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Properties of time delay and S-matrix for chaotic scattering on a leaky surface of constant negative curvature

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Abstract. *Properties of a model quantum scattering system displaying hard classical chaos*—'elastic' scattering on a leaky surface of constant negative curvature—are analysed theoretically and serve to interpret previously obtained numerical results. The low energy scattering behaviour is shown to be influenced, in the usual fashion, by a bound state just below the scattering continuum threshold. A connection between the widths of the infinite number of simple poles of the S-matrix and the Lyapunov exponent for classical trajectories is analysed. At high energies, the scattering is characterized by fluctuations in the S-matrix (via its phase) and the time delay. Analytic expressions for the autocorrelation function of the S-matrix and of the time delay are obtained using Montgomery's conjecture for the pair correlation function of the celebrated Riemann zeros whose values correspond to the positions of the S-matrix poles in momentum space. The autocorrelation function for the S-matrix is found to be Lorentzian asymptotically (at large energy differences ΔE), that is, to decrease as ΔE^{-2}, but that for the time delay is not. The distribution of fluctuations of S-matrix phases is likely to be Gaussian.

1. Introduction

Stochastic properties of quantum scattering models and in particular the manifestation of stochasticity in scattering observables have been investigated with increasing frequency in the past decade [1, 2]. Whereas stochastic properties of bound systems are quite well understood, this is not yet the case for scattering processes. This is primarily due to the fact that characteristics of stochastic properties of such systems (at least in the classical and semiclassical limits) have rigorous formulations only asymptotically in time ($t \to \infty$), for example the Lyapunov exponent. Scattering processes are usually characterized by finite interaction time so that most results concerning bound systems cannot be applied directly to scattering processes.

Due to the fundamental importance of the problem of chaotic scattering for theories of nuclear [1, 3, 4] and molecular [5] reactions, a number of different approaches have been developed for description of this phenomenon. Two types of approaches are now widely accepted: semiclassical [5] and stochastic [1, 3, 4]. Neither can be considered as complete and each has its advantages and drawbacks. The semiclassical approach appeals to a number of well established chaotic properties of classical dynamical systems but is restricted by the condition of rather high collision energies. On the other hand, the statistical approach is capable, in principle, of describing purely quantum features of chaotic scattering but is based on the *ad hoc* introduction of stochasticity.

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Recently there has been important progress in the development and justification of both approaches [5-8]. However, in order to understand details and peculiarities of the manifestation of chaos in quantum scattering it is of interest to investigate properties of some analytically solved problems even if they are so greatly simplified as to be far from physical reality. One such problem is scattering on a leaky surface of constant negative curvature [9-11]. There are several papers concerning analysis of this problem [11, 12] but in all of them the effect of stochasticity, in particular on the behaviour of the time delay, has been explored numerically and without analytical treatment of such characteristics as the pair correlation function, the distribution of fluctuations, etc.

It is well known that the stochastic properties of scattering on a leaky surface of negative curvature are closely connected to those of the non-trivial zeros of the Riemann ζ-function but this connection has not yet been explicitly exploited. This paper is devoted to thorough discussion of properties of time delay and quantum phases utilizing the known properties of ζ-function zeros. The possible consequences for realistic systems are also mentioned.

2. Formulation of the problem

Scattering of a particle on a leaky surface of negative curvature (half-plane $L\{(x, y)\in R^2 | y>0\}$) is described by the Hamiltonian

$$H=-(\hbar^2/2mR^2)y^2(\partial^2/\partial x^2+\partial^2/\partial y^2)-\hbar^2/8mR^2 \tag{2.1}$$

where m is the mass of the particle and R is a radius of curvature. For brevity we henceforth put $\hbar=m=R=1$. Free motion on negative curvature surfaces is quite different from that on conventional zero curvature ones in that it corresponds to rapidly divergent 'plane' waves (for details see [13]). In such a case boundary conditions of the tesselation type result in stochastic dynamics. In the problem of scattering on a leaky surface with tesselation, as described in [11], the following expression for the scattering wave has been derived:

$$\psi_k(y)=y^{1/2}[y^{-ik}+S(k)y^{ik}] \qquad \text{as } y\to\infty \tag{2.2}$$

where $k=(2E)^{1/2}$ is the wavevector corresponding to the energy E of scattered particle. The S-matrix $S(k)$ is determined by the expression

$$\begin{aligned} S(k)&=\pi^{-2ik}\frac{\Gamma(\frac{1}{2}+ik)}{\Gamma(\frac{1}{2}-ik)}\frac{\zeta(1+2ik)}{\zeta(1-2ik)} \\ &=\pi^{-2ik}\,e^{4ibk}\left(\frac{\frac{1}{2}-ik}{\frac{1}{2}+ik}\right)\prod_{w_\nu>0}\frac{(k+\xi_\nu)(k-\xi_\nu^*)}{(k+\xi_\nu^*)(k-\xi_\nu)}\exp[ik/(w_\nu^2+\tfrac{1}{16})] \end{aligned} \tag{2.3}$$

where $\xi_\nu=w_\nu-i/4$ and $b=\ln(2\pi)-1-\gamma/2$ (γ is the Euler constant). The values $w_\nu\in R$ ($-\infty<w_\nu<\infty$) are the coordinates of the non-degenerate Riemann zeros along the line $\mathrm{Re}\,k=\frac{1}{2}$: $\nu=\frac{1}{2}-2iw_\nu$. Here the scattering is 'elastic' since $|S(k)|=1$ and scattering is manifested only in a phaseshift, i.e.

$$S(k)=\exp[i\phi(k)]. \tag{2.4}$$

The values under study are the phaseshift $\phi(k)$ and the time delay $T(k)$, expressed by the well known formula [12, 14]

$$T(k)=-iS^*\,dS/dE=d\phi/dE=(1/k)\,d\phi/dk. \tag{2.5}$$

For convenience of future presentation we introduce the parameter

$$\tau(k(E)) = T(E)k(E) = \mathrm{d}\phi/\mathrm{d}k. \tag{2.6}$$

There is a simple relation between $\tau(k)$ and the zeros of the ζ-function [12]

$$\tau(k) = 4b - 2\ln(\pi) - \frac{1}{\frac{1}{4}+k^2} + \tfrac{1}{2}\sum_{w_\nu}\frac{1}{(\frac{1}{4})^2+w_\nu^2} + \tfrac{1}{2}\sum_{w_\nu}\frac{1}{(\frac{1}{4})^2+(k+w_\nu)^2}. \tag{2.7}$$

It is easy to understand that the behaviour of $\tau(k)$ is directly determined by the characteristic properties of the distribution of zeros of the ζ-function. Indeed, let us introduce a density of zeros

$$\rho(k) = \sum_{w_\nu}\delta(k-w_\nu). \tag{2.8}$$

Using equation (2.8) we can rewrite the expression (2.7) in the following way:

$$\tau(k) = 4b - 2\ln(\pi) - \frac{1}{\frac{1}{4}+k^2} + \tfrac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}w\,\rho(w)f(w) + \tfrac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}w\,\rho(w)f(w-k) \tag{2.9}$$

where

$$f(k) = [(\tfrac{1}{4})^2+k^2]^{-1}. \tag{2.10}$$

The phaseshift $\phi(k)$, whose value can (in principle) be observed experimentally for realistic systems, can now be expressed through $\tau(k)$. It is clear that the phaseshift is defined up to an arbitrary constant reference phase. That is, the physical meaning can be ascribed not to $\phi(k)$ itself but, for example, to

$$\phi(k) - \phi(k_0) = \int_{k_0}^{k}\mathrm{d}w\,\tau(w) = \beta(k-k_0) - 2[\tanh^{-1}(2k) - \tanh^{-1}(2k_0)]$$
$$+\tfrac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}w f(w)[N(w+k) - N(w+k_0)]. \tag{2.11}$$

Here

$$\beta = 4b - 2\ln(\pi) + \tfrac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}w\,\rho(w)f(w) \tag{2.12}$$

and

$$N(k) = \int_0^k \mathrm{d}w\,\rho(w) \tag{2.13}$$

is the total number of zeros in the interval $(0, k)$. In deriving equation (2.11) we took into account the obvious relation

$$\int_{-\infty}^{\infty}\mathrm{d}w\,\rho(w)f(w-k) = \int_{-\infty}^{\infty}\mathrm{d}w\,\rho(w+k)f(w). \tag{2.14}$$

The formulae (2.8)-(2.11) clearly show that properties of both phaseshift $\phi(k)$ and time delay $\tau(k)$ are completely governed by the density of zeros $\rho(k)$.

The stochastic properties of the distribution of zeros have been investigated both analytically and numerically [15, 16]. A large number of exact results and different asymptotic relations were derived some years ago and, more recently, computationally intensive numerical studies have been undertaken to check these various analytical

results [16]. It is evident that many of these results can be used for deriving corresponding relations for $\tau(k)$ and $\phi(k)$. This is the primary goal of the paper. However, we shall start our discussion with the limit of low scattering energy. The stochasticity of scattering does not show itself in this limit, but nevertheless this analysis will enable us to understand some characteristic peculiarities of the behaviour of $\tau(k)$ and $\phi(k)$ at low k and will demonstrate a close relation of the rather artificial model system to conventional scattering systems.

3. Low energy scattering limit

In spite of the absence of stochasticity the low energy scattering limit is nevertheless interesting because the S-matrix (2.3) and time delay clearly display resonance-like behaviour in the region $k<1$. Indeed, the expression (2.3) shows that at low $k<\frac{1}{2}$ ($E<\frac{1}{8}$)

$$S(k)\simeq -\mathrm{e}^{-\beta k}\frac{\frac{1}{2}-\mathrm{i}k}{\frac{1}{2}+\mathrm{i}k}\simeq -\frac{\frac{1}{2}-\mathrm{i}k}{\frac{1}{2}+\mathrm{i}k} \tag{3.1}$$

and

$$\tau(k)\simeq -\frac{1}{\frac{1}{4}+k^2}+\beta_0 \tag{3.2}$$

where β_0 is a constant approximately independent of k. At low energies ($E<\frac{1}{8}$) all other terms in expression (2.3) as well as the dependence of β_0 on k are negligible to an accuracy $1/k_1\simeq 0.15$, where k_1 is the coordinate of the first non-trivial zero of the ζ-function (closest to $w=0$). To the same accuracy $\exp(-k\beta)$ is neglected in equation (3.1).

The origin of the pole in (3.1) as well as the Lorentzian dependence in (3.2) are physically very natural. We know that among those eigenstates of equation (2.1) below the continuum threshold and satisfying the tesselation boundary condition, there is one which is closest to the continuum. This is the eigenstate $\psi_b(y)=$ constant, corresponding to the eigenenergy $E_b=-\frac{1}{8}$. The negative sign of E_b indicates the energy is below the continuum threshold.

It is well known [17, 18] that in the presence of an eigenstate with negative energy near the continuum, the S-matrix has a singularity on the complex energy plane near the point $E=0$ (on the physical sheet). Here we shall show that such a singularity is consistent with the analytical expression (3.1).

First we note that in spite of the fact that the problem considered is actually 2D, all waves inhomogeneous in the x direction are highly localized at $y<1$ (i.e. correspond to bound states [11]) whereas at large $y>1$ the problem for delocalized states becomes effectively 1D. This reveals that the strongly chaotic scattering region is localized at $y\simeq 1$. Therefore at small $k<\frac{1}{2}$ (corresponding to small energy $E<\frac{1}{8}$) we can restrict ourselves to investigation of 1D solutions of type (1.2) and replace the effect of the region of strong scattering by a proper boundary condition. The boundary condition can be found by a well known method in the theory of low energy resonance scattering [17, 18].

In order to employ conventional quantum scattering theory it is worth reducing equation (2.1) to a Schrödinger-type equation in flat space. After the change of variables:

$$y=\ln(z) \qquad \text{and} \qquad \psi=\exp(z/2)\phi \tag{3.3}$$

we have

$$-\tfrac{1}{2}[\partial^2/\partial z^2+\exp(2z)\partial^2/\partial x^2]\phi_k = k^2\phi_k. \tag{3.4}$$

A solution of equation (3.4) is the state

$$\phi_b(z)=\exp(-z/2)\psi_b(z)=\exp(-\kappa_b z) \qquad \kappa_b=(2|E_b|)^{1/2}=\tfrac{1}{2} \tag{3.5}$$

which resembles a bound one since ϕ_b decreases exponentially as $z\to\infty$ (ψ_b = constant).

Now we briefly recall the basic points of low energy resonance scattering theory. Let us consider the 1D scattering of particles by a potential $V(z)$ located at $z\simeq 0$ and which possesses a bound state $\phi_b(z)$ close to the continuum. Closeness to the continuum is defined by two conditions: first, the characteristic size $l\simeq\kappa_b^{-1}$ of the wavefunction $\phi_b(z)$ is much larger than the range α of the potential and, second, the energy $|E_b|$ of the bound state is much closer to the continuum threshold than to all other characteristic singularities of the S-matrix (other bound or quasibound states, etc). It is noted that the first point is in fact the consequence of the second one so that the second point can be considered as a definition of closeness.

If the positive energy E_k of the scattered particle is also low so that $E_k|E_b|$, then the effect of the potential $V(z)$ on ϕ_k can be described by the boundary condition at $z=0$:

$$\phi_k^{-1}(z)\,\mathrm{d}\phi_k/\mathrm{d}z|_{z\to 0}=1/\lambda \tag{3.6}$$

where λ is a constant. To find this constant we notice that both states ϕ_b and ϕ_k are closer to each other than to all other singularities (except for that at $E=0$). This means that logarithmic derivatives of ϕ_b and ϕ_k at $z\to 0$ coincide with each other with an accuracy $\kappa_b/k_1\ll 1$, where $k_1=(2|E_1|)^{1/2}$ is the wavevector, corresponding to the S-matrix singularity closest in energy to ϕ_b:

$$\phi_k^{-1}\,\mathrm{d}\phi_k/\mathrm{d}z|_{z\to 0}=\phi_b^{-1}\,\mathrm{d}\phi_b/\mathrm{d}z|_{z\to 0}. \tag{3.7}$$

The relation (3.7) enables us to obtain the characteristic behaviour of the S-matrix at small k [17, 18].

Let us return to our scattering problem determined by equation (3.4). Strictly speaking there are no small parameters in the theory which would ensure that the energies of all singularities of the S-matrix other than E_b are much higher in absolute value than $|E_b|=\frac{1}{8}$. However, numerical solution of the problem (in fact, numerical calculation of the lowest zeros of the ζ-function) shows that all resonances are actually much higher in energy than $|E_b|$. Thus the second condition is fortuitously fulfilled in our process. As for the first condition, it is also fulfilled in the process under study. Indeed, the only parameters whose dimension is length (except for the wavelength) are the curvature radius $R=1$ and the size of the region of strong scattering (which is equivalent to the size of the potential in the problem of potential scattering) which is given by the radii of boundary semicircles of the tesselation cell [11, 13]: $R_0=\frac{1}{2}$. Thus we get for the parameter characterizing the first condition: $\kappa_b R_0=\frac{1}{4}$. Again the smallness of this parameter should be considered as fortuitous. It leads to approximate independence of equation (3.7) on the particular choice of $|z|<1$.

Expressing ϕ_k through ψ_k by change of variables (3.3) and substituting it in equation (3.7) we obtain the expression

$$S(k)=-\frac{\kappa_b-\mathrm{i}k}{\kappa_b+\mathrm{i}k}\simeq-\frac{\frac{1}{2}-\mathrm{i}k}{\frac{1}{2}+\mathrm{i}k} \tag{3.8}$$

which coincides with equation (3.1) derived from the exact expression (2.3). Consequently we conclude that both the pole of $S(k)$ and the resonance of $\tau(k)$ at $k=0$ are actually due to resonance scattering by the 'bound' state ϕ_b. Now we understand that the width $\frac{1}{4}$ of this threshold resonance of $\tau(k)$ is nothing else but $2|E_b|$, twice the 'binding' energy in the state ϕ_b. The sense of the condition $\kappa_b/k_1 \ll 1$ also becomes quite clear: it means that the resonance at $k=0$ can be considered as isolated from all other resonances. The validity of this condition was clearly demonstrated by numerical calculation in [12].

In principle, the theory of low energy resonance scattering could also be applied to a representation in terms of ψ-functions: ψ_b and ψ_k. Repeating all previous arguments one can derive

$$\psi_k^{-1}\, d\psi_k/dy|_{y\sim 1} = \psi_b^{-1}\, d\psi_b/dy|_{y\sim 1} = 0 \tag{3.9}$$

and after that derive the same expression (3.8) for $S(k)$.

It is seen from equation (2.7) that low energy resonance scattering results in a negative contribution to the time delay $\tau(k)$. Such an effect is easily understood if we take into consideration the fact that in the presence of a bound state near the continuum the low energy particle is scattered not by the region of effective scattering itself but by this weakly bounded state which is of greater extent. Scattering by the bound state means that the particle does not spend as much time in the region as it would in the absence of this state. In other words, the contribution of this effect to $\tau(k)$ should be negative.

4. High energy scattering limit

The most interesting limit, from a physical point of view, is the high energy one in which scattering shows stochastic properties. We begin investigation of this limit with discussion of a general characteristic feature of the S-matrix and time delay before addressing a few selected attributes of each.

4.1. A connection between resonance width and the Lyapunov exponent

Expression (1.3) shows that the S-matrix has an infinite number of simple poles at coordinates of the Riemann zeros of the ζ-function. Up to moderately high energies the poles are well separated and can be interpreted as resonances of the S-matrix due to the presence of some quasibound states in the system resulting from a delicate interference of scattering waves after tesselation. These poles make Lorentzian contributions to the time delay $\tau(k)$. An interesting feature is that the halfwidth Δ of all such Lorentzians is independent of k: $\Delta = \frac{1}{4}$.

In order to understand the halfwidth we can apply the theory of quantization of semiclassical orbits developed in [11, 12]. It is well known that in negative curvature space all classical trajectories are unstable and the corresponding Lyapunov exponent is [13]

$$\omega(E) = (2E)^{1/2}.$$

It is shown in [19, 20] that an unstable quasiperiodic orbit j gives a contribution to the Green function, and thus to the S-matrix, of type

$$\delta S_j(E) \sim [S_a(E) - S_{aj} + i\omega_j T_j/2]^{-1} \tag{4.1}$$

where $S_a(E)$ is the action along the quasiperiodic trajectory with the energy E, S_{aj} is the quantized action corresponding to jth quasistationary state, $\omega_j \simeq \omega(E_j)$ is the Lyapunov exponent of the jth orbit with the energy E_j, and $T_j = \partial S_a/\partial E|_{E_j}$ is the period of this orbit. Expanding the denominator of ∂S_j in $\Delta E = E - E_j$ we get

$$\delta S_j(E) \sim (\Delta E + i\omega_j/2)^{-1}. \tag{4.2}$$

Now we can compare this contribution with the exact one

$$\delta S_{ej} \sim (k - \xi_j)^{-1} \tag{4.3}$$

where $\xi_j = k_j - i/4$ and $k_j = (2E_j)^{1/2}$ corresponds to jth Riemann zero. Expanding $k = [2(k_j^2 + \Delta E)]^{1/2}$ in ΔE one obtains

$$\delta S_{ej} \sim [\Delta E + (i/4)(2E_j)^{1/2}]^{-1} = (\Delta E + i\omega_j/4)^{-1}. \tag{4.4}$$

The expression (4.4) is very close to equation (4.2). This means that the parameters of the S-matrix poles (2.3) (except for their positions) can actually be understood in terms of the theory developed in [20] for physically realistic systems. The origin of the factor of 2 difference between imaginary terms in equations (4.2) and (4.4) is unknown but we believe it is due to some difference between the dynamics of the realistic systems considered in [20] and 'dynamics' resulting from tesselation in the model under study. It is clear that in explaining the characteristic parameters of the poles we thus explain simultaneously the unexpected independence of the halfwidth of Lorentzians in the time delay $\tau(k)$ on k.

At this point some comments are needed. In order to find the characteristics of the S-matrix poles we have used Gutzwiller's semiclassical approach [20]. It is known [21] that in general this approach fails to predict correctly the eigenvalues, i.e. poles of the Green function, at high energies when the associated resonances in the density of states strongly overlap. In this case any analysis of individual resonances (in our problem in the k-dependence of the time delay $\tau(k)$) becomes senseless. Numerical results show, however [12], that at moderately high energies, corresponding to about the first 50 poles of $S(k)$, the above-mentioned resonances are still well resolved yet the energy is high enough for the validity of the semiclassical approximation and thus Gutzwiller's approach. The analysis carried out here is accordingly valid for separated poles at moderately high energies.

4.2. Correlation function of $\tau(k)$

Now let us consider stochastic properties of $\tau(k)$ at large k and thus high energies E. Formula (2.9) shows that these properties are determined by those of the density of the Riemann zeros. It is convenient to divide $\tau(k)$ into two parts: a smooth regular part $\bar{\tau}(k)$

$$\bar{\tau}(k) = \beta - (\tfrac{1}{4} + k^2)^{-1} + \tfrac{1}{2}\int_{-\infty}^{\infty} dw\, \bar{\rho}(w) f(w-k) \tag{4.5}$$

and a fluctuating part

$$\tau_f(k) = \tfrac{1}{2}\int_{-\infty}^{\infty} dw\, \sigma(w) f(w-k). \tag{4.6}$$

In equations (4.5) and (4.6)

$$\bar{\rho}(k) \overset{k\to\infty}{=} \pi^{-1}\ln(k/\pi) \tag{4.7}$$

is the average density of zeros [4, 7] and

$$\sigma(k) = \rho(k) - \bar{\rho}(k) \tag{4.8}$$

is the fluctuating part of the density. In what follows we shall discuss only the properties of $\tau_f(k)$.

The basic characteristics of $\tau_f(k)$ are embodied in its pair correlation function

$$C(k, k') = \langle \tau_f(k)\tau_f(k')\rangle_{\Delta k} / \langle \tau_f^2(k)\rangle_{\Delta k} \tag{4.9}$$

where

$$\begin{aligned}\langle \tau_f(k)\tau_f(k')\rangle_{\Delta k} &= (\Delta k)^{-1}\int_{k_0}^{k_0+\Delta k} dw\, \tau_f(k+w)\tau_f(k'+w) \\ &\overset{k_0\gg\Delta k\gg\bar{\rho}(k_0)^{-1}}{\simeq} \int_{-\infty}^{\infty} dw\, f(k-w)\int_{-\infty}^{\infty} dw'\, f(w'-k')\langle\sigma(w)\sigma(w')\rangle_{\Delta k}.\end{aligned} \tag{4.10}$$

The last line of equation (4.10) is clearly valid because $f(w)$ is highly localized in the region $w < 1$ and $\langle\sigma(w)\sigma(w')\rangle$ is a slowly varying function of k_0 ($\ln(k_0)$). The averaging interval in (4.10) is assumed to be much smaller than k_0 but much larger than the average spacing between zeros: $k_0 \gg \Delta k \gg \bar{\rho}(k_0)^{-1}$. After averaging (4.10) $C(k, k')$ becomes dependent on k and k' only through the difference $k - k'$ (see below).

For some values of k_0 and Δk the correlation function $C(k, k')$ has been calculated numerically in [12]. Here we obtain this function analytically. An analytical expression for the correlation function $\langle\sigma(k)\sigma(k')\rangle$ at $k, k' \to \infty$ has been conjectured by Montgomery [22] on the basis of rather reasonable 'heuristic' arguments and appears to coincide with that for energy levels of the Gaussian unitary ensemble (GUE)

$$K(x-x') = \langle\sigma(x)\sigma(x')\rangle = \delta(x-x') - \frac{\sin^2\pi(x-x')}{\pi^2(x-x')^2}. \tag{4.11}$$

In equation (4.11) x is the k-variable scaled so as to have unit mean spacing.

The function has important properties:

$$\int_{-\infty}^{\infty} dx\, K(x) = 0 \tag{4.12}$$

and

$$\int_0^X dx \int_0^X dx'\, K(x-x') \overset{X\to\infty}{\sim} \ln(X). \tag{4.13}$$

The second one is closely connected to the fact that the rigidity of GUE energy levels is proportional to $\ln(X)$ [23].

Substituting (4.10) into (4.9) we find that $C(k, k')$ depends only on the difference $Q = k - k'$ and

$$C(Q) = \frac{\frac{1}{4}}{1-\exp(-\pi\bar{\rho})}\left[\frac{\frac{1}{4}-Q^2}{(\frac{1}{4}+Q^2)^2}(1-e^{-\pi\bar{\rho}}\cos 2\pi q) + \frac{Q}{(\frac{1}{4}+Q^2)^2}e^{-\pi\bar{\rho}}\sin 2\pi q\right] \tag{4.14}$$

where $q = \bar{\rho}Q$. For $k, k' \to \infty$ the density $\bar{\rho}(k) \to \infty$ (see equation (4.7)) so that in this limit

$$C_\infty(Q) = (\tfrac{1}{4})(\tfrac{1}{4} - Q^2)/(\tfrac{1}{4} + Q^2)^2. \tag{4.15}$$

Comparison of a numerically calculated $C(Q)$ [12] with that obtained by equations (4.14) and (4.15) is shown in figure 1; equations (4.14) and (4.15) are indistinguishable on the scale of plot. The baseline ($C = 0$) for the numerically calculated $C(Q)$ is obtained by choosing $C(\frac{1}{2}) = 0$; the line determined by equating the integral of $C(Q)$ over Q to zero is located slightly higher (corresponding to $C \simeq 0.05$).

The agreement is quite reasonable if we take into account the fact that numerical calculations were carried out for large but finite k and k' while the expression (4.11) is valid asymptotically at $k, k' \to \infty$. It is well known that the convergence of all characteristics of the Riemann zeros to the asymptotic ones is extremely slow (as $1/\ln k$ or even $1/(\ln k)^{1/2}$ [15]). We see that the two curves differ somewhat only for $Q > 2$. The main contribution to $C(Q)$ at such Q comes from $K(x-x')$ at large $|x-x'|$. The deviation of the conjectured $K(x-x')$ (4.11) from the actual correlation function, as determined by numerical analysis of the Riemann zeros, is well known for $|x-x'| \gg 1$ [16]. The corresponding difference for $C(Q)$ is even more pronounced than for $K(x-x')$. The high frequency fluctuations of $\rho(k)$, whose correlation function is reasonably described by Montgomery's formula (4.11), are significantly suppressed in $\tau(k)$ due to convolution with the smooth function $f(w)$ in (4.6). The fluctuations of $\tau(k)$ at $k > 1$ seem instead to be determined by lower frequency fluctuations of $\rho(k)$ at large k, whose contribution to the correlation function $K(x-x')$ is not taken into account by the Montgomery conjecture [8]. The deviation, very small and almost indistinguishable in $K(x-x')$, becomes quite noticeable in $C(Q)$.

The most convincing explanation of this situation is provided by investigating the function

$$R(t) = \sum_n e^{it x_n} \sim \int dx\, e^{itx} \rho(x) \tag{4.16}$$

which is nothing else but the Fourier transform of the density of the zeros. This function

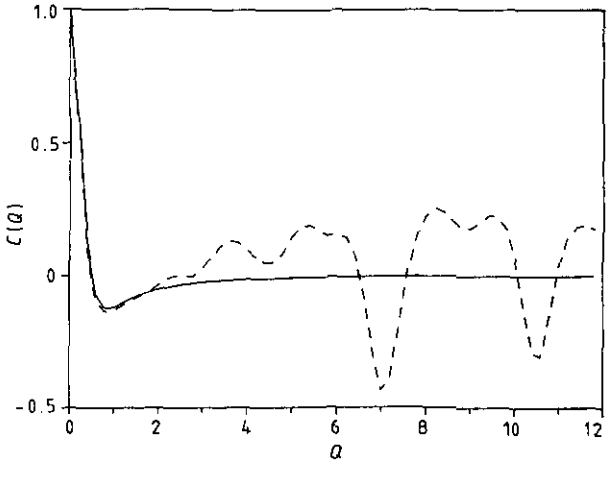

Figure 1. Comparison of the numerically calculated (broken curve) and analytical (full curve, equation (4.15)) time delay correlation functions. The numerical calculation has been made by averaging over 10^4 Riemann zeros near the 10^{12} zero which corresponds to $w = 133\,826\,702\,823.5$.

has recently been studied numerically [16] and the results show (in complete agreement with theoretical considerations [16]) that $R(t)$ has pronounced δ-type singularities at $t_m = \ln(p^m)$, where p are prime numbers and $m \in Z^+$. Note that the t_m coincide with the periods of 'orbits' in the semiclassical interpretation of the ζ-function, as proposed by Berry [24]. The presence of such singularities means that $\rho(w)$ can be expressed in the form

$$\rho(x) = \rho_0(x) + \mathrm{Re}\left[\sum_m A_m \, \mathrm{e}^{\mathrm{i}t_m x}\right] \tag{4.17}$$

where $\rho_0(x)$ is the non-oscillating part of $\rho_0(x)$. The oscillating terms of (4.17) apparently give rise to oscillating contributions to $K(x-x')$ of type

$$K_{nm}(x-x') = \mathrm{Re}\{A_{nm} \exp[\mathrm{i}(t_n - t_m)(x-x')]\} \tag{4.18}$$

and thus a corresponding contribution to $C(Q)$ of type

$$C_{nm}(Q) = \mathrm{Re}\{A_{nm} \exp[-2|t_n \pm t_m|\bar{\rho} + \mathrm{i}(t_n \pm t_m)\bar{\rho}Q]\}. \tag{4.19}$$

We see that the low frequency oscillating terms actually manifest themselves much more prominently than high frequency ones of the same amplitude. The oscillating structure of the numerically calculated $C(Q)$ shown in figure 1 results from the superposition of some lower frequency terms $C_{nm}(Q)$. The effect of damping of high frequency fluctuations and strong manifestation of low frequency ones observed here is quite general and may be important in analysis of realistic chaotic processes in which an observable is usually a functional of a fluctuating density of quasibound states (or more generally a density of resonances of the S-matrix) with a Lorentzian-type smoothing function [1].

It is easily seen that as $\bar{\rho} \to \infty$ the function $C(Q)$ (4.14) very rapidly converges to the limiting one $C_\infty(Q)$. This means that the main properties of $C(Q)$ can be understood by the analysis of limiting expression (4.15). First of all $C_\infty(Q)$ changes its sign at $Q = Q_* = \frac{1}{2}$, so that a Lorentzian approximation [12] is in principle incorrect because it does not take into account the fundamental property (4.12) of the distribution of zeros. The effect of a change of sign of correlation functions is of general significance for the theory of scattering by systems with stochastic behaviour (heavy nuclei, highly excited molecules, etc).

4.3. Stochastic properties of the phase $\phi(k)$

Now let us discuss the stochastic properties of the phase of the S-matrix $\phi(k)$. The expression for the pair correlation function of $\phi(k)$ can be obtained by double integration of $C(k-k')$ over k and k' but it is more convenient and useful to exploit equation (2.11). As for $\tau(k)$, we separate $\Delta\phi(k, k_0) = \phi(k) - \phi(k_0)$ into two parts: a smooth regular part $\overline{\Delta\phi}$ and a fluctuating part $\Delta\phi_\mathrm{f}$. For the more interesting fluctuating part we have

$$\Delta\phi_\mathrm{f}(k_0 + k, k_0) = \int_{k_0}^{k_0+k} \mathrm{d}w \, \tau_\mathrm{f}(w) = \tfrac{1}{2} \int_{-\infty}^{\infty} \mathrm{d}w \, f(w)[n(w + k_0 + k) - n(w + k_0)] \tag{4.20}$$

where

$$n(k) = \int_0^k \mathrm{d}w \, \sigma(w) \tag{4.21}$$

is the fluctuating part of $N(k)$ (equation (2.13)).

Using equation (4.20) one can find

$$\langle \Delta\phi_f^2(k)\rangle = \tfrac{1}{4}\int_{-\infty}^{\infty} dw\, f(w) \int_{-\infty}^{\infty} dw'\, f(w')\langle \Delta n(k, w)\Delta n(k, w')\rangle. \tag{4.22}$$

Here

$$\Delta n(k, w) = n(k+k_0+w) - n(k_0+w) = \int_{k_0+w}^{k+k_0+w} dw'\, \sigma(w'). \tag{4.23}$$

Averaging in equation (4.22) is made by integration over k_0 in the interval $\Delta k \ll k_0$. Hereafter for simplicity of notation we omit the argument k_0 of averaged functions, taking into account that, after averaging, correlation functions depend only on the difference of their arguments.

Characteristic values of w and w' giving dominant contributions to the integral (4.22) are determined by the width of the highly localized function $f(w)$ defined by equation (2.10). It is easy to see that for $k \gg w \sim w' \sim 1$

$$\langle \Delta n(k, w)\Delta n(k, w')\rangle \simeq \langle \Delta n(k, 0)^2\rangle + O(\ln(\bar{\rho}w)). \tag{4.24}$$

As for $\langle \Delta n(k, 0)^2\rangle$, it can be simply calculated at $k\bar{\rho} \gg 1$ by using (4.23) and (4.11):

$$\langle \Delta n(k, 0)^2\rangle \overset{k\bar{\rho}\gg 1}{\simeq} \pi^{-2}\ln(k\bar{\rho}). \tag{4.25}$$

Thus for $k \gg w$ the correction term in equation (4.24) is smaller than the main first one and can be neglected. Substituting (4.23) and (4.24) into equation (4.22) we obtain for $k \gg 1/\bar{\rho}$

$$\langle \Delta\phi_f(k)^2\rangle = \frac{1}{4}\left[\int_{-\infty}^{\infty} dw\, f(w)\right]^2 \langle \Delta n(k, 0)^2\rangle = 4\pi^2\langle \Delta n(k, 0)^2\rangle. \tag{4.26}$$

Similar simple relations can be derived for all even-order correlations. Indeed, it was proved in [25] that any even-order average $\langle \Delta n(k, 0)^{2m}\rangle$ obeys Gaussian statistics:

$$\langle \Delta n(k, 0)^{2m}\rangle = \frac{(2m)!}{2^m m!}\langle \Delta n(k, 0)^2\rangle. \tag{4.27}$$

By the considerations leading to (4.26), we can now obtain a similar relation for the average of any even power of $\Delta\phi_f(k)$:

$$\langle \Delta\phi_f^{2m}(k)\rangle \simeq \frac{(2m)!}{2^m m!}\langle \Delta\phi_f^2(k)\rangle. \tag{4.28}$$

This relation means that the distribution of values $\Delta\phi_f$ is probably Gaussian. Unfortunately there are no theorems concerning odd-order averages of Δn so that our statement about a Gaussian type of distribution of $\Delta\phi_f$-fluctuations is not rigorous; however the relation (4.28) is a strong argument in favour of this statement. In addition, a very detailed numerical analysis of statistical properties of the Riemann zeros [16] supports the assumption that the distribution of fluctuations of $\Delta n(k, 0)$, and thus that of $\Delta\phi_f$-fluctuations, is Gaussian.

For the case of Gaussian distributions of $\Delta\phi_f$-fluctuations, any averages of functions of $\Delta\phi$ can be easily found. We are particularly interested in the S-matrix autocorrelation

function,

$$\langle S(k+k_0)S^*(k_0)\rangle_{k_0}$$

$$\overset{k\bar{\rho}\gg 1}{=} \langle \exp(i\overline{\Delta\phi} + i\Delta\phi_f)\rangle = \exp(i\overline{\Delta\phi})\exp(-\langle\Delta\phi_f^2\rangle/2)$$

$$= \exp(i\overline{\Delta\phi}(k))\exp(-2\ln(\bar{\rho}k)) = (\bar{\rho}k)^{-2}\exp(i\overline{\Delta\phi}(k)). \tag{4.29}$$

We see that the asymptotic behaviour (at $k\bar{\rho} \gg 1$) of the function (4.29) is Lorentzian. Unfortunately we cannot describe the dependence of the average on k at small k; that is, it is impossible to make any statement about its behaviour in the region $k < 1$. It is worth noting that for the rather small increments $k \ll k_0$ considered, k is proportional to the increment of energy ΔE: $k \simeq \Delta E/k_0$ and therefore the dependence of the average (4.29) on ΔE is also Lorentzian. However, we should remember that equations (4.25)-(4.29) have been derived under the condition $k \gg 1$, that is, $\Delta E \gg k_0$. This means that at large k_0, a ΔE^{-2}-dependence is valid only for ΔE larger than the width Γ_E of resonances on an energy scale which increases with energy $\Gamma_E \sim (E)^{1/2} \sim k_0$ (see equation (4.4)).

Many years ago Ericson [26] proposed a Lorentzian dependence of the S-matrix autocorrelation function on ΔE. The same dependence was obtained later in a semi-classical treatment [5]. At the same time, quantum stochastic theory based on the Gaussian orthogonal ensemble approximation [8, 27] predicts a strong deviation from a Lorentzian dependence on ΔE for the autocorrelation function in one-channel scattering processes. Unfortunately our results do not enable us to make any definite conclusions about the ΔE-dependence of the autocorrelation function for $\Delta E \leqslant \Gamma_E$. If this dependence were to turn out to be Lorentzian, the origin of this dependence in our model would be more subtle than Ericson's assumption of strong uncorrelated fluctuations of amplitudes of the S-matrix resonances with change of energy. In the model under study the predicted asymptotic Lorentzian-like dependence arises from strongly correlated fluctuations of the density of states (in our case, density of zeros).

5. Conclusions

In this paper we have discussed some characteristic properties of chaotic scattering on a leaky surface of negative curvature. It is shown that a peculiarity of low-energy scattering (resonance type behaviour) is due to resonance scattering by a 'bound' state close to the continuum threshold. The major thrust of the paper is the analysis of stochastic properties of high energy scattering in the model under study. These properties are determined by those of the Riemann zeros of the ζ-function. Recent success in the mathematical description of stochastic aspects of the distribution of zeros has made it possible to investigate some important characteristics of stochastic scattering: the pair correlation function of time delay, the distribution function of phaseshifts, and the pair correlation function of the S-matrix at different scattering energies.

The pair correlation function of the S-matrix appears to depend on energy differences ΔE at large ΔE according to the inverse square law, that is, asymptotically it is Lorentzian. This fact is remarkable since a similar Lorentzian dependence was obtained earlier [26] for the correlation function of the S-matrix for a realistic scattering problem from totally different assumptions (strong uncorrelated stochastic changes of the amplitudes of resonances at different energies). Another way to derive the Lorentzian

dependence has recently been proposed by Smilansky (see review in [5]). At the same time a very strong deviation from a Lorentzian-type dependence for one-channel scattering is predicted by a statistical model based on the Gaussian orthogonal ensemble approximation [27]. Unfortunately our results do not enable us to check the predictions of these theories as applied to the model considered here because our results concern only the asymptotic behaviour of the correlation function at ΔE larger than the resonance width Γ_E.

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