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FAST TRACK COMMUNICATION

A comment on the Gelfand–Yaglom theorem, zeta functions and heat kernels for PT-symmetric Hamiltonians

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Abstract
We propose a numerical method for computing zeta functions for general classes of Hamiltonians, based on the Gelfand–Yaglom theorem, which computes the determinant without needing to compute the eigenvalues. We verify that this agrees with known analytic results for certain Hermitean Hamiltonians, and we present numerical evidence that it may extend also to non-Hermitean PT-symmetric Hamiltonians.

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(Some figures in this article are in colour only in the electronic version)

Consider a Hamiltonian H, with a spectrum of eigenvalues λ. Define the associated zeta function [1] as

$$\zeta_H(s) = \mathrm{tr}\frac{1}{H^s} = \sum_\lambda \frac{1}{\lambda^s}. \tag{1}$$

Our analysis is based on the simple observation that the log determinant of H, with a spectral parameter m^2, acts as a generating function for the zeta functions:

$$\ln\left(\frac{\det(H+m^2)}{\det(H)}\right) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} m^{2n}\zeta_H(n). \tag{2}$$

There exist certain soluble cases, some examples of which are recalled below, for which this relation can be evaluated analytically, because the relevant determinants and zeta functions can be computed in closed form [2, 3]. These soluble cases reveal a beautiful structure of functional relations satisfied by the determinants and a deep relation with number theory. Functional relations such as these also lie at the heart of the remarkable relationship between integrable models and ordinary differential equations [4]. Here we propose using a *numerical* evaluation of the log determinant, using the Gelfand–Yaglom theorem [5–8] as a numerical method for computing zeta functions. This can be applied to a large class of Hamiltonians, extending

beyond the known soluble cases. The Gelfand–Yaglom theorem, in its simplest form for Dirichlet boundary conditions on an interval $x \in [a, b]$, states that to evaluate the determinant one does not need to compute any eigenvalues; rather, one solves the homogeneous equation with simple initial-value boundary conditions:

$$H\phi = 0, \qquad \phi(a) = 0, \qquad \phi'(a) = 1 \quad \Rightarrow \quad \det H = \phi(b). \tag{3}$$

In addition to its intrinsic simplicity and geometric interpretation [9], this result is numerically practical, as it is trivial to implement numerically, even including a spectral parameter m^2 as in (2). On an infinite interval, the theorem is understood as applied to ratios of determinants, in which case the numerical integrations yield finite ratios.

A simple soluble example that illustrates the basic idea is provided by the one-dimensional free Hamiltonian, $H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$, defined on the interval $x \in [-L, L]$, with Dirichlet boundary conditions. Using (3), we find

$$\ln\left(\frac{\det(H+m^2)}{\det(H)}\right) = \ln\left(\frac{\sinh(2mL)}{2mL}\right) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \frac{\zeta_R(2n)}{\pi^{2n}} (2mL)^{2n}, \tag{4}$$

from which we easily recognize the Riemann zeta function form of the zeta functions for H:

$$\zeta_H(n) = \sum_{k=1}^{\infty} \frac{1}{(k\pi/(2L))^{2n}} = \frac{(2L)^{2n}}{\pi^{2n}} \zeta_R(2n). \tag{5}$$

A less-trivial soluble example is provided by the free radial Hamiltonian in two dimensions on a disc of radius R, in a given partial wave of angular momentum l: $H = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{l^2-1/4}{r^2}$. The eigenvalues of H are expressed in terms of the zeros $j_k^{(l)}$ of the Bessel function $J_l(r)$: $\lambda_k = 1/\left(j_k^{(l)} R\right)^2, k = 1, 2, \ldots$. Applying the Gelfand–Yaglom theorem on the interval $r \in [0, R]$ we find

$$\ln\left(\frac{\det(H+m^2)}{\det(H)}\right) = \ln\left(\frac{l! I_l(mR)}{(mR/2)^l}\right) = 1 + \frac{(mR)^2}{4(l+1)} - \frac{(mR)^4}{32(l+2)(l+1)^2} + \cdots \tag{6}$$

from which we deduce the relevant zeta functions. Note the remarkable fact that there are simple expressions for the sums of inverse powers of the Bessel zeros, known already to Euler [10], even though there is no simple expression for the Bessel zeros themselves. It is straightforward to generalize this free radial example to d dimensions.

So far, these examples were for *free* Hamiltonians. There is a class of Hamiltonians with nontrivial potentials for which the zeta functions can also be obtained in closed form, once again even though there is no closed expression for the individual eigenvalues. For the homogeneous potentials $V = x^{2N}$ these have been evaluated by Voros [2, 3]. These results are based on a construction of the associated Green function, and hence of the zeta function, from solutions to the homogeneous equation, whose solutions for such a potential are just Bessel functions. This idea was extended to PT-symmetric potentials by Mezincescu [11], and by Bender and Wang [12]. For more complicated potentials that are not homogeneous functions of x it is not usually possible to solve the homogeneous equation exactly, and so neither the eigenvalues nor the zeta functions can be computed exactly. However, the Gelfand–Yaglom side of the generating function relation (2) is still simple to evaluate numerically, and this can be used to extract numerical values for the associated zeta functions. We first show how this works for the soluble Hermitean cases mentioned above and then extend it to some nontrivial cases.

Consider the Hamiltonians

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + gx^{2N}. \tag{7}$$

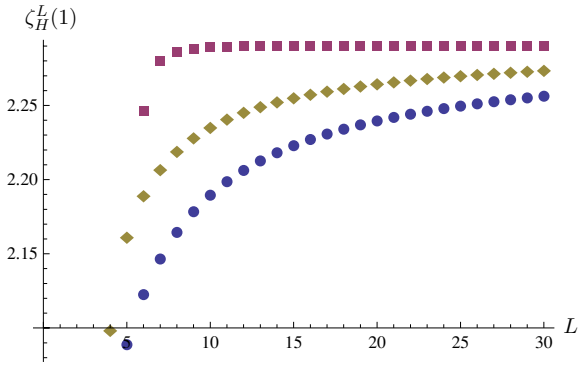

Figure 1. Plot of the zeta function $\zeta_H^L(1)$ for the quartic potential $V = x^4$ as a function of L. Lowest (blue) dots denote the raw numerical data from (8) and show a slow convergence in the large L limit. The (green) diamonds in the middle and the (red) squares at top represent the data after one and two iterations respectively of the VBS extrapolation procedure described in the text. They clearly show better and better convergence at large L.

Scaling out the coupling g, the eigenvalues scale as $\lambda \propto g^{2/(N+2)}$, so we can drop the g dependence and just consider the numerical value of the eigenvalues, and associated spectral functions, at $g = 1$. We integrate the Gelfand–Yaglom equation (3), now combined with the spectral parameter m^2,

$$(H + m^2)\phi_{m^2} = \left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^{2N} + m^2\right)\phi_{m^2} = 0 \tag{8}$$

from $x = -L$ to $x = +L$, with the initial value conditions in (3). This can be done for any value of the spectral parameter m^2. The first and second zeta functions correspond to the leading two coefficients in the small m^2-expansion in (2). Hence they are simply determined by taking one and two derivatives of the functional determinant (i.e., the end point value of the Gelfand–Yaglom solution $\phi_{m^2}(L)$) with respect to m^2 as

$$\zeta_H^L(1) = \frac{\partial}{\partial m^2} \ln \phi_{m^2}(L)\bigg|_{m^2=0}, \qquad \zeta_H^L(2) = -\left(\frac{\partial}{\partial m^2}\right)^2 \ln \phi_{m^2}(L)\bigg|_{m^2=0}. \tag{9}$$

We have evaluated these numerical derivatives for each value of L for $L = 1, 2, \ldots, L_{\max}$. In the cases studied in this paper, we have taken $L_{\max} = 30$–50 to obtain convergence, depending on the specific form of the potential. In order to find the values with infinite size ($L \to \infty$), we use the VBS extrapolation method, proposed by van den Broeck and Schwartz [13], and first applied to critical phenomena by Hamer and Barber [14]. It permits the extraction of a reliable asymptotic value from a sequence of finite-size data. The procedure of the algorithm can be explained as follows.

Suppose that we have a sequence of data f_L for $L = 1, 2, \ldots, L_{\max}$. After identifying theses data as zeroth level values, $f_L^{(0)}$, we can construct $(k+1)$ th level data $f_L^{(k+1)}$ from $f_L^{(k)}$ and $f_L^{(k-1)}$ using the recurrence relation

$$\left[f_L^{(k+1)} - f_L^{(k)}\right]^{-1} + \alpha\left[f_L^{(k-1)} - f_L^{(k)}\right]^{-1} = \left[f_{L+1}^{(k)} - f_L^{(k)}\right]^{-1} + \left[f_{L-1}^{(k)} - f_L^{(k)}\right]^{-1} \tag{10}$$

with the supplementary data $f_L^{(-1)} = \infty$. In (10), the free parameter α can be chosen to optimize the convergence. In this paper, we have chosen $\alpha = -(1 - (-1)^L)/2$ following the suggestion in [14]. As an illustration, in figure 1 we plot $\zeta_H(1)$ in the case of the quartic

Table 1. Zeta function values for x^{2N} potentials.

Potential	Numerical $\zeta_H(1)$	Exact $\zeta_H(1)$	Numerical $\zeta_H(2)$	Exact $\zeta_H(2)$
x^2	Divergent	Divergent	1.2337	$\frac{\pi^2}{8} = 1.233\,701$
x^4	2.289 91	2.289 909	0.996 32	0.996 320
x^6	1.721 35	1.721 346	0.838 750	0.838 749
x^8	1.4940	1.493 996	0.726 49	0.726 491

Table 2. Zeta function values for $\mathrm{i}x^3$ potential.

Potential	Numerical $\zeta_H(1)$	Exact $\zeta_H(1)$	Heat kernel approx $\zeta_H^{hk}(1)$	Numerical $\zeta_H(2)$	Exact $\zeta_H(2)$	Heat kernel approx $\zeta_H^{hk}(2)$
$\mathrm{i}x^3$	2.835 09	2.835 094	2.826 17	0.845 70	–	0.839 887

potential $V = x^4$. The first and second iterations of VBS algorithm clearly show good convergence for sufficiently large values of L. The values for the first two zeta functions from the VBS extrapolation are shown in table 1. The agreement with the exact values of Voros is excellent. This numerical method is straightforward to apply to more complicated potentials, for example of non-homogenous or non-polynomial form.

We now observe that for PT-symmetric Hamiltonians [15], a direct application of the Gelfand–Yaglom theorem still yields a real value of the determinant. To illustrate this, we consider cases with potentials involving complex part $\mathrm{i}x^3$, for which the principal Stokes wedge includes the real axis. Then the initial value at $x = -L$ is real, and hence by PT symmetry so is the final value at $x = +L$, even though $\phi_{m^2}(x)$ is complex in the interior of the interval. This observation, and our numerical results below, can be viewed as motivation for a serious study of the Gelfand–Yaglom theorem for PT-symmetric Hamiltonians, taking into account the appropriate Stokes wedge structure of the complex x-plane for more general PT-symmetric Hamiltonians. It is also consistent with the fact that for a PT-symmetric Hamiltonian the energy eigenvalues are either real or come in complex conjugate pairs [15]. To test the idea, we first apply this numerical procedure to the potential $V = \mathrm{i}x^3$, and obtain a numerical value of $\zeta_H(1)$ in excellent agreement with the known exact value [11, 12], as shown in table 2. Furthermore, we are able to extract a numerical value for the second zeta value $\zeta_H(2)$. The values based on a heat kernel approximation are discussed below.

Next we apply this Gelfand–Yaglom technique to the following nontrivial PT-symmetric Hamiltonian

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{x^2}{4} + \mathrm{i}gx^3. \tag{11}$$

In this case, since $V(x)$ is not homogeneous, it is not possible to scale out the dependence on the coupling g. The spectral properties of this system have been studied using exact WKB methods [16] and large-order perturbation theory [17], providing strong evidence for reality of the spectrum for real g, and illustrating consistency with WKB analysis of the associated real potential $V(x) = \frac{x^2}{4} + gx^3$ [18–20]. For the Hamiltonian (11) there is no known exact expression for the zeta function. Our numerical results for the first two zeta function values are presented in table 3, for various values of the coupling g.

Table 3. Zeta function values for $\frac{x^2}{4} + igx^3$ potential for various values of the coupling g.

Potential $x^2/4 + Igx^3$	Numerical $\zeta_H(1)$	Heat kernel approx $\zeta_H^{hk}(1)$	Numerical $\zeta_H(2)$	Heat kernel approx $\zeta_H^{hk}(2)$
$g = 1/64$	10.3388	10.3396	4.8395	5.016 17
$g = 1/32$	8.8856	8.912 79	4.642 31	4.721 61
$g = 1/16$	7.4778	7.477 15	4.152 39	4.146 12
$g = 1/8$	6.087 40	6.074 87	3.279 46	3.250 66
$g = 1/4$	4.798 37	4.783 23	2.254 56	2.230 42
$g = 1/2$	3.701 18	3.688 06	1.405 27	1.3895
$g = 1$	2.824 37	2.810 97	0.833 557	0.824 069
$g = 2$	2.1458	2.137 89	0.484 39	0.478 854

Since there are no other published results with which to compare, we make the following *approximate* comparison based on an approximation for the heat kernel trace. Recall that the heat kernel trace is related to the zeta function by a Mellin transform [2, 3]:

$$Z(t) \equiv \operatorname{tr} \mathrm{e}^{-Ht} \quad \Rightarrow \quad \zeta_H(s) = \frac{1}{\Gamma(s)} \int_0^\infty \mathrm{d}t\, t^{s-1} Z(t). \tag{12}$$

At large t, the behavior of the heat kernel $Z(t)$ is determined by the lowest eigenvalue λ_0 of H. On the other hand, at small t, the behavior can be extracted from the exponentiated form of the Seeley–DeWitt expansion [8, 21, 22]:

$$Z(t) \sim \frac{1}{\sqrt{4\pi t}} \int \mathrm{d}x \exp\left[-tV(x) - t^2 \frac{1}{6} V''(x) + t^3 \left(\frac{1}{12}(V'(x))^2 - \frac{1}{60} V^{(4)}(x)\right)\right.$$
$$\left. + t^4 \left(\frac{1}{90}(V''(x))^2 + \frac{1}{30} V'(x) V^{(3)}(x) - \frac{1}{840} V^{(6)}(x)\right) + \cdots\right]. \tag{13}$$

For one-dimensional systems, it is straightforward to generate as many terms in this series as desired. For a PT-symmetric potential, we note that even though $V(x)$ may be complex, the PT symmetry ensures that the Seeley–DeWitt expansion is real.

The heat kernel expansion (13) gives information about the small t behavior of $Z(t)$, which is related to the large eigenvalues of H, while the large t behavior of $Z(t)$ is related to the small eigenvalues of H. But to evaluate the zeta function from (12) we need $Z(t)$ for all t. We can therefore approximate the heat kernel trace, and hence the zeta function, by making an interpolation of $Z(t)$, matching its behavior at small and large t. The simplest way to do this is to match the large t behavior $Z(t) \sim \mathrm{e}^{-\lambda_0 t}$, based on just the lowest eigenvalue λ_0, to the small t behavior of $Z(t)$ obtained from the first few terms of (13). For the PT-symmetric Hamiltonian in (11):

$$Z(t, g) \sim \begin{cases} \mathrm{e}^{-\lambda_0(g)t}, & t \to \infty \\ \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} \mathrm{d}x \exp\left[-\frac{x^2 t}{4} - \frac{t^2}{12} + \frac{x^2 t^3}{48} - \frac{3g^2 x^4 t^3}{4}\right] \cos\left(gx^3 t + gxt^2 - \frac{1}{4} gx^3 t^3\right), & t \to 0 \end{cases} \tag{14}$$

We use values for $\lambda_0(g)$ from [17] to define the large t behavior of $Z(t, g)$, as a function of the coupling g. We interpolate between the asymptotic small and large t behaviors by joining the two curves, truncating them where they meet. Surprisingly, the small and large t asymptotic behaviors fit together relatively smoothly, even with such a crude approximation. Some typical

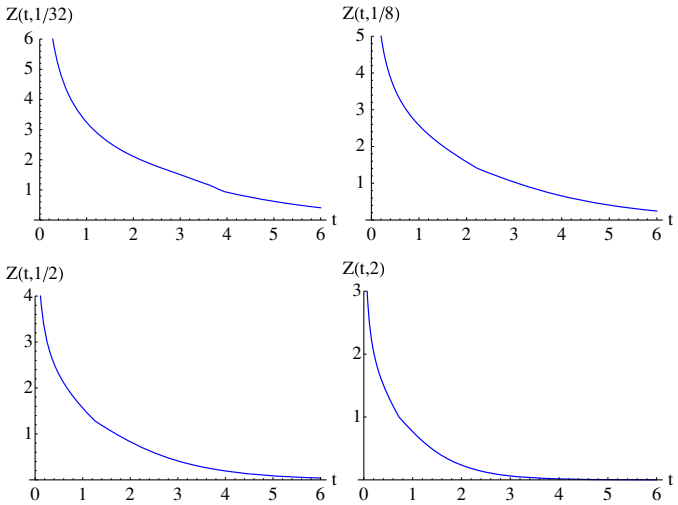

Figure 2. Interpolations of the heat kernel traces for the Hamiltonian in (11), based on the asymptotic forms in (14), for various values of the coupling g: $g = 1/32$, $g = 1/8$, $g = 1/2$, $g = 2$. Note that even this very crude approximation is quite smooth.

examples are shown in figure 2, for various values of g. Of course, better precision could be achieved by including more of the low eigenvalues in the large t behavior, and more terms of the Seeley–De Witt expansion in the small t behavior. The results for the zeta function for the simple PT potential $V = \mathrm{i}x^3$ are given in table 2 and show that this very simple approximation already yields good agreement, within a few percent. For the more complicated PT-symmetric Hamiltonian in (11), the heat kernel approximation results for the zeta function are given in table 3, and once again show good agreement with the numerical values obtained from our Gelfand–Yaglom method.

To conclude, in this paper we make two observations. First, the Gelfand–Yaglom theorem can be used as a *numerical* tool to evaluate zeta functions for general classes of quantum-mechanical Hamiltonians, without needing to find any eigenvalues. For conventional Hermitean cases this yields excellent agreement with known results for soluble cases, and can be extended to a broader class of Hamiltonians than those studied analytically [2, 3]. Second, we propose that the Gelfand–Yaglom theorem, and also the Seeley–DeWitt expansion of the heat kernel trace, could be extended to PT-symmetric Hamiltonians. Our results lend numerical support to this idea and suggest that a careful analytic study of these ideas would be worthwhile, taking into account the rich monodromy structure already found in PT models [4, 15, 16].

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