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# **Resurgence in quasi-classical scattering**

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#### Abstract

In quasi-classical studies of closed systems, e.g. a billiard, resurgence means that the contribution of long periodic orbits to the spectral determinant can be expressed in terms of composites of short orbits, and the resulting expression for the determinant is manifestly real. The question has thus long been posed whether something like resurgence applies to a scattering system with its resonances. We find here a resurgent expression for Wigner's *R*-matrix (which gives the *S*-matrix by a Cayley transform) in which long scattering pseudo-orbits are expressed in terms of composites of short pseudo-orbits, both scattering and periodic, and the result is manifestly Hermitian, giving a unitary expression for the *S*-matrix. This is particularly useful in the case that the resonance width is comparable with the resonance spacing. The pseudo-orbits are defined in terms of a fictitious and to some extent arbitrary closed reference system. We relate the results to other formulations. We give a simple but non-trivial approximation for a particular example which illustrates the phenomenon of 'resonance trapping'.

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## 1. Introduction

The quasi-classical (=semiclassical) approximation (QCA) is important in the study of scattering. Miller's QCA formula for the *S*-matrix [1],

$$S_{ij}(E) = \sum a_p \exp[iS_p(E)/\hbar], \qquad (1)$$

has an intuitive appeal since the sum is over all classical scattering orbits at energy E. They are, for example, from an incoming direction  $\hat{n}_i$  to an outgoing direction  $\hat{n}_i$  and are labelled p.  $S_p/\hbar$  is the ratio of classical action for that orbit to the Dirac constant. The prefactors  $a_p$  are proportional to the square root of the classical probability of the orbit. In QCA there are many expressions similar to equation (1). We call such expressions a sum over 'action terms'. (We shall not dwell on the prefactors in this communication. They depend on what is calculated,

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but we use the same symbol  $a_p$  in all cases. We also keep in mind two-dimensional cases only. By 'orbit' we always mean an orbit of the 'underlying' classical system.)

The nature of the convergence of the Miller series has many possibilities. See Jensen [2] for a discussion based on the fractal dimension of the classical scattering. The simplest possibility is a finite number of terms in the series, perhaps just one, as for example, the scattering from the outside of a Bunimovich stadium billiard. Scattering from three well separated discs gives an infinite, but rapidly convergent series (for real E). There are non-scattering periodic orbits in this case, and scattering orbits related to these which stay for an arbitrarily long time in the scatterer are possible, if not probable. Technically, there are resonances, complex energies in the lower half plane at which the *S*-matrix has a pole, and where the series thus diverges. These poles might not be discernible as such at real energies, but they are of theoretical interest. There is no obvious correspondence to a closed system, however.

Next, the series may not converge absolutely, but it does converge to a meaningful result if summed in the correct order. A microwave cavity or quantum dot with relatively narrow leads or antennas to the outside are examples. If the resonance widths are small compared to their spacing, it corresponds to an experimental set-up designed to study a closed system. For this purpose, it is desirable to perturb the closed system as little as possible, so usually the spatial scale of the antennas is small compared with the wavelength, and the external signal must tunnel to enter the cavity. Equation (1) does not apply then, at least in its simplest form. Since there is a crucial length small compared with the wavelength, one must take into account ray splitting or use imaginary orbits. However, a sort of quasi-classical perturbation description easily applies.

We are interested in the most difficult case not involving diffraction: namely the exitentrance channels are open in the sense that diffraction (or tunnelling) of waves entering or exiting a channel is not qualitatively important, but still narrow in the sense that the total width of the channels is small compared with the length scale, e.g. the circumference, of the scatterer. (To obtain quantitative results, it might be possible to include ray-splitting orbits [3] to account for diffraction.) The widths of the resonances are then comparable to or even somewhat greater, on average, than their spacing, but there can well be cases, amenable to a quasi-classical approach, in which a few resonances are very broad, and the rest are quite well defined. There are many important periodic orbits and a scattering orbit typically bounces around quite a while before exiting. There is some arbitrariness in the definition of the closed system, but the idea of a closed system related to the resonances is still natural.

In the limit of a closed system, there is no scattering, the resonances move to the real energy axis, and their positions are the energy levels of the closed system. The first and still the main quasi-classical tool for this case is the Gutzwiller trace formula (GTF) [4]. The GTF also takes the form equation (1), but p now labels the periodic orbits, and  $S_{ij}(E)$  is replaced by  $d_{osc}(E)$ , the oscillating part of the density of states. The sum for the GTF, if not smoothed over energy somehow, of necessity diverges for real E, since it represents a sequence of Dirac  $\delta$ -functions. For many important purposes, in particular for the study of energy level correlations, a smoothed GTF is indeed appropriate. However, for other purposes, the fact that many terms are needed in the sum presents a crucial difficulty, since the number of periodic orbits increases exponentially with their length, and it is not easy to find their numerical properties.

It was a major theoretical challenge to show that the ideas behind the GTF could in fact lead to procedures which led to definite energy levels in the quasi-classical approximation. This challenge was met by techniques known as 'resurgence'. The present paper adapts these techniques to the study of scattering and scattering resonances. The main results have been reported in [5]. We begin by reviewing the results for closed systems.



**Figure 1.** Scattering processes associated with a Bunimovich stadium billiard. (*a*) Three possible scattering orbits from the outside. The figure suggests how  $\text{Tr } S^3$  is related to an inside period three orbit. (*b*) A billiard with a lead attached. A natural choice of SSE is shown, but another possibility SSE' is given. The SSI can be taken as the billiard boundary. (*c*) Billiard with two leads attached. Use of the billiard boundary as SSI' allows direct transmission from the left to the right lead. An SSI can be chosen to eliminate the direct scattering between leads.

### 2. Resurgence in closed systems

## 2.1. 'Inside-outside duality'

A major insight called 'inside-outside duality' was developed by Doron, Dietz and Smilansky [6], who were at the time mainly interested in finding the levels of a closed system, e.g. a Bunimovich stadium. They related the spectrum of the billiard to scattering problems in several ways. First, one or more leads can be attached to the stadium [7], as in figures 1(b), (c). The scattering matrix is then an  $N_E \times N_E$  matrix because in a given energy range there are only  $N_E$  outgoing waves in the leads. It was found that the appropriately defined scattering matrix  $\mathbf{S}(E)$  gives the inside spectrum when

$$D_{\mathcal{S}}(E,\lambda) = \det(\mathbf{1} - \lambda \mathbf{S}(E)) = 0.$$
<sup>(2)</sup>

Here  $\lambda$  is a bookkeeping parameter whose physical value is unity. This is an interesting result, but not of great utility in numerical calculations of the closed system, since S is quite complicated.

However, they went on to show that the *same* result holds if **S** represents the scattering from the outside of the stadium, no leads at all, which is quasi-classically approximated by *one* term since there is only one classical orbit bouncing from the billiard with a given initial and final direction. (More precisely, except for orbits scattering from the flat sides. These orbits, for a given scattering angle, have the same action, however, so they give just one term in equation (1) with, however, a much larger prefactor than the other scattering orbits. There are interesting effects connected with this [8].)

It is remarkable that nevertheless the scattering matrix has the same (in fact even more) content as the GTF, a divergent sum of similar terms. (The scattering matrix also gives the wavefunctions.) In this case, **S** is a continuous matrix or operator and the determinant is interpreted as a Fredholm determinant. It was possible to show that Im d ln  $D(E, \lambda m)/dE$  expanded in powers of  $\lambda$ , i.e., in traces of powers of S(E) which in turn are expressed (in QCA) as a sum over periodic orbit action terms, is just term by term the GTF. There is another related operator or matrix **T** due to Bogomolny [9], calculated from orbits entirely inside the billiard, whose spectral determinant det(1 - T(E)) also vanishes on the spectrum. Figure 1(*a*)

suggests how Tr  $\mathbf{T}^3$  could equal Tr  $\mathbf{S}^3$ . We shall find a generalization of this duality below, in which there is no inside system initially defined in the problem.

Another simple scattering approach is to cut the billiard in half and attach wide leads to the halves, thus giving two scattering problems which have no resonances and are quite simple to represent in QCA [6]. For example, figure 1(c) could be cut on the dashed line (assuming the leads are closed off.) The two pieces can be pasted together again, and it can be shown that the spectrum of the closed billiard is given by (2) with  $\mathbf{S} = \mathbf{S}_L \mathbf{S}_R$ , the S-matrices from the two scattering problems. This corresponds to the use of a surface of section at the cut line in the Bogomolny approach (see below). Usually, the simplest exact formulation of this type of problem is in terms of a compact operator, which adds to the  $\mathbf{S}$  matrix the rapidly converging contribution of an infinite number of evanescent modes. These are diffraction corrections which are quasi-classically small, and we shall ignore them here, although they are of considerable interest. In any case, Prosen has shown how, in most cases, one can define generalized unitary scattering matrices, taking into account the most important evanescent modes [10]. Similarly, there are usually exact versions of the Bogomolny technique.

An important aspect of the Fredholm determinant is that it is the zeros of D(E) which are desired, not the poles, so there is no difficulty with expressing D as a convergent series. In fact, from the Fredholm theory, the Plemelj–Smithies expansion,  $D(E) = \sum_n \lambda^n d_n(E)$ is guaranteed to be absolutely convergent for all  $\lambda$ , including the physical value  $\lambda = 1$ . The  $d_n$ s can be found in terms of the traces of powers of **S** by the recursion relation  $d_n = (-1/n)\sum_{m=1}^n d_{n-m} \operatorname{Tr} \mathbf{S}^m \cdot (d_0 = 1)$ . The traces  $\operatorname{Tr} \mathbf{S}^m$  can be expressed quasi-classically in terms of periodic orbits of the inside problem which have 'surface of section (SS) length' m. The  $d_n$ s are a sum of action terms composed of composite periodic orbits whose SS lengths add up to n. This was a major advance in the problem of obtaining good quasi-classical approximations to the energy levels. This is roughly the level of approximation achieved in the pioneering work of Cvitanovic and Eckhardt [11].

## 2.2. The rank of the S matrix

For the scattering matrix in the case of leads, it is clear that in a given energy range **S** is a finite  $N_E \times N_E$  matrix, where  $N_E$  is the number of open outgoing modes of the leads. For scattering from the outside of a billiard, it is easily seen in the angular momentum representation, that  $\mathbf{S}_{ll'} - \delta_{ll'}$  is quasi-classically a matrix of finite rank *N*. That is because a classical orbit whose angular momentum *l* is greater than the wavenumber *k* times the maximum radius  $R_{\text{max}}$  of the billiard will not scatter. Thus, one may truncate the trivial part of **S** to find that the truncated **S** is equivalent to an  $N \times N$  matrix. That means that  $d_n$  is quasi-classically small for n > N, and the series of composite orbits is *finite*. The longest orbits needed have periods about equal to the Heisenberg time,  $\hbar/\Delta$ , where  $\Delta$  is the mean level spacing. Thus, the exterior scattering matrix or the **T** operator can be said to 'resum' the divergent Gutzwiller series into a well defined, indeed a finite sum of composite orbits in QCA. However, since there are usually exponentially many periodic orbits with period shorter than the Heisenberg time, finding the zeros of  $D_S$  can present formidable difficulties, especially since  $D_S$  is a complex function. Also, keeping just the first few  $d_n$ s gives a meaningless result.

#### 2.3. Resurgence

However, in addition to the finite rank, there is *resurgence* [12]. Taking the complex conjugate of D(E), (for real E and  $\lambda$ ) it is easily seen, using the unitarity of **S**, that  $D(E, \lambda)^* = e^{-2i\Phi(E)}\lambda^N D(E, 1/\lambda)$ , where  $e^{2i\Phi(E)} = \det(-\mathbf{S}(E))$ , and  $\Phi(E)$  can be identified

as  $\pi \mathcal{N}(E)$ , the integrated smoothed (Weyl) density of states. Thus,  $d_{N-n}$  can be expressed in terms of  $d_n^*$  and  $D(E) = e^{i\Phi} \Delta(E)$ , with

$$\Delta(E) = \operatorname{Re} e^{-i\Phi} \sum_{n=0}^{N/2} d_n(E).$$
(3)

Because *longer* composite orbits, n > N/2 are expressed in terms of *shorter* ones, this consequence of the unitarity is termed 'resurgence'. (This terminology was introduced by Berry and Keating [12] as analogous to existing mathematical usage. It is also noteworthy that Berry and Keating obtained the result by using ideas based on the Riemann–Siegal formula in the theory of the Riemann zeta function, not unitarity. A more precise mathematical relation between these two approaches is not known to me.)

Resurgence makes three important improvements to the theory. First, it reduces the maximum SS length of the orbits by a factor 2, which for chaotic systems means that the number of orbits needed with resurgence is about the square root of the number needed without. Thus, if an attempt is made to find all the needed orbits and their actions, and add them up numerically, it is a great help.

Second, it ensures that the output of the calculation has *manifestly* the right character. In this case the energy levels can be found as the zeros of a *real* function of real *E*, *even if errors are made in approximating action terms*.

Third, because of this, essential features are preserved even if rather gross approximations are made. For example, if only the term  $d_0 = 1$  is kept in equation (3), the result is  $\Delta(E) \approx 2 \cos \pi \mathcal{N}(E)$  which has zeros when  $\mathcal{N}(E)$  is half-odd integer. In the usual case for billiards,  $\mathcal{N}(E) \approx E\mathcal{A}/4\pi = E/\Delta$  where  $\mathcal{A}$  is the area of the billiard. This approximation predicts 'equally spaced' energy levels with the correct average density. That is quite adequate for the many cases where one is not especially interested in correlations between nearby energy levels. Note that keeping only the first term of the Plemelj–Smithies expansion is totally inadequate. Keeping a few more terms in the resurgent case supplies some level correlations at specific spacings.

These results are a systematic way of taking into account the fact that orbits or even pieces of orbits which are very close to one another, 'within a wavelength of one another', should not be distinguished quantum mechanically. Also included is the fact that longer periodic orbits are well approximated as compositions of shorter ones, and the different possible compositions tend to cancel in calculating a determinant or 'zeta function'.

#### 2.4. Surfaces of section

This main set of results was obtained independently and at about the same time by other methods [9, 12], methods which are superficially at least quite different from one another. One way of summarizing the situation is that the quantities of interest can be obtained from an exact Fredholm integral equation,  $\psi(s) = \int ds' \mathbf{K}(s, s'|E)\psi(s')$ , where the integral runs over a surface of section, (SS) or rather, the configuration space part of a surface of section. Knowing two positions s, s', on the configuration part of the SS is equivalent to knowing both position and momentum, from which the entire orbit can be found. The wavefunction  $\psi$  on the SS can be used to obtain, quasi-classically, the full wavefunction. The SS is well chosen if the exact kernel **K** is (a) easily and well approximated in QCA, after which (b) it has finite rank N and (c) is unitary [13]. By easily and well approximated, we mean that  $\mathbf{K}(s, s')$  is well approximated by the sum of a few action terms, preferably none or one. The actions are those of classical orbits beginning on the SS at coordinate s', and ending at the next encounter with the SS at coordinate s. An important example for the stadium billiard is the choice of surface of section given by the Birkhoff coordinates, where s measures distance along the

circumference of the billiard. Then **K** is given by a Hankel function, according to the boundary integral method, and the matrix corresponding to **T** just replaces **K** by its asymptotic form. **K** describes pieces of orbit by one or more terms like  $\mathbf{K}(s, s') \approx a_p \exp ikL(s, s')$ , where the momentum  $p = \hbar k$  and L is the chord distance between the two points s, s' on the boundary.

There are, for any given problem, many such formulations, some more convenient than others. The main distinction between formulations is that the variable s runs over a surface of section, and surfaces of section can be chosen in many ways. Sometimes the difference between the results for two surfaces of section is just equivalent to a unitary change of representation of the generalized scattering matrix **S**, which would not change the rank of the matrix. In other cases, the rank could be reduced, which is typically paid for by the necessity of having several or even an infinite number of terms in a sum like (1) required to represent a given element of **S**. We shall encounter such a case below. We call this method, for short, the unitary kernels surface of section method.

#### 2.5. Numerical QCA calculations

Numerical QCA calculations of energy levels, based on resurgence, have been successfully carried out [14]. These considerations have been extended to study Wigner functions [15], Green's functions and wavefunctions [16] of closed systems. Although the results are sometimes termed 'resummed' GTF or Miller series, they can also be regarded as providing derivations of the GTF starting from exact Fredholm integral equations which do not rely on Feynman's path integral formulation of quantum mechanics.

If one is willing to forego whatever insights are provided by orbit expansions, Haggerty [17] has shown that excellent numerical results are obtained by numerical diagonalization of the **T** operator. The continuous operator is approximated as a matrix of dimension rather larger than N, the quasi-classical rank of the matrix. Let the eigenvalues be  $t_a(E)$ . These are found to fall into two classes. Class 0 eigenvalues have  $|t_a(E)| \ll 1$ . Class 1 eigenvalues are of the form  $t_b(E) = b_b \exp(i\theta_b)$ , where  $|b_b - 1| \ll 1$ , and there are N class 1 eigenvalues.

The criterion that *E* is on the spectrum was originally taken to be  $D(E) = \det(1-T(E)) = 0$ . In general, because of QCA errors, D(E) never vanishes for real *E*. The criterion that  $|\det(1 - T(E))|$  be a minimum is numerically not very good: it is ambiguous and inaccurate. However, Haggerty's main conclusion is that the criterion  $\theta_b(E) = 0$  is robust and gives excellent and unambiguous results.

We would like to argue that this is related to resurgence. From this point of view, one should find the zeros of  $\Delta(E) = 2\text{Re}\,e^{-i\Phi}D(E)$ , where  $e^{2i\Phi} = \det(-T)$ . Note that any overall non-vanishing real factors in the formula for  $\Delta$  are irrelevant. Since  $\Delta$  is a real function of a real variable, there is no ambiguity about its zeros. Now  $D(E) = \prod_{a \in 0} (1 - t_a) \prod_{b \in 1} (1 - b_b \exp(i\theta_b))$ . The first factor coming from the class 0 eigenvalues has a very small phase, so the factor is nearly real, and we can drop it. Assume now that just one eigenphase,  $\theta_B$ , for b = B, vanishes for  $E = E_B$ . We assume that all the other class 1 eigenvalues, labelled b', can for the following estimate be placed on the unit circle. Then  $D(E) \propto (-i)^{N-1} \exp\left(\frac{1}{2}i\sum_{b'}\theta_{b'}\right)(1 - b_B \exp i\theta_B)$  where we have dropped the non-vanishing real factor  $\prod_{b'} 2 \sin \frac{1}{2}\theta_{b'}$ . Next note that  $\det(-T) = (-1)^N \exp\left(i\sum_{b'}\theta_{b'} + i\theta_B\right)$  up to a non-vanishing real factor, so  $e^{-i\Phi} = i(i)^{N-1} \exp\left(-\frac{1}{2}i\sum_{b'}\theta_{b'}\right) \exp\left(-\frac{1}{2}i\theta_B$ . This leads to the estimate  $\Delta = 2 \operatorname{Re}[i(\exp(-\frac{1}{2}i\theta_B) - b_B \exp(\frac{1}{2}i\theta_B))] = 2(1 + b_B) \sin \frac{1}{2}\theta_B$ . Thus, we expect  $\Delta$  to vanish when one of the phases  $\theta_b$  does.

This argument is probably good in most cases, but it can happen from time to time that two phases,  $\theta_B(E)$ ,  $\theta_{B'}(E)$  vanish at energies  $E_B$ ,  $E_{B'}$  which are unusually close together. This is rare for chaotic systems because the phase shifts repel each other. However, to our

knowledge there has been no study of the properties of nearly degenerate pairs of levels in the various quasi-classical approximations.

## 3. Unitary kernels for scattering

Scattering systems are interesting in and of themselves, not just as a tool to study closed systems. In the important case of resonances, where there are poles of the scattering matrix at complex energy  $E = E_n - i\Gamma_n$ , the roles are reversed, namely, the resonance centres  $E_n$  are often understood in relation to the energy levels of a closed system. It is the purpose of this paper to study open scattering systems and in particular to formulate resurgence in that context, as well as to find a 'resummed' Miller series which is manifestly unitary. Figures 1(b), (c) illustrate scattering systems simulating those realized by microwave or quantum dot experiments and in which we are interested, since we expect them to have resonances whose widths are on average of the order of the spacing.

The method of unitary kernels on surfaces of section has been formulated for scattering systems. A surface of section in this case consists of two parts, the 'external' part, SSE, and the 'internal' part, SSI [18]. All scattering orbits pass through the SSE just twice, namely upon entering and leaving. They encounter the SSI  $0, 1, ... \infty$  times. Figure 1(*b*) illustrates a case where the SSI is the billiard boundary, less the opening, and the SSE is an imaginary surface across the opening. Another possibility is to move the SSE out to SSE'. Figure 1(*c*) illustrates three choices of SSI, two associated with the imaginary surface (SSI) dividing the billiard into two, or the boundary of the billiard (SSI)' that is left after opening the leads. The former can be regarded as either a 'two-sided SSI', meaning that a particle crossing the surface from either direction is regarded as 'encountering' the surface, or it can be 'one-sided', meaning only crossings from the left, say, are counted. The second possibility is usually chosen because the length of the SS is shorter. We shall find it good to take the two-sided definition, where the SSI is encountered from either direction. With this choice a particle going from the right SSE to the left SSE must cross the SSI and therefore there are no rays that go from SSE to SSE without encountering the SSI.

We can then introduce a closed reference system by changing the interpretation of the SSE. Namely, we forget about the outside, and say that a particle striking the SSE from the inside does not escape, but is reflected according to some rule. For example, either Neumann or Dirichlet conditions could be imposed there. (That is, the piece of orbit arriving at SSE would acquire an addition phase  $a\pi$ , a = 0 for Neumann, a = 1 for Dirichlet.) The choice of SSE together with the reflection rule naturally affects the definition of the reference closed system and its spectrum, but of course should not affect the physics of the scattering. Thus the predicted scattering matrices for the different choices of SSE should be equivalent, for example just differ by a constant phase. The phase of the scattering matrix is, after all, a matter of convention. (It is of course true that the accuracy of the leading order QCA may depend on the choice of SSE and the reflection rule, e.g. the diffraction corrections might differ in the two cases.)

In any case, a kernel U is introduced, which may be considered either an exact formulation of the problem or a quasi-classical approximation [19]. This unitary kernel has the form

$$\mathbf{U}(E) = \begin{pmatrix} \mathbf{U}_{EE} & \mathbf{U}_{EI} \\ \mathbf{U}_{IE} & \mathbf{U}_{II} \end{pmatrix}$$
(4)

and it represents both the scattering system *and* the closed reference system. The energy dependence of elements of the kernel is assumed to be like that of short sums of action terms, with actions such that  $dS/dE \ge 0$ . For billiards, the actions are of the form  $S = \hbar kL$ , where

 $\hbar k = \sqrt{E}$ . The choice of sign for dS/dE is conventional; it could be chosen non-positive equally well. However, complications arise if some S's have positive action derivatives while others are negative. The prefactors  $a_p$  are taken to be analytic except for a possible cut along the -k axis. The determinant whose zeros give the spectrum of the closed system is  $D_U(E, \lambda) = \det(1 - \lambda \mathbf{U}(E))$ .

Other assumptions, for example that the elements are constants, can be made with somewhat different interpretations of the formulae [20]. In fact, very similar ideas, not motivated by quasi-classics and surfaces of section (and not noted by physicists until recently), were developed more than 25 years ago in system theory and engineering mathematics as a general theory of the input–output approach to linear dynamic open systems [21]. These ideas were discovered, brought to the attention of physicists and further developed by Fyodorov and Sommers [20]. They are also related to a standard approach in scattering theory [22]. In this approach Hilbert space is broken into two or three parts, an interior part, and a scattering part (incoming and outgoing). Operators connecting these parts are postulated, and an evolution operator is postulated for the interior part. These more abstract models are particularly convenient if one is content with a statistical treatment. The definition of the inside system is taken for granted and there is no arbitrariness with choices of SS.

The S-matrix in the scattering interpretation is written as [18]

$$\mathbf{S} = \mathbf{U}_{EE} + \mathbf{U}_{EI} \frac{1}{1 - \mathbf{U}_{II}} \mathbf{U}_{IE}.$$
 (5)

(From the QCA perspective, equation (5) was obtained before equation (4).) Formula (5) organizes the scattering into four pieces.  $U_{EE}$  is the *direct* scattering which in QCA takes into account orbits which come in at an SSE and which leave again without ever encountering SSI. The process of crossing the SSE and going directly to the SSI is given by  $U_{IE}$ , and the process of going to the SSE and escaping after the last encounter with the SSI is given by  $U_{EI}$ . The crossings of the SSI are given by  $[1 - U_{II}]^{-1} = \sum_{n=0}^{\infty} U_{II}^n$ .

If the SS's are astutely chosen [19], and the system is simple enough, the operators  $U_{MN}$  will be quite simple in QCA. The rank of these matrices is dependent on the choice of SS, e.g., the rank of  $U_{II}$  is proportional to the length of SSI. In particular, the two-sided interpretation of the SSI in figure 1(*c*) has a corresponding matrix  $U_{II}$  that has twice the rank of the matrix associated with the one-sided interpretation of the SSI. However, the bigger matrix has half its elements zero, and the elements are simpler when expressed in QCA. We shall see that there can be other simplifications in choosing the two-sided case. Quasi-classically, in the configuration space orbit representation,  $U_{MN}$  is a kernel or operator given by one or a few action terms with short classical orbits from a point on the SS going to a next encounter with some piece of the SS. Equation (1) is recovered by expanding  $[1 - U_{II}]^{-1}$  and doing the integrals in the operator products by stationary phase. This groups the terms of the Miller sum according to the number of crossings of the SSI, and when summed in this order, the series converges. However, the convergence may be slow. Further, if the energy is considered to have a negative imaginary part, the actions  $S_p$  also acquire that feature and the series does not converge near the complex resonance energies.

We next show that the zeros of  $D_S(E) = \det(1 - \mathbf{S}(E))$  also give the closed spectrum. Indeed, suppose the energy is such that **U** has an eigenvalue unity. Then, there exists a non-trivial eigenvector  $(u_E, u_I)$  of **U** which satisfies

$$\mathbf{U}_{EE}\boldsymbol{u}_E + \mathbf{U}_{EI}\boldsymbol{u}_I = \boldsymbol{u}_E,\tag{6}$$

$$\mathbf{U}_{IE}\boldsymbol{u}_E + \mathbf{U}_{II}\boldsymbol{u}_I = \boldsymbol{u}_I. \tag{7}$$

Now,  $U_{II}$  is a subunitary matrix, a truncation of a unitary matrix, so its eigenvalues have magnitude less than 1 for real energy, unless some sector is completely decoupled from the rest of the U matrix. Putting aside this trivial case, we see from equation (7) that

$$u_I = \frac{1}{1 - \mathbf{U}_{II}} \mathbf{U}_{IE} u_E \tag{8}$$

is well defined and thus from (6),

$$\mathbf{U}_{EE}\boldsymbol{u}_{E} + \mathbf{U}_{EI}\frac{1}{1 - \mathbf{U}_{II}}\mathbf{U}_{IE}\boldsymbol{u}_{E} = \boldsymbol{u}_{E} = \mathbf{S}\boldsymbol{u}_{E}.$$
(9)

This shows that **S** has unit eigenvalue when **U** does. Conversely, if equation (9) holds with  $u_E \neq 0$ , one can define  $u_I$  by equation (8) and thus obtain equation (6). Note that the rank of **S** can be much different from that of **U**, which typically means that in the interesting case of resonances where  $\mathbf{U}_{II} \neq 0$ , there are an infinite number of terms in the Miller expansion of **S**.

What is more, we may define a matrix **W** which is just equation (5) with the interchange  $E \leftrightarrow I$ . It is then obvious that **W** is unitary and  $D_W(E)$  vanishes if and only if *E* is on the spectrum of the closed system. The matrix **W** can often be interpreted as a scattering matrix. In any case, it is useful, as we shall see below.

Thus we have three matrices,  $\mathbf{U}$ ,  $\mathbf{S}$  and  $\mathbf{W}$ , which generally have quite different ranks, whose spectral determinants yield the same spectrum, the spectrum of a particular choice of closing the system. The spectral determinants can be evaluated using resurgence, since the matrices are unitary.

The resonances cannot be identified with the spectrum thus found. Rather, resonances are given by the zeros of  $D_I(E, \lambda) = \det(1 - \lambda \mathbf{U}_{II}(E))$  for complex *E* (in the lower half plane). However, the operators  $\mathbf{U}_{MN}$  are of finite rank, and thus equivalent to ordinary matrices. This implies that the expansion of  $D_I$  in powers of  $\lambda$  terminates at some dimension,  $N_I$ . The rank of **S** is taken to be  $N_E$ , the rank of **W** and  $\mathbf{U}_{II}$  is  $N_I$  and the rank of **U** is  $N = N_E + N_I$ .

Since  $\mathbf{U}_{II}$  is subunitary, resurgence does not directly apply to the calculation of  $D_I(E)$ , or to  $(1 - \mathbf{U}_{II})^{-1}$ . If one is interested only in real energy, then if the resonance widths are broad compared with their spacing, the geometric series for  $[1 - \mathbf{U}_{II}]^{-1}$  converges rapidly, so the use of resurgence is not essential, although even here, the grouping of terms as found in the Fredholm expression may be helpful [11].

The conditions on the  $U_{MN}$ s required to make U unitary are sufficient to make S and W unitary. If we regard the scattering system as given, the choice of the SSE is to some extent arbitrary so the closed system is also arbitrary. For example, the difference between Dirichlet and Neumann conditions is a change in sign of orbits reaching the SSE, so  $U_{EI} \rightarrow -U_{EI}, U_{EE} \rightarrow -U_{EE}$  interchanges Dirichlet and Neumann conditions on the part of the boundary of the closed reference system consisting of the SSE. This sign change leads to nothing more than a sign change of S although the spectrum of the closed system does depend on the reflection rule.

## 4. No direct scattering

Even though the direct scattering specified by  $U_{EE}$  tends to be fairly simple in and of itself, it presents complications which we want to avoid. With the choice of SS of figure 1(*b*), the only direct scattering would be a possible reflection from the corners when the entering particle first encounters the SSE. That would be a diffraction effect, which we consider to be small in this paper. Of the three choices of surface of section for figure 1(*c*) mentioned above, the first two would allow direct scattering from the left lead to the right lead, but the use of the double-sided SSI forces all orbits to cross the SSI before escaping. The simplification of treating the 'ideal' case of no direct scattering is often made [22, 25, 26], (for reasons apparently quite different from ours) and we shall start with that case too, that is, we shall consider  $U_{EE} = 0$ .

We would like to apply the resurgence ideas to calculate  $[\mathbf{1}_I - \mathbf{U}_{II}]^{-1}$ , but since  $\mathbf{U}_{II}$  is not unitary, this cannot be done directly. However, with no direct scattering the matrix **W** simplifies greatly and becomes

$$\mathbf{W} = \mathbf{U}_{II} + \mathbf{U}_{IE}\mathbf{U}_{EI}.$$
 (10)

Quasi-classically,  $\mathbf{U}_{II}$  is not unitary because it omits orbits reflecting from the closure of the SSE. The term  $\mathbf{U}_{IE}\mathbf{U}_{EI}$  exactly takes care of this 'deficiency', and all periodic orbits in the closed system are included in det(1 – W). The SS length of the orbits, using W, differs from those given by U, however, so the meaning of the expansion coefficients  $d_n$  differs in the two cases.

The scattering matrix is thus

$$\mathbf{S} = \mathbf{U}_{EI} \frac{1}{1 - \mathbf{W} + \mathbf{U}_{IE} \mathbf{U}_{EI}} \mathbf{U}_{IE}.$$
(11)

Factoring out  $(1 - W)^{-1}$  and using  $A(1 - BA)^{-1} = (1 - AB)^{-1}A$ , we may express S in terms of

$$\mathbf{L} = \mathbf{U}_{EI} \frac{1}{1 - \mathbf{W}} \mathbf{U}_{IE} \tag{12}$$

as

$$\mathbf{S} = \frac{\mathbf{L}}{\mathbf{L}+1}.\tag{13}$$

If the energy is almost on the spectrum of the closed system, then L will be large and det(1-S) will vanish, as noted above. Note that L is defined on the external space, as is S, and that diagonalizing L is the same as diagonalizing S. The condition on L that makes S unitary is

$$\mathbf{L} + \mathbf{L}^{\dagger} + \mathbf{1} = \mathbf{0}. \tag{14}$$

It is known [16] how to extend the ideas of resurgence to  $[\mathbf{1} - \lambda \mathbf{W}]^{-1} = \mathbf{X}/Y$  where  $Y = D_W(E) = \sum_{n=0}^{N_I} \lambda^n Y_n(E)$  and  $\mathbf{X} = \sum_{n=0}^{N_I-1} \lambda^n \mathbf{X}_n(E)$ . The recursion relation for  $Y_n$  is the same as for  $d_n$ , with Tr U<sup>m</sup> replaced by Tr W<sup>m</sup>. The resurgence relation  $Y_n = e^{2i\Phi} Y_{N_I-n}^*$  holds, with  $e^{2i\Phi} = \det(-\mathbf{W})$  and again,  $\Phi(E) = \pi \mathcal{N}(E)$ . Thus Y is related to the real function  $\Delta_W(E)$  by  $\Delta_W = e^{-i\Phi}Y = 2 \operatorname{Re} \tilde{\Delta}_W$  with  $\tilde{\Delta}_W = e^{-i\Phi} \sum_{n=0}^{[N_I/2]} Y_n$ . (We assume that  $N_I$  is even. The formulae are slightly different if  $N_I$  is odd. The notation  $\sum_{n=0}^{[M]}$  means that an extra factor  $\frac{1}{2}$  multiplies the last term n = M.)

The recursion relation for **X** is  $\mathbf{X}_n = Y_n \mathbf{1} + \mathbf{W} \mathbf{X}_{n-1}$ , so  $\mathbf{X}_n = \sum_{j=0}^n Y_j \mathbf{W}^{n-j}$ . The resurgence relations for  $\mathbf{X}_n$  are found from  $\mathbf{X}^{\dagger} / Y^* = [1 - \lambda \mathbf{W}^{-1}]^{-1} = -(\mathbf{W}/\lambda)/[1 - \mathbf{W}/\lambda]$ 

$$\mathbf{X}_{n}^{\dagger} = -\mathbf{e}^{-2\mathbf{i}\Phi}\mathbf{W}\mathbf{X}_{N_{l}-n-1}.$$
(15)

Following [16], we find after a little algebra

$$\mathbf{L} = \frac{1}{Y} \mathbf{U}_{EI} \mathbf{X} \mathbf{U}_{IE}$$
$$= \left(\mathbf{L}_{1} - \mathbf{L}_{1}^{\dagger} - \tilde{\Delta}_{W}^{*} \mathbf{1}_{E}\right) / \Delta_{W}, \qquad (16)$$

where

$$\mathbf{L}_{1} = \mathbf{e}^{-\mathrm{i}\Phi} \mathbf{U}_{EI} \left[ \sum_{n=0}^{[N_{I}/2]} \mathbf{X}_{n} \right] \mathbf{U}_{IE}.$$
(17)

The formula, equation (16), manifestly satisfies the condition  $\mathbf{L} + \mathbf{L}^{\dagger} + \mathbf{1} = 0$ , or equivalently,  $\mathbf{K} = \mathbf{K}^{\dagger}$ , where  $\mathbf{L} = -\frac{1}{2}\mathbf{1}_{E} + \frac{1}{2}\mathbf{i}\mathbf{K}$ ,

$$\mathbf{i}\mathbf{K} = \left[2\left(\mathbf{L}_{1} - \mathbf{L}_{1}^{\dagger}\right) + \mathbf{1}_{E}(\tilde{\Delta}_{W} - \tilde{\Delta}_{W}^{*})\right] / \Delta_{W}$$
(18)

and S has the form

$$\mathbf{S} = -\frac{1 - \mathrm{i}\mathbf{K}}{1 + \mathrm{i}\mathbf{K}}.\tag{19}$$

The matrix **K** is essentially the **R** matrix introduced by Wigner.

Semiclassically,  $\mathbf{U}_{EI}\mathbf{X}_{n}\mathbf{U}_{IE}$  is a sum over composite orbits which are made up in part of fictitious scattering orbits (or scattering pseudo-orbits) from SSE to SSE, composed with periodic pseudo-orbits. By pseudo-orbit we mean one which does not exist in the original scattering system, because it involves a reflection from the SSE. (Note that we use 'pseudoorbit' in a sense different from Berry and Keating [12], who use the term for what we call composite orbits. It is also different from the pseudo-orbits of [27] who use this terminology for what we call diffractive ray-splitting orbits.) The periodic pseudo-orbits appear in the factors  $Y_{n-r}$ , and the scattering pseudo-orbits are part of the expression for  $\mathbf{U}_{EI}\mathbf{W}^{r}\mathbf{U}_{IE}$ .

A periodic pseudo-orbit of SS length *n* (as determined by **W**) has *n* encounters with SSI. As determined by **U**, the length of a periodic pseudo-orbit which has *i* encounters with SSI and *e* encounters with SSE is n = i + e. Similarly, scattering orbits contributing to **L**<sub>1</sub>, for example, will include fictitious orbits (arising from the term  $\mathbf{U}_{IE}\mathbf{U}_{EI}$  in **W**) which are reflected from the SSE. That is, for the scattering interpretation,  $\mathbf{U}_{EI}$  and  $\mathbf{U}_{IE}$  only appear once, since the particle enters and escapes just once. However, the term  $\mathbf{U}_{IE}\mathbf{U}_{EI}$  in **W** is interpreted as a reflection at SSE. So, **L** and **K** mix these interpretations and are calculated on the basis of orbits which do not exist in the original problem.

#### 5. General scattering case

The existence or absence of direct scattering has no particular physical significance: it is an artefact of the choice of surface of section. Of course, prompt scattering, quickly in and quickly out, might naturally be written as direct scattering, but it is not necessary to do so. We believe, although we have no formal proof, that one can always choose surfaces of section for which  $U_{EE} = 0$ . If the entrance channel *E* is physically at some distance from the exit channel *E'*, then the SSI can always be arranged to intervene between the two for all orbits. If the entrance and exit channels are the same, then one can introduce a piece of SSI just inside SSE through which all incoming orbits must pass. These manipulations have the necessary defect that they increase the rank of the matrices  $U_{II}$  and W, but there does not seem to be any formal objection. Indeed, if  $U_{EE} = 0$ , it can be shown that unitarity of U requires that  $N_I \ge N_E$ .

This is the main result of this paper. We have arrived at a formula, equations (18) and (19), for the scattering matrix, which can be expressed in terms of composite orbits which encounter the SSI  $N_I/2$  or fewer times. Thus, many fewer orbits are needed (in the case that the expansion of  $(1 - \lambda U_{II})^{-1}$  does not converge rapidly) than without resurgence. However, the orbits are more complicated. They are composed of scattering orbits together with periodic orbits. The scattering orbits are pseudo-orbits which are made up of pieces which come in through the SSE, bounce around on the SSI *and* SSE and eventually escape through the SSE. The periodic orbits are also pseudo-orbits, which have the possibility of reflecting from the SSE rather than escaping. The formulation guarantees a unitary **S** matrix even if the quasiclassical approximation has errors. In addition, we have generalized the inside–outside

duality to an inside–outside *triality*, since we find three matrices **S**, **W** and **U**, whose spectral determinants vanish on the spectrum of the same closed system. Clearly, **W** can also be regarded as a sort of scattering matrix, and there are problems where this is a very natural interpretation.

#### 6. Relation to other theories

We continue with some further manipulations to make contact with other theories. There are important formulae for scattering in the literature [22] which are written in terms of a rectangular matrix V (something like  $U_{IE}$ ) and its Hermitian conjugate  $V^{\dagger}$ . The latter involves, in QCA, action terms with negative action,  $a_p^* \exp(-iS_p(E))$ . Although such terms can be treated in QCA, the interpretation in terms of orbits is more complex.

Continuing with the restriction  $\mathbf{U}_{EE} = \mathbf{0}$ , we note relations between the  $\mathbf{U}_{MN}$  required to make **U** and thus **S** and **W** unitary, e.g.  $\mathbf{U}_{EI}\mathbf{U}_{II}^{\dagger} = \mathbf{0}$  and  $\mathbf{U}_{IE}\mathbf{U}_{IE}^{\dagger} + \mathbf{U}_{II}\mathbf{U}_{II}^{\dagger} = \mathbf{1}$ . This also leads to equations like  $\mathbf{W}^{\dagger}\mathbf{U}_{IE} = \mathbf{U}_{EI}^{\dagger}$ .

We replace S by  $\tilde{S} = -S$ , which in other contexts is more usual. Thus  $\tilde{S} = 1 - 2iK/[1 + iK]$ . Using the unitarity of W and the relations just mentioned we find  $iK = U_{IE}^{\dagger}[(1 + W)/(1 - W)/]U_{IE}$  and

$$\tilde{\mathbf{S}} = \mathbf{1} - 2\mathrm{i}\mathbf{U}_{IE}^{\dagger} \frac{\mathbf{1}}{\mathbf{R}(\mathbf{E}) + \mathrm{i}\mathbf{U}_{IE}\mathbf{U}_{IE}^{\dagger}} \mathbf{U}_{IE},\tag{20}$$

where  $\mathbf{R} = i(\mathbf{1} - \mathbf{W})/(\mathbf{1} + \mathbf{W})$ . Note that  $\mathbf{R}(E)$  is an Hermitian matrix, the *R*-matrix for  $\mathbf{W}$ , whose determinant vanishes with  $\Delta_W$ , that is, on the spectrum of the closed system. An advantage of doing things this way is that  $\mathbf{U}_{IE}\mathbf{U}_{IE}^{\dagger}$  may have a weak energy dependence, and it contains the geometry essentially necessary for the widths of the resonances.

Other work [22] starts from the formula  $\tilde{\mathbf{S}} \approx \mathbf{1} - 2i\mathbf{V}_{IE}^{\dagger} \left(E - \mathbf{H}_0 + i\mathbf{V}_{IE}\mathbf{V}_{IE}^{\dagger}\right)^{-1}\mathbf{V}_{IE}$ . (See references [23, 24] for further discussion of this scattering formulation.) To compare, we imagine that, in some energy region, **R** can be diagonalized to **R** = diag  $\left(\tan\left(\frac{1}{2}\delta_i(E)\right)\right) \approx$ diag $\left((E - E_i)\tau_i\right)$  where the  $E_i$  are the energies of the closed interior region. The  $\tau_i$ s are approximately half the phase derivatives,  $\frac{1}{2}d\delta_i(E)/dE|_{E=E_i}$  where **W** diagonalizes to diag  $(\exp(i\delta_i(E)))$  and  $\delta_i$  vanishes at  $E = E_i$ . The  $N_I$  eigenphases  $\delta_i$  of **W** will be roughly equally spaced, so they must advance by an angle of order  $2\pi/N_I$  when the energy is incremented by  $E \rightarrow E + \Delta$ , leading to the estimate  $\tau_i^{-1} \approx N_I \Delta/\pi$ . In this representation, we may define  $\mathbf{V}_{iE} = \sqrt{\tau_i^{-1}}\mathbf{U}_{iE}$  to obtain the standard formula, where  $\mathbf{H}_0$  has eigenvalues  $E_i$ .

we may define  $\mathbf{V}_{jE} = \sqrt{\tau_j^{-1}} \mathbf{U}_{jE}$  to obtain the standard formula, where  $\mathbf{H}_0$  has eigenvalues  $E_i$ . The widths of the states are not directly given by  $\tau_i^{-1}$  but are rather distributed over the different states via the diagonalization of  $\mathbf{H}_0 - i\mathbf{V}_{IE}\mathbf{V}_{IE}^{\dagger}$ . The average magnitude of the widths is a property of the closed system, but the distribution of widths over the different states is given by the geometrical matrix  $\mathbf{U}_{IE}\mathbf{U}_{IE}^{\dagger}$ . This is a version of what is sometimes called 'Howland's Razor' [28].

We note that there is a sort of sum rule on the widths, since  $\mathbf{U}_{IE}\mathbf{U}_{IE}^{\dagger}$  is an  $N_I \times N_I$ idempotent matrix with trace  $N_E$  so it has  $N_E$  eigenvalues unity, and the rest vanish. This sum rule is not so obvious in terms of the matrix  $\mathbf{V}_{IE}\mathbf{V}_{IE}^{\dagger}$ . If upon diagonalization of the non-Hermitian matrix  $\mathbf{H}_0 - i\mathbf{V}_{IE}\mathbf{V}_{IE}^{\dagger}$  the imaginary parts are distributed more or less equally for all states, the resulting resonance widths will be of order  $N_E\Delta/2\pi$ . If  $\mathbf{V}_{IE}\mathbf{V}_{IE}^{\dagger}$  can be almost simultaneously diagonalized with  $\mathbf{H}_0$  then there will be  $N_E$  states with large widths of order  $N_I\Delta/2\pi$ , and the rest will be small. This is a case known as 'resonance trapping' [29].

Another formulation is due to Fyodorov and Sommers [20] who do not assume that  $U_{EE} = 0$ . They find a representation of U, such that  $U_{EE}$  is of the form  $U_{EE} = \sqrt{1 - \sigma \sigma^{\dagger}}$ ,

 $\sigma^{\dagger}$  being a 'diagonal' rectangular  $N_E \times N_I$  matrix. In this representation U is

$$\mathbf{U} = \begin{pmatrix} \sqrt{1 - \sigma^{\dagger}\sigma} & -\sigma^{\dagger} \\ \mathbf{Y}\sigma & \mathbf{Y}\sqrt{1 - \sigma\sigma^{\dagger}}, \end{pmatrix}$$
(21)

where  $\mathbf{U}_{EI} = -\sigma^{\dagger}$ ,  $\mathbf{U}_{IE} = \mathbf{Y}\sigma$ . If  $\sigma = 0$ , then inside and outside are decoupled, so  $\det(1 - \mathbf{Y}) = \mathbf{0}$  is the condition that there is a stationary internal state, or from a quantum perspective, there is an internal eigenstate. The spectrum of  $\mathbf{U}$  is clearly the same as that of  $\mathbf{Y}$ . This is easy to show, since  $\mathbf{Y} = \mathbf{W}$ , i.e.  $\mathbf{W} = \mathbf{U}_{II} + \mathbf{U}_{IE} (1 - \mathbf{U}_{EE})^{-1} \mathbf{U}_{EI} = \mathbf{Y}\sqrt{1 - \sigma\sigma^{\dagger}} - \mathbf{Y}\sigma(1 - \sqrt{1 - \sigma^{\dagger}\sigma})^{-1}\sigma^{\dagger} = \mathbf{Y}$ .

In much of the work to date, only statistics are considered to be of interest. Therefore, no attempt was made to specify what the Hamiltonian  $\mathbf{H}_0$  is or which closed system was being studied. Rather, it is assumed that  $\mathbf{H}_0$  is a member of a random matrix ensemble. In the unitary kernels approach, one could take  $\mathbf{W}$  as a random unitary matrix, although it is clear from the equation  $\mathbf{W}^{\dagger}\mathbf{U}_{IE} = \mathbf{U}_{EI}^{\dagger}$  that  $\mathbf{W}$  has an important relationship to  $\mathbf{U}_{IE}$ . Alternatively, one could study random subunitary matrices, in particular  $\mathbf{U}_{II}$  which again would depend essentially on  $\mathbf{U}_{IE}$ . Some steps have been taken in this direction [30]. An interesting case [31] is to study the distribution of eigenvalues of a subunitary matrix of the form  $\mathbf{W}\sqrt{1-\sigma\sigma^{\dagger}}$  where  $\mathbf{W}$  is random unitary, and  $\sigma$  is given.

#### 7. Applications of scattering resurgence

#### 7.1. Numerical results

The importance of resurgence as a numerical method in the calculation of scattering properties is somewhat doubtful. Aside from statistical quantities, the things most often calculated are the length spectrum, the complex energies of the resonances, and particularly in the context of weak localization, the transmission and reflection coefficients. The underlying classical orbit structure shows up most clearly in the *length spectrum*, which is found from correlations of the S-matrix as peaks in  $p(l) = |\int dk e^{ikl} S_{ij}(k)|^2$ . The Miller series is usually used directly in this formula, followed by a diagonal approximation, and that can give good results, with peaks at the lengths of the scattering orbits. However, the use of additional diffractive ray-splitting orbits is often necessary [27]. One could also consider correlations of K or L, e.g. of S/(1 - S). This could be studied by expanding L in powers of W and making the diagonal approximation, which would yield the lengths of periodic orbits of the closed system in addition to the scattering orbits. This is interesting, but does not rely on resurgence.

The complex resonance positions are probably best obtained numerically by the method of complex scaling [28, 29]. We are not aware of QCA approximations applied to that method, or of any relationship to resurgence.

## 7.2. Qualitative results

7.2.1. Weak localization. The transmission and reflection coefficients (e.g. for electrons entering a scattering region) are basically absolute squares of *S*-matrix elements. The reflection is increased by coherent backscattering, because some backscattered orbits and their distinct time reversed partners have the same classical action if the system is time reversal invariant and add coherently. Removing the time reversal invariance property by adding a weak magnetic field eliminates the coherent backscattering, reducing the total reflection coefficient. This is nicely calculated in the diagonal approximation, i.e. by expanding the *S*-matrix in the Miller series and then in the *S*-matrix product, keeping just the pairs of terms with the same+time



**Figure 2.** (*a*) A 'quarter Sinai billiard' with lead attached. A short reflected 'prompt' ray is shown, as well as a 'chaotic' ray with a long path. (*b*) A variable tunnelling barrier near the cavity entrance is added. The effect of this barrier is indicated.

reversed orbit. If the transmission amplitude is estimated in the diagonal approximation, this effect does not exist, since pairs of time reversed orbits do not exist for transmission. Because of unitarity however, the transmission amplitude must increase if the reflection amplitude decreases. Thus the QCA plus diagonal approximation fails. This long standing puzzle was largely cleared up in a beautiful paper by Richter and Sieber [32] who show that taking account of 'slightly' off-diagonal contributions solves this problem, at least for uniformly hyperbolic dynamics. It is clear that the present approach, which obtains a manifestly unitary *S*-matrix, must also solve the problem. However, the basic quantity is  $\mathbf{K}$  rather than  $\mathbf{S}$ , so there are complications and the comparison with [32] is not straightforward. Detailed results will be presented in a future contribution.

7.2.2. Toy models. The QCA is mainly valuable for the insight it gives, and the further approximations that it affords. Many phenomena are best understood by producing a toy model which displays the effect, together with numerical studies of a more realistic model. The graph scattering models introduced by Kottos and Smilansky [33] are interesting for this reason. Simple, although rather extreme approximations to resurgence formulae for scattering also fall into this class. These can give highly non-trivial results which serve as a basis for understanding particular phenomena, both experimental and numerical.

As an example, we consider a Sinai scatterer, with a single entrance–exit channel, as shown in figure 2(*a*). If we knew all the scattering and periodic orbits up to half the Heisenberg time, we could solve this problem quasi-classically from equation (19) but that would be rather like the numerical solution of the original problem. A toy model which captures interesting features of the system is as follows: we make the extreme approximation of throwing away all the  $Y_n$ s except for  $Y_0 = 1$ , in equation (16). This approximation was mentioned in section 2.3. We also discard all  $\mathbf{X}_n$ s except  $\mathbf{X}_0 = \mathbf{1}$ . Then  $\tilde{\Delta}^* = e^{i\Phi}$ , and  $\mathbf{L}_1 = e^{-i\Phi}\mathbf{U}_{EI}\mathbf{U}_{IE}$ . This operator describes prompt scattering orbits, as illustrated, entering and leaving again after one reflection from the SSI. Interesting results are obtained if that process is not too improbable. The reflection is assumed to come from the side of the square parallel to the SSE. We estimate (using the theory of the prefactors, not discussed here)

$$\mathbf{U}_{EI}\mathbf{U}_{IE} \approx \sqrt{\frac{kL_E^2}{4\pi i L_S}} \,\mathrm{e}^{2ikL_S} \equiv \beta \,\mathrm{e}^{2ikL_S}. \tag{22}$$

Here  $L_E$  is the width of the lead, and  $kL_E/\pi \approx 1$ , under the assumption that there is just one scattering mode.  $L_S$  is the square side, so the orbits contributing to equation (22) are approximately of length  $2L_S$ . The prefactor  $L_E$  comes from estimating the number of orbits which make this bouncing ball round trip. Exactly how this estimate is made is probably not too important in view of the overall gross simplifications of the model. However, we do find that  $|\beta| \approx \sqrt{L_E/L_S} \ll 1$ .

(This approximation is related to a graph scattering model in which the incoming wave has a choice of two paths a, b on entering the system. The **U** matrix for such a model could be

$$\mathbf{U}(k) = \begin{pmatrix} 0 & c & s \\ cD_a & s^2D_a & -csD_a \\ sD_b & -csD_b & c^2D_b. \end{pmatrix}$$
(23)

One path *a* is the quick in and out path of length  $2L_s$ , i.e.  $D_a = e^{ika} = e^{2ikL_s}$ . The other path is much longer, and intuitively represents a typical chaotic path. Our approximation does not assign this path a definite length as is usual for graph scattering, but suggests an action  $D_b = e^{2i\Phi(k)}$ . The parameters *c*, *s* can be taken as constants with  $c^2 + s^2 = 1$ . In this model the **W** matrix is diag $(D_a, D_b)$ .)

Continuing with the resurgence approximation we find that the poles of the scattering matrix are given by the zeros of

$$e^{i\Phi}\Delta_W(E)(1+L) = 1 + \beta e^{2ikL_s} - \beta^* e^{2i\Phi - 2ikL_s}.$$
(24)

(Note *L* is infinite when  $\Delta_W(E)$  vanishes.) The many chaotic orbits are crudely accounted for in the last, resurgent, term through the quantity  $\Phi$ . Since  $2\Phi = 2\pi \mathcal{N}(E) \approx \frac{1}{2}\mathcal{A}k^2$ , where  $\mathcal{A} = L_S^2 - \pi R^2/4$  is the area of the billiard, we see that for  $kL_S \gg 1$ ,  $\Phi \gg kL_S$ . There are resonances when  $\beta^* e^{2i\Phi} \approx 1$ , when *k* has a negative imaginary part. The term  $\beta e^{2ikL_S}$  in equation (24) gives a small correction to the position of these poles. There is no resonance associated with this term, i.e. if the energy is sufficiently imaginary that the term is of order unity, then  $e^{2i\Phi}$  is huge. The factor  $e^{-2ikL_S}$  also just gives a small correction. It reduces the mean spacing of resonances slightly as compared with the mean spacing of energy levels of a closed chaotic system given by  $\cos \Phi(E) = 0$ .

It is interesting to modify the system slightly by putting a tunnel barrier at the entrance to the scatterer, whose reflection amplitude is r and transmission amplitude is t, where  $|r|^2 + |t|^2 = 1$ . See figure 2(b). The S-matrix  $S_r$  with the barrier is related to the  $S = S_{r=0}$ matrix just found by

$$S_r = r + t \frac{S}{1 - rS} t. \tag{25}$$

Note that near r = 1, the poles of  $S_r(E)$  are near the zeros of 1 - S(E), the energy levels of the closed system.

We plot in figure 3, the position and width of a few resonances of  $\dot{S}_r$ , i.e. the zeros of (1 - rS), easily obtained from an expression similar to equation (24). For t = 0, the closed system, the levels have no width. As t increases, all the levels acquire some width, but as t approaches unity, a number of levels (of which just one is shown) acquire large width; while the other resonances are trapped, their width decreases after the initial increase.

The actual resonances of Sinai and similar billiards show this phenomenon, and it is confirmed by complex scaling numerical calculations of billiard systems modelling the



Figure 3. Numerical results for this model. Three successive energy levels of the closed system were chosen, and their positions in the complex plane followed as the system was opened, i.e. for tunnelling t going from zero to unity. One mode ceases to be resonant, while the other two are 'trapped'.

experiments [29]. It is interesting that the very crude approximation to the QCA scattering shows the effect, although it of course does not give the correct centres of the resonances. Resonance trapping thus appears as an effect of competition between sufficiently numerous prompt in and out orbits and the much longer chaotic orbits, together with the resonance width 'sum rule' noted in section 6.

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