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The smooth spectral counting function and the total phase shift for quantum billiards

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Abstract. The interior–exterior duality provides a means to extract spectral information (for the interior problem) from the scattering matrix (which is relevant to the exterior problem). We study the smooth spectral counting function for the interior, and compare it to the smooth total phase shift in the exterior. To leading order in the semiclassical approximation these functions are known to coincide. Using various techniques, we study the higher-order corrections of the two functions and discuss the difference between them.

1. Introduction

A billiard boundary can serve to define two seemingly unrelated physical systems. It may bind a particle (or a wavefunction) to the *interior*, or act as an obstacle when particles (or waves) scatter from the *exterior*. During the past few years, an intimate duality between the interior and the exterior problems was established on both the classical and the quantum (wave) levels. In the quantum domain, this implies a link between the spectrum of the interior problem and the properties of the scattering matrix $S(k)$, where k is the wave number. Stated in crude terms, it says that whenever k approaches an eigenvalue k_n from below, an eigenvalue of $S(k)$ approaches unity from the upper half plane (the scattering matrix is unitary and its eigenvalues are on the unit circle). The reverse is also true—the approach of an eigenvalue of the $S(k)$ matrix to 1 marks the approach of k to an eigenvalue of the interior problem. The interior–exterior duality is reviewed in [1] and various aspects and applications are given in [2–4]. The rigorous formulation is presented in [5].

Denoting the eigenvalues of $S(k)$ by $\exp[-\mathrm{i}\theta_l(k)]$, and making use of the interior–exterior duality, the interior spectral density, $d(k)$, is expressed as

$$d(k) = \sum_{n=1}^{\infty} \delta(k - k_n) = \lim_{\epsilon \to 0^+} \sum_l \delta_{2\pi}[\theta_l(k) + \epsilon]\theta_l'(k) \tag{1}$$

where $\delta_{2\pi}(x)$ is the 2π periodic Dirac δ function. It is assumed that $\theta_l'(k) > 0$ (at least in a region $-\epsilon < \theta_l \bmod 2\pi < 0$ for some positive ϵ). Equation (1) can be expressed in an alternative way by using the Poisson summation formula, and by taking the limit as

$$d(k) = \frac{1}{2\pi}\Theta'(k) + \frac{1}{\pi}\,\mathrm{Im}\sum_{m=1}^{\infty}\frac{1}{m}\,\mathrm{Tr}\left[\frac{\mathrm{d}}{\mathrm{d}k}S^{\dagger m}(k)\right] \tag{2}$$

where $\Theta(k)$ is the total phase shift, defined by $\det[S(k)] = \exp[-\mathrm{i}\Theta(k)]$. It is a continuous function of k, and $\Theta(0) = 0$. For further use it is convenient to introduce

$$\eta(k) = \frac{1}{2\pi}\,\Theta(k)\,. \tag{3}$$

One can get a physical interpretation and a leading-order estimate of $\eta(k)$ by recalling the definition of the Wigner mean delay time [1] as

$$\tau(E) = \frac{\hbar}{\mathrm{i}\Lambda}\,\mathrm{Tr}\left[S^{\dagger}(E)\frac{\mathrm{d}S(E)}{\mathrm{d}E}\right] \tag{4}$$

where Λ is the number of effective scattering modes. It is given by the integer part of kL/π, where L is the circumference of the billiard. To get the leading-order estimate for $\eta(k)$, we assume for simplicity that the billiard is convex, and estimate the mean delay time by $-\langle c\rangle/v$, where $\langle c\rangle$ is the mean chord length of the billiard. (Note that the mean delay time is negative because in this case one actually saves time, on average.) The mean chord length is given by $\langle c\rangle = A\pi/L$, where A is the area of the billiard. Finally, we have

$$\eta'(k) = \hbar v\frac{\mathrm{d}\eta(E)}{\mathrm{d}E} \approx \frac{\Lambda\langle c\rangle}{2\pi} \approx \frac{Ak}{2\pi}\,. \tag{5}$$

This coincides with the leading term in Weyl's formula for the smooth level density of the interior billiard problem. The coincidence (to leading order) between the asymptotic expression (5) and the Weyl formula is not surprising. Due to the Kreĭn spectral shift formula [6] we can interpret $\eta'(k)$ as the excess spectral density in the continuum due to the introduction of the scatterer. To leading order, this is equal to the volume of phase space excluded because of the presence of the scatterer, measured in units of $2\pi\hbar$. However, this is also the estimate of the interior spectral density. This identity was first shown in the mathematical literature in [7]. They derived (5) for quite a general class of billiard shapes in any number of dimensions. Several authors [8–10] obtained similar results and also considered higher terms in the asymptotic series for $\eta(k)$.

Semiclassically, the density of states is divided into a smooth part $\bar{d}(k)$, described by Weyl's formula, and an oscillatory part, described as a sum over periodic orbits (the Gutzwiller sum). This description can be derived by semiclassical arguments from (2). The smooth part is described by Weyl's law from (5), and the sum over periodic orbits comes from the infinite sum on the right. In addition, both terms in (2) have oscillatory contributions of classical orbits which are trapped in the exterior (which exactly cancel each other). The function $\eta(k)$ is thus not a smooth function, but may be divided into a smooth part $\bar{\eta}(k)$ and an oscillatory part. The smooth part $\bar{\eta}(k)$ will be properly defined in the next section.

The surprise, which is the main concern of the present work, comes when one compares the next terms in the high-k asymptotic expansion of $\bar{\eta}'(k)$ and the corresponding terms in the Weyl asymptotic expansion for the smooth spectral density $\bar{d}(k)$: the circumference terms are opposite in sign! Moreover, we provide convincing evidence that *all* the coefficients, except for the area term, in the asymptotic expansion of $\eta'(k)$ are equal in magnitude to the corresponding terms in the asymptotic expansion of $\bar{d}(k)$ but are of opposite sign. The circumference term is just the first of this kind. To illustrate this point, consider a circle billiard of unit radius with Dirichlet boundary conditions. Then,

$$\bar{d}_{\mathrm{c,D}}(k) \approx \frac{k}{2} - \frac{1}{2} - \frac{1}{128k^2} + \frac{111}{32\,768k^4} + \cdots \tag{6}$$

to be compared with

$$\bar{\eta}'_{\mathrm{c,D}}(k) \approx \frac{k}{2} + \frac{1}{2} + \frac{1}{128k^2} - \frac{111}{32\,768k^4} + \cdots. \tag{7}$$

Note that for the circle $\eta(k)$ is asymptotically equal to its smooth part $\bar{\eta}(k)$ (this point is elaborated in section 3). The corresponding expressions for a circular billiard with Neumann boundary conditions are

$$\bar{d}_{\mathrm{c,N}}(k) \approx \frac{k}{2} + \frac{1}{2} - \frac{5}{128k^2} + \frac{807}{32\,768k^4} + \cdots \tag{8}$$

to be compared with

$$\bar{\eta}'_{\mathrm{c,N}}(k) \approx \frac{k}{2} - \frac{1}{2} + \frac{5}{128k^2} - \frac{807}{32\,768k^4} + \cdots. \tag{9}$$

Note that the expressions for $\bar{d}_{\mathrm{c,D}}(k)$ and $\bar{\eta}'_{\mathrm{c,N}}(k)$ coincide up to the second term. The magnitude of the coefficients is different from the third term and beyond.

Various authors in the mathematical literature estimated the second term in the asymptotic series and compared it to the corresponding term in the Weyl series [8–10]. The sign in the second term of the asymptotic expansion of $\eta(k)$ in [8] differs from the sign in [9, 10], and in (7). We cannot trace the origin of this difference. (We assume that the sign of the second term in the expression for $N(k)$ in [10] is a misprint, because it contradicts well known results [11].)

In the next section we shall derive $\bar{\eta}'_{\mathrm{c,D}}(k)$ (equation (7)) and will show that for the circle, all the coefficients, except for the area term, differ in sign from the corresponding terms in the asymptotic expansion of $\bar{d}_{\mathrm{c,D}}(k)$ (equation (6)). For any other smooth shape, we cannot prove this statement in full generality, but can use results of Berry and Howls [12] to show that it holds at least for the leading 13 terms (for Dirichlet boundary conditions).

Another problem which we should address originates from the following observation. If $\bar{\eta}(k)$ does not provide the entire smooth counting function, the deficit, which (to leading order) is twice the circumference term (and hence proportional to k), must come from the infinite sum on the right-hand side of (2). However, this was argued previously to yield the oscillatory contributions to the spectral functions. At the end of the next section we consider this problem for the circular billiard.

The interior–exterior duality does not apply exclusively to scattering problems in the plane. As a matter of fact, one can define similar relations where the scattering is defined by attaching waveguides to the billiard, [1, 2, 13, 14]. The total phase for such systems plays a similar role in this formulation, and we shall compare its asymptotic expansion with that of the corresponding Weyl series. This topic, together with a few other relevant points, will be discussed in section 3.

2. The smooth part of the total phase shift

We shall start by defining what we mean by the smooth part of total phase shift. For this purpose, we adapt the method of [12, 15] to the present problem. The starting point is Kreĭn's spectral shift formula

$$-\frac{1}{\pi}\,\mathrm{Im}\lim_{\epsilon\to 0^+}\mathrm{Tr}[G^+(k+\mathrm{i}\epsilon) - G_0^+(k+\mathrm{i}\epsilon)] = \frac{1}{2k}\eta'(k) \tag{10}$$

where $G_0^+(k)$ is the free Green function with outgoing boundary conditions, and $G^+(k)$ is the Green function for the *exterior* of the billiard, with the appropriate condition on the billiard boundary, and outgoing boundary conditions at infinity. The *trace* operation in (10) is understood as an integration over the *entire* plane, and $G^+(\boldsymbol{r},\boldsymbol{r},k) = 0$ for $\boldsymbol{r} \in \Omega$. To extract $\bar{\eta}(k)$ we first derive an asymptotic expression for $\mathrm{Tr}[G^+(k) - G_0^+(k)]$ for imaginary $k = \mathrm{i}s$, and $s > 0$. We define

$$g^{\mathrm{out}}(s) \equiv \mathrm{Tr}[G^+(k = \mathrm{i}s) - G_0^+(k = \mathrm{i}s)] \tag{11}$$

and assume an asymptotic expansion of the form

$$g^{\mathrm{out}}(s) \approx -\frac{\mathrm{i}A}{4} + \sum_{m=1}^{\infty} \frac{C_m^{\mathrm{out}}}{s^m}\,. \tag{12}$$

The expansion is led by the area term which we discussed above. (Technically, it comes from the integral of $-\operatorname{Im} G_0^+$ over the interior domain, where G^+ vanishes.) One then defines the smooth part of the total phase shift by

$$\bar{\eta}'(k) \equiv -\frac{2k}{\pi} \operatorname{Im} g^{\mathrm{out}}(s = -\mathrm{i}k)\,. \tag{13}$$

The oscillatory terms of $\eta(k)$ are exponentially small for imaginary k, and are neglected in the asymptotic expansion (12). The smooth part $\bar{\eta}(k)$ is the quantity that remains after transforming to the imaginary axis, making the asymptotic approximation, and transforming back to the real axis.

The smoothing operation as defined above follows closely the method of [12, 15] to extract the smooth part of the spectral density of the interior billiard. Their starting point is

$$d(k) = \frac{Ak}{2\pi} + \frac{2k}{\pi} \operatorname{Im} \lim_{\epsilon \to 0^+} \mathrm{Tr}[G(k + \mathrm{i}\epsilon) - G_0^+(k + \mathrm{i}\epsilon)] \tag{14}$$

where $G(k)$ is now the Green function for the *interior* problem with the appropriate condition on the billiard boundary. One defines the function

$$g^{\mathrm{in}}(s) \equiv \mathrm{Tr}[G(k = \mathrm{i}s) - G_0^+(k = \mathrm{i}s)] \tag{15}$$

assumes an asymptotic expansion of the form

$$g^{\mathrm{in}}(s) \approx \sum_{m=1}^{\infty} \frac{C_m^{\mathrm{in}}}{s^m} \tag{16}$$

and proceeds as before. The main contribution to (12) and (16) comes from the close vicinity of the boundary [16]. Hence one would expect that the corresponding asymptotic expansions will be related, the difference might be due only to the change of the sign of the curvature when one goes from the interior to the exterior. This is indeed the case, and in the following we shall demonstrate this by a detailed analysis.

2.1. The circle billiard

We calculate explicitly the smooth total phase shift for the circle billiard (centred at the origin and of unit radius) with Dirichlet boundary conditions. The Green function is explicitly known, and after some manipulation one gets

$$g^{\mathrm{out}}(s) = -\frac{1}{2} \sum_{l=-\infty}^{\infty} \left[-\left(1 + \frac{l^2}{s^2}\right) K_l(s) I_l(s) + I_l'(s) K_l'(s) - \frac{K_l'(s)}{s K_l(s)} \right] \tag{17}$$

where the functions $I_l(z)$, $K_l(z)$ are the modified Bessel functions [17]. The asymptotic expansion for $g^{\mathrm{out}}(s)$ is found by replacing the summation over l by an integral (a step which introduces exponentially small errors), and by using the uniform asymptotic expansions of

$I_l(s)$ and $K_l(s)$ (see equations (9.7.7), (9.7.8) in [17]). This gives the following expression for the coefficients C_m^{out} in the asymptotic series (12):

$$C_m^{\text{out}} = \int_0^\infty \mathrm{d}x \frac{\sqrt{1+x^2}}{x^m} B_m^{\text{out}}\left(\frac{x}{\sqrt{1+x^2}}\right). \tag{18}$$

The functions $B_m^{\text{out}}(t)$ are defined implicitly as the coefficients of l^{-m} of the resulting expansion,

$$\begin{aligned}\sum_{m=1}^{\infty} \frac{B_m^{\text{out}}(t)}{l^m} = {}& \frac{1}{2}\left(\sum_{m=0}^{\infty} \frac{u_m(t)}{l^m}\right)\left(\sum_{m=0}^{\infty} \frac{(-1)^m u_m(t)}{l^m}\right) + \frac{1}{2}\left(\sum_{m=0}^{\infty} \frac{v_m(t)}{l^m}\right)\left(\sum_{m=0}^{\infty} \frac{(-1)^m v_m(t)}{l^m}\right) \\ & - \left(\sum_{m=0}^{\infty} \frac{(-1)^m v_m(t)}{l^m}\right) \Bigg/ \left(\sum_{m=0}^{\infty} \frac{(-1)^m u_m(t)}{l^m}\right)\end{aligned} \tag{19}$$

where the polynomials $u(t)$ and $v(t)$ are defined in the uniform asymptotic expansion for the Bessel functions. Once the functions $B_m^{\text{out}}(t)$ are derived from the above, substituting them in (18) yields the desired expansion of $g^{\text{out}}(s)$. Using the Kreĭn spectral shift formula (10), the asymptotic expansion for $\bar{\eta}_{\text{c,D}}(k)$ (equation (7)) immediately follows.

The results of the above calculation may now be compared with the results for the interior problem [15, 12]. Using the known expressions for the interior Green function for the circle one gets

$$g^{\text{in}}(s) = -\frac{1}{2} \sum_{l=-\infty}^{\infty} \left[\left(1 + \frac{l^2}{s^2}\right) K_l(s) I_l(s) - I_l'(s) K_l'(s) - \frac{I_l'(s)}{s I_l(s)}\right]. \tag{20}$$

From here one obtains the asymptotic expansion for $g^{\text{in}}(s)$ by following the same steps as in the exterior case. A straightforward calculation shows that

$$C_m^{\text{out}} = (-1)^{m+1} C_m^{\text{in}}. \tag{21}$$

This provides the desired relation between the asymptotic series for the smooth level density (6) and the k derivative of the smooth total phase shift (7) for the circle billiard. All the coefficients of the even powers of k are equal in sign but opposite in magnitude. The coefficients of all odd powers, except the area term, vanish (because of the Im operation). The two series are thus opposite in sign beyond the area term. The results for the numerical values of the first 31 coefficients C_m^{in} are given in [12].

2.2. *General smooth boundary*

The methods developed to calculate the asymptotic expansion of $g^{\text{in}}(s)$ for general smooth boundaries rely heavily on the fact that the main contribution for large s comes from the close vicinity of the boundary $\partial\Omega$. In this vicinity, the Green function can be locally expressed using the local curvature $\kappa(q)$ where q is the arc length along $\partial\Omega$. These same methods can also be applied for the calculation of the asymptotic series for $g^{\text{out}}(s)$, since, here too, the main contribution comes from the vicinity of $\partial\Omega$. As a matter of fact, one can read off the asymptotic expansion for $g^{\text{out}}(s)$, by replacing the sign of $\kappa(q)$ in the expansion for $g^{\text{in}}(s)$.

Balian and Bloch [16] were the first to provide a systematic derivation. Their method uses the Born series for $G(r, r') - G_0^+(r, r')$ which is a multiple reflection series. This method has a severe difficulty since the number of reflections does not determine a unique power of $1/s$ in the expansion, and hence, to get the C_m coefficients, one has to perform cumbersome book-keeping which gets complicated as m increases.

Stewartson and Waechter [15, 12] proposed a convenient variant of the method of Balian and Bloch, which circumvents some of its difficulties. The Green function in the vicinity of a point σ on the boundary is expressed in terms of a charge distribution on the line tangential to the boundary at σ. The boundary is expanded as a series, with coefficients which depend on the curvature $\kappa(\sigma)$ and its derivatives. Successive approximations improve the accuracy by which the Green function satisfies the boundary conditions in the vicinity of σ on $\partial\Omega$. Finally, the coefficients $C_m^{\rm in}$ are expressed as

$$C_m^{\rm in} = \oint \mathrm{d}\sigma\, c_m(\sigma) \tag{22}$$

where $c_m(\sigma)$ depends on the curvature and its derivatives. Berry and Howls [12] calculated explicit expressions for the leading c_m for $m \leqslant 13$. One can check that by changing the sign of $\kappa(\sigma)$, the coefficient c_m is multiplied by $(-1)^{m+1}$. Hence when one changes the sign of κ for the calculation of $C_m^{\rm out}$ one finds that (21) holds for arbitrary (smooth) billiards, at least for $m \leqslant 13$.

2.3. The smooth part of the rest

Now that we know that the smooth part of the spectral counting function does indeed differ from the smooth part of the total phase shift (divided by 2π), we have to go back to our starting point (2) and show how the infinite sum on the right-hand side provides the difference, in spite of the fact that it is usually considered only for its oscillatory part. Unfortunately, we do not have a general result, and we shall therefore concentrate on the circle billiard as an example.

For the circle billiard, as the scattering matrix is diagonal in the angular momentum representation, and using the Poisson summation formula, equation (2) may be expressed as

$$d(k) = \eta'(k) + \frac{1}{\pi}\,\mathrm{Im}\sum_{n=1}^{\infty}\sum_{m=-\infty}^{\infty}\frac{1}{n}\int_{-\infty}^{\infty}\mathrm{d}l\,\frac{\partial}{\partial k}\exp[\mathrm{i}n\theta_l(k) + 2\pi\mathrm{i}ml] \tag{23}$$

where the diagonal matrix elements are

$$S_l(k) = \exp[-\mathrm{i}\theta_l(k)] = -\frac{H_l^-(k)}{H_l^+(k)} \tag{24}$$

(and is defined for non-integer l by the usual definition of the Bessel functions). The contribution of the periodic orbit manifolds is derived from the terms with $1 \leqslant m \leqslant n-1$ by a saddle-point approximation. The result is a purely oscillatory function. The rest of the terms are neglected in the semiclassical approximation. It is then reasonable to assume that it may be possible, by a more careful calculation, to associate with each term a smooth contribution such that the smooth contributions add up to give the correct difference between the smooth density of states and the total phase shift. We now show that this is not the case.

First, consider the terms with $1 \leqslant m \leqslant n-1$. These terms are calculated using the saddle-point approximation, yielding an asymptotic expansion for the integral. All terms in the asymptotic expansion are oscillatory. We therefore conclude that any smooth contribution must be exponentially small.

The terms with $m < 0$ ($m > n$) may be calculated by closing the contour of integration in the lower (upper) complex l plane. The method of calculation is similar to the one used in obtaining the contribution of creeping trajectories [18, 19]. The calculations are given in [20], with the final result that the contribution of these terms is exponentially small (as is typical to creeping orbit calculations).

Finally, we consider the terms with $m = 0$ and $m = n$. For $n = 1$ the contribution is related to the forward scattering amplitude, and by adapting the calculations of [19], we have

$$\int_{-\infty}^{\infty} \mathrm{d}l \, \frac{\partial}{\partial k} S_l(k) = -1 - \frac{C}{3k^{2/3}} \tag{25}$$

where $C \approx 0.9962\mathrm{e}^{\mathrm{i}\pi/3}$. This term is indeed smooth, but has an unexpected dependence on k, and is of the wrong sign (with respect to the correction we are looking for). The arguments used in these calculations fail for high values of n, and for these values numerical calculations give the only available data. These calculations suggest that the behaviour of the contribution found for $n = 1$ is typical for higher n values as well. The $m = 0$ and $m = n$ thus do not account for the difference in the length term of the smooth part.

It is clear that by adding the smooth terms extracted from each term in the infinite sum separately finally gives the wrong result. Yet we wish to show that the infinite sum does have a smooth part which correctly balances the difference between $\bar{d}(k)$ and $\bar{\eta}'(k)$. This will be done by considering complex k in the upper half plane (which is the same idea behind the previous calculations for the smooth part of $\bar{d}(k)$ and $\bar{\eta}'(k)$).

We first note that the derivative of the total phase shift may be written as

$$\eta'(k) = \frac{2}{\pi^2 k} \sum_{l=-\infty}^{\infty} \frac{1}{H_l^-(k) H_l^+(k)} \,. \tag{26}$$

We now consider k to be in the upper half plane. For such k we have that $|S_l^*(k)| < 1$, and the sum over n in (2) may be resummed, leading to

$$\frac{1}{\pi} \operatorname{Im} \sum_{l=-\infty}^{\infty} \frac{1}{1 - S_l^*(k)} \frac{\partial S_l^*(k)}{\partial k} = -\operatorname{Im} \frac{2\mathrm{i}}{\pi^2 k} \sum_{l=-\infty}^{\infty} \frac{1}{H_l^-(k) J_l(k)} \tag{27}$$

where the Im operation has a meaning only when (eventually) returning to the real k axis. Adding the contributions of (26) and (27) one gets for the density of states

$$d(k) = \frac{2}{\pi^2 k} \operatorname{Im} \sum_{l=-\infty}^{\infty} \frac{Y_l(k)}{J_l(k) H_l^+(k) H_l^-(k)} \,. \tag{28}$$

This is indeed 0 except when $J_l(k) = 0$, i.e. when the circle has an eigenvalue. Taking $k = k_0 + \mathrm{i}\epsilon$, where k_0 is an eigenvalue of the circle, the sum over δ functions is immediately recovered. Alternatively, one could evaluate the smooth part of (27) directly. To do this we write the result of (27) as

$$\operatorname{Im} \frac{2\mathrm{i}}{\pi^2 k} \sum_{l=-\infty}^{\infty} \frac{1}{H_l^+(k) J_l(k)} \,. \tag{29}$$

The quantity in front of the Im operation, for $k = \mathrm{i}s$ (negative energy), is equal to

$$-\frac{1}{\pi k} \sum_{l=-\infty}^{\infty} \frac{1}{I_l(s) K_l(s)} \,. \tag{30}$$

This expression may be expanded as an asymptotic series for $s \to \infty$, using the methods of section 2.1. The result coincides with the asymptotic series for

$$-\frac{2k}{\pi} \left[g^{\mathrm{in}}(s) + g^{\mathrm{out}}(s) \right] \tag{31}$$

in all odd terms. This shows that the smooth part of the infinite sum exactly accounts for the difference between the smooth parts of the density of states and the total phase shift.

3. Discussion

The main difference between the total phase shift of the exterior problem, and the smooth spectral counting function of the interior problem, is the sign difference between the corresponding length terms. This amounts to $kL/2\pi$, where L is the circumference of the billiard. One should bear in mind, however, that kL/π is the area (in units of $2\pi\hbar$) of the phase space domain where the classical bounce map acts. Hence, the integer part of this number, Λ, is the dimension of the Hilbert space where the quantum analogue of the bounce map is defined. In other words, Λ is the number of scattering phase shifts which are substantially different from zero, or the effective dimension of the S matrix.

In the early discussions of the interior–exterior duality [2], it was argued that one should consider $\Theta(k) - \pi\Lambda(k)$ as the effective total phase shift, and therefore its smooth part (divided by 2π) provides correctly the two leading terms in the smooth counting function for the interior billiard problem. A simple way to see this is to assume that the Λ contributing phase shifts increase linearly with k, while the rest are negligible. Consider one contributing phase shift $\theta(k)$, and the corresponding staircase $N_\theta(k)$ of those eigenvalues which are found by $\theta(k)$ becoming an integer multiple of 2π. It is then obvious that the smooth part, if it is to represent some averaging of $N_\theta(k)$, should be given by $\bar{N}_\theta(k) = [\theta(k) - \pi]/2\pi$. The combined effect of the Λ contributing phase shifts adds up to the corresponding expression for $\bar{N}(k)$. The results of the present paper substantiate the previous heuristic arguments.

The next sign difference occurs only in the fourth term which decreases as k^{-1}. For most applications this is a negligible correction, but it is not too small to find if it is systematically looked for. We demonstrate this point by a numerical example.

In order to find high-order terms in the asymptotic expansion of the smooth density of states numerically, we need to apply an appropriate smoothing procedure. We use the method of repeated integration [11]. Define

$$F_n(k) = \int_0^k \mathrm{d}k_1 \int_0^{k_1} \mathrm{d}k_2 \ldots \int_0^{k_{n-1}} \mathrm{d}k_n\, d(k_n)\,. \tag{32}$$

Note that $F_1(k)$ is just the number-counting function $N(k)$. Each integration smooths the function, i.e. more terms in the asymptotic expansion for the smooth part may be compared. However, each integration of the asymptotic series introduces an additional constant of integration. For $\bar{F}_1(k) = \bar{N}(k)$ the additional constant of integration, for the unit circle, is $\frac{1}{6}$. We do not know how to generally find the constants of integrations introduced with each integration.

The number-counting function can only be compared (without additional smoothing) to the first two terms of the smooth part, as fluctuations are larger than unity. For comparing the constant term in $\bar{N}(k)$, $F_2(k)$ is needed, and for comparing the third term in $\bar{d}(k)$ (equation (6)), $F_3(k)$ is needed. For the unit circle with Dirichlet boundary conditions, its smooth part is given by

$$\bar{F}_3(k) = \frac{k^4}{48} - \frac{k^3}{12} + \frac{k^2}{12} + \frac{k\ln k - k}{128} + ck + \cdots. \tag{33}$$

In figure 1(a) we present results for comparing $F_3(k)$ with the first three terms in $\bar{F}_3(k)$ (equation (33)). ($F_3(k)$ was calculated for $k < 600$ using the first 89 699 eigenvalues of the circle.) The curve grows asymptotically as the fourth term in the expansion (33), and by subtracting it (see figure 1(b)) the constant c is determined to be approximately -0.002.

It was stated in section 1 that for the circle $\eta(k)$ and $\bar{\eta}(k)$ are asymptotically equal. In the general case, $\eta(k)$ contains oscillatory contributions from trapped periodic orbits. There are no trapped classical orbits in the circle, but there are non-classical trapped periodic

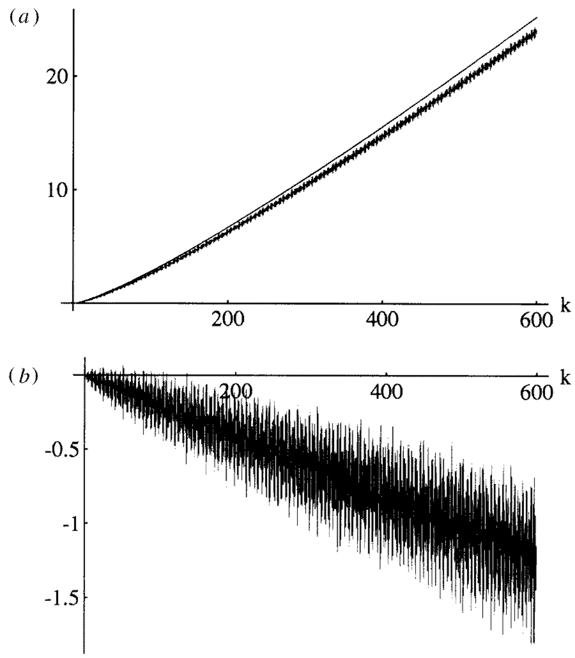

Figure 1. (*a*) The function $F_3(k) - k^4/48 + k^3/12 - k^2/12$ for the unit circle with Dirichlet boundary conditions, as calculated from the exact eigenvalues, compared with the fourth term in the expansion (33) $(k \ln k - k)/128$. (*b*) The difference between the two curves, which has large fluctuations around a straight line with a slope of approximately $c = -0.002$.

orbits, namely creeping orbits which go around the circle. (Creeping orbits were described in [18], and introduced in the Gutzwiller trace formula in [21].) To obtain the contribution of the creeping orbits to the total phase shift, one should consider the terms neglected when calculating $\eta(k)$ by changing the sum in (26) into an integral,

$$\eta'_m(k) = \frac{2}{\pi^2 k} \int_{-\infty}^{\infty} \mathrm{d}l \, \frac{1}{H_l^-(k) H_l^+(k)} \exp(2\pi \mathrm{i} m l) \tag{34}$$

for $m \neq 0$. The integral may be calculated by the method used in [18, 19] for creeping wave contributions. The result for $\eta'_m(k)$ is oscillatory, and corresponds to a creeping orbit which goes around the circle $|m|$ times. The contribution is exponentially small, and therefore vanishes asymptotically to any order. However, in practice these oscillations are observed in numerical calculations of the total phase shift for low k.

The last point to be addressed is an issue raised in a recent work [22], where the Fredholm determinant of the integral kernel of the boundary integral equation was studied. It was pointed out that up to terms of order k^{-1} the smooth interior counting function for Dirichlet boundary conditions $\bar{N}_{\mathrm{D}}(k)$ coincides with $1/2\pi$ times the smooth total phase shift for the exterior problem with Neumann boundary conditions $\bar{\eta}_N(k)$. Our work confirms the above result, and states further that the agreement between the two functions breaks at exactly the term of order k^{-1}.

So far we have dealt exclusively with the consequences of the interior–exterior duality where the exterior problem is defined in the plane. Another variant of the same principle is the scattering system defined by connecting a ‘waveguide’ to the billiard in a way that is discussed and explained in [1, 2]. Here also, the spectrum of the billiard is determined by locating the values of the wavenumber k for which one of the eigenvalues of the scattering matrix obtains the value 1. In this set-up, however, one has to consider the generalized S matrix [23], namely, the matrix which describes also transitions between evanescent modes in the waveguide. Using the analogue of (2) one expects to get a relation between the total phase shift and the interior counting function. We cannot present here a detailed theory, but would like to examine one simple case, namely the quantization of a square billiard, by the waveguide method.

Consider a square billiard of size a. The scattering problem is formed by connecting a waveguide of width a to one of the edges of the square [2] (the square thus forms an extension of length a to the waveguide). The scattering matrix is diagonal, and is given by

$$S_{n,n'}(k) = -\exp(2\pi \mathrm{i}\sqrt{(ka/\pi)^2 - n^2})\delta_{nn'}\,. \tag{35}$$

One can easily check that the spectrum of the square is obtained by requiring that any of the phases in (35) is an integer multiple of 2π. The number of conducting modes Λ is equal to the integer part of ka/π. The total phase shift is given by

$$\eta(k) = \sum_{n=1}^{\Lambda} \sqrt{(ka/\pi)^2 - n^2} - \frac{\Lambda}{2}\,. \tag{36}$$

Using the Poisson summation formula and other standard relations, one gets

$$\eta(k) = \frac{(ka)^2}{4\pi} - \frac{ka}{\pi} + \frac{1}{4} + \frac{ka}{2\pi}\sum_{m=1}^{\infty}\frac{1}{m}J_1(2mka) - \frac{1}{2\pi}\sum_{m=1}^{\infty}\frac{1}{m}\sin(2mka)\,. \tag{37}$$

This is an exact equality which can be interpreted in the following way. The expression appearing in the upper line of (37) is the smooth part of $\eta(k)$. It coincides with the spectral counting function $\bar{N}(k)$ for the square which consists of three terms only—the area, circumference and corners terms [11]. We thus see that in this method of quantization, the problem which was discussed throughout this paper does not arise, at least for the leading contributions. The other terms in (37) are the oscillatory contributions to $\eta(k)$. They can be interpreted as due to trapped periodic manifolds. The first infinite sum is the contribution of the (open) manifold of periodic orbits which are parallel to the transverse motion in the waveguide. The last sum is due to the limiting periodic orbits which run along the transverse edges of the billiard. These two limiting orbits are the closure of the manifold mentioned previously. We thus see that the oscillatory part of (37) consists of contributions which exhaust all possible *trapped* periodic motion in the open billiard. We would like to emphasize again that this result is exact.

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References

[1] Smilansky U *Mesoscopic Quantum Physics (Proc. Les Houches Summer School, Session LXI, 1994)* ed E Akkermans, G Montambaux and J L Pichard (Amsterdam: North-Holland) to be published
[2] Doron E and Smilansky U 1992 *Nonlinearity* **5** 1055–84
[3] Dietz B and Smilansky U 1993 *Chaos* **3** 581–90
[4] Dietz B, Eckmann J-P, Pillet C-A, Smilansky U and Ussishkin I 1995 *Phys. Rev.* E **51** 4222–31
[5] Eckmann J-P and Pillet C-A 1995 *Commun. Math. Phys.* **170** 283–313
[6] Birman M Sh and Yafaev D R 1993 *St Petersburg Math. J.* **4** 833–70
[7] Jensen A and Kato T 1978 *Commun. Part. Diff. Equ.* **3** 1165–95
[8] Majda A and Ralston J 1978 *Duke Math. J.* **45** 183–96, 513–36, 1979 *Duke Math. J.* **46** 725–31
[9] Petkov V and Popov G 1982 *Ann. Inst. Fourier, Grenoble* **32** 111–49

[10] Melrose R B 1988 *Commun. Part. Diff. Equ.* **13** 1431–39
[11] Baltes H P and Hilf E R 1976 *Spectra of Finite Systems* (Mannheim: Bibliographisches Institut)
[12] Berry M V and Howls C J 1994 *Proc. R. Soc.* A **447** 527–55
[13] Schanz H and Smilansky U 1995 *Chaos, Solitons, Fractals* **5** 1289–309
[14] Prosen T 1995 *J. Phys. A: Math. Gen.* **28** 4133–55
[15] Stewartson K and Waechter R T 1971 *Proc. Camb. Phil. Soc.* **69** 353–63
[16] Balian R and Bloch C 1970 *Ann. Phys.* **60** 401–47; errata 1974 *Ann. Phys.* **84** 559
[17] Abramowitz M and Stegun I A (eds) 1965 *Handbook of Mathematical Functions* (New York: Dover)
[18] Levy B R and Keller J B 1959 *Commun. Pure Appl. Math.* **12** 159–209
[19] Nussenzveig H M 1965 *Ann. Phys.* **34** 23–95
[20] Ussishkin I 1994 *Master's Thesis* Weizmann Institute
[21] Vattay G, Wirzba A and Rosenqvist P E 1994 *Phys. Rev. Lett.* **73** 2304–7
[22] Steiner F Private communication
[23] Weidenmüller H A 1964 *Ann. Phys.* **28** 60–115