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Exact and approximate energy sums in potential wells

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Abstract

Sums of the N lowest energy levels for quantum particles bound by potentials are calculated, emphasising the semiclassical regime $N \gg 1$. Euler-Maclaurin summation, together with a regularisation, gives a formula for these energy sums, involving only the levels $N+1$, $N+2$…. For the harmonic oscillator and the particle in a box, the formula is exact. For wells where the levels are known approximately (e.g. as a WKB series), with the higher levels being more accurate, the formula improves accuracy by avoiding the lower levels. For a linear potential, the formula gives the first Airy zero with an error of order 10^{-7}. For the Pöschl–Teller potential, regularisation is not immediately applicable but the energy sum can be calculated exactly; its semiclassical approximation depends on how N and the well depth are linked. In more dimensions, the Euler–Maclaurin technique is applied to give an analytical formula for the energy sum for a free particle on a torus, using levels determined by the smoothed spectral staircase plus some oscillatory corrections from short periodic orbits.

Keywords: semiclassical, Euler–Maclaurin, WKB

(Some figures may appear in colour only in the online journal)

1. Introduction

This is a study of sums of the first N energies E_1, E_2... of quantum systems with discrete spectra, that is

$$S(N) = \sum_{1}^{N} E_n, \tag{1.1}$$

concentrating on the asymptotics for large N. This work was motivated by applications in density-functional theory [1, 2]. A sufficiently accurate and robust approximation to the sum of the lowest N levels of a potential could avoid the need to solve the Kohn–Sham equations, thereby increasing the number of electrons that can be treated. An independent interest is the combination of techniques we employ.

The sum $S(N)$ is a function of the discrete index N. We will need to represent it for continuous N. One way is simply to interpolate linearly between the integers, i.e.

$$S\left(N\right)=\sum_{1}^{\infty}\Theta\left(N+1-n\right)\left(N+1-n\right)\left(E_{n}-E_{n-1}\right)\quad\left(E_{0}=0\right). \tag{1.2}$$

This function is continuous but not smooth: its slope is discontinuous at integers N. Our aim here is to find formulas for $S(N)$ that are smooth, while still coinciding with, or being close to, the exact or approximate $S(N)$ at integers. Figure 1 displays the difference between the integer, linearly interpolated, and smooth functions $S(N)$.

Our technique, which works when all states are bound, is explained in section 2. A regularisation procedure enables the sum of the first N energies to be replaced by the sum of levels $N+1, N+2$.... In the usual cases, where the levels are known only approximately, with the levels below N being less accurate than those above, this has the advantage of avoiding contamination of the sum by the lower energies.

Sections 3–5 describe preliminary examples: simple cases where the levels are known and $S(N)$ can be evaluated analytically. We include the harmonic oscillator (section 3), and the particle in a 1D box (section 4), simply to illustrate the general technique. For the Pöschl–Teller potential (section 5), whose depth is finite and which binds a finite number of levels, the technique is not obviously applicable; the reason for including this additional exactly solvable case is because the potential contains a parameter (its depth), whose asymptotics interact interestingly with N.

The heart of the paper is section 6, where $S(N)$ is calculated for the odd energies of the linear potential $|x|$; these are the zeros of the Airy function [3, 4]. This is an explicit example where the approximate evaluation of $S(N)$ yields extraordinary accuracy when the individual levels are given, by WKB theory, in the form of a divergent series.

In more than one dimension, the energies fluctuate pseudo-randomly about those of a smoothed spectrum. This is the case whether the classical motion is integrable (level fluctuations Poissonian [5]) or chaotic (levels distributed according to random-matrix theory [6–8]). Then $S(N)$ can still be evaluated using the method of section 2, with the energies being those of the fully or partially smoothed spectrum. In section 7 we illustrate this for particles on a 2-torus.

In a complementary study [9], the statistics of the energy sum (1.1) has been calculated using random-matrix theory; we thank a referee for bringing this paper to our attention.

Although some of our approximations are semiclassical, we will save writing by setting Planck's constant $\hbar=1$. In the examples we treat, $\hbar$ can be eliminated by scaling; when this is not immediately obvious, it will be explained.

2. General method

The lower levels in $S(N)$ can be eliminated by writing the sum in (1.1) formally as the difference of two infinite divergent sums:

$$S\left(N\right)=S\left(\infty\right)-\sum_{N+1}^{\infty}E_{n}. \tag{2.1}$$

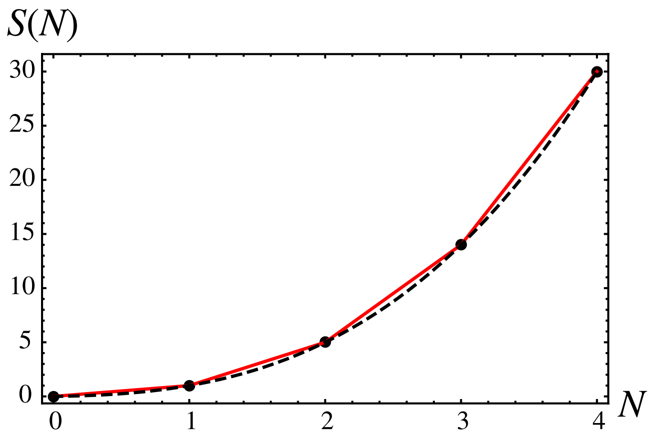

Figure 1. Discrete sum (dots), linearly interpolated sum (red online), and smooth energy sum (dashed curve) for a particle in a box (see section 4).

Both sums must be regularised by analytic continuation. For $S(\infty)$, which contributes a constant to $S(N)$, we accomplish this via the partition function [10] (also called the propagator for the heat equation, i.e. heat kernel); for a Hamiltonian H, this is

$$K(t) = Tr\left[\exp(-Ht)\right] = \sum_{1}^{\infty} \exp(-E_n t). \tag{2.2}$$

Usually this diverges as $t \to 0$, but its Laurent expansion may include a term proportional to t; hence the regularisation

$$S(\infty) = -\text{coefficient of } t \text{ in } K(t). \tag{2.3}$$

(Equivalently, $S(\infty)$ is the spectral zeta function $Z(s) = \sum_1^\infty E_n^{-s}$ [10], evaluated at $s = -1$.)

For the infinite sum over $N+1 \leqslant n < \infty$, we use the Euler–Maclaurin formula [3]. In this, the discrete energies E_n are represented by any interpolation for continuous n, and the discrete sum is expressed as an integral over continuous n, corrected by derivatives at the summation limit. Thus our theoretical expression for the energy sum is

$$S_{\text{th}}(N;K) = S(\infty) - \int_{N+1}^{\infty} \mathrm{d}nE_n - \tfrac{1}{2}E_{N+1} + \sum_{1}^{K} \frac{B_{2k}}{(2k)!}\partial_N^{2k-1}E_{N+1}. \tag{2.4}$$

B_{2k} are the Bernoulli numbers [3], expressed in terms of the Riemann zeta function $\zeta(s)$ for even integers:

$$B_{2k} = \frac{2\,(2k)!(-1)^{k+1}\zeta(2k)}{(2\pi)^{2k}} : B_2 = \tfrac{1}{6}, \quad B_4 = -\tfrac{1}{30}, \quad B_6 = \tfrac{1}{42}, \; \cdots . \tag{2.5}$$

The formally divergent integral over n must also be interpreted by the same regularisation. This is accomplished by the continuous-variable counterpart of the partition function procedure. In all cases we encounter, E_n involves monomials, whose interpretation, intuitively clear but explained in detail in appendix A, is

$$-\int_{N+1}^{\infty} \mathrm{d}n(n-\mu)^{\nu} = \frac{(N+1-\mu)^{\nu+1}}{\nu+1}. \tag{2.6}$$

In a few cases, described in the next two sections, the series involving k in (2.4) terminates, and Euler–Maclaurin is exact. More generally, as in the case described in section 6, the series over k is semiconvergent: it is an asymptotic series, whose terms get smaller and then increase [11].

An alternative representation of $S(N)$ follows from transforming the sum (1.1) using the Poisson summation formula [12]. This yields a series of integrals over n that are then approximated by expanding about their endpoints $n = N$. But this is simply a complicated way of reproducing the result of the Euler–Maclaurin representation (2.4). Poisson summation will however play a role in section 7, not in calculating the energy sum but in calculating the energies E_n involved in the sum, which will include some oscillatory contributions to the level counting function [13, 14] (spectral staircase). A different alternative would be to regularise not by using $S(\infty)$ but demanding $S(0) = 0$; this makes no difference for the examples in sections 3–5 and negligible difference in sections 6 and 7.

3. Harmonic oscillator

The energies, and the sum (1.1), are

$$E_n = n - \tfrac{1}{2} \Rightarrow S(N) = \tfrac{1}{2}N^2. \tag{3.1}$$

To interpret this in terms of the Euler–Maclaurin representation (2.4), we need the regularised sum over all n, in terms of the partition function (2.2) and (2.3). For this case, $K(t)$, and its Laurent expansion, can be evaluated explicitly:

$$\begin{aligned} K(t) &= \sum_1^\infty \exp\left(-\left(n-\tfrac{1}{2}\right)t\right) = \frac{1}{2\sinh\left(\tfrac{1}{2}t\right)} \\ &= t^{-1} - \tfrac{1}{24}t + \tfrac{7}{5760}t^3 + \cdots \Rightarrow S(\infty) = \tfrac{1}{24}. \end{aligned} \tag{3.2}$$

In the theoretical expression (2.4), we need (2.6) to interpret the infinite integral, leading to contributions that add to reproduce the exact energy sum:

$$S_{th}(N;1) = \tfrac{1}{24} + \tfrac{1}{2}\left(N+\tfrac{1}{2}\right)^2 - \tfrac{1}{2}\left(N+\tfrac{1}{2}\right) + \tfrac{1}{12} = \tfrac{1}{2}N^2. \tag{3.3}$$

An interesting minor variant is the spectrum without the zero-point energy (or, equivalently, the positive eigenvalues of an angular-momentum component), where $S(N)$ is the sum over the positive integers:

$$E_n = n \Rightarrow S(N) = \tfrac{1}{2}N(N+1). \tag{3.4}$$

The constant is $S(\infty) = 1 + 2 + 3 + \cdots$, discussed in recreational mathematics [15]. The regularisation (2.2) gives one interpretation of the old result in terms of the Riemann zeta function $\zeta(s)$, i.e. $S(\infty) = \zeta(-1) = -\frac{1}{12}$:

$$K(t) = \frac{1}{\exp t - 1} = t^{-1} - \tfrac{1}{2} + \tfrac{1}{12}t - \tfrac{1}{720}t^3 + \cdots \Rightarrow S(\infty) = \zeta(-1) = -\tfrac{1}{12}. \tag{3.5}$$

Thus (2.4) gives

$$S_{\mathrm{th}}(N;1) = -\tfrac{1}{12} + \tfrac{1}{2}(N+1)^2 - \tfrac{1}{2}(N+1) + \tfrac{1}{12} = \tfrac{1}{2}N(N+1). \tag{3.6}$$

4. 1D box

For a free particle in the space $0 \leqslant x \leqslant \pi$ between hard walls, the energies (with $\hbar = 2 \times \text{mass} = 1$), and the energy sum, are

$$E_n = n^2 \Rightarrow S(N) = \tfrac{1}{3}N^3 + \tfrac{1}{2}N^2 + \tfrac{1}{6}N. \tag{4.1}$$

For this case, the partition function is a theta function θ_3 [3], whose Poisson transformation shows that its expansion contains no term proportional to t, so the sum over all energies is zero:

$$\begin{aligned} K(t) &= \sum_1^\infty \exp\left(-n^2 t\right) = \tfrac{1}{2}\left(\theta_3\left(0, \exp(-t)\right) - 1\right) \\ &= \tfrac{1}{2}\left(-1 + \sqrt{\tfrac{\pi}{t}}\right) + \sqrt{\tfrac{\pi}{t}} \sum_1^\infty \exp\left(-\tfrac{m^2\pi^2}{t}\right) \Rightarrow S(\infty) = 0. \end{aligned} \tag{4.2}$$

Again, Euler–Maclaurin representation reproduces the exact $S(N)$:

$$S_{\text{th}}(N;1) = 0 + \tfrac{1}{3}(N+1)^3 - \tfrac{1}{2}(N+1)^2 + \tfrac{1}{6}(N+1) = \tfrac{1}{3}N^3 + \tfrac{1}{2}N^2 + \tfrac{1}{6}N. \tag{4.3}$$

5. Pöschl-Teller potential

This exactly solvable potential, with finite depth D supporting discrete energy levels between $E = 0$ and $E = D$, is

$$V(x) = D\left(1 - \frac{1}{\cosh^2 x}\right). \tag{5.1}$$

The energies (with $\hbar = \text{mass} = 1$), and the energy sum, are [16]

$$\begin{aligned} E_n(D) &= -\tfrac{1}{2}\left(n - \tfrac{1}{2}\right)^2 + \left(n - \tfrac{1}{2}\right)\sqrt{2D + \tfrac{1}{4}} - \tfrac{1}{8}, \\ S(N;D) &= -\tfrac{1}{6}N^3 + \tfrac{1}{2}N^2\sqrt{2D + \tfrac{1}{4}} - \tfrac{1}{12}N. \end{aligned} \tag{5.2}$$

For this potential, the number of bound states is finite, so the regularisation technique of section 2 is not immediately applicable—and regularisation would bring no advantage, because the system is exactly solvable. The Euler–Maclaurin formula can be applied in its conventional form [3], involving the lower limit $n = 1$ of (1.1), and is easily confirmed to reproduce the exact $S(N)$.

Temporarily reinstating $\hbar$, it is clear from the Schrödinger equation that it can be eliminated by the scaling $D \to D/\hbar$ (and corresponding scalings for E_n and $S(N)$). Thus the semiclassical regime ($\hbar$ small) is $D \gg 1$. We are interested only in the bound states, so the total number $n_{\max}(D)$ of energies in the sum (1.1), and the corresponding maximum value $S_{\max}(D)$ of the energy sum, and their leading-order large D approximations, are

$$\begin{aligned} E_n(D) = D \Rightarrow n = n_{\max}(D) &= \sqrt{2D + \tfrac{1}{4}} + \tfrac{1}{2} \approx \sqrt{2D} \equiv n_{\max 0}(D), \\ S(n_{\max}; D) = S_{\max}(D) &= \tfrac{2}{3}D\left(\sqrt{2D + \tfrac{1}{4}} + \tfrac{3}{4}\right) \approx \tfrac{\sqrt{8}}{3}D^{3/2} \equiv S_{\max 0}(D). \end{aligned} \tag{5.3}$$

For this exactly solvable potential, large D approximations do not lead to divergent series, as for the WKB approximations for general potentials [11] (an example is explored in the following section). Instead, the series is convergent, and associated with the expansion

Table 1. Ground state energies E_1 for Pöschl–Teller well depths $D = 1, 2, 3$, calculated directly from the expansion (5.6), and from the scaled energy sum (5.5).

D	1	2	3
$E_1(D)$	0.5	0.78078	1
$E_{1,0}(D)$	0.70710	1	1.22474
$E_{1,1}(D)$	0.45711	0.75	0.97475
$E_{1,2}(D)$	0.50130	0.78125	1.00026
$E_{1,3}(D)$	0.49992	0.78076	0.99999
$S_{sc0}(\nu_1;D)$	0.54044	0.83333	1.05808
$S_{sc1}(\nu_1;D)$	0.50130	0.78125	1.00026
$S_{sc2}(\nu_1;D)$	0.49992	0.78076	0.99999

$\sqrt{2D+\frac{1}{4}} = \sqrt{2D} + 1/\left(8\sqrt{2D}\right) + \cdots$ There are many ways to implement the large D (semiclassical) approximation of $S(N;D)$, depending on whether and how N is incorporated by linking it to D. With no linkage, i.e. approximating $S(N;D)$ with N fixed, all energies below N lie in the range $0 < E < \mathrm{O}(\sqrt{D})$, that is, near the bottom of the well. More natural is to scale N with the total number of bound states, and S with its maximum value. Again this can be done in several ways, depending on whether the scalings are done with $n_{\max}$ and $S_{\max}$ or $n_{\max0}$ and $S_{\max0}$ in (5.3). The scalings $n_{\max0}$ and $S_{\max0}$ lead to simpler and faster-converging large D approximations. Therefore we represent the level indices and the Pöschl–Teller energy sum in the form

$$\nu \equiv \frac{N}{n_{\max 0}}, \quad S_{sc}(\nu;D) \equiv \frac{S(\nu n_{\max 0}(D);D)}{S_{\max 0}(D)}. \tag{5.4}$$

With these scalings, the ranges of the level indices and the sum are $0 < \nu < 1$ and $0 < S_{sc} < 1$, and the semiclassical regime corresponds to D large, ν fixed. Explicitly,

$$S_{sc}(\nu;D) = \underbrace{\underbrace{\underbrace{\frac{\nu^2}{2}(3-\nu)}_{S_{sc0}(\nu)} - \frac{\nu(4-3\nu)}{32D}}_{S_{sc1}(\nu;D)} - \frac{3\nu^2}{1024D^2}}_{S_{sc2}(\nu;D)} + O\left(\frac{1}{D^3}\right). \tag{5.5}$$

This large D expansion is extraordinarily accurate, even for $D = 1$, as figure 2 illustrates. (The alternative scaling, using $n_{\max}$ and $S_{\max}$, introduces additional terms, of order $D^{1/2}$, $D^{-1/2}$, $D^{-3/2}$...).

The case $N = 1$ is interesting. Since $S(1) = E_1$, the energy sum is an alternative way of approximating the ground-state energy, to be compared with the direct large D expansion

$$E_1(D) = \tfrac{1}{2}\sqrt{2D+\tfrac{1}{4}} - \tfrac{1}{4}$$
$$= \underbrace{\underbrace{\underbrace{\underbrace{\sqrt{\tfrac{1}{2}D}}_{E_{1,0}(D)} - \tfrac{1}{4}}_{E_{1,1}(D)} + \tfrac{1}{16\sqrt{2}}D^{-1/2}}_{E_{1,2}(D)} + \tfrac{1}{512\sqrt{2}}D^{-3/2}}_{E_{1,3}(D)} + O\left(D^{-5/2}\right). \tag{5.6}$$

The first three approximations differ by half-integer powers of D, in contrast to the energy sum (5.5), whose approximations differ by integer powers of D. Therefore, as table 1 illustrates, the

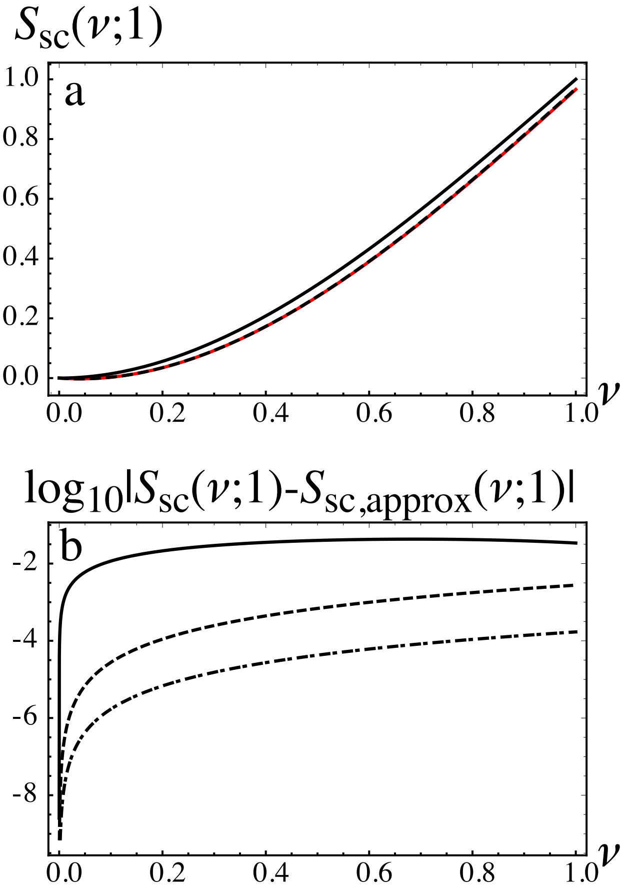

Figure 2. Energy sums for Pöschl–Teller potential for $D = 1$. (a) The full red curve (colour online) is the exact scaled sum S_{sc} from (5.3) and (5.4); the full black curve is the leading approximation S_{sc0} in (5.5), and the dashed black curve (visually indistinguishable from the exact sum) is the next approximation S_{sc1}. (b) Errors S_{sc}–$S_{sc,\ approx}$, where $S_{sc,\ approx} = S_{sc0}$ (full curve), $S_{sc,\ approx} = S_{sc1}$ (dashed curve), and $S_{sc,\ approx} = S_{sc2}$ (dot-dashed curve).

early terms of the energy sum provide a more efficient way of approximating E_1: S_{sc1} and S_{sc2} give the same approximation as E_{12} and E_{13}.

6. Hard-wall linear potential

General 1D potential wells are not exactly solvable, and semiclassical approximations, in terms of series in powers of $\hbar$, are given by the WKB approximation [17, 18]. These explicit series take the form of a 'quantum action' $I\,(E;\hbar)$, where $I(E;0)$ is the classical action. The energies E_n that must be summed to obtain $S(N)$ are determined implicitly by a quantum condition $I\,(E_n;\hbar) = n - \mu$, where μ (a Keller–Maslov index [19]) depends on boundary conditions. Getting the energies E_n requires reversion of the semiclassical series. We illustrate the essential features of approximations to the energy sum with the levels of a linear potential, about which much is known [4].

The potential is $V(x) = |x|$, whose wavefunction $\psi(x)$ is the Airy function [3], and the odd and even energy levels (with $\hbar = 2 \times \text{mass} = 1$) are given by the zeros a_n and a_n' of the Airy function and its derivative. We consider just the odd levels, corresponding to a linear potential on the half-line $x > 0$ and a hard wall at $x = 0$:

$$V(x) = \begin{Bmatrix} x \ (x \geqslant 0) \\ \infty \ (x \leqslant 0) \end{Bmatrix} \Rightarrow \psi(x) = Ai(x - E) \Rightarrow E_n = -a_n. \tag{6.1}$$

The similar formalism for the even levels, and the totality of even and odd levels, is described at the end of appendix B. By elementary $\hbar$ scaling, the semiclassical approximation corresponds to $n \gg 1$.

For the nth zero, the approximation of order M is given [3, 20] by

$$\begin{aligned} E_n(M) &= \sum_0^M T_m \left(\tfrac{3}{2}\pi\left(n - \tfrac{1}{4}\right)\right)^{2/3-2m} \\ T_0 = 1, T_1 &= \tfrac{5}{48}, T_2 = -\tfrac{5}{36}, T_3 = \tfrac{77125}{82944}, \cdots. \end{aligned} \tag{6.2}$$

In the literature [20], the coefficients T_0 to T_9 are listed. We needed many more; appendix B describes the way we calculated them, and lists T_0 to T_{20}. The asymptotics of the coefficients is given in (B.8), indicating that the terms in the series (6.2) have the generic 'factorial/power' form [11]. Therefore the smallest term is near

$$M = M^*(n) = \lfloor \pi n \rfloor, \tag{6.3}$$

in which $\lfloor ... \rfloor$ denotes the floor function (integer part of ...). To illustrate the accuracy of the asymptotics (B.8) for T_m for the terms in (6.2), the ratio approximate term/exact term for $M = M^*$ is 0.992 for $n = 5$, 0.9988 for $n = 10$, and 0.999 96 for $n = 50$.

For the energy sum, we use the Euler–Maclaurin representation (2.4). This will extend the cases considered in sections 3 and 4, where Euler–Maclaurin summation is exact because the sums over m and k terminate, to the present situation, in which the energies are known only approximately. We require the regularised sum $S(\infty)$, whose value is known [4, 21] to be zero. We apply (2.4) to the sum of contributions m in (6.2), using (2.6) for the regularised integrals over n, and explicitly evaluate the elementary derivatives with respect to n, and collect terms of the same order in $1/N$. Thus

$$\begin{aligned} S_{\text{th}}(N; M) &= \left(\frac{3}{2}\pi\left(N + \frac{3}{4}\right)\right)^{5/3} \frac{2}{3\pi} \times \\ \sum_{m=0}^{M} &\frac{1}{\left(\frac{3}{2}\pi\left(N + \frac{3}{4}\right)\right)^{2m}} \left[T_m \left(\frac{1}{5/3 - 2m} - \frac{1}{2\left(N + \frac{3}{4}\right)}\right)\right. \\ &\left. - \left(\frac{3}{2}\pi\right)^{2m} \left(2m - \frac{8}{3}\right)! \sum_{k=0}^{m-1} \frac{T_k B_{2(m-k)} \left(\frac{3}{2}\pi\right)^{-2k}}{\left(2k - \frac{5}{3}\right)! \left(2(m-k)\right)!}\right]. \end{aligned} \tag{6.4}$$

The first few terms of the series are

$$S_{\text{th}}(N; 3) = \left(\tfrac{3\pi}{2}\right)^{2/3} \left(\tfrac{3}{5}\left(N + \tfrac{3}{4}\right)^{5/3} - \tfrac{1}{2}\left(N + \tfrac{3}{4}\right)^{2/3} + \tfrac{1}{36\pi^2}\left(2\pi^2 - 5\right)\left(N + \tfrac{3}{4}\right)^{-1/3}\right). \tag{6.5}$$

Figure 3 illustrates the accuracy of the formula (6.4) for different values of the truncation M, for $N = 5$. The least term occurs near $M_{\text{opt}}(N) = \left\lfloor \pi\left(N + \frac{3}{4}\right)\right\rfloor$. Naive optimal truncation simply neglects all the terms with $M > M_{\text{opt}}(N)$. But for the series (6.4), whose terms alternate in sign, an intuitive way to increase the accuracy by several orders of magnitude is simply to add half of the next term, i.e. the term with $M = M_{\text{opt}}(N) + 1$. This procedure (which can

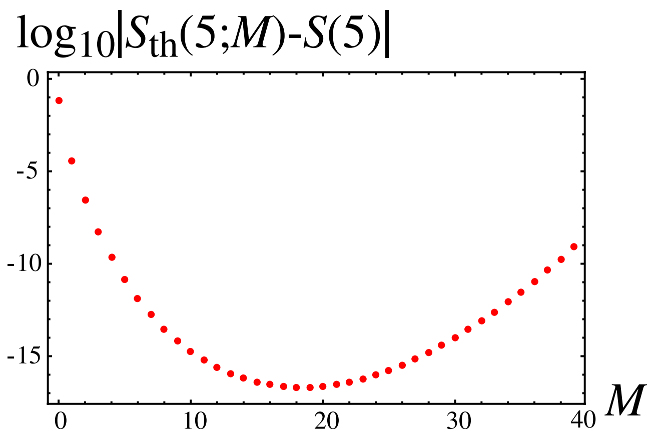

Figure 3. Errors of the approximation S_{th} (equation (6.4)) for the sum of odd energies (Airy zeros) for the potential $|x|$, for $N = 5$, as a function of the Euler–Maclaurin truncation index M.

Table 2. Energy sums $S(N)$ for the potential $|x|$, and asymptotically optimal errors of the approximation $S_{\mathrm{opt}}(N)$ (equation (6.6)).

N	$S(N)$	$S_{\mathrm{opt}}(N) - S(N)$	$\lfloor \pi\left(N + \frac{3}{4}\right) \rfloor$
1	2.33811	8.7007×10^{-8}	5
2	6.42606	-1.5273×10^{-10}	8
3	11.9466	2.8647×10^{-13}	11
4	18.7333	-5.4150×10^{-16}	14
5	26.6775	1.6617×10^{-19}	18
6	35.7001	-1.6626×10^{-23}	21
7	45.7403	-4.0013×10^{-25}	24
8	56.7488	1.4039×10^{-27}	27
9	68.6848	-3.6505×10^{-30}	30
10	81.5136	8.4660×10^{-33}	33

be justified by Borel Summation of the divergent tail of the series over M) corresponds to calculating

$$S_{\mathrm{opt}}(N) = \tfrac{1}{2}\left(S_{\mathrm{th}}(N; M_{\mathrm{opt}}(N) + 1) + S_{\mathrm{th}}(N; M_{\mathrm{opt}}(N))\right). \tag{6.6}$$

Table 2 shows the optimal errors for different N, calculated in this way. Even for relatively small values of N the accuracy is extraordinary, and the fractional error agrees well with the elementary asymptotic estimate $\exp(-2\pi(N + 3/4))/(2\pi(N + 3/4))^{3/2}$ obtained from the leading terms in (6.4), the estimate (B.8) for T_m, and Stirling's formula.

Note in particular the optimal error for $S_1 = E_1$ in table 2. Its magnitude, of order 10^{-7}, should be compared with the errors in the ground-state energy calculated directly from the series (6.2) for the Airy zeros, also terminated by adding half the smallest term. Table 3 shows the comparison, indicating that the large N series for $S(N)$, when applied to $N = 1$, outperforms the direct WKB eigenvalue asymptotics (6.2). The reason is that the energy sum for $N = 1$, when evaluated by the method of section 2, involves the energies E_2, E_3, ... , whose WKB approximations are more accurate than that for E_1.

Table 3. Errors in the approximations (6.2) and (6.6) for the lowest odd energy (smallest Airy zero) for the potential |x|; smallest errors bold.

M	0	1	2	3	4	5	6	7
$E_1 - (E_1(M+1) + E_1(M))/2$	0.008	4.6×10^{-4}	$\mathbf{-1.9\times10^{-5}}$	-2.1×10^{-4}	9.1×10^{-4}	-4.7×10^{-3}	-0.032	-0.29
$S(1) - (S_{\text{th}}(1;M+1) + S_{\text{th}}(1;M))/2$	-0.046	2.4×10^{-4}	-1.5×10^{-5}	2.3×10^{-6}	-5.3×10^{-7}	$\mathbf{8.7\times10^{-8}}$	1.7×10^{-7}	-5.7×10^{-7}

7. Towards more dimensons: quantum particle on a torus

The Euler–Maclaurin representation (2.4) for the energy sum requires the energies E_n to be represented analytically in terms of a monotonic function of continuous n. Achieving this in $d > 1$ dimensions is problematic, because the successive energies fluctuate pseudo-randomly. For separable d-dimensional Hamiltonians, the energies can be represented (exactly or approximately) in terms of a set of d quantum numbers, but the successive energies usually involve very different numbers in the set, and the statistics of the fluctuations is Poissonian [5]. For general nonseparable Hamiltonians (e.g. when the classical trajectories are chaotic), there are no quantum numbers, no explicit expressions are available for the individual energies E_n in increasing order, and the statistics are those of random-matrix theory [6, 7].

However, it is always possible to represent the spectrum in terms of a level counting function (spectral staircase) $\mathcal{N}(E)$, that is the sum of two contributions [14]. These are determined uniquely within semiclassical approximation schemes: a series of terms that are smooth functions of energy (monomials in $\hbar$), arising from gross features of the classical phase space; and a series of terms that are oscillatory in $\hbar$, arising from classical periodic orbits [13, 22] and representing fluctuations about the smoothed staircase. Thus, with Θ denoting the unit step, the staircase is

$$\mathcal{N}(E) = \sum_{1}^{\infty} \Theta(E - E_n) = \mathcal{N}_{\text{sm}}(E) + \mathcal{N}_{\text{osc}}(E). \tag{7.1}$$

With the natural convention $\Theta(0) = ½$ the exact levels are determined by the values of $\mathcal{N}(E)$ halfway up the steps, i.e.

$$\mathcal{N}(E_n) = n - \tfrac{1}{2}. \tag{7.2}$$

Key to using the representation (7.1) to calculate the energy sum is the observation that the two contributions depend differently on $\hbar$:

$$\mathcal{N}_{\text{sm}}(E) \approx \frac{\Omega(E)}{\hbar^d}, \quad \mathcal{N}_{\text{osc}}(E) \approx \sum_{\text{periodic orbits } j} \frac{A_j(E)}{\hbar^\mu} \exp\left(\frac{iS_j(E)}{\hbar}\right), \tag{7.3}$$

in which [14] $\Omega(E)$ is the phase space volume enclosed by the energy surface E, $S_j(E)$ is the action of the periodic orbit labelled j, the amplitude $A_j(E)$ depends on the stability of the orbit, and the exponent μ is a rational fraction between 0 (for chaotic dynamics) and $(d-1)/2$ (for completely integrable dynamics). The quantum condition (7.2) must be a monotonic function of E, so the derivative $\partial\mathcal{N}/\partial E$ (i.e. the level density) must be positive. The contribution $\mathcal{N}_{\text{sm}}(E)$ is always positive and $O(\hbar^{-d})$, and this must dominate the contributions to $\mathcal{N}_{\text{osc}}(E)$, which are $O\left(T_j(E)\,\hbar^{-(\mu+1)}\right)$, in which T_j is the period of the orbit j. Since $\mu + 1 < d$, the desired monotonicity will hold for orbits whose period is not too long, that is, whose periods are smaller than $O\left(\hbar^{d-\mu-1}\right)$. Therefore in calculating the energy sum using (2.4) we can use approximate energy levels incorporating these short orbits in the semiclassical representation

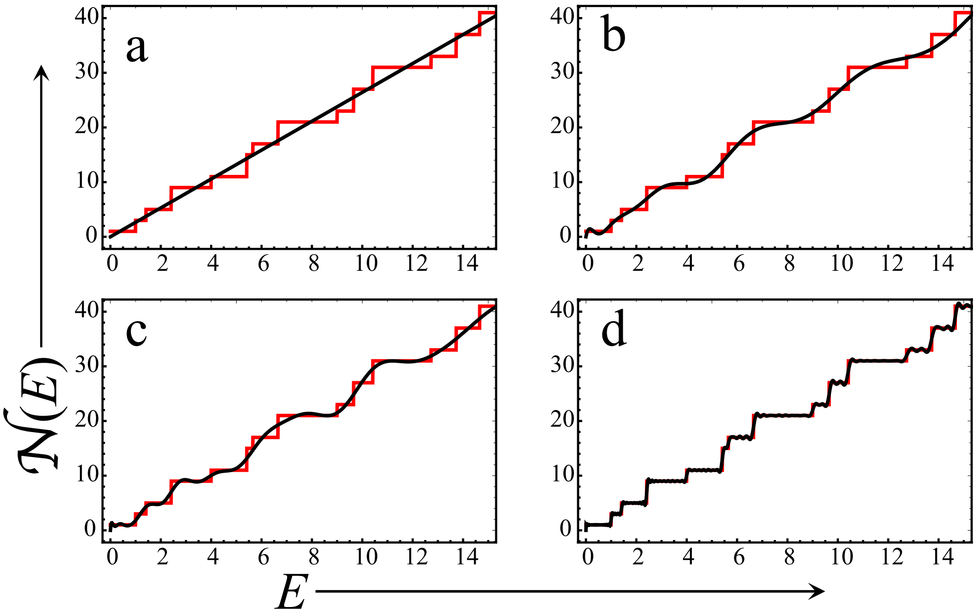

Figure 4. Staircase function (7.5) for $\alpha = 1/2^{1/4}$, including periodic orbits with $|j|,|k| \leqslant K$, where (a) $K = 0$, (b) $K = 1$, (c) $K = 2$, (d) $K = 20$; stepped curves (red online): exact stair; black curves: approximate stairs.

of $\mathcal{N}(E)$. (The long orbits, excluded here, play the crucial role of generating the sharp steps in $\mathcal{N}(E)$.)

To illustrate this, we employ the simplest nontrivial example: a quantum particle moving freely on a 2-torus, that is a rectangle of side lengths 2π and $2\pi\alpha$ with opposite sides identified, or, equivalently, the periodised plane with the rectangle as unit cell. The exact energies are

$$E_{l,m} = l^2 + \frac{m^2}{\alpha^2} \quad (-\infty < l,\ m < +\infty). \tag{7.4}$$

These are easy to compute and arrange in order, to give the sequence E_n. This case is particularly challenging for semiclassical approximations because there are many degeneracies (e.g. $\pm l$, $\pm m$, exchanging l and m), so the spectral fluctuations are large. Its simplicity has the advantage of avoiding complications, irrelevant for our purpose here, from perimeters, curvatures, and corners [23], that occur for 'quantum billiards' with boundaries.

For this system, the spectral staircase function, in the form (7.1) can be calculated exactly using the Poisson summation formula:

$$\begin{aligned}\mathcal{N}(E) &= \sum_{l,m=-\infty}^{+\infty} \Theta\left(E - l^2 - \tfrac{m^2}{\alpha^2}\right)\\ &= \sum_{j,k=-\infty}^{+\infty} \int_{-\infty}^{\infty} \mathrm{d}l \int_{-\infty}^{\infty} \mathrm{d}m \Theta\left(E - l^2 - \tfrac{m^2}{\alpha^2}\right) \exp\left(2\pi i\left(jl + km\right)\right)\\ &= \pi\alpha E + 2\pi\alpha\sqrt{E} \sum_{\substack{j,k=-\infty\\ j=k\neq 0}}^{+\infty} \frac{J_1\left(\sqrt{E}L_{jk}\right)}{L_{jk}},\end{aligned} \tag{7.5}$$

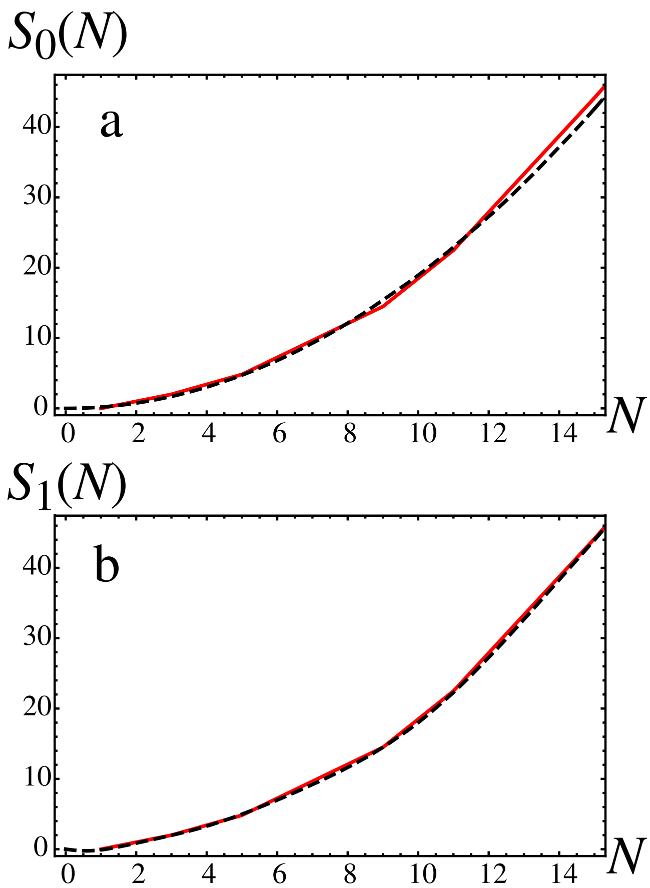

Figure 5. Energy sums (7.9) for $\alpha = 1/2^{1/4}$, including periodic orbits (a) $K = 0$ (no periodic orbits), (b) $K = 1$ (8 periodic orbits).

in which $\mathcal{N}_{\rm sm}(E) = \pi\alpha E$ comes from the term $j = k = 0$ in the sum, and in $\mathcal{N}_{\rm osc}(E)$, involving the Bessel functions,

$$L_{jk} = 2\pi\sqrt{j^2 + \alpha^2 k^2} \tag{7.6}$$

is the length of the periodic orbit labelled j,k. (These orbits form continuous families, each consisting of paths in the periodised plane from points x, y in the rectangle to points $x + 2\pi j$, $y + 2\pi\alpha k$.) Figure 4 shows the emergence of the steps as increasing numbers of periodic orbits are included, with the concomitant loss of monotonicity, arising from the fact that although the strengths of the contributions from the longer orbits decrease, they also oscillate faster.

To determine the ordered energies E_n, it is necessary to invert the quantization condition (7.2), incorporating a number of periodic orbits small enough to ensure that the staircase is monotonic. We accomplish this approximately, using the fact that the oscillatory contributions are smaller than the smooth contributions. We start with the zero-order energies $E_{0,n}$, i.e.

$$\mathcal{N}_{\rm sm}(E_{0,n}) = n - \tfrac{1}{2} \Rightarrow E_{0,n} = \frac{\left(n - \frac{1}{2}\right)}{\pi\alpha}, \tag{7.7}$$

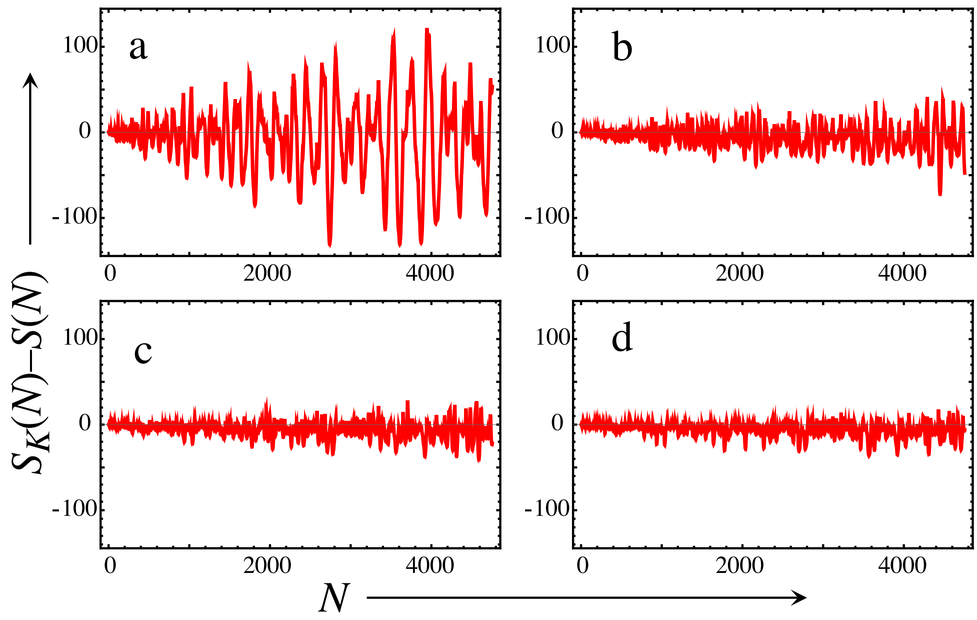

Figure 6. Errors in the energy sum calculated from (7.9) for $\alpha = 1/2^{1/4}$, including periodic orbits with $|j|,|k| \leqslant K$, where (a) $K = 0$ (no periodic orbits), (b) $K = 1$ (8 periodic orbits), (c) $K = 2$ (24 Periodic orbits), (d) $K = 3$ (48 periodic orbits).

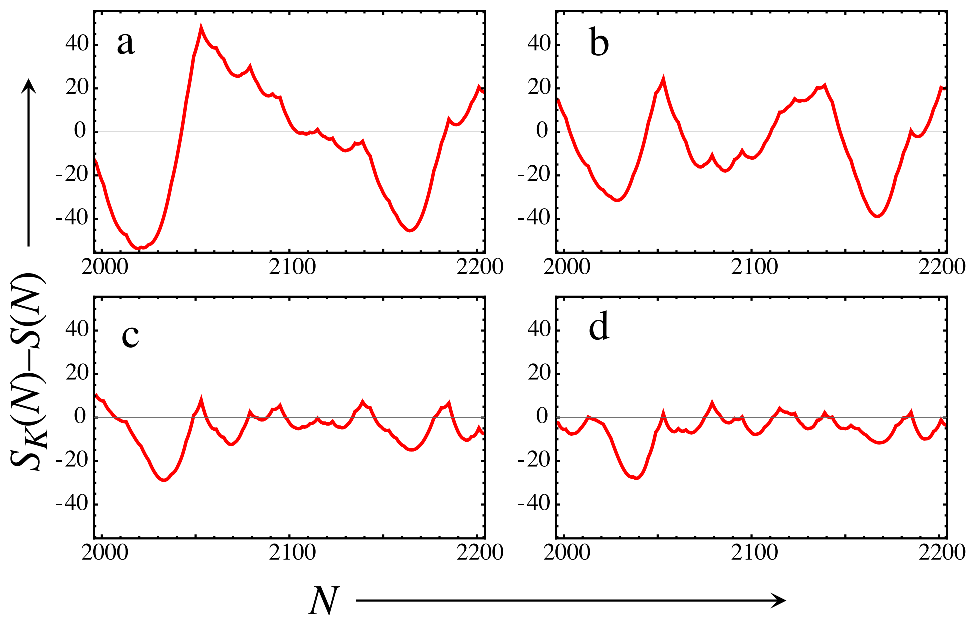

Figure 7. Magnifications of central regions of figures 6.

and include the oscillatory contributions, with a finite number of periodic orbits, by solving (7.2) iteratively. The first iteration suffices, yielding the approximate energies

$$E_{K,n} = E_{0,n} - 2\sqrt{E_{0,n}} \sum_{\substack{j,k=-K \\ j=k\neq 0}}^{+K} \frac{J_1\left(\sqrt{E_{0,n}} L_{jk}\right)}{L_{jk}}. \tag{7.8}$$

These are the energies to be included in the Euler–Maclaurin formula (2.4). We also require $S(\infty)$; this is zero, because the partition function is the product of two factors of the 1D form (4.2). We have confirmed numerically that at the present level of approximation, it is not necessary to include the derivative terms in (2.4). Thus the energy sum, including periodic orbits with $|j|,|k| \leqslant K$, is

$$\begin{aligned} S_K(N) = \frac{N^2}{2\pi\alpha} - 4\pi\alpha E_{0,N+1} \sum_{\substack{j,k=-K \\ j=k\neq 0}}^{+K} \frac{J_2\left(\sqrt{E_{0,N+1}} L_{jk}\right)}{L_{j,k}^2} \\ + \sqrt{E_{0,N+1}} \sum_{\substack{j,k=-K \\ j=k\neq 0}}^{+K} \frac{J_1\left(\sqrt{E_{0,N+1}} L_{jk}\right)}{L_{j,k}}. \end{aligned} \tag{7.9}$$

Figure 5 shows the exact and approximate energy sums for $N \leqslant 15$. Even for these small values of N, the curves are hard to distinguish, even for $K = 0$, i.e. when no periodic orbits are included. Figure 6 shows the errors over a much larger range; as described below, these increase with N, because of the fluctuations, but are much smaller when periodic orbits are included. The errors are larger than the mean spacing between adjacent energies, which is constant ($\sim 1/\pi\alpha = 0.379$), but are always very small compared with the value of $S(N) \sim N^2/2\pi\alpha$: e.g. $S(5000) \sim 4.73 \times 10^6$. Figure 7 shows magnified regions of figures 6, illustrating how the scale of the fluctuations gets smaller as more orbits are included. These calculations are for side ratio $\alpha^2 = 1/\sqrt{2}$. For different α, other calculations (not shown) give similar results.

We can estimate the increase of the fluctuations with N by calculating the r.m.s. error $\sigma_K(N)$, where the variance $\sigma_K(N)^2$ is calculated by averaging over the oscillations in $S_K(N)$. Thus, using asymptotics of the Bessel functions, using (7.7) for $E_{0,n}$, and noting that a similar calculation shows that the second sum in (7.9) grows more slowly with N,

$$\begin{aligned} \sigma_K(N)^2 = \left\langle \left(S_K(N) - S(N)\right)^2 \right\rangle \approx 16\left(N + \tfrac{1}{2}\right)^2 \sum_{\text{excluded}(K)} \frac{\left\langle J_2\left(\sqrt{E_{0,N+1}} L_{jk}\right)^2 \right\rangle}{L_{j,k}^4} \\ \approx \tfrac{1}{2}\sqrt{\tfrac{\alpha}{\pi^{11}}}\left(N + \tfrac{1}{2}\right)^{3/2} \sum_{\text{excluded}(K)} \frac{1}{\left(j^2 + \alpha^2 k^2\right)^{5/2}}, \end{aligned} \tag{7.10}$$

where the sum is over all j, k excluded by the square of side K in (7.9); this sum converges, and is $O((K+1)^{-3})$. Thus $S_K(N)$ grows as $N^{3/4}$, consistent with the calculations illustrated in figures 6. From the argument of the Bessel functions, the oscillation frequency as N increases scales as $(K+1)^2$.

As a check of (7.9), we also calculated the sum energy directly from the individual approximate levels given by (7.8). The results are indistinguishable in every detail from figures 6 and 7, probably because any improvement is masked by the fluctuations. The close similarity indicates the effectiveness of the analytical sum (7.9), generated from the Euler–Maclaurin procedure.

Table 4. Exact sums, and errors for periodic-orbit truncations K, for 2-torus levels with α =00201/$2^{1/4}$.

N	$S(N)$	$S_0(N) - S(N)$	$S_1(N) - S(N)$	$S_2(N) - S(N)$	$S_3(N) - S(N)$
1	0	0.189	−0.086	−0.074	−0.041
2	1	−0.243	−0.133	−0.209	−0.221
3	2	−0.297	−0.020	0.113	0.074
4	3.414	−0.386	−0.129	−0.187	−0.098
5	4.828	−0.097	0.153	0.040	−0.074

The numerical values in table 4 show the energy sum, and the errors for increasing periodic-orbit truncation K, for small values of N. All errors (except one) are small in comparison with the mean level spacing. For such such small N it is hard to see a consistent picture, though there is a tendency for the errors to decrease with increasing K.

8. Concluding remarks

We have shown that the technique of section 2, in which regularisation is combined with Euler–Maclaurin summation, is a widely applicable and effective way to evaluate the energy sum $S(N)$ defined by (1.1). In some cases (sections 3 and 4) it is exact, and for 1D potentials where the energies are approximately known it can give the semiclassical energy sum with high accuracy, as illustrated (section 6) for the Airy zeros. In more dimensions, the method is effective for the energy sum of levels of the partially smoothed spectrum, when some periodic orbits are included, as illustrated (section 7) for the particle on a 2-torus. For finite-depth wells, unregularised Euler–Maclaurin works, at least for the exactly solvable Pöschl–Teller potential; for this case the natural semiclassical expansion parameter is a combination of N and the well depth.

Our preliminary analysis suggests several avenues for further research.

- Extending the linear-potential analysis of section 6 to general infinite potential wells, by applying the known [24] WKB series for the quantization condition analogous to (B.4), thus building on the leading-order correction already obtained [25], where some of the formulas were obtained by elementary means. This would incorporate the regularised sums $S(\infty)$ for general potentials [10, 18, 26, 27].
- For finite-depth wells, going beyond the Pöschl–Teller example of section 5 to include WKB-generated energies for potentials that are not exactly solvable. In cases where the sum of all the bound states (the counterpart of $S(\infty)$) is not known, this would require application of the Euler–Maclaurin formula directly to (1.1) in its familiar (i.e. not regularised) form, possibly incorporating the requirement $S(0) = 0$.
- Where WKB is applied, further increasing the accuracy of the summations beyond that illustrated in section 5, by employing asymptotic techniques [11, 28–31] involving resummation of the divergent tail of the relevant series beyond their smallest terms.
- For nonanalytic potentials, for example a smooth well truncated at finite depth, summing the energies would require modification of (6.4), incorporating techniques recently developed elsewhere [32].
- For higher-dimensional potential wells more general than the particle on a 2-torus, incorporating multidimensional semiclassical techniques [33] to get explicit formulas for the correction terms ('Weyl series') in the series for the smoothed spectrum $\mathcal{N}_{\mathrm{sm}}(E)$ and the periodic-orbit terms $\mathcal{N}_{\mathrm{osc}}(E)$.

Acknowledgment

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Appendix A. Derivation of the regularisation (2.6)

By analogy with the partition function procedure (2.2) and (2.3), we define the integral in (2.6) as

$$I = -\text{coefficient of } t \text{ in} \int_{N+1}^{\infty} \mathrm{d}n \exp\left(-t(n+\mu)^{\nu}\right). \tag{A.1}$$

Thus we require the small t expansion of the following integral, where $N+1$ is replaced by N to save writing, and we make elementary changes of variable:

$$\begin{aligned} J &= -\textstyle\int_N^{\infty} \mathrm{d}x \exp\left(-t(n+\mu)^{\nu}\right) \\ &= -\tfrac{1}{t\nu}(N+\mu)^{1-\nu} \exp\left(-t(N+\mu)^{\nu}\right) \textstyle\int_0^{\infty} \mathrm{d}y \exp(-y) \left(1+\tfrac{y}{t(N+\mu)^{\nu}}\right)^{1/\nu-1}. \end{aligned} \tag{A.2}$$

Next, we use the expansion

$$(1+\xi)^{1/\nu-1} = \sum_0^{\infty} c_n \xi^n \to c_n = \frac{1}{2\pi i} \oint \frac{\mathrm{d}\xi}{\xi^{n+1}} (1+\xi)^{1/\nu-1}. \tag{A.3}$$

Thus

$$\int_0^{\infty} \mathrm{d}y \exp(-y) \left(1+\frac{y}{t(N+\mu)^{\nu}}\right)^{1/\nu-1} = \sum_0^{\infty} c_n \frac{n!}{t^n (N+\mu)^{\nu n}}, \tag{A.4}$$

and J can be written as a double sum:

$$J = -\frac{1}{t\nu}(N+\mu)^{1-\nu} \sum_{m=0}^{\infty} \frac{(-1)^m}{m!} t^m (N+\mu)^{m\nu} \sum_0^{\infty} c_n \frac{n!}{t^n (N+\mu)^{\nu n}}. \tag{A.5}$$

The coefficient of t in (A.1) is the contribution with $m = n+2$, so, using the contour integral in (A.3),

$$\begin{aligned} I &= -\tfrac{1}{\nu}(N+\mu)^{1+\nu} \textstyle\sum_0^{\infty} \tfrac{(-1)^n c_n}{(n+2)(n+1)} \\ &= -\tfrac{1}{\nu}(N+\mu)^{1+\nu} \tfrac{1}{2\pi i} \oint \mathrm{d}\xi (1+\xi)^{1/\nu-1} \textstyle\sum_0^{\infty} \tfrac{(-1)^n}{\xi^{n+1}(n+2)(n+1)} \\ &= \tfrac{1}{\nu}(N+\mu)^{1+\nu} \tfrac{1}{2\pi i} \oint \mathrm{d}\xi (1+\xi)^{1/\nu-1} \left(1-(1+\xi)\log\left(1+\tfrac{1}{\xi}\right)\right). \end{aligned} \tag{A.6}$$

A double integration by parts eliminates the logarithm, enabling the contour integal to be evaluated by the residue at $\xi = 0$. Its value is $\nu/(\nu+1)$, completing the derivation of (2.6). This way of getting what seems an intuitively obvious result seems complicated; perhaps there is a simpler one.

Appendix B. Calculation of T_m coefficients in (6.2)

This follows and extends the discussion in [20]. We start from the following combination of the standard asymptotic series [3, 4] for the Airy functions Ai and Bi:

$$Bi_M(-E) + iAi_M(-E) = \frac{\exp\left(i\left(z(E) + \frac{1}{4}\pi\right)\right)}{\sqrt{\pi}E^{1/4}} \sum\nolimits_M (z(E)) \quad \left(z(E) \equiv \tfrac{2}{3}E^{3/2}\right), \tag{B.1}$$

where Σ_M denotes the formal asymptotic series to Mth order

$$\Sigma_M(z) = \frac{1}{2\pi}\sum_0^M \frac{\left(m-\frac{1}{6}\right)!\left(m-\frac{5}{6}\right)!}{m!}\left(\frac{-i}{2z}\right)^m = 1 - \frac{5i}{72z} - \frac{385}{10368z^2} + \cdots. \tag{B.2}$$

The 'quantum condition' determining the levels (Airy zeros) implicitly is thus

$$z(E_n) + \mathrm{Im}\left[\log\left(\Sigma_M\left(z\left(E_n(M)\right)\right)\right)\right] = \left(n - \tfrac{1}{4}\right)\pi. \tag{B.3}$$

From Stirling's approximation, the large m 'asymptotics of the asymptotics' in the sum (B.2) is

$$\frac{\left(m-\frac{1}{6}\right)!\left(m-\frac{5}{6}\right)!}{m!} \approx (m-1)! \quad (m \gg 1), \tag{B.4}$$

Therefore the series for z has the form

$$z + \cdots - \frac{(-1)^k (2k)!}{2\pi(2z)^{2k+1}} + \cdots = \left(n - \tfrac{1}{4}\right)\pi, \tag{B.5}$$

in which ... and ... are separated by the asymptotic ($k \gg 1$) approximation for the terms. Inverting this expression, to get the energies E_n explicitly as functions of continuous n, requires reversion of series [20], for which the asymptotics of a function (here the inverse) of a function that is itself given as an asymptotic series [34], leads to

$$\tfrac{2}{3}E_n^{3/2} = \left(n - \tfrac{1}{4}\right)\pi\left(1 + \cdots + (-1)^k \frac{(2k)!}{\pi\left(2\pi\left(n-\frac{1}{4}\right)\right)^{2k+2}} + \cdots\right), \tag{B.6}$$

and hence, by further asymptotics of the 2/3 power function, to the desired form (6.2), with the coefficients T_m:

$$E_n = \left(\tfrac{3\pi}{2}\left(n - \tfrac{1}{4}\right)\right)^{2/3}\left(1 + \cdots + (-1)^k \frac{2(2k)!}{3\pi\left(2\pi\left(n-\frac{1}{4}\right)\right)^{2k+2}} + \cdots\right). \tag{B.7}$$

With computer algebra (e.g. Mathematica's `InverseSeries` function), it is not difficult to calculate hundreds of coefficients. As m increases, the T_m are represented by ratios of integers that increase very rapidly; table B1 shows T_1 to T_{20}.

The asymptotic form (B.5) implies the following asymptotics for the corefficients T_m:

$$T_m \approx (-1)^{m+1}\left(\tfrac{2\pi}{3}\right)(2m-2)!\left(\tfrac{3}{4}\right)^{2m} \quad (m \gg 1). \tag{B.8}$$

For the even levels in the potential $|x|$, the energy levels $E_{n,\mathrm{even}}$ are given by the zeros $-a'_n$ of $Ai'(-E)$. Again using standard Airy asymptotics, replacing (B.1)–(B.4) are

Table B1. Coefficients T_m.

m	T_m
0	1
1	5/48
2	−5/36
3	77 125/82 944
4	−108 056 875/6967 296
5	162 375 596 875/334 430 208
6	−1622 671 914 671 875/66 217 181 184
7	1501 264 787 795 732 65 625/82 639 042 117 632
8	−644 932 726 927 939 889 453 125/3470 839 768 940 544
9	13042116997445589075044921875/520200964553048064
10	−569 789 860 268 573 944 980 176 052 734 375/132 083 753 999 696 658 432
11	25 716 195 883 508 7358 239 821 956 396 181 640 625/278 960 888 447 359 342 608 384
12	−4260 043 450 658 439 625 615 850 895 889 732 425 107 421 875/ 1778 543 040 384 984 224 734 0130 304
13	9069 017 047 957 395 268 381 316 695 903 125 939 513 916 015 625/ 121 957 237 054 970 346 838 903 750 656
14	−1810 271 277 633 586 533 592 120 646 709 512 524 415 775 650 634 765 625/ 66 588 651 432 013 809 374 041 447 858 176
15	378 176 119 842 183 032 100 868 306 594 392 061 376 826 060 531 219 482 421 875/ 3271 461 275 059 878 446 423 4951 324 205 056
16	−71164840343520829497340335316126166138638002879118637084960937 5/ 12 580 554 030 695 452 292 600 901 926 0731 392
17	626876081188948978827514046969796801390686073071553852349709777832 03125/ 19 861 172 259 339 524 443 374 895 888 730 186 317 824
18	−(699 119 570 892 539 684 566 217 052 495 289 521 135 102 491 608 432 776 053 948 216 646 57 5 927 734 375)/(350 976 705 580 918 406 201 099 472 697 695 487 515 426 816)
19	(370 516 876 625 582 057 246 579 990 165 313 241 890 240 457 948 238 284 887 457 895 774 546 2 83 721 923 828 125)/(262 456 685 941 773 090 279 222 174 109 939 867 716 799 168 512)
20	−(5519 033 892 983 537 417 011 056 251 284 086 528 764 711 502 879 616 5130 794 916 225 525 906 328 777 313 232 421 875)/(4943 314 623 912 004 465 606 915 035 844 6065 519 529 304 260 608)

$$Bi'_M(-E) + iAi'_M(-E) = -\frac{iE^{1/4}\exp\left(i\left(z(E)+\frac{1}{4}\pi\right)\right)}{\sqrt{\pi}}\sum\nolimits'(z(E)), \tag{B.9}$$

$$\Sigma'(z) = -\tfrac{1}{2\pi}\sum_0^\infty \frac{\left(m-\frac{7}{6}\right)!\left(m+\frac{1}{6}\right)!}{m!}\left(\frac{-i}{2z}\right)^m = 1 + \frac{7i}{72z} - \frac{455}{10368z^2} + \cdots, \tag{B.10}$$

$$z(E_{n,\mathrm{even}}) + \mathrm{Im}\left[\log\left(\Sigma'\left(z\left(E_{n,\mathrm{even}}(M)\right)\right)\right)\right] = \left(n-\tfrac{3}{4}\right)\pi. \tag{B.11}$$

The reversion of series, and evaluation of the energy sum, are essentially the same as for the odd states. A formal combined quantum condition, including both cases, is

$$\begin{gathered} z(E_n) = \left(n-\tfrac{1}{2}\right)\tfrac{1}{2}\pi - \tfrac{1}{2}\mathrm{Im}\left[\log\left(\Sigma_{n,M}\Sigma'_{n,M}\right) + (-1)^n\log\left(\Sigma_{n,M}/\Sigma'_{n,M}\right)\right], \\ \Sigma_{n,M} = \Sigma\left(z\left(E_n(M)\right)\right), \quad \Sigma'_{n,M} = \Sigma'\left(z\left(E_n(M)\right)\right), \end{gathered} \tag{B.12}$$

in which $n = 1,2,3...$, with even n giving the odd levels and odd n giving the even levels.

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