

## Semiclassical spectra and diagonal matrix elements by harmonic inversion of cross-correlated periodic orbit sums

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Semiclassical spectra weighted with products of diagonal matrix elements of operators  $\hat{A}_\alpha$ , i.e.,  $g_{\alpha\alpha'}(E) = \sum_n \langle n | \hat{A}_\alpha | n \rangle \langle n | \hat{A}_{\alpha'} | n \rangle / (E - E_n)$ , are obtained by harmonic inversion of a cross-correlation signal constructed of classical periodic orbits. The method provides highly resolved semiclassical spectra even in situations of nearly degenerate states, and opens the way to reducing the required signal lengths to shorter than the Heisenberg time. This implies a significant reduction of the number of orbits required for periodic orbit quantization by harmonic inversion. [S1063-651X(99)07908-8]

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The semiclassical quantization of periodic orbits is of fundamental interest for both regular [1] and chaotic [2,3] dynamical systems. In both cases the semiclassical density of states is obtained by summing over the periodic orbits of the underlying classical system. However, periodic orbit sums of this type usually diverge. Various techniques have been developed in recent years to overcome this problem. Most of these techniques are especially designed for hyperbolic (chaotic) systems [4–6] and cannot be applied to systems with regular or mixed regular-chaotic dynamics. Recently a new technique, based on *harmonic inversion* of semiclassical signals [7,8], was shown to be both very powerful and universal for the problem of periodic orbit quantization in that it does not depend on special properties of the system such as ergodicity or the existence of a symbolic dynamics. The method only requires the knowledge of periodic orbits and their physical quantities up to a certain maximum period, which depends on the average local density of states. Unfortunately, this method is not free of the general drawback of most semiclassical approaches, which suffer from a rapid (exponential for chaotic systems) proliferation of periodic orbits with their period, which in turn requires an enormous number of orbits to be taken into account.

In this paper we propose to implement an extension of the *filter-diagonalization method*, which is a method of solving the harmonic inversion problem [9,10], to the case of time cross-correlation functions [9,11,12], i.e., the one-dimensional time signal  $C(t)$  is extended to a  $D \times D$  matrix of cross-correlated time signals  $C_{\alpha\alpha'}(t)$ , with  $\alpha, \alpha' = 1, \dots, D$ . This method has recently also served as a powerful tool for the semiclassical calculation of tunneling splittings [13]. The informational content of a  $D \times D$  time signal is increased roughly by a factor of  $D$  as compared to a  $1 \times 1$  signal. Here we demonstrate that the required amount of periodic orbits can be significantly reduced when a cross-correlated periodic orbit sum (signal) is inverted instead of a single periodic orbit sum. The power of the method is demonstrated for the circle billiard, as an example of a completely integrable system.

Consider a quantum Hamiltonian  $\hat{H}$  whose eigenvalues are  $w_n$  and eigenstates  $|n\rangle$ . We introduce a set of  $D$  smooth

and linearly independent operators (there is no need to choose commuting observables) and define a non-trace-type cross-correlated function [14]

$$g_{\alpha\alpha'}(w) = \sum_n \frac{b_{\alpha n} b_{\alpha' n}}{w - w_n + i\epsilon}, \quad (1)$$

where  $b_{\alpha n}$  and  $b_{\alpha' n}$  are the diagonal matrix elements of operators  $\hat{A}_\alpha$  and  $\hat{A}_{\alpha'}$ , respectively, i.e.,

$$b_{\alpha n} = \langle n | \hat{A}_\alpha | n \rangle. \quad (2)$$

Note that Eq. (1) can only be written as a trace formula,

$$g_{\alpha\alpha'}(w) = \text{tr} \{ \hat{A}_\alpha \hat{G}^+(w) \hat{A}_{\alpha'} \},$$

with the Green function  $\hat{G}^+(w) = (w - \hat{H} + i\epsilon)^{-1}$ , if either  $\hat{A}_\alpha$  or  $\hat{A}_{\alpha'}$  commutes with  $\hat{H}$  [14]. The weighted density of states is given by

$$\varrho_{\alpha\alpha'}(w) = -\frac{1}{\pi} \text{Im} g_{\alpha\alpha'}(w). \quad (3)$$

Until recently the periodic orbit quantization would involve the use of periodic orbit expressions for functions  $g_{\alpha\alpha'}(w)$  similar to that in Eq. (1). The problem one would then encounter when trying to extract the semiclassical eigenenergies (poles) is that of the analytic continuation of  $g_{\alpha\alpha'}^{\text{sc}}(w)$  to the real axis, where the latter diverges. A general procedure proposed in Refs. [7,8] introduced aspects of signal processing into the solution of this problem. It was suggested to perform a spectral analysis (harmonic inversion) of a “time” (more precisely, action  $s$ ) signal constructed of the same set of periodic orbits. Here we extend the harmonic inversion procedure of Refs. [7,8] to the analysis of a semiclassical cross-correlation signal

$$C_{\alpha\alpha'}(s) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} g_{\alpha\alpha'}(w) e^{-isw} dw, \quad (4)$$

defined as the Fourier transform of  $g_{\alpha\alpha'}(w)$ . When applied to the quantum expression (1), this yields

$$C_{\alpha\alpha'}(s) = -i \sum_n b_{\alpha n} b_{\alpha' n} e^{-i w_n s}. \quad (5)$$

Let us assume that  $C_{\alpha\alpha'}(s)$  is given, and the spectral parameters (e.g.,  $w_n$  and  $d_{\alpha\alpha',n} = b_{\alpha n} b_{\alpha' n}$ ) are to be extracted. This can be done by solving the conventional harmonic inversion problem [9,10], which is formulated as a nonlinear fit of the signal  $C(s)$  by the sum of sinusoidal terms,

$$C(s) = \sum_n d_n e^{-i s w_n}, \quad (6)$$

with the set of, in general, complex variational parameters  $\{w_n, d_n\}$ . Simple information theoretical considerations [10,8] then yield an estimate for the required signal length,  $s_{\max} \sim 4\pi\bar{\varrho}(w)$ , for poles  $w_n \leq w$  which can be extracted by this method. When a periodic orbit approximation of the quantum signal  $C(s)$  is used, this estimate results sometimes in a very unfavorable scaling because of a rapid (exponential for chaotic systems) proliferation of periodic orbits with increasing period.

Consider a generalized harmonic inversion problem, which assumes that the whole  $s$ -dependent  $D \times D$  signal  $C_{\alpha\alpha'}(s)$  is adjusted simultaneously to the form of Eq. (5), with  $b_{\alpha n}$  and  $w_n$  being the variational parameters. The advantage of using the cross-correlation approach [9,11,12] is based on the simple argument that the total amount of independent information contained in the  $D \times D$  signal is  $D(D+1)$  multiplied by the length of the signal, while the total number of unknowns (here  $b_{\alpha n}$  and  $w_n$ ) is  $(D+1)$  times the total number of poles  $w_n$ . Therefore the informational content of the  $D \times D$  signal per unknown parameter is increased [compared to the case of Eq. (6)] by a factor of  $D$ . (Of course, this scaling holds only approximately and for sufficiently small numbers  $D$  of operators  $\hat{A}_\alpha$  chosen.)

The calculation of a semiclassical approximation to  $C_{\alpha\alpha'}(s)$  is significantly simplified for systems with a scaling property, i.e., where the shape of periodic orbits does not depend on the scaling parameter  $w$  and the classical action scales as  $S_{\text{PO}} = w s_{\text{PO}}$ . For the identity operator  $\hat{A}_1 = I$  the element  $C_{11}^{\text{sc}}(s)$  is the Fourier transform of Gutzwiller's trace formula [2,3] for chaotic systems, and of the Berry-Tabor formula [1] for regular systems, i.e. (see Refs. [7,8]),

$$C_{11}^{\text{sc}}(s) = \sum_{\text{PO}} \mathcal{A}_{\text{PO}} \delta(s - s_{\text{PO}}), \quad (7)$$

where  $s_{\text{PO}}$  are the periods of the orbits and  $\mathcal{A}_{\text{PO}}$  the amplitudes (recurrence strengths) of the periodic orbit contributions including phase information. For  $\hat{A}_1 = I$  and an arbitrary smooth operator  $\hat{A}_\alpha$  the elements  $C_{\alpha 1}^{\text{sc}}(s)$  are obtained from a semiclassical approximation to the generalized trace formula  $\text{tr}\{\hat{G}^+ \hat{A}_\alpha\}$  [15,8]. The result is that the amplitudes  $\mathcal{A}_{\text{PO}}$  in Eq. (7) have to be multiplied by the classical average of the observable  $A_\alpha$  along the periodic orbit,

$$a_{\alpha, \text{PO}} = \frac{1}{s_{\text{PO}}} \int_0^{s_{\text{PO}}} A_\alpha(\mathbf{q}(s), \mathbf{p}(s)) ds, \quad (8)$$

with  $A_\alpha(\mathbf{q}, \mathbf{p})$  the Wigner transform of the operator  $\hat{A}_\alpha$ . The problem of finding a semiclassical approximation to Eq. (9) for the general case of two arbitrary smooth operators  $\hat{A}_\alpha$  and  $\hat{A}_{\alpha'}$  is investigated in Ref. [14], where numerical evidence is presented that the amplitudes  $\mathcal{A}_{\text{PO}}$  in Eq. (7) have to be multiplied by the product of the classical averages,  $a_{\alpha, \text{PO}} a_{\alpha', \text{PO}}$ , of the two corresponding classical observables, i.e.,

$$C_{\alpha\alpha'}^{\text{sc}}(s) = \sum_{\text{PO}} a_{\alpha, \text{PO}} a_{\alpha', \text{PO}} \mathcal{A}_{\text{PO}} \delta(s - s_{\text{PO}}). \quad (9)$$

We here adopt the results of Ref. [14] and use Eq. (9) as the starting point for the following application of harmonic inversion of cross-correlation functions. Note that all quantities in Eq. (9) are obtained from the classical periodic orbits.

The idea of periodic orbit quantization by harmonic inversion [7,8,11] is to fit the semiclassical functions  $C_{\alpha\alpha'}^{\text{sc}}(s)$  given in a finite range  $0 < s < s_{\max}$  by the functional form of the quantum expression (5). The frequencies of the harmonic inversion analysis are then identified with the semiclassical eigenvalues  $w_n$  and the amplitudes  $b_{\alpha n}$  with the semiclassical approximations to the diagonal matrix elements  $\langle n | \hat{A}_\alpha | n \rangle$ . We will show that for a given number of periodic orbits the accuracy of semiclassical spectra can be significantly improved with the help of the cross-correlation approach, or, alternatively, spectra with similar accuracy can be obtained from a periodic orbit cross-correlation signal with significantly reduced signal length.

Here we only give a qualitative and brief description of the method. The details of the numerical procedure of solving the harmonic inversion problem (6) and the generalized harmonic inversion problem (5) are presented in Refs. [9–12]. The idea is to recast the nonlinear fit problem as a linear algebraic problem [9]. This is done by associating the signal  $C_{\alpha\alpha'}(s)$  (to be inverted) with a time cross-correlation function between an initial state  $\Phi_\alpha$  and a final state  $\Phi_{\alpha'}$ ,

$$C_{\alpha\alpha'}(s) = \langle \Phi_{\alpha'} | e^{-i s \hat{H}_{\text{eff}}} | \Phi_\alpha \rangle, \quad (10)$$

where the fictitious quantum dynamical system is described by an effective Hamiltonian  $\hat{H}_{\text{eff}}$ . The latter is defined implicitly by relating its spectrum to the set of unknown spectral parameters  $w_n$  and  $b_{\alpha n}$ . Diagonalization of  $\hat{H}_{\text{eff}}$  would yield the desired  $w_n$  and  $b_{\alpha n}$ . This is done by introducing an appropriate basis set in which the matrix elements of  $\hat{H}_{\text{eff}}$  are available only in terms of the known signals  $C_{\alpha\alpha'}(s)$ . The Hamiltonian  $\hat{H}_{\text{eff}}$  is assumed to be complex symmetric even in the case of a bound system. This makes the harmonic inversion stable with respect to ‘‘noise’’ due to the imperfections of the semiclassical approximation. The most efficient numerical and practical implementation of the harmonic inversion method with all relevant formulas can be found in Refs. [10–12].

We now demonstrate the method of harmonic inversion of cross-correlated periodic orbit sums for the example of the

circle billiard. This is a regular physical system, and the periodic orbits and their physical quantities can be obtained analytically. We choose this system for the sake of simplicity and it will be evident that the procedure works equally well with more complex systems where periodic orbits have to be searched numerically. The nearest neighbor level statistics of integrable systems is a Poisson distribution, with a high probability for nearly degenerate states, and we will demonstrate the power of our new method by fully resolving those nearly degenerate states. The exact quantum mechanical eigenvalues  $E = \hbar^2 k^2 / 2M$  of the circle billiard are given as zeros of Bessel functions  $J_{|m|}(kR) = 0$ , where  $m$  is the angular momentum quantum number and  $R$ , the radius of the circle. In the following we choose  $R = 1$ . Semiclassical eigenvalues can be obtained by an EBK (Einstein-Brillouin-Keller) torus quantization resulting in the quantization condition [16]

$$kR \sqrt{1 - (m/kR)^2} - |m| \arccos \frac{|m|}{kR} = \pi \left( n + \frac{3}{4} \right), \quad (11)$$

with  $m = 0, \pm 1, \pm 2, \dots$  being the angular momentum quantum number and  $n = 0, 1, 2, \dots$  the radial quantum number. States with angular momentum quantum number  $m \neq 0$  are twofold degenerate.

For billiard systems the scaling parameter is the absolute value of the wave vector,  $w \equiv k = |\mathbf{p}|/\hbar$ , and the action is proportional to the length of the orbit,  $S_{\text{PO}} = \hbar k \ell_{\text{PO}}$ . The periodic orbits of the circle billiard are those orbits for which the angle between two bounces is a rational multiple of  $2\pi$ , i.e., the periods  $\ell_{\text{PO}}$  are obtained from the condition

$$\ell_{\text{PO}} = 2m_r \sin \gamma, \quad (12)$$

with  $\gamma \equiv \pi m_\phi / m_r$ ,  $m_\phi = 1, 2, \dots$  the number of turns of the orbit around the origin, and  $m_r = 2m_\phi, 2m_\phi + 1, \dots$  the number of reflections at the boundary of the circle. Periodic orbits with  $m_r \neq 2m_\phi$  can be traversed in two directions and thus have multiplicity 2. To construct a periodic orbit cross-correlation signal  $C_{\alpha\alpha'}^{\text{sc}}(\ell)$ , as defined by Eq. (9), we choose three different operators,  $\hat{A}_1 = I$  the identity,  $\hat{A}_2 = r$  the distance from the origin, and  $\hat{A}_3 = (L/k)^2$  the square of the scaled angular momentum. For these operators the classical weights  $a_{\alpha, \text{PO}}$  [Eq. (8)] are obtained as

$$\begin{aligned} a_{1, \text{PO}} &= 1, \\ a_{2, \text{PO}} &= \frac{1}{2} \left( 1 + \frac{\cos \gamma}{\tan \gamma} \operatorname{arcsinh} \tan \gamma \right), \\ a_{3, \text{PO}} &= \cos^2 \gamma. \end{aligned} \quad (13)$$

The calculation of the weights  $\mathcal{A}_{\text{PO}}$  in Eq. (9) depends on whether the classical dynamics is regular or chaotic. For the circle billiard with regular dynamics we start from the Berry-Tabor formula [1] and obtain

$$\mathcal{A}_{\text{PO}} = \sqrt{\frac{\pi}{2}} \frac{\ell_{\text{PO}}^{3/2}}{m_r^2} e^{-i[(\pi/2)\mu_{\text{PO}} + \pi/4]}, \quad (14)$$

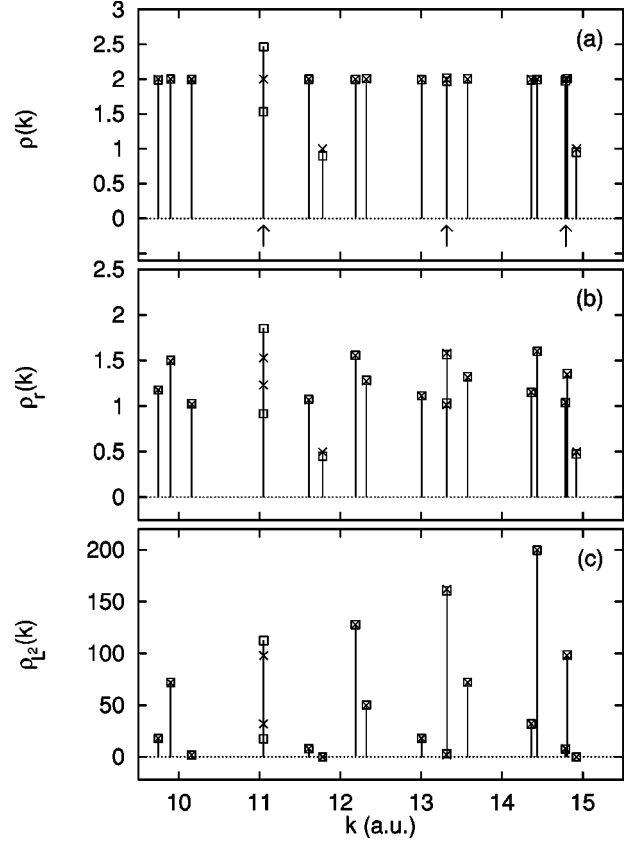


FIG. 1. Density of states weighted with the diagonal matrix elements of the operators (a)  $\hat{A} = I$ , (b)  $\hat{A} = r$ , (c)  $\hat{A} = L^2$  for the circle billiard with radius  $R = 1$  as functions of the wave number  $k = |\mathbf{p}|/\hbar$  (in atomic units). Crosses, EBK eigenvalues and quantum matrix elements. Squares, eigenvalues and matrix elements obtained by harmonic inversion of cross-correlated periodic orbit sums. Three nearly degenerate states are marked by arrows.

where  $\mu_{\text{PO}} = 3m_r$  is the Maslov index. Note that the formalism is directly applicable to chaotic systems with the amplitudes  $\mathcal{A}_{\text{PO}}$  in Eq. (9) computed according to Gutzwiller's trace formula [2,3].

Once all the ingredients of Eq. (9) for the circle billiard are available, the  $3 \times 3$  periodic orbit cross-correlation signal  $C_{\alpha\alpha'}^{\text{sc}}(\ell)$  can easily be constructed and inverted by the generalized filter-diagonalization method. Results obtained from the periodic orbits with maximum length  $s_{\text{max}} = 100$  are presented in Fig. 1. Figure 1(a) is part of the density of states,  $\varrho(k)$ , and Figs. 1(b) and 1(c) are the density of states weighted with the diagonal matrix elements of the operators  $\hat{A} = r$  and  $\hat{A} = L^2$ , respectively. The squares are the results from the harmonic inversion of the periodic orbit cross-correlation signals. For comparison the crosses mark the matrix elements obtained by exact quantum calculations at positions  $k^{\text{EBK}}$  obtained from the EBK quantization condition (11). We do not compare with the exact zeros of the Bessel functions because Eq. (9) is correct only to first order in  $\hbar$  and thus the harmonic inversion of  $C_{\alpha\alpha'}^{\text{sc}}(s)$  cannot provide the exact quantum mechanical eigenvalues. A discussion of the semiclassical accuracy can be found in [16], and higher order  $\hbar$  corrections to the periodic orbit sum are considered in [17]. However, the perfect agreement between the eigen-

TABLE I. Nearly degenerate semiclassical states of the circle billiard.  $k^{\text{EBK}}$ , results from EBK quantization.  $k^{\text{HI}}$ , eigenvalues obtained by harmonic inversion of cross-correlated periodic orbit sums. States are labeled by the radial and angular momentum quantum numbers  $(n, m)$ .

$n$	$m$	$k^{\text{EBK}}$	$k^{\text{HI}}$
1	4	11.048664	11.048569
0	7	11.049268	11.049239
3	1	13.314197	13.314216
0	9	13.315852	13.315869
3	2	14.787105	14.787036
1	7	14.805435	14.805345
1	11	19.599795	19.599863
5	1	19.609451	19.608981
1	15	24.252501	24.252721
6	2	24.264873	24.264887

values  $k^{\text{HI}}$  obtained by harmonic inversion and the EBK eigenvalues  $k^{\text{EBK}}$  is remarkable, and this is even true for nearly degenerate states marked by arrows in Fig. 1(a). The eigenvalues of some nearly degenerate states are presented in Table I. It is important to emphasize that these states with level splittings of, e.g.,  $\Delta k = 6 \times 10^{-4}$  cannot be resolved by the originally proposed method of periodic orbit quantization by harmonic inversion [7,8] with a periodic orbit signal length  $s_{\text{max}} = 100$ . To resolve the two levels at  $k \approx 11.049$  (see Table I) a signal length of at least  $s_{\text{max}} \approx 500$  is required if a single periodic orbit function  $C^{\text{sc}}(s)$  is used instead of a cross-correlation function. The method presented in this paper can therefore be used to significantly reduce the required signal length and thus the required number of periodic orbits for periodic orbit quantization by harmonic inversion. As

such the part of the spectrum shown in Fig. 1 can even be resolved, despite the splittings of the nearly degenerate states marked by the arrows, from a short cross-correlation signal with  $s_{\text{max}} = 30$ , which is about the Heisenberg period  $s_H = 2\pi\bar{Q}(k)$ , i.e., half of the signal length required for the harmonic inversion of a  $1 \times 1$  signal [8]. The reduction of the signal length is especially important if the periodic orbit parameters are not given analytically, as in our example of the circle billiard, but must be obtained from a numerical periodic orbit search. Note also that the density of periodic orbits increases with the period and in chaotic systems the proliferation of periodic orbits is exponential. How small can  $s_{\text{max}}$  get as one uses more and more operators in the method? It might be that half of the Heisenberg period is a fundamental barrier for bound systems with chaotic dynamics in analogy to the Riemann-Siegel formula [6] while for regular systems an even further reduction of the signal length should in principle be possible. However, further investigations are necessary to clarify this point.

In conclusion, we have introduced a method of periodic orbit quantization and calculation of diagonal matrix elements based on the construction of a cross-correlated periodic orbit sum followed by its harmonic inversion. The method is not restricted to bound regular systems but is universal and can be applied to open and chaotic systems as well. It opens the way to reducing the required signal lengths to shorter than the Heisenberg time and therefore significantly reduces the number of orbits required for periodic orbit quantization by harmonic inversion.

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