HEAT KERNEL ASYMPTOTICS FOR OPERATOR VALUED STURM-LIOUVILLE EQUATIONS

Jochen Brüning

Dedicated to Alexander Peyerimhoff on the occasion of his sixtieth birthday

Received: October 27, 1986

Abstract: For operator Sturm-Liouville problems with commutative potentials we derive a local expansion for the operator heat kernel which is asymptotic in the trace norm. We give explicit formulae for the coefficients in an important special case and derive some consequences for index calculations concerning regular singular operators.

AMS-Classification: 34G10, 34B25, 35P05, 35J10

1. Introduction. The analysis of second order elliptic equations is most complete in the simplest case of a one-dimensional operator of Sturm-Liouville type; by this we mean a differential expression

$$\tau := -\partial_z^2 + A(z), \quad z \text{ in some interval } I.$$  \hspace{1cm} (1.1)

The very precise and well known methods developed for these equations do not, in general, extend to elliptic equations in several variables. It has been noted, however, that many elliptic problems can be reduced to the form (1.1) if we allow \(A(z)\) to be an operator valued function, the most prominent example being the Laplacean in polar coordinates. This approach made it possible to use suitably modified methods from the Sturm-Liouville case in the analysis of second order elliptic equations in several variables. For example, R. Seeley and the author have derived the resolvent expansion for operators of this type, even with singularities ([2], [3]), and applied it to index
computations in various singular situations ([4]), ([5]). More precisely, we have studied (1.1) with
\[ \tilde{A}(x) = x^{-2} A(x) \]
where \( A(x) \) satisfies the following conditions:

For all \( x \geq 0 \), \( A(x) \) is a self-adjoint operator in the Hilbert space \( H \) with domain \( H_A \), independent of \( x \), and the function \( R_x \exists x \mapsto A(x) \in \mathcal{L}(H_A, H) \) is smooth;
\[ A(x) \geq -c + 1 \text{ for some } c \text{ and all } x \geq 0, \] (1.3)
\[ A(0) \geq -1/4; \]
(1.4)
\[ (A(0) + 1)^{-1} \in C_p(H), \text{ the von Neumann-Schatten class,} \]
for some \( p > 0 \);
\[ \| A(0) (A(x) + c)^{-1} \|_H \leq C \text{ for all } x \geq 0; \]
(1.5)
\[ \| A(b)(x)(A(0) + 1)^{-1}\|_H \leq C \text{ for all } x \geq 0. \]
(1.6)

From these assumptions it follows that \( r \) in (1.1), regarded as an operator in \( L^2(R^n, H) \) with domain \( C_c^\infty(R^n, H_A) \) is symmetric and semibounded (cf. [3] Section 2) hence the Friedmisch extension \( T \) exists and is self-adjoint and semibounded in \( L^2(R^n, H) \). Using two more assumptions, namely

for any monomial \( Q(A(x), \ldots, A^{(j)}(x), (A(x) + \lambda)^{-1}) \) where the powers of \( (A(x) + \lambda)^{-1} \) at least balance the others we have
\[ \sup_{\lambda > 0, \lambda \in \mathbb{R}} \| Q(A(x), \ldots, A^{(j)}(x), (A(x) + \lambda)^{-1}) \|_H < \infty \]
(1.7)
where \( \Gamma \) is a suitable sector in the complex plane;

For any monomial \( Q(x, \lambda) \) as in (1.7) where the powers of \( (A(x) + \lambda)^{-1} \) exceed the others at least by \( p + 1/2 \) (with \( p \) from (1.4)) \( Q(x, \lambda) \) is trace class in \( H \) and we have an asymptotic expansion
\[ \text{tr}_H Q(x, x^2) \sim \sum \sigma_{\alpha}(x) x^\alpha \log^j x \]
as \( x \to \infty \) and \( x^2 \in \Gamma \); (1.8)
we have proved in [3] that for any \( \varphi \in C_0^\infty(R) \) and any \( m \geq p + 1 \) \( \text{tr}_X \varphi(T + x^2)^{-m} \) exists and has an asymptotic expansion of the type described in (1.8). This means that an assumption on the resolvent of \( A(x) \) leads to an expansion theorem for the resolvent of \( T \). If one is interested in the heat kernel expansion, i.e. the asymptotic expansion of \( \text{tr}_X \varphi e^{-tX} \), then this follows from the analytic expansion using a Cauchy integral (cf. [3] Theorem 7.1). However, in certain applications it is inconvenient to derive the heat kernel expansion from assumptions on the resolvent of \( A(x) \) which one would like to replace by an assumption on the heat kernel of \( A(x) \). It is the purpose of this note to do this. We have to impose, however, an additional restriction on \( A(x) \), namely that the family \( (A(x))_{x \geq 0} \) is commutative. Thus we assume

For any \( n \in \mathbb{N} \) and any choice of \( x := (x_1, \ldots, x_n) \in R^n_+ \) the operator \( A_x := A(x_1) \ldots A(x_n) \) is self-adjoint in \( H \) with domain \( H_n \) independent of \( x \), and for any permutation \( \sigma \) we have with \( \sigma(x) := (x_{\sigma(1)}, \ldots, x_{\sigma(n)}) \)
\[ A_{\sigma(x)} = A_{\sigma(1)}. \]
(1.9)
The assumption (1.9) can be relaxed to certain commutator estimates, at the expense of complicating the proofs and the presentation. Since the constant coefficient case is of considerable interest we have chosen to work with (1.9).

The plan of the paper is as follows. In Section 2 we generalize the well known Hadamard–Minakshisundaram–Pleijel expansion to obtain a local expansion of the operator kernel of \( e^{-tX} \) using the assumptions (1.2) through (1.6) and (1.9); the coefficients in this expansion are defined recursively. Then we indicate how the expansion of \( \text{tr}_X \varphi e^{-tX} \) follows from this if an assumption parallel to (1.8) is introduced. In Section 3 we give explicit formulae for the coefficients in the case that \( A(x) = A(0) \). Our results are applied to certain computations involving \( \eta \)-functions in Section 4.

I am indebted to Bob Seeley for innumerable discussions concerning this subject and related questions. Thanks are also due to Herbert Schröder for help with the computations.

2. The asymptotic expansion of the operator heat kernel is based on the ansatz
\[ e^{-tT}(x, y) \sim (4\pi t)^{-1/2} e^{-(x-y)^2/4t} \sum_{j \geq 0} t^j U_j(x, y) e^{-t^{j/4} A(y)} \]
(2.1)
for \( x, y, t > 0 \). This imitates the Hadamard–Minakshisundaram–Pleijel construction except for the factor \( e^{-t^{j/4} A(y)} \) which we are forced to introduce in order to obtain trace class operators. A formal computation gives
Let $H_k$ be the domain of $A_k = A(x_1) \cdots A(x_j)$ for certain $x_i \in \mathbb{R}^+$, $1 \leq i \leq j$, independent of the choice $x_i$ and

$$H_{j+1} \subset H_j \subset H_0 := H,$$

for $j \in \mathbb{N}$. Each $H_j$ is a Hilbert space with the graph norm of some operator $A(x_1, \ldots, x_j)$, and by the closed graph theorem the embeddings $H_{j+1} \subset H_j$ are all continuous.

For the solution of (2.3) we have

**Lemma 2.1** The recursion formulae (2.3) have a unique solution $U_j$

$$U_j(x,y) = \int_0^1 s^{j-1} R_{j-1}(y + s(x-y), y) dy,$$

$x, y > 0, j \in \mathbb{N}$ Moreover, $U_j \in C^\infty(\mathbb{R}^+ \times \mathbb{R}^+)$ for all $k \in \mathbb{Z}_+$ and for $x, y, z > 0, \epsilon \in H_{j+1}$

$$U_j(x, y) A(\epsilon) = A(x) U_j(x, y) e.$$

**Proof.** The assertion is obvious for $j = 0$. Suppose it has been proved for $j - 1 \geq 0$. By assumption we have for $k \in \mathbb{Z}_+$

$$R_{j-1}(x, y) = \frac{\partial^2}{x^2} U_{j-1}(x, y) - (x^{-2} A(x) - y^{-2} A(y)) U_{j-1}(x, y) \in C^\infty(\mathbb{R}^+ \times \mathbb{R}^+, \mathcal{L}(H_{j+k}, H_k)).$$

Thus defining $U_j(x, y)$ by (2.5) we also have $U_j \in C^\infty(\mathbb{R}^+ \times \mathbb{R}^+, \mathcal{L}(H_{j+k}, H_k))$, and it is easily seen that we obtain a smooth solution of (2.6b). Substituting $V_j(x, y) := (x-y) U_j(x, y)$ we see that $V_j$ is the unique solution of the initial value problem

$$\partial_v V_j(x, y) = (x-y)^{-1} R_j(x, y), \quad V_j(y, y) = 0.$$

Finally, (2.6) follows from (2.5) and the induction hypothesis.

To prove that (2.1) is asymptotic in a suitable sense we have to examine the continuity properties of the coefficients $U_j$ more closely; at this point we make use of the commutativity assumption in a crucial way. We introduce the operators

$$U_{jk}(y) := \frac{1}{k!} \partial^k_x |_{x=y} U_j(x, y), \quad x, y \in \mathbb{R}^+, \quad j, k \in \mathbb{Z}_+.$$ 

The recursion (2.3) implies the following recursion for the $U_{jk}$.

**Lemma 2.2** The operators $U_{jk}$ satisfy the recursion

$$U_{00}(y) = 1, \quad U_{0k}(y) = 0 \quad \text{if} \ k \geq 1,$$

$$U_{j+1,k}(y) = (j + k + 1)^{-1} [(k + 1)(k + 2) U_{j,k+2}(y)$$

$$- \sum_{\ell=0}^{k-1} U_{j,\ell}(y) \sum_{m=0}^{k-\ell} (-1)^m \frac{m+1}{(k-\ell-m)!} y^{-m-2} A^{k-\ell-m}(y)]$$

Letting

$$\alpha_{jk} := \left[ \frac{2}{3} j + \frac{1}{3} k \right] = \text{the greatest integer} \leq \frac{2}{3} j + \frac{1}{3} k$$

$U_{jk}$ is a universal polynomial in the variables $A(y), A'(y), \ldots$ of degree $d_{jk} \leq \min\{\alpha_{jk}, j\}$

**Proof.** The formulae (2.8) follow immediately from

$$U_{j+1,k}(y) = (j + k + 1)^{-1} \frac{1}{k!} \partial^k_x |_{x=y} R_j(x, y)$$

and (2.3). The second assertion is obvious if $j = 0$ and it is also obvious that $d_{jk} \leq j$ for all $k$ if the assertion holds for $0 \leq \ell \leq j$ and all $k$ we obtain from (2.8b) that $U_{j+1,k}(y)$ is a universal polynomial in the variables $A(y), A'(y), \ldots$. For its degree $d_{j+1,k}$ we have the inequality

$$d_{j+1,k} \leq \max\{\alpha_{j,k+2}, \max_{0 \leq \ell \leq k-1} (\alpha_{j,\ell} + 1)\}.$$

But

$$\alpha_{j,k+2} = \left[ \frac{2}{3} j + \frac{1}{3} (k + 2) \right] = \alpha_{j+1,k},$$

$$\alpha_{j,\ell} + 1 \leq \left[ \frac{2}{3} j + \frac{1}{3} (k - 1) \right] + 1 = \alpha_{j+1,k},$$
and the assertion follows.

Now we choose \( \varphi, \psi \in C_0^\infty(\mathbb{R}^*) \) such that \( \psi = 1 \) in a neighborhood of \( \text{supp} \varphi \). As a parametrix for the heat operator \( \partial_t + T \) we then try

\[
H_t^{N} u(z) := \int_0^\infty H_t^{N}(z, y)(u(y))dy, \ u \in L^2(\mathbb{R}_+, H),
\]

where

\[
H_t^{N}(z, y) = (4\pi t)^{-1/2}e^{-(z-y)^2/4t} \sum_{j=0}^N t^j \psi(z) U_j(z, y) \varphi(y)e^{-t\varphi^{-1}A(y)}. \tag{2.10}
\]

From Lemma 2.1 and (1.5), (1.6), and (1.9) we see that

\[
F_j(z, y)(A(y) + C_0)^{-j} \in C^\infty(\mathbb{R}^* \times \mathbb{R}^*, \mathcal{L}(H))
\]

hence

\[
H_t^{N}(z, y) \in C^\infty(\mathbb{R}^* \times \mathbb{R}^*, \mathcal{L}(H)).
\]

Also, \( H_t^{N} \) is a bounded operator in \( L^2(\mathbb{R}_+, H) \) and the \( L^2 \) norm can be bounded independent of \( t \in (0, 1] \). In fact, it follows from the spectral theorem and the Cauchy-Schwarz inequality that

\[
\left\| \int_0^\infty H_t^{N}(z, y)(u(y))dy \right\|_H \leq CN(4\pi t)^{-1/2} \int_0^\infty e^{-(z-y)^2/4t} \|u(y)\|_H dy.
\]

Next we check the initial condition.

**Lemma 2.3** For \( u \in L^2(\mathbb{R}_+, H) \) we have

\[
\lim_{t \to 0} H_t^{N} u = u \quad \text{in} \quad L^2(\mathbb{R}_+, H).
\]

**Proof.** By the uniform boundedness of \( \|H_t^{N}\|_{L^2} \) for \( t \in (0, 1] \) we may assume that \( u \in C_0^\infty(\mathbb{R}^*, H) \). We first estimate the operator norm of a term in the sum (2.10) with \( j \geq 1 \). To do so we use the Taylor expansion of \( U_j(z, y) \) near \( z = y \),

\[
U_j(z, y) = \sum_{k=0}^M U_{jk}(y)(z-y)^k
+ \frac{(z-y)^{M+1}}{M!} \int_0^1 (1-u)^m \partial_x^{M+1} U_j(y + u(z-y), y)du.
\]

From Lemma 2.2 we find that

\[
\psi(z) U_j(z, y)(A(y) + C_0)^{-j} \varphi(y)e^{-t\varphi^{-1}A(y)}
\]

is uniformly bounded in \( z \) and \( y \). Since \( U_j \in C^\infty(\mathbb{R}^* \times \mathbb{R}^*, \mathcal{L}(H)) \) we obtain similarly that the remainder term is \( O((M+1)/2)(4\pi t)^{-1/2}e^{-(z-y)^2/4t} \). Thus we infer that

\[
\lim_{t \to 0} \|H_t^{N} u - (4\pi t)^{-1/2} \int_0^\infty e^{-(z-y)^2/4t} \psi(z) \varphi(y)e^{-t\varphi^{-1}A(y)}(u(y))dy \|_{L^2(\mathbb{R}_+, H)} = 0.
\]

Now if \( z \in \mathbb{R}^* \) is fixed, we may estimate

\[
\int_0^\infty e^{-(z-y)^2/4t} \psi(z)(\varphi(y) - \varphi(z))e^{-t\varphi^{-1}A(y)}(u(y))dy \leq \|\varphi\|_H \|u\|_2
\]

as \( H \)-norm as small as we please if \( y \) is sufficiently close to \( z \) and \( t \) is sufficiently small. Since \( u \in C^\infty(\mathbb{R}_+, H) \) the assertion is obvious for the second and third term on the right. The first term is estimated by standard semigroup theory (cf. [7], §7.3) using the continuity of \( y \mapsto A(y) \).

Thus

\[
\lim_{t \to 0} (4\pi t)^{-1/2} \int_0^\infty e^{-(z-y)^2/4t} \psi(z)(\varphi(y) - \varphi(z))e^{-t\varphi^{-1}A(y)}(u(y))dy
\]

completing the proof of the lemma.

Now we compare \( H_t^{N} \) and \( e^{\pm t\varphi} \) following Duhamel's principle as usual. Note first that the operator functions \( t \mapsto (A(y) + C_0)e^{-t\varphi^{-1}A(y)} \in \mathcal{L}(H) \) are smooth for all \( j \geq 0 \). This follows again from the arguments in [7] §7.3 quoted above, and the commutativity of the family \( A(y) \) implies that

\[
\partial_y e^{-tA(y)} = -A'(y)e^{-tA(y)}.
\]

Since \( C_0^\infty(\mathbb{R}_+, H) \subset \mathcal{D}(t) \) it is then easy to see that \( t \mapsto H_t^{N} u \in \mathcal{D}(t) \) is smooth in \( t > 0 \) for all \( u \in C_0^\infty(\mathbb{R}_+, H) \). Using (2.2) and (2.3) one computes that writing

\[
(\partial_t + T)H_t^{N} u =: R_t^{N} u
\]
we have
\[ R_t^N u(x) = \int_0^\infty R_t^N(x, y)(u(y)) dy \]
with
\[
R_t^N(x, y) = -\psi'(x)H_t^N(z, y)\psi(y) - 2\psi'(z)\partial_x H_t^N(z, y)\psi(y)
+ (4\pi t)^{-1/2} e^{-\frac{(x-y)^2}{4t}} T^N_0(x, y)\partial_x H_t^N(x, y)
+ \left(4(x-y) - 2A(y)\right) U_t^N(x, y) e^{-t\psi(x)} A(x) \psi(y).
\]
Thus we obtain from Lemma 2.3 and [7] Theorem 6.1.
\[
H_t^N u = e^{-tT} \varphi u + \int_0^t e^{-(t-s)T} R_s^N u ds,
\]
and this holds for all \( u \in L^2(R_+, H) \). Pick \( \chi \in C_0^\infty(R^+) \) such that \( \chi \supset \psi \) in the sense that \( \chi = 1 \) in a neighborhood of supp \( \psi \). Then
\[
H_t^N - \chi e^{-tT} \varphi = \int_0^t \chi e^{-(t-s)T} R_s^N u ds
\]
as operator equality in \( L^2(R_+, H) \). Now we choose \( \tilde{\psi}, \tilde{\varphi} \in C_0^\infty(R^+) \) such that \( \chi \supset \tilde{\psi}, \tilde{\varphi} \supset \varphi \). Then
\[
\int_0^t \chi e^{-(t-s)T} R_s^N u ds = \int_0^t \chi e^{-(t-s)T} \tilde{\varphi} R_s^N u ds.
\]
We construct \( \tilde{H}_t^N, \tilde{R}_t^N \) in the same way as \( H_t^N, R_t^N \) with \( \psi, \varphi \) replaced by \( \tilde{\psi}, \tilde{\varphi} \). Then we obtain from (2.14) with \( \varphi \) and \( \tilde{\varphi} \)
\[
\chi e^{-tT} \varphi = H_t^N - \int_0^t \chi e^{-(t-s)T} \tilde{\varphi} R_s^N u ds
= H_t^N - \int_0^t \tilde{H}_s^N R_s^N u ds + \int_0^t \int_0^s \chi e^{-(t-s)T} \tilde{R}_s^N u ds ds
=: H_t^N - \int_0^t \tilde{H}_s^N R_s^N u ds + U_t^N.
\]
Now we want to apply the Trace Lemma in [3] to conclude that \( U_t^N \) has a continuous kernel with values in the trace class \( C_1(H) \). To see this and to estimate the trace norm of this kernel we only have to prove the following

**Lemma 2.4** We have \( [\partial_x, U_t^N] \in C_1(L^2(R_+, H)) \) for \( N \) sufficiently large and
\[
\| [\partial_x, U_t^N] \|_{tr} = O(t^{\mu_N})
\]
with \( 0 < \mu_N \to \infty \) as \( N \to \infty \).
\[
\|e^{-tT(z,y)} - H_t(z,y) - \int_0^t \int_0^t \tilde{H}_{t,s}^N(z,y) R_s^N(z,y) ds \, ds \|_{C_1(H)} \\
\leq C \mu^N
\]

where \(\mu^N \to \infty\) as \(N \to \infty\). But estimating as in Lemma 2.3 we see that

\[
\|e^{-tT(z,y)} - H_t(z,y) - \int_0^t \int_0^t \tilde{H}_{t,s}^N(z,y) R_s^N(z,y) ds \, ds \|_{C_1(H)} \\
\leq C_N (4\pi(t-s))^{-1/2} e^{-(z-s)^2}/4(t-s) \| R_s^N(z,y) \|_{C_1(H)},
\]

so (2.19) follows from (2.15).

The main interest of Theorem 2.1 is of course in its application to the expansion of the heat kernel on the diagonal. For \(\varphi \in C^0_0(\mathbb{R}^+)\) we obtain from the Trace Lemma and Theorem 2.1 the asymptotic expansion

\[
\text{tr}_{L^2} \varphi e^{-tT} = \int_0^\infty \varphi(z) \text{tr}_H e^{-tT(z,z)} dz \\
\sim (4\pi)^{-1/2} \sum_{j \geq 0} t^j \int_0^\infty \varphi(z) \text{tr}_H U_j(z,z) e^{-z/4A(z)} dz.
\]

So away from the singularity the asymptotic expansion of \(\text{tr} e^{-tT}\) is reduced to the expansion of

\[
\text{tr}_H Q_j(A(z), \cdots, A^{(k)}(z)) e^{-z/4A(z)}
\]

(2.21)

**Heat Kernel Asymptotics**

For certain polynomials \(Q_j\) in the derivatives of \(A\) which can be computed recursively from (2.8). Moreover, by [3] Theorem 7.1 also some singular contributions to \(\text{tr}_{L^2} \varphi e^{-tT}\) with \(\varphi \in C^0_0(\mathbb{R})\) are determined by the expansions in (2.21), as it stands.

For the Friedrichs extension we can obtain the Expansion Theorem 7.1 in [3] directly from Theorem 2.1 as follows. The scaling property of \(T\) (cf. [3] §4 for these facts and the notation) gives

\[
e^{-tT(z,z)} = z^{-1} e^{-t s^{-2} T(z,1)}
\]

(2.22)

and (2.20) becomes

\[
\text{tr}_{L^2} \varphi e^{-tT} = \int_0^\infty \varphi(z) z^{-1} \text{tr}_H e^{-t z/4z} T(z,1) dz.
\]

(2.23)

Now it is easily checked that in view of Theorem 2.1 the Singular Asymptotics Lemma of [2] can be applied to

\[
\sigma(z,s) := \varphi(z) z^{-1} \text{tr}_H e^{-t z/4z} T(z,1)
\]

and thus gives the asymptotic expansion of (2.23). It is to be noted, however, that this approach uses commutativity or, more generally, commutator assumptions and thus is less general than the method of [3].

### 3. Explicit computations

The coefficient functions \(U_j(z,y)\) are of considerable interest even in the constant coefficient case. Thus we now assume

\[
A(z) = A(0) =: A, z \geq 0.
\]

(3.1)

Let us write

\[
U_{jk} := U_{jk}(1); \quad U_{jk} \in A^0_+ (\mathbb{R}^+)
\]

(3.2)

by Lemma 2.2 \(U_{jk}\) is a universal polynomial in \(A\) of degree \(d_{jk} \leq \min\{\frac{3}{2}j + \frac{1}{2}k, j\}\) and the recursion (2.9) specializes to

\[
\begin{align}
U_{00} = I, \quad U_{0k} = 0 \quad &\text{if } k \geq 1, \\
U_{j+1,k} = (j + k + 1)^{-1}[(k + 1)(k + 2)U_{j,k+2} + \sum_{\ell=0}^{k-1}(-1)^{k-1-\ell}(k + 1 - \ell)A_{j,\ell}].
\end{align}
\]

(3.3a, 3.3b)

Writing
and inserting this in (3.3) leads to the following recursion for the coefficients $U_{jk}$:

\[
U_{jk} = \sum_{i=0}^{d_{jk}} U_{jk}^i A^i. \tag{3.4}
\]

and inserting this in (3.3) leads to the following recursion for the coefficients $U_{jk}$:

\[
U_{jk}^i = 0 \quad \text{if } i, j, \text{ or } k < 0, \tag{3.5a}
\]

\[
U_{00}^0 = 1, \quad U_{0k}^i = 0 \quad \text{if } k \geq 1, \text{ and } i \geq 0, \tag{3.5b}
\]

\[
U_{j+1,k}^i = (j + k + 1)^{-1}(k + 1)(k + 2)U_{j+1,k+2}^i + \sum_{\ell=0}^{k-1} (-1)^{k-1-\ell}(k + 1 - \ell)U_{j+1,\ell}^i \quad \text{if } i, j, k \geq 0. \tag{3.5c}
\]

A straightforward computation gives the following formulae for the first few $U_{jk}$.

**Lemma 3.1**

\[
U_{10} = 0, \quad U_{1k} = (-1)^{k-1} A \quad \text{if } k \geq 1;
\]

\[
U_{20} = -A, \quad U_{2k} = (-1)^{k+1}(k + 1)A + (-1)^{k}(k-1) A^2 \quad \text{if } k \geq 1;
\]

\[
U_{30} = -A + \frac{1}{3} A^2;
\]

\[
U_{3k} = (-1)^{k+1}(k + 1)(k + 2)A + \frac{(-1)^k}{6}(2k + 1)(2k + 2)A^2 + \frac{(-1)^{k+1}}{12}(k-1)(k-2)A^3 \quad \text{if } k \geq 1;
\]

\[
U_{40} = -6A + \frac{5}{2} A^2;
\]

\[
U_{50} = -24A + \frac{66}{5} A^2 - \frac{11}{15} A^3;
\]

\[
U_{60} = -120A + 76A^2 - \frac{49}{6} A^3 + \frac{1}{18} A^4.
\]

Next we single out two easy special cases.

**Lemma 3.2** We have

\[
U_{jk}^j = \begin{cases} 
0 & \text{if } j + k \leq 1, \\
(-1)^{k+1}(j-1)! \binom{k+j-1}{j-1} & \text{if } j + k > 1,
\end{cases} \tag{3.6}
\]

and

\[
U_{jk}^j = \begin{cases} 
1 & \text{if } j = k = 0, \\
0 & \text{if } j = 0, k > 0, \\
\frac{(-1)^{k+j}}{j!} \binom{k+j-1}{j-1} & \text{if } j \geq 1.
\end{cases} \tag{3.7}
\]

**Proof.** We start with the proof of (3.6) using induction on $j$. It is clear from (3.5a,b) and Lemma 3.1 that $U_{jk}^j = 0$ if $j + k \leq 1$. Also, it is easily seen that for $j, k \geq 0$

\[
U_{jk}^j = \begin{cases} 
1 & \text{if } j = k = 0, \\
0 & \text{otherwise.}
\end{cases} \tag{3.8}
\]

Thus the recursion (3.5c) reduces to

\[
U_{j+1,k}^i = (j + k + 1)^{-1}(k + 1)(k + 2)U_{j+1,k+2}^i + (-1)^{k-1}(k + 1)\delta_{j0}
\]

\[
= (j + k + 1)^{-1}(k + 1)(k + 2)U_{j,k+2}^i
\]

if $j \geq 1$. But

\[
(j + k + 1)^{-1}(k + 1)(k + 2)(-1)^{k+j}(j-1)! \binom{k+j}{j-1}
\]

\[
= (-1)^{k+j+1}(k + j)(k + j - 1) \cdots (k + 1)
\]

\[
= (-1)^{k+j+1} \binom{k+j}{j}.
\]

For the proof of (3.7) we use induction on $j$, too. The assertion for $j = 0, 1$ is proved above, and for $j \geq 1$ we have by $d_{jk} \leq j$ the recursion

\[
U_{j+1,k}^{j+1} = (j + k + 1)^{-1} \sum_{\ell=0}^{k-1} (-1)^{k-1-\ell}(k + 1 - \ell)U_{j+1,\ell}^{j+1}
\]

\[
= (-1)^{k+j+1}(j + 1 + k)^{-1} \sum_{\ell=0}^{k-1} \frac{(k + 1 - \ell)}{j!} \binom{j-1}{j-1}
\]

\[
= (-1)^{k+j+1} \frac{1}{j!(j + 1 + k)} \left[ (k + 1) \sum_{\ell=j}^{k-1} \binom{j-1}{j-1} - j \sum_{\ell=0}^{k-1} \binom{j-1}{j-1} \right]
\]

\[
= (-1)^{k+j+1} \frac{1}{j!(j + 1 + k)} \left[ (k + 1) \binom{k-1}{j-1} - j \binom{k}{j + 1} \right]
\]

To see the common structure of (3.6) and (3.7) we note the identity
valid for all \( j, k \geq 0 \). Thus we are lead to the ansatz

\[
U^i_{jk} = (-1)^{k+i} \sum_{\ell = j-i}^{j-1} \alpha_i^j \ell \binom{k+\ell}{\ell}
\]

(3.10)

in the range \( 1 \leq i \leq j, \ k \geq 0 \). This does in fact result in the following explicit formulae which give the \( U^i_{jk} \) in terms of derivatives of rational functions evaluated at 0.

**Theorem 3.1** For \( 1 \leq i \leq j \) and \( k \geq 0 \) we have

\[
U^i_{jk} = (-1)^{k+i} \sum_{\ell = j-i}^{j-1} \frac{(-1)^{j+i+1}}{(j-\ell-1)!(\ell+1)!} \partial \frac{\partial}{\partial x} \bigg|_{x=0} [z(1-z)^{-1} D^{j-i}(1)]
\]

(3.11)

where \( D \) is the differential operator

\[
D = \partial_x^2 x^3 (1-z)^{-1}.
\]

(3.12)

**Proof.** To prove (3.11) we start with the ansatz (3.10). Combining it with the recursion (3.5) with the additional definition

\[
\alpha_i^j \ell = 0 \quad \text{if} \quad \ell < j - i \text{ or } \ell > j - 1
\]

and observing the identity

\[
\sum_{\ell = 0}^{k-1} \binom{k+\ell}{m} = \binom{k+m+2}{m+2} - \binom{k+m}{m}
\]

we obtain for \( k \geq 0 \)

\[
\sum_{\ell = j+1-i}^{j+i-1} \left( (\ell + 1) \alpha^{j+1}_j \ell - \ell (\ell - 1) \alpha^{j+1}_j \ell - 2 \right) + \alpha^{j+1}_j \ell - 2 - i - 1 = 0.
\]

(3.13a)

Since this can only be true if the coefficient of \( \binom{k+\ell}{\ell} \) vanishes for all \( \ell \) the \( \alpha_i^j \ell \) have to satisfy the recursion

\[
\begin{align*}
\alpha_i^{j+1}_j \ell - 1 + (j-\ell) \alpha_i^{j+1}_j \ell - 2 \\
+ \alpha_i^{j+1}_j \ell - 2 - i - 1 = 0, \quad 1 \leq i \leq j, \ i + 1 - i \leq \ell \leq j.
\end{align*}
\]

(3.13b)

\section*{Heat Kernel Asymptotics}

A moment’s reflection shows that the equations (3.13) have a unique solution: in fact, restricting the range of \( \ell \) first to \( j - i \leq \ell \leq j - 2 \) we obtain the \( \alpha_i^j \ell \) inductively from (3.13); taking \( \ell = j \) in (3.13b) shows that the coefficients \( \alpha_i^{j+1}_j \ell \) are also determined. To solve the scheme some experimental computations suggest a further ansatz, namely

\[
\alpha_i^j \ell := \frac{(-1)^i+j+1}{(j-\ell-1)!(\ell+1)!} \beta_i^{j+1} \ell
\]

(3.14)

with certain coefficients \( \beta_i^m \) defined for \( 0 \leq m \leq \ell \). Comparing with (3.12) we must have

\[
\beta_0^m = 0, \quad \beta_i^m = 1, \quad \ell \geq 1,
\]

(3.15a)

and inserting (3.14) into (3.13) gives (setting \( m = j - i \))

\[
\beta_i^{m+1} = (\ell - 1) \beta_i^m + \beta_i^{m+1}
\]

or

\[
\beta_i^{m+1} - \beta_i^m = \beta_i^{m+1} - \beta_i^m.
\]

(3.15b)

It is convenient to define

\[
\beta_i^m = 0 \quad \text{if} \quad \ell < m.
\]

(3.15b) gives immediately for \( \ell > m + 1 \)

\[
\beta_i^{m+1} = \beta_i^{m+1} + \sum_{n=m+2}^{\ell} (\beta_i^{m+1} - \beta_i^{m+1})
\]

\[
= \beta_i^{m+1} + \sum_{n=m+1}^{\ell} (n+1)(n+2) \beta_i^m,
\]

and with \( \ell = m + 1 \) we obtain from (3.15a)

\[
\beta_i^{m+1} = (m+1)(m+2) \beta_i^m = 0
\]

i.e.

\[
\beta_i^{m+1} = \sum_{n=m+1}^{\ell} (n+1)(n+2) \beta_i^m.
\]

(3.16)

Now it is natural to introduce the generating functions

\[
P_m(z) := \sum_{n \geq 0} \beta_i^m x^n.
\]

(3.17)

By (3.15a) we have
\[ P_0(z) = z(1 - z)^{-1}, \quad (3.18) \]

and an easy computation shows that

\[ P_{m+1}(z) = P_0(z) \partial_z^2 z^2 P_m(z). \quad (3.19) \]

Introducing the differential operator \( D \) defined by (3.12) we see by induction on \( m \) that

\[ P_m(z) = P_0(z) D^m(1)(z) \quad \text{for} \quad m \geq 0, \quad (3.20) \]

where the notation means application of \( D^m \) to the constant function 1. From (3.18) and (3.20) it is also clear that the functions \( P_m \) are analytic in \( |z| < 1 \) hence it follows from (3.17) that

\[ \beta\alpha = \frac{1}{m!} \beta^n \bigg|_{z=0} P_m(z). \]

The proof is complete. \( \square \)

4. An application of the pointwise expansion will be given to index computations. The index theorem for regular singular operators derived in [4] requires the calculation of the constant terms in two expansions of the type (2.19); this has been carried out in [3] §7 and [4] §4. With further applications in mind we will use Theorem 2.1 to deal with a more general situation. Recall that a first order elliptic differential operator \( D : C^\infty(E) \rightarrow C^\infty(F) \) between sections of two hermitian bundles \( E, F \) over a Riemannian manifold \( M \) was called "regular singular" in [4] if the following is true: there is an open subset \( U \subset M \) such that \( M \setminus U \) is a smooth compact manifold with boundary and \( D \mid C^\infty(E \mid U) \) is unitarily equivalent to an operator valued ordinary differential operator

\[ \partial_z + z^{-1}(S_0 + S_1(z)) =: T \quad (4.1) \]

with domain \( C^\infty((0, z_0), H_1) \) in the Hilbert space \( L^2((0, z_0), H) \). Here \( H \) is a Hilbert space, \( H_1 \) is a compactly embedded dense subspace, \( S_0 \) is self-adjoint with domain \( H_1 \) (in fact, \( S_0 \) is an elliptic differential operator of first order), and \( S_1(z) \) is a smooth function in \( (0, z_0) \) with values in the continuous linear maps from \( H_1 \) to \( H \), such that for some \( \beta > 1/2 \)

\[ \| S_0(z) + S_1(z) \| + \| S_1(z)(z_0 + 1)^{-1} \| = O(z^{\beta}), \quad z \rightarrow 0. \quad (4.2) \]

In computing the index of \( D \) we may assume that \( S_1(z) \equiv 0 \) for \( z < \delta \), and we are lead to consider the difference

\[ \text{tr}_H \varphi(e^{-iTT^*} - e^{-iT^*}) \quad (4.3) \]

for \( \varphi \in C^\infty([-\delta, \delta]) \) with \( \varphi = 1 \) near 0; the constant term in the asymptotic expansion as \( t \rightarrow 0 \) will then contribute to the index. A simple computation shows that

\[ T^*T = -\partial_z^2 + z^{-2}(S_0^2 + S_0), \quad (4.4a) \]

\[ TT^* = -\partial_z^2 + z^{-2}(S_0^2 - S_0), \quad (4.4b) \]

acting on \( C^\infty((0, \delta), H_2), H_2 := D(S_0^2). \) Since \( S_0^2 \pm S_0 + \frac{1}{4} = (S_0 \pm \frac{1}{2})^2 \geq 0 \) the assumptions of §1 are satisfied. Let us write for \( |z| \leq 1 \)

\[ A_e = S_0^2 - \varepsilon S_0, \]

\[ U_e := \text{Friedrichs extension of} -\partial_z^2 + z^{-2}A_e \text{ with domain} C^\infty(R^*, H_2) \text{ in} L^2(R^+, H). \]

According to Theorem 2.1 we have for \( x > 0 \) an asymptotic expansion

\[ \text{tr}_H e^{-itU_e(x, z)} \sim (4\pi t)^{-1/2} \sum_{j=0}^\infty i^j \text{tr}_H Q_j(x, A_e) e^{-ix^2/2A_e} \]

with certain polynomials \( Q_j \) in \( A_e \) of order \( \leq \frac{3}{2} j \). Since \( A_e \) is an elliptic operator it follows that we have an expansion of the type

\[ \text{tr}_H e^{-itU_e(x, z)} \sim \sum_{j=0}^\infty i^j \delta_j^0 \varphi^0_0(z) \]

as \( t \rightarrow 0 \). The index calculation connected with (4.3) then requires the knowledge of

\[ \delta_j^0(x) - \delta_j^0 \varphi(x) \]

cf. [4] §4. We will now generalize this situation in assuming that instead of (4.1) we have

\[ T = \partial_z + z^{-1} \varphi(x) S_0 \quad (4.5) \]

\( \in C^\infty((0, z_0), H_1) \) where \( \varphi \in C^\infty(R) \) is positive and \( \equiv 1 \) for large \( |x| \), and \( S_0 \) is such that the assumptions of §1 are satisfied by \( S_0^2 \pm S_0 \). Then we obtain

\[ T^*T = -\partial_z^2 + z^{-2}(\varphi(x)^2 S_0^2 + (\varphi(x) - x \varphi'(x)) S_0), \]

\[ TT^* = -\partial_z^2 + z^{-2}(\varphi(x)^2 S_0^2 - (\varphi(x) - x \varphi'(x)) S_0). \]

Writing

\[ S(x) := \varphi(x) S_0, \quad \psi(x) := \varphi(x)^{-1} (\varphi(x) - x \varphi'(x)) \]

we have \( \psi \in C^\infty(R) \) and
As before we put for \( |\varepsilon| \leq 1, \varepsilon \in [0, x_0) \)

\[ A_\varepsilon (x) := S(x)^2 - \varepsilon \psi(x) S(x), \]

\[ U_\varepsilon := \text{Friedrichs extension of } -\partial_x^2 + x^{-2} A_\varepsilon (x) \text{ with domain } C_0^\infty (\mathbb{R}^*, H_2) \text{ in } L^2(\mathbb{R}^+, H), \]

which makes sense since \( A_\varepsilon (x) \) satisfies the assumptions of §1, too. Starting from Theorem 2.1 we have

\[ \text{tr}_H e^{-tU_\varepsilon (x,z)} \sim (4\pi t)^{-1/2} \sum_{j\geq 0} t^j \text{tr}_H (U_j (x, z) e^{-t \varepsilon \partial_x^2 A_\varepsilon (x)}), \]  

(4.7)

and by Lemma 2.2 \( U_j (x, z) \) is a universal polynomial in \( A_\varepsilon (x), A'_\varepsilon (x), \ldots \) of degree \( d_j \leq \frac{3}{2} j \) and with coefficients in \( C^\infty (\mathbb{R}^*) \). Since \( \psi(x) > 0 \) for all \( x \) it is easy to see that we have

\[ U_j (x, z) = \sum_{k, l \leq 3/2 j} c_{k,l} e^{2k(x)} S(x)^{2k} \psi(x)^{2k} \]  

(4.8)

where \( c_{k,l} \in C^\infty (\mathbb{R}^*) \) depends universally on \( \varphi \) but not on \( S_0 \). To derive an asymptotic expansion of (4.7) it is, therefore, enough to study the expansion of each term in the sum which arises from (4.7) if we plug in (4.8). Now we claim that we have the expansion

\[ \sum_{m \geq 0} \frac{\psi(x)}{x^2} \cdot \frac{t^m}{m!} (\frac{x}{x^2})^m \text{tr}_H (S(x)^{2k+t+m} e^{-t x^{-2} S(x)}). \]  

(4.9)

where \( S(x)^{2k+t} e^{-t x^{-2} S(x)} \) is a universal polynomial in \( A_\varepsilon (x), A'_\varepsilon (x), \ldots \) of degree \( d_j \leq \frac{3}{2} j \) and with coefficients in \( C^\infty (\mathbb{R}^*) \). Since \( \psi(x) > 0 \) for all \( x \) it is easy to see that we have

\[ U_j (x, z) = \sum_{k, l \leq 3/2 j} c_{k,l} e^{2k(x)} S(x)^{2k} \psi(x)^{2k} \]  

(4.8)

where \( c_{k,l} \in C^\infty (\mathbb{R}^*) \) depends universally on \( \varphi \) but not on \( S_0 \). To derive an asymptotic expansion of (4.7) it is, therefore, enough to study the expansion of each term in the sum which arises from (4.7) if we plug in (4.8). Now we claim that we have the expansion

\[ e^{2k+t} \text{tr}_H (S(x)^{2k+t} e^{-t x^{-2} S(x)}) \]

\[ \sim \sum_{m \geq 0} \frac{\psi(x)}{x^2} \cdot \frac{t^m}{m!} (\frac{x}{x^2})^m \text{tr}_H (S(x)^{2k+t+m} e^{-t x^{-2} S(x)}). \]  

(4.9)

This follows from

\[ e^{-t x^{-2} S(x)} \sum_{j=0}^{N-1} \frac{t^j \psi(x)}{j!} \]

\[ + \frac{\psi(x)}{N!} \int_0^1 (1-u)^{N-1} \text{tr}_H (S(x)^{2k+t} e^{-t x^{-2} S(x)}) du \]

and

\[ \| S(x)^N e^{-t x^{-2} S(x)} \| \text{tr} = O(t^{-N/2 - p_0}) \]  

(4.11)

for \( x > 0 \) and \( N \in \mathbb{Z}_+ \). Denoting by \( P_\varepsilon \) the orthogonal projection onto \( \text{ker}(S(x) - z) \) (4.10) follows from Taylor's formula for \( S_\varepsilon (x) := P_\varepsilon S(x) \) and in general by letting \( x \) go to infinity; (4.11) is a consequence of the spectral theorem and (2.16).

Combining (4.7), (4.8), and (4.9) we deduce

\[ \text{tr}_H e^{-tU_\varepsilon (x,z)} - \text{tr}_H e^{-tU_\varepsilon (z,x)} \]

\[ \sim -x^{-1/2} \sum_{j,k,m \geq 0} \frac{\psi(x)}{j!} \frac{t^m}{m!} c_{k,l} (x^{-2} \psi(x))^m \]

\[ \cdot \text{tr}_H (S(x)^{2k+t+m} e^{-t x^{-2} S(x)}). \]  

(4.12)

We now relate this expansion to the \( \eta \)-function

\[ \eta_S (x) := \sum_{\lambda \in \text{spec} (S(x))) \{ 0 \} } \pm \lambda \lambda \sim \]  

of the operator \( S(x) \). Assuming now as in the beginning of this section that \( S_0 \) is a self-adjoint elliptic differential operator of first order we have the following statement.

**Lemma 4.1** \( \eta_S (x) \) is meromorphic in \( C \) with poles on the real line, and holomorphic in some right halfplane. In each set \( \{ x \mid \Re x \geq c \} \), \( \eta_S (x) \) grows polynomially. Moreover, for \( q \in \mathbb{Z}_+ \) and \( c \) sufficiently large

\[ \text{tr}_H S(x)^{2q+1} e^{-t x^{-2} S(x)} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} (t z^{-2})^{-2} (z^{-2} \Gamma(z) \eta_S (z)(z - 2q - 1)dz. \]  

(4.13)

**Proof.** From our assumptions on \( S_0 \) and [4] (4.19) the meromorphy and the growth properties of \( \eta_S (x) \) are evident. (4.13) follows from summing the identity

\[ \lambda^{2q+1} e^{-t x^{-2} \lambda^2} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} (t z^{-2})^{-2} (z^{-2} \Gamma(z) \lambda^{2q+1} - 1 - 2z - 1)dz. \]  

(4.14)

The integral in (4.13) can now be expanded by the residue theorem, shifting the path of integration to the left and using the exponential decay of \( \Gamma(z) \eta_S (z)(z - 2q - 1) \) in vertical strips. The resulting expansion in \( t \) involves powers of \( t \) and possibly \( \log t \) if a pole of the shifted \( \eta \)-function coincides with a pole of \( \Gamma \). To avoid this complication we restrict attention to nonpositive \( t \)-powers. Thus let \( \alpha \leq 0 \), then the coefficients of \( t^\alpha \) and \( t^\alpha \log t \) in (4.12) can in view of (4.13) only come from
\[ \pi^{-1/2} \sum_{j,k,l,m \geq 0} \varepsilon^{j+m-1/2} \frac{t^{j+m} c_{jkm}(z)}{m!} x^{-2m} \cdot \]
\[ \text{Res}_{z=x+j+m-a-1/2} \left[ t(z^{-2})^{j/2} \Gamma(z) \eta_S(z)(2z-2k-m-\ell) \right]. \]

Since \( \alpha \leq 0 \) we have \( j + m - \alpha - 1/2 \geq 1/2 \) if \( j \geq 1 \); if \( j = 0 \) we have \( \ell = 0 \) and hence \( m \geq 1 \) since \( m + \ell \) is odd so in general
\[ j + m - \alpha - 1/2 \geq \frac{1}{2}. \]

Thus we encounter no poles of \( \Gamma \) and only simple poles of \( \eta_S(z) \). Therefore, the coefficient of \( t^a \) is zero and the coefficient of \( t^a \) is given by
\[ \pi^{-1/2} \sum_{j,k,l,m \geq 0} \varepsilon^{j+m} c_{jkl}(z) \frac{\psi(x)^m}{m!} x^{2j-2a-1} \cdot \]
\[ \cdot \Gamma(j + m - a - 1/2) \frac{1}{2} \text{Res}_{\eta_S(z)}(2j - k - \ell + m + \ell - 1 - 2\alpha). \] (4.14)

Since \( j - k - \ell \geq \frac{1}{2} \) and \( m + \ell \) is odd we have
\[ 2(j - k - \ell) + m + \ell - 1 - 2\alpha \geq -2\alpha \] (4.15)
and we can have equality only if \( j = 0 \), \( m = 1 \). Since in (4.7) \( U_0(x,y) \equiv 1 \) we obtain for the contribution from \( j = 0 \), \( m = 1 \) the expression
\[ (4\pi)^{-1/2} \varepsilon \psi(x) x^{-2a-1} \Gamma(1/2 - \alpha) \text{Res}_{\eta_S(z)}(-2\alpha) \]
\[ = \varepsilon (4\pi)^{-1/2} \varepsilon \psi(x) \varphi(x)^{2a} x^{-2a-1} \Gamma(1/2 - \alpha) \text{Res}_{\eta_S(z)}(-2\alpha) \]
and all other contributions come from poles of \( \eta_S \) of the form \(-2\alpha + 2k \), \( k \in \mathbb{N} \).

Summing up our results we obtain

**Theorem 4.1** For \( x > 0 \), \( |\varepsilon| \leq 1 \) we have an asymptotic expansion
\[ \text{tr}_H e^{-\tau U}(x, x) - \text{tr}_H e^{-\tau U}(x, x) \sim \sum_{\alpha \geq 0} g_\alpha(x, \varepsilon) t^\alpha + o_\alpha(1) \]
(4.16)
as \( t \to 0 \). The coefficients are given by
\[ g_\alpha(x, \varepsilon) = (4\pi)^{-1/2} \varepsilon \psi(x) \varphi(x)^{2a} x^{-2a-1} \Gamma(1/2 - \alpha) \text{Res}_{\eta_S(z)}(-2\alpha) \]
\[ + \sum_{k \geq 1} h_{\alpha k}(x, \varepsilon) \text{Res}_{\eta_S(z)}(-2\alpha + 2k) \]
where \( h_{\alpha k} \) is a universal polynomial in \( \varepsilon^{-1}, \varphi, \varphi', \ldots \).