$\hbar$ expansion for the periodic orbit quantization by harmonic inversion

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(Received 3 March 1998)

Semiclassical spectra beyond the Gutzwiller and Berry-Tabor approximation for chaotic and regular systems, respectively, are obtained by harmonic inversion of the $\hbar$ expansion of the periodic orbit signal. The method is illustrated for the circle billiard, where the semiclassical error is reduced by one to several orders of magnitude with respect to the lowest order approximation used previously. [S1063-651X(98)13410-4]

PACS number(s): 05.45.+b, 03.65.Sq

Semiclassical spectra can be obtained for both regular and chaotic systems in terms of the periodic orbits of the system. For chaotic dynamics the semiclassical trace formula was derived by Gutzwiller [1,2], and for integrable systems the Berry-Tabor formula [3] is well known to be precisely equivalent to the Einstein-Brillouin-Keller (EBK) torus quantization [4]. However, the semiclassical trace formulas are exact only in exceptional cases, e.g., the geodesic motion on the constant negative curvature surface. In general they are just the leading order terms of an infinite series in powers of the Planck constant and the accuracy of semiclassical quantization is still an object of intense investigation [5–7]. Methods for the calculation of the higher order periodic orbit contributions were developed in [8–10]. However, the $\hbar$ expansion of the periodic orbit sum does not solve the general problem of the construction of the analytic continuation of the trace formula. The semiclassical trace formula usually does not converge in the physically interesting region even when only the leading order terms in $\hbar$ are considered, and special techniques are necessary to overcome the convergence problems [11–13]. Up to now the $\hbar$ expansion for periodic orbit quantization is restricted to systems with known symbolic dynamics, like the three disk scattering problem, where cycle expansion techniques can be applied [9,10].

Recently the *harmonic inversion* technique [14,15] was proposed as a universal method for periodic orbit quantization [16,17], which allows the analytic continuation of the non-convergent periodic orbit sum to the region where the semiclassical eigenvalues and resonances are located. The power of this method was demonstrated by its wide applicability to open and bound systems with both regular and chaotic classical dynamics. However, the method was restricted to the conventional lowest order $\hbar$ approximation of the periodic orbit sum, i.e., it cannot be applied straightforwardly to the $\hbar$ expansion of the periodic orbit sum. In this paper we overcome these problems and extend the method of periodic orbit quantization by harmonic inversion to the analysis of the $\hbar$ expansion of the periodic orbit sum. When applied to the circle billiard, as a first example, the accuracy of semiclassical eigenvalues is improved by at least one to several orders of magnitude. The method can be applied to a large variety of systems, i.e., it is not restricted to problems which can be solved with cycle expansion techniques.

As previously [16] we consider systems with a scaling property, i.e., where the shape of periodic orbits (PO) does not depend on the scaling parameter w and the classical action S_{PO} scales as

$$S_{PO}=ws_{PO}\,. \tag{1}$$

The scaling parameter plays the role of an inverse effective Planck constant, i.e., $w\equiv\hbar_{\rm eff}^{-1}$, and the $\hbar$ expansion of the periodic orbit sum can therefore be written as a power series in w^{-1}. The semiclassical spectrum is given by

$$\varrho(w)=-\frac{1}{\pi}\mathrm{Im}\,g(w), \tag{2}$$

with

$$g(w)=\sum_{n=0}^{\infty}g_n(w)=\sum_{n=0}^{\infty}\frac{1}{w^n}\sum_{PO}\mathcal{A}_{PO}^{(n)}e^{is_{PO}w} \tag{3}$$

the fluctuating part of the semiclassical response function. The $\mathcal{A}_{PO}^{(n)}$ are the complex amplitudes of the nth order periodic orbit contributions including phase information from the Maslov indices. Usually the zeroth order contributions $\mathcal{A}_{PO}^{(0)}$ are considered only. The Fourier transform of the principal periodic orbit sum

$$C_0(s)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}g_0(w)e^{-isw}dw=\sum_{PO}\mathcal{A}_{PO}^{(0)}\delta(s-s_{PO}) \tag{4}$$

is adjusted by application of the *harmonic inversion* technique [16,17] to the functional form of the exact quantum expression

$$C(s)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\sum_k\frac{d_k}{w-w_k+i\epsilon}e^{-iws}dw=-i\sum_k d_ke^{-iw_ks}, \tag{5}$$

with $\{w_k,d_k\}$ the eigenvalues and multiplicities. The frequencies $w_{k,0}$ obtained by harmonic inversion of Eq. (4) are the zeroth order $\hbar$ approximation to the semiclassical eigenvalues. We will now demonstrate how the higher order correction terms to the semiclassical eigenvalues can be extracted from the periodic orbit sum (3). We first remark that the asymptotic expansion (3) of the semiclassical response function suffers, for $n \geqslant 1$, from the singularities at $w=0$, and it is therefore not appropriate to harmonically invert the Fourier transform of Eq. (3), although the Fourier transform formally exists. This means that the method of periodic orbit quantization by harmonic inversion cannot straightforwardly be extended to the $\hbar$ expansion of the periodic orbit sum. Instead we will calculate the correction terms to the semiclassical eigenvalues separately, order by order, as described in the following.

Let us assume that the $(n-1)$st order approximations $w_{k,n-1}$ to the semiclassical eigenvalues are already obtained and the $w_{k,n}$ are to be calculated. The difference between the two subsequent approximations to the quantum mechanical response function reads

$$g_n(w) = \sum_k \left(\frac{d_k}{w - w_{k,n} + i\epsilon} - \frac{d_k}{w - w_{k,n-1} + i\epsilon} \right) \approx \sum_k \frac{d_k \Delta w_{k,n}}{(w - \overline{w}_{k,n} + i\epsilon)^2}, \tag{6}$$

with $\overline{w}_{k,n} = (w_{k,n} + w_{k,n-1})/2$ and $\Delta w_{k,n} = w_{k,n} - w_{k,n-1}$. Integration of Eq. (6) and multiplication by w^n yields

$$\mathcal{G}_n(w) = w^n \int g_n(w)\, dw = \sum_k \frac{-d_k w^n \Delta w_{k,n}}{w - \overline{w}_{k,n} + i\epsilon}, \tag{7}$$

which has the functional form of a quantum mechanical response function but with residues proportional to the nth order corrections $\Delta w_{k,n}$ to the semiclassical eigenvalues. The semiclassical approximation to Eq. (7) is obtained from the term $g_n(w)$ in the periodic orbit sum (3) by integration and multiplication by w^n, i.e.,

$$\mathcal{G}_n(w) = w^n \int g_n(w)\, dw = -i \sum_{PO} \frac{1}{s_{PO}} \mathcal{A}_{PO}^{(n)} e^{i w s_{PO}} + \mathcal{O}\left(\frac{1}{w}\right). \tag{8}$$

We can now Fourier transform both Eqs. (7) and (8), and obtain $(n \geqslant 1)$

$$C_n(s) \equiv \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathcal{G}_n(w) e^{-iws}\, dw = i \sum_k d_k (w_k)^n \Delta w_{k,n} e^{-i w_k s} \tag{9}$$

$$\overset{\text{hi}}{=} -i \sum_{PO} \frac{1}{s_{PO}} \mathcal{A}_{PO}^{(n)} \delta(s - s_{PO}). \tag{10}$$

Equations (9) and (10) are the main result of this paper. They imply that the $\hbar$ expansion of the semiclassical eigenvalues can be obtained, order by order, by harmonic inversion (hi) of the periodic orbit signal in Eq. (10) to the functional form of Eq. (9). The frequencies of the periodic orbit signal (10) are the semiclassical eigenvalues w_k. Note that the accuracy of the semiclassical eigenvalues does not necessarily increase with increasing order n. We indicate this in Eq. (9) by omitting the index n at the eigenvalues w_k. The corrections $\Delta w_{k,n}$ to the eigenvalues are obtained from the *amplitudes*, $d_k(w_k)^n \Delta w_{k,n}$, of the periodic orbit signal.

The method requires as input the periodic orbits of the classical system up to a maximum period (scaled action) $s_{\max}$, determined by the average density of states [16,17]. The amplitudes $\mathcal{A}_{PO}^{(0)}$ are obtained from Gutzwiller's trace formula [1,2] and the Berry-Tabor formula [3] for chaotic and regular systems, respectively. For the next order correction $\mathcal{A}_{PO}^{(1)}$ explicit formulas were derived by Gaspard and Alonso for chaotic systems with smooth potentials [8] and in Refs. [9,10] for billiards. With appropriate modifications [18] the formulas can be used for regular systems as well.

We now demonstrate the $\hbar$ expansion of the periodic orbit sum for the example of the circle billiard. We choose this system mainly for the sake of simplicity, since all the periodic orbits and the relevant physical quantities can be obtained analytically. It will be evident that the procedure works equally well with more complex systems where periodic orbits have to be searched numerically. Furthermore this system has served recently as a showpiece example for solving the fundamental problem of reducing the number of orbits required for periodic orbit quantization [19]. 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 $R=1$. The lowest order semiclassical eigenvalues can be obtained by an EBK torus quantization resulting in the quantization condition [5]

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

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

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, $S_{PO} = \hbar k \ell_{PO}$. The periodic orbits of the circle billiard are those orbits for which the angle between two bounces is a rational multiple of 2π, i.e., the periods ℓ_{PO} are obtained from the condition

$$\ell_{PO} = 2 m_r \sin \gamma, \tag{12}$$

with $\gamma \equiv \pi m_\phi / m_r$, $m_\phi = 1,2, \ldots$ the number of turns of the orbit around the origin, and $m_r = 2m_\phi, 2m_\phi + 1, \ldots$ 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. As mentioned before the calculation of the zeroth order amplitudes $\mathcal{A}_{PO}^{(0)}$ in Eq. (3) depends on whether the classical dynamics is regular or chaotic. For the circle billiard with regular dynamics we start from the Berry-Tabor formula [3] and obtain

$$\mathcal{A}_{PO}^{(0)} = \sqrt{\frac{\pi}{2}} \frac{\ell_{PO}^{3/2}}{m_r^2} e^{-i[(\pi/2)\mu_{PO} + \pi/4]}, \tag{13}$$

where $\mu_{PO} = 3m_r$ is the Maslov index. [Note that the factor w^{-n} in Eq. (3) must be replaced by $w^{-(n-1/2)}$ for the regular circle billiard.] For the calculation of the first order periodic

TABLE I. The 20 lowest eigenstates of the circle billiard with radius $R=1$. n,m: Radial and angular momentum quantum numbers; $k^{\rm EBK}$: Results from EBK quantization; $k^{(0)}$: Eigenvalues obtained by harmonic inversion of the periodic orbit signal without $\hbar$ corrections (nearly degenerate states marked by asterisks are not fully resolved); $k^{(1)}$: Eigenvalues obtained by harmonic inversion of the periodic orbit signal including $\hbar$ correction; $k^{\rm ex}$: Exact eigenvalues, i.e., zeros of the Bessel functions $J_m(kR)=0$.

n	m	$k^{\rm EBK}$	$k^{(0)}$	$k^{(1)}$	$k^{\rm ex}$
0	0	2.356194	2.356187	2.409239	2.404826
0	1	3.794440	3.794430	3.834226	3.831706
0	2	5.100386	5.100379	5.138108	5.135622
1	0	5.497787	5.497782	5.520501	5.520078
0	3	6.345186	6.345180	6.382687	6.380162
1	1	6.997002	6.996999	7.015857	7.015587
0	4	7.553060	7.553053	7.590944	7.588342
1	2	8.400144	8.400140	8.417477	8.417244
2	0	8.639380	8.639370	8.653839	8.653728
0	5	8.735670	8.735652	8.774088	8.771484
1	3	9.744628	9.744619	9.761243	9.761023
0	6	9.899671	9.899663	9.938844	9.936110
2	1	10.160928	10.160925	10.173526	10.173468
1	4	11.048664	11.048966*	11.077169*	11.064709
0	7	11.049268	11.048966*	11.077169*	11.086370
2	2	11.608251	11.608248	11.619883	11.619841
3	0	11.780972	11.780968	11.791546	11.791534
0	8	12.187316	12.187318	12.228099	12.225092
1	5	12.322723	12.322717	12.338791	12.338604
2	3	13.004166	13.004163	13.015235	13.015201

orbit contribution $g_1(w)$ in Eq. (3) we adopt the method of Alonso and Gaspard [9] and obtain the first order periodic orbit amplitudes

$$\mathcal{A}_{PO}^{(1)}=\sqrt{\pi m_r}\frac{5-2\sin^2\gamma}{6\sqrt{\sin^3\gamma}}e^{-i[(\pi/2)\mu_{PO}-\pi/4]}. \qquad (14)$$

We plan to give a detailed derivation of Eq. (14) elsewhere [18]. With the periodic orbit amplitudes, Eqs. (13) and (14), at hand we have all the ingredients necessary for the harmonic inversion of the zeroth and first order periodic orbit signal. For the technical details of the harmonic inversion technique see Refs. [14,15,17]. We considered periodic orbits up to maximum length $\ell_{\rm max}=200$, which was sufficient to resolve the low lying states, despite a few near degeneracies. The zeroth order semiclassical approximations $k^{(0)}$ to the eigenvalues are obtained by harmonic inversion of the signal $C_0(s)$ [Eq. (4)], and are presented in Table I. They agree (despite the near degenerate states at $k\approx 11.05$ marked by asterisks) within the numerical accuracy with the results of the torus quantization, Eq. (11) (see eigenvalues $k^{\rm EBK}$ in Table I). However, the semiclassical eigenvalues deviate significantly, especially for states with low radial quantum numbers n, from the exact quantum mechanical eigenvalues $k^{\rm ex}$ in Table I.

The first order corrections to the semiclassical eigenvalues $k^{(0)}$ are obtained by harmonic inversion of the periodic orbit signal $C_1(s)$ [Eq. (10)]. The resulting spectrum, i.e., the

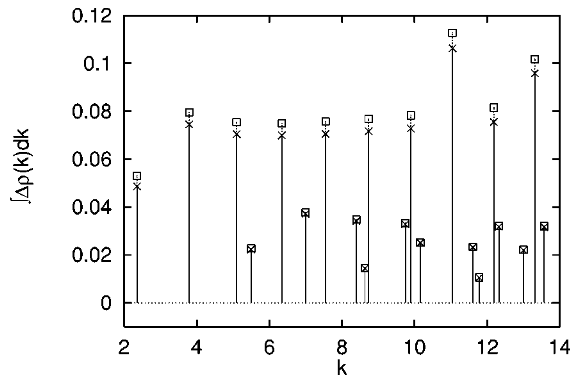

FIG. 1. Integrated difference of the density of states, $\int\Delta\varrho(k)dk$, for the circle billiard with radius $R=1$. Crosses: $\Delta\varrho(k)=\varrho^{\rm ex}(k)-\varrho^{\rm EBK}(k)$. Squares: $\Delta\varrho(k)=\varrho^{(1)}(k)-\varrho^{(0)}(k)$ obtained from the $\hbar$ expansion of the periodic orbit signal.

integrated differences of the density of states $\int\Delta\varrho(k)dk$, are shown in Fig. 1. The squares mark the spectrum for $\Delta\varrho(k)=\varrho^{(1)}(k)-\varrho^{(0)}(k)$ obtained from the harmonic inversion of the signal $C_1(s)$. For comparison the crosses present the same spectrum but for the difference $\Delta\varrho(k)=\varrho^{\rm ex}(k)-\varrho^{\rm EBK}(k)$ between the exact quantum mechanical and the EBK spectrum. The deviations between the peak heights exhibit the contributions of terms of the $\hbar$ expansion series beyond the first order approximation.

The peak heights of the levels in Fig. 1 (dashed lines and squares) are, up to a multiplicity factor for the degenerate states, the shifts Δk between the zeroth and first order semiclassical approximations to the eigenvalues k. The first order eigenvalues $k^{(1)}=k^{(0)}+\Delta k$ are presented in Table I, and are in excellent agreement with the exact eigenvalues $k^{\rm ex}$. An appropriate measure for the accuracy of semiclassical eigenvalues is the deviation from the exact quantum eigenvalues in units of the average level spacings, $\langle\Delta k\rangle_{\rm av}=1/\overline{\varrho}(k)$. Figure 2 presents the semiclassical error in units of the average level spacings $\langle\Delta k\rangle_{\rm av}\approx 4/k$ for the zeroth order (diamonds) and first order (crosses) approximations to the eigenvalues. States are labeled by the radial and angular momentum quantum numbers (n,m). In the zeroth order approximation the semiclassical error for the low lying states is about 3–10% of the mean level spacing. This error is reduced in the first order

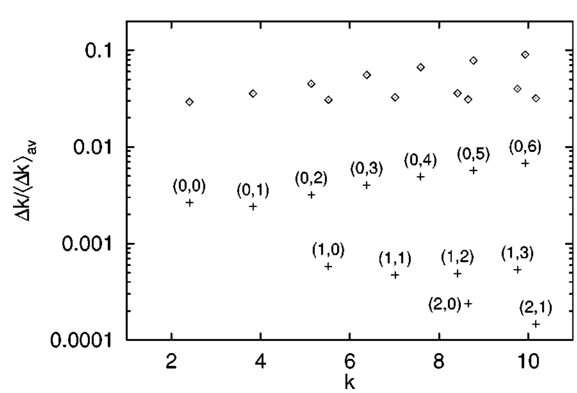

FIG. 2. Semiclassical error $|k^{(0)}-k^{\rm ex}|$ (diamonds) and $|k^{(1)}-k^{\rm ex}|$ (crosses) in units of the average level spacing $\langle\Delta k\rangle_{\rm av}\approx 4/k$. States are labeled by quantum numbers (n,m).

approximation by at least one order of magnitude for the least semiclassical states with radial quantum number $n=0$. The accuracy of states with $n \geqslant 1$ is improved by two or more orders of magnitude.

As mentioned above the general technique developed in this paper is not restricted to the circle billiard but can in general be applied to the whole variety of systems which can be quantized semiclassically by harmonic inversion of the periodic orbit sum. While for the circle billiard the periodic orbit parameters can be calculated analytically the orbits must be obtained from a numerical periodic orbit search in general. However, no additional periodic orbits need to be searched for the $\hbar$ expansion of the periodic orbit sum, i.e., it is sufficient to calculate the amplitudes in Eq. (3) for the given set of orbits as described in Refs. [8–10].

In conclusion, we have demonstrated that semiclassical spectra beyond the Gutzwiller and Berry-Tabor approximation can be obtained by harmonic inversion of the $\hbar$ expansion of the periodic orbit signal. For the circle billiard, as a first example, the semiclassical error is reduced by at least one to several orders of magnitude by just including the lowest order periodic orbit correction terms. The method proposed in this paper opens the way to the calculation of high precision semiclassical eigenvalues directly from periodic orbit data for both regular and chaotic systems. It is not restricted to bound systems but can be applied to open systems as well.

This work was supported by the Deutsche Forschungsgemeinschaft (Sonderforschungsbereich No. 237).

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