (2009)

19. Hess, H., Schrader, R., Uhlenbrock, D.A.: Kato's inequality and the spectral distribution of Laplacians on compact Riemannian manifolds. *J. Differ. Geom.* **15**(1), 27–37 (1980)
20. Hsu, E.P.: *Stochastic Analysis on Manifolds*, vol. 38. American Mathematical Society, Providence (2002)
21. Inahama, Y., Taniguchi, S.: Short time full asymptotic expansion of hypoelliptic heat kernel at the cut locus. *Forum Math. Sigma* **5**, e16 (2017)
22. Kannai, Y.: Off diagonal short time asymptotics for fundamental solutions of diffusion equations. *Commun. Partial Differ. Equ.* **2**(8), 781–830 (1977)
23. Klingenberg, W.P.A.: *Riemannian Geometry*, volume 1 of De Gruyter Studies in Mathematics. Walter de Gruyter & Co., Berlin (1995)
24. Melrose, R.B.: *The Atiyah–Patodi–Singer Index Theorem*, vol. 4. A K Peters Ltd., Wellesley (1993)
25. Milnor, J.: *Morse Theory*. Based on Lecture Notes by M. Spivak and R. Wells. *Annals of Mathematics Studies*, No. 51. Princeton University Press, Princeton (1963)
26. Molchanov, S.A.: Diffusion processes, and Riemannian geometry. *Uspehi Mat. Nauk* **30**(1), 3–59 (1975)
27. Moretti, V.: Proof of the symmetry of the off-diagonal heat-kernel and Hadamard's expansion coefficients in general C^∞ Riemannian manifolds. *Comm. Math. Phys.* **208**(2), 283–308 (1999)
28. Moretti, V.: Proof of the symmetry of the off-diagonal Hadamard/Seeley–DeWitt's coefficients in C^∞ Lorentzian manifolds by a local Wick rotation. *Commun. Math. Phys.* **212**(1), 165–189 (2000)
29. Neel, R., Stroock, D.: *Analysis of the cut locus via the heat kernel*. *Surveys in Differential Geometry*, vol. 9, pp. 337–349. International Press, Somerville (2004)
30. Roe, J.: *Elliptic Operators Topology and Asymptotic Methods*, volume 395 of Pitman Research Notes in Mathematics Series, 2nd edn. Longman, Harlow (1998)
31. Rosenberg, S.: *The Laplacian on a Riemannian Manifold*, volume 31 of London Mathematical Society Student Texts. Cambridge University Press, Cambridge. An introduction to analysis on manifolds (1997)
32. Simon, B.: A Feynman–Kac formula for unbounded semigroups. In: *Stochastic Processes, Physics and Geometry: New Interplays, I* (Leipzig, 1999), volume 28 of CMS Conference Proceedings, pp. 317–321. American Mathematical Society, Providence (2000)
33. Strichartz, R.S.: Analysis of the Laplacian on the complete Riemannian manifold. *J. Funct. Anal.* **52**(1), 48–79 (1983)
34. Taylor, M.E.: *Partial Differential Equations II Qualitative Studies of Linear Equations*, volume 116 of Applied Mathematical Sciences. Springer, New York (2011)
35. Werner, D.: *Functional Analysis*, extended edn. Springer, Berlin (2000)
36. Wolf, J.A.: Essential self-adjointness for the Dirac operator and its square. *Indiana Univ. Math. J.* **22**, 611–640 (1972/1973)