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On the quantum zeta function

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Abstract. It is remarkable that the quantum zeta function, defined as a sum over energy eigenvalues E:

$$Z(s) = \sum \frac{1}{E^s}$$

admits of exact evaluation in some situations for which not a single E be known. Herein we show how to evaluate instances of $Z(s)$, and of an associated parity zeta function $Y(s)$, for various quantum systems. For some systems both $Z(n), Y(n)$ can be evaluated for infinitely many integers n. Such Z, Y values can be used, for example, to effect sharp numerical estimates of a system's ground energy. The difficult problem of evaluating the analytic continuation $Z(s)$ for arbitrary complex s is discussed within the contexts of perturbation expansions, path integration, and quantum chaos.

1. Introduction

We define the quantum zeta function as a formal sum over system eigenvalues E:

$$Z(s) = \sum \frac{1}{E^s} \tag{1.1}$$

when such a sum exists. Z is of course reminiscent of the celebrated Riemann zeta function

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}. \tag{1.2}$$

When the ordered energy eigenvalues E are discrete, non-vanishing, and sufficiently divergent, we expect the literal sum for the function $Z(s)$ to converge for sufficiently large $\mathrm{Re}(s)$. Indeed, the Riemann sum converges for $\mathrm{Re}(s) > 1$, this observation being the historical starting point for analytic continuation to general complex s. Presumably $Z(s)$ will, in most situations, likewise possess an analytic continuation. It is remarkable that $Z(s)$ can be evaluated in terms of fundamental constants (such as π and various algebraic constants) and values of standard functions (such as, say, the gamma function or ζ itself) in certain quantum settings for which not a single isolated E has been so evaluated. When eigenstates can be assigned definite parity, we define also a companion entity called the parity zeta function $Y(s)$:

$$Y(s) = \sum \frac{\pm 1}{E^s} \tag{1.3}$$

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where the sign ($\pm$) of a term is the parity of the eigenstate associated with the given E. We shall also be able to provide exact evaluations of Y for certain systems.

Previous results on the quantum zeta function include those of Voros (1980) and Berry (1986), who made use of various identities involving quantum theoretical constructs such as resolvent operators and Green functions. Zeta function regularization and physical applications of the quantum zeta functon are discussed in Elizalde (1994). There is a zeta function field theory literature exemplified in the work of Steiner (1987). Herein we concentrate on systems characterized by a non-relativistic, real-valued one-dimensional potential $V(x)$, adopting the standard Green function expressed in terms of orthonormal eigenstate wavefunctions ψ_n as

$$G(x, x_0, E) = \sum_n \frac{\psi_n(x)\psi_n^*(x_0)}{E - E_n} \tag{1.4}$$

which stands as a particular solution of the Schrödinger equation (we adopt atomic units $m = \hbar = 1$ throughout)

$$-\frac{1}{2}\frac{\partial^2 G}{\partial x^2} + V(x)G - EG = -\delta(x - x_0). \tag{1.5}$$

It is fortuitous that many exact evaluations of Z can be obtained via knowledge of the zero-energy Green function $G(x, x_0, 0)$ or of E-derivatives of G at $E = 0$. On the notion of orthonormality of the wavefunctions it is formally immediate from (1.4) that

$$Z(1) = -\int G(x, x, 0)\, \mathrm{d}x \tag{1.6}$$

with the integral taken over the one-dimensional domain on which the eigensystem is defined (for example $V(x) = x^2$ relegated to the domain $x \in (0, \infty)$ would be an appropriate setting for an harmonic oscillator system with infinite reflecting wall at the origin). More generally, for positive integers n

$$Z(n) = -\frac{1}{(n-1)!}\int G^{(n-1)}(x, x, 0)\, \mathrm{d}x \tag{1.7}$$

where $G^{(m)}$ denotes the mth partial derivative of G with respect to the energy argument. Another representation for $Z(n), n \in Z^+$ amounts to an attractive trace relation of Itzykson *et al* (1986), following again from orthonormality, to the effect that

$$Z(n) = (-1)^n \int G(x_1, x_2, 0)G(x_2, x_3, 0)\cdots G(x_n, x_1, 0)\, \mathrm{d}x_1\, \mathrm{d}x_2\, \cdots\, \mathrm{d}x_n\,. \tag{1.8}$$

For symmetric potentials V the parity zeta function enjoys the formal relation

$$Y(1) = -\int G(x, -x, 0)\, \mathrm{d}x \tag{1.9}$$

as follows immediately, again, from the eigenstate sum for G. Relations for $Y(n)$ for larger integers n may be obtained in straightforward fashion, in the partial-derivative or Itzykson *et al* trace forms.

It is more difficult to evaluate $Z(s)$ or $Y(s)$ for general complex s. One idea we shall exploit is to transform the spacetime propagator K, defined as

$$\theta(t)K(x,t|x_0,0) = \frac{\mathrm{i}}{2\pi}\int_{-\infty}^{\infty} G(x,x_0,E)\mathrm{e}^{-\mathrm{i}Et}\,\mathrm{d}E \tag{1.10}$$

where the E-integral is taken just above the real axis so to avoid the E-poles (Crandall 1993). The eigenstate representation of the spacetime propagator is

$$K(x,t|x_0,0) = \sum_n \psi_n(x)\psi_n^*(x_0)\mathrm{e}^{-\mathrm{i}E_n t}\,. \tag{1.11}$$

Formally, the quantum zeta function can be cast as a Mellin transform

$$Z(s) = \frac{\mathrm{i}^s}{\Gamma(s)}\int_0^{\infty} t^{s-1}\int K(x,t|x,0)\,\mathrm{d}x\,\,\mathrm{d}t\,. \tag{1.12}$$

This representation is often referred to as the heat-kernel form of the zeta function. It is of interest that the inverse transform yields the quantum partition function

$$\sum_n \mathrm{e}^{-\tau E_n} = \frac{1}{2\pi\mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \frac{Z(s)\Gamma(s)\mathrm{d}s}{\tau^s} \tag{1.13}$$

where the real parameter c is to the right of all Z poles. Exact knowledge of K, as may sometimes be achieved through path integration, can give rise to exact quantum zeta evaluations. When a potential is time-dependent, the problem of ill-defined steady-state eigenvalues E can be circumvented by defining the quantum zeta function in heat-kernel form, that is, in terms of the complete time-domain integral (1.12). It is therefore natural to propose this Mellin transform as the very definition of the quantum zeta function. What is more the Mellin transform, by conveying information about zeros of Z, may find future application to the problem of quantum chaos. We further discuss this Mellin transform representation at the end of the paper.

A word on the practical applications of the quantum zeta function is in order. We have the classical observation of Waring, exploited previously by Berry (1986), that when $0 < E_0 < E_1 < E_2 < \cdots$, the ground energy E_0 can be extracted in principle from

$$E_0 = \lim_{s\to\infty} Z(s)^{-1/s}\,. \tag{1.14}$$

Thus sufficient knowledge of the large-s behaviour of $Z(s)$ will yield information about the ground state. As early as 1781, Euler used

$$Z(s)^{-1/s} < E_0 < \frac{Z(s)}{Z(s+1)} \tag{1.15}$$

together with extrapolation methods, to resolve to one part per million a certain Bessel zero, which zero happens to be the lowest-lying eigenvalue for a vibrating disc (Berry 1986). When the potential V is symmetric, a sharp ground energy estimate can often be obtained from the apparently new asymptotic relation

$$E_0 \sim \frac{1}{2}\left(\frac{Z(s)}{Z(s+1)} + \frac{Y(s)}{Y(s+1)}\right) \tag{1.16}$$

in which the influence of the first excited energy, E_1, decays rapidly as $s \to \infty$.

There is also the possibility of extracting ground-state information by analysing the leading asymptotic behaviour of the inverse transform (1.13). If enough be known about the line integral's behaviour for large real τ, the ground energy E_0 can be extracted. This procedure is reminiscent of the Feynman–Kac technique of extracting the ground energy from the spacetime propagtor itself (Schulman 1981).

In situations where an explicit set of excited-state energies $E_1, E_2, \ldots, E_m$ are known to some numerical precision, one can alternatively estimate the ground energy via

$$\frac{1}{E_0^s} \sim Z(s) - \sum_{n=1}^{m} \frac{1}{E_n^s} - \sum_{n=m+1}^{\infty} \frac{1}{W_n^s} \tag{1.17}$$

where W_n denotes, say, a WKB approximation to E_n. Similar relations using the parity zeta function $Y(s)$ are possible; in fact the employment of Y evaluations tends to be a superior numerical strategy because of the cancellations inherent in Y. It has been observed previously (Berry 1986) that quantum zeta approximation strategies can yield surprisingly good ground state estimates. We demonstrate this phenomenon in some of our examples to follow.

2. The perturbed oscillator

Here we determine $Z(s)$, for arbitrary complex s, for the singularly-perturbed oscillator specified by

$$V(x) = \frac{1}{2}\omega^2 x^2 + \frac{g}{x^2} \tag{2.1}$$

where the perturbation parameter g satisfies $g > -\frac{1}{8}$. This restriction turns out to be necessary to prevent a 'fall to the centre', i.e. to allow a well-defined eigensystem.

We consider first the simple harmonic case ($g = 0$). For spatial domain $(-\infty, \infty)$ the system is possessed of well known eigenvalues $E_n = (n + \frac{1}{2})\omega$, so that for $\mathrm{Re}(s) > 1$ we have

$$\begin{aligned} Z(s) &= \sum_{n=0}^{\infty} \frac{1}{E_n^s} \\ &= \frac{1}{\omega^s}\left(\frac{1}{\left(\frac{1}{2}\right)^s} + \frac{1}{\left(\frac{3}{2}\right)^s} + \frac{1}{\left(\frac{5}{2}\right)^s} + \cdots\right) \\ &= \frac{2^s - 1}{\omega^s}\zeta(s) \,. \end{aligned} \tag{2.2}$$

We infer by analytic continuation that the Z of the simple harmonic oscillator is thus related directly to the Riemann zeta function, for arbitrary complex s.

Now consider $g \neq 0$. The relevant spatial domain is now $(0, \infty)$, with all wavefunctions vanishing at the $x = 0$ singularity. The exact spacetime propagator for arbitrary $x, x_0 \geqslant 0$ has been developed via path integration (Khandekar and Lawande 1975) as

$$K(x, t|x_0, 0) = \frac{\omega\sqrt{x x_0}}{\mathrm{i}\sin\omega t}\, \mathrm{e}^{\frac{1}{2}\mathrm{i}\omega\left(x^2 + {x_0}^2\right)\cot\omega t}\, I_a\left(\frac{\omega x x_0}{\mathrm{i}\sin\omega t}\right) \tag{2.3}$$

where I_ν is the modified Bessel function of order ν, and a natural parameter

$$a = \tfrac{1}{2}\sqrt{1+8g} \tag{2.4}$$

has entered the theory. The ensuing steps of analysis proceed most smoothly (i.e. relevant integrals clearly exist) if the oscillator frequency ω be assigned an infinitesimal negative imaginary part. A relevant K-integral is

$$\int_0^\infty K(x,t|x,0)\,\mathrm{d}x = \frac{\mathrm{e}^{-\mathrm{i}a\omega t}}{\mathrm{e}^{\mathrm{i}\omega t}-\mathrm{e}^{-\mathrm{i}\omega t}} \tag{2.5}$$

which when used in the Mellin transform representation (1.12) yields the quantum zeta function for $\mathrm{Re}(s) > 0$ as

$$Z(s) = \frac{\mathrm{i}^s}{\Gamma(s)}\int_0^\infty \frac{t^{s-1}\mathrm{e}^{-\mathrm{i}\omega(a+1)t}}{1-\mathrm{e}^{-2\mathrm{i}\omega t}}\,\mathrm{d}t \tag{2.6}$$

$$= \frac{1}{(2\omega)^s}\zeta\left(s,\frac{a+1}{2}\right) \tag{2.7}$$

where $\zeta(s,a)$ is the Hurwitz zeta function, defined as

$$\zeta(s,\rho) = \sum_{n=0}^{\infty}\frac{1}{(n+\rho)^s} \tag{2.8}$$

when the literal sum exists. The Hurwitz zeta function also has a well-studied analytic continuation (Apostol 1976), and we conclude that the quantum zeta function of the perturbed oscillator has been determined, for arbitrary complex s, in terms of standard functions. Note that in the 'simple harmonic limit' $a \to \frac{1}{2}$ we obtain the Dirichlet series

$$Z(s) = \left(\frac{2}{\omega}\right)^s\left(\frac{1}{3^s}+\frac{1}{7^s}+\frac{1}{11^s}+\cdots\right) \tag{2.9}$$

which is precisely the zeta sum over the simple harmonic oscillator's odd-parity states, for the even states are extinguished by the origin singularity.

3. Power potentials

Consider the power potential

$$V(x) = |x|^\nu \tag{3.1}$$

where ν is any positive real number. Herein we derive exact evaluations of $Z(1)$ and $Y(1)$. While previous treatments (Voros 1980) contain such results for positive even integers ν, we shall not need this restriction. Accordingly, on the assumption of ν-analyticity, we arrive at some compelling conjectures.

Except for the simple harmonic oscillator ($\nu = 2$) and the absolute-linear potential ($\nu = 1$), energy eigenvalues have so far eluded closed-form evaluation in terms of standard functions or fundamental constants. Even when $\nu = 1$ the energies are related to zeros and derivative-zeros of the Airy function, and whether these special real numbers can be called fundamental is perhaps a question of taste. In many ways the canonical unsolved eigenvalue problem is that of the quartic oscillator, $V(x) = x^4$. This system has been tirelessly studied over the decades, but again, not a single E for the quartic has been successfully cast in closed form. An interesting anecdote in this regard runs as follows. Some years ago Turschner (1979) announced a closed-form evaluation for *every* quartic eigenvalue. Though this result appeared sufficiently erudite, involving values of the gamma function, the eigenvalues were subsequently shown by numerical techniques to be wrong. Turschner's effort, though, as an approximation scheme brought about renewed interest in the art of estimating and bounding the elusive eigenvalues, as exemplified in the work of Crandall and Reno (1980).

Within the present context the general ν-dependent evaluations of $Z(1)$ and $Y(1)$ may be derived in the following way. We resort to the zero-energy Green function. Happily, though the power-potential Schrödinger equation has (except for $\nu = 1, 2$) not been solved explicitly, it is nevertheless possible to give the general solution for the zero-energy equation

$$-\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + x^\nu\psi = 0 \tag{3.1}$$

as (Abramowitz and Stegun 1965)

$$\psi(x) = \sqrt{x}(AI_{1/p}(\alpha x^{p/2}) + BK_{1/p}(\alpha x^{p/2})) \tag{3.2}$$

where I, K are the standard modified Bessel functions, we define $p = \nu+2, \alpha = \sqrt{8}/p$, and A, B are undetermined superposition constants. One may now fabricate a Green function G by presuming it to be the product of two such general solutions (one in x, one in x_0), then invoking boundary conditions. There are four conditions that, taken together, completely specify the zero-energy Green function. One condition is that G be well behaved for fixed x_0 and $x \to \infty$. Two more conditions are: continuity of G, and of $\partial G/\partial x_0$ when $x_0 = 0, x \neq 0$. A fourth condition is the necessary discontinuity relation for any system's Green function (Crandall 1993)

$$\operatorname*{Disc}_{x=x_0} \frac{\partial G}{\partial x} = 2 \tag{3.3}$$

which relation is necessitated by the delta-function source term in (1.5). These conditions can be applied, together with known asymptotic behaviour of I, K and knowledge of the Wronskian of I, K (Abramowitz and Stegun 1965) to yield the following form for the exact zero-energy Green function. The result is, for $|x| \geqslant |x_0|$

$$G(x, x_0, 0) = -\frac{4}{p}\sqrt{|xx_0|}K_{1/p}(\alpha|x|^{p/2})\Bigg(S(x, x_0)I_{1/p}(\alpha|x_0|^{p/2}) + \frac{\sin(\pi/p)}{\pi}K_{1/p}(\alpha|x_0|^{p/2})\Bigg) \tag{3.4}$$

where $S(x, x_0) = 1$ if x, x_0 have the same sign, otherwise $S(x, x_0) = 0$. As with Green functions generally, one obtains G in the case $|x| \leqslant |x_0|$ by swapping coordinates in (3.4). It is possible now to integrate either $G(x, x, 0)$ or $G(x, -x, 0)$ over $x \in (-\infty, \infty)$ (these procedures are somewhat intricate, involving the formidable Weber–Schafheitlin integrals of

Bessel functions) to arrive at the zeta values (we use superscript (ν) to specify the potential in question)

$$Y^{(\nu)}(1) = \left(\frac{2}{(\nu+2)^2}\right)^{\nu/(\nu+2)} \frac{\Gamma^2\left(\frac{2}{\nu+2}\right)\Gamma\left(\frac{3}{\nu+2}\right)}{\Gamma\left(\frac{4}{\nu+2}\right)\Gamma\left(1-\frac{1}{\nu+2}\right)} \tag{3.5}$$

$$Z^{(\nu)}(1) = \left(1 + \sec\frac{2\pi}{\nu+2}\right) Y^{(\nu)}(1)\,. \tag{3.6}$$

For ν a positive even integer, these results agree with those of Voros (1980). Let us analyse some special cases. First, for the simple harmonic oscillator ($\nu = 2$), $Z^{(2)}(1)$ is singular (indeed, equation (2.2) indicates a pole for this system's $Z^{(2)}(s)$ at $s = 1$). Yet the parity zeta function according to equation (3.5) is

$$Y^{(2)}(1) = \frac{\pi}{\sqrt{8}}\,. \tag{3.7}$$

This is reasonable, because (taking $\omega = \sqrt{2}$, $g = 0$ in (2.1)) the oscillating sum for Y, namely

$$\frac{1}{\sqrt{2}}\left(\frac{1}{\frac{1}{2}} - \frac{1}{\frac{3}{2}} + \frac{1}{\frac{5}{2}} - \cdots\right) \tag{3.8}$$

is likewise seen to be $\pi/\sqrt{8}$.

For the absolute-linear potential ($\nu = 1$) the literal sum for $Z^{(1)}(1)$ does not exist (the E values for this system diverge, but too slowly), yet on the assumption that $Z^{(\nu)}(1)$ be *analytic* in ν we arrive at

$$Z^{(1)}(1) = -\left(\frac{2}{9}\right)^{1/3} \frac{\Gamma\left(\frac{2}{3}\right)}{\Gamma\left(\frac{4}{3}\right)}\,. \tag{3.9}$$

It is natural to conjecture that this (negative) value represents the correct analytic continuation of the system's quantum zeta function to the location $s = 1$. Easier to grasp intuitively is the evaluation

$$Y^{(1)}(1) = -Z(1) \tag{3.10}$$

which is a positive real number corresponding to the alternating sum of reciprocal energies for $V(x) = |x|$. We shall have more to say about this system's eigenvalues in the next section, in which the quantum bouncer (linear potential relegated to positive spatial axis) is analysed.

It is evident from equation (3.5) that $Y^{(\nu)}(1)$ is a positive real number for *every* positive ν. This is reasonable, since an alternating sum of reciprocal energies (if the series be summed in natural order) is expected to converge to a positive limit as long as the energies themselves diverge. From equation (3.6) we see that only for the simple harmonic oscillator ($\nu = 2$) is $Z^{(\nu)}(1)$ singular. Thus, on the assumption of ν-analyticity, we have established a continuation value $Z^{(\nu)}(1)$ for every positive power ν. It is interesting that, for every potential 'under' the harmonic (i.e. $\nu < 2$) the continued value $Z^{(\nu)}(1)$ is negative, while it is positive for all potentials 'above' the harmonic (i.e. $\nu > 2$). The physical meaning, if any, of this phenomenon is obscure.

The limit $\nu \to \infty$ deserves mention, for in this limit the system is that of an infinite well, with relevant domain $x \in (-1, 1)$ at whose ends stand infinite reflecting barriers. Indeed, on the basis of standard gamma function asymptotics (Henrici 1977) the limiting values are

$$\begin{aligned} Y^{(\infty)}(1) &= \tfrac{2}{3} \\ Z^{(\infty)}(1) &= \tfrac{4}{3}\,. \end{aligned} \tag{3.11}$$

Indeed, these limits are reasonable because the relevant Z sum for this infinite potential well is an even-state sum plus an odd-state sum:

$$\begin{aligned} Z^{(\infty)}(1) &= \sum_{m=0}^{\infty} \frac{1}{\pi^2(2m+1)^2/8} + \sum_{m=1}^{\infty} \frac{1}{\pi^2 m^2/2} \\ &= 1 + \tfrac{1}{3} \end{aligned} \tag{3.12}$$

with $Y^{(\infty)}(1)$ obtained in similar fashion as $(1 - \frac{1}{3})$.

For the quartic oscillator ($\nu = 4$) the beautiful evaluation for $Z^{(4)}(1)$, originally found by Voros (1980) as

$$\begin{aligned} Z^{(4)}(1) &= \frac{3^{2/3}}{8\pi^2}\Gamma^5\left(\tfrac{1}{3}\right) \\ &= 3Y^{(4)}(1) \end{aligned} \tag{3.13}$$

with value $Z^{(4)} \sim 3.635\ 003\ 644\ 88\ldots$, may be verified numerically in the following, instructive way. The standard WKB approximations to E_n for the quartic are

$$W_n = (c(n + \tfrac{1}{2}))^{4/3} \tag{3.14}$$

where the constant is

$$c = \sqrt{8\pi}\,\frac{\Gamma\left(\frac{7}{4}\right)}{\Gamma\left(\frac{1}{4}\right)}\,. \tag{3.15}$$

The following numerical test was carried out. Using 140 experimental (i.e. differential equation solution) values $1/E_0, 1/E_1, \ldots, 1/E_{139}$, and the WKB values $1/W_{140}, \ldots, 1/W_{9000}$, all of these were summed (Moore and Vajk 1995). Then a 'tail,' an integral of $1/W_x$, over $x \in (9001, \infty)$, was finally added to give what might be called an 'experimental' value $Z^{(4)}(1) \sim 3.635\ 0017\ldots$. This experimental value is correct to better than one part per million.

Beyond the numerical verification, the calculation is indicative of the opportunity to estimate the ground energy itself. It is interesting that, using *only* the excited WKB approximations and the relation

$$\frac{1}{E_0} \sim Y(1) + \frac{1}{W_1} - \frac{1}{W_2} + \frac{1}{W_3} - \cdots \tag{3.16}$$

one obtains a quartic ground energy E_0 estimate with an error of less than 0.1 per cent.

4. The quantum bouncer

The quantum bouncer is a system for which the potential is linear but an infinite reflecting wall resides at the origin. That is, for a positive real λ and $x \geqslant 0$

$$V(x) = \lambda x \tag{4.1}$$

while the potential is taken to be infinite for negative x. This system is the quantum theoretical version of a mass m bouncing off the origin under the force of uniform gravity g, with physical energies ϵ related to our dimensionless eigenvalues by $\epsilon = (m\hbar^2 g^2/\lambda^2)^{1/3}E$. For this system we shall be able to evaluate $Z(n)$ for any integer $n > 1$. The explicit sum for $Z(1)$ diverges, although an analytic continuation of $Z(s)$ to $s = 1$ is believed to exist as we explain at the end of this section.

All wavefunctions, and the Green function, must vanish at $x = 0$. The Schrödinger equation

$$-\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + \lambda x\psi - E\psi = 0 \tag{4.2}$$

is essentially the Airy differential equation whose general solution for arbitrary E involves the standard Airy functions Ai, Bi (Abramowitz and Stegun 1965). By careful boundary condition matching as in the last section one can obtain the exact Green function, for $x \geqslant x_0 \geqslant 0$, as

$$G(x, x_0, E) = \pi\sqrt{2b}\,\mathrm{Ai}(b(\lambda x - E))\left(\frac{\mathrm{Ai}(b(\lambda x_0 - E))\,\mathrm{Bi}(-bE)}{\mathrm{Ai}(-bE)} - \mathrm{Bi}(b(\lambda x_0 - E)\right) \tag{4.3}$$

where $b = (2/\lambda^2)^{1/3}$. We note that this Green function may also be derived in a completely different way, using the path integral and perturbation expansion approach in Crandall (1993). In every order of perturbation theory G can be explicitly evaluated, and the perturbation series summed by way of hypergeometric function theory.

As usual the energy eigenvalues correspond to E-poles of G. These poles occur when $\mathrm{Ai}(-bE) = 0$, so that for $n = 0, 1, 2, \ldots$ we have

$$E_n = (\lambda^2/2)^{1/3}|a_{n+1}| \tag{4.4}$$

where a_m is the mth zero (ordered by magnitude) of $\mathrm{Ai}(z)$.

To obtain $Z(n)$ it is enough to obtain the integral (over $x \in (0, \infty)$) of the E-derivative $G^{(n-1)}(x, x, E)$ at $E = 0$. The procedure is somewhat intricate, so we simply list the relevant relations as follows:

$$Z(n) = -\frac{\pi 2^{n/3} T_{n-1}(0)}{\Gamma(n)\lambda^{2n/3}} \tag{4.5}$$

where the T-function is defined by

$$(-1)^n T_n(z) = C^{(n)}(z)\int_0^\infty \mathrm{Ai}(u)^2\,\mathrm{d}u - \sum_{j=1}^{n}\binom{n}{j} C^{(n-j)}(z)\frac{\mathrm{d}^{j-1}}{\mathrm{d}z^{j-1}}\mathrm{Ai}(z)^2 + \frac{\mathrm{d}^{n-1}}{\mathrm{d}z^{n-1}}(\mathrm{Ai}(z)\,\mathrm{Bi}(z)) \tag{4.6}$$

with C defined by

$$C(z) = \mathrm{Bi}(z)/\,\mathrm{Ai}(z)\,. \tag{4.7}$$

We then invoke explicit derivative evaluations for the Airy functions, valid for $m = 0, 1, 2, \ldots$

$$\mathrm{Ai}^{(m)}(0) = f_m(-1)^m \sin(\pi(m+1)/3) \tag{4.8}$$

$$\mathrm{Bi}^{(m)}(0) = f_m(1 + \sin(\pi(4m+1)/6) \tag{4.9}$$

where the constants f_m are defined as

$$f_m = \frac{3^{(m-2)/3}\Gamma\left(\frac{m+1}{3}\right)}{\pi}\,. \tag{4.10}$$

The last two derivative relations can be obtained by appropriate contour integration, starting with integral representations (Abramowitz and Stegun 1965) of Ai, Bi. We shall need one final relation, namely

$$\int_0^\infty \mathrm{Ai}(u)^2\,\mathrm{d}u = \frac{\Gamma\left(\frac{5}{6}\right)}{2\pi^{5/6}12^{1/6}} \tag{4.11}$$

again derivable via contour integration. Putting all of this knowledge together allows evaluation of $Z(n)$ for any integer $n > 1$, as in the following cases (for $\lambda = \frac{1}{2}$, which choice allows a little simplification):

$$Z(2) = \frac{3^{5/3}\Gamma^4\left(\frac{2}{3}\right)}{\pi^2} \tag{4.12}$$

$$Z(3) = 4 - \frac{3^{5/2}\Gamma^6\left(\frac{2}{3}\right)}{\pi^3} \tag{4.13}$$

$$Z(4) = \frac{3^{10/3}\Gamma^8\left(\frac{2}{3}\right)}{\pi^4} - \frac{3^{-1/6}8\Gamma^2\left(\frac{2}{3}\right)}{\pi} \tag{4.14}$$

$$Z(5) = \frac{3^{2/3}10\Gamma^4\left(\frac{2}{3}\right)}{\pi^2} - \frac{3^{25/6}\Gamma^{10}\left(\frac{2}{3}\right)}{\pi^5} \tag{4.15}$$

$$Z(6) = \frac{16}{5} - \frac{3^{5/2}4\Gamma^6\left(\frac{2}{3}\right)}{\pi^3} + \frac{3^5\Gamma^{12}\left(\frac{2}{3}\right)}{\pi^6} \tag{4.16}$$

and so on. On the appearance of such formulae we are moved to conjecture that each $Z(n)$ is always a polynomial, with rational coefficients, in the curious number

$$\frac{\Gamma^2\left(\frac{2}{3}\right)}{3^{1/6}\pi}\,. \tag{4.17}$$

Here is how one may test the Waring limiting scheme (1.14) numerically for the ground state. First, for $\lambda = \frac{1}{2}$ the ground-state energy is known (from tables of Airy zeros) to be

$$E_0 \sim 1.169\,053\,705\ldots\,. \tag{4.18}$$

Consider $Z(30)$, which as expected is a formidable but finite series. The numerical value of the Waring approximation to E_0 turns out to be

$$Z(30)^{-1/30} \sim 1.169\,053\,703\ldots \tag{4.19}$$

which gives a fractional error of order 10^{-9}.

One byproduct of this quantum zeta analysis is a set of identities involving the time-honoured Airy zeros a_n. Using the proportionality of the quantum bouncer's eigenvalues to these zeros we establish the attractive identity

$$\sum_{n=1}^{\infty} \frac{1}{a_n^2} = \frac{3^{5/3}\Gamma^4\left(\frac{2}{3}\right)}{4\pi^2} \tag{4.20}$$

with analogous identites, involving higher even powers of $1/a_n$, following immediately from the other exact Z evaluations.

The potential $V(x) = |x|$, where now as in Section 3 the spatial domain is $(-\infty, \infty)$, has energy eigenvalues proportional to $|a_n|$ (for odd states) but proportional to $|a_n'|$ (for even states), where a_n' denotes the nth zero of the derivative Ai'. From (3.10), then, we arrive at another evaluation

$$\sum_{n=1}^{\infty} \left(\frac{1}{a_n} - \frac{1}{a_n'}\right) = 3^{-2/3}\frac{\Gamma\left(\frac{2}{3}\right)}{\Gamma\left(\frac{4}{3}\right)}\,. \tag{4.21}$$

On subtraction of equation (3.10) from (3.9), and again scaling properly from energy eigenvalues to Airy zeros, we develop a conjecture: the analytic continuation of the function

$$z(s) = \sum_{n=1}^{\infty} \frac{1}{|a_n|^s} \tag{4.22}$$

valid as an explicit sum for $\mathrm{Re}(s) > \frac{3}{2}$, has

$$z(1) = -3^{-2/3}\frac{\Gamma\left(\frac{2}{3}\right)}{\Gamma\left(\frac{4}{3}\right)} \tag{4.23}$$

and that the $Z(s)$ of the quantum bouncer (with $\lambda = \frac{1}{2}$) has the (negative) continuation value

$$Z(1) = 2z(1)\,. \tag{4.24}$$

5. The delta ring

We turn to another system for which exact evaluation of $Z(n)$ is possible for any positive integer n. The 'delta ring' is a system for which a particle moves freely on a circle (angle $x \in (-\pi, \pi]$), save for the influence of a delta function well of coupling A at angle $x = 0$. The desired Green function, call it $G^{(A)}(x, x_0, E)$, will be a particular solution to a periodicized version of (1.5)

$$-\frac{1}{2}\frac{\partial^2 G}{\partial x^2} + V(x)G - EG = -\sum_{n\in Z} \delta(x - x_0 - 2\pi n)\,. \tag{5.1}$$

where the periodic potential with coupling A is given by

$$V(x) = -A \sum_{n\in Z} \delta(x - 2\pi n)\,. \tag{5.2}$$

When $A = 0$ the system is a free rotor whose Green function, call it $G^{(0)}$, is a simple superposition of free particle Green functions

$$\begin{aligned} G^{(0)}(x, x_0, E) &= -\frac{\mathrm{i}}{k} \sum_{n\in Z} \mathrm{e}^{\mathrm{i}k|x+2\pi n - x_0|} \\ &= \frac{1}{k} \frac{\cos(k(\pi - |x - x_0|))}{\sin(k\pi)} \end{aligned} \tag{5.3}$$

where $E = k^2/2$. As usual the energy eigenvalues are pole locations, which occur for $k \in Z$

$$E = 0, \frac{1^2}{2}, \frac{2^2}{2}, \frac{3^2}{2}, \ldots \tag{5.4}$$

where it is important to observe that each positive E value is two-fold degenerate: there are two eigenstates (one even, one odd parity) for each positive eigenvalue. Clearly, the quantum zeta function is ill-defined for the $A = 0$ free rotor, because E_0 vanishes. However, for non-zero A we may proceed to evaluate $Z(n)$.

Consider first a system defined on the full axis ($x \in (-\infty, \infty)$) and with potential (5.2). (The defining Schrödinger equation, however, is to have only a single source term $-\delta(x - x_0)$ on the right.) This system is envisioned as a particle moving freely save for the influence of an infinitely wide delta-function comb of separation 2π. Using the path integral approach of Crandall (1993) we may formally expand the Green function, call it $H^{(A)}$ to distinguish it from $G^{(A)}$, as

$$\begin{aligned} H^{(A)}(x, x_0, E) = -\frac{\mathrm{i}}{k} \sum_{j=0}^{\infty} \left(\frac{\mathrm{i}A}{k}\right)^j \sum_{\mu_1,\ldots,\mu_j\in Z} \exp\big(&\mathrm{i}k(|x - 2\pi\mu_j| + |2\pi\mu_j - 2\pi\mu_{j-1}| \\ &+ \cdots + |2\pi\mu_1 - x_0|\big) \end{aligned} \tag{5.5}$$

where the $j = 0$ summation is understood to be just $\mathrm{e}^{\mathrm{i}k|x-x_0|}$. Convergence issues for the infinite μ sums can be successfully addressed by assigning to k a positive imaginary part. Now to obtain the delta ring Green function $G^{(A)}$ we can periodicize according to

$$G^{(A)}(x, x_0, E) = \sum_{n\in Z} H^{(A)}(x + 2\pi n, x_0, E)\,. \tag{5.6}$$

Happily, it turns out that the entire perturbation sum now collapses because of the n-summation. Let both $x, x_0 \in (-\pi, \pi]$, and consider the first sum encountered in the development of (5.6), namely

$$\sum_{n\in Z} \mathrm{e}^{\mathrm{i}k|x+2\pi n-2\pi\mu_j|}\,. \tag{5.7}$$

This sum is patently independent of μ_j. This means the μ_j sum itself can be performed, which sum is independent of μ_{j-1}, and so on. The perturbation sum thus boils down to

$$G^{(A)}(x, x_0, E) = G^{(0)}(x, x_0, E) - \frac{AG^{(0)}(x, 0, E)G^{(0)}(0, x_0, E)}{1 + AG^{(0)}(0, 0, E)}\,. \tag{5.8}$$

Explicitly, then, the exact delta ring Green function for $x, x_0 \in (-\pi, \pi]$ is

$$
\begin{aligned}
G^{(A)}(x, x_0, E) = {}& \frac{1}{k}\frac{\cos(k(\pi - |x - x_0|))}{\sin(k\pi)} \\
& - \frac{A}{2k^2}\frac{\csc^2(\pi k)}{1 + (A/k)\cot(\pi k)}\left(\cos\big(k(|x| - |x_0|)\big) + \cos\big(k(|x| + |x_0| - 2\pi)\big)\right) .
\end{aligned}
$$

Assuming A be non-zero, the energy eigenvalues are now the pole locations given by either of the two conditions

$$
\begin{aligned}
& \frac{\sin(k\pi)}{k} = 0 \\
& \tan(\pi k) = -\frac{A}{k} .
\end{aligned}
\tag{5.10}
$$

The former condition specifies odd parity states, whose energies incidentally are unchanged by any delta function because the odd parity wavefunctions vanish at the delta location. The second relation determines the even parity states, these states generally being shifted in a direction depending on the sign of the coupling constant A. Note that, due to delicate cancellation of singularities in (5.9) when A is non-zero, there is no pole at $k = 0$.

Consider now a function $Z(1; k)$ defined as

$$
\begin{aligned}
Z(1; k) &= \sum_n \frac{1}{E_n - k^2/2} \\
&= -2\int_0^\pi G^{(A)}(x, x, E)\, \mathrm{d}x \\
&= \frac{1}{k^2} - \frac{\pi}{k}\cot(\pi k) - \frac{\pi}{A} + \frac{\pi\left(\frac{A}{k} + \frac{k}{A}\right) - \frac{1}{k}}{k + A\cot(\pi k)} .
\end{aligned}
\tag{5.11}
$$

It is this function whose k-derivatives at $k = 0$ will give exact quantum zeta evaluations. Evidently the number $Z(n)$ can always be cast as a polynomial in $1/A$, with coefficients being rational multiples of powers of π. In particular,

$$Z(1) = -\frac{2\pi}{A} + \frac{4}{3}\pi^2 \tag{5.12}$$

$$Z(2) = \frac{4\pi^2}{A^2} - \frac{8}{3}\frac{\pi^3}{A} + \frac{32}{45}\pi^4 \tag{5.13}$$

$$Z(3) = -\frac{8\pi^3}{A^3} + \frac{8\pi^4}{A^2} - \frac{16}{5}\frac{\pi^5}{A} + \frac{512}{945}\pi^6 \tag{5.14}$$

and so on. Because odd-parity states are unperturbed by the delta potential, an evaluation of Y is immediate

$$Y(s) = Z(s) - 4\zeta(2s) . \tag{5.15}$$

As we can resolve $Z(n), Y(n)$ for any positive integer n, it is intriguing to contemplate the use of the asymptotic relation (1.16) to effect an A-expansion of the ground-state energy. Symbolic computation suggests that the approximation

$$E_0 \sim \frac{1}{2}\left(\frac{Z(n)}{Z(n+1)} + \frac{Y(n)}{Y(n+1)}\right) \tag{5.16}$$

gives a series for the delta ring ground energy, to $O(A^{n+1})$. Thus for example the employment of exact evaluations $Z(4)$, $Z(5)$, $Y(4)$, $Y(5)$ yields

$$E_0 \sim -\frac{A}{2\pi} - \frac{1}{6}A^2 - \frac{2\pi}{45}A^3 - \frac{8\pi^2}{945}A^4 + O(A^5) \tag{5.17}$$

corresponding to the least solution to the tangent relation of (5.10) with $E = k^2/2$.

6. The quantum pendulum

We turn to a difficult but illuminating system, the 'quantum pendulum' specified by

$$V(x) = -A\cos x \tag{6.1}$$

where $x \in (-\pi, \pi]$ and all wavefunctions have period 2π. This system is again a free rotor, save for directed gravitational force acting on the motion. For uniform gravity g, particle mass m, and pendulum rod length L, the coupling A can be taken to be the dimensionless structure constant

$$A = \frac{gm^2L^3}{\hbar^2}\,. \tag{6.2}$$

Though closed forms for quantum zetas are yet unattainable, we shall at least be able to provide convergent series for calculation of $Z(1)$ and $Y(1)$. In particular, the series for $Y(1)$ will enjoy rapid convergence.

We shall employ an infinite-dimensional matrix approach. Assume first that the Green function appropriate to the periodicized Schrödinger equation (5.1) with $V(x) = -A\cos x$ can be written as the *ansatz*

$$G(x, x_0, E) = -\frac{1}{\pi}\sum_{n\in Z} g_n(x_0, E)\mathrm{e}^{\mathrm{i}n(x-x_0)}\,. \tag{6.3}$$

Now equation (5.1) is formally satisfied if, for $n \in Z$ and $E = k^2/2$ we have

$$(n^2 - k^2)g_n(x_0) - A(g_{n-1}(x_0)\mathrm{e}^{\mathrm{i}x_0} + g_{n+1}(x_0)\mathrm{e}^{-\mathrm{i}x_0}) = 1\,. \tag{6.4}$$

This leads to a formal representation of the Green function as

$$G(x, x_0, E) = -\frac{1}{\pi}\sum_{m,n\in Z} \mathrm{e}^{\mathrm{i}mx}(D^{-1})_{mn}\mathrm{e}^{-\mathrm{i}nx_0} \tag{6.5}$$

where D is the infinite-dimensional matrix

$$D = \begin{bmatrix} \ddots & & & & & & \\ & -k^2+2^2 & -A & 0 & 0 & 0 & \\ & -A & -k^2+1^2 & -A & 0 & 0 & \\ & 0 & -A & -k^2 & -A & 0 & \\ & 0 & 0 & -A & -k^2+1^2 & -A & \\ & 0 & 0 & 0 & -A & -k^2+2^2 & \\ & & & & & & \ddots \end{bmatrix} \tag{6.6}$$

Explicitly

$$D_{mn} = (-k^2 + m^2)\delta_{mn} - A\delta_{m,n-1} - A\delta_{m,n+1}\,. \tag{6.7}$$

Consider for the moment a finite version D_N of the matrix D, which version is $(2N+1)$-by-$(2N+1)$, so that the diagonal elements of D_N run from $-k^2 + (-N)^2$ to $-k^2 + (N^2)$ inclusive. We shall ultimately take the limit $N \to \infty$. What will drive the ensuing analysis is a set of key numbers e_j defined as determinants of partial, $(N-j+1)$-by-$(N-j+1)$ matrices (we now suppress zero entries in the visual display)

$$e_j = \mathrm{Det}\begin{bmatrix} -k^2 + j^2 & -A & & & \\ -A & -k^2 + (j+1)^2 & -A & & \\ & -A & \ddots & & \\ & & & -k^2 + (N-1)^2 & -A \\ & & & -A & -k^2 + N^2 \end{bmatrix} \tag{6.8}$$

and we assign the value $e_{N+1} = 1$ for convenience in what follows. It is evident on the basis of matrix manipulation that

$$\mathrm{Det}(D_N) = -k^2 e_1^2 - 2A^2 e_1 e_2 \tag{6.9}$$

and furthermore that the number $F = e_1/e_2$ will be, in the large-N limit, the continued fraction

$$F(k) = (1 - k^2) - \cfrac{A^2}{(4 - k^2) - \cfrac{A^2}{(9 - k^2) - \cdots}}\,. \tag{6.10}$$

The quantum pendulum eigenvalues occur as E-singularities of the D matrix. It follows from the relation (6.9) for $\mathrm{Det}(D_N)$ that for even parity states an eigenvalue E is a solution to the relation

$$0 = -2E - \cfrac{2A^2}{(1 - 2E) - \cfrac{A^2}{(4 - 2E) - \cdots}} \tag{6.11}$$

while for odd parity states E the relevant relation is

$$0 = 1 - 2E - \cfrac{A^2}{(4 - 2E) - \cfrac{A^2}{(9 - 2E) - \cdots}}\,. \tag{6.12}$$

These continued fraction zeros are (up to a proportionality constant) classical Mathieu eigenvalues (Abramowitz and Stegun 1965), which is expected because the pendulum Schrödinger equation is a manifestation of the Mathieu equation.

Using the Green function representation (6.5) we have the trace relations:

$$\begin{aligned} Z(1) &= \frac{1}{\pi}\int_{-\pi}^{\pi} \sum_{m,n\in Z} \mathrm{e}^{\mathrm{i}mx}(D^{-1})_{mn}\mathrm{e}^{-\mathrm{i}nx}\,\mathrm{d}x \\ &= 2\,\mathrm{Tr}(D^{-1}) \end{aligned} \tag{6.13}$$

where Tr denotes matrix trace, and

$$Y(1) = \frac{1}{\pi} \int_{-\pi}^{\pi} \sum_{m,n \in Z} \mathrm{e}^{\mathrm{i}mx} (D^{-1})_{mn} \mathrm{e}^{\mathrm{i}nx} \, \mathrm{d}x$$
$$= 2\,\mathrm{Cr}(D^{-1}) \tag{6.14}$$

where Cr denotes the 'counter-trace;' i.e. the sum of the elements of the perpendicular diagonal, or $\sum_m D^{-1}_{m,-m}$.

Happily, it is possible to express the inverse of D_N in convenient form. By analysing minors, for $i \geqslant j$ one obtains

$$(D_N^{-1})_{ij} = \frac{(-1)^{i+j}(-A)^{i-j} e_{1-j} e_{i+1}}{\mathrm{Det}(D_N)} \tag{6.15}$$

with each of i, j running through $[-N, N]$. All other elements of the inverse may be obtained from Hermitian symmetry. Thus we have

$$\mathrm{Tr}(D_N^{-1}) = \frac{1}{\mathrm{Det}(D_N)} \left(e_1^2 + 2(e_0 e_2 + e_{-1} e_3 + e_{-2} e_4 + \cdots)\right) \tag{6.16}$$

$$\mathrm{Cr}(D_N^{-1}) = \frac{1}{\mathrm{Det}(D_N)} \left(e_1^2 + 2(A^2 e_2^2 + A^4 e_3^2 + A^6 e_4^2 + \cdots)\right) . \tag{6.17}$$

Convergent series for the zeta functions can now be formulated on the basis of recursion relations for the key numbers e_j. Let p_n, q_n be the convergents to the continued fraction for $F(k)$. Specifically, $p_{-1} = 1, q_{-1} = 0$, $p_0 = 1 - k^2, q_0 = 1$, and for $n > 1$

$$p_{n-1} = (n^2 - k^2) p_{n-2} - A^2 p_{n-3} \tag{6.18}$$

$$q_{n-1} = (n^2 - k^2) q_{n-2} - A^2 q_{n-3} . \tag{6.19}$$

Now the e_j satisfy the same recursion relations (except for an index offset), and for non-negative n we have superposition formulae

$$e_{-n} = (-k^2 e_1 - A^2 e_2) p_{n-1} - A^2 e_1 q_{n-1} \tag{6.20}$$

$$e_{n+2} = A^{-2n} (e_2 p_{n-1} - e_1 q_{n-1}) . \tag{6.21}$$

The resulting zeta series now follow from (6.9) and the trace formulae (6.16), (6.17) as (for these series, p_m, q_m denote the convergents to the number $F(0)$)

$$Z(1) = -\frac{F(0)}{A^2} + \frac{2}{F(0)} \sum_{n=0}^{\infty} \frac{p_{n-1}^2 - F(0)^2 q_{n-1}^2}{A^{2n}} \tag{6.22}$$

$$Y(1) = -\frac{F(0)}{A^2} - \frac{2}{F(0)} \sum_{n=0}^{\infty} \frac{(p_{n-1} - F(0) q_{n-1})^2}{A^{2n}} . \tag{6.23}$$

Both zeta functions here are well defined unless the pendulum with coupling A happens to have a zero eigenvalue. Stated another way: if neither $F(0) = 1 - A^2/(4 - A^2/(9 - A^2 \cdots))$ nor $A^2/F(0)$ vanishes, the sums exist and $Z(1), Y(1)$ are both well defined. The series for

$Y(1)$ is quite convergent, due to the rapidity with which $p_n/q_n \to F(0)$. A numerical evaluation of the parity zeta function is, for pendulum coupling $A = 1$,

$$Y(1) \sim -3.615\,644\,253\,507\,767\,293\,665\,116\,737\,324\,139\,287\,349\,999\,562\,811\,928\,0509\ldots. \tag{6.24}$$

Actually, due to the satisfactory convergence it is possible to obtain typical $Y(1)$ evaluations to thousands of digits in a convenient time span. The $Z(1)$ series, however, converges slowly as is. But convergence can be accelerated via detailed analysis of the continued fraction asymptotics. An example of an accelerated series for this quantum zeta function is

$$\begin{aligned} Z(1) = {} & -\frac{F(0)}{A^2} + 4\zeta(2) + 8A^2\zeta(6) + 24A^2\zeta(8) \\ & + \frac{2}{F(0)} \sum_{n=1}^{\infty} \left(\frac{p_{n-2}^2 - F(0)^2 q_{n-2}^2}{A^{2n-2}} - 2F(0) \left(\frac{1}{n^2} + \frac{2A^2}{n^6} + \frac{6A^2}{n^8} \right) \right). \end{aligned} \tag{6.25}$$

Such acceleration techniques were used to calculate $Z(1)$ for coupling $A = 1$, as

$$Z(1) \sim 4.757\,888\,110\,183\,612\,153\,949\,189\,635\,865\,216\,502\,181\,005\,204\,662\,108\,093\,48\ldots. \tag{6.26}$$

It is hard to imagine attaining such high precision through, say, direct summation of reciprocals of calculated Mathieu eigenvalues.

A more general Y series can in fact be used to extract isolated Mathieu eigenvalues themselves. The generalized version of (6.23) is

$$\begin{aligned} Y(1; k) &= \sum_{n=0}^{\infty} \frac{(-1)^n}{E_n - k^2/2} \\ &= \frac{1}{1 + (k^2 F(k)/2A^2)} \left(-\frac{F(k)}{A^2} - \frac{2}{F(k)} \sum_{n=0}^{\infty} \frac{(p_{n-1} - F(k) q_{n-1})^2}{A^{2n}} \right) \end{aligned} \tag{6.27}$$

where now p_m, q_m are understood to be convergents to $F(k)$. Set $A = \frac{5}{4}$, so that the standard Mathieu nomenclature (Abramowitz and Stegun 1965) has $q = 4A = 5$, and $b_2(q) = 8E_1$, where E_1 is the first excited energy of the quantum pendulum. For this A it turns out that E_1 is the smallest (in magnitude) system eigenvalue. Traditional tables have $b_2(5) \sim 2.099\,460\,45\ldots$. Now taking *numerical* derivatives of $Y(1; \sqrt{2E})$ at $E = 0$ allows, in the spirit of (1.7) and (1.14), a Waring estimation of E_1. For $n = 40$ this procedure was carried out, giving the Mathieu eigenvalue estimate

$$b_2(5) \sim 2.099\,460\,445\,486\,665\,364\ldots \tag{6.27}$$

presumed correct to the implied precision.

7. Matrix methods

Among the systems we have analysed stand two quantum scenarios for ring domain $x \in (-\pi, \pi]$. Consider the general ring system defined by

$$-\frac{1}{2}\frac{\partial^2 G}{\partial x^2} + V(x)G - EG = -\sum_{n\in Z}\delta(x - x_0 - 2\pi n) \tag{7.1}$$

where the potential

$$V(x) = \sum_{m\in Z} a_m \cos(mx) \tag{7.2}$$

is manifestly periodic. In this notation the delta ring of section 5 has $a_m = -A/(2\pi)$ for all m, while the quantum pendulum of section 6 has $a_1 = a_{-1} = -A/2$ and all other a_m zero.

We could have studied the quantum zeta function for the delta ring using the general formal solution

$$G(x, x_0, E) = -\frac{1}{\pi}\sum_{m,n\in Z} \mathrm{e}^{\mathrm{i}mx}(D^{-1})_{mn}\mathrm{e}^{-\mathrm{i}nx_0} \tag{7.3}$$

where the D matrix is cast in terms of the Fourier coefficients of the potential:

$$D = \begin{bmatrix} \ddots & & & & \\ & 1^2 - k^2 & 0 & 0 & \\ & 0 & -k^2 & 0 & \\ & 0 & 0 & 1^2 - k^2 & \\ & & & & \ddots \end{bmatrix} + 2\begin{bmatrix} \ddots & & & & \\ & a_0 & a_1 & a_2 & \\ & a_{-1} & a_0 & a_1 & \\ & a_{-2} & a_{-1} & a_0 & \\ & & & & \ddots \end{bmatrix}. \tag{7.4}$$

Within this matrix formalism, then, the delta ring could have been analysed in terms of determinants of matrices of the form

$$M = \Delta + \begin{bmatrix} \ddots & & & & \\ & c & c & c & \\ & c & c & c & \\ & c & c & c & \\ & & & & \ddots \end{bmatrix} \tag{7.5}$$

where Δ is a diagonal matrix and $c = -A/\pi$. Indeed, the determinant of any such matrix has an elegant symbolic representation:

$$\mathrm{Det}(M) = -z^2\frac{\partial}{\partial z}\left(\frac{1}{z}\prod_i(\Delta_{ii} + c - z)\right)\Bigg|_{z=c}. \tag{7.6}$$

This representation can actually be used (in fact the algebraic details are instructive) to establish the exact diagonal elements of D^{-1} for the delta ring, and therefore to recover the function $Z(1; k)$ defined in (5.11).

For application to other, as yet unexplored periodic ring systems, we describe an algorithm due to Wheeler (1995) for trace computation. This method has the feature of requiring neither determinantal calculations nor matrix inversions. The Wheeler algorithm runs so:

To obtain $\mathrm{Tr}(D^{-1})$, where D is N-by-N,

(i) Define $T_m := \mathrm{Tr}(D^m)$, for $m = 0, 1, 2, \ldots, N$;
(ii) Define $Q_0 := 1$ and for $m = 1, 2, \ldots, N$

$$Q_m := \sum_{j=1}^{m} (-1)^{j-1} \frac{(m-1)!}{(m-j)!} T_j Q_{m-j}; \tag{7.7}$$

(iii) Define $P_i := (-1)^i Q_{N-i}/(N-i)!$, for $i = 0, \ldots, N$.

Then

$$\mathrm{Tr}(D^{-1}) = -\frac{1}{P_0} \sum_{i=0}^{N-1} T_i P_{i+1}\,. \tag{7.8}$$

We present a numerical calulation based on the algorithm. Consider the periodic potential

$$V(x) = -\cos(x) + 2\cos(2x) - \cos(3x) \tag{7.9}$$

which specifies what might be called a 'rippled pendulum' system. A quantum zeta function evaluation is

$$Z(1) = 2\,\mathrm{Tr}(D^{-1}) \tag{7.10}$$

where D is the seven-banded infinite matrix

$$D = \begin{bmatrix} \ddots & & & & & & \\ & 2^2 & -1 & 2 & -1 & 0 & \\ & -1 & 1^2 & -1 & 2 & -1 & \\ & 2 & -1 & 0 & -1 & 2 & \\ & -1 & 2 & -1 & 1^2 & -1 & \\ & 0 & -1 & 2 & -1 & 2^2 & \\ & & & & & & \ddots \end{bmatrix}. \tag{7.11}$$

Using the Wheeler algorithm which, again, invokes only matrix powering and rational arithmetic, we obtain (for finite $(2N+1)$-by-$(2N+1)$ versions of D and Romberg extrapolation over various N up to $N = 100$) the estimate $Z(1) \sim 1.315\,96$. It would be good to get independent verification of this Z value for the rippled pendulum.

8. Open problems

An outstanding open problem is that of providing exact evaluation of $Z(n)$, for some integer $n > 1$, for the quartic oscillator. It should be mentioned that Voros (1980) has evaluated analytic continuation values such as $Z(0), Z'(0)$; and also given numerical values of other $Z(s)$. Clearly, the larger a real argument of Z, the more information is conveyed about the quartic's elusive ground-state energy.

Though we have presented a prescription for resolving all $Z(n), n > 1$ for the quantum bouncer, and conjectured an analytic continuation value $Z(1)$, it would be of interest to evaluate $Z(s)$ for non-integral s. Being as the nth Airy zero rises in magnitude as $cn^{2/3}$, one wonders, for example, whether the analytic continuation $Z(s)$ has a solitary pole at $s = \frac{3}{2}$. There is also the open polynomial conjecture ending with (4.17).

For the delta ring we have likewise shown how to evaluate $Z(n)$ for all positive integers n, yet we do not know $Z(s)$ for any other s. On the basis of the asymptotic growth $E_n \sim n^2/2$ for any coupling A, one may expect a pole of Z at $s = \frac{1}{2}$.

For the quantum pendulum it is evidently difficult to develop highly efficient series for any $Z(n)$. One wonders whether it be *generally* true across systems that $Y(1)$ appear more numerically tractable than $Z(1)$. Another open problem is to derive quantum zeta results for the pendulum on the basis of a perturbation expansion of which (5.5) is indicative. Though this approach has worked out for the delta ring, the analogous perturbation series for the pendulum has so far, due presumably to its extreme complexity, resisted attack.

Now to the issue of quantum chaos. First consider the circular billiard, whose defining Schrödinger equation is taken to be the two-dimensional form

$$-\tfrac{1}{2}\nabla^2 G - EG = -\delta^2(r - r_0) \tag{8.1}$$

with the caveat that the Green function $G(r, r_0, E)$ vanish everywhere on the unit circle; i.e. $G = 0$ whenever $|r| = 1$ or $|r_0| = 1$. This system (with and without magnetic flux) has been studied by Berry (1986), Elizalde (1993) and Leseduarte (1994). The quantum zeta function is, for sufficiently large $\mathrm{Re}(s)$

$$Z(s) = \sum \frac{1}{E^s} = 2^s \sum_{\nu \in Z} \sum_{n \in Z^+} \frac{1}{j_{|\nu|,n}^{2s}} \tag{8.2}$$

where $j_{\mu,n}$ is the nth positive zero of J_μ. One may employ the identity (Watson 1922)

$$J_\nu(z) = \frac{(z/2)^\nu}{\Gamma(\nu + 1)} \prod_{n=1}^{\infty} \left(1 - \frac{z^2}{j_{\nu,n}^2}\right) \tag{8.3}$$

and the standard ascending series for J_ν to obtain such evaluations as

$$Z(2) = \tfrac{1}{12}\pi^2 - \tfrac{5}{8} \tag{8.4}$$

$$Z(3) = \tfrac{1}{4}\zeta(3) - \tfrac{1}{16}\pi^2 + \tfrac{35}{96} \tag{8.5}$$

and so on. Berry (1986) has shown how to obtain such integer-argument evaluations from the Itzykson *et al* trace formulae applied to the zero-energy Green function (which function for the circular billiard can actually be written down in an elegant, logarithmic form). On the other hand the work of Elizalde (1993) reveals a clever method for extracting zeta values without recourse to a Green function, Bessel sum rules being used instead.

Though the numbers $Z(n), n = 2, 3, \ldots$ are tractable for the billiard, we know little about the analytic continuation $Z(s)$, although the continuation to the negative real axis has been effectively studied in Leseduarte (1994). The open problem of general analytic comtinuation is important in regard to quantum chaos. There is the possibility that quantum zeta functions $Z(s)$ for *classically* chaotic systems will possess special analytic properties. For example, some characteristic distribution of zeros of $Z(s)$ in the complex s-plane might be a 'signature' for a chaotic Hamiltonian. In particular, the 'heart' and 'Africa' billiards (each having non-circular boundary) exhibit classical chaos (Robnik 1983). It is for these reasons that further results on $Z(s)$ for classically chaotic billiard systems, and even for the circular billiard, would be welcome indeed.

Another possible approach to an analytic theory of quantum chaos is the following. An anharmonic oscillator Hamiltonian, such as yields the quantum bouncer or quantum pendulum, can be expected to exhibit classical chaos under the influence of a time-dependent driving force (an object bouncing under gravity on an undulating platform is one of the oldest and easiest demonstrations of chaos). Therefore the proposed Mellin transform definition (1.12) might be adopted in order to resolve some asymptotic property of the analytic continuation of $Z(s)$. In this way, characteristic quantum-chaotic properties of Z might be revealed. One looks longingly at the Mellin transform and wonders whether path integration might allow for sufficiently fine analytical approximations. Indeed, it is theoretically possible to integrate over the time domain very early on in the Feynman path integration development of K. The procedure yields a pure-geometric (i.e. devoid of time-dependence) path integral representation for $Z(s)$. Work on this formalism is in progress.

Finally, when the potential is symmetric there is an interesting, as yet unexplored perturbation theory approach to evaluation of the parity zeta function $Y(s)$. This is to use the formal Green function representation, derivable via path integration (Crandall 1993)

$$G(x, x_0, E) = -\frac{i}{k} \sum_{j=0}^{\infty} \left(\frac{-\mathrm{i}}{k}\right)^j \int \exp\big(\mathrm{i}k(|x - x_j| + |x_j - x_{j-1}| + \cdots + |x_1 - x_0|)\big) \prod_{m=1}^{j} (V(x_m)\,\mathrm{d}x_m) \tag{8.6}$$

with the $j = 0$ integral interpreted as $\mathrm{e}^{\mathrm{i}k|x-x_0|}$, and as usual $E = k^2/2$. Since Y can be obtained in principle from the integral of $G(x, -x, E)$ over the spatial domain, one may perform this x-integral *first*. This removes all spatial dependence from the perturbation expansion, leaving only a set of E-dependent, j−dimensional integrals for $j = 1, 2, \ldots$. What is especially intriguing is that for many potentials, such as power potentials, exponential potentials $V(x) = \mathrm{e}^{\lambda|x|}$, and many other forms, each j-integral can be cast in closed form. Thus there is hope for new evaluations of $Y(n), n \in Z^+$ based on exact summation of perturbation series.

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