

## Semiclassical cross section correlations

Bruno Eckhardt,<sup>1</sup> Shmuel Fishman,<sup>2</sup> and Imre Varga<sup>1,3</sup>

<sup>1</sup>*Fachbereich Physik, Philipps Universität Marburg, D-35032 Marburg, Germany*

<sup>2</sup>*Department of Physics, Technion, Haifa 32000, Israel*

<sup>3</sup>*Elméleti Fizika Tanszék, Fizikai Intézet, Budapesti Műszaki és Gazdaságtudományi Egyetem, H-1524 Budapest, Hungary*

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We calculate within a semiclassical approximation the autocorrelation function of cross sections. The starting point is the semiclassical expression for the diagonal matrix elements of an operator. For general operators with a smooth classical limit the autocorrelation function of such matrix elements has two contributions with relative weights determined by classical dynamics. We show how the random matrix result can be obtained if the operator approaches a projector onto a single initial state. The expressions are verified in calculations for the kicked rotor.

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### I. INTRODUCTION

Quantum systems whose classical limit is chaotic show fluctuations in cross sections and eigenvalue positions whose statistical properties seem to fall into a few universality classes [1–3]. Among the many measures that have been applied to characterize these statistical features, much attention has been given to two-point correlation functions since they can under certain assumptions be related to the classical dynamics [4]. For the case of spectra of bounded systems this has worked remarkably well and in addition one of the main predictions of the semiclassical analysis, the existence of long range correlations due to periodic orbits [4,5], has been confirmed many times [1,6].

More recently investigations of the statistical behavior of directly observable quantities, such as cross sections, have been worked out within the nonlinear  $\sigma$  model for disordered systems [7,8]. The correlation function was found to have two contributions, a Lorentzian and a derivative of a Lorentzian with respect to its parameter. The ratio between the two terms is fixed and depends on symmetry only. Since there is no semiclassical expression for the individual wave functions from which the cross sections could be calculated, the derivation of such correlation functions within semiclassics poses a serious challenge. A first step in this direction was undertaken by Agam [9], who exploited quantum properties of the matrix elements and did not use previously established formulas for diagonal matrix elements [10,11]. The derivation presented here is similar in spirit but starts from the semiclassical expression for diagonal matrix elements and specializes to the case of the cross section in the end. In particular, we show how the relative weight between the two contributions to the correlation function can be changed. The final expressions are compared with data for cross sections in an open kicked rotor model.

In Sec. II we present the semiclassical derivation of the correlation function between cross sections. This calculation is actually straightforward and closely patterned after calculations for other two-point correlations [4]. In Sec. III we discuss the limit that has to be taken in the observable to arrive at the correlation function for cross sections. In Sec. IV we discuss numerical simulations for an open kicked rotor. Some concluding comments are given in Sec. V.

### II. SEMICLASSICAL CORRELATION FUNCTIONS FOR SMOOTH OPERATORS

Quantum cross sections for the transition from an initial state  $|i\rangle$  to a set of final states  $|n\rangle$  which are eigenstates of a Hamiltonian  $H|n\rangle = E_n|n\rangle$  are proportional to

$$\sigma(E) \propto \sum_n \langle n|D|i\rangle \langle i|D|n\rangle \delta(E-H), \quad (1)$$

where  $D$  denotes the dipole operator. Using the projection operator

$$A = D|i\rangle \langle i|D \quad (2)$$

and Green's function  $G = 1/(E-H)$  the cross section becomes [dropping the proportionality factors implied in Eq. (1)]

$$\sigma_A(E) = -\frac{1}{\pi} \text{Im} \text{tr}(GA). \quad (3)$$

If the operator  $A$  is sufficiently smooth and has a nonsingular classical limit, there is a semiclassical expression for  $\sigma(E)$  that naturally divides into two pieces [10,11],

$$\sigma_A^{(sc)}(E) = \sigma_0(E) + \sigma_{A,fl}(E). \quad (4)$$

The first term, a smoothly varying background contribution from paths of “zero length,” is determined by integration over the energy shell of the Wigner transform  $A_W$  of the observable with the measure  $d\mu = d^d p d^d q / h^d$  (in  $d$  degrees of freedom),

$$\sigma_0(E) = \int d\mu A_W \delta(E-H). \quad (5)$$

The second term describes the fluctuations around it and is determined by classical periodic orbits,

$$\sigma_{A,fl}(E) = \frac{1}{\pi\hbar} \text{Re} \sum_p A_p w_p e^{iS_p/\hbar}, \quad (6)$$

where  $S_p$ ,  $T_p$ , and  $w_p$  are the action, period, and weight of the periodic orbit  $p$ , respectively, and

$$A_p = \int_0^{T_p} dt A_W(p(t), q(t)) \quad (7)$$

is the integral of the observable (again the Wigner transform of  $A$ ) over the periodic orbit  $p$ . This result is derived under the condition that the observable is sufficiently smooth so that it does not affect the stationary phase evaluation that singles out periodic orbits. Wigner transformations of projection operators are critical in this respect since they typically approach  $\delta$  functions in momenta as  $\hbar$  goes to zero, i.e., they become rather singular. This is the main limitation that prevents a direct application of the above expression to the calculation of the autocorrelation function of the cross sections. We therefore adopt the following strategy: We first calculate the autocorrelation function for  $\sigma_A(E)$  within a semiclassical approximation for a smooth observable  $A$  and then discuss the limit of a singular operator.

The object we want to calculate is the normalized autocorrelation function of the fluctuations around the mean cross section  $\sigma_0(E)$ ,

$$C(\varepsilon) = \langle \sigma_{A,fl}(E + \varepsilon/2) \sigma_{A,fl}(E - \varepsilon/2) \rangle / \langle \sigma_0 \rangle^2, \quad (8)$$

where  $\langle \dots \rangle$  denotes an average over energy. The energy scale is set quantum mechanically by the mean spacing  $\Delta$  between neighboring levels, calculated from the mean density of states

$$\rho_0 = 1/\Delta = \int d\mu \delta(E - H). \quad (9)$$

The associated time scale is the Heisenberg time  $T_H = 2\pi\hbar\rho_0 = h/\Delta$ . The scale for the observable is set by the phase space average of its Wigner transform,

$$\bar{A} = \frac{\int d\mu A_W \delta(E - H)}{\int d\mu \delta(E - H)} \quad (10)$$

so that  $\sigma_0 = \bar{A}\rho_0 = \bar{A}/\Delta$ .

Substituting the fluctuating part from the periodic orbits gives

$$C(\varepsilon) = \frac{\Delta^2}{2\bar{A}^2\pi^2\hbar^2} \times \text{Re} \left\langle \sum_{p,p'} A_p^* A_{p'} w_p^* w_{p'} e^{i[S_p(E+\varepsilon/2) - S_{p'}(E-\varepsilon/2)]/\hbar} \right\rangle.$$

The classical action in the exponent can be expanded for small  $\varepsilon$ ,

$$\begin{aligned} S_p(E + \varepsilon/2) - S_{p'}(E - \varepsilon/2) \\ \approx S_p(E) - S_{p'}(E) + \varepsilon(T_p + T_{p'})/2. \end{aligned}$$

In the diagonal approximation [4] the correlation function becomes

$$C_{diag}(\varepsilon) = \frac{g\Delta^2}{2\bar{A}^2\pi^2\hbar^2} \text{Re} \sum_p |A_p|^2 |w_p|^2 e^{iT_p\varepsilon/\hbar}; \quad (11)$$

the factor  $g$  accounts, as usual, for degeneracies. In the case of real symmetric Hamiltonians,  $g=2$ , while for Hermitian Hamiltonians  $g=1$ .

For the next step we use the periodic orbit sum rule [12] and follow the steps in [13]. The periodic orbits proliferate exponentially with time so that the sum on  $p$  can be replaced by an integral over time. The density of orbits is given by  $e^{\mu T}/T$  with  $\mu$  the topological entropy and their weight by  $|w_p|^2 = e^{-\lambda T}$  with  $\lambda$  the Lyapunov exponent. The difference between the Lyapunov exponent and the topological entropy is the classical escape rate,

$$\Gamma = \lambda - \mu. \quad (12)$$

The integrals  $A_p$  of the observable along the orbit vary considerably among orbits of similar length. The high density of periodic orbits allows us to capture this probabilistically through the distribution  $P(A)$  of values obtained for all orbits with periods in a small interval around  $T$ . If the correlations in the classical dynamics fall off sufficiently rapidly, the distribution will be Gaussian,

$$P(A) = \frac{1}{\sqrt{\pi s_A}} e^{-(A - \bar{A})^2/s_A^2} \quad (13)$$

with a mean  $\bar{A} = \bar{A}T$  following from ergodicity and a variance  $s_A^2 = \alpha T$  that increases linearly with time. With this distribution function and the assumption that there are no correlations between weights  $w_p$  and observables  $A_p$ , the mean square average of the  $A_p$ 's from orbits with periods near  $T$  changes with time like

$$\langle |A_p|^2 \rangle(T) = \bar{A}^2 T^2 + \alpha T. \quad (14)$$

Thus, summing the contributions of orbits in the diagonal approximation, we obtain

$$\begin{aligned} C_{diag}(\varepsilon) &= \frac{g\Delta^2}{2\bar{A}^2\pi^2\hbar^2} \\ &\times \text{Re} \int_0^{T_H} dT \frac{e^{(\mu - \lambda + i\varepsilon/\hbar)T}}{T} (\bar{A}^2 T^2 + \alpha T). \end{aligned}$$

For bounded systems ( $\mu = \lambda$ ) and for  $\varepsilon = 0$  we obtain the expression for the variance of matrix elements derived in [13] and tested and verified in many situations [14–16]. If the system is sufficiently open so that  $\Gamma T_H \gg 1$  the contributions from the off-diagonal terms can be neglected and the integration continued to infinity (as explained in the next paragraph). Then

$$C_{diag}(\varepsilon) \approx \frac{g\Delta^2}{2\bar{A}^2\pi^2\hbar^2} \text{Re} \left( \alpha \frac{1}{\Gamma - i\varepsilon/\hbar} + \bar{A}^2 \frac{1}{(\Gamma - i\varepsilon/\hbar)^2} \right). \quad (15)$$

With the energy and time scales mentioned above, i.e.,  $\varepsilon = \tilde{\varepsilon}\Delta$  and  $\Gamma = 2\pi\tilde{\Gamma}/T_H = \tilde{\Gamma}\Delta/\hbar$ , the correlation function becomes

$$C(\varepsilon) \approx \frac{g}{\pi} \left( \frac{\alpha}{\bar{A}^2 T_H} \frac{\tilde{\Gamma}}{\tilde{\Gamma}^2 + \tilde{\varepsilon}^2} + \frac{1}{2\pi} \frac{\tilde{\Gamma}^2 - \tilde{\varepsilon}^2}{(\tilde{\Gamma}^2 + \tilde{\varepsilon}^2)^2} \right). \quad (16)$$

As in the calculation of Fyodorov and Alhassid [7] the correlation function has two terms, a Lorentzian and a derivative of a Lorentzian with respect to the width. However, in contrast to their formula, where the relative weight between the two terms was fixed, it here depends on the observable and the Heisenberg time. This point will be taken up again in the next section.

The above derivation is based on the usual assumptions on the diagonal approximation, the validity of a periodic orbit sum rule and the replacement of a sum over orbits by an integral in time. As a consequence deviations can be expected for short times where isolated periodic orbits dominate, an effect that should be particularly noticeable near bifurcations. Deviations from the diagonal approximations are strong for the orthogonal ensemble and absent for the unitary ensemble, at least up to the Heisenberg time [17]. The extension of the time integration up to infinity rather than the Heisenberg time is justified if the system is very open, i.e., if  $\Gamma T_H \gg 1$ , so that the corrections due to off-diagonal terms for times beyond the Heisenberg time can be neglected. When approaching bounded systems  $\Gamma$  vanishes and the corrections have to be taken into account. The final expression is thus reasonable only for sufficiently open systems where  $\Gamma/\hbar \gg \Delta$ . In this limit the contributions from long orbits are quickly suppressed and the differences between the unitary and orthogonal ensembles should disappear, except of course for the factor of 2. It is possible to go beyond this by assuming that the form factor is the random matrix form factor times an exponential damping, as suggested also by Alhassid and Fyodorov [8,18].

The derivative of the Lorentzian in the second term, weighted by the mean of the operator, can be traced back to the autocorrelation function of the density of states (without operator) as calculated earlier [19]. The width  $\Gamma$  that enters here is the classical escape rate, since that is what determines the modification of the classical sum rule. The prediction then is that the quantum resonances have half that width, since it is the probabilities and not the amplitudes that have to follow the classical behavior. In many cases, especially with a finite number of channels, the situation presumably is more complex, since the quantum resonances have a distribution of widths and it is not clear which quantity (average width, maximum of distribution, longest lifetime, etc.) dominates the form factor [20]. In the semiclassical limit of an infinite number of channels some information can be drawn from the results of Fyodorov and Sommers for random matrix models with fixed transmission [21] and from the distribution of resonance widths calculated by Haake *et al.* [22]: in both cases a single width parameter, given by half the classical escape rate in the first case and by half the gap in the distribution in the second case, suffices to describe the correlation function.

Finally, we note that if the classical correlations do not decay sufficiently rapidly the average of the square of the integrals along the orbits can be expressed as an integral over the correlation function as in the previous calculation of matrix elements [13].

### III. THE LIMIT OF PROJECTION OPERATORS

The final result for the correlation function given in Eq. (16) has the two functional dependencies also identified by Alhassid and Fyodorov [7], but the relative weighting depends on the observable. Even worse, the first term contains  $T_H$  in the denominator and therefore seems to vanish in the semiclassical limit where  $T_H$  diverges. Then the correlation function is of the form of a derivative of the Lorentzian only. So how can one obtain Alhassid and Fyodorov's result  $\alpha/\bar{A}^2 T_H = 1$  within this semiclassical approach?

The key to the problem is the observation that the semiclassical approximation assumes the observable to have a nonsingular classical limit whereas the quantum cross sections are obtained from observables that are projectors on the initial state (weighted with the dipole operator). The Wigner transform of a projector is itself a function of Planck's constant and becomes singular in the semiclassical limit. More specifically, one can visualize the Wigner transform of a projector as a characteristic function that in  $d$  dimensions exists on a phase space cell of volume  $h^d$ , since that is the phase space volume occupied by a single state. The observables for which the semiclassical trace formula was derived were smooth with a nonsingular limit, that is to say, they covered an increasing number of quantum states in the semiclassical limit. This smearing over many states suppresses the first term in the correlation function.

It is possible to estimate the consequences of this observation on the operator  $A$  in a simple model of a uniformly damped quantum map. Consider a two-dimensional chaotic map on a finite phase space and its quantum representation by an  $N \times N$  unitary operator  $U$ . The dimension  $N$  of  $U$ , Planck's constant  $h$ , and the volume  $\Omega_0$  of the classical phase space are connected by  $h = \Omega_0/N$ . Damping is introduced uniformly everywhere in phase space and on all quantum states. The projector is modeled by an observable that takes on the value  $a_0$  in some part of phase space of area  $\Omega_A$  and vanishes everywhere else.

On the classical side the integrals of the observable along the periodic orbit are replaced by sums over the points of the orbit. If there are no correlations between different time steps, the average value of the  $A_p$  over all orbits with period  $n$  is given by  $\langle A_p \rangle = n a_0 p$ , where  $p = \Omega_A/\Omega_0$  is the probability for a randomly chosen point to lie in the phase space area where the observable does not vanish. The second moment of the distribution is given by

$$\langle A_p^2 \rangle = a_0^2 p^2 n^2 + a_0^2 p(1-p)n. \quad (17)$$

By comparison with Eq. (14) we read off  $\bar{A} = a_0 p$  and  $\alpha = a_0^2 p(1-p)$ . The Heisenberg time is  $T_H = N$ , the dimension of the Hilbert space. Therefore,

$$\frac{\alpha}{\bar{A}^2 T_H} = \frac{a_0^2 p(1-p)}{a_0^2 p^2 N} = \frac{1-p}{pN}. \quad (18)$$

With an escape rate  $\bar{\Gamma}$  expressed in units of the Heisenberg time the correlation function then becomes

$$C(\varepsilon) = \frac{g}{\pi} \left( \frac{1-p}{pN} \frac{\bar{\Gamma}}{\bar{\Gamma}^2 + \varepsilon^2} + \frac{1}{2\pi} \frac{\bar{\Gamma}^2 - \varepsilon^2}{(\bar{\Gamma}^2 + \varepsilon^2)^2} \right). \quad (19)$$

This expression clearly shows the suppression of the first term in the semiclassical limit of large  $N$  if  $p$  is fixed.

However, if the observable is a projector onto a single state its Wigner transform should localize on a cell of phase space volume  $h$ . Thus,  $\Omega_A = \Omega_0/N$  and  $p = 1/N$ , so that the product  $pN = 1$ . Except for the tiny correction  $1/N$  to the correct ratio of 1 this is the result obtained by Alhassid and Fyodorov [7]. In addition, it suggests a way to modify the relative weighting between the two terms: consider transitions not from a single state but from  $M$  states in an incoherent superposition, i.e.,

$$A = D \sum_m |m\rangle\langle m| D. \quad (20)$$

Then the phase space area covered by  $A$  will increase  $M$ -fold and the weight of the Lorentzian will decrease correspondingly,

$$C(\varepsilon) \approx \frac{g}{\pi} \left( \frac{1}{M} \frac{\bar{\Gamma}}{\bar{\Gamma}^2 + \varepsilon^2} + \frac{1}{2\pi} \frac{\bar{\Gamma}^2 - \varepsilon^2}{(\bar{\Gamma}^2 + \varepsilon^2)^2} \right) \quad (21)$$

(where it is assumed that  $M \ll N$ ). The resolution to the problem of the relative weight between the two terms in the correlation function posed at the beginning of this section is thus that, by focusing on initial states that are projectors, the classical observable also depends on  $\hbar$ , and this  $\hbar$  dependence influences the classical quantities as well. Indeed, if the classical observable becomes very localized in phase space, it is rarely visited, the return time becomes large, and the variance increases much more slowly, on a time scale also set by the return time. In this way the Heisenberg time enters the classical quantities.

#### IV. NUMERICAL TESTS ON THE KICKED ROTOR

The model of the previous section clearly stretches the applicability of the semiclassical expressions for the matrix elements to their limits and requires numerical tests. We use the kicked rotor in the momentum space quantization of Izrailev [23] for this purpose,

$$U_{nm} = \frac{1}{N} \sum_{l=0}^{N-1} e^{-iKNV(2\pi l/N)} e^{-2i\pi l(n-m)/N} e^{-i2\pi m^2/N}, \quad (22)$$

where [18]  $V(\phi) = \cos \phi - \sin(2\phi)$  is the kicking potential. This model is known to belong to the unitary universality class ( $g=1$ ) due to the second term in the potential that breaks the conjugation symmetry [24,25]. If the kicking strength is sufficiently large the correlations decay very

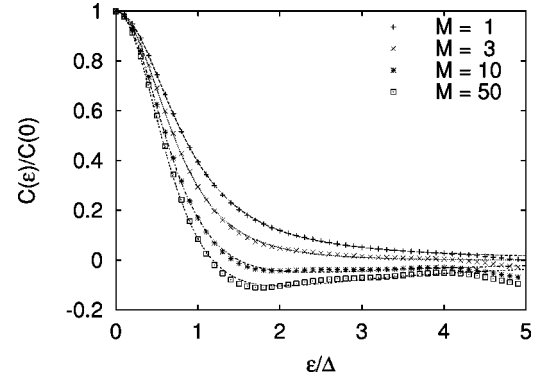


FIG. 1. Cross section correlation function for different widths of the observable, increasing from  $M=1$  (top curve) to 3, 10, and 50 (bottom curve). The width of the resonances was uniform throughout the quantum spectrum:  $\Gamma = \Delta$  [see Eq. (23)]. The continuous curves are fits to the functional form of Eq. (16) with  $\bar{\Gamma}$  and the coefficient of the Lorentzian as fitting parameters with the condition  $C(0) = 1$ .

quickly and one ends up with essentially random values for the momenta. The calculations were done for  $K=7$  [26] and matrix sizes  $N=101, 201, 401, 801,$  and  $1601$ . The initial states were taken to be momentum eigenstates of the unperturbed map. From the eigenstates  $|\nu\rangle$  and eigenphases  $\phi_\nu$  a cross section was formed with the operator  $A$  from Eq. (20) according to

$$\sigma(\phi) = \text{Re} \sum_\nu \frac{\langle \nu | A | \nu \rangle}{1 - \exp[i(\phi - \phi_\nu) - \Gamma/2]}. \quad (23)$$

The damping  $\Gamma/2$  is uniform for all eigenstates and models the coupling of the system to a continuum (for a discussion of this point see the previous section and the references cited there). The role of the energy is now taken over by the phase  $\phi$  and the mean and correlation function are calculated over the periodicity interval  $2\pi$ . The mean separation between eigenphases is  $\Delta = 2\pi/N$ . Figure 1 shows the correlation function obtained for different numbers of initial states and constant damping. For a single initial state the contribution from the derivative of a Lorentzian is barely noticeable, but as the number of initial states increases the deviations from the Lorentzian become larger. In particular, the correlation

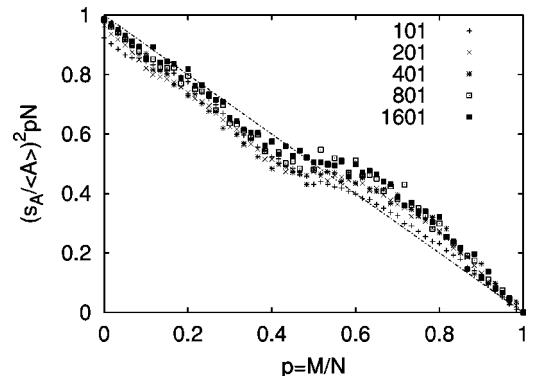


FIG. 2. Ratio between variance and average squared for observables of different widths. The different symbols correspond to different sizes of the matrix and thus to different values of  $\hbar$ .



function develops a zero for  $M/2\pi > \bar{\Gamma}$ . Fitting Eq. (16) with the coefficient of the Lorentzian and  $\bar{\Gamma}$  as free parameters yields a broadening  $\bar{\Gamma} \approx \Gamma$  independent of  $M$  and the coefficient of the Lorentzian in Eq. (16) is proportional to  $M^{-1}$  as expected from Eq. (21).

A random matrix calculation [25] shows that the quantity that controls the relative weight between the two terms is the ratio between the variance  $s_A^2$  of the matrix elements and the square of the average for different matrix sizes. This quantity,  $(s_A/\langle A \rangle)^2$  should equal  $(1-p)/pN$ . As shown in Fig. 2, the renormalized quantity  $(s_A/\langle A \rangle)^2 pN$  follows the expected  $1-p$  behavior rather closely, albeit with large fluctuations. It thus seems that the assumptions that enter in our semiclassical derivation of the correlation function can be satisfied in chaotic systems.

### V. FINAL REMARKS

We have shown how within a semiclassical approximation correlation functions for cross sections in open systems can be calculated. The calculations could be supported with simulations in the standard map and in particular the changes in the relative weight between the two contributions to the correlation function could be demonstrated.

Actually, the calculation works much better than can reasonably be expected: it is well known that the calculation of wave functions usually requires in addition to periodic orbits

also recurrent orbits [27,28]. Their importance depends on the width of the initial state [11]. It may happen, however, that in a statistical sense the differences between the contributions from recurrent and periodic orbits cancel. A related problem concerns the higher moments of the distribution and thus the form of the full distribution. Even in the singular limit of small  $p$  considered in the model, the distribution of classical contributions remains Gaussian, or perhaps Poissonian [25], but the distribution for transition strengths expected from random matrix theory is exponential (for the unitary ensemble) or Porter-Thomas (for the orthogonal ensemble). Further calculations indeed show that, while the first and second moments agree, the higher moments and the full distributions differ [25].

Among the consequences that seem worthwhile to pursue are the dependence on the initial state and the possibility of highlighting the non-Lorentzian part, the modification to allow for nonexponential classical escape [18,25], and the singular contributions from periodic orbits near bifurcations [29].

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