HEAT KERNEL ASYMPTOTICS FOR ROOTS OF GENERALIZED LAPLACIANS

CHRISTIAN BÄR AND SERGIU MOROIANU

ABSTRACT. We describe the heat kernel asymptotics for roots of a Laplace type operator Δ on a closed manifold. A previously known relation between the Wodzicki residue of Δ and heat trace asymptotics is shown to hold pointwise for the corresponding densities.

1. INTRODUCTION

Let Δ be a positive self-adjoint differential operator of Laplace type acting on sections in a Hermitian vector bundle over a compact Riemannian manifold M. Then the corresponding heat operator $e^{-t\Delta}$, $t > 0$, is smoothing and its Schwartz kernel $p_t(x, y)$ is known to have an asymptotic short time expansion along the diagonal of the form $p_t(x, x) \sim \sum_{j=0}^{\infty} t^{j-n/2} a_{2j-n}(x)$, $t \searrow 0$. The coefficients $a_{2j-n}(x)$ can in principle be computed recursively in terms of curvature, the total symbol of Δ and their derivatives. In this paper we study the short time asymptotics of the Schwartz kernel of $e^{-t\sqrt{\Delta}}$. For example, if D is an invertible self-adjoint operator of Dirac type, then $\Delta := D^2$ is of Laplace type and we can apply our analysis to $e^{-t|D|}$. It turns out that the behavior of the heat kernel $h_t(x, y)$ of $\sqrt{\Delta}$ depends in a crucial manner on the parity of the dimension n of the underlying manifold M. If n is even, then there is an expansion

$$h_t(x,x) \overset{t\searrow 0}{\sim} \sum_{j=0}^{n/2} t^{2j-n} A_{2j-n}(x) + \sum_{j=1}^{\infty} t^j A_j(x)$$

where some of the coefficients $A_j(x)$ are directly related to the heat coefficients $a_j(x)$ for Δ itself. In the odd-dimensional case logarithmic terms appear

$$h_t(x,x) \overset{t\searrow 0}{\sim} \sum_{j=0}^{\infty} t^{2j-n} A_{2j-n}(x) + \sum_{j=0}^{\infty} t^{2j+1} \log t \, B_{2j+1}(x).$$

Date: August 14, 2002.

2000 *Mathematics Subject Classification.* 58J40, 58J42.

Key words and phrases. Laplace type operators, heat kernel, complex powers, Mellin transformation, Wodzicki residue.

The authors have been partially supported by the Research and Training Network HPRN-CT-1999-00118 "Geometric Analysis" funded by the European Commission.

All coefficients $B_j(x)$ and some of the $A_j(x)$ can again be obtained from the $a_j(x)$. The remaining coefficients are apparently not locally computable. Conversely, all heat coefficients $a_*(x)$ of Δ can be obtained from those of $\sqrt{\Delta}$, so that the short time expansion for $\sqrt{\Delta}$ contains more information than that for Δ, contrary to statements occasionally found in the literature, see e. g. [10, Sec. 4]. The details can be found in Theorem 7.

In order to relate $e^{-t\Delta}$ and $e^{-t\sqrt{\Delta}}$ we look at the complex powers Δ^{-s} of Δ. The Mellin transformation $\Delta^{-s} = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} e^{-t\Delta} dt$ implies that the heat coefficients $a_*(x)$ can be obtained as residues of poles of the Schwartz kernel $q_{-s}(x,y)$ of Δ^{-s}, more precisely,

$$\mathrm{Res}_{s=n/2-k}\left(\Gamma(s) q_{-s}(x,x)\right) = a_{2k-n}(x),$$

see Proposition 3. For complex powers it is trivial to pass from Δ to $\sqrt{\Delta}$ since $\sqrt{\Delta}^{-s} = \Delta^{-s/2}$. The inverse Mellin transform $e^{-tQ} = \frac{1}{2\pi i} \int_{\mathrm{Re}(s)=\tau} t^{-s} \Gamma(s) Q^{-s} ds$ for $Q = \sqrt{\Delta}$ then brings us back to heat operators. The logarithmic terms arise because in odd dimensions $\Gamma(s) q_{-s/2}(x,x)$ has double poles.

Our method also allows us to determine the short time heat asymptotics for $\Delta^{1/m}$, $m = 1, 2, \ldots$. Logarithmic terms appear only if n is odd and m is even. See Theorem 8 for details.

An alternative approach could have used the resolvent $(\Delta - \lambda)^{-1}$ instead of complex powers. This has been proposed e. g. in [10]. For $m = 2$ one could also have used the trace of the wave operator $e^{it\Delta^{1/2}}$ whose structure as a distribution is well understood, see [5, 8]. But the approach used here seems to be simpler.

In the last section we relate the Wodzicki residue density and heat coefficients. The Wodzicki residue is the unique trace on the algebra of pseudodifferential operators which extends the Dixmier trace on operators of order $\leq -n$. Kalau and Walze [12] and Kastler [13] independently showed that the Wodzicki residue of $\Delta^{-n/2+1}$ is essentially given by the integral of the second heat coefficient $\int_M \mathrm{Tr}(a_{-n+2}(x)) dx$. This fact has attracted attention in noncommutative geometry since it yields an operator-theoretic characterization of the Einstein-Hilbert action in general relativity, see e. g. [6]. Ackermann [1] noted that this is a special case of a more general relation between integrals of the heat coefficients and the Wodzicki residue of suitable powers of Δ. We show in Theorem 13 that the corresponding equality holds already on the level of densities, i. e. for each $x \in M$ the heat coefficient $a_{-2j}(x)$ is up to a universal factor the same as $\mathrm{wres}(\Delta^{-j})(x)$. Taking traces and integrating over M then yields the results of Kalau, Walze, Kastler, and Ackermann.

We tried to keep the presentation as self-contained as possible. For this reason we recall some definitions and include a few analytic basics which will be quite standard to the expert. However, we think that this way the text is much more coherent.

2. From the heat kernel to complex powers

Let (M, g) be a closed Riemannian manifold, let E be a Hermitian vector bundle over M and let Δ be a second-order differential operator acting on the sections of E. We assume that Δ is self-adjoint and of Laplace type, i. e. its principal symbol satisfies

$$\sigma_2(\Delta)(\xi) = g(\xi, \xi).$$

The Schwartz kernel $p_t(x, y)$ of the heat operator $e^{-t\Delta}$ has the following asymptotic behavior as $t \searrow 0$, where $n := \dim(M)$:

$$(t, x) \mapsto t^{n/2} p_t(x, x), \quad (t, x) \in [0, \infty) \times M, \tag{1}$$

is a smooth section of $E \otimes E^*$ over $[0, \infty) \times M$, and

$$(t, x, y) \mapsto p_t(x, y), \quad (t, x, y) \in [0, \infty) \times (M \times M \setminus \mathrm{Diag}), \tag{2}$$

is a smooth section of $E \boxtimes E^*$ and vanishes at $t = 0$ together with all its derivatives. A more standard way of writing (1) is the asymptotic expansion for p_t on the diagonal:

$$p_t(x, x) \overset{t \searrow 0}{\sim} \sum_{j=0}^{\infty} t^{j-n/2} a_{2j-n}(x). \tag{3}$$

These properties of the Schwartz kernel were first established for the Laplace-Beltrami operator acting on functions in the fundamental paper [14]. The version for generalized Laplacians that we use here can be found e. g. in [2, Ch. 2].

For simplicity we assume throughout the paper that Δ is strictly positive, unless otherwise stated. In this case $e^{-t\Delta}$ is a continuous family of bounded operators for $t \in [0, \infty)$ and vanishes exponentially fast in the operator norm as $t \to \infty$. Thus, for $\mathrm{Re}(s) > 0$ the complex powers of Δ are well-defined via the Mellin transformation formula

$$\Delta^{-s} := \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} e^{-t\Delta} dt, \tag{4}$$

the integral converging absolutely in the operator norm.

Proposition 1. *Let $K \subset M \times M \setminus \mathrm{Diag}$ be compact and let $\ell \in \mathbb{N}$. Then the restriction of the Schwartz kernel q_{-s} of Δ^{-s} to K is an entire function in s with values in the Banach space $C^\ell(K, E \boxtimes E^*)$ and vanishes for $s \in -\mathbb{N}$, $\mathbb{N} = \{0, 1, 2, \ldots\}$.*

Proof. We show this by deriving a relationship between the Schwartz kernels $p_t(x, y)$ of $e^{-t\Delta}$ and $q_{-s}(x, y)$ of Δ^{-s}. Consider the δ-function δ_x as a distribution in E^* with values in E_x and similarly δ_y as a distribution in E with values in E_y^*. Then we can write the following element of $E_x \otimes E_y^*$ as

$$p_t(x, y) = \delta_x(e^{-t\Delta}(\delta_y)) = (e^{-t\Delta/2}(\delta_y), e^{-t\Delta/2}(\delta_x))_{L^2}$$

hence

$$|p_t(x, y)| \leq \|e^{-(t-1)\Delta}\| \cdot \|e^{-\Delta/2}(\delta_x)\|_{L^2} \cdot \|e^{-\Delta/2}(\delta_y)\|_{L^2}.$$

Since $e^{-\Delta/2}$ is smoothing $\|e^{-\Delta/2}(\delta_x)\|_{L^2}$ and $\|e^{-\Delta/2}(\delta_y)\|_{L^2}$ are finite, thus $p_t(x,y)$ decays exponentially fast. Similarly,

$$|\tfrac{\partial^k}{\partial t^k} p_t(x,y)| \leq \|e^{-(t-1)\Delta}\| \cdot \|\Delta^k e^{-\Delta/2}(\delta_x)\|_{L^2} \cdot \|e^{-\Delta/2}(\delta_y)\|_{L^2},$$

so that all t-derivatives of $p_t(x,y)$ decay exponentially fast. Since $e^{-\Delta/2}(\delta_x)$ depends smoothly on x the estimates are uniform in x and y. Moreover, replacing the δ-functions by suitable derivatives of the δ-function we obtain the corresponding estimates for all derivatives of p_t in x and y. This means that for each $k, \ell \in \mathbb{N}$ there is a constant $C_{k,\ell}$ such that

$$\|\tfrac{\partial^k}{\partial t^k} p_t\|_{C^\ell(M\times M, E\boxtimes E^*)} \leq C_{k,\ell}\, \|e^{-(t-1)\Delta}\|$$

for $t \geq 1$. In particular, for any $s \in \mathbb{C}$ the integral

$$\int_1^\infty t^{s-1} p_t \, dt$$

converges absolutely in all Banach spaces $C^\ell(M \times M, E \boxtimes E^*)$.

For $K \subset M \times M \setminus \mathrm{Diag}$ we see from (2) that

$$\int_0^1 t^{s-1} p_t \, dt$$

is also absolutely convergent in $C^\ell(K, E \boxtimes E^*)$ for all $s \in \mathbb{C}$. By (4) it is clear that

$$q_{-s}(x,y) := \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} p_t(x,y) dt \tag{5}$$

defines the Schwartz kernel of Δ^{-s} wherever the integral converges absolutely. The vanishing statement for $s \in -\mathbb{N}$ follows from the poles of the Gamma function. □

Vanishing of q_{-s} off the diagonal for $s \in -\mathbb{N}$ reflects the fact that for these s the operator Δ^{-s} is *differential*. We fix our attention now to the diagonal. From (1) we see that for all $(x,y) \in M \times M$ the integral in (5) is absolutely convergent for $\mathrm{Re}(s) > \frac{n}{2}$. For such s we have therefore

$$\begin{aligned}
\Gamma(s) q_{-s}(x,x) &= \int_0^\infty t^{s-n/2-1} t^{n/2} p_t(x,x) dt \\
&= \frac{-1}{s-n/2} \int_0^\infty t^{s-n/2} \tfrac{\partial}{\partial t} \left(t^{n/2} p_t(x,x) \right) dt \\
&= \frac{(-1)^k}{\prod_{j=0}^{k-1}(s-n/2+j)} \int_0^\infty t^{s-n/2+k-1} \tfrac{\partial^k}{\partial t^k} \left(t^{n/2} p_t(x,x) \right) dt \qquad (6)
\end{aligned}$$

where we have repeatedly integrated by parts. The asymptotic properties of p_t ensure that there are no boundary terms. Now the k^{th} derivative of a smooth function is again a smooth function, in particular bounded as $t \searrow 0$, so the integral in (6) is absolutely convergent (hence analytic) for $\mathrm{Re}(s) > \frac{n}{2} - k$ in all Banach spaces $C^\ell(\mathrm{Diag}, E \boxtimes E^*)$. The right-hand side of (6) has simple poles at $s \in n/2 - \mathbb{N}$. We have shown

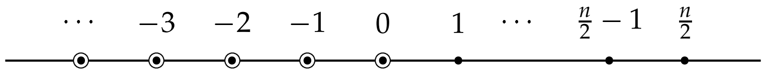
Proposition 2. *For each $x \in M$ the function $\{s \in \mathbb{C}; \mathrm{Re}(s) > \frac{n}{2}\} \ni s \mapsto q_{-s}(x,x)$ extends meromorphically to $\mathbb{C}$ with simple poles. This defines meromorphic functions with values in the Banach space $C^\ell(\mathrm{Diag}, E \boxtimes E^*)$ for all $\ell \in \mathbb{N}$.*

- *If n is even, then the poles of $q_{-s}(x,x)$ arise at*
$$s = n/2, n/2-1, \ldots, 1.$$
In particular, the number of poles is finite.
- *If n is odd, then the poles of $q_{-s}(x,x)$ arise at*
$$s \in n/2 - \mathbb{N}.$$
Moreover, $q_{-s}(x,x)$ has zeroes at $s \in -\mathbb{N}$.

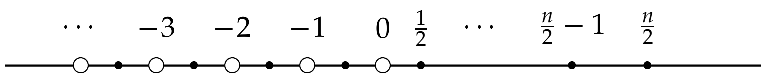
□

Poles of $\Gamma(s)$: ○ Poles of $\Gamma(s)q_{-s}(x,x)$: •

n even:



n odd:



One crucial observation is now that the coefficients in the asymptotic expansion (3) of the heat kernel can be read off from the poles of the complex powers. More precisely, we have

Proposition 3. *For all $x \in M$ we have*
$$\mathrm{Res}_{s=n/2-k}\Gamma(s)q_{-s}(x,x) = a_{2k-n}(x)$$
where $a_{2k-n}(x)$ are the heat coefficients in (3).

PROOF. From (6) with $k+1$ instead of k and from (3) we see that
$$\begin{aligned}\mathrm{Res}_{s=n/2-k}\Gamma(s)q_{-s}(x,x) &= \frac{-1}{k!}\int_0^\infty \frac{\partial^{k+1}}{\partial t^{k+1}}(t^{n/2}p_t(x,x))dt \\ &= \frac{1}{k!}\frac{\partial^k}{\partial t^k}(t^{n/2}p_t(x,x))|_{t=0} \\ &= a_{2k-n}(x).\end{aligned}$$

□

Another technical consequence to be used later is the following

Proposition 4. *Let $\alpha < \beta$ and let $K \subset M \times M \setminus \mathrm{Diag}$ be compact. Then the restriction to K of the meromorphic function $s \mapsto \Gamma(s)q_{-s}$ is uniformly bounded on $\{s \in \mathbb{C};\ \alpha \le \mathrm{Re}(s) \le \beta\}$ in each of the Banach spaces $C^\ell(K, E \boxtimes E^*)$.*

Moreover, for any $\varepsilon > 0$ *the restriction of* $s \mapsto \Gamma(s) q_{-s}$ *to the diagonal* Diag *is uniformly bounded on* $\{s \in \mathbb{C};\ \alpha \le \mathrm{Re}(s) \le \beta,\ |\mathrm{Im}(s)| \ge \varepsilon\}$ *in each of the Banach spaces* $C^\ell(\mathrm{Diag}, E \boxtimes E^*)$. *If* $\beta > \alpha > \frac{n}{2}$, *then the same holds on* $\{s \in \mathbb{C};\ \alpha \le \mathrm{Re}(s) \le \beta\}$.

PROOF. The first statement is clear from (5), (2) and the asymptotic properties of p_t. For the second statement choose $k \in \mathbb{N}$ so large that $\alpha > \frac{n}{2} - k$. Then the integral in (6) converges absolutely in $C^\ell(\mathrm{Diag}, E \boxtimes E^*)$ on the region under consideration and the proposition follows. □

3. FROM COMPLEX POWERS TO THE HEAT KERNEL

Let $Q := \Delta^{1/2}$. Through the inverse Mellin transform we write for $t > 0$, $\tau > 0$,

$$e^{-tQ} = \frac{1}{2\pi i} \int_{\mathrm{Re}(s)=\tau} t^{-s} \Gamma(s) Q^{-s} ds. \tag{7}$$

Lemma 5. *The function* $\Gamma(s)$ *is rapidly decreasing on the lines* $\mathrm{Re}(s) = \tau$ *for all* $\tau \in \mathbb{R}$, *uniformly in each strip* $\{s \in \mathbb{C};\ \alpha \le \mathrm{Re}(s) \le \beta\}$ *for all* $\alpha < \beta$.

PROOF. For $\mathrm{Re}(s) > 0$ make the change of variable $t = e^v$ in the integral defining the Gamma function,

$$\Gamma(s) := \int_0^\infty t^{s-1} e^{-t} dt.$$

Writing $s = \tau + i\sigma$ we get

$$\Gamma(s) = \int_{\mathbb{R}} e^{iv\sigma} e^{v\tau - e^v} dv$$

which is the inverse Fourier transform of a Schwartz function, hence Schwartz itself (in σ). For $\mathrm{Re}(s) \le 0$ use the functional equation of the Gamma function. □

The integral (7) is therefore absolutely convergent in the operator norm for $\tau > 0$ and is independent of such τ by the Cauchy residue formula. This implies that $Q^k e^{-tQ}$ is bounded for all $k \in \mathbb{N}$ and so e^{-tQ} is smoothing (always for $t > 0$).

We want now to derive from (7) an identity relating Schwartz kernels. Since $Q^{-s} = \Delta^{-s/2}$ we can use the results of the previous section. For $\mathrm{Re}(s) > n$ the operators Q^{-s} have continuous Schwartz kernels $q_{-s/2}(x,y)$. Recall the *Legendre duplication formula* for the Gamma function:

$$\frac{\Gamma(s)}{\Gamma(s/2)} = (2\pi)^{-1/2} 2^{s-1/2} \Gamma\left(\tfrac{s+1}{2}\right).$$

Together with Proposition 4 and Lemma 5 we see that the heat kernel $h_t(x,y)$ of Q satisfies

$$\begin{aligned} h_t(x,y) &= \frac{1}{2\pi i} \int_{\mathrm{Re}(s)=\tau} t^{-s} \Gamma(s) q_{-s/2}(x,y) ds \\ &= \frac{1}{4\pi^{3/2} i} \int_{\mathrm{Re}(s)=\tau} \left(\tfrac{t}{2}\right)^{-s} \Gamma\left(\tfrac{s+1}{2}\right) \Gamma(s/2) q_{-s/2}(x,y) ds \end{aligned} \tag{8}$$

for all $\tau > n$. The point is now that the integrand in the right-hand side has an analytic extension which decays rapidly in all vertical strips $\alpha \le \mathrm{Re}(s) \le \beta$. This follows again from Proposition 4 and Lemma 5. Thus we can move the line of integration in (8) to the left across poles, provided that we account for these poles using the residue formula:

$$\begin{aligned} h_t(x,y) &= \frac{1}{2\pi i}\int_{\mathrm{Re}(s)=n-k+\varepsilon} t^{-s}\Gamma(s) q_{-s/2}(x,y)ds \\ &\quad + \sum_{j=0}^{k-1} \mathrm{Res}_{s=n-j}(t^{-s}\Gamma(s)q_{-s/2}(x,y)). \end{aligned} \tag{9}$$

Note that all the poles are of the form $s = n - j$ but some of these points are in fact regular. We first examine the off-diagonal behavior.

Proposition 6. *The heat kernel $h_t(x,y)$ of $\Delta^{1/2}$ is smooth for $(t,x,y) \in [0,\infty) \times (M \times M \setminus \mathrm{Diag})$ with only odd Taylor coefficients at $t = 0$.*

PROOF. Let K be a compact subset of $M \times M \setminus \mathrm{Diag}$. Then the integral in

$$\frac{\partial^k}{\partial t^k} h_t = \int_{\mathrm{Re}(s)=n+\varepsilon} \tfrac{(-1)^k s(s+1)\cdots(s+k-1))}{2^{k+2}\pi^{3/2} i} \left(\tfrac{t}{2}\right)^{-s-k} \Gamma\left(\tfrac{s+1}{2}\right)\Gamma(s/2) q_{-s/2}\, ds$$

converges absolutely in $C^\ell(K, E \boxtimes E^*)$ by Proposition 4. Thus $h_t(x,y)$ is smooth for $(t,x,y) \in (0,\infty) \times (M \times M \setminus \mathrm{Diag})$. The integral term in (9) is of order $\mathrm{O}(t^{k-n-\varepsilon})$ and $q_{-s/2}|_K$ is entire by Proposition 1. Thus (9) yields an asymptotic expansion in $C^\ell(K, E \boxtimes E^*)$

$$h_t|_K \overset{t\searrow 0}{\sim} \sum_{j=0}^{\infty} t^j\, q_{j/2}|_K\, \tfrac{(-1)^j}{j!}$$

where we used $\mathrm{Res}_{s=-j}(\Gamma(s)) = (-1)^j/j!$. This shows that $h_t|_K$ is also smooth at $t = 0$. Since $q_{j/2}|_K$ vanishes for even j by Proposition 1 only odd Taylor coefficients occur at $t = 0$. □

The behavior on the diagonal of $h_t(x,x)$ depends on parity. Again the restriction to Diag of the integral in the right-hand side of (9) is of order $\mathrm{O}(t^{k-n-\varepsilon})$ in $C^\ell(\mathrm{Diag}, E \boxtimes E^*)$ for all ℓ. Assume first that n is even. From Proposition 2 we know that $\Gamma(s)q_{-s/2}(x,x)$ has simple poles at $s \in \{n, n-2, \dots, 2\} \cup -\mathbb{N}$, thus the residue at $s = n - j$ in (9) is a multiple of t^{j-n}. However, if n is odd then $\Gamma(s)q_{-s/2}(x,x)$ has simple poles at $s = n, n-2, \dots, 1$ and *double* poles at $s = -1, -3, \dots$. Accordingly, $h_t(x,x)$ will have an asymptotic expansion containing singular terms $t^{-n}, t^{-n+2}, \dots, t^{-1}$, odd Taylor terms $t, t^3, t^5, \dots$ and log terms $t \log t, t^3 \log t, t^5 \log t, \dots$. Moreover, some of the coefficients can be written down in terms of the coefficients (3) of the asymptotic expansion of p_t.

Theorem 7. *Let M be an n-dimensional compact Riemannian manifold, let Δ be a positive self-adjoint differential operator of Laplace type acting on sections in a Hermitian vector bundle over M. Let a_j be the heat kernel coefficients for Δ and let q_{-s} be the Schwartz kernel of Δ^{-s}.*

Then the heat kernel h_t of the operator $\Delta^{1/2}$ restricted to Diag *has the following asymptotic expansion as $t \searrow 0$:*

- *For even n*

$$h_t(x,x) \overset{t\searrow 0}{\sim} \sum_{j=0}^{n/2-1} t^{2j-n} A_{2j-n}(x) + \sum_{j=0}^{\infty} t^j A_j(x)$$

where the smooth coefficient functions A_* are

$$\begin{aligned} A_{2j-n}(x) &= a_{2j-n}(x)\, 2^{n/2-j}(n-2j-1)!! \text{ for } j=0,\dots,n/2-1,\\ A_{2j}(x) &= a_{2j}(x)\,\frac{(-2)^{-j}}{(2j-1)!!} \text{ for } j\geq 0,\\ A_{2j+1}(x) &= -\frac{q_{j+1/2}(x,x)}{(2j+1)!} \text{ for } j\geq 0. \end{aligned}$$

- *For odd n*

$$h_t(x,x) \overset{t\searrow 0}{\sim} \sum_{j=0}^{\infty} t^{2j-n} A_{2j-n}(x) + \sum_{j=0}^{\infty} t^{2j+1}\log t\; B_{2j+1}(x)$$

where

$$\begin{aligned} A_{2j-n}(x) &= a_{2j-n}(x)\frac{2^{n-2j}}{\sqrt{\pi}}\left(\frac{n-2j-1}{2}\right)! \text{ for } j=0,\dots,\tfrac{n-1}{2},\\ B_{2j+1}(x) &= a_{2j+1}(x)\,\frac{(-1)^{j+1}}{2^{2j}\sqrt{\pi}j!} \text{ for } j\geq 0,\\ A_{2j+1}(x) &= a_{2j+1}(x)\left(\frac{(-1)^j\log 2}{2^{2j}\sqrt{\pi}j!} + \frac{\mathrm{FP}_{s=-2j-1}(\Gamma(\frac{s+1}{2}))}{2^{2j+1}\sqrt{\pi}}\right)\\ &\quad +\mathrm{FP}_{s=-2j-1}(\Gamma(\tfrac{s}{2})q_{-s/2}(x,x))\frac{(-1)^j}{2^{2j+1}\sqrt{\pi}j!} \text{ for } j\geq 0, \end{aligned}$$

where FP *denotes the finite part.*

PROOF. It was noted above that the integral term from (9) is of order $O(t^{k-n-\varepsilon})$ in $C^\ell(\mathrm{Diag}, E\boxtimes E^*)$ for all ℓ. Clearly the residues in (9) are some powers of t, possibly multiplied with $\log t$ when the poles are double, and our task is to identify the coefficients. For this we use Proposition 3 and (8), where $\Gamma(s)$ has been substituted by the Legendre duplication formula. Assume first n is even. Then for $j\in\{0,1,\dots,n/2-1\}$ we have

$$\begin{aligned} \mathrm{Res}_{s=n-2j}(t^{-s}\Gamma(s)q_{-s/2}(x,x)) &= \tfrac{1}{2\sqrt{\pi}}\mathrm{Res}_{s=n-2j}\left(\tfrac{t}{2}\right)^{-s}\Gamma\left(\tfrac{s+1}{2}\right)\Gamma(\tfrac{s}{2})q_{-s/2}(x,x)\\ &= \left(\tfrac{t}{2}\right)^{2j-n}\tfrac{1}{2\sqrt{\pi}}\Gamma\left(\tfrac{n-2j+1}{2}\right)2a_{2j-n}(x). \end{aligned}$$

This gives the asymptotic term $t^{2j-n}A_{2j-n}(x)$ if we use the functional equation of the Gamma function to write

$$\Gamma\left(\tfrac{n-2j+1}{2}\right) = \Gamma\left(\tfrac{1}{2}\right)2^{j-\frac{n}{2}}(n-2j-1)!!$$

and the identity $\Gamma(\frac{1}{2}) = \sqrt{\pi}$. Similarly for $j \geq 0$,

$$\begin{aligned} \mathrm{Res}_{s=-2j}(t^{-s}\Gamma(s)q_{-s/2}(x,x)) &= \left(\tfrac{t}{2}\right)^{2j} \tfrac{1}{2\sqrt{\pi}}\Gamma(-j+1/2)2a_{2j}(x) \\ &= t^{2j}A_{2j}(x) \end{aligned}$$

because of the identity

$$\Gamma\left(\tfrac{-2j+1}{2}\right) = \Gamma\left(\tfrac{1}{2}\right)\frac{(-2)^j}{(2j-1)!!}.$$

Finally around the pole $s = -2j-1$, $j \geq 0$ we do not use the duplication formula but rather we write

$$\begin{aligned} \mathrm{Res}_{s=-2j-1}(t^{-s}\Gamma(s)q_{-s/2}(x,x)) &= t^{2j+1}q_{j+1/2}(x,x)\mathrm{Res}_{s=-2j-1}(\Gamma(s)) \\ &= t^{2j+1}q_{j+1/2}(x,x)\frac{(-1)^{2j+1}}{(2j+1)!}. \end{aligned}$$

This yields the asymptotic term $t^{2j+1}A_{2j+1}(x)$.

Let us now pass to the odd-dimensional case. For $j \in \{0,\dots,\frac{n-1}{2}\}$

$$\mathrm{Res}_{s=n-2j}(t^{-s}\Gamma(s)q_{-s/2}(x,x)) = \left(\frac{t}{2}\right)^{2j-n}\frac{1}{2\sqrt{\pi}}\Gamma\left(\tfrac{n-2j+1}{2}\right)2a_{2j-n}(x).$$

Since $n-2j+1$ is even we have $\Gamma\left(\frac{n-2j+1}{2}\right) = \left(\frac{n-2j-1}{2}\right)!$ so the residue is $t^{2j-n}A_{2j-n}(x)$. The most complicated case is at $s = -2j-1$, $j \geq 0$ since the pole there is double. We write the limited development around $s = -2j-1$ of the functions involved:

$$\begin{aligned} (\frac{t}{2})^{-s} &= (\frac{t}{2})^{2j+1}(1-(s+2j+1)\log\tfrac{t}{2}) + O(s+2j+1)^2, \\ \Gamma\left(\tfrac{s+1}{2}\right) &= \frac{2(-1)^j}{j!}(s+2j+1)^{-1} + \mathrm{FP}_{s=-2j-1}(\Gamma(\tfrac{s+1}{2})) + O(s+2j+1), \\ \Gamma\left(\tfrac{s}{2}\right)q_{-s/2}(x,x) &= \frac{2a_{2j+1}(x)}{s+2j+1} + \mathrm{FP}_{s=-2j-1}(\Gamma(\tfrac{s}{2})q_{-s/2}(x,x)) + O(s+2j+1). \end{aligned}$$

From this one computes

$$\begin{aligned} &\mathrm{Res}_{s=-2j-1}\left(\frac{1}{2\sqrt{\pi}}(\frac{t}{2})^{-s}\Gamma\left(\tfrac{s+1}{2}\right)\Gamma\left(\tfrac{s}{2}\right)q_{-s/2}(x,x)\right) \\ &= t^{2j+1}A_{2j+1}(x) + t^{2j+1}\log t B_{2j+1}(x) \end{aligned}$$

as claimed. □

It is remarkable that in the even-dimensional case there are no logarithmic terms in the expansion.

Note that all the heat invariants of Δ appear among the asymptotic terms of Theorem 7, but the converse is not true since $A_{2j+1}(x)$ is not expressible in terms of the $a_*(x)$ alone.

The asymptotic heat coefficients $a_*(x)$ of a Laplace type operator can in principle be computed recursively and be expressed in terms of curvature, the total symbol of Δ and their derivatives at x. This has been worked out in many cases, see e. g. [3, 4, 7, 9, 11].

Let us look at the Dirac operator D on a closed Riemannian spin manifold acting on sections in the spinor bundle $E = \Sigma M$. Then $\Delta := D^2$ is of Laplace type and we can apply Theorem 7 to $Q := |D|$ provided D has trivial kernel so that Δ is positive. It is well-known that in this case

$$\begin{aligned} a_{-n}(x) &= (4\pi)^{-n/2} \cdot \mathrm{id}_{\Sigma_x M}, \\ a_{-n+2}(x) &= -(4\pi)^{-n/2} \cdot \frac{\mathrm{scal}(x)}{12} \cdot \mathrm{id}_{\Sigma_x M}, \end{aligned}$$

where $\mathrm{scal}(x)$ denotes scalar curvature at x. Hence in the even-dimensional case the asymptotic expansion in Theorem 7 for the kernel of $e^{-t|D|}$ starts as

$$\begin{aligned} h_t(x,x) \overset{t\searrow 0}{\sim} \; & t^{-n} \cdot (2\pi)^{-n/2} \cdot (n-1)!! \cdot \mathrm{id}_{\Sigma_x M} \\ & - t^{-n+2} \cdot (2\pi)^{-n/2} \cdot (n-3)!! \cdot \frac{\mathrm{scal}(x)}{24} \cdot \mathrm{id}_{\Sigma_x M} + \cdots \end{aligned}$$

Our method can be applied to show the existence of and examine the small-time asymptotic expansion for the heat kernel of $\Delta^{1/m}$ for all $m > 0$. The only difference from the above analysis is the use of the Gauss multiplication formula

$$\Gamma(z)\Gamma(z + \tfrac{1}{m}) \cdots \Gamma(z + \tfrac{m-1}{m}) = (2\pi)^{(m-1)/2} m^{1/2 - mz} \Gamma(mz).$$

We state the result without proof.

Theorem 8. *Let M be an n-dimensional compact Riemannian manifold, let Δ be a positive self-adjoint differential operator of Laplace type acting on sections in a Hermitian vector bundle over M, let m be a positive integer. Let a_j be the heat kernel coefficients for Δ and let q_{-s} be the Schwartz kernel of Δ^{-s}.*

Then the heat kernel $h_{m,t}$ of the operator $\Delta^{1/m}$ restricted to Diag *has the following asymptotic expansion as $t \searrow 0$:*

- *For n even*

$$\begin{aligned} h_{m,t}(x,x) \overset{t\searrow 0}{\sim} & \sum_{j=0}^{n/2-1} t^{m(j-n/2)} \cdot \frac{(m(n/2-j))!}{(n/2-j)!} \cdot a_{2j-n}(x) \\ & + \sum_{j=0}^{\infty} t^j \cdot \frac{(-1)^j}{j!} \cdot q_{j/m}(x,x) \end{aligned}$$

  with $q_k(x,x) = (-1)^k \cdot k! \cdot a_{2k}(x)$ for all integral $k \geq 0$.
- *For n and m odd*

$$\begin{aligned} h_{m,t}(x,x) \overset{t\searrow 0}{\sim} & \sum_{j=0}^{\infty} t^{m(j-n/2)} \cdot m \cdot \frac{\Gamma(m(n/2-j))}{\Gamma(n/2-j)} \cdot a_{2j-n}(x) \\ & + \sum_{j=0}^{\infty} t^j \cdot \frac{(-1)^j}{j!} \cdot q_{j/m}(x,x) \end{aligned}$$

  with $q_k(x,x) = 0$ for all integral $k \geq 0$.

- *For n odd and m even*

$$
\begin{aligned}
h_{m,t}(x,x) \overset{t\searrow 0}{\sim} & \sum_{j=0}^{(n-1)/2} t^{m(j-n/2)} \cdot m \cdot \frac{\Gamma(m(n/2-j))}{\Gamma(n/2-j)} \cdot a_{2j-n}(x) \\
& + \sum_{\substack{j=0 \\ j/m+n/2 \notin \mathbb{N}}}^{\infty} t^j \cdot \frac{(-1)^j}{j!} \cdot q_{j/m}(x,x) \\
& + \sum_{j=(n+1)/2}^{\infty} t^{m(j-n/2)} \cdot \left(\frac{(-1)^{m/2}}{(m(j-n/2))!} \cdot \mathrm{FP}_{s=m(n/2-j)}(q_{-s/m}(x,x)) \right. \\
& \qquad \left. + \frac{m \cdot a_{2j-n}(x)}{\Gamma(n/2-j)} \cdot \mathrm{FP}_{s=m(n/2-j)}(\Gamma(s)) \right) \\
& - \sum_{j=(n+1)/2}^{\infty} t^{m(j-n/2)} \log t \cdot \frac{(-1)^{m/2}}{(m(j-n/2))!} \cdot \frac{m \cdot a_{2j-n}(x)}{\Gamma(n/2-j)}
\end{aligned}
$$

with $q_k(x,x) = 0$ for all integral $k \geq 0$.

In particular, we see that logarithmic terms appear only for odd n and even m. Some of the values in these expansions seem to have been computed in [10].

4. The Wodzicki residue

For the sake of completeness we recall the definition of classical pseudodifferential operators. We identify densities with functions on M using the fixed metric g.

Definition 9. Let $p : V \to M$ be a vector bundle with Riemannian metric h and $E \to M$ another vector bundle. A *classical symbol* on V with coefficients in E of order $s \in \mathbb{C}$ is a smooth section f in $p^*(\mathrm{End}(E))$ over V admitting an asymptotic expansion

$$f(x,\xi) \overset{|\xi|\nearrow\infty}{\sim} \sum_{j=0}^{\infty} \sigma_{-j}(x, \tfrac{\xi}{|\xi|}) |\xi|^{s-j}$$

for suitable smooth sections σ_{-j} in $p^*(\mathrm{End}(E))$ on the h-unit-sphere bundle in V.

The definition is independent of h. Let now $\phi : M \times M \to \mathbb{R}$ be a cut-off function such that $\phi \equiv 1$ in a neighborhood of Diag and the support of ϕ is contained in an open set diffeomorphic to a neighborhood of the zero section of the normal bundle NDiag. For any distribution k on $M \times M$ with singular support on Diag and wave front set in N^*Diag (i. e. k conormal to Diag) we denote by $\mathcal{F}(\phi k)$ the Fourier transform of the pull-back of ϕk to NDiag.

Definition 10. An operator $A : C^\infty(M,E) \to C^\infty(M,E)$ is called *classical pseudodifferential* of order s if its Schwartz kernel $k_A(x,y)$ satisfies

- k_A is conormal to Diag.

- The Fourier transform of ϕk_A in the fibers of NDiag is a classical symbol of order s on N^*Diag.

The definition is independent of the choice of ϕ, of the collar neighborhood diffeomorphism and of the trivialization of $E \boxtimes E^*$ over the fibers of NDiag needed for the purpose of Fourier transform. We fix these choices and call $\sigma_A := \mathcal{F}(\phi k_A)$ the full symbol of A. Note that the full symbol does depend on the choices.

Let $A(s)$ be an entire family of classical pseudodifferential operators of order $-s$. By this we mean that for all $k \in \mathbb{Z}$, $\frac{\partial A(s)}{\partial \bar{s}} = 0$ for $\mathrm{Re}(-s) < k$ inside the Banach space of bounded operators between Sobolev spaces $L(H^k(M,E), H^0(M,E))$. For such a family it follows that $(1-\phi)k_{A(s)}$ is an entire family of sections of $E \boxtimes E^*$ over $M \times M$ and that the family of symbols $\sigma_{A(s)}$ is entire in s. In turn this implies that the coefficients $\sigma_{-j}(s)$ are entire families of sections in $p^*(\mathrm{End}(E))$ over the sphere in the conormal bundle:

$$\sigma_{A(s)}(x,\xi) \overset{|\xi| \nearrow \infty}{\sim} \sum_{j=0}^{\infty} \sigma_{-j}(s, x, \tfrac{\xi}{|\xi|})|\xi|^{-s-j}. \tag{10}$$

Proposition 11. *The restriction to* Diag *of the Schwartz kernel of an entire family* $A(s)$ *of classical pseudodifferential operators of order* $-s$ *is well-defined and holomorphic for* $\mathrm{Re}(s) > n = \dim(M)$*, with values in the space of smooth sections of* $\mathrm{End}(E)$ *over* Diag*. This family extends analytically to* $\mathbb{C}$ *with possible simple poles at* $s \in n - \mathbb{N}$*. The residues are given by*

$$\mathrm{Res}_{s=n-j}\left(k_{A(s)}(x,x)\right) = \frac{1}{(2\pi)^n}\int_{S_x^*\mathrm{Diag}} \sigma_{-j}(n-j, x, \theta)d\theta. \tag{11}$$

PROOF. It is a well-known fact that an operator $A(s)$ of order $-s$ with $\mathrm{Re}(s) > n$ has a continuous Schwartz kernel $k_{A(s)}(x,y)$ so the restriction makes sense. For classical pseudodifferential operators this fact can be seen as follows: the Fourier transform of the kernel $\phi k_{A(s)}$ is a symbol of order $-s$, thus it is in L^1 for $\mathrm{Re}(s) > n$. Therefore $\phi k_{A(s)}$ is continuous since it is the inverse Fourier transform of an L^1-function. Using the inverse Fourier transform in the normal directions we write

$$k_{A(s)}(x,x) = \frac{1}{(2\pi)^n}\int_{N_x^*\mathrm{Diag}} \sigma_{A(s)}(x,\xi)d\xi.$$

Let us show that for all $k \in \mathbb{N}$, $k_{A(s)}|_{\mathrm{Diag}}$ extends to $\{\mathrm{Re}(s) > n-k\}$ with possible poles at $s = n, n-1, \dots, n-k+1$. Let $\psi : \mathbb{R} \to \mathbb{R}$ be a smooth function so that $\psi(r) = 0$ for $r \le \frac{1}{2}$ and $\psi(r) = 1$ for $r \ge 1$. Formula (10) implies the limited expansion

$$\sigma_{A(s)}(x,\xi) = \sum_{j=0}^{k-1} \sigma_{-j}(s,x,\tfrac{\xi}{|\xi|})|\xi|^{-s-j}\psi(|\xi|) + w_{-k}(s,x,\xi)$$

where $w_{-k}(s,x,\xi)$ is defined by the above equality and is an entire family of classical symbols of order $-s-k$. We have already seen that $\int_{N_x^*\mathrm{Diag}} w_{-k}(s,x,\xi)d\xi$ is analytic for $\mathrm{Re}(s+k) > n$, i. e. for $\mathrm{Re}(s) > n-k$. Let us examine the integrals $\int_{N_x^*\mathrm{Diag}} \sigma_{-j}(s,x,\frac{\xi}{|\xi|})|\xi|^{-s-j}\psi(|\xi|)d\xi$. The integral on the unit ball $\{|\xi| \le 1\}$ is uniformly convergent for all s, hence it is entire. For the integral on the complement of the unit ball in $N_x^*\mathrm{Diag}$ introduce polar coordinates $r := |\xi|$, $\theta := \frac{\xi}{|\xi|}$. Notice that $\psi(|\xi|)$ is identically 1 on $|\xi| \ge 1$, thus we are left with

$$\begin{aligned}&\int_{\{|\xi|\ge 1\}} \sigma_{-j}(s,x,\tfrac{\xi}{|\xi|})|\xi|^{-s-j}\psi(|\xi|)d\xi \\ &= \int_{S_x^*\mathrm{Diag}} \sigma_{-j}(s,x,\theta)d\theta \int_1^\infty r^{-s-j}r^{n-1}dr \\ &= \frac{1}{s-n+j}\int_{S_x^*\mathrm{Diag}} a_{-j}(s,x,\theta)d\theta.\end{aligned}$$

The integral on the sphere is entire in s so the whole thing extends to $\mathbb{C}$ with a simple pole at $s = n - j$. □

Definition 12. Let $A(s)$ be any entire family of classical pseudodifferential operators of order $-s$ such that $A(0) = \mathrm{id}_E$. For any classical pseudodifferential operator P define the *Wodzicki residue density* of P by

$$\mathrm{wres}(P)(x) := \mathrm{Res}_{s=0}(k_{A(s)P}(x,x)).$$

We have applied Proposition 11 to the entire family $A(s)P$ of order $-s+k$. Let

$$\sigma_P(x,\xi) \overset{|\xi|\nearrow\infty}{\sim} \sum_{j=0}^{\infty} p_{k-j}(x,\tfrac{\xi}{|\xi|})|\xi|^{k-j}$$

be the asymptotic expansion of the full symbol σ_P. Clearly $\sigma_P(x,\xi) = \sigma_{A(0)P}(x,\xi)$. Formula (11) at $s = 0$ shows that

$$\mathrm{wres}(P)(x) = \frac{1}{(2\pi)^n}\int_{S_x^*\mathrm{Diag}} p_{-n}(x,\theta)d\theta.$$

So $\mathrm{wres}(P)(x)$ is independent of the family $A(s)$ used in the definition and coincides with the Wodzicki residue density defined in [16] up to a constant.

Let A be an elliptic self-adjoint positive classical pseudodifferential operator of order $m > 0$. It was proved by Seeley [15] that the family of complex powers A^{-s} is an entire family of classical pseudodifferential operators of order $-s$. Since $A^0 = \mathrm{id}_E$ we can use the family $A(s) := A^{-s}$ to construct the Wodzicki residue density.

Combining Proposition 3 and the above facts we can refine the results of Kalau and Walze [12], Kastler [13] and Ackermann [1].

Theorem 13. *Let M be an n-dimensional compact Riemannian manifold, let Δ be a positive self-adjoint differential operator of Laplace type acting on sections in a Hermitian vector bundle over M. Let a_j be the heat kernel coefficients for Δ.*

If n is even then for $j = n/2, n/2-1, \dots, 1$ we have

$$\mathrm{wres}(\Delta^{-j})(x) = \frac{2a_{-2j}(x)}{\Gamma(j)}. \tag{12}$$

If n is odd then the same identity holds for $j \in n/2 - \mathbb{N}$.

PROOF. Use the complex powers of $A := Q = \Delta^{1/2}$ in the definition of wres. Then for $j \in \mathbb{C}$ and $P = \Delta^{-j}$ we have

$$\text{wres}(\Delta^{-j})(x) = \text{Res}_{s=0}(q_{-s/2+j}(x,x)) = \text{Res}_{s=2j}(q_{-s/2}(x,x)) \tag{13}$$

in the notation of Section 2. From Proposition 2 we see that the poles occur only for $j = n/2, n/2-1, \ldots, 1$ if n is even, respectively for $j \in n/2 - \mathbb{N}$ if n is odd. Moreover, for such j (12) follows immediately from Proposition 3 and (13). □

Through integration over M our results transform into statements regarding the zeta function and the heat trace asymptotics. The Wodzicki residue is defined by

$$\text{Wres}(P) := \text{Res}_{s=0}\text{Tr}(A(s)P)$$

for any entire family of order $-s$ with $A(0) = \text{id}_E$ as above. Clearly then $\text{Wres}(P) = \int_M \text{wres}(P)(x)dx$. Thus Theorem 13 implies the main result of [12, 13, 1]:

$$\text{Res}_{s=2j}\zeta(\Delta, s) = \text{Wres}(\Delta^{-j}) = \frac{2}{\Gamma(j)} \int_M \text{Tr}(a_{-2j}(x))dx$$

for j depending on parity as above (recall the definition $\zeta(\Delta, s) := \text{Tr}(\Delta^{-s/2})$).

REFERENCES

[1] T. Ackermann, *A note on the Wodzicki residue,* J. Geom. Phys. **20** (1996), 404–406.

[2] N. Berline, E. Getzler, M. Vergne, *Heat Kernels and Dirac Operators,* Springer-Verlag, Berlin Heidelberg 1991.

[3] T. Branson, P. Gilkey, K. Kirsten, D. Vassilevich, *Heat kernel asymptotics with mixed boundary conditions,* Nucl. Phys. B **563** (1999), 603–626.

[4] T. Branson, P. Gilkey, B. Ørsted, *Leading terms in the heat invariants,* Proc. Am. Math. Soc. **109** (1990), 437–450.

[5] J. Chazarain, *Formule de Poisson pour les variétés riemanniennes,* Invent. Math. **24** (1974), 65–82.

[6] A. Connes, *Gravity coupled with matter and the foundation of non-commutative geometry,* Commun. Math. Phys. **182** (1996), 155–176.

[7] H. Donnelly, *Heat equation asymptotics with torsion,* Indiana Univ. Math. J. **34** (1985), 105–113.

[8] J. J. Duistermaat, V. W. Guillemin, *The spectrum of positive elliptic operators and periodic geodesics,* Differ. Geom., Proc. Symp. Pure Math. **27** (1975), Part 2, Stanford 1973, 205–209.

[9] P. Gilkey, *Invariance theory, the heat equation and the Atiyah-Singer index theorem,* 2nd edition, Studies in Advanced Mathematics. Boca Raton, FL: CRC Press 1995.

[10] E. V. Gorbar, *Heat kernel expansion for operators containing a root of the Laplace operator,* J. Math. Phys. **38** (1997), 1692–1699.

[11] V. P. Gusynin, V. V. Kornyak, *Symbolic computation of DeWitt-Seeley-Gilkey coefficients on curved manifolds,* J. Symb. Comput. **17** (1994), 283–294.

[12] W. Kalau, M. Walze, *Gravity, non-commutative geometry and the Wodzicki residue,* J. Geom. Phys. **16** (1995), 327–344.

[13] D. Kastler, *The Dirac operator and gravitation,* Commun. Math. Phys. **166** (1995), 633–643.

[14] S. Minakshisundaram, A. Pleijel, *Some properties of the eigenfunctions of the Laplace operator on Riemannian manifolds,* Canad. J. Math. **1** (1949), 242–256.

[15] R. Seeley, *Complex powers of an elliptic operator,* Proc. Sympos. Pure Math. (Singular integrals), Chicago, Ill., 1966, Amer. Math. Soc. (1967), 288–307.
[16] M. Wodzicki, *Noncommutative residue. I: Fundamentals,* K-theory, arithmetic and geometry Semin., Moscow Univ. 1984–1986, Lect. Notes Math. **1289** (1987), 320–399.

UNIVERSITÄT HAMBURG, FACHBEREICH MATHEMATIK, BUNDESSTR. 55, D-20146 HAMBURG, GERMANY

E-mail address: baer@math.uni-hamburg.de

INSTITUTUL DE MATEMATICĂ AL ACADEMIEI ROMÂNE, P.O. BOX 1-764, RO-70700 BUCHAREST, ROMANIA

E-mail address: moroianu@alum.mit.edu