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A case study of an exactly solvable heat kernel

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Abstract. The heat kernel $K(s)=\mathrm{Tr}(\mathrm{e}^{-sH(\lambda)}-\mathrm{e}^{-sH(0)})$ is determined exactly for the operator $H(\lambda)=-\partial_x^2-\lambda(\lambda+1)\,\mathrm{sech}^2\,x$. The behaviour of $K(s)$ is extracted for both large and small s. It is shown that for all $s<\infty$, $K(s)$ is a continuous function of λ although new bound states are formed when λ passes through the positive integers. This implies that the scattering states provide a discontinuous contribution to the heat kernel such that the sum of bound and scattering contributions is continuous. For small s, a general expression is derived for the coefficients K_m in the small s expansion of the heat kernel: $K(s)=\Sigma\, K_m s^{m-1/2}$. With $E_n(\lambda)$ denoting the eigenvalues of $H(\lambda)$, the spectral function $N(E)=\Sigma\,\{\Theta(E-E_n(\lambda))-\Theta(E-E_n(0))\}$ is found. It is proved for general potentials that the coefficients of the large E expansion of $N(E)$, N_m, given by $N(E)=\Sigma\, N_m E^{-(m-1/2)}$ are related to those of the small s expansion of $K(s)$ by $N_m=K_m/\Gamma(3/2-m)$ and this is demonstrated explicitly for $H(\lambda)$ given above. A discussion is given on the use of the small s expansion to reproduce $K(s)$.

1. Introduction

Consider a Hamiltonian operator $H(\lambda)$ that depends on the parameter λ. This parameter characterizes the strength of the potential appearing in the Hamiltonian. The heat kernel associated with this operator is defined in the present work to be

$$K(s)=\mathrm{Tr}(\mathrm{e}^{-sH(\lambda)}-\mathrm{e}^{-sH(0)}) \tag{1.1}$$

where Tr denotes the trace over a complete set of states. Quantities of this type appear in a number of areas of physics including gravitation and various field theory applications. The interest of the present authors lies in the fact that logarithms of functional determinants may be found once the heat kernel is known. This follows from the work of Schwinger [1] who used the following representation

$$\ln\det[H(\lambda)/H(0)]=-\int_0^\infty \mathrm{d}s/s\, K(s) \tag{1.2}$$

which is valid for operators with positive spectra. The logarithm of functional determinants appears, for example, in the free energy of condensed matter systems when fermions are explicitly integrated out of mean-field type theories (see for example [2]). In reference [2] an approach based on the work of D'yakanov *et al* [3] was used to find an approximation of the logarithm of a functional determinant ratio. The approach of D'yakanov *et al* was to approximate $\ln\det[H(\lambda)/H(0)]$ by using two different approximations to the heat kernel appearing in equation (1.2). Thus for s less than a partition point δ, a truncated small s expansion was used while for s larger than δ the

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heat kernel was approximated by its low-lying modes. In [2] the low-lying modes were, in fact, bound states and we shall refer to the low-lying modes as bound states in what follows. The partition point δ was determined in [3] by requiring the approximation to $\ln\det[H(\lambda)/H(0)]$ to be stationary under variations of δ, some further discussion of this can be found in [2]. The above procedure seems to give an accurate approximation to $\ln\det[H(\lambda)/H(0)]$ over a range of values of λ but it does seem to have one failing. When the parameter λ is varied to such an extent that the number of bound states changes, it leads to a discontinuous approximation to $\ln\det[H(\lambda)/H(0)]$. This comes about since the small s expansion of $K(s)$ depends only on the potential and its derivatives and is a smooth function of λ (if the potential is) while the large s, bound state contribution is discontinuous (reasonable choices of δ do not change the discontinuous behaviour of the approximation). Given that in a soluble problem that uses exact results for the functional determinant ratio [4], continuous behaviour in λ is found, it suggests that the discontinuity in the bound state contribution to the heat kernel may be healed by contributions from scattering states that were neglected in the approximation used.

One of the purposes of the present work is to expose the detailed way the scattering states yield a discontinuous contribution to the heat kernel—thereby compensating for the discontinuity associated with the bound states. We shall do this by investigating a problem that exhibits the above behaviour and yet is simple enough to be solved exactly. An interesting result that follows from an exact determination of the heat kernel is that a general formula for the coefficient of s^n in the small s expansion can be given.

As a warning to the mathematically knowledgeable reader, we note that the level of mathematical precision employed in the present work is that commonly practised in much of theoretical physics. We shall therefore make a number of assumptions which are not, in a strict mathematical sense, justified but which we believe to be correct. We shall furthermore freely interchange orders of summation and integration.

Sections 2, 3 and 4 of this work are concerned with defining and calculating the heat kernel for an exactly soluble problem. Section 5 looks at limiting cases of the exact result. Section 6 relates the small s expansion of the heat kernel to the high energy expansion of the spectral function (which is essentially the integrated density of states). Section 7 consists of a discussion and there are two appendices.

2. Definition of the problem

Let us define one-dimensional Schrödinger operators ($\partial_x \equiv \partial/\partial x$)

$$H(\lambda) = -\partial_x^2 - \lambda(\lambda+1)\operatorname{sech}^2 x \tag{2.1a}$$

$$H(0) = -\partial_x^2 \tag{2.1b}$$

subject to Dirichlet boundary conditions at $(-L, L)$. This corresponds to a particle being restricted to the interval $(-L, L)$ of the x axis (in following sections we shall consider the limit $L\to\infty$). We shall restrict our discussion to the range $\lambda \geqslant 0$.

We define the heat kernel associated with this problem by

$$K_L(s) = \mathrm{Tr}[\exp(-sH(\lambda)) - \exp(-sH(0))] \tag{2.2}$$

where Tr denotes the trace over a complete set of states. We note that the heat kernel $K_L(s)$ is finite because of the rapid fall-off of the potential $-\lambda(\lambda+1)\operatorname{sech}^2 x$ with x.

If the eigenvalues of $H(\lambda)$ and $H(0)$ are $E_n(\lambda)$ and $E_n(0)$ respectively, then we can write

$$K_L(s)=\sum_n [\exp(-sE_n(\lambda))-\exp(-sE_n(0))]. \tag{2.3}$$

If, for example, $\Sigma_n \exp(-sE_n(0))]$ was not finite then there is a possible ambiguity in going from (2.2) to (2.3). In this case the sum in (2.3) would change on an infinite reordering of the $\exp(-sE_n(0))$. It turns out that for finite s and L, $\Sigma_n \exp(-sE_n(0))]$ exists (the sum is calculable and may be expressed in terms of the Jacobi theta function). Presumably the corresponding sum with λ finite also exists and hence the passage from (2.2) to (2.3) is unambiguous.

In order to calculate $K_L(s)$ let us introduce the spectral function $N_L(E)$ defined in terms of the eigenvalues of $H(\lambda)$ and $H(0)$ by

$$N_L(E)=\sum_n \{\Theta(E-E_n(\lambda))-\Theta(E-E_n(0))\} \tag{2.4}$$

where Θ is the Heaviside step function:

$$\begin{aligned}\Theta(x)&=1, && x>0\\ &=\tfrac{1}{2} && x=0\\ &=0 && x<0.\end{aligned} \tag{2.5}$$

The potential in (2.1a) results in the eigenvalues of $H(\lambda)$ moving relative to those of $H(0)$ but not in their creation or destruction. In particular, it drags down one or more eigenvalues below $E=0$. At energies more negative than the lowest of these, corresponding to the ground state of $H(\lambda)$, $N_L(E)$ vanishes sharply. This allows us to perform an integration by parts and write

$$K_L(s)=\int \mathrm{d}E\, sN_L(E)\,\mathrm{e}^{-sE}. \tag{2.6}$$

It thus remains to find a convenient form for $N_L(E)$.

3. Determination of the spectral function $N(E)$ in the limit $L\to\infty$

The spectral function $N_L(E)$ can be determined from knowledge of the functional determinant

$$D_L(z)=\det[(H(\lambda)-z)(H(0)-z)^{-1}]. \tag{3.1}$$

The subscript L on D reminds us that Dirichlet boundary conditions are imposed on the eigenfunctions at $\pm L$; for finite L the spectra of $H(\lambda)$ and $H(0)$ are discrete. In terms of the eigenvalues, we take the definition of the determinant as

$$D_L(z)=\prod_n \frac{(E_n(\lambda)-z)}{(E_n(0)-z)} \tag{3.2}$$

assuming the product is convergent.

Noting that

$$\lim_{\delta\to 0+} \operatorname{Im}\ln(E_n-E+\mathrm{i}\delta)=\pi\Theta(E-E_n) \tag{3.3}$$

(with $\Theta(x)$ as defined in (2.5)) allows us to write

$$N_L(E) = \lim_{\delta\to 0+} \frac{1}{\pi} \operatorname{Im} \ln D_L(E - \mathrm{i}\delta). \tag{3.4}$$

As is often the case, the simplest results are obtained in the limit $L\to\infty$. The limit is slightly subtle in that the limits $L\to\infty$ and $\delta\to 0$ do not commute. The conventional treatment (see for example section 49 of the textbook by Gottfried [5]) is to define the appropriate quantity by taking first the limit $L\to\infty$ and then allowing δ to tend to zero. Thus we define

$$N(E) = \lim_{\delta\to 0+} \lim_{L\to\infty} \frac{1}{\pi} \operatorname{Im} \ln D_L(E - \mathrm{i}\delta). \tag{3.5}$$

The result of taking this order of limits is that $N(E)$ is, in general, no longer an integer valued function of E. For negative energies (where the bound states contribute) it is integer valued, however for positive energies (scattering states) it is a continuous function of E. Our understanding is that keeping δ finite during the 'infinite volume' limit $L\to\infty$ implements an averaging over the scattering states resulting in a continuous spectral function, $N(E)$. The function

$$D(z) = \lim_{L\to\infty} D_L(z) \qquad z \text{ a general complex number} \tag{3.6}$$

for the operator of (2.1) is well known in the literature (in appendix C of [4] a derivation is given, using a theorem from scattering theory that directly relates the transmission amplitude to the functional determinant ratio, (3.1)). It is given by

$$\begin{aligned} D(z) &= \frac{\Gamma(1+\sqrt{-z})\Gamma(\sqrt{-z})}{\Gamma(1+\lambda+\sqrt{-z})\Gamma(\sqrt{-z}-\lambda)} \\ &\equiv \frac{1}{\sqrt{-z}} \frac{\{\Gamma(1+\sqrt{-z})\}^2}{\Gamma(1+\lambda+\sqrt{-z})\Gamma(\sqrt{-z}-\lambda)} \end{aligned} \tag{3.7}$$

where the square roots are cut along the negative real axis and the branch selected is such that $\sqrt{w}$ is positive when w is real and positive. Thus we obtain $N(E)$ from (3.5) by making the replacement of z by $E - \mathrm{i}\delta$ and taking the limit $\delta\to 0+$.

Proceeding with the calculation (the limit $\delta\to 0+$ being implicit in what follows) we write

$$N(E) = N_1 + N_2 + N_3 + N_4 \tag{3.8a}$$

where

$$N_1 = -\frac{1}{\pi} \operatorname{Im} \ln[\sqrt{-E+\mathrm{i}\delta}] \tag{3.8b}$$

$$N_2 = \frac{2}{\pi} \operatorname{Im} \ln \Gamma(1+\sqrt{-E+\mathrm{i}\delta}) \tag{3.8c}$$

$$N_3 = -\frac{1}{\pi} \operatorname{Im} \ln \Gamma(1+\lambda+\sqrt{-E+\mathrm{i}\delta}) \tag{3.8d}$$

$$N_4 = -\frac{1}{\pi} \operatorname{Im} \ln \Gamma(\sqrt{-E+\mathrm{i}\delta}-\lambda). \tag{3.8e}$$

We can write N_1 in the form

$$\frac{-1}{\pi}\tan^{-1}\left(\frac{\sqrt{E^2+\delta^2}+E}{\sqrt{E^2+\delta^2}-E}\right)^{1/2}$$

and this is recognizable, in the limit where δ tends to zero, as

$$N_1=-\tfrac{1}{2}\Theta(E). \tag{3.9}$$

For N_2, N_3 and N_4 let us distinguish their contributions for positive and negative E.

(a) Negative E

N_2 and N_3 may be seen to make no contribution to N. Using the recursion relation of the gamma function we can rewrite N_4 as

$$N_4=-\frac{1}{\pi}\,\mathrm{Im}\ln\Gamma(\sqrt{-E+\mathrm{i}\delta}+[\lambda]-\lambda+1)+\frac{1}{\pi}\,\mathrm{Im}\sum_{n=0}^{[\lambda]}\ln\{\sqrt{-E+\mathrm{i}\delta}-\lambda+n\}. \tag{3.10}$$

It may be quickly verified that for negative E only the sum in this equation makes a contribution which is

$$N_4=\sum_{n=0}^{[\lambda]}\Theta(E+(\lambda-n)^2). \tag{3.11a}$$

This is the bound state contribution to $N(E)$, the bound states lying at energies

$$E_n=-(\lambda-n)^2 \qquad n=0,1,\ldots,[\lambda]. \tag{3.11b}$$

There are $[\lambda]+1$ bound states and as λ passes through the positive integers, $[\lambda]$ jumps discontinuously, signalling the formation of new bound states.

(b) Positive E

For positive E we can replace $\sqrt{-E+\mathrm{i}\delta}$ by $\mathrm{i}\sqrt{E}$. Using the standard result [6] in which ψ is the digamma function

$$\mathrm{Im}\ln\Gamma(x+\mathrm{i}y)=y\psi(x)+\sum_{n=0}^{\infty}[y/(x+n)-\tan^{-1}[y/(x+n)]] \tag{3.12}$$

we can write for positive E

$$\begin{aligned}N_2+N_3+N_4={}&([\lambda]+1)+\frac{\sqrt{E}}{\pi}\left[2\psi(1)-\psi(1+\lambda)-\psi(-\lambda)\right.\\&\left.+\sum_{n=0}^{\infty}\left(\frac{2}{1+n}-\frac{1}{1+\lambda+n}-\frac{1}{-\lambda+n}\right)\right]\\&-\frac{1}{\pi}\sum_{n=0}^{\infty}\left\{2\tan^{-1}\left(\frac{\sqrt{E}}{1+n}\right)-\tan^{-1}\left(\frac{\sqrt{E}}{1+\lambda+n}\right)\right.\\&\left.-\tan^{-1}\left(\frac{\sqrt{E}}{-\lambda+n}\right)\right\}.\end{aligned} \tag{3.13}$$

It may be shown, using the properties of the digamma function that the coefficient of $\sqrt{E}$ on the RHS of this equation vanishes identically.

(c) General E

Putting the above results for positive and negative E together, we can write, for general E,

$$N(E)=\sum_{n=0}^{[\lambda]}\Theta(E+(\lambda-n)^2)-\tfrac{1}{2}\Theta(E)-\frac{\Theta(E)}{\pi}\times\sum_{n=0}^{\infty}\left\{2\tan^{-1}\left(\frac{\sqrt{E}}{1+n}\right)-\tan^{-1}\left(\frac{\sqrt{E}}{1+\lambda+n}\right)-\tan^{-1}\left(\frac{\sqrt{E}}{-\lambda+n}\right)\right\}. \tag{3.14}$$

Note that an alternative way of writing $N(E)$ follows from using

$$\tan^{-1}(a/b)=\pi/2\,\mathrm{sgn}(a/b)-\tan^{-1}(b/a). \tag{3.15}$$

It quickly follows that we can write

$$N(E)=\sum_{n=0}^{[\lambda]}\Theta(E+(\lambda-n)^2)-\Theta(E)([\lambda]+1)-\tfrac{1}{2}\Theta(E)+\frac{\Theta(E)}{\pi}\times\sum_{n=1}^{\infty}\left\{2\tan^{-1}\left(\frac{n}{\sqrt{E}}\right)-\tan^{-1}\left(\frac{(n+\lambda)}{\sqrt{E}}\right)-\tan^{-1}\left(\frac{(n-1-\lambda)}{\sqrt{E}}\right)\right\}. \tag{3.16}$$

When $N(E)$ is written in this form, the Euler–Maclaurin summation formula may be applied to obtain a high-energy expansion. In appendix 1, we derive the leading terms in the high-energy expansion of $N(E)$. Here we simply note that for $E\to\infty$, $N(E)$ vanishes (as $E^{-1/2}$).

4. Calculation of the heat kernel

We shall now calculate the heat kernel given by (2.6) in the limit $L\to\infty$. We assume that this follows from the sequence of limits used in (3.5), thus we take

$$K(s)=\int \mathrm{d}E\, sN(E)\,\mathrm{e}^{-sE} \tag{4.1}$$

with the spectral function $N(E)$ given by (3.14). To evaluate the heat kernel we use the following result (a derivation of this is given in appendix 2)

$$\int_0^\infty \mathrm{d}E\, s\,\mathrm{e}^{-sE}\tan^{-1}\left(\frac{\sqrt{E}}{a}\right)=\sqrt{\pi}\,\mathrm{sgn}(a)\int_0^\infty \mathrm{d}u\,\exp[-u^2-2u\sqrt{s}|a|]. \tag{4.2}$$

Thus

$$K(s)=\sum_{n=0}^{[\lambda]}\mathrm{e}^{s(\lambda-n)^2}-\tfrac{1}{2}-\frac{1}{\sqrt{\pi}}\sum_{n=0}^{\infty}\int_0^\infty \mathrm{d}u\,\exp(-u^2)\{2\exp[-2u\sqrt{s}(n+1)]-\exp[-2u\sqrt{s}(n+\lambda+1)]-\mathrm{sgn}(n-\lambda)\exp[-2u\sqrt{s}|n-\lambda|]\}. \tag{4.3}$$

It is possible to simplify this expression by using the identity

$$\mathrm{sgn}(n-\lambda)\exp[-2u\sqrt{s}|n-\lambda|]\equiv-\{\exp[2u\sqrt{s}(n-\lambda)]+\exp[-2u\sqrt{s}(n-\lambda)]\}\Theta(n-\lambda)+\exp[-2u\sqrt{s}(n-\lambda)]. \tag{4.4}$$

Using this identity in equation (4.3), it is straightforward to show that the terms of (4.4) multiplied by the step function cancel, after the integration in (4.3), with the bound state contributions from the leading sum in (4.3) leaving

$$K(s)=-\frac{1}{2}-\frac{1}{\sqrt{\pi}}\sum_{n=0}^{\infty}\int_0^{\infty}du\,\exp(-u^2)\{2\exp[-2u\sqrt{s}(n+1)]$$
$$-\exp[-2u\sqrt{s}(n+\lambda+1)]-\exp[-2u\sqrt{s}(n-\lambda)]\}. \quad (4.5)$$

Finally the sum may be carried out and we obtain, after a few simple manipulations, the following exact integral representation for the heat kernel which contains the explicit s and λ dependence

$$K(s)=\frac{2}{\sqrt{\pi}}\int_0^{\infty}du\,e^{-u^2}\frac{\sinh[u\sqrt{s}\lambda]\sinh[u\sqrt{s}(\lambda+1)]}{\sinh[u\sqrt{s}]}. \quad (4.6)$$

We shall make use of this exact result in later sections.

For future reference let us note that if λ equals an integer, say m, the heat kernel can be obtained in terms of a finite sum of known functions. To see this we use the identity

$$\frac{\sinh[u\sqrt{s}m]\sinh[u\sqrt{s}(m+1)]}{\sinh[u\sqrt{s}]}\equiv\sum_{n=0}^{m-1}\sinh[2u\sqrt{s}(m-n)] \quad (4.7)$$

and use the following integral involving the complementary error function erfc(z) [6]

$$\frac{2}{\sqrt{\pi}}\int_0^{\infty}du\,\exp[-u^{-2}-2uz]=\exp[z^2]\,\mathrm{erfc}(z) \quad (4.8)$$

to obtain

$$K(s)=\sum_{n=0}^{m-1}e^{s(m-n)^2}\tfrac{1}{2}(\mathrm{erfc}[-\sqrt{s}(m-n)]-\mathrm{erfc}[\sqrt{s}(m-n)]) \qquad (\lambda \text{ is an integer, } m). \quad (4.9)$$

5. Limiting behaviour of the heat kernel

Let us investigate the behaviour of the heat kernel as a function of λ in the limit where s is either large or small compared with unity.

(a) Large s

To obtain the large s limit we use

$$\frac{1}{\sinh[u\sqrt{s}]}=2\sum_{n=0}^{\infty}\exp[-(2n+1)u\sqrt{s}]. \quad (5.1)$$

Next we replace the sinh's appearing in the numerator of (4.6) by their definition in terms of exponentials. We obtain

$$K(s)=\tfrac{1}{2}\sum_{n=0}^{\infty}\{\exp[(n-\lambda)^2s]\,\mathrm{erfc}((n-\lambda)\sqrt{s})-\exp[(n+1)^2s]\,\mathrm{erfc}((n+1)\sqrt{s})$$
$$-\exp[n^2s]\,\mathrm{erfc}(n\sqrt{s})+\exp[(n+\lambda)^2s]\,\mathrm{erfc}((n+\lambda)\sqrt{s})\}. \quad (5.2)$$

Then in terms of ν, the deviation of λ from an integer

$$\nu=\lambda-[\lambda] \qquad \nu\in[0,1] \tag{5.3}$$

we find we can write

$$K(s)=\sum_{n=0}^{[\lambda]-1} e^{s(n-\lambda)^2}\tfrac{1}{2}\operatorname{erfc}(-\sqrt{s}(\lambda-n))+\tfrac{1}{2}e^{s\nu^2}\operatorname{erfc}(-\sqrt{s}\,\nu)$$
$$+\tfrac{1}{2}e^{s(1-\nu)^2}\operatorname{erfc}[\sqrt{s}(1-\nu)]-\tfrac{1}{2}+O(s^{-1/2}) \tag{5.4a}$$

where a sum over the leading term in the asymptotic expansion of the error functions with large arguments in (5.2) has led to the $O(s^{-1/2})$ corrections in this equation. We note that within the sum in (5.4a), all terms have $\sqrt{s}(\lambda-n)\gg 1$, so we can replace the erfc by 2 (and generate additional $O(s^{-1/2})$ corrections to $K(s)$):

$$K(s)=\sum_{n=0}^{[\lambda]-1} e^{s(n-\lambda)^2}+\tfrac{1}{2}e^{s\nu^2}\operatorname{erfc}(-\sqrt{s}\,\nu)$$
$$+\tfrac{1}{2}e^{s(1-\nu)^2}\operatorname{erfc}[\sqrt{s}(1-\nu)]-\tfrac{1}{2}+O(s^{-1/2}). \tag{5.4b}$$

It is evident from (4.6) that $K(s)$ is a continuous function of λ however from (5.4b) it follows that $K(s)$ takes two different forms depending on how far λ is from an integer (we recall that every time λ passes through an integer from below a new bound state is formed).

(i) provided λ does not lie within $O(s^{-1/2})$ of an integer, i.e.

$$\nu\gg 1/\sqrt{s} \qquad (1-\nu)\gg 1/\sqrt{s} \tag{5.5}$$

we may approximate the erfcs in the second and third terms by 2 and zero respectively (with the generation of additional $O(s^{-1/2})$ corrections). This leaves contributions only from bound states and the scattering states at the edge of the continuum:

$$K(s)=\sum_{n=0}^{[\lambda]} e^{s(n-\lambda)^2}-\tfrac{1}{2}+O(s^{-1/2}) \qquad \nu,1-\nu\gg s^{-1/2}. \tag{5.6}$$

(ii) If λ lies within $O(s^{-1/2})$ of an integer, say m, then it is straightforward to show that irrespective of whether λ is larger or smaller than m, we have

$$K(s)=\sum_{n=0}^{m-1} e^{s(n-\lambda)^2}+e^{s(\lambda-m)^2}\tfrac{1}{2}\operatorname{erfc}(-\sqrt{s}(\lambda-m))-\tfrac{1}{2}+O(s^{-1/2}). \tag{5.7}$$

(This should be compared with the exact result, given in equation (4.9) for all s.) Given that all quantities in (5.7) are, to $O(s^{-1/2})$, continuous functions of λ we recover a heat kernel that is continuous function of λ (to this order). With additional work one can shown, order by order, that $K(s)$ is continuous but this is obvious from equation (4.6) already. Note that we have continuity even when λ passes through an integer and the number of bound states changes. Thus when λ goes from just below to just above the integer m, a new bound state is formed and the bound state contribution to $K(s)$ is discontinuous. The only way a continuous variation of $K(s)$ can occur is by a discontinuous rearrangement of the scattering states that screens or compensates the effect of the number of bound states changing. We can explicitly compute the discontinuity in the scattering contribution by defining the scattering part of the heat kernel as

$$K_{sc}(s)\equiv K(s)-\sum_{n=0}^{[\lambda]} e^{s(n-\lambda)^2} \tag{5.8}$$

the sum on the right-hand side being the bound state contribution. It follows from continuity of $K(s)$ that for all s,

$$K_{sc}(s)|_{\lambda=m+} - K_{sc}(s)|_{\lambda=m-} = -1. \tag{5.9}$$

(b) Small s

To obtain the small s limit we use [6]

$$\frac{1}{\sinh(u\sqrt{s})} = -2\sum_{n=0}^{\infty} s^{n-1/2}u^{2n-1}\frac{(2^{2n-1}-1)}{(2n)!}B_{2n} \tag{5.10}$$

where B_n are the Bernoulli numbers. Furthermore we write the sinh product of appearing in (4.6) for the heat kernel as a difference of two cosh terms which we also expand about zero argument. We obtain, on evaluating the u integral

$$K(s) = -\frac{1}{\sqrt{\pi}}\sum_{n=1}^{\infty}\sum_{m=0}^{\infty} s^{n+m-1/2}[(2\lambda+1)^{2n}-1]\frac{(2^{2m-1}-1)B_{2m}\Gamma(m+n)}{(2n)!(2m)!}. \tag{5.11}$$

Writing

$$K(s) = \sum_{n=1}^{\infty} K_n s^{n-1/2} \tag{5.12}$$

and expressing the Bernoulli numbers in terms of the Riemann zeta function

$$B_{2m} = \frac{(-1)^{m-1}2(2m)!\zeta(2m)}{(2\pi)^{2m}} \tag{5.13}$$

we obtain the general expression for the expansion coefficients K_n

$$K_n = \frac{2\Gamma(n)}{\sqrt{\pi}}\sum_{m=0}^{n-1}(-1)^m\frac{(2^{2m-1}-1)[(2\lambda+1)^{2(n-m)}-1]\zeta(2m)}{[2(n-m)]!(2\pi)^{2m}}. \tag{5.14}$$

Up to a normalization convention, the expansion of (5.12) is termed the Minakshisundarem-Seeley expansion [7] or the Schwinger-De-Witt expansion [8]. We shall refer to the coefficients K_n as the MS coefficients. Let us note that the quantity in the square brackets in (5.14) can be written in terms of the strength of the potential V_0 defined by

$$V_0 = -\lambda(\lambda+1) \tag{5.15}$$

as

$$[(2\lambda+1)^{2(n-m)}-1] \equiv [(1-4V_0)^{n-m}-1]. \tag{5.16}$$

This last form makes it obvious that K_n is a polynomial of degree n in V_0, a fact not immediately obvious from the exact result of (4.6).

6. Relation of the small *s* expansion of the heat kernel to the high energy expansion of the spectral function

In section 3 of this work we derived an expression for the spectral function $N(E)$. By virtue of (4.1) there is an intimate relation between the heat kernel and the spectral function. We note that the heat kernel is closely related to the partition function of statistical physics. It is clear that the parameter s plays the role of an inverse temperature, thus small s correspond to high temperatures and hence high energies. It therefore follows that the small s expansion of the heat kernel is related to a high-energy expansion of the spectral function [9]. In this section we shall, for completeness, use 'physicists methods' to make explicit the connection of the higher terms of the small s expansion of the heat kernel and the high-energy expansion of the spectral function. Let us note that we do not prove that the resulting series is genuinely asymptotic to the heat kernel. A recent more rigorous analysis is contained in [10].

Before we give a proof of the result for general potentials, let us look at the relation between the small s expansion of $K(s)$ and the large E expansion of $N(E)$. From equations (5.12) and (5.14) we have

$$K(s)=\sum_{n=1}^{\infty} K_n s^{(n-1/2)} \tag{6.1a}$$

$$K_1=\frac{1}{\sqrt{\pi}}\lambda(\lambda+1) \tag{6.1b}$$

$$K_2=\frac{1}{\sqrt{\pi}}\tfrac{1}{3}[\lambda(\lambda+1)]^2 \tag{6.1c}$$

$$K_3=\frac{1}{\sqrt{\pi}}\tfrac{2}{45}[2\{\lambda(\lambda+1)\}^3-\{\lambda(\lambda+1)\}^2] \tag{6.1d}$$

whereas from the results of appendix 1, we have

$$N(E)=\sum_{n=1}^{\infty} N_n E^{-(n-1/2)} \tag{6.2a}$$

$$N_1=\frac{1}{\pi}\lambda(\lambda+1) \tag{6.2b}$$

$$N_2=-\frac{1}{6\pi}[\lambda(\lambda+1)]^2 \tag{6.2c}$$

$$N_3=\frac{1}{30\pi}[2\{\lambda(\lambda+1)\}^3-\{\lambda(\lambda+1)\}^2]. \tag{6.2d}$$

An inspection of equations (6.1) and (6.2) indicates that, at least as far as the leading coefficients are concerned, the coefficients K_n and N_n differ only by a factor that depends on n which is given by

$$N_n=\frac{K_n}{\Gamma(\frac{3}{2}-n)}. \tag{6.3}$$

In the proof of this for general n and for a reasonably general class of potentials we shall use similar notation to the previous sections, with the exception that the operators are denoted by H and H_0 and their eigenvalues are E_n and E_{n_0}, respectively. We shall also implicitly use the sequence of limits for L and δ used in section 3. The proof is as follows.

Using equation (3.4) we can write

$$\begin{aligned}N(E)&\equiv\sum\{\Theta(E-E_n)-\Theta(E-E_{n0})\}\\&=-\frac{1}{\pi}\operatorname{Im}\operatorname{Tr}\{\ln[(H-(E+\mathrm{i}\delta)]-\ln[(H_0-(E+\mathrm{i}\delta)]\}.\end{aligned} \tag{6.4}$$

In terms of

$$G(z)=[H-z]^{-1} \qquad G_0(z)=[H_0-z]^{-1} \tag{6.5}$$

we have

$$N(E)=-\frac{1}{\pi}\,\mathrm{Im}\,\mathrm{Tr}[\ln G(E+\mathrm{i}\delta)-\ln G_0(E+\mathrm{i}\delta)]. \tag{6.6}$$

It is convenient, at this point, to introduce the function

$$C(-m^2)=-\mathrm{Tr}[\ln G(-m^2)-\ln G_0(-m^2)]. \tag{6.7}$$

On the assumption that both H and H_0 have positive spectra, as can be arranged by a common additive shift of all their energy levels (we always assume that the spectra of H and H_0 are bounded from below), we can use the 'Schwinger representation' of the logarithm given in equation (1.2) and write

$$\begin{aligned} C(-m^2)&=\mathrm{Tr}\int_0^\infty \frac{\mathrm{d}s}{s}\{\exp[-s(m^2+H)]-\exp[-s(m^2+H_0)]\} \\ &=\int_0^\infty \frac{\mathrm{d}s}{s}\,\mathrm{e}^{-sm^2}\,\mathrm{Tr}[\exp(-sH)-\exp(-sH_0)] \\ &\equiv\int_0^\infty \frac{\mathrm{d}s}{s}\,\mathrm{e}^{-sm^2}K(s). \end{aligned} \tag{6.8}$$

Then given

$$K(s)=\sum_{n=1}^{\infty} K_n s^{(n-1/2)} \tag{6.9}$$

we find

$$C(-m^2)=\sum_{n=1}^{\infty}\frac{\Gamma(n-\frac{1}{2})K}{(m^2)^{(n-1/2)}}K_n. \tag{6.10}$$

By analytic continuation

$$C(z)=\sum_{n=1}^{\infty}\frac{\Gamma(n-\frac{1}{2})}{(\sqrt{-z})^{(2n-1)}}K_n \tag{6.11}$$

(the square root is cut along the negative real axis and is positive on the positive real axis). It then follows from equations (6.6) and (6.7) that

$$\begin{aligned} N(E)&=\frac{1}{\pi}\,\mathrm{Im}\,C(E+\mathrm{i}\delta) \\ &=\frac{1}{\pi}\sum_{n=1}^{\infty}(-1)^{n+1}\frac{\Gamma(n-\frac{1}{2})}{E^{(n-1/2)}}K_n. \end{aligned} \tag{6.12}$$

Lastly, we use the standard result [6]

$$\Gamma(x)\Gamma(1-x)=\frac{\pi}{\sin(\pi x)} \tag{6.13}$$

with $x = n - \frac{1}{2}$, yielding the high-energy expansion of $N(E)$ in terms of the MS coefficients of $K(s)$:

$$N(E) = \sum_{n=1}^{\infty} \frac{K_n}{\Gamma(\frac{3}{2} - n)} E^{-(n-1/2)}. \tag{6.14}$$

Note that we have proved this result for operators with positive spectra. However the MS coefficients, K_n, depend only on integrals of various powers of the potential $H - H_0$ and its derivatives and these may be analytically continued to operators having spectra beginning at a finite negative energy.

The result (6.14) depends on the small s expansion of $K(s)$ having only half odd integral powers of s (equation (6.9)). This holds for non-singular potentials which are infinitely differentiable. An example where it does not hold is for delta function potentials which yield both half integer and integer powers of s.

7. Discussion

In this work we have exactly evaluated the heat kernel for a particular, one-dimensional, Schrödinger operator. This exact result has provided an explicit example of the discontinuous rearrangement of the scattering states when the number of bound states changes. Equation (5.9) gives the discontinuity of the scattering part of the heat kernel, it yields, for all s,

$$K_{sc}(s)|_{\lambda=m_+} - K_{sc}(s)|_{\lambda=m_-} = -1. \tag{7.1}$$

In the limit $s \to 0_+$ the left-hand side of this equation measures the change in the number of scattering states when the number of bound states increases from m to $(m+1)$. It is thus an example of the conversion of scattering states into bound states (cf Levinsons theorem).

The result of the explicit evaluation of the MS coefficients in the small s expansion of the heat kernel, equation (5.14) deserves further comment. Ordinarily, one is not in the fortunate position of having knowledge of all the MS coefficients of a heat kernel. The principal reason is that in a general problem, their complexity increases rapidly with order and their calculation becomes increasingly time consuming. It is interesting to see whether the effort of calculating a large number of MS terms is justified. In the present section we shall investigate the ability of the MS expansion to reproduce the large s (predominantly bound state) behaviour of the heat kernel. We do this from the naive approach of simply summing a finite, number of terms of the MS series. In view of the asymptotic nature of the expansion (cf comments in section 5) it makes no sense to sum an arbitrarily large number of terms. Rather, the procedure is to truncate the expansion at an appropriate point.

7.1. Heat kernel as a function of s at fixed λ

We shall, for simplicity, consider the heat kernel as a function of s when λ is held fixed. We consider non-integral values of λ since exceptional behaviour occurs at the integers. We take λ to have the values $\lambda = 1.2$ and $\lambda = 2.7$. In order to see the ability of the MS expansion to reproduce the large s part of the heat kernel we provide a number of plots. In figure 1(a) and 1(b) the crude large s approximation of (5.6) is presented along with a small s expansion, (5.12), in which 10 terms have been included.

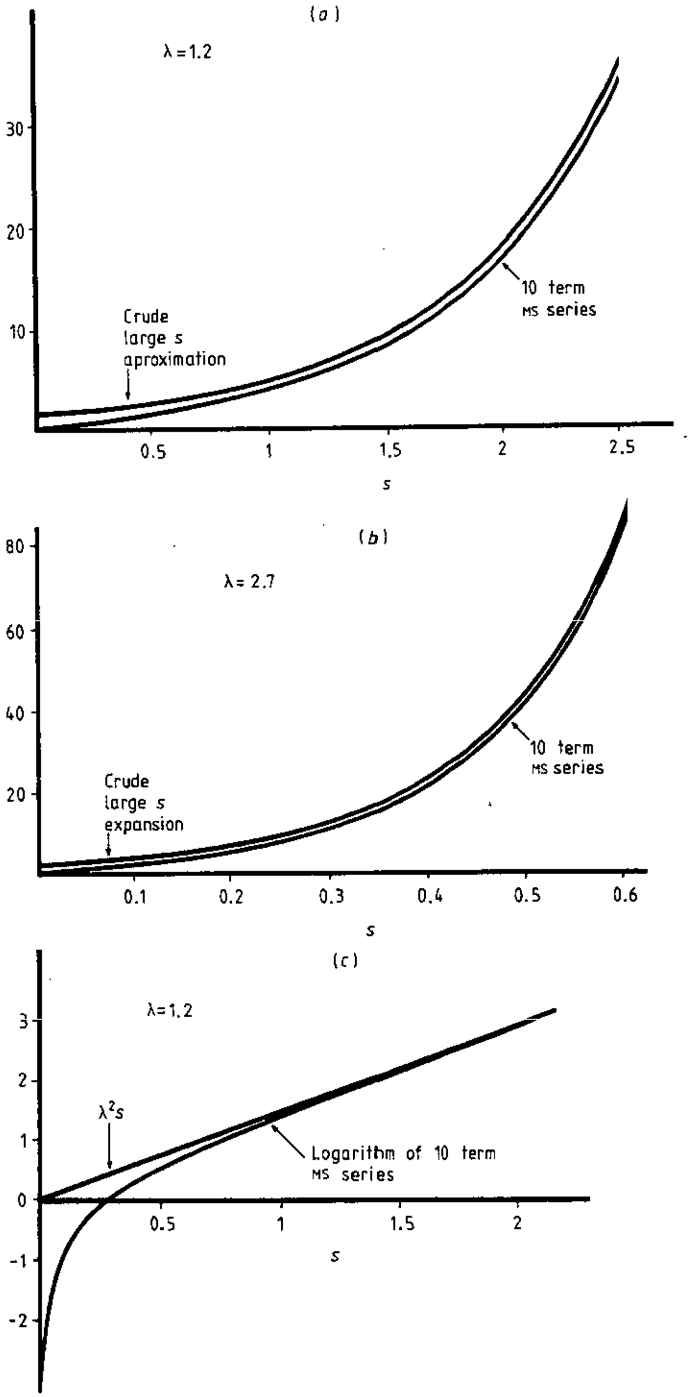

Figure 1. Heat kernel as a function of s at fixed λ. Plots of the crude large s expansion to the heat kernel $\Sigma_{n=0}^{[\lambda]} \mathrm{e}^{s(n-\lambda)^2} - \frac{1}{2}$ and the 10-term MS expansion $\Sigma_{n=1}^{10} K_n s^{(n-1/2)}$: ($a$) for $\lambda = 1.2$; (b) for $\lambda = 2.7$. (c) Logarithm of the heat kernel as a function of s at fixed λ. Plots of the logarithm of the 10-term MS expansion and the lowest bound state contribution to this quantity, $\lambda^2 s$ for $\lambda = 1.2$.

This number of terms is before the point in the asymptotic expansion where successive terms start increasing. In figure (1*c*) we plot the logarithm of the above small *s* approximation to the heat kernel for $\lambda=1.2$ along with the straight line $\lambda^2 s$; at sufficiently large *s* we know $K(s)\sim e^{s\lambda^2}$ and thus the logarithm should become approximately linear in *s*. The figures show that at fixed λ there is a very strong overlap between the truncated MS series and the large *s* behaviour of the heat kernel.

7.2. *Heat kernel as a function of λ at fixed s*

Let us now consider the behaviour of the heat kernel as a function of λ at large values of *s*. We note that the MS series is an expansion in powers of *s*. Consequently, on varying λ when the number of terms (and *s*) is held fixed may lead to spurious behaviour. This follows since different values of λ may require different numbers of

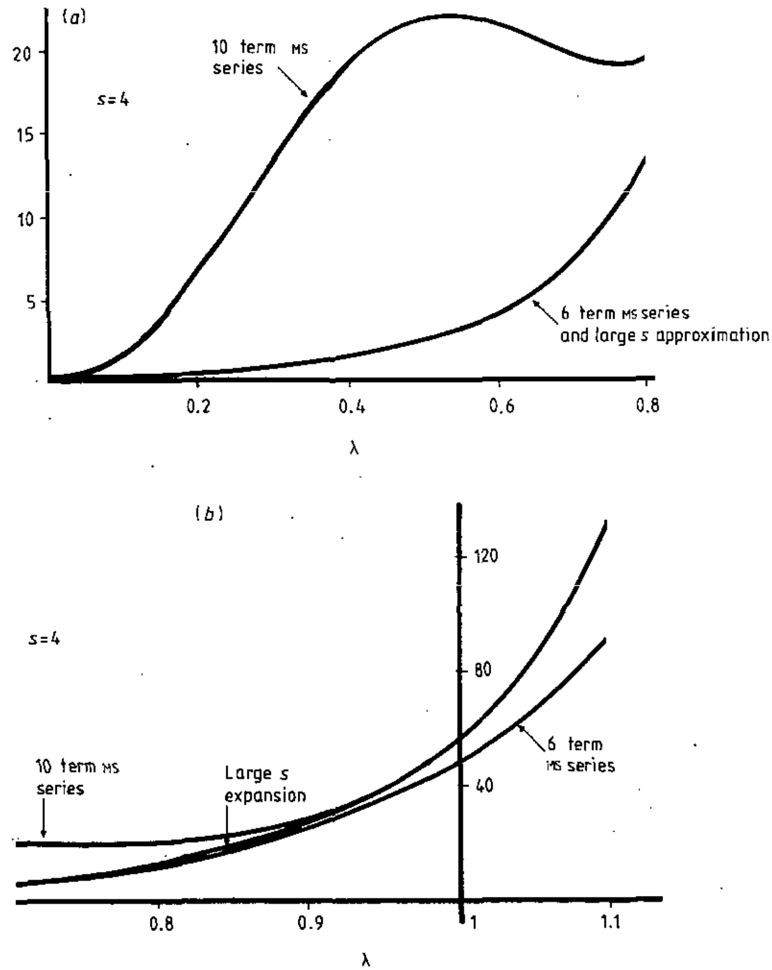

Figure 2. Heat kernel as a function of λ at fixed *s*. A plot of the large *s* expansion to the heat kernel given in equation (5.4) alongside 6 and 10 term MS expansions for $s=4$. The 6 term MS expansion and the large *s* approximation are indistinguishable (on the scale used) in the region $\lambda=0$ to $\lambda=0.8$. The peak in the 10 term MS expansion around $\lambda=\frac{1}{2}$ is a spurious feature caused by the inclusion of too many terms in the MS expansion near this value of λ.

terms in the asymptotic series for an accurate approximation of the heat kernel. We illustrate this for a reasonably large value of s, namely $s=4$. In figures 2(a) and 2(b) we plot the large s approximation to $K(s)$ given in (5.4) and two differently truncated MS approximations, (5.12), in which 6 and 10 terms have been included. The peak in figure 2(a) (at about $\lambda \sim 0.5$) that arises from the MS expansion with 10 terms is clearly a spurious feature that follows from the inclusion of too many terms in the expansion (in this region of λ values). By contrast in figure 2(b) the 10-term series matches smoothly onto the large s approximation for $\lambda \sim 1$ whereas the 6-term series begins to drop off in this region.

It appears then, that with suitable care, the MS expansion of the heat kernel can yield not only information about the small s behaviour but also a significant amount of information about the large s, predominantly bound state, behaviour.

Acknowledgments

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Appendix 1. High energy expansion of the spectral function $N(E)$

In this appendix we perform a high energy expansion of the spectral function $N(E)$ given in equation (3.16).

For $E>0$, equation (3.16) reads

$$N(E>0)=-\tfrac{1}{2}+\frac{1}{\pi}\sum_{n=1}^{\infty}[2\tan^{-1}(n\sqrt{E})-\tan^{-1}((n+\lambda)/\sqrt{E}) -\tan^{-1}((n-1-\lambda)/\sqrt{E})] \tag{A1.1}$$

Using the Euler-Maclaurin summation formula [6], we can write

$$N(E>0)=-\tfrac{1}{2}+\frac{(\sqrt{E})}{\pi}\int_0^{\infty}\mathrm{d}u\, f(u)-\frac{1}{2\pi}f(0)-\frac{1}{(12\pi\sqrt{E})}f'(0) +\frac{1}{(720\pi E^{3/2})}f'''(0)+\ldots \tag{A1.2}$$

where a prime denotes differentiation with respect to argument and

$$f(u)=2\tan^{-1}(u)-\tan^{-1}(u+\lambda/\sqrt{E})-\tan^{-1}(u-(1+\lambda)/\sqrt{E}). \tag{A1.3}$$

If we define

$$I(x)=\int_0^{\infty}\mathrm{d}u[\tan^{-1}u-\tan^{-1}(u+x)] =-(\pi/2)x+(x^2/2-x^4/12+x^6/30-\ldots) \tag{A1.4}$$

we can write

$$N(E>0)=-\tfrac{1}{2}+\frac{(\sqrt{E})}{\pi}\{I(\lambda/\sqrt{E})+I(-(1+\lambda)/\sqrt{E})\} -\frac{1}{(2\pi)}f(0)-\frac{1}{(12\pi\sqrt{E})}f'(0)+\frac{1}{(720\pi E^{3/2})}f'''(0)+\ldots \tag{A1.5}$$

The large E expansion of $N(E)$ now follows by expanding all terms in this equation in powers of $1/\sqrt{E}$ up to a given order. We find

$$N(E>0)=\frac{1}{\pi}\lambda(\lambda+1)E^{-1/2}-\frac{1}{6\pi}[\lambda(\lambda+1)]^2E^{-3/2}$$
$$+\frac{1}{30\pi}\{2[\lambda(\lambda+1)]^3-[\lambda(\lambda+1)]^2\}E^{-5/2}+\mathrm{O}(E^{-7/2}). \tag{A1.6}$$

Appendix 2. Proof of: $\int_0^\infty \mathrm{d}E\, s\, \mathrm{e}^{-sE}\tan^{-1}(\sqrt{E}/a)=\sqrt{\pi}\,\mathrm{sgn}(a)\int_0^\infty \mathrm{d}u\, \exp[-(u^2+2u|a|\sqrt{s})]$

To prove this result we write $s\,\mathrm{e}^{-sE}=-\mathrm{d}/\mathrm{d}E\;\mathrm{e}^{-sE}$ and integrate the left-hand side, which we call $I(a)$, by parts

$$I(a)\equiv\int_0^\infty \mathrm{d}E\, s\,\mathrm{e}^{-sE}\tan^{-1}(\sqrt{E}/a)=\frac{a}{2}\int_0^\infty \frac{\mathrm{d}E}{\sqrt{E}}\frac{\mathrm{e}^{-sE}}{E+a^2}$$
$$=a\int_0^\infty \mathrm{d}v\frac{\mathrm{e}^{-sv^2}}{v^2+a^2}. \tag{A2.1}$$

Next we make the replacement

$$1/(v^2+a^2)=\int_0^\infty \mathrm{d}\lambda\, \exp[-\lambda(v^2+a^2)] \tag{A2.2}$$

in equation (A2.1) and carry out the v integration first. Lastly we change variables from λ to u:

$$\lambda=(u/|a|+\sqrt{s})^2-s \tag{A2.3}$$

and obtain the result given in the title to this appendix.

References

[1] Schwinger J 1951 *Phys. Rev.* **82** 664
[2] Nakahara M, Waxman D and Williams G 1991 *J. Phys. C: Solid State Phys.* **3** 6743
[3] D'yakanov D I, Petrov V Yu and Yung A V 1984 *Sov. J. Nucl. Phys.* **39** 150
[4] Nakahara M, Waxman D and Williams G 1990 *J. Phys. A: Math. Gen.* **23** 5017
[5] Gottfried K 1966 *Quantum Mechanics* (New York: Benjamin)
[6] Abramowitz M and Stegun I A 1965 *Handbook of Mathematical Functions* (New York: Dover)
[7] Minakshisundaram S 1949 *J. Indian Math. Soc.* **41** 6
Seeley R T 1967 *Proc. Symp. Pure Appl. Math. AMS* **10** 288
[8] DeWitt B S 1975 *Phys. Rep.* **19** 295
[9] Baltes H P and Hilf E R 1976 *Spectra of Finite Systems* (Mannheim: Bibliographisches Institut)
[10] Osborn T A and Wong R 1983 *J. Math. Phys.* **24** 1487; 1985 *J. Math. Phys.* **26** 753