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# The Heat Equation with Singular Coefficients

## I. Operators of the Form $-\frac{d^2}{dx^2}+\frac{\kappa}{x^2}$ in Dimension 1*

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**Abstract.** The small time asymptotics of the kernel of $e^{-tH}$ is defined and derived for $H=\frac{d^2}{dx^2}+\frac{\kappa}{x^2}$ on $\mathbb{R}^1$. Lemmas on singular asymptotics in the sense of distributions are formulated and used. The results are applied to derive an index formula on $\mathbb{R}^1$.

## 1. Introduction

In this and a few subsequent papers I intend to discuss the heat equation with coefficients containing singularities of the kind exemplified by $\frac{\kappa}{x^2}$. I shall study some general properties and asymptotic behavior with an eye toward applications in spectral theory and in quantum theory. From the point of view of the latter, one only needs to concentrate on Euclidean space, but our discussion will eventually be extended to arbitrary manifolds in a straightforward way.

My motivation for this study originated in an earlier attempt to compute quantum corrections to classical solutions in Euclidean Yang-Mills theory [1]. In a steepest descent approximation scheme one has to calculate the determinant of a second order expansion operator about the extremum of the exponential in a function space integral. The operator in question is a second order differential operator on $\mathbb{R}^4$ and the determinant is defined by the derivative of the analytic continuation of the zeta function

$$\zeta(\lambda)=\frac{1}{\Gamma(\lambda)}\int_0^\infty ds\, s^{\lambda-1}\,\mathrm{Tr}(e^{-sH}-e^{-sH_0}) \tag{1.1}$$

to $\lambda=0$ according to the formula

$$\ln\det H=-\zeta'(0). \tag{1.2}$$

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Here $H_0$ is a fixed operator used, roughly speaking, to normalize the determinant. The heat equation enters the picture at this point and in our work we unavoidably had to deal with the case of singular coefficients.

In the case where $H$ is an elliptic operator with smooth coefficients on a compact manifold without boundary it is known that the heat equation exhibits some convenient and attractive features [2]. For example, if $H$ is a second order operator which is also self-adjoint on a suitable domain (the second Sobolev space), it is known that $e^{-sH}$ is an infinitely smoothing operator for $\mathrm{Re}\, s>0$ and the kernel $e^{-sH}(x,y)$ of $e^{-sH}$ as an integral operator, is smooth as a function of $x$ and $y$ for $\mathrm{Re}\, s>0$. Further, as $s\to 0+$ one obtains an asymptotic expansion of the diagonal $x=y$ of the form

$$e^{-sH}(x,x) \sim s^{-d/2}(a_0(x)+a_1(x)\cdot s+\ldots), \tag{1.3}$$

where the $a_k(x)$ are functions of the coefficients of the differential operator $H$ and their derivatives evaluated at the point $x$. Here $d$ is the dimension of the manifold. This asymptotic expansion is responsible for a lot of useful applications of the heat equation to spectral theory.

One can see from this asymptotic expansion that the situation is going to be drastically different for operators whose coefficients are allowed a certain singular behavior. For example, if $H$ is again an elliptic (according to the highest order term) self-adjoint second order differential operator whose zero$^{\text{th}}$ order coefficient has singularities like $1/|x|^2$ near some point on the manifold, it follows from the fact that $a_k(x)$ are polynomials of increasing order as $k\to\infty$ in the derivatives of the coefficients of $H$ that $a_k(x)\sim 1/|x|^{n_k}$ near the singular point where $n_k$ increases with $k$. This renders the asymptotic expansion useless (or almost useless) when one tries to compute a quantity like $\int e^{-sH}(x,x)dx$ over the manifold.

It was conjectured in [1] that $e^{-sH}(x,x)$ has in a situation of this kind an asymptotic expansion in the sense of distributions containing terms with a different $s$-behavior from what appears in (1.3), for example, terms with different powers of $s$ and perhaps $\ln s$. The presence of a $\ln s$ term was actually demonstrated there by making use of some previous calculations on the model at hand. The present work will prove that conjecture and it will also introduce calculational schemes that are general and quite manageable at least for the first few orders.

In the present paper we discuss the operators

$$H_\kappa = -\frac{d^2}{dx^2}+\frac{\kappa}{x^2}, \tag{1.4}$$

where $\kappa \geqq 3/4$ as differential operators on the real line $\mathbb{R}$. They deserve special treatment, not as illuminating examples, but rather as fundamental operators that will be used to generate the general theory. In Sect. 2, I shall discuss (1.4) as an operator in the Hilbert space $L^2(\mathbb{R}_+)$ or $L^2(\mathbb{R})$. In Sect. 3, I shall describe the behavior of the kernel $e^{-sH_\kappa}(x,y)$ as a function of $x$ and $y$ away from and on the diagonal $x=y$. In Sect. 5, I use a theorem of Sect. 4 to prove an asymptotic expansion in the sense of distributions of the form

$$e^{-sH_\kappa}(x,y) \sim \sum_{k=0}^{\infty} c_k(\kappa)u_k s^{k-1/2} + \sum_{k=0}^{\infty} d_k(\kappa) w_k \cdot s^k, \tag{1.5}$$

where $c_k(\kappa)$, $d_k(\kappa)$ are real functions of $\kappa \geqq 3/4$, $u_k$ and $w_k$ are distributions, $w_k$ being a combination of Dirac distributions and their derivatives. The coefficients will also be computed there as compact algebraic expressions in $\kappa$ and $k$ by using formulas for traces like

$$\operatorname{Tr} x^k(e^{-sH_\kappa} - \text{leading behavior}), \tag{1.6}$$

where $x$ is treated on a multiplication operator by $x$ and "leading behavior" is a combination of operators that have kernels which cancel $e^{-sH_\kappa}(x,x)$, when evaluated on the diagonal, to order $|x|^{-1}$ as $|x| \to \infty$. It is shown that (1.6) isolates the $\delta^{(k)}$ term in (1.5). The prototype of a formula for a trace like (1.6) is the striking identity

$$\operatorname{Tr}(e^{-sH_\kappa} - e^{-sH_0}) = (\kappa + 1/4)^{1/2}, \tag{1.7}$$

where $H_0 = -\frac{d^2}{dx^2}$. In Sect. 7, I discuss the trace formula (1.7), which was originally derived using the properties of Bessel functions.

In Sect. 6, I apply the results to the derivation of an index formula on the line. Some results from the next paper in the series are used there, to the effect that the asymptotic expansion of the heat kernel as $s \to 0$ for operators having the same leading behavior as (1.4) agrees with that of (1.5) to order $s^0$.

## 2. The Operators $H_\kappa$ on $L^2(\mathbb{R})$

Because of the singularity at $x=0$, one begins by defining $H_\kappa$ as an operator on $C_0^\infty(\mathbb{R}\backslash\{0\})$, the smooth functions with compact support away from 0. If $\kappa \geqq 3/4$, this definition uniquely determines a self-adjoint operator on $L^2(\mathbb{R})$, precisely:

**Proposition (2.1).** *The operator $H_\kappa$ on $C_0^\infty(\mathbb{R}_+\backslash\{0\})$ defined by*

$$(H_\kappa \phi)(x) = -\frac{d^2\phi(x)}{dx} + \frac{\kappa}{x^2}\phi(x)$$

*is essentially self-adjoint if $\kappa \geqq 3/4$.*

*Proof* [3]. The equation $-\phi''(x) + \frac{\kappa}{x^2}\phi(x) = 0$ has the two linearly independent solutions $\phi_\pm(x) = x^{\alpha_+}$, $\alpha_\pm = \frac{1 \pm (4\kappa+1)^{1/2}}{2}$. If $\kappa \geqq 3/4$, we have $\alpha_+ \geqq 3/2$ and $\alpha_- \leqq -1/2$. Thus $\phi_+$ is not square integrable near $\infty$ and $\phi_-$ is not $L^2$ near 0, which means that $\frac{\kappa}{x^2}$ is in the limit point case near both 0 and infinity. This implies that $H_\kappa$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}_+\backslash\{0\})$ by Weyl's criterion (see [3, Theorem X.7]).

For the construction of functions of the operator $H_\kappa$ we need to characterize the domain of the closed operator. The following proposition is not the strongest possible result but is sufficient for the present purposes (see also [3, Proposition X.2]).

**Proposition (2.2).** *Let $\kappa \geqq 3/4$. Let $\phi \in L^2(\mathbb{R}_+)$ be in the domain of the closure of the operator $H_\kappa$ defined on $C_0^\infty(\mathbb{R}_+\backslash\{0\})$. Extend $\phi$ to $\mathbb{R}_-$ by $\phi|_{\mathbb{R}_-}=0$. Then we have $\phi \in H^1(\mathbb{R}) = \{\psi \in L^2(\mathbb{R}) | (1+k^2)^{1/2}\hat{\psi}(k) \in L^2(\mathbb{R})\}$, $\phi'$ is absolutely continuous on* $(0, \infty)$ *and* $\lim_{x\to 0} \phi(x) = 0$. *($\hat{\psi}$ is the Fourier transform of $\psi$.)*

*Proof.* Since $H_\kappa$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}_+\backslash\{0\})$ the closure is self-adjoint. Thus $\phi \in D_\kappa$ if and only if there exists a vector $H_\kappa\phi$ such that

$$(\psi, H_\kappa\phi) = \left(-\frac{d^2}{dx^2}\psi + \frac{\kappa}{x^2}\psi, \phi\right) = \left(-\frac{d^2}{dx^2}\psi, \phi\right) + \left(\frac{\kappa}{x^2}\psi, \phi\right)$$

for each $\psi \in C_0^\infty(\mathbb{R}_+\backslash\{0\})$. Thus the second derivative of $\phi$ in the sense of distributions is a distribution, say $u$, such that $|u(\psi)| \leqq C \cdot \|\psi\|_2$, locally. This means that $\frac{d^2}{dx^2}\phi$ is locally $L^2$, and it follows by Sobolev's lemma that $\phi$ belongs to $C^1$. Therefore $\phi'$ is absolutely continuous and $-\phi'' + \frac{\kappa}{x^2}\phi \in L^2(\mathbb{R}_+)$. Now we have for $\phi \in C_0^\infty(\mathbb{R}\backslash\{0\}) \|\phi'\|^2 + \kappa \left\|\frac{1}{x}\phi\right\|^2 = (\phi, H_\kappa\phi) \leqq \|\phi\| \cdot \|H_\kappa\phi\|$, so that $\|\phi'\|^2 \leqq \|\phi\| \cdot \|H_\kappa\|$ and $\left\|\frac{1}{x}\phi\right\|^2 \leqq \|\phi\| \cdot \|H_\kappa\phi\|$. Since any $\phi \in D$ can be approximated from $C_0^\infty(\mathbb{R}\backslash\{0\})$ in the norm $\|\cdot\|^2 + \|H_\kappa \cdot\|^2$, we see that $\left\|\frac{1}{x}\phi\right\|^2 < \infty$ and $\phi \in H^1(\mathbb{R})$ for all $\phi \in D$. It follows that $\phi$ is continuous on $\mathbb{R}$, so that $\phi(0) \equiv \lim_{x\to 0} \phi(x) = 0$.

Henceforth we assume $\kappa \geqq 3/4$ and let $H_\kappa$ denote a closed operator. The spectrum of the operator $H_\kappa$ is a subset of $\mathbb{R}_+$. Consider now the solutions of the differential equation

$$\left[-\frac{d^2}{dx^2} + \frac{\kappa}{x^2} + z\right]\psi = 0 \qquad x > 0, \tag{2.1}$$

where $z \notin \mathbb{R}_-$. It is then clear that $\psi$ cannot be in $L^2(\mathbb{R}_+)$ and if $\psi \in L^2$ near 0 (respectively, near $\infty$) we must have $\lim_{x\to 0} \psi(x) = 0$ $\left(\text{respectively, } \lim_{x\to\infty} \psi(x) = 0\right)$. With the substitution $\psi = x^{1/2}\tilde{\psi}$ we get Bessel's equation for $\tilde{\psi}$:

$$-\frac{d^2}{dx^2}\tilde{\psi} - \frac{1}{x}\frac{d}{dx}\tilde{\psi} + \frac{\kappa + 1/4}{x^2}\tilde{\psi} + z\tilde{\psi} = 0, \tag{2.1'}$$

so that the solutions of (2.1) are given in terms of the so-called modified Bessel functions $I_\nu$ and $K_\nu$ as ($\mathrm{Re}\sqrt{z} > 0$) [4].

$$\begin{aligned}\psi_1(x) &= (\sqrt{z}x)^{1/2} K_\nu(\sqrt{z}x) = (\sqrt{z}x)^{1/2} \frac{1}{2}\pi \frac{I_{-\nu}(\sqrt{z}|x|) - I_\nu(\sqrt{z}|x|)}{\sin(\nu\pi)},\\ \psi_2(x) &= (\sqrt{z}x)^{1/2} I_\nu(\sqrt{z}x) = (\sqrt{z}x)^{1/2} \cdot \left(\frac{\sqrt{z}x}{2}\right)^\nu \cdot \sum_{k=0}^{\infty} \frac{(z/4)^k \cdot x^{2k}}{k!\Gamma(\nu+k+1)}.\end{aligned} \tag{2.2}$$

We shall describe the necessary properties of $I_\nu$ and $K_\nu$ below. Here

$$\nu = (\kappa + \tfrac{1}{4})^{1/2}. \tag{2.3}$$

We assume at this point and in the following that $\nu$ is not an integer. First we note (see below) that $\psi_1(x)\to 0$ as $x\to\infty$ and $\psi_2(x)\to 0$ as $x\to 0$. Since $\psi_1$ and $\psi_2$ are solutions of the differential equations (2.1) their Wronskian must be a constant:

$$\psi_1(x)\psi_2'(x)-\psi_2(x)\psi_1'(x)=\sqrt{z}\,.$$

This is obtained by evaluating the left-hand side asymptotically as $x\to 0$ from (2.2). Form the function of two variables:

$$G_z(x,y)=\frac{1}{\sqrt{z}}\left[\theta(x-y)\psi_1(x)\psi_2(y)+\theta(y-x)\psi_1(y)\psi_2(x)\right], \tag{2.4}$$

where $\theta(x)=1$, $x\geqq 0$ and $\theta(x)=0$, $x<0$. $G_z$ satisfies

$$\int((z+H_\kappa)\phi)(x)G_z(x,y)\psi(y)dxdy=\int\phi(x)\psi(x)dx\,,$$

where $\phi\in C_0^\infty(0,\infty)$, $\psi\in C_0^\infty(0,\infty)$, as can be seen from the differential equation satisfied by $\psi_1$ and $\psi_2$. Thus for $z\notin\mathbb{R}_-$, $G_z(x,y)$ is the kernel of an integral operator representing the bounded operator $(H_\kappa+z)^{-1}$.

Let us describe the behavior of $G_z(x,y)$ more precisely as a function of $x$ and $y$. We need to know some of the properties of the modified Bessel functions which have been studied exhaustively in the literature. As a consequence of their definition which is contained in (2.2), we have the leading order

$$\left.\begin{aligned}&K_\nu(\varrho)\sim\tfrac{1}{2}\Gamma(\nu)(\tfrac{1}{2}\varrho)^{-\nu},\\&I_\nu(\varrho)\sim(\tfrac{1}{2}\varrho)^{\nu}/\Gamma(\nu+1).\end{aligned}\right.\quad\text{as}\quad\varrho\to 0 \tag{2.5}$$

On the other hand it is known that as $\varrho\to\infty$ one obtains

$$\begin{aligned}K_\nu(\varrho)&\sim\sqrt{\frac{\pi}{2\varrho}}\,e^{-\varrho},\\I_\nu(\varrho)&\sim\frac{1}{\sqrt{2\pi\varrho}}\,e^{\varrho}.\end{aligned} \tag{2.6}$$

The entire asymptotic expansion, as $\varrho\to\infty$, is given by

$$\begin{aligned}K_\nu(\varrho)&\sim\frac{\pi}{\sqrt{2\varrho}}e^{-\varrho}\left\{1+\frac{4\nu^2-1}{8\varrho}+\frac{(4\nu^2-1)(4\nu^2-9)}{2!(8\varrho)^2}\right.\\&\qquad\left.+\frac{(4\nu^2-1)(4\nu^2-9)(4\nu^2-25)}{3!(8\varrho)^3}+\dots\right\},\\I_\nu(\varrho)&\sim\frac{e^{\varrho}}{\sqrt{2\pi\varrho}}\left\{1-\frac{4\nu^2-1}{8\varrho}+\frac{(4\nu^2-1)(4\nu^2-9)}{2!(8\varrho)}-\dots\right\},\end{aligned} \tag{2.7}$$

from which we obtain a useful asymptotic expansion of the product as $\varrho\to\infty$:

$$K_\nu(\varrho)I_\nu(\varrho)\sim\frac{1}{2\varrho}\left\{1-\frac{1}{2}\frac{4\nu^2-1}{(2\varrho)^2}+\frac{1}{2}\cdot\frac{3}{4}\frac{(4\nu^2-1)(4\nu^2-9)}{(2\varrho)^4}-\dots\right\}. \tag{2.8}$$

If we write $G_z(x,y)$ in terms of the Bessel functions

$$G_z(x,y)=(xy)^{1/2}[\theta(x-y)K_\nu(\sqrt{z}\,x)I_\nu(\sqrt{z}\,y)+\theta(y-x)K_\nu(\sqrt{z}\,y)I_\nu(\sqrt{z}\,x)]\,, \qquad (2.9)$$

we can prove the following properties ($\mathrm{Re}\sqrt{z}>0$):

a) $G_z(x,y)$ is continuous as a function of two variables.

b) $G_z(x,y)$ is smooth for $0<x<y$ or $0<y<x$.

c) $G_z(x,y)\sim\left(\frac{1}{2}\sqrt{z}\right)^\nu\cdot x^{\nu+1/2}y^{1/2}K_\nu(\sqrt{z}\,y)$ as $x\to 0$; $G_z(x,y)\sim\pi^{1/2}(2\sqrt{z})^{-1/2}y^{1/2}\cdot I_\nu(\sqrt{z}\,y)e^{-\sqrt{z}x}$ as $x\to\infty$.

d) $G_z(x,y)=l_1(z,x,y)+z^\nu x^{\nu+1/2}l_2(z,x,y)$, where $l_1$ and $l_2$ are analytic in $z,x,y$ for $x$ in a neighborhood of 0.

e) $G_z(x,x)\sim\frac{x}{\nu}$ as $x\to 0$; $G_z(x,x)\sim\frac{1}{\sqrt{z}}$ as $x\to\infty$.

f) $G_z(x,x)=l_1(z,x,x)+z^\nu x^{2\nu+1}\tilde{l}_2(z,x)$, where $l_1$ and $l_2$ are analytic in $x$ and $z$ for $x$ in a neighborhood of 0.

g) $(H_\kappa+z)G_z(x,y)=\delta_y$, the Dirac distribution at the point $y$ with respect to the variable $x$, in the sense of distributions.

The last property repeats the definition of $G_z$ as the Green's function for $H_\kappa$, i.e., the kernel of $(H_\kappa+z)^{-1}$ as an integral operator. To indicate the dependence of $G_z$ on $\kappa$ we shall write sometimes $G_z(x,y;\kappa)$.

We conclude this section by an easy extension to operators on the entire real line $\mathbb{R}$.

Let $H_{\kappa_-,\kappa_+}$ be the operator defined by

$$(H_{\kappa_-,\kappa_+}\phi)(x)=\begin{cases}-\dfrac{d^2\phi}{dx^2}+\dfrac{\kappa_-}{x^2}\phi(x) & \text{if}\quad x<0\,,\\[2mm] -\dfrac{d^2\phi(x)}{dx^2}+\dfrac{\kappa_+}{x^2}\phi(x) & \text{if}\quad x>0\,,\end{cases}$$

for $\phi\in C_0^\infty(\mathbb{R}\backslash\{0\})$. We have

**Proposition (2.3).** *$H_{\kappa_-,\kappa_+}$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}\backslash\{0\})$ if $\kappa_\pm\geqq 3/4$. The domain of the closed operator is $D^-\oplus D$, where $D^-$ is $D$ reflected through the origin. The Green's function is given by*

$$\begin{aligned}G_z(x,y);\kappa_-,\kappa_+)=(H_{\kappa_-,\kappa_+}+z)^{-1}(x,y)&=\theta(x)\theta(y)G_z(x,y;\kappa_+)\\ &\quad+\theta(-x)\theta(-y)\cdot G_z(-x,-y;\kappa_-)\,.\end{aligned}$$

The proof is straightforward.

## 3. The Heat Kernel Function for $H_\kappa$

### *a) Definition of the Heat Kernel*

Let $H$ be a self-adjoint operator on a Hilbert space with a discrete or continuous spectrum which is a subset of the positive real axis. By the spectral theorem, $e^{-sH}$ can be defined as a bounded operator on the Hilbert space if $\mathrm{Re}\,s>0$; if $z\notin\mathbb{R}_-$,

$(H+z)^{-1}$ is also defined as a bounded operator and we have the relation via an inverse Laplace transform:

$$e^{-sH}=\int \frac{dz}{2\pi i} e^{sz}(H+z)^{-1}, \tag{3.1}$$

where the contour of integration is indicated in the figure

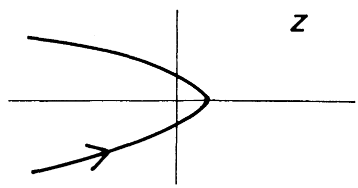


**Fig. 1**

For an operator on $L^2(\mathbb{R})$ where $(H+z)^{-1}$ is an integral operator such as $G_z$ of the previous section, we can write (3.1) as a relation between the kernels. Thus

$$e^{-sH_\kappa}(x,y)=\int \frac{dz}{2\pi i} e^{sz} G_z(x,y;\kappa). \tag{3.2}$$

One can study the heat kernel from the already known properties of $G_z(x,y;\kappa)$. Using the expression (2.9) we may write

$$\begin{aligned} e^{-sH_\kappa}(x,y)=(xy)^{1/2}\int \frac{dz}{2\pi i} e^{sz}[&\theta(x-y)K_\nu(\sqrt{z}\,x)I_\nu(\sqrt{z}\,y) \\ &+\theta(y-x)K_\nu(\sqrt{z}\,y)I_\nu(\sqrt{z}\,x)]. \end{aligned} \tag{3.3}$$

**Lemma (3.1).** *We can write* $K_\nu(\sqrt{z}x)I_\nu(\sqrt{z}y)=x^{-\nu}y^{\nu}g_1(zx^2)g_2(zy^2)+z^{\nu}x^{\nu}y^{\nu}\cdot g_2(zx^2)$ $g_2(zy^2)$, *where* $g_1(zx^2)$ *and* $g_2(xy^2)$ *are analytic functions of their arguments (depending on* $\nu$*) for* $\nu$ *not an integer.*

*Proof.* From the definition of $I_\nu$ in (2.2), we see that $I_\nu(\sqrt{z}x)\propto(\sqrt{z}x)^\nu g_2(zx^2)$, where $g_2$ is entire and remains entire if $\nu$ is replaced by $-\nu$ (in which case we write it as $g_1$). The lemma follows.

If we now apply the lemma to (3.3) we see that the $g_1g_2$ term vanishes for $x,y>0$ by analyticity: the exponential $e^{sz}$ allows us to close the contour at $-\infty$, if $\operatorname{Re}s>0$, and obtain 0 by Cauchy's theorem. Thus we can write

$$e^{-sH_\kappa}(x,y)=(xy)^{1/2}\int \frac{dz}{2\pi i} e^{sz}(xy)^\nu z^\nu g(zx^2)g(zy^2), \tag{3.4}$$

where $g$ $(=g_2)$ is an entire function of its argument. Thus

**Proposition (3.2).** $e^{-sH_\kappa}(x,y)$ *is* $C^\infty$ *as a function of the two variables* $x$ *and* $y$ *for* $x>0$, $y>0$ *if* $\operatorname{Re}s>0$.

*b) Behavior of the Heat Kernel off the Diagonal*

**Proposition (3.3).** *For fixed $y$ $e^{-sH_\kappa}(x,y)$ is $C^k$ for $x$ in a neighborhood of 0 including 0 if $k<\nu+\frac{1}{2}$, $\nu=(\kappa+\frac{1}{4})^{1/2}$, and*

$$e^{-sH_\kappa}(x,y) \sim x^{\nu+1/2}\left(-\frac{\pi}{2^{\nu+1}\Gamma(\nu+1)\sin\nu\pi}\right)\int \frac{dz}{2\pi i} e^{sz} z^{\nu/2} I_\nu(\sqrt{z}\, y) y^{1/2}$$

*as $x\to 0$. As $x\to\infty$, we have*

$$e^{-sH_\kappa}(x,y) \sim c\cdot e^{-x^2/s}\cdot\frac{1}{s^{1/2}},$$

*where $c$ depends on $y$, $\kappa$.*

*Proof.* The differentiability property at $x=0$ follows from Lemma (3.1). The asymptotic estimates follow from the corresponding estimates for the Bessel functions given in the previous section. For the estimate near $x=0$ we keep in mind that Lemma (3.1) effectively says that the $I_{-\nu}$ term in the definition of $K_\nu$ by (2.2) is dropped when writing down the heat kernel. Finally, I remark that one can integrate the asymptotic estimates for the Bessel functions to obtain the leading behavior of $e^{-sH_\kappa}(x,y)$ because they are essentially Taylor expansions about $\varrho=0$ as $\varrho\to 0$ and about 0 in $\frac{1}{\varrho}$ as $\varrho\to\infty$.

As we shall not need the behavior of $e^{-sH_\kappa}(x,y)$ off the diagonal for small $s$, I defer the precise statement and proof of the exponential decay as $s\to 0$ to the next paper.

### *c) Behavior on the Diagonal*

The crucial property of $e^{-sH_\kappa}(x,y)$ that makes a treatment by the classical asymptotic expansion (1.3) of the heat operator impossible is a scaling property in the $s,x,y$ variables, which is stated in the following theorem. In the next section, it is explained how scaling of this kind necessitates an asymptotic expansion in the sense of distribution. On the other hand it is this exact scaling that makes $H_\kappa$ a fundamental operator more tractable than other operators with similar singular behavior.

**Theorem (3.4).** *We have for $\kappa\geqq 3/4$*

$$e^{-sH_\kappa}(x,y)=s^{-1/2}e^{-H_\kappa}\left(\frac{x}{s^{1/2}},\frac{y}{s^{1/2}}\right).$$

*Proof.* Make a change of variable $z\to s^{-1}z$ in (3.3).

The ultimate objective of this paper is to derive an asymptotic expansion for $e^{-sH_\kappa}(x,x)$ as $s\to 0$. Consider therefore the function:

$$e^{-sH_\kappa}(x,x)=s^{-1/2}e^{-H_\kappa}\left(\frac{x}{s^{1/2}},\frac{x}{s^{1/2}}\right).$$

The asymptotic behavior for fixed $x>0$ as $s\to 0$ is completely equivalent to the behavior for fixed $s$ as $x\to\infty$. A similar duality holds between $s\to\infty$ and $x\to 0$. It suffices therefore to look at the function $e^{-H_\kappa}(w,w)$ for $w\geqq 0$.

**Proposition (3.5).** *$e^{-H_\kappa}(w,w)$ is analytic in $w$ for $w>0$. It is $C^k$ for $k<2\nu+1$, $\nu=(\kappa+\frac{1}{4})^{1/2}$ for $w$ in a neighborhood of 0. Asymptotically,*

$$e^{-H_\kappa}(w,w)\sim w^{2\nu+1}\cdot c(\kappa) \qquad as \quad w\to 0,$$

$$e^{-H_\kappa}(w,w)\sim \frac{1}{2\sqrt{\pi}}\left\{1-\frac{1}{2\cdot 4}\cdot 2\cdot\frac{4\kappa}{w^2}+\ldots\right\} \quad as \quad w\to\infty.$$

*Proof.* Analyticity follows from the analyticity of $I_\nu$ and $K_\nu$. Differentiability and the asymptotic behavior as $w\to 0$ follow from (3.4). The asymptotic expansion as $w\to\infty$ follows by term-by-term integration of (2.8) (where $\varrho$ is replaced by $\sqrt{z}\,w$), remembering that the latter is the Taylor series in $\frac{1}{\varrho}$ about 0.

The proof of Proposition (3.5) tells us how to work out the asymptotic expansion as $w\to\infty$ to all orders. This expansion together with the rest of the information contained in Proposition (3.5) and the scaling property of Theorem (3.4) is all we need to prove the term-by-term $s$-behavior of $e^{-sH_\kappa}(x,x)$ as $s\to 0$. The coefficients in the expansion require more detailed information about the heat kernel and they will be derived in Sect. 5.

## 4. Singular Asymptotics of Functions on the Real Line

In this section I study the asymptotics of a function of two real variables, $f(x,s)$, as $s\to 0+$ in the sense of distributions if $f(x,s)$ is of the form $F\left(\frac{s}{x^2}\right)$, where $F(y)$ is $C^\infty$ in a neighborhood of $y=0$. It is then clear that the asymptotic expansion of $F\left(\frac{s}{x^2}\right)$ as $s\to 0$ for $x\neq 0$, which is just a Taylor series, becomes singular when extended to $x=0$. Theorem (3.4) and Proposition (3.5) show that $e^{-sH_\kappa}(x,x)$ can be written as $s^{-1/2}f(x,s)$ where $f$ is a function of the kind just described for $x\geqq 0$. I prefer to consider functions $f((x,s)$ with $x$ ranging over the entire real line with $f(x,s)=0$ for $x<0$. The asymptotics will be studied in $D'(\mathbb{R})$. In other words we do not want our test functions to have support away from zero even though $f$ is a function on the half-line. In this way we shall be able to apply the one-dimensional results to higher dimensions by using spherical coordinates. It will also be possible to treat the operator $H_{\kappa_-,\kappa_+}$ (see the end of Sect. 2), which are unsymmetric about the origin, because by Proposition (2.3) we can write $e^{-sH_{\kappa_-,\kappa_+}}(x,x)=s^{-1/2}[f_-(-x,s)+f_+(x,s)]$, where $f_\pm$ are again functions of the kind treated in this section.

The present results will later be generalized in different directions. First, to functions $f(x,s)$ with singular asymptotic behavior but not necessarily of the exact form $F\left(\frac{s}{x^2}\right)$. Second, to functions of $x$ in higher dimensional space, which will be treated, as mentioned by using the half-line results. An easy generalization to functions $f$ of the form $\chi(x)F\left(\frac{s}{x^2}\right)$, where $\chi$ is $C^\infty$, will be worked out at the end of this section. The general expressions for the asymptotic coefficients and a detailed derivation are given in the appendix to the paper because they are not needed for my present or later purposes.

**Theorem (4.1).** *Let $f(x,s)$ be a family of functions of $x\in\mathbb{R}$ with $s>0$ and suppose that $f(x,s)=0$ for $x<0$ and $f(x,s)=F\left(\frac{s}{x^2}\right)$ for $x>0$, where $F(y)$ is $C^\infty$, $y\geqq 0$. Assume further that*

$$F(y)\sim\sum_{k=0}^{\infty}F_k y^k \quad as \quad y\to 0\,,$$

$$F(y)\leqq B<\infty \qquad as \quad y\to\infty\,.$$

*Consider the distribution $f_s$ defined in the canonical way by the functions $f(x,s)$ of $x$ in $D'(\mathbb{R})$. We then have in $D'(\mathbb{R})$ as $s\to 0+$*

$$f_s\sim\sum_{m=0}^{\infty}u_m s^m+\sum_{m=1}^{\infty}w_m s^m\ln s+\sum_{m=1}^{\infty}v_m s^{m-1/2}\,.$$

*If $\delta_0$ denotes the Dirac distribution at 0, we have:*

*a) $u_m$ is a linear combination of the $2m^{\text{th}}$ distribution derivative of $\ln x$ and the distribution $\delta_0^{(2m-1)}$ if $m>0$.*

*$u_0$ is a distribution of order 0 with $\operatorname{sing\,supp} u_0=\{0\}$.*

*b) $w_m$ is a constant times $\delta_0^{(2m-1)}$.*

*c) $v_m$ is a constant times $\delta_0^{(2m-2)}$.*

*Finally, we have for each $m$ that $w_m=0$ if and only if $F_m=0$ and $\operatorname{supp} u_m=\{0\}$ if and only if $F_m=0$.*

*Proof.* One could perhaps argue abstractly but since my approach is oriented toward calculations, I give a proof that also derives formulas for the $u$'s, $w$'s, and $v$'s. Consider the asymptotic expansion of $F(y)$ as $y\to 0$. We can write

$$F(y)=\sum_{k=0}^{m-1}F_k y^k+R_m(y) \tag{4.1}$$

for some fixed $m$, where $R_m(y)$ is the remainder after $m$ terms. The assumptions on $F$ imply that

$$\begin{aligned}|y^{-(m-1)}R_m(y)|&\leqq c(m) &&\text{as}\quad y\to\infty\,,\\ |y^{-(m-1)}R_m(y)|&\leqq y\cdot c'(m) &&\text{as}\quad y\to 0\,.\end{aligned} \tag{4.2}$$

If we then look at the function $x^{2(m-1)}f(x,s)$, where $f(x,s)=F\left(\frac{s}{x^2}\right)$ is rewritten in terms of the expansion (4.1) we see that each term in the resulting representation is smooth. By (4.2) the term $x^{2(m-1)}R_m\left(\frac{s}{x^2}\right)$, for fixed $s$, is bounded by a constant as $x\to 0$ and by $\frac{1}{x^2}$ as $x\to\infty$. Now to study $f_s(x)\equiv f(x,s)$ asymptotically in $D'(\mathbb{R})$ as $s\to 0+$, we have to find an expansion in $s$ of

$$\int dx\,\phi(x)f(x,s) \tag{4.3}$$

for each $\phi\in C_0^\infty(\mathbb{R})$.

At this point, make the simplifying assumption

$$\left(\frac{\partial}{\partial x}\right)^k F\left(\frac{1}{x^2}\right) \leqq b_k \cdot (x^{-k}+1) \tag{4.4}$$

for some constant $b_k$, $k=0,1,\ldots$. The condition (4.4) will ensure that boundary terms in the integration by parts below and in the appendix vanish at $x=0$. Inequality (4.4) will also ensure convergence of the integrals at the different stages in the proof. At the end of the proof in the appendix, however, it will be shown that the results of the theorem remain unchanged even without (4.4) or any other condition on the derivatives of $f(x,s)$ near $x=0$.

Assuming (4.4), rewrite (4.3) as

$$\begin{aligned}\int dx \frac{1}{x^{2(m-1)}}(x^{2(m-1)}\phi(x)f(x,s)) &= -\frac{1}{(2m-3)!}\int_0^\infty \ln x \cdot dx \\ &\quad \cdot \left(\frac{\partial}{\partial x}\right)^{2m-2}(x^{2(m-1)}\phi(x)f(x,s)) \\ &= -\frac{1}{(2m-3)!}\int_0^\infty dx \cdot \ln x \cdot \left(\frac{\partial}{\partial x}\right)^{2(m-1)} \\ &\quad \cdot \left\{\phi(x)x^{2(m-1)}\left(\sum_{k=0}^{m-1} F_k\left(\frac{s}{x^2}\right)^k + R_m\left(\frac{s}{x^2}\right)\right)\right\}.\end{aligned}$$

By the remarks above one can see that the sum in the last expression can be differentiated term-by-term. The part involving the summation will give the part of $u_k$ which is the $2k^{\text{th}}$ distribution derivative of $\ln x$ for $0 \leqq k \leqq m-1$. One then shows that what would have been the remainder, $R_m$, yields a sum of Dirac distributions and their derivatives plus a new remainder of order $s^{m-1/2}$. In this manner one obtains the asymptotics through order $s^{m-1}$, but the details that are given in the appendix are necessary for the more precise statement of theorem.

*Example.* Let $f(x,s)=e^{-x^2/s}$ for $-\infty<x<\infty$. Now $\int_{-\infty}^{\infty} dx\,\phi(x)f(x,s)$ can be found asymptotically by a Taylor expansion of $\phi$ if $\phi \in C_0^\infty(\mathbb{R})$. Thus

$$\int \phi(x)e^{-x^2/s}dx = s^{1/2}\int \phi(s^{1/2}x)e^{-x^2}dx \sim s^{1/2}\sum_{k=0}^{\infty}\frac{1}{k!}\phi^{(k)}(0)\int_{-\infty}^{\infty} x^k e^{-x^2}dx \cdot s^k.$$

Thus

$$e^{-x^2/s} \sim \sum_{\substack{k=0\\ k\ \text{even}}}^{\infty} s^{k+1/2}\frac{(-1)^k}{k!}\cdot 2\Gamma\left(\frac{k+1}{2}\right)\delta_0^{(k)}.$$

In this case only the $v$-terms given in Theorem (4.1) are present and the result is evidently consistent with the conclusion of the theorem. It can also be verified that the formulas given in the appendix yield the same exact constants for the coefficients of the asymptotic terms.

A more complicated example is worked out in the appendix using Theorem (4.1).

As promised, I give an easy extension of Theorem (4.1):

**Theorem (4.2).** *Let* $f(x,s)=\chi(x)F\left(\frac{s}{x^2}\right)$, *where* $\chi\in C^\infty(\mathbb{R})$. *Let* $f_s\in D'(\mathbb{R})$ *be defined by* $f_s(\phi)=\int_0^\infty f(x,s)\phi(x)dx$. *Then, if F satisfies the same conditions as in Theorem* (4.1),

$$f_s\sim\sum_{m=0}^\infty u_m s^m+\sum_{m=1}^\infty w_m s^m\ln s+\sum_{m=1}^\infty v_m s^{m-1/2}.$$

a) $u_0\in D'(\mathbb{R})$, of order 0, $\operatorname{sing\,supp} u_0=\{0\}$.
b) For $m>1$, $u_m\in D'(\mathbb{R})$, of order $2m$, $\operatorname{sing\,supp} u_m=\{0\}$.
c) $w_m$ is a linear combination of $\delta_0^{(k)}$, $k\leqq 2m-1$.
d) $v_m$ is a linear combination of $\delta_0^{(k)}$, $k\leqq 2m-2$.

*Proof.* The asymptotic expansion is the same as in Theorem (4.1) with $u_m$, $w_m$, $v_m$ replaced by $\chi\cdot u_m$, $\chi\cdot w_m$, $\chi\cdot v_m$. The theorem follows from the structure of the $u$'s, $w$'s, and $v$'s of Theorem (4.1).

*Remarks.* The condition on $F(y)$ as $y\to\infty$ in Theorem (4.1) can be relaxed significantly. One needs to assume, instead of $|F(y)|\leqq B$ as $y\to\infty$,

$$\int_0^c d\zeta\left|F\left(\frac{1}{\zeta^2}\right)\right|<\infty.$$

i.e. integrability instead of boundedness. The proof of the theorem is exactly the same.

It is striking in Theorem (4.1) that no restriction is needed on the derivatives of $F\left(\frac{s}{x^2}\right)$ as $x\to 0$. From the proof of the theroem it appears at first that condition (4.4) is necessary. In the appendix to this paper, it is shown how this condition is dispensed with.

Consider for example the function

$$f(x,s)=e^{is^{1/2}/x},\qquad x>0. \tag{4.5}$$

We have, clearly,

$$\left(\frac{\partial}{\partial x}\right)^k f(x,1)=O(x^{-2k})$$

and not $o(x^{-2k})$, so that (4.4) is violated. Nevertheless we still obtain the kind of asymptotic expansion described in Theorem (4.1). Equation (4.5) essentially appears in a recent paper by Uhlmann [6] on a mathematical derivation of some classical phenomena in conical refraction, where the author has independently derived an asymptotic expansion in the sense of distributions by methods similar to those of the present paper. Lemma (3.10) of [6] can also be proved by using Theorem (4.1) of this work.

## 5. Asymptotics of $e^{-sH_\kappa}(x,x)$; the Trace Formulas

Theorem (3.4) and Proposition (3.5) show that $s^{1/2}e^{-sH_\kappa}(x,x)$ is of the type of function $f(x,s)$ considered in Theorem (4.1). We obtain therefore

**Theorem (5.$\kappa$).** *Let $H_\kappa$ be the operator defined by Proposition* (2.1) *on $L^2(\mathbb{R}_+)$. Then we have an asymptotic expansion in $D'(\mathbb{R})$ (distribution in $x$) as $s \to 0+$ of the form*

$$e^{-sH_\kappa}(x,x) \sim \sum_{m=0}^{\infty} u_m s^{m-1/2} + \sum_{m=1}^{\infty} w_m s^{m-1/2} \ln s + \sum_{m=0}^{\infty} v_m s^m,$$

*where $u_m$, $w_m$, $v_m$ have the same general properties as are described in* a)–c) *of Theorem* (4.1).

Since the present paper is restricted to dimension one, I shall demonstrate the computability of the coefficients in such an expansion by a real one-dimensional problem, i.e. one extending over $\mathbb{R}$, and defer the study on the half-line. One obtains:

**Theorem (5.$\kappa,\kappa$).** *Let $H_{\kappa,\kappa}$ be as defined at the end of Sect. 2. We have asymptotically as $s \to 0$*

$$e^{-sH_{\kappa,\kappa}}(x,x) \sim \sum_{m=0}^{\infty} c_m(\kappa) u_m \cdot s^{m-1/2} + \sum_{m=0}^{\infty} d_m(\kappa) \delta_0^{(2m)} \cdot s^m,$$

*where $u_m$ is the distribution defined by $u_m(\phi) = \int dx \cdot \ln x \left(\frac{\partial}{\partial x}\right)^{2m} \phi$.*

*Proof.* By the symmetry of $H_{\kappa,\kappa}$ under the transformation $x \to -x$ on the real line, we can conclude that $e^{-sH_{\kappa,\kappa}}(x,x) = s^{1/2}(f(x,s) + f(-x,s))$, where $f$ is some function satisfying the conditions of Theorem (4.1). Thus the terms in the asymptotic expansion of $f(x,s)$ that are odd under $x \to -x$ will not appear in the expansion of $e^{-sH_{\kappa,\kappa}}(x,x)$. The odd terms are precisely the ones containing $\delta_0^{(2m-1)}$. It follows that only the terms indicated in the theorem are present. For the precise form of $u_m$ we have to resort to the formulas in the appendix.

The coefficients $c_m(\kappa)$ are proportional to the asymptotic coefficients in the expansion of Proposition (3.5) for large $w$ and are easy to compute. It is striking and important that the $d_m(\kappa)$ can also be computed. It is striking because the formulas in the appendix for them proved totally fruitless. And it is important because they also give the leading behavior of the kernels of more general operators.

**Theorem (5.$\kappa,\kappa'$).** *The coefficients $d_m(\kappa)$ in Theorem* (5.$\kappa,\kappa$) *are given by*

$$d_m(\kappa) = 2^{2m} \cdot \frac{(m+1)!}{(2m)!\,(2m+1)!} \cdot \prod_{j=-m}^{m} (v+j),$$

*where $v = (\kappa + \frac{1}{4})^{1/2}$.*

*Proof.* The theorem will follow from Lemma (5.1) and Proposition (5.2) below.

**Lemma (5.1).** *Let $F_k$ be the coefficients in the asymptotic expansion*

$$e^{-sH_{\kappa,\kappa}}(w,w) \sim \sum_{k=0}^{\infty} F_k \left(\frac{1}{w}\right)^{2k} \quad as \quad w \to \infty.$$

*Then the coefficients $d_m(\kappa)$ are given by*

$$\frac{1}{(2m)!}\int_{-\infty}^{\infty} dx\cdot x^{2m}\left[e^{-sH_{\kappa,\kappa}}(x,x)-s^{-1/2}\sum_{k=0}^{m} F_k\left(\frac{s}{x^2}\right)^k\right]\sim d_k(\kappa)s^m.$$

**Proposition (5.2)** (the trace formulas).

$$\int_{-\infty}^{\infty} dx\cdot x^{2m}\left[e^{-sH_{\kappa,\kappa}}(x,x)-s^{1/2}\sum_{k=0}^{m} F_k\left(\frac{s}{x^2}\right)^k\right]=s^m\cdot 2^{2m}\frac{(m+1)!}{(2m+1)!}\cdot\prod_{j=-m}^{m}(\nu+j).$$

*In particular,*

$$\mathrm{Tr}(e^{-sH_{\kappa,\kappa}}-e^{-sH_0})=\nu,$$

*where $H_0$ is the operator $-\frac{d^2}{dx^2}$ with domain $H^2(\mathbb{R})$.*

*Proof of the Lemma* (5.1). Consider the function $f$ defined by

$$s^{-1/2}f(x,s)=e^{-sH_{\kappa,\kappa}}(x,x)-\sum_{k=0}^{m} F_k\left(\frac{s}{x^2}\right)^k s^{-1/2}.$$

The function $\left(\frac{x^2}{s}\right)^m f(x,s)$ is a function of $\frac{s}{x^2}$ alone and satisfies

$$\begin{aligned}\left(\frac{x^2}{s}\right)^m f(x,s)&\sim -F_m \quad\text{as}\quad \frac{x^2}{s}\to 0,\\ &\sim c\cdot\frac{s}{x^2}\quad\text{as}\quad\frac{s}{x^2}\to 0.\end{aligned}\tag{5.1}$$

Thus is satisfies the hypotheses of Theorem (4.1). Furthermore, if we write

$$\left(\frac{x^2}{s}\right)^m f(x,s)\sim\sum_{k=0}^{\infty} G_k\left(\frac{s}{x^2}\right)^k\quad\text{as}\quad\frac{s}{x^2}\to 0,$$

we have $G_0=0$. Theorem (4.1) then implies that, for $\psi\in C_0^\infty(\mathbb{R})$.

$$\int_{-\infty}^{\infty} dx\,\psi(x)\left(\frac{x^2}{s}\right)^m f(x,s)\sim O(s^{1/2})\cdot\psi(0)+O(s),$$

so that

$$\int_{-\infty}^{\infty} dx\,\psi(x)x^{2m}f(x,s)\sim O(s^{m+1/2})\cdot\psi(0)+O(s^{m+1}).\tag{5.2}$$

Now choose $\chi\in C_0^\infty(\mathbb{R})$ with $\chi=1$ in a neighborhood of 0, and write

$$\int dx\,s^{-1/2}f(x,s)\cdot x^{2m}=\int dx\cdot\chi(x)x^{2m}f(x,s)s^{-1/2}+\int dx(1-\chi(x))x^{2m}f(x,s)s^{-1/2}.\tag{5.3}$$

The left-hand side is exactly the quantity we wish to estimate to order $s^m$. Consider each term on the right-hand side. The term

$$\int dx\,\chi(x)x^{2m}f(x,s)s^{-1/2}\tag{5.4}$$

is $O(s^m)$ by the discussion above. Now we can show that the coefficient of the $s^m$-asymptotic term is precisely $(2m)!\,d_m(x)$. In fact, write (5.4) as

$$\begin{aligned}\int dx(\chi(x)x^{2m})e^{-sH}(x,x)-\sum_{k=0}^{m}F_k\cdot s^{-1/2}\int dx\,\chi(x)x^{2(m-k)}s^k\\ \sim\sum_{k=0}^{\infty}d_k(\kappa)\delta_0^{(2k)}(x^{2m}\chi(x))s^k+\sum_{k=0}^{\infty}c_k(\kappa)u_k(\chi)s^{k-1/2}\\ -\sum_{k=0}^{m}F_k\int dx\,\chi(x)x^{2(m-k)}s^{k-1/2},\end{aligned}$$

by Theorem $(5.\kappa,\kappa)$, and we can see by inspection that the coefficient of $s^m$ is $d_m(\kappa)\delta_0^{(2m)}(x^{2m}\chi(x))=(2m)!\,d_m(\kappa)$. We then have for (5.4)

$$\int dx\,\chi(x)\cdot x^{2m}f(x,s)s^{-1/2}=(2m)!\,d_m(\kappa)s^m+O(s^{m+1/2}).$$

For the second term in (5.3), note that (5.2) suggests that it is $O(s^{m+1/2})$, since $(1-\chi(0))=0$. This is not exactly rigorous, since $1-\chi(x)$ is not of compact support. But (5.1) implies that given $d>0$, we have for $|x|\geqq d$,

$$|f(x,s)s^{-1/2}|\leqq c\cdot s^{-1/2}\left(\frac{s}{x^2}\right)^{m+1}$$

for some constant $C$. Since $1-\chi(x)=0$ in $|x|<d$ for some $d>0$, we have for the second term in (5.3)

$$\begin{aligned}\left|\int dx(1-\chi(x))x^{2m}f(x,s)s^{-1/2}\right|&\leqq c\cdot\int_d \frac{dx}{x^2}\cdot s^{m+1/2}\\ &=c'\cdot s^{m+1/2},\end{aligned}$$

so that this term gives no contribution to $O(s^m)$ and the lemma is proved.

*Proof of the Proposition* (5.2). One has to use special properties of the Bessel functions.

First we represent $e^{-sH_{\kappa,\kappa}}(x,x)$ in terms of Bessel functions (see the end of Sect. 2):

$$e^{-sH_{\kappa,\kappa}}(x,x)=|x|\cdot\int\frac{dz}{2\pi i}K_\nu(\sqrt{z}\,|x|)I_\nu(\sqrt{z}\,|x|)e^{sz},$$

and make use of the following integral representation of the product of modified Bessel functions [4]:

$$K_\nu(b\varrho)I_\nu(b\varrho)=\frac{\Gamma(2\nu+1)}{\Gamma(\nu+1)}\left(\frac{b^2}{4\varrho}\right)^{\nu}\int_0^{\infty}dt\frac{J_\nu(2\varrho t)}{t^\nu(t^2+b^2)^{\nu+1/2}},\tag{5.5}$$

where $J_\nu$ is the Bessel function of order $\nu$. The term $F_k\left(\frac{s}{x^2}\right)^{2k}$ in the asymptotic expansion of $e^{-sH_{\kappa,\kappa}}(x,x)$ as $x\to\infty$ is given by the $k^{\text{th}}$ order term in the binomial expansion of $(t^2+b^2)^{-(\nu+1/2)}$ (where $b=\sqrt{z}$) in (5.5) in powers of $\frac{t^2}{z}$:

$$F_k\left(\frac{s}{x^2}\right)^k=|x|\int\frac{dz}{2\pi i}e^{sz}\frac{\Gamma(2\nu+1)}{\Gamma(\nu+1)}\left(\frac{z}{4|x|}\right)^\nu\int_0^\infty dt\frac{J_\nu(2|x|t)}{t^\nu}\cdot\frac{\Gamma(-\nu+\frac{1}{2})}{\Gamma(-\nu+\frac{1}{2}-k)k!}\left(\frac{t^2}{z}\right)^k.$$

After substitution in the quantity we want to compute we perform the $x,t,z$ integration in that order. For the $x$ integration we use the formula [4]

$$\int_0^\infty dx\,x^\mu J_\nu(x)=\frac{2^\mu\Gamma\left(\frac{\nu+\mu+1}{2}\right)}{\Gamma\left(\frac{\nu-\mu+1}{2}\right)}.$$

For the $t$-integration, we use

$$\int_0^\infty\frac{dt}{t}\frac{\partial^{2k+1}}{\partial t^{2k+1}}\frac{1}{(t^2+z)^{\nu+1/2}}=z^{-\nu-k-1}\frac{\Gamma(\nu+k+1)}{\Gamma(\nu+\frac{1}{2})}(-1)^k\sqrt{\pi}\,2^{2k}(k+1)!$$

The contour integration then becomes trivial and yields the result.

## 6. The Index of Some Differential Operators on $\mathbb{R}$

Consider the following first order differential operator defined on $[C_0^\infty(\mathbb{R}\backslash\{0\})]^M \subset [L^2(\mathbb{R})]^M$ (a direct sum of $M$ copies of $L^2$), $M$ an integer:

$$L=i\frac{d}{dx}+i\frac{1}{x}A(x), \tag{6.1}$$

where $A(x)$ is an hermitian $M\times M$ $C^\infty$ matrix of functions satisfying

$$\lim_{x\to\pm\infty}\frac{1}{x}A(x)=A_\pm, \tag{6.2}$$

where $A_\pm$ are non-singular matrices of finite numbers. Assume further that the eigenvalues of the hermitian matrix $A(0)$ are outside the interval $(-\frac{1}{2},\frac{3}{4})$. The significance of this condition is seen when we form the operators

$$\begin{aligned} L^+L&=-\frac{d^2}{dx^2}+\frac{A(x)^2+A(x)}{x^2}-\frac{A'(x)}{x},\\ LL^+&=-\frac{d^2}{dx^2}+\frac{A(x)^2-A(x)}{x^2}+\frac{A'(x)}{x}, \end{aligned}\tag{6.3}$$

defined for functions $C_0^\infty$ on $\mathbb{R}\backslash\{0\}$. The approximations of these operators by their leading behavior near $x=0$, i.e., the operators

$$H_\pm=-\frac{d^2}{dx^2}+\frac{A(0)^2\pm A(0)}{x^2} \tag{6.4}$$

can be written in diagonal form in the representation that makes $A(0)$ diagonal:

$$\bigoplus_{k=1}^{M}\left(-\frac{d^2}{dx^2}+\frac{\lambda_k^2\pm\lambda_k}{x^2}\right), \tag{6.4'}$$

where $\lambda_k$ are the eigenvalues of $A(0)$. By virtue of the condition above, $\lambda_k^2\pm\lambda_k\geqq\frac{3}{4}$, so that the operators (6.4) are self-adjoint on the domain

$$D^M=\left\{\psi\in[H^2(\mathbb{R})]^M\,\left|\,\left\|\frac{1}{x^2}\psi\right\|_2<\infty\right.\right\}. \tag{6.5}$$

We obtain by comparison:

**Theorem (6.1).** *Let $L$ be defined by* (6.1) *and all the conditions above. Then the operators* (6.3) *are essentially self-adjoint on the domain $[C_0^\infty(\mathbb{R}\backslash\{0\})]^M$ and the domain of their closure is* (6.5). *Further, the closed operators so defined are Fredholm.*

*Proof.* The proof uses an easy perturbation argument by the Kato-Rellich theorem in the following version [3]: if $H_0, H$ are symmetric unbounded operators and $D\subset D(H)\cap D(H_0)$ such that for some $a<1$,

$$\|(H-H_0)\phi\|\leqq a\{\|H\phi\|+\|H_0\phi\|\}+b\|\phi\| \quad \text{for all} \quad \phi\in D,$$

then $H$ is essentially self-adjoint on $D$ if and only if $H_0$ is, and in that case the self-adjoint extensions of $H$ and $H_0$ are defined on the same domain.

Now let $H$ be $L^+L$ or $LL^+$, as given by (6.3), and let $H_0$ be $H_+$ or $H_-$, given by (6.4), respectively. Take $D=[C_0^\infty(\mathbb{R}\backslash\{0\})]^M$. It is easy to see that in either case $H-H_0=B(x)+\frac{c}{x}$, where $c$ is constant and $B(x)$ is $C^\infty$ and bounded. It is then clear that $H$ and $H_0$ satisfy the condition of the Kato-Rellich theorem and the statements about the domains of the operators (6.3) follow.

That $L^+L$ and $LL^+$ are Fredholm follows from the fact that they are bounded below by Hermitian operators that are identical to $L^+L$ and $LL^+$ outside a compact set and have no singularity at the origin. The condition (6.2) implies via a theorem of Seeley [5] that these lower bound operators are Fredholm. This proves the theorem.

It now follows by simple arguments that (6.1) is a closable operator and the closure is Fredholm under all the conditions above.

We can therefore try to compute the index of $L$ in (6.1). I use a technique developed in [5] for computing the index of operators on open manifolds in terms of the resolvent or the heat operator (see also Appendix B of [1]). The basic result is the following proposition:

**Proposition (6.2).** *Let $L$ be a first order elliptic differential operator on the Hilbert space $\bigoplus_1^M L^2(\mathbb{R}^n)$:*

$$L=i\delta^i(x)\partial_i+i\Phi(x), \tag{6.6}$$

where $\delta_i(x)$, $\Phi(x)$ are $M\times M$ matrices of smooth functions. Let $\delta_i$, $\Phi$ denote multiplication operators by $\delta^i(x)$, $\Phi(x)$. Suppose $z\notin\mathbb{R}_-$, and let $(LL^++z)^{-1}(x,y)$,

$(L^+L+z)^{-1}(x,y)$ denote the kernel functions of the indicated integral operators. Then, for $x \neq y$

$$2z\,\mathrm{tr}((D^+D+z)^{-1}-(DD^+ +z)^{-1})(x,y)=\left(\frac{\partial}{\partial x^i}+\frac{\partial}{\partial y^i}\right)J_z^i(x,y)+A_z(x,y)\,, \quad (6.7)$$

where tr denotes trace over the matrix indices, $J_z^i(x,y)$ is the kernel of the integral operator

$$J_z^i = i\,\mathrm{tr}[D(D^+D+z)^{-1}\delta^{i+} - D^+(DD^+ +z)^{-1}\delta^i]\,,$$

and $A_z(x,y)$ is the kernel of an integral operator on $L^2(\mathbb{R}^n)$ that can be represented as the trace of commutators of multiplication operators by smooth functions and the integral operators $D(D^+D+z)^{-1}$ and $D^+(DD^+ +z)^{-1}$.

The multiplication operators in the last statement are basically $\delta^i$ and $\Phi$. The theorem is a local one and it is derived by using the differential equations satisfied by the resolvents. It can therefore be extended to operators with singularities such as are studied in this section. Equation (6.7) will then be valid for $x$ and $y$ away from the singularity. The following two lemmas show how the singular points can be included in the range of validity.

**Lemma (6.1).** *Let* $L_1 = i\frac{d}{dx} + i\frac{1}{x}A(x)$ *be an operator of the form* (6.1), *where* $A_1(x) = A(x)$ *for* $|x| \geqq R$ *and* $A_1(x) = A(0)$ *for* $|x| \leqq r$, $0<r<R$. *Then index* $L =$ *index* $L_1$.

*Proof.* We can write $L_1 = L + B(x)$, where $B(x) = i\frac{1}{x}(A_1(x)-A(x))$ is $C^\infty$ and of compact support. We can then show that $B$, the multiplication operator by $B(x)$, is compact relative to $L_1$; in other words that the operator $B: D(L_1) \to [L^2(\mathbb{R})]^M$ is a compact operator, where $D(L_1)$ is equipped with the norm $\|L_1\cdot\| + \|\cdot\|$. It will then follow, by basic index theory [7], that $L_1$ and $L_1 - B = L$ have the same index.

To prove the compactness property, note first that $B$ is compact relative to $i\frac{d}{dx}$ with domain $H^1(\mathbb{R})$ by the Rellich lemma [8]. This is equivalent to saying that bounded sets in $D\left(i\frac{d}{dx}\right)$ $\left[\text{with norm } \left\|i\frac{d}{dx}\cdot\right\| + \|\cdot\|\right]$ are mapped to precompact sets by $B$. But note that we have the inequality, valid for $\psi \in C_0^\infty(\mathbb{R}\backslash\{0\})$,

$$\begin{aligned}\left\|i\frac{d}{dx}\psi\right\|^2 &= \left(\psi, -\frac{d^2}{dx^2}\psi\right) \leqq \left(\psi, \left[-\frac{d^2}{dx^2} + \frac{A(0)^2 + A(0)}{x^2}\right]\psi\right)\\ &\leqq \left(\psi, \left[-\frac{d^2}{dx^2} + \frac{A_1(x)^2 + A_1(x)}{x^2}\right]\psi\right) + C\cdot(\psi,\psi)\\ &= \|L_1\psi\|^2 + C\|\psi\|^2\,,\end{aligned}$$

where $C$ is an upper bound for the function

$$\frac{A_1(x)^2 + A_1(x)}{x^2} - \frac{A_1(0)^2 + A_1(0)}{x^2} \in C^\infty(\mathbb{R})\,.$$

Since $C_0^\infty(\mathbb{R}\setminus\{0\})$ is dense in $D(L_1)$, it follows that, for all $\psi\in D(L_1)$,

$$\left\| i\frac{d}{dx}\psi\right\|^2 \leqq C\cdot(\|L_1\psi\|+\|\psi\|)$$

for some constant $C$. Thus a bounded set in $D(L_1)$ is bounded with respect to the norm of $D\left(i\frac{d}{dx}\right)$ and is therefore mapped to a precompact set under $B$. It follows that $B$ is $L_1$-compact, hence the lemma.

**Lemma (6.2).** *Let $L_1$ be as in Lemma* (6.1). *Given a fixed $t>0$, we have* $\exp(-tL_1^+L_1)(x,y)=O(x^\nu)$, *as $x\to 0$ for fixed $y$, and* $\exp(-tL_1^+L_1)(x,x)=O(x^{2\nu})$ *as $x\to 0$ for some $\nu\geqq 1$. Similar estimates hold for* $\exp(-tL_1L_1^+)$.

*Proof.* The heat kernel in the case of both $\exp(-tL_1^+L_1)$ and $\exp(-tL_1L_1^+)$ can be represented by using (3.2) and (2.4), which are generally true for a second order differential operator on $\mathbb{R}$ (with first order term equal to 0) and not just for the special operator of (2.1). Now in the neighborhood of $x=0$ the $\psi_1(x)$, $\psi_2(x)$ of (2.4) will still be linear combinations of the modified Bessel function of (2.2). Because $\psi_2(x)$ has to be $L^2$ near 0, it should only contain terms involving the $I_\nu$ Bessel functions. For linear independence of $\psi_1$ and $\psi_2$, $\psi_1$ must contain $K_\nu$'s. For $x, y$ in the neighborhood of 0 we will still have a representation of the form (3.4). This proves the required estimates as in Propositions (3.3) and (3.5).

We would like to evaluate (6.7) on the diagonal but the resolvents become usually singular there, so it is more convenient to work with heat operators. A direct complex integration of (6.7) along the contour of Sect. 3 then yields

$$\begin{aligned}-\frac{\partial}{\partial s}\operatorname{tr}(e^{-sL^+L}-e^{-sLL^+})(x,y)&=\frac{1}{2}\left(\frac{\partial}{\partial x^i}+\frac{\partial}{\partial y^i}\right)\operatorname{tr}[Le^{-L^+L}\delta^{i^+}-L^+e^{-sLL^+}\delta^i]\cdot(x,y)\\&\quad+\int\frac{dz}{2\pi i}e^{sz}A_z(x,y).\end{aligned}\tag{6.8}$$

It is then argued (Appendix B of [1]) that the last term goes to zero as $x\to y$ because it is now represented as the matrix trace of commutators of multiplication operators with the integral operators $e^{-sL^+L}$ and $e^{-sLL^+}$ which are smooth on the diagonal. This argument will work in the present case as well for the operator (6.1), because the heat kernels will behave sufficiently well even at the singularity, according to Lemma (6.2). Equation (6.7) therefore gives for $x=y$:

$$-\frac{\partial}{\partial s}\operatorname{Tr}(e^{-sL^+L}-e^{-sLL^+})=\int\frac{dze^{sz}}{2\pi i}\int_{-\infty}^{\infty}dx\frac{1}{2}\frac{\partial}{\partial x^i}\operatorname{tr}J_z^i(x,x).\tag{6.9}$$

More remarks are in order. It is argued in [5] that the $A_z$ term in (6.8) goes to zero as $x\to y$ in dimension 1, basically because the singular parts of the two resolvents cancel. This does not apply here because of the additional non-differentiability at $x=0$. On the other hand we could not have divided (6.7) by $z$ to obtain an equation for the trace of the difference of the heat operators rather than for its derivative with respect to $s$ as in (6.9), because the heat operators in the expression for $\int A_z \frac{dz}{2\pi i} e^{sz}$ would be replaced by operators of the type

$$\int \frac{dz}{2\pi i} e^{sz} \frac{1}{z} \frac{1}{z+L^+L} = \frac{1}{L^+L} - \frac{1}{L^+L} e^{-sL^+L},$$

which are much more singular than $e^{-sL^+L}$.

Now the right-hand side of (6.9) has been computed in [5] [see, e.g., (3.14) of that work]. We then obtain by making use of those results

$$-\frac{\partial}{\partial s}\mathrm{Tr}(e^{-sL^+L} - e^{-sLL^+}) = \int \frac{dz}{2\pi i} e^{sz}\left(-\frac{1}{2}\right)\mathrm{tr}\left(\frac{A_+}{(z+A_+^2)^{1/2}} - \frac{A_-}{(z+A_-^2)^{1/2}}\right), \quad (6.10)$$

where $A_\pm$ are given by (6.2). Now it is also shown in [5] that the limit as $s\to\infty$ of the trace that appears on the left hand side of (6.10) is precisely the index of $L$ if $L$ is Fredholm. Thus, integrate (6.10) with respect to $s$ from 0 to $\infty$. Now let $\tilde{L}$ be an operator that looks exactly like $L$ everywhere except that $A(x)$ in (6.1) is deformed to vanish like $x$ as $x\to 0$. By the results of [5] again [Eq. (3.14)] the right hand side of (6.10) is equal to $-\frac{\partial}{\partial s}\mathrm{Tr}(e^{-s\tilde{L}^+\tilde{L}} - e^{-s\tilde{L}\tilde{L}^+})$. Since $L$ is a smooth operator on odd dimensional space, the latter trace is 0 in the limit $s\to 0+$. We obtain, therefore,

$$\mathrm{index}\, L = \mathrm{index}\, \tilde{L} + \lim_{s\to 0+} \mathrm{Tr}(e^{-sL^+L} - e^{-sLL^+}). \quad (6.11)$$

If we anticipate the results of the next paper again, we see that we can evaluate the limit on the right hand side by approximating $L$ by its leading behavior near the singularity. This statement asserts the validity, in a special case, of a natural generalization of the fact, well-known for the case of smooth coefficients, that the asymptotics of $e^{-sH}(x,x)$ and $e^{-sH'}(x,x)$ will agree up to a given order $s^k$ if the derivatives of the coefficients of $H$ and $H'$ at $x$ agree up to some order $m$ (depending on $k$). Thus we need the coefficient of $s^0$ in the asymptotic expansion of

$$\mathrm{Tr}(e^{-sH_+} - e^{-sH_-})$$

as $s\to 0+$ where $H_\pm$ are given by (6.4). Using the representation (6.4′) and Theorem $(5.\kappa,\kappa')$ for $m=0$, we obtain for this coefficient

$$\sum_{k=1}^{M} ((\lambda_k^2+\lambda_k+\tfrac{1}{4})^{1/2} - (\lambda_k^2-\lambda_k+\tfrac{1}{4})^{1/2}),$$

each $\lambda_k \geqq 3/2$ or $\leqq -1/2$, by assumption. If $\lambda_k \geqq 3/2$ the quantity in brackets is $|\lambda_k+\frac{1}{2}| - |\lambda_k - \frac{1}{2}| = 1$. If $\lambda_k \leqq -1/2$ the same expression gives $-\lambda_k - \frac{1}{2} - (\frac{1}{2}-\lambda_k) = -1$. Thus the limit on the right hand side of (6.11) is precisely the signature of the matrix $A(0)$, $\mathrm{sign}\, A(0)$, i.e., the number of positive minus the number of negative eigenvalues. We summarize:

**Theorem (6.3)** [Index theorem for (6.1)]. *Let $L$ be defined and satisfy all the properties as described in the beginning of this section. Let $\tilde{L}$ be obtained from $L$ by deformation in a neighborhood of* 0 *to a smooth lower order term in* (6.1). *Then $L$, $\tilde{L}$ are closable and their closures are Fredholm and*

$$\begin{aligned}\mathrm{index}\,(L) = \mathrm{index}\,\tilde{L} + \mathrm{sign}\, A(0) = &-\tfrac{1}{2}\mathrm{tr}(A_+|A_+|^{-1} - A_-|A_-|^{-1}) \\ &+ \mathrm{tr}\, A(0)|A(0)|^{-1}.\end{aligned}$$

## 7. Discussion of the Trace Formula [9]

It would be very interesting to understand the origin and significance of the trace formulas of Proposition (5.2). In particular, it would be desirable to understand why the traces have a power dependence on $s$ (the $m^{\text{th}}$ trace is proportional to $s^m$) and why the dependence on $v$ is again polynomial. The first question is easy to answer by using the fact that the heat kernel can be expressed in the form given by Theorem (3.4). I also give a derivation of a partial answer to this question that points to a generalization of the trace formula to operators of the more general form of Sect. 6. I cannot see any illuminating answer to the second question.

Consider operators of the type (6.1) with $M=1$ and let $A(x)$ be the constant $v-\frac{1}{2}$. We then obtain from (6.3)

$$L^+L=-\frac{d^2}{dx^2}+\left(v^2-\frac{1}{4}\right)\frac{1}{x^2},$$

$$LL^+=-\frac{d^2}{dx^2}+\left((v-1)^2-\frac{1}{4}\right)\cdot\frac{1}{x^2}$$

for $v\geqq 3/2$. Let $H(v)$ denote the operator $H_{\kappa,\kappa}$ with $\kappa=v^2-\frac{1}{4}$. The results of [5], as explained in the previous section yield

$$\frac{\partial}{\partial s}\operatorname{Tr}(e^{-sH(v)}-e^{-sH(v-1)})=0,$$

because the $A_\pm$ of Eq. (6.2) are now 0. This shows that

$$\frac{\partial}{\partial s}\operatorname{Tr}(e^{-sH(v)}-e^{-sH_0}),$$

where $H_0=-\dfrac{d^2}{dx^2}$ is a periodic function of $v$ with period 1. There is obviously quite a gap between this statement and the conclusion of Proposition (5.2) that it is actually zero.

If $v$ is an integer, the Bessel functions appropriate to the problem are of half-integer order. They are then expressed in terms of elementary functions and as a check one can verify the first few trace formulas (for small $v$ and small $m$) explicitly.

## Appendix. Derivation of Singular Asymptotics on the Half-Line

I give more details about the derivation of Theorem (4.1) in this appendix as well as formulas for the distribution coefficients of the different terms in the asymptotic expansion.

Start with the assumption in the theorem of Sect. 4 and write, as already indicated in the sketch-of-proof of the theorem given there

$$\int dx\,\phi(x)f(x,s)=-\frac{1}{(2m-3)!}\int_0^\infty dx\ln x\left(\frac{\partial}{\partial x}\right)^{2m-3}$$
$$\cdot\left\{\phi(x)x^{2(m-1)}\left(\sum_{k=0}^{m-1}F_k\left(\frac{s}{x^2}\right)^k+R_m\left(\frac{s}{x^2}\right)\right)\right\}. \tag{A.1}$$

In the term with the summation it will be enough to point out the term of highest order:

$$-\frac{1}{(2m-3)!}\cdot s^{m-1}\int_0^\infty dx\cdot \ln x\cdot \frac{\partial^{2m-3}}{\partial x^{2m-3}}\phi(x). \tag{A.2}$$

Next we show that the term containing $R_m$ can be written as a sum of derivatives of the Dirac distribution at 0 evaluated for the test function $\phi$ plus a remainder which is of order $s^{m-1/2}$. We rewrite the term in (A.1) containing $R_m$ as

$$\int_0^\infty dx \ln x \frac{\partial}{\partial x}\cdot \sum_{k=0}^{2m-4}\binom{2m-4}{k}\cdot \phi^{(k)}(x)\cdot\left(\frac{\partial}{\partial x}\right)^{2m-4-k}\left(x^{2(m-1)}R_m\left(\frac{s}{x^2}\right)\right). \tag{A.3}$$

Now write

$$\phi^{(k)}(x)=\phi^{(k)}(0)+[\phi^{(k)}(x)-\phi^{(k)}(0)], \tag{A.4}$$

and substitute in (A.3). The first term in (A.4) will give a contribution that cannot be reduced any further in terms of $\phi$. After rescaling $x$ by $x\to xs^{1/2}$ it will yield the $\ln s$ terms, among others, in the expansion of Theorem (4.1). We note that the second term in (A.4) vanishes for $x=0$ like $x$ and, therefore, it is possible to do an integration by parts in (A.3) because the $\frac{1}{x}$ singularity from the $\ln x$ will be cancelled. To isolate the remainder, one then only needs the following lemma:

**Lemma (A.1).** *Let $\phi\in C_0^\infty(\mathbb{R})$. Then*

$$\int_0^\infty dx\,\phi(x)\left(\frac{\partial}{\partial x}\right)^p x^{2(m-1)}R_m\left(\frac{s}{x^2}\right)=\sum_{k=0}^{\left(\frac{p-1}{2}\right)}(-1)^p\phi^{(p-2k-1)}(0)\cdot F_{m-1-k}\cdot(2k)!\cdot s^{m-1-k}+c_s[\phi]s^{m-1/2},$$

*where $c_s[\phi]$ is bounded in $s$.*

*Proof.* Use integration by parts, repeated $p$ times until the differentiation is transferred to $\phi(x)$ in the integral. Because the integral extends over the half-line, we pick up some boundary terms at the origin, which give the sum on the right-hand side of the equation in the lemma. What is left is proportional to

$$\int_0^\infty dx\,\phi^{(p)}(x)x^{2(m-1)}R_m\left(\frac{s}{x^2}\right),$$

which is estimated by

$$\sup_x|\phi^{(p)}(x)|\cdot\int_0^\infty dx\,x^{2(m-1)}\left|R_m\left(\frac{s}{x^2}\right)\right|.$$

By a single rescaling $x\to x\cdot s^{1/2}$, the last integral is seen to be proportional to $s^{m-1/2}$, which proves the lemma.

Thus we have shown that we have isolated terms through orders $s^{m-1}\cdot\ln s$ in the expansion, with a remainder of order $s^{m-1/2}$. We do this for each $m$ and then pick out the highest order terms, i.e., the terms of orders $s^{m-1}$, $s^{m-3/2}$ and $s^{m-1}\cdot\ln s$.

We can then write down the distribution coefficients for each $m$ in the expansion of Theorem (4.1):

$$\begin{aligned}
u_0 &= F_0\theta(x),\\
u_m &= -\frac{F_m}{(2m-1)!}\left(\frac{\partial}{\partial x}\right)^{2m}[\theta(x)\ln x]\\
&\quad+\frac{1}{(2m-2)!}F_m\left(\frac{\partial}{\partial x}\right)^{2m-1}\delta_0\cdot\int_0^1 dt\ln t(1-t)^{2m-2}\\
&\quad-\frac{1}{(2m-1)!}\left(\frac{\partial}{\partial x}\right)^{2m-1}\delta_0\int_0^\infty d\zeta\ln\zeta\frac{\partial}{\partial\zeta}\left[\zeta^{2m}R_{m+1}\left(\frac{1}{\zeta^2}\right)\right], \qquad \text{(A.5)}\\
w_m &= -\frac{1}{2}\cdot\frac{1}{(2m-1)!}F_m\cdot\left(\frac{\partial}{\partial x}\right)^{2m-1}\delta_0,\\
v_m &= -\frac{1}{(2m-2)!}\left(\frac{\partial}{\partial x}\right)^{2m-2}\delta_0\int_0^\infty d\zeta\cdot\ln\zeta\frac{\partial^2}{\partial\zeta^2}\left[\zeta^{2m}R_{2m}\left(\frac{1}{\zeta^2}\right)\right],
\end{aligned}$$

where the derivatives $\left[\frac{\partial}{\partial x}\right]^{2m}\ln x$, $\left[\frac{\partial}{\partial x}\right]^{p}\delta_0$ are understood in the sense of distributions.

Before proceeding to the general case where the condition (4.4) is not satisfied by $F(y)$, it will be shown that the formulas above for $u_m$, $v_m$, $w_m$ can be cast into a form that does not explicitly involve the derivatives of $F\left(\frac{1}{x^2}\right)$ in the neighborhood of $x=0$. We see by inspection that we need to deal with the following two integrals in the formulas for $u_m$ and $v_m$:

$$L_{1,m}[F]\equiv\int_0^\infty d\zeta\ln\zeta\frac{\partial}{\partial\zeta}\left[\zeta^{2m}R_{m+1}\left(\frac{1}{\zeta^2}\right)\right], \qquad \text{(A.6)}$$

$$L_{2,m}[F]\equiv\int_0^\infty d\zeta\ln\zeta\left(\frac{\partial}{\partial\zeta}\right)^2\left[\zeta^{2m}R_{m+1}\left(\frac{1}{\zeta^2}\right)\right], \qquad \text{(A.7)}$$

($F$ enters the right-hand side through $R_{m+1}$). In view of (4.4), differentiation of $F$ in $R_{m+1}$ does not make the integrand too singular and (A.6) and (A.7) converge nicely near $\zeta=0$. Now start with (A.6), cut-off the integral at $\zeta=\varepsilon$ and integrate by parts:

$$\begin{aligned}
L_{1,m}[F] &= \lim_{\varepsilon\to0+}\int_\varepsilon^\infty d\zeta\ln\zeta\frac{\partial}{\partial\zeta}\left[\zeta^{2m}R_{m+1}\left(\frac{1}{\zeta^2}\right)\right]\\
&= \lim_{\varepsilon\to0}\left\{-\ln\varepsilon\cdot\varepsilon^{2m}R_{m+1}\left(\frac{1}{\varepsilon^2}\right)-\int_\varepsilon^\infty d\zeta\cdot\zeta^{2m-1}R_{m+1}\left(\frac{1}{\zeta^2}\right)\right\}\\
&= \lim_{\varepsilon\to0}\left\{F_m\ln\varepsilon-\int_\varepsilon^\infty d\zeta\cdot\zeta^{2m-1}R_{m+1}\left(\frac{1}{\zeta^2}\right)\right\}\\
&\equiv \lim_{\varepsilon\to0}L_{1,\varepsilon,m}[F], \qquad \text{(A.8)}
\end{aligned}$$

where we define $L_{1,\varepsilon,m}[F]$, and the last step uses the definition (4.1) for $R_{m+1}(y)$ and the condition (4.4). Similarly, we can write for (A.7)

$$L_{2,m}[F]=\lim_{\varepsilon\to 0} L_{2,\varepsilon,m}[F],$$

where

$$L_{2,\varepsilon,m}[F]=-\int_{\varepsilon}^{\infty} d\zeta\,\zeta^{2(m-1)}R_{m+1}\left(\frac{1}{\zeta^2}\right)-\frac{F_m}{\varepsilon}. \tag{A.9}$$

Finally define the "cutoff" distributions $u_{\varepsilon,m}$, $v_{\varepsilon,m}$ by replacing $L_{1,m}[F]$, $L_{2,m}[F]$ appearing in (A.5) by $L_{1,\varepsilon,m}[F]$, $L_{2,\varepsilon,m}[F]$, and $\theta(x)$ by $\theta(x-\varepsilon)$.

We are now ready to work out the proof for the case where (4.4) is removed. First write

$$\int_0^{\infty} dx\,F\left(\frac{s}{x^2}\right)\psi(x)=\lim_{\varepsilon\to 0}\int_{\varepsilon}^{\infty} dx\,F\left(\frac{s}{x^2}\right)\psi(x),$$

and apply exactly the same integrations by parts, including those of Lemma (A.1), to obtain

$$\begin{aligned}\int_{\varepsilon}^{\infty} dx\,F\left(\frac{s}{x^2}\right)\psi(x)=&\left\{u_{\varepsilon,0}(\psi)+\sum_{k=1}^{m-1}s^k(u_{\varepsilon,k}(\psi)+s^{-1/2}v_{\varepsilon,k}(\psi)+\ln s\,w_k(\psi))\right\}\\ &+\int_{\varepsilon}^{\infty} d\zeta\,\Phi(\zeta)\zeta^{2(m-1)}R_m\left(\frac{s}{\zeta^2}\right)\\ &+B_{s,\varepsilon}\left(\psi(\varepsilon),\partial_x\psi(\varepsilon),\partial_x^2\psi(\varepsilon),\dots;F\left(\frac{s}{\varepsilon^2}\right),\partial_x F\left(\frac{s}{\varepsilon^2}\right),\dots\right),\end{aligned} \tag{A.10}$$

where $\Phi(\zeta)$ is linear in $\psi(\zeta)$ and bounded as a function of $\zeta$; $B_{s,\varepsilon}$ contains all the boundary terms at $\zeta=\varepsilon$ resulting from the various integrations by parts. The terms in brackets will give the asymptotic terms to order $s^{m-1}\ln s$. The next term is the remainder obtained by applying the proof of Lemma (A.1). It is readily seen that all the terms on the right hand side of (A.10), which is an exact identity, have a limit as $\varepsilon\to 0$, except perhaps for the $B_{s,\varepsilon}$ term. But the left-hand side of (A.10) also has a limit as $\varepsilon\to 0$, so that $B_{s,\varepsilon}$ does as well. In fact, although $B_{s,\varepsilon}$ is a complicated combination of many terms, many of them apparently singular as $\varepsilon\to 0$, a lengthy calculation reveals that all the singular parts cancel out nicely, so that

$$\lim_{\varepsilon\to 0} B_{s,\varepsilon}\left(\psi(\varepsilon),\dots;F\left(\frac{s}{\varepsilon^2}\right),\dots\right)=0.$$

Finally, we still obtain

$$\left|\int_0^{\infty} d\zeta\,\Phi(\zeta)\zeta^{2(m-1)}R_m\left(\frac{s}{\zeta^2}\right)\right|\leqq c\cdot\|\Phi\|_{\infty}\cdot s^{m-1/2}.$$

Thus the asymptotic expansion is proved again and the coefficients are given by (A.5) if we effect the replacements

$$\int_0^{\infty} d\zeta\,\ln\zeta\,\frac{\partial}{\partial\zeta}\left[\zeta^{2m}R_{m+1}\left(\frac{1}{\zeta^2}\right)\right]\to\lim_{\varepsilon\to 0} L_{1,\varepsilon,m}[F],$$

$$\int_0^{\infty} d\zeta\,\ln\zeta\left(\frac{\partial}{\partial\zeta}\right)^2\left[\zeta^{2m}R_{m+1}\left(\frac{1}{\zeta^2}\right)\right]\to\lim_{\varepsilon\to 0} L_{2,\varepsilon,m}[F].$$

*1. Examples*

As an illustration of some of the details of the proof above, the case $m=1$ can be worked out easily assuming the conditions (4.4). Write

$$\begin{aligned}\int_0^\infty dx F\left(\frac{s}{x^2}\right)\psi(x) &= -\int_0^\infty dx\left(\frac{\partial^2}{\partial x^2}\ln x\right)x^2\left[F_0+F_1\cdot\frac{s}{x^2}+R_2\left(\frac{s}{x^2}\right)\right]\psi(x)\\ &= -\int_0^\infty dx\ln x\partial_x^2\left[\left(x^2F_0+sF_1+x^2R_2\left(\frac{s}{x^2}\right)\right)\psi(x)\right]\\ &= F_0\int_0^\infty dx\psi(x)-s\cdot F_1\int_0^\infty dx\ln x\partial_x^2\psi(x)-\int_0^\infty dx\ln x\partial_x\\ &\quad\cdot\partial_x\left[x^2R_2\left(\frac{s}{x^2}\right)\psi(x)\right].\end{aligned}\tag{A.11}$$

The last term is now written as

$$\begin{aligned}&\int_0^\infty dx\ln x\partial_x\left[\psi(x)\partial_x\left(x^2R_2\left(\frac{s}{x^2}\right)\right)+x^2R_2\left(\frac{s}{x^2}\right)\partial_x\psi(x)\right]\\ &\quad=\psi(0)\int_0^\infty dx\ln x\partial_x^2\left[x^2R_2\left(\frac{s}{x^2}\right)\right]+\partial_x\psi(0)\int_0^\infty dx\ln x\partial_x\left[x^2R_2\left(\frac{s}{x^2}\right)\right]\\ &\quad+\int_0^\infty dx\ln x\partial_x\left[(\psi(x)-\psi(0))\partial_x\left(x^2R_2\left(\frac{s}{x^2}\right)\right)\right]\\ &\quad+\int_0^\infty dx\ln x\partial_x\left[x^2R_2\left(\frac{s}{x^2}\right)(\partial_x\psi(x)-\partial_x\psi(0))\right].\end{aligned}\tag{A.12}$$

The last two terms here can be written, after integration by parts, as

$$\begin{aligned}&-\int_0^\infty dx\frac{\psi(x)-\psi(0)}{x}\partial_x\left[R_2\left(\frac{s}{x^2}\right)x^2\right]-\int_0^\infty dx\frac{\partial_x\psi(x)-\partial_x\psi(0)}{x}x^2R_2\left(\frac{s}{x^2}\right)\\ &=\left[\frac{\psi(x)-\psi(0)}{x}x^2R_2\left(\frac{s}{x^2}\right)\right]_{x=0}+\int_0^\infty dx\left[\partial_x\frac{\psi(x)-\psi(0)}{x}-\frac{\partial_x\psi(x)-\partial_x\psi(0)}{x}\right]x^2R_2\left(\frac{s}{x^2}\right)\\ &=\partial_x\psi(0)(-F_1\cdot s)+\int_0^\infty dx\Phi(x)x^2R_2\left(\frac{s}{x^2}\right),\end{aligned}\tag{A.13}$$

where the integrated term has been evaluated and $\Phi(x)$, defined here in the obvious way, is bounded. Write the last term in (A.13) as

$$-\varrho_2(s)=\int_0^\infty dx\Phi(x)x^2R_2\left(\frac{s}{x^2}\right).$$

Then

$$|\varrho_2(s)|\leqq\|\Phi\|_\infty\int_0^\infty dx\left|x^2R_2\left(\frac{s}{x^2}\right)\right|=s^{3/2}\|\Phi\|_\infty\int_0^\infty dx\left|x^2R_2\left(\frac{1}{x^2}\right)\right|.\tag{A.14}$$

The integral in (A.14) comverges because

$$\left|x^2R_2\left(\frac{1}{x^2}\right)\right| = \left|x^2F\left(\frac{1}{x^2}\right)-x^2F_0-F_1\right| \leqq \text{const} \quad \text{as} \quad x\to 0$$

$$\leqq x^2\cdot\frac{c}{x^4}=\frac{c}{x^2} \qquad\qquad \text{as} \quad x\to\infty\,.$$

Thus there exists a $c>0$ such that $|\varrho_2(s)|\leqq c\cdot s^{3/2}\|\Phi\|_\infty$. We still need to simplity the first two terms in (A.12). We have

$$\begin{aligned}\int_0^\infty dx\ln x\partial_x^2\left[x^2R_2\left(\frac{s}{x^2}\right)\right] &= s^{1/2}\int_0^\infty dx\ln(xs^{1/2})\partial_x^2\left[x^2R_2\left(\frac{1}{x^2}\right)\right]\\ &= s^{1/2}\int_0^\infty dx\ln x\partial_x^2\left[x^2R_2\left(\frac{1}{x^2}\right)\right]+s^{1/2}\ln s^{1/2}\int_0^\infty dx\partial_x^2\left[x^2R_2\left(\frac{1}{x^2}\right)\right]\\ &= s^{1/2}L_{2,1}[F]+\frac{1}{2}s^{1/2}\ln s\,\partial_x\left[x^2F\left(\frac{1}{x^2}\right)-F_0x^2-F_1\right]\Bigg|_{x=0}^{\infty}\\ &= s^{1/2}L_{2,1}[F]+O\left(\frac{1}{x^5}\right)\Bigg|_{x=\infty}-O(x)|_{x=0}\\ &= s^{1/2}L_{2,1}[F]\,. \end{aligned} \tag{A.15}$$

[The $O(x)$ for $x\to 0$ follows from

$$\left|\partial_x x^2R_2\left(\frac{1}{x^2}\right)\right| = \left|2xF\left(\frac{1}{x^2}\right)-2xF_0+x^2\partial_xF\left(\frac{1}{x^2}\right)\right|$$

$$\leqq 2b_0x+2|F_0|x+b_1x\,,$$

where $b_0$, $b_1$ are defined in (4.4).] Similarly we find

$$\begin{aligned}\int_0^\infty dx\ln x\partial_x\left[x^2R_2\left(\frac{s}{x^2}\right)\right] &= s\int_0^\infty dx\ln x\partial_x\left[x^2R_2\left(\frac{1}{x^2}\right)\right]\\ &\quad+\frac{1}{2}s\ln s\int_0^\infty dx\partial_x\left[x^2R_2\left(\frac{1}{x^2}\right)\right]\\ &= sL_{1,1}[F]+\frac{1}{2}s\ln s\left[x^2R_2\left(\frac{1}{x^2}\right)\right]_{x=0}^{\infty}\\ &= sL_{1,1}[F]+O\left(\frac{1}{x^2}\right)\Bigg|_{x=\infty}+\frac{1}{2}s\ln s\cdot F_1\\ &= sL_{1,1}[F]+\frac{1}{2}s\ln sF_1\,. \end{aligned} \tag{A.16}$$

Substituting (A.13), (A.15), (A.16) back into (A.12) and then (A.12) into (A.11) we obtain

$$\begin{aligned}
\int_0^\infty dx F\left(\frac{s}{x^2}\right)\psi(x) &= F_0 \int_0^\infty dx\psi(x) + s\left\{-F_1 \cdot \int_0^\infty dx \ln x \partial_x^2 \psi(x) + F_1 \partial_x \psi(0)\right\} \\
&\quad - s^{1/2}\psi(0) L_{2,1}[F] + s \cdot \partial_x \psi(0) L_{1,1}[F] \\
&\quad + \frac{F_1}{2} s \ln s \partial_x \psi(0) + \varrho_2(s) \\
&= F_0 \int_0^\infty dx \psi(x) \\
&\quad + s\left\{-F_1 \int_0^\infty dx \ln x \partial_x^2 \psi(x) + F_1 \partial_x \psi(0) + \partial_x \psi(0) L_{1,1}[F]\right\} \\
&\quad - s^{1/2}\psi(0) L_{2,1}[F] + \frac{F_1}{2} \partial_x \psi(0) s \ln s + \varrho_2(s) \\
&= F_0 \langle \theta(x), \psi(x)\rangle \\
&\quad + s\langle -F_1 \partial_x^2 \theta(x) \ln z - F_1 \partial_x \delta_0 - L_{1,1}[F]\partial_x \delta_0, \psi(x)\rangle \\
&\quad + s^{1/2}\langle -L_{2,1}[F]\delta_0, \psi(x)\rangle + s \ln s \left\langle -\frac{F_1}{2}\partial_x \delta_0, \psi(x)\right\rangle \\
&\quad + \varrho_2(s)\,. 
\end{aligned} \tag{A.17}$$

Since $\varrho_2(s)$ satisfies the estimate (A.14), we have verified our asymptotic expansion to $O(s \ln s)$. It can be seen that the coefficients agree with (A.5). In particular, the coefficient of $F_1 \partial_x \delta_0$ in the $s$-asymptotic term should be, according to (A.5), $\int_0^1 dt \ln t = [t \ln t - t]_{t=0}^1 = -1$, which agrees with (A.17).

## 2. *A particular Example of Asymptotics to all Orders*

Consider the following concrete instance for $f(x,s)$:

$$f(x,s) = F\left(\frac{s}{x^2}\right) = \frac{1}{1+\frac{s}{x^2}}\,, \quad x>0\,. \tag{A.18}$$

To apply (A.5) we need to compute $F_m$ and $R_{m+1}(y)$ for each $m = 0, 1, \ldots$. Note that

$$\begin{aligned}
F(y) &= \frac{1}{1+y} = \sum_{m=0}^\infty (-1)^m y^m, \quad y \to 0 \\
&\Rightarrow F_m = (-1)^m\,.
\end{aligned}$$

The remainder after $m+1$ terms is also easy to write down:

$$R_{m+1}(y) = \frac{1}{1+y} - \sum_{k=0}^m (-1)^k y^k = \frac{1}{1+y} - \frac{y^{m+1}+1}{1+y} = -\frac{y^{m+1}}{1+y}\,.$$

Now we can evaluate $L_{1,m}$, $L_{2,m}$ defined by (A.6) and (A.7):

$$L_{1,m}\left[\frac{1}{1+y}\right] = -\int_0^\infty d\zeta \ln\zeta \frac{\partial}{\partial\zeta}\zeta^{2m}\frac{(1/\zeta^2)^{m+1}}{1+\frac{1}{\zeta^2}}$$

$$= -\int_0^\infty d\zeta \ln\zeta \frac{\partial}{\partial\zeta}\frac{1}{\zeta^2+1}$$

$$= -\int_0^\infty d\zeta \ln\zeta \frac{\partial}{\partial\zeta}\left(\frac{1}{\zeta^2+1}-1\right) = \left[-\int_0^M d\zeta \frac{\zeta^2}{\zeta^2+1} + \ln M\right]_{M=\infty}$$

$$= \left[-\frac{1}{2}\ln(M^2+1)+\ln M\right]_{M=\infty} = \left[-\ln M - \frac{1}{2}\cdot\frac{1}{M^2} + \ldots + \ln M\right]_{M=\infty} = 0.$$

On the other hand,

$$L_{2,m}\left[\frac{1}{1+y}\right] = -\int_0^\infty d\zeta \ln\zeta \frac{\partial^2}{\partial\zeta^2}\frac{1}{\zeta^2+1} = -\int_0^\infty d\zeta \ln\zeta \frac{\partial^2}{\partial\zeta^2}\left(\frac{1}{1+\zeta^2}-1\right)$$

$$= +\int_0^\infty d\zeta \frac{1}{\zeta^2}\frac{-\zeta^2}{\zeta^2+1} = -\int_0^\infty d\zeta \frac{1}{1+\zeta^2} = -\frac{\pi}{2}.$$

Finally, apart from this particular example, we note as a general result:

**Lemma (A.2).** $\int_0^1 dt \ln t(1-t)^{2m-2} = -\frac{1}{2m-1}\sum_{k=1}^{2m-1}\frac{1}{k}.$

I found that this is true by deriving Theorem (4.1) in a completely different way (see subsequent papers). It can be checked for a few small values of $m$. I have been unable to find a direct elementary proof!

We can now write down the full asymptotic expansion for (A.18):

$$\left\langle \frac{\theta(x)}{1+\frac{s}{x^2}}, \psi(x)\right\rangle \sim \langle\theta(x), \psi(x)\rangle$$

$$+\sum_{m=1}^\infty s^m\left\langle -\frac{(-1)^m}{(2m-1)!}\partial_x^{2m}\theta(x)\ln x - \frac{1}{(2m-1)!}(-1)^m\sum_{k=1}^{2m-1}\frac{1}{k}\partial_x^{2m-1}\delta_0, \psi(x)\right\rangle$$

$$+\sum_{m=1}^\infty s^{m-1/2}\left\langle\frac{1}{(2m-2)!}\frac{\pi}{2}\partial_x^{2m-2}\delta_0, \psi(x)\right\rangle$$

$$+\sum_{m=1}^\infty s^m \ln s\left\langle -\frac{1}{2}\frac{1}{(2m-1)!}(-1)^m\partial_x^{2m-1}\delta_0, \psi(x)\right\rangle.$$

By letting $s\to s\lambda$ or $s\to s\lambda^{-1}$ we can differentiate this asymptotic expansion with respect to $\lambda$ to obtain one for

$$\frac{p\left(\frac{s}{x^2}\right)}{\left(1+\frac{s}{x^2}\right)^n},$$

where $p\left(\frac{s}{x^2}\right)$ is a given polynomial of degree $\leqq n-1$.

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