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COMMENT

A note on the energy moments

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Abstract. The relationship between the Buslaev–Faddeev and Percival methods for studying the moments $\mathrm{Tr}(H^p)$ is shown explicitly by analytic continuation of the generalised zeta function written in terms of the partition function.

Dikii (1961) has studied relations for the moments $\mathrm{Tr}(H^p)$ for a Sturm–Liouville problem in a finite interval using a method based on the analytic continuation of a generalised zeta function. Buslaev and Faddeev (1960) have extended this treatment to systems with a continuous or mixed spectrum and Percival (1962) used the expansion of the partition function $Z(-\beta) = \mathrm{Tr}\, \mathrm{e}^{-\beta H}$ and by taking successive derivations of it with respect to β and letting $\beta \to 0^+$ he obtained the different energy moments for integer $p \geqslant 0$.

As these moments turn out to be divergent for $\beta \to 0^+$, he defined a new derivative operation which amounts to taking the usual derivative (of any order) and subtracting from it all the singular terms for $\beta \to 0^+$; in this way he obtained the same results as previous authors, who used an analytic continuation procedure for the generalised zeta function.

In order to clarify the connection between these procedures, in this comment we shall perform the analytic continuation of the generalised zeta function by expressing it in terms of the partition function. For this purpose, let us recall that the Riemann zeta function can be written as (see, for example, Titchmarch 1951)

$$\Gamma(s)\zeta(s) = \int_0^\infty x^{s-1} \sum_{n=1}^{\infty} \mathrm{e}^{-nx}\, \mathrm{d}x \tag{1}$$

valid for $\mathrm{Re}\, s > 1$. A convenient way to make the analytic continuation for $\mathrm{Re}\, s < 1$ is by means of the finite part à la Hadamard (see Guelfand and Shilov 1962); this amounts to subtracting from the 'partition function' $\Sigma\, \mathrm{e}^{-nx}$ which appears in equation (1) as many terms from its Laurent expansion (around $x = 0$) as are necessary to make the integral convergent. (For more details see, for instance, appendix A of Ruggiero *et al* 1977.)

We shall consider the problem treated by Percival, that is, a non-relativistic particle in a spherical potential $V(r)$ in the s state. Let us consider the partition function

$$Z_I(-\beta) = Z(-\beta) - Z_T(-\beta) = \mathrm{Tr}\, \mathrm{e}^{-\beta H} - \mathrm{Tr}\, \mathrm{e}^{-\beta T} \tag{2}$$

where $H = T + V$ (V is of short range and is analytic in r).

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We have (see Percival 1962)

$$Z_I(-\beta)=\sum_\lambda e^{-\beta E_\lambda}+\frac{1}{\pi}\int_0^\infty e^{-\beta E}\frac{d\delta(E)}{dE}\,dE \tag{3}$$

or

$$Z_I(-\beta)=Z_I^B(-\beta)+Z_I^c(-\beta) \tag{4}$$

where $Z_I^B(-\beta)$ corresponds to the bound states (whose number N is finite) and $Z_I^c(-\beta)$ to the continuum of states. $\delta(E)$ is the phase-shift function.

Writing

$$\mathrm{Tr}(H^{-s}-T^{-s})=\sum_\lambda E_\lambda^{-s}+\frac{1}{\pi}\int_0^\infty E^{-s}\frac{d\delta(E)}{dE}\,dE, \tag{5}$$

the first term on the RHS of equation (5), which corresponds to the bound states, is analytic in the whole complex s plane. Now for the second term we can write

$$\mathrm{Tr}(H^{-s}-T^{-s})_c=\frac{1}{\Gamma(s)}\int_0^\infty \beta^{s-1}Z_I^c(-\beta)\,d\beta. \tag{6}$$

Since

$$Z_I^B(-\beta)=\sum_\lambda e^{-\beta E_\lambda}=N-\beta\sum_\lambda E_\lambda+\ldots+\frac{\beta^p}{p!}(-1)^p\sum_\lambda E_\lambda^p+\ldots, \tag{7}$$

it follows from equation (17) of Percival (1962) that

$$Z_I^c(-\beta)=[\pi]^{1/2}\left(-2a_1\beta^{1/2}+4a_2\beta^{3/2}+\ldots+\frac{(-1)^p2^{2p}p!\,a_p\beta^{p-\frac{1}{2}}}{(2p)!}+\ldots\right)$$
$$+\left(b_0'-\frac{b_1'}{1!}\beta+\ldots+\frac{(-1)^pb_p'}{p!}\beta^p+\ldots\right) \tag{8}$$

with

$$b_p'=b_p-\sum_\lambda E_\lambda^p. \tag{9}$$

The coefficients a_p and b_p can be found in Percival (1962).

Equation (6) is valid for Re $s>0$, and therefore it defines the left-hand side which is analytic in this region.

We can write equation (6) as:

$$\mathrm{Tr}(H^{-s}-T^{-s})_c=\frac{1}{\Gamma(s)}\int_0^1 \beta^{s-1}Z_I^c(-\beta)\,d\beta+\frac{1}{\Gamma(s)}\int_1^\infty \beta^{s-1}Z_I^c(-\beta)\,d\beta. \tag{10}$$

The second term of equation (10) is analytic in the whole s plane. In order to continue analytically the first term for Re $s<0$, we note that for Re $s>0$ we have

$$\frac{1}{\Gamma(s)}\int_0^1 \beta^{s-1}Z_I^c(-\beta)\,d\beta=\frac{1}{\Gamma(s)}\left(\int_0^1 \beta^{s-1}(Z_I^c(-\beta)-b_0')\,d\beta+\frac{b_0'}{s}\right). \tag{11}$$

The right-hand side can be continued analytically up to Re $s=-\frac{1}{2}$. In this region it defines the finite part of the left-hand side of equation (11) (see Guelfand and Shilov 1962).

In a similar way, the analytic continuation of the left-hand side of equation (11) up to $s=-p-\frac{1}{2}$ is given by

$$\frac{1}{\Gamma(s)}\Big[\Big[\int_0^1 \beta^{s-1}\Big(Z_I^c(-\beta)+2\pi^{1/2}a_1\beta^{1/2}-\ldots-\frac{(-1)^p\pi^{1/2}p!\,a_p\beta^{p-\frac{1}{2}}}{(2p)!}$$
$$-b_0'+\frac{b_1'}{1!}\beta-\ldots-\frac{(-1)^p b_p'\beta^p}{p!}\Big)\,\mathrm{d}\beta$$
$$-\frac{2\pi^{1/2}a_1}{s+\frac{1}{2}}+\ldots+\frac{(-1)^p\pi^{1/2}p!\,a_p}{(2p)!\,(s+p-\frac{3}{2})}+\frac{b_0'}{s}-\frac{b_1'}{1!}\frac{1}{s+1}+\ldots+\frac{(-1)^p b_p'}{p!\,(s+p)}\Big]. \tag{12}$$

For $s=-p$ with p an integer greater than or equal to zero, $(\Gamma(-p))^{-1}=0$ and therefore the second term on the RHS of equation (10) does not contribute, while the analytic continuation of the first term receives only the contribution of the last term of equation (12), which is equal to

$$\frac{1}{\Gamma(s)}\frac{(-1)^p b_p'}{(s+p)p!}\Big|_{s=-p}=b_p'. \tag{13}$$

Therefore the analytic continuation of equation (10) for $s=-p$ gives

$$\mathrm{Tr}(H^p-T^p)_c=b_p'=b_p-\sum_\lambda E_\lambda^p \tag{14}$$

and the analytic continuation of equation (5) for $s=-p$ gives

$$\mathrm{Tr}(H^p-T^p)=b_p, \tag{15}$$

which is the result given by Percival. Formally, it is obtained from equation (17) of Percival (1962) by taking

$$\lim_{\beta\to 0^+}(-1)^p\frac{\mathrm{d}^pZ_I(-\beta)}{\mathrm{d}\beta^p}$$

and subtracting from it all the singular terms in $\beta=0$.

The process of analytic continuation in the variable s used above is also called analytic regularisation (see Guelfand and Shilov 1962).

Now we have

$$Z_T(-\beta)=\mathrm{Tr}\,\mathrm{e}^{-\beta T}=(m/2\pi\beta)^{1/2},$$

which, according to the discussion given above, will give $\mathrm{Tr}(T^{-s})=0$ for $s=-p$ as a negative integer. But in general we have

$$\mathrm{Tr}(T^{-s})\sim\int_0^\infty k^{-2s}\,\mathrm{d}k$$

which is zero by analytic regularisation (see p 70 of Guelfand and Shilov 1962).

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