Resurgence in Quasiclassical Scattering

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(Received 28 August 2002; published 19 February 2003)

In quasiclassical spectral theory, "resurgence" means that long periodic orbits can be expressed by short ones in such a way that the spectral determinant is real. The question has thus long been posed whether long scattering orbits can be expressed by short orbits in such a way as to make the quasiclassical scattering matrix unitary. We here find a resurgent and manifestly Hermitean expression for Wigner's R matrix, implying a unitary scattering matrix. The result is particularly important if the average resonance width is comparable with the average resonance spacing.

DOI: 10.1103/PhysRevLett.90.070401 PACS numbers: 03.65.Nk, 03.65.Sq, 05.45.Mt, 73.50.Bk

Scattering is a fundamental experimental and theoretical tool in nearly all branches of physics. If the geometry of the scatterer is of interest, the wavelength of the scattering probe must be short, thus the importance of the classical and quasiclassical approximations (QCA). Miller's QCA formula [1] for the scattering S matrix

$$\mathbf{S}_{ij}(E) = \sum a_p \exp[iS_p(E)/\hbar], \tag{1}$$

has an intuitive appeal: it sums over all classical *scattering* orbits p at energy E from, for example, an incoming direction $\hat{\boldsymbol{n}}_j$ into an outgoing direction $\hat{\boldsymbol{n}}_i$ and $S_p(E)$ is a classical action for that orbit. The prefactors a_p are proportional to the square root of the classical probability of the orbit. Expressions like (1) are characteristic of quasiclassics: we call them sums over "action terms." (We do not discuss the prefactors here, and we use the same symbol a_p in all cases. We keep in mind two-dimensional billiards as examples.) At one extreme, e.g., scattering from the outside of a stadium billiard, Fig. 1(a), Eq. (1) has but one or a few terms and there are no periodic orbits and no resonances. At the other extreme of a completely closed system, the Gutzwiller trace formula [2] (GTF) is a divergent series like Eq. (1), a sum over *periodic* orbits. Since the mathematical and computational problems posed by the GTF are now largely understood by methods briefly recalled below, the most challenging problem remaining for the QCA is intermediate, the case of many resonances whose widths are comparable to their spacing. Figures 1(b) and 1(c) show a typical situation: billiards with open leads that support relatively few scattering channels. The question is, "Can the insights developed for the GTF be extended to scattering and scattering resonances in the case that the Miller series is not absolutely convergent?" That question is here answered in the affirmative, namely, we find a resurgent expression which makes the scattering matrix manifestly unitary.

A major insight called "inside-outside" duality was developed by Doron, Dietz, and Smilansky [3] who related the spectrum of the billiard to scattering problems in several ways, e.g., one or more leads can be attached to the billiard [4], as in Figs. 1(b) and 1(c). The scattering matrix $\mathbf{S}(E)$ gives the closed spectrum when E is such that

$$D_S(E, \lambda) = \det[\mathbf{1} - \lambda \mathbf{S}(E)] = 0. \tag{2}$$

$D_S(E)$ is the Fredholm or spectral determinant. [λ is a bookkeeping parameter set to unity. The GTF is given by the QCA expansion of $d\ln D(E)/dE$.] Reference [3] showed the *same* result holds if $\mathbf{S}$ represents the scattering from the outside of the billiard, no leads at all, which is quasiclassically approximated by one action term. We find a generalization of duality below, where there is no inside system initially defined in the problem.

From Fredholm theory, the Plemelj-Smithies expansion, $D_S(E) = \Sigma_n \lambda^n s_n(E)$ is absolutely convergent for all λ. The s_n's are found from the recursion relation $s_n = (-1/n)\Sigma_{m=1}^{n} s_{n-m} \mathrm{Tr}\mathbf{S}^m$ ($s_0 = 1$). $\mathrm{Tr}\mathbf{S}^m$ in QCA is a sum of action terms over periodic orbits of "surface of section (SS) length" m. The s_n's are then a sum of action terms

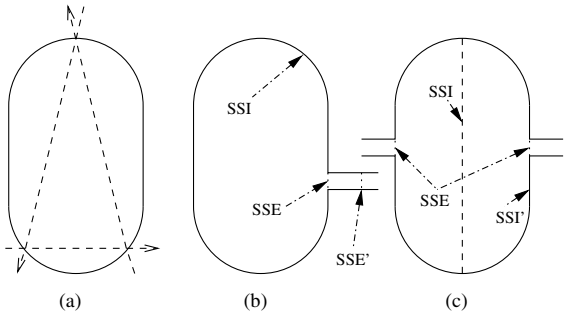

FIG. 1. Scattering processes associated with a Bunimovich stadium billiard. (a) Three possible scattering orbits from the outside. The figure suggests how $\mathrm{Tr}\mathbf{S}^3$ is related to an inside period three orbit. (b) A billiard with a lead attached. The most natural choice of SSE is shown,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

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made up of "composite" periodic orbits whose composite SS length is n.

Further, the $\mathbf{S}$ matrix has finite rank in QCA, so $s_n = 0$, $n > N$ (e.g., N is the number of outgoing waves in the leads). Thus, Eq. (2) "resums," in QCA, the divergent Gutzwiller series as a finite sum of action terms with composite orbits. However, since there are often exponentially many periodic orbits needed, finding the zeros of D_S can present formidable difficulties, especially since $D_S(E)$ is not real.

But, there is *resurgence* [5]. The complex conjugate of $D_S(E, \lambda)$, for real E and λ, using $\mathbf{S}^\dagger = \mathbf{S}^{-1}$, is $D_S(E, \lambda)^* = e^{-2i\Phi(E)}\lambda^N D(E, 1/\lambda)$, where $e^{2i\Phi(E)} = \det[-\mathbf{S}(E)]$, and $\Phi(E)$ is $\pi\mathcal{N}(E)$, the integrated smoothed (Weyl) density of states. Thus s_{N-n} can be expressed in terms of s_n^* and $D(E) = e^{i\Phi}\Delta(E)$, with $\Delta(E) = 2\mathrm{Re}e^{-i\Phi}\Sigma_{n=0}^{N/2} s_n(E) = 2\mathrm{Re}\tilde{\Delta}(E)$. Resurgence makes three improvements: (i) it greatly reduces the number of orbits needed, (ii) the result has *manifestly* the right character: Δ is a *real* function of real E, *even if errors are made in approximating action terms,* and (iii) essential features are preserved even if rather gross approximations are made. For example, if only $s_0 = 1$ is kept, $\Delta(E) \approx 2\cos\pi\mathcal{N}(E)$, giving the correct mean density.

These results were obtained independently and at about the same time by other methods [6,5], superficially quite different from one another. There are many ways of organizing such calculations. The most important, following Bogomolny [6], is by a generalization of Poincaré's *surface of section* to the quantum case. A way of summarizing the situation is that there are (many) exact Fredholm integral equations, $\psi(s) = \int ds' \mathbf{K}(s, s'|E)\psi(s')$, nontrivially solvable if E is on the spectrum, where the integral runs over (the coordinate part) of an SS. The SS is well chosen if $\mathbf{K}$ is (a) easily and well approximated in QCA by the sum of a few action terms, after which, in QCA (b) it has finite rank N, and (c) is unitary [7]. 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. Numerical QCA calculations of energy levels, based on resurgence, have been successfully carried out [8]. Direct diagonalization of $\mathbf{K}$ after the approximation of step (a) is also very successful, especially when using a technique to analyze the eigenvalues [9] which is related to resurgence [10]. These considerations have been extended to study Wigner functions, Green's functions, and wave functions [11,12] of closed systems. We call this method the "unitary kernels on surfaces of section" (UKSS) method.

Scattering systems are interesting in and of themselves, not just as a tool to study closed systems. In the important case of resonances, poles of the S matrix at complex energy $E = E_n - i\Gamma_n$, the roles are reversed; namely, the resonances are often understood in relation to a closed system. It is the purpose of this Letter 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) and 1(c) illustrate scattering systems simulating those realized by microwave or quantum dot experiments. Such systems are especially challenging since their resonance widths Γ_n are on average comparable to or a little larger than their average spacing $\overline{\delta E_n}$. [If $\overline{\Gamma}_n \gg \overline{\delta E}_n$, Eq. (1) converges rapidly. If $\overline{\Gamma}_n \ll \overline{\delta E}_n$, ray-splitting and tunneling orbits must be added to Eq. (1), but a sort of perturbation theory works.]

The UKSS has been formulated for scattering. A SS is in this case divided into two parts, the "external" part, SSE, and the "internal" part, SSI [13]. All scattering orbits pass through the SSE just twice, upon entering and leaving, but encounter the SSI any number of times. Figures 1(b) and 1(c) show examples.

We can 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 does not escape, but is reflected according to some rule. For example, either Neumann or Dirichlet conditions could be imposed there. 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 S matrices for the different choices of SSE should be equivalent, for example, just differ by a constant phase.

A unitary kernel $\mathbf{U}$ is introduced, in block form, which may be either exact or a QCA [14],

$$\mathbf{U}(E) = \begin{pmatrix} \mathbf{U}_{EE} & \mathbf{U}_{EI} \\ \mathbf{U}_{IE} & \mathbf{U}_{II} \end{pmatrix}. \tag{3}$$

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 $dS/dE = S' \geq 0$. The determinant whose zeros give the spectrum of the closed system is $D_U(E) = \det[1 - \mathbf{U}(E)]$. [The sign of S' is conventional; it could be chosen nonpositive equally well. However, complications arise if the S''s have both signs. Other assumptions can be made [15]. In fact, very similar ideas, not motivated by the QCA and SS's (and not noted by physicists until recently) were developed long ago in engineering mathematics as a general theory of the input-output approach to linear dynamic open systems [16]. These ideas were discovered, brought to the attention of physicists, and further developed in Ref. [15]. They are also related to a standard approach in scattering theory [17].]

The S matrix in the scattering interpretation is [13]

$$\mathbf{S} = \mathbf{U}_{EE} + \mathbf{U}_{EI}\frac{1}{1 - \mathbf{U}_{II}}\mathbf{U}_{IE}. \tag{4}$$

Equation (4) organizes the scattering into four pieces.

$\mathbf{U}_{EE}$ is the *direct* scattering of orbits entering and leaving the SSE without encountering SSI. Orbits crossing SSE and going directly to the SSI are given by $\mathbf{U}_{IE}$, and similarly for $\mathbf{U}_{EI}$. The intermediate crossings of the SSI are given by $[1 - \mathbf{U}_{II}]^{-1}$.

The ranks of these matrices depend on the choice of SS; e.g., the rank of U_{II} is proportional to the length of SSI. Quasiclassically, $\mathbf{U}_{MN}$ is a kernel 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 $[1 - \mathbf{U}_{II}]^{-1}$ 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 $D_S(E) = \det[1 - \mathrm{S}(E)]$ *also* give the closed spectrum. Indeed, take E so that $D_U(E) = 0$; i.e., $\mathbf{U}$ has an eigenvalue unity. Then, there is a nontrivial eigenvector (u_E, u_I) satisfying $\mathbf{U}_{EE}u_E + \mathbf{U}_{EI}u_I = u_E$, $\mathbf{U}_{IE}u_E + \mathbf{U}_{II}u_I = u_I$. Putting aside trivial cases, we see that $u_I = [1 - \mathbf{U}_{II}]^{-1}\mathbf{U}_{IE}u_E$ and thus $u_E = \mathbf{S}u_E$; i.e., $\mathbf{S}$ has unit eigenvalue when $\mathbf{U}$ does. The converse also holds.

Define a "scattering" matrix $\mathbf{W}$ which is just Eq. (4) with the interchange $E \leftrightarrow I$. It is then obvious that $\mathbf{W}$ is unitary and $D_W(E)$ vanishes if and only if E is on the spectrum of the closed system. The conditions on the $\mathbf{U}_{MN}$'s required to make $\mathbf{U}$ unitary are sufficient to make $\mathbf{S}$ and $\mathbf{W}$ 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 $\mathbf{U}_{EI} \to -\mathbf{U}_{EI}$, $\mathbf{U}_{EE} \to -\mathbf{U}_{EE}$ 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 $\mathbf{S}$ although the spectrum of the reference system of course depends on the reflection rule.

From Eq. (4) the *resonances* are given by the zeros of $D_I(E, \lambda) = \det[1 - \lambda\mathbf{U}_{II}(E)]$ for *complex* E. The expansion of D_I in powers of λ *does* terminate at some dimension, N_I. (The rank of $\mathbf{S}$ is N_E, the rank of $\mathbf{W}$ and $\mathbf{U}_{II}$ is N_I, and the rank of $\mathbf{U}$ is $N = N_E + N_I$.) However, resurgence does *not* work since $\mathbf{U}_{II}$ is *subunitary*(eigenvalues inside the unit circle), not unitary.

Even though the direct scattering specified by $\mathbf{U}_{EE} \neq 0$ tends to be simple in and of itself, we can make progress, if the SS is such or can be chosen so that $\mathbf{U}_{EE} = 0$. This simplification of treating the "ideal" case of no direct scattering is often made [17–19] (for reasons apparently quite different from ours) and we do so, too, in this Letter. More generally, diffraction effects lead to ray splitting, in particular, to direct backscattering. If this is numerically small, it can be studied by a sort of perturbation theory, as we will show in a future publication[10].

In the ideal case, $\mathbf{W} = \mathbf{U}_{II} + \mathbf{U}_{IE}\mathbf{U}_{EI}$ and $\mathbf{S} = \mathbf{U}_{EI}[1_I - \mathbf{W} + \mathbf{U}_{IE}\mathbf{U}_{EI}]^{-1}\mathbf{U}_{IE}$. This nice structure for $\mathbf{S}$ leads to $\mathbf{S} = \mathbf{L}/(\mathbf{L} + 1_E)$, where $\mathbf{L} = \mathbf{U}_{EI}[1_I - \mathbf{W}]^{-1}\mathbf{U}_{IE}$. We can use the Fredholm formula and resurgence to obtain $\mathbf{1}_I/(\mathbf{1}_I - \mathbf{W}) = e^{-i\Phi}(\mathbf{\Sigma}_{n=q}^{N_I-1}\mathbf{X}_n)/\Delta_W(E)$, where $\Delta_W(E) = \tilde{\Delta}_W + \tilde{\Delta}_W^*$, $\tilde{\Delta}_W = e^{-i\Phi}\sum_{m=0}^{N_I/2} w_m$, $\mathbf{X}_n = \mathbf{\Sigma}_{m=0}^{n}\mathbf{W}^m w_{n-m}$. [The w_n's are the expansion coefficients of $D_W(E, \lambda)$.] After a little algebra, also using relations like $\mathbf{W}^\dagger\mathbf{U}_{IE} = \mathbf{U}_{EI}^\dagger$ coming from $\mathbf{U}^\dagger = \mathbf{U}^{-1}$ and defining $i\mathbf{K} = 2\mathbf{L} + \mathbf{1}_E$, the result is obtained:

$$\mathbf{S} = -\frac{\mathbf{1}_E - i\mathbf{K}}{\mathbf{1}_E + i\mathbf{K}}, \tag{5}$$

$$i\mathbf{K} = [2(\mathbf{L}_1 - \mathbf{L}_1^\dagger) + \mathbf{1}_E(\tilde{\Delta}_W - \tilde{\Delta}_W^*)]/\Delta_W, \tag{6}$$

where $\mathbf{L}_1 = e^{-i\Phi}\mathbf{U}_{EI}[\sum_{n=0}^{(N_I/2)}\mathbf{X}_n]\mathbf{U}_{IE}$. Equation (6) manifestly satisfies the condition $\mathbf{K} = \mathbf{K}^\dagger$. The matrix $\mathbf{K}$ is close to the R matrix introduced by Wigner.

Quasiclassically, $\mathbf{U}_{EI}\mathbf{X}_n\mathbf{U}_{IE}$ is a sum over composite orbits made up in part of fictitious scattering orbits (or scattering *pseudo-orbits*) entering and leaving the 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. (We use "pseudo-orbit" in a sense different from that in Ref. [5], where Berry and Keating use the term for what we call "composite orbits.") The periodic pseudo-orbits appear in the factors w_{n-r}; the scattering pseudo-orbits are part of the expression for $\mathbf{U}_{EI}\mathbf{W}^r\mathbf{U}_{IE}$. Scattering orbits contributing to $\mathbf{L}_1$, for example, will include fictitious orbits (arising from the term $\mathbf{U}_{IE}\mathbf{U}_{EI}$ in $\mathbf{W}$) which are reflected from the SSE. That is, for the scattering interpretation, $\mathbf{U}_{EI}$ and $\mathbf{U}_{IE}$ appear only once, since the particle enters and escapes just once. However, the term $\mathbf{U}_{IE}\mathbf{U}_{EI}$ in $\mathbf{W}$ is interpreted as a reflection at SSE. So, $\mathbf{L}_1$ and $\mathbf{K}$ mix these interpretations and are calculated on the basis of orbits which do not exist in the original problem. Note also, the SS length depends on the choice of $\mathbf{U}$ or $\mathbf{W}$. A pseudo-orbit of SS length n (as determined by $\mathbf{W}$) has n encounters with SSI. As determined by $\mathbf{U}$, the length of a pseudo-orbit which has i encounters with SSI and e encounters with SSE is $n = i + e$.

This is our main result: a formula for the scattering matrix, which can be expressed in terms of composite orbits which encounter the SSI $N_I/2$ or fewer times. The orbits are composed of pieces which come in through the SSE, bounce around on the SSI *and* SSE, and eventually escape through the SSE. The formulation guarantees a unitary $\mathbf{S}$ matrix even if the QCA has errors. Extreme approximations like $\mathbf{L}_1 \approx e^{-i\Phi}\mathbf{U}_{EI}\mathbf{U}_{IE}$, $\tilde{\Delta}_W \approx e^{-i\Phi}$ have some merit [10]. 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. Further discussion will be given in a future paper [10]. We have not tested this theory numerically and indeed do not expect it to be an attractive numerical technique, since it requires finding many periodic *and* scattering orbits in the most difficult cases. However, it does have a potential for crude but qualitatively correct approximations, especially in interesting "toy" scattering models [10].

Although Wigner's R matrix has proven useful, there is still a matrix inversion needed to find **S** itself. For this reason we have not yet been able to use our results to shed light on the "weak localization" problem which depends on the unitarity of **S**. $[|\mathbf{S}_{ij}|^2$ is interpreted as a conductance from channel i to channel j. The diagonal terms $i = j$ are expected to grow as a magnetic field is turned off, i.e., as the system becomes time reversal invariant, due to "coherent backscattering." This should, by unitarity, make the off-diagonal terms decrease, but that is not at all automatic in quasiclassics based on Eq. (1) [20]].

We record a further result. We replace **S** by $\tilde{\mathbf{S}} = -\mathbf{S}$, which in other contexts is more usual. An important formula [17], $\tilde{\mathbf{S}} = \mathbf{1} - 2i\mathbf{V}^\dagger[E - \mathbf{H}_0 + i\mathbf{V}\mathbf{V}^\dagger]^{-1}\mathbf{V}$, posits a Hamiltonian $\mathbf{H}_0$ for the closed system and a rectangular matrix **V** connecting to scattering channels and no direct scattering. Using $\mathbf{U}^\dagger = \mathbf{U}^{-1}$ we find a corresponding formula in the UKSS,

$$\tilde{\mathbf{S}} = \mathbf{1} - 2i\mathbf{U}_{IE}^\dagger \frac{\mathbf{1}}{\mathbf{R} + i\mathbf{U}_{IE}\mathbf{U}_{IE}^\dagger}\mathbf{U}_{IE}, \tag{7}$$

where $\mathbf{R} = i(\mathbf{1} - \mathbf{W})/(\mathbf{1} + \mathbf{W})$. Note that $\mathbf{R}(E)$ is a Hermitian matrix, the R matrix for **W**, whose determinant vanishes with Δ_W on the reference spectrum. An advantage of this way of doing things is that $\mathbf{U}_{IE}\mathbf{U}_{IE}^\dagger$ may have a weak energy dependence. The magnitude of the resonance widths comes from the reference system, but the distribution of widths over the various states is determined by the geometrical term $\mathbf{U}_{IE}\mathbf{U}_{IE}^\dagger$. This is a version of what has been called "Howland's Razor" [21]. 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, the rest vanishing. This makes it possible to understand "resonance trapping" [22] in this formulation.

We thank Professor Peter Fulde for hospitality and support at the MPIPKS-Dresden. The work was supported in part by the U.S.–Israel Binational Science Foundation (BSF). Discussions with Bertrand Georgeot, Ed Ott, Tom Antonsen, Shmuel Fishman, Alfredo Ozorio de Almeida, Steve Tomsovic, Ingrid Rotter, and Klaus Richter were very helpful. We thank Henning Schomerus for pointing out Ref. [15].

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