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Krein's formula and heat-kernel expansion for some differential operators with a regular singularity

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Abstract

We get a generalization of Krein's formula—which relates the resolvents of different self-adjoint extensions of a differential operator with regular coefficients—to the non-regular case $A = -\partial_x^2 + (v^2 - 1/4)/x^2 + V(x)$, where $0 < v < 1$, and $V(x)$ is an analytic function of $x \in \mathbb{R}^+$ bounded from below. We show that the trace of the heat kernel e^{-tA} admits a non-standard small- t asymptotic expansion which contains, in general, integer powers of t^v . In particular, these powers are present for those self-adjoint extensions of A which are characterized by boundary conditions that break the local formal scale invariance at the singularity.

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1. Introduction

In quantum field theory the effective action, the free energy and other physical quantities related to the vacuum state are generically divergent and require a renormalization procedure. A powerful and elegant regularization scheme relies on the small- t asymptotic expansion of the trace of the heat kernel e^{-tA} corresponding to an elliptic differential operator A determined by the Lagrangian of the theory (see, e.g. [1–3].)

It is well known [4] that for an elliptic boundary value problem in an m -dimensional compact manifold with boundary, described by a differential operator A of order d , with smooth coefficients and defined on a domain of functions subject to local boundary conditions, the heat-kernel trace admits a small- t asymptotic expansion given by

$$\mathrm{Tr}\{e^{-tA}\} \sim \sum_{n=0}^{\infty} a_n(A) t^{(n-m)/d}, \quad (1.1)$$

where the coefficients $a_n(A)$ are integrals on the manifold and its boundary of geometrical invariants [5].

However, not much is known about the heat-kernel trace asymptotic expansion for the case of differential operators with singular coefficients (see chapter 6 of [3].)

In 1980 Callias and Taubes [6] have pointed out that for some differential operators with singular coefficients the heat-kernel trace asymptotic expansion in terms of powers of the form $t^{(n-m)/d}$ is ill-defined and conjectured that more general powers of t , as well as $\log t$ terms, could appear.

In the present paper we will study the small- t asymptotic expansion of the heat-kernel trace of the differential operator

$$A = -\partial_x^2 + \frac{v^2 - 1/4}{x^2} + V(x), \quad (1.2)$$

where $v \in (0, 1) \subset \mathbb{R}$ and $V(x)$ is an analytic function of $x \in \mathbb{R}^+$.

The operator (1.2) defined on $\mathcal{D}(A) := \mathcal{C}_0^\infty(\mathbb{R}^+)$, the set of smooth functions on \mathbb{R}^+ with compact support out of the origin, admits a one-parameter family of self-adjoint extensions, A^θ with $\theta \in \mathbb{R}$. These self-adjoint extensions are characterized by the *boundary condition* the functions in their domains satisfy at the singular point $x = 0$. Each of them describes a different physical system whose spectral properties depend on the behaviour of the functions at the singularity.

Since the heat kernel e^{-tA^θ} corresponding to an arbitrary self-adjoint extension A^θ is not trace class, we will study the trace of the difference $e^{-tA^\theta} - e^{-tA^\infty}$, where A^∞ denotes the Friedrichs extension. We will show in section 4 that this trace admits an asymptotic expansion of the form

$$\mathrm{Tr}\{e^{-tA^\theta} - e^{-tA^\infty}\} \sim \sum_{n=0}^{\infty} a_n(v, V)t^{\frac{n}{2}} + \sum_{N,n=1}^{\infty} b_{N,n}(v, V)\theta^N t^{\nu N + \frac{n}{2} - \frac{1}{2}}. \quad (1.3)$$

The coefficients $a_n(v, V)$, $b_{N,n}(v, V)$ can be recursively computed for each potential $V(x)$. Note that the singular term in (1.2) not only contributes to the coefficients $a_n(v, V)$ of the standard terms but also leads to the presence of powers of t whose exponents are not half-integers but depend on the ‘external’ parameter v .

It is also remarkable that these terms are absent only for $\theta = 0$ and $\theta = \infty$, which correspond to the self-adjoint extensions characterized by scale invariant boundary conditions at the singular point $x = 0$. Indeed, the first two terms in the rhs of equation (1.2), which are dominant for $x \simeq 0$, present the same scaling dimension. However, the behaviour of the wave functions at the origin breaks, in general, this local scale invariance. Only for the self-adjoint extensions characterized by $\theta = 0$ or $\theta = \infty$ is the boundary condition also scale invariant (see equation (2.1).)

There is a dimensional argument in favour of the plausibility of the result in (1.3). Note that the parameter θ in (2.1) has dimensions $[\text{length}]^{-2\nu}$ and, due to the analyticity of $V(x)$, the dimensions of any other parameter in the problem is an integer power of the length. Since t has dimensions $[\text{length}]^2$, if the coefficients of the asymptotic expansion of the heat-kernel trace were to depend on the boundary conditions by means of a polynomial dependence on θ , then this expansion should contain integer powers of t^ν . Consequently, the only self-adjoint extensions for which these powers are to be absent are $\theta = 0$ and $\theta = \infty$.

As a matter of fact, the ‘functorial method’ [2, 3, 7] which has been widely used to determine the coefficients of the heat-kernel expansion in the regular case can be also applied to operator (1.2) to determine some of the $a_n(v, V)$ and $b_{N,n}(v, V)$ in expression (1.3). The asymptotic expansion (1.3) generalizes the results in [8, 9] where some singular Schrödinger and Dirac operators were considered.

There is a second new result in the present paper which leads us to the derivation of the asymptotic expansion (1.3). By generalizing Krein’s formula [10] (see also [11]) we find a

relation between the resolvents corresponding to different self-adjoint extensions of operator (1.2). Since there exist two self-adjoint extensions, namely A^0 and A^∞ , for which the ν -dependent exponents of t in (1.3) are absent, expansion (1.3) will come out as a consequence of this relation.

Schrödinger operators defined by a singular potential whose leading behaviour near the singularity is given by (1.2) have been studied as models of conformal invariance in quantum mechanics [12], Calogero models [13], SUSY breaking in quantum mechanics [9] and cosmic strings [14]. Since the dynamics of quantum fields on black holes' backgrounds is described by operators similar to (1.2), there exists a microscopic description of black holes in the vicinity of the horizon in terms of conformal models [15]. In this context, in which the operator (1.2) is relevant, particular attention to the most general boundary conditions has been given in [16].

Differential operators with a singular coefficient given by (1.2) are also obtained from the Laplacian on manifolds with conical singularities where the parameter ν is related to the deficiency angle. The asymptotic expansion of the heat kernel of the Laplacian on manifolds with conical singularities has been considered, probably for the first time, in [17]. This problem has been also studied in [18]; however, the most general boundary conditions at the singularity were not considered there.

More recently, Mooers [19] studied the self-adjoint extensions of the Laplacian acting on differential forms on a manifold with a conical singularity and showed that the asymptotic expansion of the heat-kernel trace contains powers of t whose exponents depend on the deficiency angle of the singularity¹.

In section 2 we describe the self-adjoint extensions of operator (1.2) and in section 3 we generalize Krein's formula to this type of singular operators. Finally, in section 4, we use this generalization to establish expansion (1.3) that describes the small- t asymptotic expansion of the heat-kernel trace.

2. Self-adjoint extensions

Let us consider the one-dimensional differential operator A given by (1.2) defined on $\mathcal{D}(A) := C_0^\infty(\mathbb{R}^+) \subset \mathbf{L}_2(\mathbb{R}^+)$. First, note that the first two terms in the rhs of expression (1.2) have the same scaling properties at the singular point $x = 0$. This fact will be essential in the following.

Next, we describe the behaviour at the singular point $x = 0$ of the functions in $\mathcal{D}(A^\dagger)$.

Theorem 2.1.

$$\psi \in \mathcal{D}(A^\dagger) \rightarrow \psi(x) = C[\psi](x^{-\nu+1/2} + \theta_\psi x^{\nu+1/2}) + O(x^{3/2}), \quad (2.1)$$

for $x \rightarrow 0^+$ and some constants $C[\psi], \theta_\psi \in \mathbb{C}$.

Proof. See the appendix. \square

Corollary 2.2.

$$\phi, \psi \in \mathcal{D}(A^\dagger) \rightarrow (\phi, A^\dagger \psi) - (A^\dagger \phi, \psi) = C^*[\phi]C[\psi](\theta_\phi^* - \theta_\psi). \quad (2.2)$$

Remark 2.3. By choosing $\psi = \phi$ we conclude that for all $\psi \in \mathcal{D}(A^\dagger)$ the parameter θ_ψ defined by theorem 2.1 is real.

Proof. Expression (2.2) follows from an integration by parts in its lhs using theorem 2.1. \square

¹ Although this result is confirmed by our calculations we obtain a different value for the corresponding coefficient (see page (4) of [19]).

As a consequence of corollary 2.2 the self-adjoint extensions A^θ of the differential operator A are characterized by a real parameter θ , being their domains defined by

$$\mathcal{D}(A^\theta) := \{\phi \in \mathcal{D}(A^\dagger) : \theta_\phi = \theta\}, \quad (2.3)$$

where θ_ϕ is defined according to theorem 2.1. The parameter θ thus determines the boundary condition at the singularity.

There exists another self-adjoint extension (see the appendix), which we denote by A^∞ , whose domain is given by

$$\mathcal{D}(A^\infty) = \{\phi \in \mathcal{D}(A^\dagger) : \phi(x) = C[\phi]x^{\nu+1/2} + O(x^{3/2}), \quad \text{with } C[\phi] \in \mathbb{C}\}. \quad (2.4)$$

3. Generalization of Krein's formula

The non-regular differential operator A , given by expression (1.2), defined on $\mathcal{D}(A) := \mathcal{C}_0^\infty(\mathbb{R}^+)$ admits an infinite family of self-adjoint extensions A^θ characterized by a real parameter θ . As we have shown, this parameter describes the boundary condition at the singularity. The purpose of this section is to establish a relation between the resolvents corresponding to these self-adjoint extensions. We will consequently obtain a generalization of Krein's formula.

The kernel $G_\theta(x, x', \lambda)$ of the resolvent $(A^\theta - \lambda)^{-1}$ can be written as

$$G_\theta(x, x', \lambda) = -\frac{1}{W(\lambda)} \{\Theta(x' - x)L_\theta(x, \lambda)R(x', \lambda) + \Theta(x - x')L_\theta(x', \lambda)R(x, \lambda)\}, \quad (3.1)$$

where $\Theta(x)$ is the Heaviside function and $L_\theta(x, \lambda), R(x, \lambda) \in \text{Ker}(A^\dagger - \lambda)$. The latter is square integrable at $x \rightarrow \infty$ and the former satisfies the boundary condition

$$L_\theta(x, \lambda) = x^{-\nu+1/2} + \theta x^{\nu+1/2} + O(x^{3/2}), \quad (3.2)$$

at $x \rightarrow 0^+$. $W(\lambda)$ is their Wronskian, which is independent of x .

As a first step, we will find a relation between the resolvents corresponding to $\theta = \infty$ and $\theta = 0$. In order to do this, we consider the equation

$$(A^\theta - \lambda)\phi^\theta(x, \lambda) = f(x) \quad (3.3)$$

whose solutions for $\theta = 0$ and $\theta = \infty$ are given by

$$\phi^\infty(x, \lambda) = \int_0^\infty G_\infty(x, x', \lambda) f(x') dx' = \phi^\infty(\lambda)x^{\nu+1/2} + O(x^{3/2}), \quad (3.4)$$

$$\phi^0(x, \lambda) = \int_0^\infty G_0(x, x', \lambda) f(x') dx' = \phi^0(\lambda)x^{-\nu+1/2} + O(x^{3/2}). \quad (3.5)$$

Note that

$$\phi^\infty(\lambda) = \int_0^\infty G_\infty(x', \lambda) f(x') dx', \quad \phi^0(\lambda) = \int_0^\infty G_0(x', \lambda) f(x') dx', \quad (3.6)$$

where

$$G_\infty(x', \lambda) := \lim_{x \rightarrow 0} x^{-\nu-1/2} G_\infty(x, x', \lambda), \quad G_0(x', \lambda) := \lim_{x \rightarrow 0} x^{\nu-1/2} G_0(x, x', \lambda). \quad (3.7)$$

Lemma 3.1.

$$\phi^0(x, \lambda) = \phi^\infty(x, \lambda) + 2\nu G_\infty(x, \lambda)\phi^0(\lambda). \quad (3.8)$$

Proof.

$$\begin{aligned}\phi^0(x, \lambda) - \phi^\infty(x, \lambda) &= \int_0^\infty [G_0(x, x', \lambda) - G_\infty(x, x', \lambda)](A^0 - \lambda)\phi^0(x', \lambda) dx' \\ &= - \lim_{x' \rightarrow 0^+} \{[G_0(x, x', \lambda) - G_\infty(x, x', \lambda)]\partial_{x'}\phi^0(x', \lambda) \\ &\quad - \partial_{x'}[G_0(x, x', \lambda) - G_\infty(x, x', \lambda)]\phi^0(x', \lambda)\} = 2\nu G_\infty(x, \lambda)\phi^0(\lambda). \quad \square\end{aligned}$$

Taking the limit $x \rightarrow 0^+$ in equation (3.8) we obtain

$$G_\infty(x, \lambda) = \frac{1}{2\nu}(x^{-\nu+1/2} - K(\lambda)^{-1}x^{\nu+1/2}) + O(x^{3/2}), \quad (3.9)$$

where

$$K(\lambda) := \frac{\phi^0(\lambda)}{\phi^\infty(\lambda)}. \quad (3.10)$$

Note that $K(\lambda)$ can be computed by studying the behaviour at the singularity of the kernel of the resolvent corresponding to the extension $\theta = \infty$.

Replacing $\phi^0(\lambda)$ from equation (3.10) into equation (3.8) one can express the solution $\phi^0(x, \lambda)$ corresponding to $\theta = 0$ by means of data related to the self-adjoint extension corresponding to $\theta = \infty$,

$$\phi^0(x, \lambda) = \phi^\infty(x, \lambda) + 2\nu K(\lambda)G_\infty(x, \lambda)\phi^\infty(\lambda). \quad (3.11)$$

Next, we will establish a similar expression giving the resolvent for an arbitrary self-adjoint extension in terms of data related to the boundary conditions corresponding to $\theta = \infty$.

Lemma 3.2.

$$\phi^\theta(x, \lambda) = \phi^\infty(x, \lambda) + 2\nu(K(\lambda)^{-1} + \theta)^{-1}G_\infty(x, \lambda)\phi^\infty(\lambda). \quad (3.12)$$

Proof. Equation (3.8) shows that the difference between both sides of expression (3.12) belongs to $\text{Ker}(A^\dagger - \lambda)$. Moreover, equations (3.4) and (3.9) show that both sides of (3.12) belong to $\mathcal{D}(A^\theta)$. The proof follows by virtue of the uniqueness of the solution of equation (3.3). \square

Finally, from equations (3.11) and (3.12) it is straightforward to obtain the following theorem.

Theorem 3.3 (Generalization of Krein's formula).

$$(A^\theta - \lambda)^{-1} - (A^\infty - \lambda)^{-1} = \frac{(A^0 - \lambda)^{-1} - (A^\infty - \lambda)^{-1}}{1 + \theta K(\lambda)}. \quad (3.13)$$

In the next section we will show that the asymptotic expansion of $K(\lambda)$ for large $|\lambda|$ presents powers of λ whose exponents depend on the parameter ν . This leads, due to the relation between the resolvent and the heat kernel, to the asymptotic series (1.3).

4. Asymptotic expansion of the resolvent

In this section we will show that $K(\lambda)$ admits a large- $|\lambda|$ asymptotic expansion in powers of λ with ν -dependent exponents. Since we can consider λ in the negative real semi-axis of the complex plane, we will study the solutions ψ of equation

$$(A + z)\psi(x, z) = 0, \quad (4.1)$$

for large $z \in \mathbb{R}^+$. In particular, due to equations (3.9) and (3.13) we just need to consider solutions satisfying the boundary conditions corresponding to $\theta = \infty$ and $\theta = 0$.

Taking into account the scaling properties of the first two terms in (1.2) it is convenient to define a new variable $y := \sqrt{z}x \in \mathbb{R}^+$. Equation (4.1) can then be written as

$$\left(-\partial_y^2 + \frac{\nu^2 - 1/4}{y^2} + 1 + \frac{1}{z}V(y/\sqrt{z})\right)\psi(y/\sqrt{z}, z) = 0. \quad (4.2)$$

Assuming analyticity of $V(x)$, this equation can be iteratively solved for large z and the solution which is square integrable at $y \rightarrow \infty$ is given by

$$R(y, z) = \sqrt{y}K_\nu(y) + \sum_{n=0}^{\infty} \psi_n(y)z^{-1-n/2}, \quad (4.3)$$

where $K_\nu(y)$ is the modified Bessel function and $\psi_n(y)$ depend polynomially on $V(x)$ and its derivatives. From this expression it can be easily seen that the behaviour of $R(y, z)$ for $x \rightarrow 0^+$ is given by

$$R(y, z) \simeq \frac{\Gamma(\nu)}{2^{1-\nu}}y^{-\nu+1/2} + \frac{\Gamma(-\nu)}{2^{1+\nu}}H(z) \cdot y^{\nu+1/2} + O(y^{3/2}), \quad (4.4)$$

where $H(z)$ admits a large- z asymptotic expansion in half-integer powers of z .

From equation (3.1) for the case $\theta = \infty$ and equations (3.9) and (4.4) we obtain

$$K(z) = 4^\nu \frac{\Gamma(1+\nu)}{\Gamma(1-\nu)} z^{-\nu} H(z)^{-1}. \quad (4.5)$$

Since $H(z)$ admits an asymptotic series in half-integer powers of z , the large- z asymptotic expansion of $K(z)$ contains powers of z whose exponents depend on the parameter ν . Proceeding in a similar way one can prove, by means of expression (4.3), that $\text{Tr}\{(A^0 + z)^{-1} - (A^\infty + z)^{-1}\}$ admits an asymptotic expansion in half-integer powers of z .

From theorem 3.3 and due to the factor $z^{-\nu}$ in equation (4.5) we conclude that the large- $|\lambda|$ asymptotic expansion of $\text{Tr}\{(A^\theta - \lambda)^{-1} - (A^\infty - \lambda)^{-1}\}$ contains integer powers of $\lambda^{-\nu}$. Finally, it can be straightforwardly shown that its inverse Laplace transform, $\text{Tr}\{e^{-tA^\theta} - e^{-tA^\infty}\}$, admits the asymptotic expansion given by (1.3).

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Note added in proof. The interesting case $\nu = 0$ —not considered in this article—leads to a different kind of unusual spectral properties. Indeed, it has been shown [21] that the corresponding zeta-function $\zeta(s)$ is not, in general, regular at $s = 0$.

Appendix. Proof of theorem 2.1

By virtue of Riesz representation lemma [20]

$$\psi \in \mathcal{D}(A^\dagger) \rightarrow \exists \tilde{\psi} \in \mathbf{L}_2(\mathbb{R}^+) : (\psi, A\phi) = (\tilde{\psi}, \phi) \quad \forall \phi \in \mathcal{D}(A). \quad (\text{A.1})$$

Consequently,

$$A^\dagger \psi := \tilde{\psi}. \quad (\text{A.2})$$

Defining $\chi := x^{-\nu-1/2}\psi$ we obtain

$$\partial_x(x^{2\nu+1}\partial_x\chi) = -x^{\nu+1/2}(\tilde{\psi} - V(x)\psi) \in \mathbf{L}_1(\mathbb{R}^+). \quad (\text{A.3})$$

Therefore, there exists a constant $C_1 \in \mathbb{C}$ such that

$$\partial_x\chi = C_1x^{-1-2\nu} - x^{-1-2\nu} \int_0^x y^{\nu+1/2} \left(-\partial_y^2 + \frac{\nu^2 - 1/4}{y^2} \right) \psi \, dy. \quad (\text{A.4})$$

The Cauchy–Schwartz inequality implies

$$\left| x^{-1-2\nu} \int_0^x y^{\nu+1/2} \left(-\partial_y^2 + \frac{\nu^2 - 1/4}{y^2} \right) \psi \, dy \right| \leq C_2 \left\| \left(-\partial_y^2 + \frac{\nu^2 - 1/4}{y^2} \right) \psi \right\|_{(0,x)} x^{-\nu}, \quad (\text{A.5})$$

for some $C_2 \in \mathbb{C}$. In consequence,

$$\left| \int^x z^{-1-2\nu} \int_0^z y^{\nu+1/2} \left(-\partial_x^2 + \frac{\nu^2 - 1/4}{x^2} \right) \psi \, dy \, dz \right| \leq C_3 + C_4x^{1-\nu}, \quad (\text{A.6})$$

where $C_3, C_4 \in \mathbb{C}$. Thus, there exist $C_5, C_6 \in \mathbb{C}$, such that

$$\tilde{\psi} = C_5x^{-\nu+1/2} + C_6x^{\nu+1/2} + O(x^{3/2}), \quad (\text{A.7})$$

for $x \rightarrow 0^+$.

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