

Spectral zeta functions for Aharonov–Bohm quantum billiards

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Abstract. This is a study of the sum $\zeta(s; \alpha) \equiv \sum_{j=1}^{\infty} [E_j(\alpha)]^{-s}$ over the eigenvalues $E_j(\alpha)$ of Schrödinger's equation in a (billiard) domain \mathcal{D} with reflecting walls, threaded by a single line of magnetic flux α . For integer s , $\zeta(s; \alpha)$ is calculated by generalising a Green function technique of Itzykson *et al* based on a conformal transformation between \mathcal{D} and the unit disc. When the transformation is generated by a polynomial of finite degree an explicit formula enables $\zeta(2; \alpha)$ to be easily computed with high accuracy. In conjunction with a semiclassical approximation the exact values of $\zeta(2; \alpha)$ can be used to calculate the ground state $E_1(\alpha)$ for a non-integrable billiard, with an error of about one per cent.

1. Introduction

The zeta function of a Hermitian operator \hat{H} with infinitely many discrete eigenvalues $\{E_j\}$ is the sum

$$\zeta(s) \equiv \sum_{j=1}^{\infty} \frac{1}{E_j^s}. \quad (1)$$

Zeta functions have been evaluated for some one-dimensional differential operators. If \hat{H} is the Hamiltonian of a quantal harmonic oscillator, then because the energy levels are equally spaced $\zeta(s)$ can be expressed simply in terms of Riemann's zeta function. If \hat{H} is the operator of Bessel's equation, $-\mathrm{d}^2/\mathrm{d}x^2 + (\nu^2 - \frac{1}{4})/x^2$, applied to functions vanishing at $x=0$ and $x=1$, then E_j is the square of the j th zero of the ν th Bessel function, from whose product formula $\zeta(s)$ has been evaluated for even integer s in studies begun by Euler two centuries ago (Watson 1944). If \hat{H} is the Hamiltonian of a particle in an even power law potential, that is $-\mathrm{d}^2/\mathrm{d}x^2 + x^{2M}$, with M a natural number, then even though, when $M > 1$, the eigenfunctions are not standard special functions it is possible to obtain analytic properties, recurrence relations and some special values of $\zeta(s)$, as shown by Voros (1983).

Itzykson *et al* (1986) have extended these studies to a class of two-dimensional operators, namely quantum billiards, in which particles are free within a domain \mathcal{D} on whose reflecting boundary wavefunctions must vanish. They are able to express $\zeta(s)$ for integer s in closed form, as $2s$ -fold integrals. This extension is important because in contrast to the one-dimensional cases the corresponding classical Hamiltonian motion (bouncing balls in \mathcal{D}) need not be integrable. Itzykson *et al*'s integrals therefore provide exact sum rules for the unknown energy levels of quantal systems whose classical motion may be chaotic.

Our purpose here is threefold. Firstly, to generalise Itzykson *et al*'s results (§ 2) so as to include the Aharonov–Bohm billiards recently introduced by Berry and Robnik

(1986, hereafter called **BR**). These are quantum billiards where the particles have charge q and where a single line of magnetic flux Φ threads \mathcal{D} . With coordinates $\mathbf{r} = (x, y)$ with the flux line at the origin, the Hamiltonian (**BR**) is

$$\hat{H} = -(\nabla - i\alpha\mathbf{A}(\mathbf{r}))^2 \tag{2}$$

where the *quantum flux parameter* α is defined by

$$\alpha \equiv q\Phi/h \tag{3}$$

(h being Planck's constant), and \mathbf{A} is any vector potential satisfying

$$\nabla \wedge \mathbf{A} = 2\pi\delta(\mathbf{r}). \tag{4}$$

The flux α breaks the time-reversal symmetry of the quantum dynamics and thereby alters the universality class of the statistics of high-lying energy levels (**BR**); here it is the α dependence of the zeta functions $\zeta(s; \alpha)$ that will be studied.

The second purpose (§ 3) is to show that Itzykson *et al*'s formulae and the present generalisation simplify considerably for domains which can be obtained by a finite-degree conformal mapping of the unit disc (these include domains for which the classical motion is chaotic). Explicit formulae will be found for $\zeta(2; \alpha)$.

The third purpose (§ 4) is to show how the exact results for $\zeta(2; \alpha)$ can be combined with semiclassical approximations to give unexpectedly good estimates of the ground-state energy E_1 as a function of α .

2. Trace formulae and Green function

We define the (zero-energy) Green function \mathcal{G}_{12} and Green operator \hat{G} by

$$\mathcal{G}_{12} \equiv \langle \mathbf{r}_1 | \hat{G} | \mathbf{r}_2 \rangle \equiv \langle \mathbf{r}_1 | \hat{H}^{-1} | \mathbf{r}_2 \rangle \quad (= \mathcal{G}_{21}^*). \tag{5}$$

Then for integer s , from (1), $\zeta(s)$ is the trace

$$\begin{aligned} \zeta(s) &= \text{Tr } \hat{H}^{-s} = \text{Tr } \hat{G}^s \\ &= \iint d\mathbf{r}_1 \dots \iint d\mathbf{r}_s \mathcal{G}_{12} \mathcal{G}_{23} \dots \mathcal{G}_{s1} \end{aligned} \tag{6}$$

where the s integrations are over the domain \mathcal{D} .

The idea of Itzykson *et al* (1986) is to express (6) in terms of integrals over the unit disc, related to \mathcal{D} by *conformal transformation*. With position in the disc plane denoted by

$$\mathbf{R} = (X, Y) = (R, \theta) \quad \text{with } Z = X + iY \tag{7}$$

and position in \mathcal{D} denoted by

$$\mathbf{r} = (x, y) = (r, \phi) \quad \text{with } z = x + iy \tag{8}$$

the transformation is defined by an analytic function $w(Z)$ by

$$z = w(Z) \quad \text{i.e.} \quad x = \text{Re } w(Z) \quad y = \text{Im } w(Z). \tag{9}$$

The boundary of \mathcal{D} is the image of the boundary of the unit disc $R = 1$, and the Jacobian is $|w'(Z)|^2$, so that (6) becomes

$$\zeta(s) = \iint d\mathbf{R}_1 |w'(Z_1)|^2 \dots \iint d\mathbf{R}_s |w'(Z_s)|^2 \mathcal{G}_{12} \dots \mathcal{G}_{s1} \tag{10}$$

where now the integrations are over the unit disc and \mathcal{G}_{12} has arguments Z_1 and Z_2 (or R_1 and R_2).

In r space \mathcal{G}_{12} is determined by $\hat{H}\hat{G} = 1$ in position representation; from (2) and (5) follow

$$\begin{aligned} -(\nabla_{r_1} - i\alpha A(r_1))^2 \mathcal{G}_{12} &= \delta(r_1 - r_2) \\ \mathcal{G}_{21} = \mathcal{G}_{12}^* \quad \mathcal{G}_{12} &= 0 \quad \text{if } r_1 \text{ or } r_2 \text{ is on the boundary of } \mathcal{D}. \end{aligned} \quad (11)$$

As explained by BR, the operator is most easily transformed to R space by choosing a gauge in which the lines of the vector potential become concentric circles (in r this corresponds to A being the velocity field of a steady incompressible irrotational flow in \mathcal{D} with a vortex of strength 2π at $r=0$). Then

$$-(\nabla_{r_1} - i\alpha A(r_1))^2 = -|w'(Z_1)|^{-2} (\nabla_{R_1} - (i\alpha \hat{\theta}/R_1))^2 \quad (12)$$

where $\hat{\theta}$ is the angular unit vector in the R plane. Now (11) becomes

$$\begin{aligned} -(\nabla_{R_1} - (i\alpha \hat{\theta}/R_1))^2 \mathcal{G}_{12} &= |w'(Z_1)|^2 \delta(r_1 - r_2) = \delta(R_1 - R_2) \\ \mathcal{G}_{21} = \mathcal{G}_{12}^* \quad \mathcal{G}_{12} &= 0 \quad \text{if } R_1 = 1 \text{ or } R_2 = 1. \end{aligned} \quad (13)$$

This is just the Aharonov-Bohm zero energy Green function for a *circular* billiard: with our gauge, all dependence on the shape of the \mathcal{D} boundary has disappeared. It follows that in (10) the zeta function depends on \mathcal{D} only through the factors $w'(Z)$, and on α only through the factors \mathcal{G} .

To solve (13) we begin with the non-magnetic billiard ($\alpha = 0$), for which \mathcal{G}_{12} satisfies Poisson's equation and is the potential at Z_1 of a line charge at Z_2 inside a conducting cylinder, namely

$$\mathcal{G}_{12} = -\frac{1}{2\pi} \ln \left| \frac{Z_1 - Z_2}{1 - Z_1^* Z_2} \right| \quad (\text{if } \alpha = 0). \quad (14)$$

Denoting by $Z_>$ and $Z_<$ the positions further from and closer to the origin and expanding in powers of $Z_</Z_>$ gives the convergent series

$$\mathcal{G}_{12} = \frac{1}{2\pi} \left[-\ln R_> + \frac{1}{2} \sum_{n=-\infty}^{\infty} \frac{\exp[in(\theta_1 - \theta_2)]}{|n|} R_<^{|n|} \left(\frac{1}{R_>^{|n|}} - R_>^{|n|} \right) \right] \quad (\text{if } \alpha = 0) \quad (15)$$

where $n=0$ is excluded.

With flux, the elementary solutions of (13) which occur in (15) are modified as follows:

$$\begin{aligned} e^{in\theta_1} R_1^{\pm n} &\text{ becomes } e^{in\theta_1} R_1^{\pm(n-\alpha)} \\ e^{-in\theta_2} R_2^{\pm n} &\text{ becomes } e^{-in\theta_2} R_2^{\pm(n-\alpha)}. \end{aligned} \quad (16)$$

The correct generalisation of (15) now gives the Aharonov-Bohm Green function as

$$\mathcal{G}_{12} = \frac{1}{4\pi} \sum_{n=-\infty}^{\infty} \frac{\exp[in(\theta_1 - \theta_2)]}{|n-\alpha|} R_<^{|n-\alpha|} \left(\frac{1}{R_>^{|n-\alpha|}} - R_>^{|n-\alpha|} \right) \quad (17)$$

where the sum now includes the term with $n=0$, whose limit as $\alpha \rightarrow 0$ gives the logarithm in (15). This is a single-valued function of R_1 and R_2 , satisfying (13) and therefore also

$$\mathcal{G}_{12}(-\alpha) = \mathcal{G}_{12}^*(\alpha) \quad \mathcal{G}_{12}(\alpha+1) = \exp[i(\theta_1 - \theta_2)] \mathcal{G}_{12}(\alpha). \quad (18)$$

The form (17) is the one we will use to calculate zeta functions from (10), but it is interesting to express the Green function in several other ways. By using

$$\frac{x^{|a|}}{|a|} = \int_0^x dt t^{|a|-1} \tag{19}$$

and evaluating the sums in (17) we obtain the integral representation

$$\mathcal{G}_{12} = \{\exp[i\alpha(\theta_1 - \theta_2)]/4\pi\} [I(Z_2^* Z_1, Z_2^*/Z_1^*) + I(1/Z_1^* Z_2, Z_1/Z_2)] \tag{20} \quad (R_1 > R_2)$$

where

$$I(u, v) \equiv \int_u^v ds s^{[\alpha]-\alpha}/(1-s). \tag{21}$$

(If $R_1 < R_2$, Hermiticity implies that the correct form for \mathcal{G}_{12} is obtained by exchanging Z_1 and Z_2 and taking the complex conjugate.) In (20) neither the exponential nor integral factors is single-valued but their product is.

Another method of evaluating the sums in (17) is by means of the Poisson formula

$$\sum_{n=-\infty}^{\infty} F(n) = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} dx F(x) \exp(2\pi i m x). \tag{22}$$

The integrals to which this gives rise are of the form

$$\int_0^{\infty} \frac{dx}{x} \cos ax (e^{-bx} - e^{-cx}) = \frac{1}{2} \ln \left(\frac{a^2 + c^2}{a^2 + b^2} \right) \tag{23}$$

and lead to

$$\mathcal{G}_{12} = \frac{1}{4\pi} \sum_{m=-\infty}^{\infty} \exp[i\alpha(\theta_1 - \theta_2 - 2\pi m)] \ln \left(\frac{(\theta_1 - \theta_2 - 2\pi m)^2 + (\ln R_1 R_2)^2}{(\theta_1 - \theta_2 - 2\pi m)^2 + (\ln R_1/R_2)^2} \right). \tag{24}$$

In the angular dependence, m evidently plays the role of a winding number labelling circuits of the flux line, so that this is a ‘whirling wave’ representation of the type introduced by Berry (1980) for the Aharonov-Bohm scattering wavefunction and by Morandi and Menossi (1984) for the Aharonov-Bohm propagator. In complex form, (24) is

$$\mathcal{G}_{12} = \frac{1}{2\pi} \sum \left(\frac{Z_1 Z_2^*}{Z_2 Z_1} \right)^{\alpha/2} \ln \left(\frac{|\ln Z_1 Z_2^*|}{|\ln Z_1/Z_2|} \right) \tag{25}$$

where the summation is over the multivalued values of the summand on all sheets of its Riemann surface. In (24) and (25) the sums are single-valued even though the individual terms are not.

3. Explicit formulae for $\zeta(2; \alpha)$

Because the average level density of billiards is asymptotically constant, $\zeta(s)$ diverges as $s \rightarrow 1$ (equation (1)) and the simplest zeta function therefore has $s = 2$. From (10) and (5),

$$\zeta(2; \alpha) = \int_0^{2\pi} d\theta_1 \int_0^{2\pi} d\theta_2 \int_0^1 dR_1 R_1 \int_0^1 dR_2 R_2 |w'(Z_1)|^2 |w'(Z_2)|^2 |\mathcal{G}_{12}|^2 \tag{26}$$

where from now on the α dependence will be indicated explicitly.

To evaluate this we must choose $w(Z)$ and hence a shape for the billiard domain \mathcal{D} . In the work of Itzykson *et al* (1986) (for which $\alpha = 0$) the main emphasis is on triangular domains, for which $w(Z)$ has algebraic singularities (at the images of the vertices). Here we will concentrate on domains with smooth boundaries, generated by conformal transformations for which $w(Z)$ is a low-order polynomial, as introduced by Robnik (1983, 1984) for flux-free billiards (classical and quantum) and applied by BR to the Aharonov-Bohm billiards.

For this type of transformation we may write

$$w'(Z) = \sum_{l=0}^{l_{\max}} d_l Z^l \quad (27)$$

involving $l_{\max} + 1$ complex coefficients d_l . In numerical examples we shall take $l_{\max} = 2$, for which a canonical form (see BR) is

$$w(Z) = Z + BZ^2 + C e^{i\chi} Z^3$$

i.e. $d_0 = 1 \quad d_1 = 2B \quad d_2 = 3C e^{i\chi}$ (28)

where B , C and χ are real.

When (27) is substituted into (26) along with the Green function (17) there results a sixfold summation, which the angular integrations immediately reduce twofold. The radial integrations are elementary but lead to complicated expressions whose reduction will not be described in detail except to state that it makes use of the identity

$$\frac{1}{a} - \frac{1}{a+b} - \frac{1}{a+c} + \frac{1}{a+b+c} = \frac{(2a+b+c)bc}{a(a+b)(a+c)(a+b+c)}. \quad (29)$$

The final result is

$$\zeta(2; \alpha) = \frac{1}{4} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{s=|m-n|}^{l_{\max}} \sum_{t=|m-n|}^{l_{\max}} g(m, n, s, t) \quad (30)$$

where

$$g(m, n, s, t) = \frac{(2a + |m - \alpha| + |n - \alpha|) \operatorname{Re} d_s d_{s-|m-n|}^* d_t^* d_{t-|m-n|}}{a(a + |m - \alpha|)(a + |n - \alpha|)[(a + |m - \alpha| + |n - \alpha|)^2 - (s - t)^2]} \quad (31)$$

in which

$$a = 2 + s + t - |m - n|. \quad (32)$$

The quadruple sum is not as bad as it looks. For fixed n the number of m, s, t terms is finite (and equal to $(l_{\max} + 1)(l_{\max} + 2)(l_{\max} + 3)/6$). The n sum is infinite but converges as $\sum |n|^{-3}$. It is therefore easy to calculate $\zeta(2; \alpha)$ on a microcomputer: when $l_{\max} = 2$, six-figure accuracy (table 1) is achieved in a few minutes for each value of α .

Consider $\zeta(2; \alpha)$ as a function of α for a given billiard, i.e. for a given choice of $\{d_l\}$ in (27). The following symmetries follow from corresponding symmetries of (18) of \mathcal{G}_{12} or of the eigenvalues $E_j(\alpha)$ (see BR):

$$\zeta(2; \alpha) = \zeta(2; -\alpha) = \zeta(2; \alpha + 1). \quad (33)$$

It is therefore necessary to consider only the range $0 \leq \alpha \leq \frac{1}{2}$. We expect $\zeta(2; \alpha)$ to be smooth apart from discontinuities of slope at integer α . These discontinuities arise from discontinuities in the slopes of the individual eigenvalues, given by

$$(\partial E_j(\alpha)/\partial \alpha) \rightarrow 2\pi \operatorname{sgn}(\alpha) \psi_j^2(r=0; \alpha=0) \quad \text{as } \alpha \rightarrow 0 \quad (34)$$

Table 1. Spectral zeta function $\zeta(2; \alpha)$ for three billiards of the type (28): the unit circle ($B = C = 0$); the heart ($B = 0.4, C = 0$) and the Africa ($B = C = 0.2, \chi = \pi/3$).

α	$10^2 \zeta(\text{circle})$	$10^2 \zeta(\text{heart})$	$10^2 \zeta(\text{Africa})$
0	4.936 68	8.308 31	6.635 13
0.05	4.580 83	7.847 25	6.235 62
0.1	4.286 65	7.462 94	5.903 94
0.15	4.044 43	7.144 14	5.629 77
0.2	3.846 64	6.882 11	5.405 13
0.25	3.687 52	6.670 11	5.223 87
0.3	3.562 63	6.502 93	5.081 24
0.35	3.468 64	6.376 64	4.973 69
0.4	3.403 14	6.288 38	4.898 62
0.45	3.364 48	6.236 17	4.854 27
0.5	3.351 69	6.218 89	4.839 59

where ψ_j is the j th normalised wavefunction, assumed non-degenerate for zero flux; this formula is derived in appendix 1.

For the (unit) *circular billiard*, $d_l = \delta_{l,0}$ and (30) gives

$$\zeta(2; \alpha) = \frac{1}{16} \sum_{n=-\infty}^{\infty} \frac{1}{(2+|n-\alpha|)(1+|n-\alpha|)^2} \tag{35}$$

This is a sum rule for the zeros of fractional-order Bessel functions, because the circle eigenfunctions (labelled l, m) are

$$\psi_{lm}(\mathbf{r}; \alpha) = N_{lm} J_{|l-\alpha|}(j_{|l-\alpha|,m} r) e^{il\phi} \quad (-\infty < l < \infty, m \geq 1) \tag{36}$$

where N_{lm} are normalisation constants and $j_{\nu,m}$ is the m th non-zero zero of the Bessel function of order ν . Thus the circle energy levels are

$$E_{lm} = j_{|l-\alpha|,m}^2 \tag{37}$$

and

$$\zeta(2; \alpha) = \sum_{l=-\infty}^{\infty} \sum_{m=1}^{\infty} j_{|l-\alpha|,m}^{-4} \tag{38}$$

By elementary arguments involving low-order Riemann zeta functions, (35) gives the limiting values

$$\begin{aligned} \zeta(2; 0) &= \frac{1}{48} \pi^2 - \frac{5}{32} = 0.049\ 3668 \\ \zeta(2; \frac{1}{2}) &= \frac{1}{16} \pi^2 - \frac{7}{12} = 0.033\ 5169 \\ \partial \zeta(2; \alpha) / \partial \alpha &\rightarrow -\frac{5}{64} \quad \text{as } \alpha \rightarrow 0_+. \end{aligned} \tag{39}$$

The function $\zeta(2; \alpha)$ obtained from the sum (35) is plotted in figure 1.

An approximation to the function $\zeta(2; \alpha)$ for the circle can be obtained from (35) by applying Poisson's formula (22). This gives, first of all, the exact results

$$\begin{aligned} \zeta(2; \alpha) &= \frac{1}{16} \sum_{m=-\infty}^{\infty} \exp(2\pi i m \alpha) \int_{-\infty}^{\infty} dx \frac{\exp(2\pi i m x)}{(|x|+1)^2(|x|+2)} \\ &= \frac{1}{8} \int_0^{\infty} \frac{dx}{(x+1)^2(x+2)} + \frac{1}{4} \sum_{m=1}^{\infty} \cos(2\pi m \alpha) \int_0^{\infty} dx \frac{\cos 2\pi m x}{(x+1)^2(x+2)} \\ &= \frac{1 - \ln 2}{8} + \frac{1}{4} \sum_{m=1}^{\infty} \cos(2\pi m \alpha) [1 + 2\pi m \text{Si}(2\pi m) + \text{Ci}(2\pi m) - \text{Ci}(4\pi m)] \end{aligned} \tag{40}$$

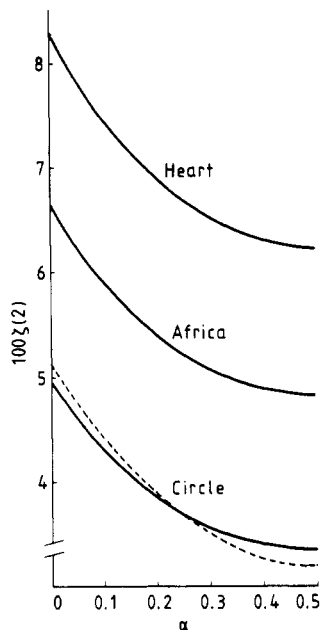


Figure 1. $\zeta(2; \alpha) \equiv \sum_{j=1}^{\infty} [E_j(\alpha)]^{-2}$ computed from (30) for the circular billiard and for the Africa and heart billiards (equations (28) and (43)). The broken curve is the approximation (42) for the circle.

where Si and Ci are the sine and cosine integrals, defined by

$$\text{Si}(x) \equiv - \int_x^{\infty} dt \frac{\sin t}{t} \quad \text{Ci}(x) \equiv - \int_x^{\infty} dt \frac{\cos t}{t}. \tag{41}$$

If these integrals are approximated by their lowest-order large x asymptotic forms, the zeta function becomes

$$\begin{aligned} \zeta(2; \alpha) &\approx \frac{1 - \ln 2}{8} + \frac{5}{16} \sum_{m=1}^{\infty} \frac{\cos(2\pi m\alpha)}{(2\pi m)^2} \\ &= \frac{1}{8}(1 - \ln 2) + \frac{5}{64}(\frac{1}{6} - \alpha + \alpha^2) \\ &= \frac{91}{768} - \frac{1}{8} \ln 2 + \frac{5}{64}(\alpha - \frac{1}{2})^2. \end{aligned} \tag{42}$$

This approximation is also plotted in figure 1 and evidently gives a qualitatively accurate description of the function $\zeta(2; \alpha)$ (the value of $-\partial\zeta(2; 0)/\partial\alpha$ is exact).

Of course the main interest lies in non-circular billiards, for which the $E_j(\alpha)$ are not expressible in terms of standard special functions, and figure 1 and table 1 also show $\zeta(2; \alpha)$ obtained from (20) for two billiards in the family (28). These are

$$\begin{aligned} B=0.4 \quad C=0 & \quad \text{('heart' billiard)} \\ B=C=0.2 \quad \chi=\pi/3 & \quad \text{('Africa' billiard)} \end{aligned} \tag{43}$$

the reason for the names being apparent from figure 2. Previous studies of these billiards (Robnik 1983, BR) indicate that the classical bouncing trajectories (the same with and without flux) are chaotic.

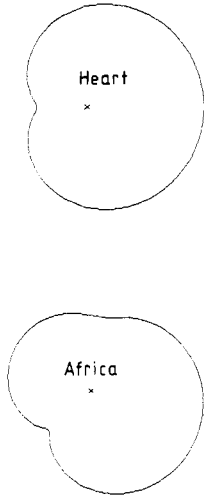


Figure 2. Boundaries of heart and Africa billiard domains (equations (28) and (43)) with crosses marking the position of the flux line.

The scale of the ζ axis in figure 1 is not significant, because for any α the numerical value of $\zeta(2; \alpha)$ can be altered simply by uniform magnification of \mathcal{D} ($\zeta(2; \alpha)$ is proportional to \mathcal{A}^2 where \mathcal{A} is the area of \mathcal{D}). It is the shape of the curves which is important, not their scale, and it is clear from figure 1 that the three zeta functions are qualitatively similar. But they are not identical, because if all three curves are scaled to have the same value at $\alpha = 0$ their values at $\alpha = \frac{1}{2}$ differ by 10%.

The qualitative similarity of ζ curves for billiards whose classical motions are very different is explained by the fact that differences of classical motion affect the *asymptotic* spectral fluctuations, whereas the series for $\zeta(2)$ is sensitive to the details of *low-lying levels* and depends only on the average locations of the high levels. To demonstrate this, we calculate $\zeta(2; \alpha)$ using a finite number of levels computed by matrix diagonalisation of \hat{H} , and approximate the remaining levels by the best semiclassical approximation which is blind to the details of the classical motion. Thus we write

$$\zeta(2; \alpha) = \sum_{j=1}^N \frac{1}{E_j^2} + \sum_{N+1}^{\infty} \frac{1}{E_j^2} \equiv \zeta_N^-(2; \alpha) + \zeta_{N+1}^+(2; \alpha). \tag{44}$$

The semiclassical approximation for the zeta tail ζ_{N+1}^+ is obtained from the smoothed spectral staircase function $\mathcal{N}_{sm}(E)$, i.e. the smoothed number of states with energies less than E , for which we use the corrected Weyl formula (Baltes and Hilf 1976), valid for simply connected \mathcal{D} with area \mathcal{A} and (smooth) boundary with length \mathcal{L} , with an extra term arising from the flux α . The derivation of this extra term is given in appendix 2. The resulting expression for $\mathcal{N}_{sm}(E)$, written for $0 \leq \alpha \leq 1$ but periodic in α , is

$$\mathcal{N}_{sm}(E) = \mathcal{A}E/4\pi - \mathcal{L}\sqrt{E}/4\pi + \frac{1}{6} - \alpha(1 - \alpha)/2. \tag{45}$$

With this formula the best approximation to the j th level is given by

$$\mathcal{N}_{sm}(E_j) = j - \frac{1}{2} \tag{46}$$

which is

$$E_j \approx \llbracket \mathcal{L} + \{ \mathcal{L}^2 + 16\pi\mathcal{A}[j - \frac{2}{3} + \alpha(1 - \alpha)/2] \}^{1/2} (2\mathcal{A})^{-1} \rrbracket^2. \tag{47}$$

As a specific numerical example we take the heart billiard (43) with the golden flux $\alpha = \frac{1}{2}(\sqrt{5} - 1)$ and $N = 125$ in (44). We have

$$\begin{aligned} \mathcal{A} &= 4.1469 & \mathcal{L} &= 7.3376 \\ \zeta_{125}^-[2; \tfrac{1}{2}(\sqrt{5} - 1)] &\approx 0.062\,387 & & \text{(matrix diagonalisation)} & (48) \\ \zeta_{126}^+[2; \tfrac{1}{2}(\sqrt{5} - 1)] &\approx 0.000\,773 & & \text{(equation (47))} \end{aligned}$$

(the value of ζ_{125}^- was kindly supplied by M Robnik). Thus (44) gives $\zeta[2; \frac{1}{2}(\sqrt{5} - 1)] \approx 0.063\,160$, in agreement with $\zeta[2; \frac{1}{2}(\sqrt{5} - 1)] = 0.063\,1597$ from (30). Comparable accuracy (better than one part in 10^5) was obtained by similar computations over the whole range $0 \leq \alpha \leq \frac{1}{2}$ with the Africa billiard. Degradation of the asymptotic formula (45) can result in a considerable loss of accuracy: if for example all three correction terms are omitted the significant digits of ζ_{125}^+ are 872 rather than 773 and $\zeta(2)$ is accurate only to one part in 10^3 .

This insensitivity to the details of high-lying levels suggests that $\zeta(2; \alpha)$ might be usefully employed to estimate the ground state, and it is to this that we now turn.

4. Estimates of the ground state

Watson (1944) gives examples of the early history of the use of sum rules to obtain approximations to low-lying eigenvalues. For example in 1776 Waring introduced

$$E_1 = \lim_{s \rightarrow \infty} [\zeta(s)]^{-1/s} \quad (49)$$

as a technique for estimating the smallest root of an equation, and in 1781 Euler used

$$[\zeta(s)]^{-1/s} < E_1 < \zeta(s)/\zeta(s+1) \quad (50)$$

to compute the lowest Bessel zero $j_{0,1}$ to one part in a million (by extrapolation based on several values of $\zeta(s)$).

For Aharonov-Bohm billiards, with $\zeta(s)$ available only for $s=2$ at present, we employ what we call the 'semiclassical zeta approximation'. This is based on (44) with $N = 1$, in which the ground state is

$$E_1(\alpha) = [\zeta(2; \alpha) - \zeta_2^+(2; \alpha)]^{-1/2} \quad (51)$$

with ζ_2^+ approximated by the semiclassical formulae (45)-(47). The semiclassical sum for ζ_2^+ converges slowly (as j^{-2}) but is rapidly evaluated by replacing its tail by the lowest Euler-Maclaurin integral, that is, by using

$$\zeta_2^+ \approx \frac{16\mathcal{A}^4}{\mathcal{L}^4} \sum_{j=1}^{\infty} T_j^{-4} = \lim_{M \rightarrow \infty} \left(\frac{16\mathcal{A}^4}{\mathcal{L}^4} \sum_{j=1}^M T_j^{-4} + \frac{\mathcal{A}^3}{\pi\mathcal{L}^2} T_{M+1/2}^{-2} (1 - 2T_{M+1/2}^{-1}) \right) \quad (52)$$

where

$$T_j \equiv 1 + [1 + (16\pi\mathcal{A}/\mathcal{L}^2)(j - \frac{2}{3} + \alpha(1 - \alpha)/2)]^{1/2}. \quad (53)$$

(This technique accelerates the convergence by a factor of 100.)

Table 2 shows the ground state calculated in this way for the Africa billiard (43) (which has $\mathcal{A} = 3.7699$, $\mathcal{L} = 7.1012$), for several values of the flux α , together with the 'exact' values of $E_1(\alpha)$ (kindly supplied by M Robnik). Figure 3 shows the same data along with two other approximations: the pure semiclassical approximation ((47) with $j = 1$) and the bare zeta approximation ((51) with ζ_2^+ set to zero). Another possibility

Table 2. Ground state of the Africa billiard.

	$E_1(\alpha)$ exact	$E_1(\alpha)$ from (51)-(53)	% error
0	5.067	5.108	0.8
$\frac{1}{2}(\sqrt{5}-1) = 0.1180$	5.678	5.710	0.6
0.25	6.279	6.268	-0.2
$\frac{1}{2}(3-\sqrt{5}) = 0.3820$	6.708	6.631	-1.1
0.5	6.849	6.743	-1.5

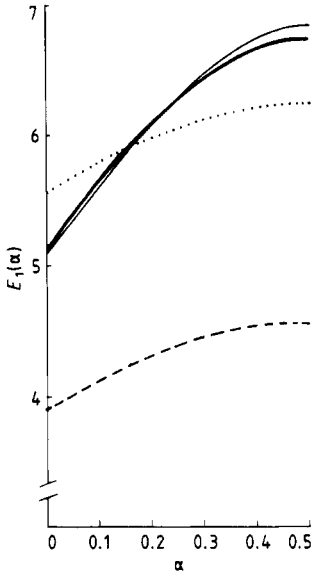


Figure 3. Ground state $E_1(\alpha)$ for the Africa billiard including the exact ground state (thin curve), the semiclassical zeta approximation based on (51)-(53) (thick curve), the pure semiclassical approximation (dotted curve) and the bare zeta approximation (broken curve).

might appear to be based on (51) with the uncorrected Weyl formula (first term of (45)), but this gives

$$\zeta_2^+ \approx \frac{\mathcal{A}^2}{4\pi^2} \sum_{j=2}^{\infty} (2j-1)^{-2} = \frac{\mathcal{A}^2}{4\pi^2} (\pi^2/8 - 1) \tag{54}$$

which for the Africa billiard exceeds the exactly known ζ_2 for all α and so is meaningless when employed in (51).

Evidently the semiclassical zeta approximation gives the ground state accurate to about one per cent over the whole range of α .

At first it is surprising to get such high accuracy from such a simple theory with no adjustable parameters (such as occur in variational procedures, for example). Some insight into the accuracy comes from the following estimate of the expected fractional error ε_1 , which arises as the result of deviations δE_j of the higher levels from the assumed semiclassical form (47). From (51) and (44) we have

$$\varepsilon_1 \equiv \frac{\delta E_1}{E_1} = \frac{E_1^2}{2} \delta \zeta_2^+ = E_1^2 \sum_{j=2}^{\infty} \frac{\delta E_j}{E_j^3} \tag{55}$$

Now we assume the errors δE_j of the different levels are independent with mean values zero, i.e. $\langle \delta E_j \rangle = 0$ and $\langle \delta E_i \delta E_j \rangle = 0$ ($i \neq j$). Then

$$\langle \varepsilon_1^2 \rangle = E_1^4 \sum_{j=1}^{\infty} \frac{\langle \delta E_j^2 \rangle}{E_j^6}. \quad (56)$$

Next we assume that $\langle \delta E_j^2 \rangle$ are the fluctuations in level spacings as described by the Gaussian unitary ensemble which is the appropriate ensemble for systems without time-reversal symmetry (see BR). In terms of the mean level spacing $4\pi/\mathcal{A}$ and the normalised fluctuating spacings S ,

$$\begin{aligned} \langle \delta E_j^2 \rangle^{1/2} &\approx 4\pi(\langle S^2 \rangle - 1)^{1/2} / \mathcal{A} = 4\pi(\frac{3}{8}\pi - 1)^{1/2} / \mathcal{A} \\ &= (0.422 \times 4\pi) / \mathcal{A}. \end{aligned} \quad (57)$$

It is adequate to approximate the series (56) by its first term, and E_1 and E_2 by (47). This gives, for the expected fractional ground-state error,

$$\langle \varepsilon_1^2 \rangle^{1/2} \approx 0.422 \times (16\pi\mathcal{A}T_1^4 / \mathcal{L}^2 T_2^6) \quad (58)$$

where T_j is defined in (53). For the Africa billiard, $\langle \varepsilon_1^2 \rangle^{1/2} \approx 0.027$ which is indeed comparable with the errors in table 1. (For $\alpha = 0$ and $\alpha = \frac{1}{2}$ the appropriate fluctuations are those of the Gaussian orthogonal ensemble; instead of 0.422 this gives $(8/\pi^{3/2} - 1)^{1/2} = 0.661$ and still leads to expected errors of a few per cent.)

One consequence of the above error analysis is that the semiclassical zeta approximation relies for its success on level repulsion (such as that occurring in the Gaussian ensembles) and especially on repulsion between E_1 and E_2 . The approximation should therefore be at its worst for billiards whose *ground state is degenerate*. This occurs for the *circular billiard* where, because of (37), *all* states are (doubly) degenerate when $\alpha = \frac{1}{2}$ (the degeneracies are between states with l and $-l+1$). The way in which this degrades the semiclassical zeta approximation for $E_1(\alpha)$ as α approaches $\frac{1}{2}$ is clear from table 3 and figure 4. For the degenerate case itself the simplest remedy is to replace (44) by

$$\begin{aligned} \zeta(2; \frac{1}{2}) &= (2/E_1^2) + \zeta_3^+(2; \frac{1}{2}) \\ \text{i.e.} \quad E_1 &= [2/(\zeta(2; \frac{1}{2}) - \zeta_3^+(2; \frac{1}{2}))]^{1/2} \end{aligned} \quad (59)$$

and then use the semiclassical approximation (47) to evaluate ζ_3^+ . This gives $E_1(\frac{1}{2}) = 9.892$ which is in error (cf table 3) by only +0.2%.

Table 3. Ground state of the circular billiard.

	$E_1(\alpha)$ exact	$E_1(\alpha)$ from (51)–(53)	% error
0	5.783	5.848	1.1
0.1	6.541	6.567	0.4
0.2	7.328	7.232	-1.3
0.3	8.146	7.783	-4.5
0.4	8.993	8.152	-9.3
0.5	9.870	8.282	-16.1

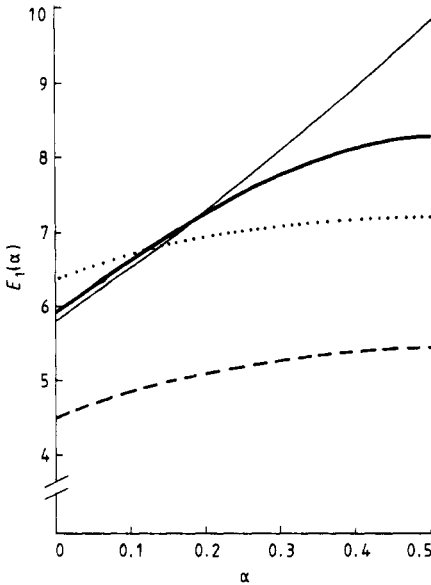


Figure 4. As figure 3, but for the circular billiard.

5. Conclusions

In this study we have concentrated on finding explicit formulae for $\zeta(2; \alpha)$, and employing them to estimate the ground state. This merely scratches the surface of what spectral zeta functions contain, and there are two obvious directions for future research.

Firstly, $\zeta(s; \alpha)$ should be studied for integer $s > 2$. The formalism already exists: equation (10) with \mathcal{G}_{12} given by (17) and $w'(Z)$ by (27). But the algebra involved in finding the generalisations of $\zeta(2; \alpha)$ as given by (30) is very heavy, even for $s = 3$, and would probably best be carried out on a computer using symbolic manipulation. If this turns out to be feasible, the resulting sequence of zeta functions could be used in Euler's procedure based on (50) to calculate $E_1(\alpha)$ with high accuracy. By extension, N zeta functions could be used to estimate the first N levels, and it would be interesting to see whether very high states could be calculated accurately in this way (probably not).

Secondly, the analytic properties of $\zeta(s; \alpha)$ in the complex s plane should be studied. The reason for doing this is that in principle the whole spectrum can be reconstructed from this complex function. For example the *partition function* is

$$\sum_{j=1}^{\infty} e^{-tE_j} = \text{Tr } e^{-t\hat{H}} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \zeta(s) \Gamma(s) t^{-s} \tag{60}$$

where $c > 1$, and the level density is

$$\sum_{j=1}^{\infty} \delta(E - E_j) = \text{Tr } \delta(E - \hat{H}) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \zeta(s) E^{s-1}. \tag{61}$$

Of course some of the information contained in the analytic structure of $\zeta(s; \alpha)$ concerns high-lying states and is therefore *semiclassical*. An elementary example is the

simple pole at $s = 1$, whose residue is the asymptotic (Weyl) level density ($\mathcal{A}/4\pi$ for billiards with and without flux). More refined properties (perhaps the distribution of zeros) would contain information distinguishing billiards with and without flux and billiards with chaotic or regular classical trajectories.

Acknowledgments

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Appendix 1

This is the derivation of equation (34). For any α , the rate of change of eigenvalue with flux is

$$\frac{\partial E_j}{\partial \alpha} = \left\langle j \left| \frac{\partial \hat{H}}{\partial \alpha} \right| j \right\rangle = \iint \mathbf{d}\mathbf{r} \psi_j^*(\mathbf{r}; \alpha) \frac{\partial \hat{H}}{\partial \alpha} \psi_j(\mathbf{r}; \alpha) \quad (\text{A1.1})$$

where the integration domain is \mathcal{D} . For \hat{H} we take (2) with the gauge in which the lines of \mathbf{A} are concentric circles. Then

$$\frac{\partial \hat{H}}{\partial \alpha} = \frac{2}{r^2} \left(i \frac{\partial}{\partial \phi} + \alpha \right). \quad (\text{A1.2})$$

For ψ_j we write a superposition of elementary solutions of Schrödinger's equation in polar coordinates, namely

$$\psi_j(\mathbf{r}; \alpha) = \sum_{l=-\infty}^{\infty} c_l(\alpha) e^{il\phi} J_{|l-\alpha|}(k_j r) \quad (\text{A1.3})$$

where $k_j \equiv \sqrt{E_j}$. Then with the boundary of \mathcal{D} denoted by $r = r_b(\phi)$ (A1.1) gives

$$\begin{aligned} \frac{\partial E_j}{\partial \alpha} &= 2 \int_0^{2\pi} d\phi \int_0^{r_b(\phi)} dr \sum_{l=-\infty}^{\infty} \sum_{l'=-\infty}^{\infty} c_l(\alpha) c_{l'}^*(\alpha) \\ &\times \exp[i(l-l')\phi] \frac{J_{|l-\alpha|}(k_j r) J_{|l'-\alpha|}(k_j r)}{r} (\alpha - l). \end{aligned} \quad (\text{A1.4})$$

We want to study $\partial E_j / \partial \alpha$ as α tends to zero (or any other integer). When α equals zero the terms multiplied by $-l$, which come from the $i \partial / \partial \phi$ term in (A1.2), must sum to zero because $i \partial / \partial \phi$ is a Hermitian operator so its contribution to $\partial E_j / \partial \alpha$ must be real, whereas the zero flux wavefunction $\psi_j(\mathbf{r}; 0)$ is real (i.e. $c_{-l}(0) = c_l^*(0)$ if as we assume, it is non-degenerate) and this implies that the terms give a contribution to (A1.4) which is imaginary.

The terms multiplied by α all tend to zero except the one with $l = l' = 0$ for which the radial integrals diverge at the origin if $\alpha = 0$. This term gives

$$\frac{\partial E_j}{\partial \alpha} \rightarrow 2 \psi_j^2(0; 0) \lim_{\alpha \rightarrow 0} \alpha \int_0^{2\pi} d\phi \int_0^{r_b(\phi)} dr \frac{J_{|\alpha|}^2(k_j r)}{r} \quad \text{as } \alpha \rightarrow 0 \quad (\text{A1.5})$$

where we have used the fact, which follows from (A1.3), that $c_0(0)$ is the (real) value of the zero flux wavefunction at $r = 0$. In the limit the integrals are dominated by the behaviour close to the origin, so

$$\begin{aligned} \lim_{\alpha \rightarrow 0} \alpha \int_0^{2\pi} d\phi \int_0^{r_b(\phi)} dr \frac{J_{|\alpha|}^2(k_j^2 r)}{r} &= \lim_{\alpha \rightarrow 0} \frac{\alpha (k_j/2)^{2|\alpha|}}{\Gamma^2(1+|\alpha|)} \int_0^{2\pi} d\phi \int_0^{r_b(\phi)} dr r^{2|\alpha|-1} \\ &= \lim_{\alpha \rightarrow 0} \frac{\alpha}{2|\alpha|\Gamma^2(1+|\alpha|)} \int_0^{2\pi} d\phi \left(\frac{k_j r_b(\phi)}{2}\right)^{2|\alpha|} = \pi \operatorname{sgn}(\alpha) \end{aligned} \tag{A1.6}$$

and when substituted into (A1.5) this gives (34).

What makes $\partial E_j/\partial \alpha$ discontinuous at $\alpha = 0$ is the singular nature of the magnetic field $\Phi \delta(r)$ of a single flux line; for a smooth magnetic field, switching on the flux would not be a singular perturbation, and $\partial E_j/\partial \alpha$ would vanish at $\alpha = 0$.

Appendix 2

This is the justification for using the corrected Weyl rule (45), with the extra term involving the flux α , as the smoothed spectral staircase function for Aharonov-Bohm billiards. The spectral staircase (unsmoothed) is defined as

$$\mathcal{N}(E) \equiv \sum_{j=1}^{\infty} \Theta(E - E_j) \tag{A2.1}$$

where Θ denotes the unit step function. Its derivative is the spectral density given in terms of the trace of the energy-dependent Green function by

$$\frac{d\mathcal{N}(E)}{dE} = -\frac{1}{\pi} \operatorname{Im} \operatorname{Tr} \frac{1}{E + i\varepsilon - \hat{H}} \equiv -\frac{1}{\pi} \iint_{\mathcal{A}} d\mathbf{r} \operatorname{Im} \mathcal{G}_E(\mathbf{r}, \mathbf{r}). \tag{A2.2}$$

Semiclassically (that is for large E) $\mathcal{G}_E(\mathbf{r}, \mathbf{r})$ consists of contributions from the classical trajectories that begin and end at \mathbf{r} and have energy E (for a review of these ideas see Berry (1983)). These trajectories are of two sorts. First, there are the (infinitely many) closed orbits which return to \mathbf{r} after a finite time. Their contributions to $\mathcal{N}(E)$ are oscillatory functions of energy whose phase is proportional to their action; this includes a term for orbits winding w times round the flux line (see BR). The closed orbits describe spectra on fine scales and are of course flux dependent.

Second, there are the trajectories which go from \mathbf{r}' to \mathbf{r} without any excursion (these are the limits as $\mathbf{r}' \rightarrow \mathbf{r}$ of the direct paths from \mathbf{r}' to \mathbf{r}). It is these trajectories which give the non-oscillatory (smoothed) contributions $\mathcal{N}_{sm}(E)$ whose flux dependence we now seek to establish.

For ordinary billiards ($\alpha = 0$) Balian and Bloch (1970) show that the non-oscillatory part of $\operatorname{Im} \mathcal{G}_E(\mathbf{r}, \mathbf{r})$ is given by that of the Green function in unbounded space unless \mathbf{r} is very close to the boundary, and this lowest-order theory gives the leading (Weyl) term in (45). When \mathbf{r} is very close to the boundary there are corrections to \mathcal{G}_E in the form of multiple integrals involving tiny closed orbits formed by clusters of neighbouring points, and these give rise to the corrections in (45). Switching on the flux leaves the boundary terms unaffected, because the only possible contribution to each tiny closed orbit would be a phase factor depending on the magnetic flux through it, but this flux is zero (the flux line α does not pierce such orbits) so that the factor is unity. (This also follows from a Feynman picture (Morandi and Menossi 1984) in which $\mathcal{G}_E(\mathbf{r}, \mathbf{r})$ is the sum of all paths—not just classical orbits—from \mathbf{r} to \mathbf{r} with flux

contributing according to the winding number, and the winding number is zero for all (tiny) paths giving rise to the asymptotic boundary contributions.)

In fact the flux term in (45) arises from the area integral of the unbounded Green function. We find this Green function by a method similar to that employed for the zero energy circle Green function in § 2. Without flux, the unbounded Green function is (with $k \equiv \sqrt{E}$)

$$\begin{aligned} \mathcal{G}_E(\mathbf{r}_1, \mathbf{r}_2) &= -\frac{1}{4i} H_0^{(1)}(k|\mathbf{r}_1 - \mathbf{r}_2|) \\ &= -\frac{1}{4i} \sum_{l=-\infty}^{\infty} \exp[i l(\theta_1 - \theta_2)] J_{|l|}(kr_{<}) H_{|l|}^{(1)}(kr_{>}) \quad (\alpha = 0). \end{aligned} \quad (\text{A2.3})$$

With flux, the correct generalisation (analogous to that of Morandi and Menossi (1984) for the time-dependent case) is

$$\mathcal{G}_E(\mathbf{r}_1, \mathbf{r}_2) = -\frac{1}{4i} \sum_{l=-\infty}^{\infty} \exp[i l(\theta_1 - \theta_2)] J_{|l-\alpha|}(kr_{<}) H_{|l-\alpha|}^{(1)}(kr_{>}). \quad (\text{A2.4})$$

The quantity appearing in (A2.2) is thus

$$-\pi^{-1} \text{Im} \mathcal{G}_E(\mathbf{r}, \mathbf{r}) = \frac{1}{4\pi} \sum_{l=-\infty}^{\infty} J_{|l-\alpha|}^2(kr). \quad (\text{A2.5})$$

When $\alpha = 0$ the Bessel sum is unity and its area integral in (A2.2) simply gives the leading (Weyl) term in (45), as stated previously. The extra number of states below energy $E \equiv K^2$ in a billiard (assumed circular without affecting the result) with area $\mathcal{A} \equiv \pi R^2$ is

$$\begin{aligned} \Delta \mathcal{N} &= 2 \int_0^K dk k \int_0^R dr 2\pi r \left(-\frac{1}{\pi} \text{Im} [\mathcal{G}_E(\mathbf{r}, \mathbf{r}) - \mathcal{G}_E(\mathbf{r}, \mathbf{r})_{(\alpha=0)}] \right) \\ &= \int_0^K dk k \int_0^R dr r \sum_{l=-\infty}^{\infty} (J_{|l-\alpha|}^2(kr) - J_{|l|}^2(kr)). \end{aligned} \quad (\text{A2.6})$$

Transforming using the Poisson formula (22) gives

$$\Delta \mathcal{N} = -8 \sum_{m=1}^{\infty} \sin^2(m\pi\alpha) \int_0^R dr r \int_0^K dk k \int_0^{\infty} dx J_x^2(kr) \cos(2\pi mx). \quad (\text{A2.7})$$

For the Bessel function we employ the smoothed Debye approximation

$$\begin{aligned} J_x^2(kr) &\approx [(kr)^2 - x^2]^{-1/2} / \pi \quad (x < kr) \\ &\approx 0 \quad (x > kr). \end{aligned} \quad (\text{A2.8})$$

The x integration can be performed and we obtain

$$\begin{aligned} \Delta \mathcal{N} &= -4 \sum_{m=1}^{\infty} \sin^2(m\pi\alpha) \int_0^R dr r \int_0^K dk k J_0(2\pi mkr) \\ &= -4 \sum_{m=1}^{\infty} \frac{\sin^2(m\pi\alpha)}{(2\pi m)^2} [1 - J_0(2\pi mKR)]. \end{aligned} \quad (\text{A2.9})$$

Smoothing eliminates the J_0 term for large KR (the semiclassical limit), giving the non-oscillatory flux contribution as

$$\begin{aligned}\Delta\mathcal{N}_{\text{sm}} &= -\frac{1}{\pi^2} \sum_{m=1}^{\infty} \frac{\sin^2(m\pi\alpha)}{m^2} \\ &= -\alpha(1-\alpha)/2 \quad (0 \leq \alpha \leq 1)\end{aligned}\tag{A2.10}$$

thereby completing the justification of (45).

The negative value of $\Delta\mathcal{N}_{\text{sm}}$ shows that the flux line acts to repel states from its neighbourhood. But this effect is small: $\Delta\mathcal{N}_{\text{sm}} < \frac{1}{8}$ and so never exceeds the curvature term $\frac{1}{6}$ in (45).

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