Amplitude ordering of the trace formula for the two-particle disk billiard

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For the periodic orbit quantization of a system of particles confined in a two-dimensional disk billiard, the proliferation of multiparticle periodic orbits with length precludes standard length truncation of the trace formula and alternative truncation schemes are necessary. An amplitude ordering of the single-particle periodic orbits reveals a quantum-classical correspondence for the angular momentum of a particle in the disk which is useful for the quantization of all the low energy states of the multiparticle problem. We explicitly show that a simple amplitude truncation of the trace formula better approximates the semiclassical density of states and in particular resolves closely spaced levels that are otherwise unresolved using the standard approach.

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Semiclassical trace formulas are Fourier expansions of the oscillating density of states expressed in terms of classical periodic orbits [1]. The great appeal of using such expansions is that the gross shell structure of many finite systems can be reproduced using only a few of the shortest orbits [2]. Full quantization, on the other hand, is generally difficult and one has to include many orbits before one obtains a good approximation to the exact result. In such cases, the convergence of these periodic orbit expansions is a central issue in semiclassical mechanics.

In integrable systems, there is also the fundamental problem of near degeneracies since the level spacing distribution has a Poisson character [3]. To achieve a sufficient resolution in energy space, one has to include contributions from orbits with very large actions. This problem is most evident in noninteracting multibody systems where the combination of independent spectra leads to many near degeneracies even at low energies. In a recent paper [4], we performed the periodic orbit quantization of the two-particle disk billiard and found a few closely spaced low-lying levels that could not be resolved using millions of two-particle periodic orbits. The convergence of the trace formula became an important consideration and this motivated the current study since we wanted to explicitly resolve these levels.

The periodic orbit quantization of the one-particle disk billiard and its convergence have been studied in Ref. [5]. Although an exact trace formula is known for the one-particle disk billiard, there remains the question of how to truncate the series most effectively [2]. The standard procedure is to specify a length cutoff $L_{\max}$ and use an ordered *subset* of the shorter orbits [5,2]. To resolve nearly degenerate levels using this scheme, one has to use a sufficiently large $L_{\max}$. For the multibody situation, this is highly impractical. The essential difficulty is that the number of multibody periodic orbits with length $L<L_{\max}$ grows rapidly with additional degrees of freedom. If one is interested in reproducing a specific set of levels, it becomes crucial to have more judicious selection criteria for choosing which orbits to include in the expansions.

In this Brief Report, we explore the convergence of the trace formula for the one- and two-particle disk billiard using an ''amplitude ordering'' technique similar to the stability ordering of cycle expansions [6,7] studied for nonintegrable systems in Refs. [8,9]. The authors of Ref. [8] use the magnitude of the terms in an expansion for their ordering scheme. Similarly, we will use only orbits whose amplitude exceeds some prescribed threshold. An immediate benefit is the possibility of more significant periodic orbit contributions at comparatively larger lengths. Since our goal is to resolve near degeneracies, this seems to be a more optimal strategy since it is the longer orbits that are responsible for short-range oscillations in the density of states. We now make this prescription more precise.

We first examine the one-particle disk billiard. Recall that the semiclassical single-particle density of states is given by [2]

$$\rho_1^{\mathrm{sc}}(k)=\overline{\rho_1}(k)+\tilde{\rho}_1(k), \tag{1}$$

where the first term is a smooth function of k arising from zero-length orbits and the second term is oscillatory in k and arises from a sum over topologically distinct families of periodic orbits. The periodic orbit families of the disk may be classified by two integers (v,w) where v is the number of vertices and w is the winding number around the center. The length of an orbit is then $L_{vw}=2vR\sin(\pi w/v)$. Using this notation, the trace formula for the oscillating part of the density of states is [5,2] ($\hbar^2/2m\equiv 1$)

$$\tilde{\rho}_1(k)=2\sqrt{\frac{kR^3}{\pi}}\sum_{vw} d_{vw}\mathcal{A}(v,w)\cos\left(kL_{vw}-3v\,\frac{\pi}{2}+\frac{\pi}{4}\right), \tag{2}$$

where the amplitude

$$\mathcal{A}(v,w)=\frac{\sin^{3/2}(\pi w/v)}{\sqrt{v}}=\frac{(L_{vw}/2R)^{3/2}}{v^2}. \tag{3}$$

The sum goes from $w=1,\ldots,\infty$ and $v=2w,\ldots,\infty$ and the degeneracy factor d_{vw}, which accounts for negative windings, is 1 for $v=2w$ and 2 for $v>2w$. Any numerical evaluation of Eq. (2) involves computing the contributions from a finite set of orbits. Since different sets will generate different results, the basic question is how to choose the best set. This depends on which specific quantum states one is interested in reproducing. The problem is that knowledge of which set of

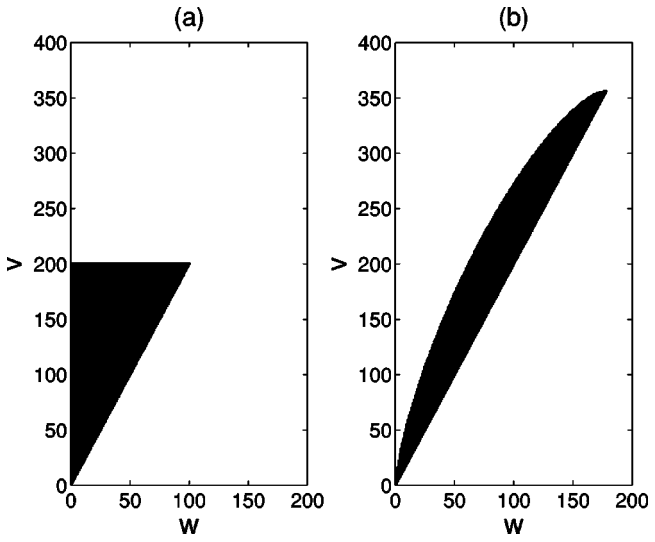

FIG. 1. The positive-winding single-particle orbits (v,w) used by the two different truncation procedures. (a) The orbits used in a standard truncation of the sum in Eq. (2) with $w_{\max}=100$, $v_{\max}=200$. (b) The set of orbits that satisfy $\mathcal{A}(v,w)>\varepsilon=0.052\,987\,25$. In each case, $N_+=10^4$.

orbits best reproduces these states is usually not available in advance and so one starts with the simplest truncation procedures.

In the following analysis, there will be three important parameters: N_+, the total number of positive-winding orbits (which indicates the computational effort involved); N_S, the total number of periodic orbits used by the standard truncation (ST) procedure; and N_A, the total number of periodic orbits used by the amplitude truncation (AT) procedure. The latter two quantities include degeneracies due to negative-winding orbits.

Suppose we use $N_+=10^4$ orbits. The most natural way [5,2] to truncate the sum in Eq. (2) is to use *only* orbits that have $w\leqslant w_{\max}=100$ and $v\leqslant v_{\max}=2w_{\max}=200$ [Fig. 1(a)]. In general, specifying $(v_{\max},w_{\max})$ determines the length of the longest orbit used in the truncated sum, $L_{\max}=2v_{\max}R$. It is important to note that one has not used all orbits that have a length $L\leqslant L_{\max}$. In fact, there is a countably infinite set of shorter periodic orbits. Nonetheless, all of the orbits that are used ($N_S=1.99\times10^4$) are shorter than $L_{\max}=400R$. In this sense, specifying $(v_{\max},w_{\max})$ is equivalent to specifying a length cutoff $L_{\max}$.

Alternatively, an amplitude truncation uses only those orbits for which $\mathcal{A}(v,w)>\varepsilon$, for some prescribed value of ε. Specifying ε determines the maximum winding number: $w_{\max}=[1/2\varepsilon^2]$. For each value of $w\leqslant w_{\max}$, one sweeps through the values of $v\geqslant 2w$ until the amplitude falls below ε. If $\varepsilon=0.052\,987\,25$, then precisely $N_+=10^4$ orbits ($N_A=1.9822\times10^4$) satisfy $\mathcal{A}(v,w)>\varepsilon$. These orbits are plotted in Fig. 1(b). We note that the significance of ε is that it can be varied to give the same number of orbits as the standard set. This allows us to directly compare the convergence of the two methods. One would expect amplitude truncation to have better convergence since one is using the most important terms in the sum. We now check this conjecture by

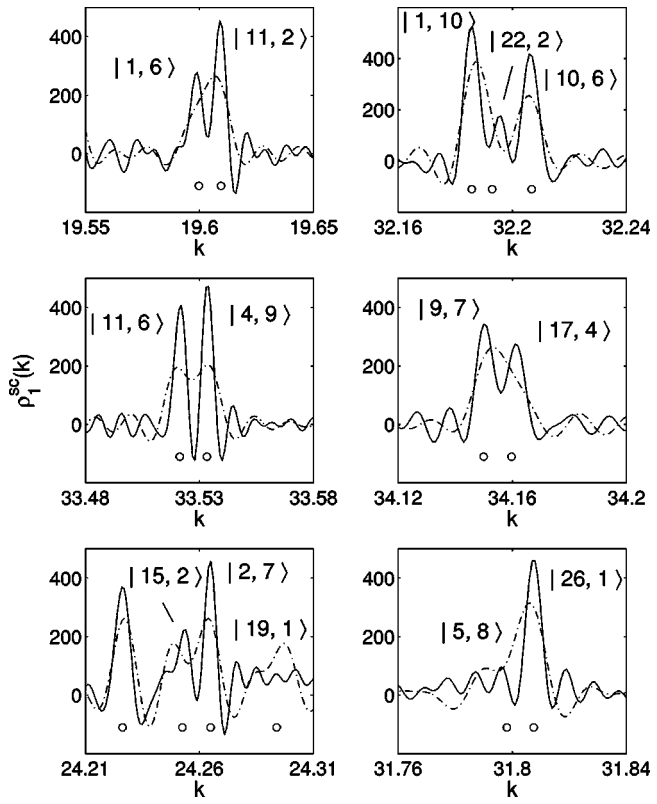

FIG. 2. The semiclassical single-particle density of states computed using the two different sets of orbits in Fig. 1. The dash-dotted line uses standard length truncation [Fig. 1(a)] and the solid line uses amplitude truncation [Fig. 1(b)]. Peaks correspond to the quantum states $|m,n\rangle$ indicated and circles denote the positions of single-particle levels obtained from torus quantization. Notice that away from peaks the two methods are generally out of phase because the set of orbits that are interfering is different in the two cases.

evaluating the trace formula (2) using these two different sets of orbits. Before presenting the results, we point out an interesting observation.

Inspection of Fig. 1 reveals a surprising result: amplitude truncation typically excludes many of the shorter orbits used in standard truncation. A common view, which is stressed in Ref. [2], is that for a low resolution of $\tilde{\rho}_1$, ''only those orbits with the smallest actions (lengths) and *simultaneously* the largest amplitudes in the Fourier decomposition of $\tilde{\rho}_1$ are important.'' This statement does not seem to apply to the amplitudes of the disk. While it is true that the shortest few orbits have the largest amplitudes, it is not generally true that shorter orbits are more important than longer orbits.

Comparing the two methods, we observe that levels with small azimuthal quantum number ($m\leqslant 5$) are more resolved using amplitude truncation. For states with higher azimuthal quantum numbers ($m\geqslant 6$), the convergence depends on the radial quantum number n; ST is better for $n\leqslant 2$, but AT is better for $n>2$. Some generic examples involving closely spaced levels are shown in Fig. 2. By ''closely spaced,'' we mean levels that have a spacing $\Delta k\ll\overline{\Delta k}$, where $\overline{\Delta k}=0.2190$ is the average level spacing for wave numbers $k<k_{\max}=35$. For the levels shown in Fig. 2, it is obvious

which method gives better resolution. In general, any level is ''more resolved'' if the peak is a better approximation to the exact result, which is a δ-function spike. In particular, the convergence of the two methods for single levels k_i (which have the property $|k_{i\pm1}-k_i|>2\overline{\Delta k}$) can be checked numerically by computing moments for each peak and comparing with the exact result.

The semiclassical approximation $S_{vw}\gg\hbar\sim kL_{vw}\gg1$ implies that both methods should improve with increasing energy. Since amplitude truncation also uses longer orbits, the approximation should be consistently more accurate, but this is not what is observed. The higher angular momentum states with the lowest energies are poorly reproduced by amplitude truncation. To understand these results, we first recognize that states with large angular momentum and small energy are ones for which the particle is furthest from the center of the disk and therefore pushed to the wall of the billiard. To replicate these states, we need to use orbits that mimic this quantum behavior. In other words, we need classical orbits that graze the wall of the billiard. These are precisely the orbits that have many more vertices than windings. AT excludes such orbits and therefore has trouble reproducing the higher-m states with small n. ST does include more of these types of orbits and thus more accurately reproduces these states. As mentioned above, this deficiency of AT for the disk is not observed for fixed m as n increases (i.e., as the energy increases). We summarize this quantum-classical correspondence for the disk billiard as follows: *The high angular momentum states with the smallest energies are reproduced semiclassically by the boundary orbits which have the property* $v\gg w$.

We now discuss the two-particle disk billiard where knowledge of this correspondence is extremely useful. The semiclassical two-particle density of states can be written as [4]

$$\rho_2^{\mathrm{sc}}(k)=(\overline{\rho_1}*\overline{\rho_1})(k)+2(\overline{\rho_1}*\widetilde{\rho}_1)(k)+(\widetilde{\rho}_1*\widetilde{\rho}_1)(k). \quad (4)$$

The formulas for the first two terms can be found in Ref. [4]. Here, we recall only the last term in the decomposition. For the disk,

$$(\widetilde{\rho}_1*\widetilde{\rho}_1)(k)\approx 2\sqrt{\frac{k^3R^5}{\pi}}\sum_{v_aw_a,v_bw_b}\mathcal{A}(v_a,w_a,v_b,w_b)$$

$$d_{v_aw_a}d_{v_bw_b}\cos\left(kL_{ab}-3(v_a+v_b)\frac{\pi}{2}+\frac{\pi}{4}\right), \quad (5)$$

where

$$\mathcal{A}(v_a,w_a,v_b,w_b)=\frac{\sin^2(\pi w_a/v_a)\sin^2(\pi w_b/v_b)}{[v_a^2\sin^2(\pi w_a/v_a)+v_b^2\sin^2(\pi w_b/v_b)]^{3/4}}. \quad (6)$$

As an illustration of the proliferation of periodic orbits that occurs in higher dimensions, we choose a length cutoff $L_{\max}=400R$. In this case, a standard length truncation implies that there are $N_+=10^4$ one-particle periodic orbits to consider in Eq. (2) and $N_+=2.470\,09\times10^7$ two-particle periodic orbits to consider in Eq. (5). In Ref. [4], we calculated the semiclassical two-particle density of states on the interval $0\leqslant k\leqslant10$ using a standard truncation of Eq. (5) ($N_+=6.25\times10^6$) and found four multiplets that could not be resolved. The preceding analysis clearly indicates that for the two-body problem an amplitude truncation is more suitable since most of the two-particle states at lower energies are states for which *each* particle is in a low angular momentum state. We now demonstrate this explicitly.

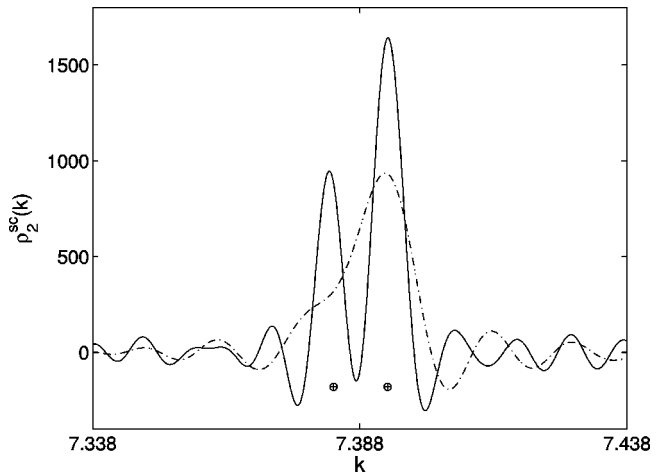

FIG. 3. The semiclassical two-particle density of states [Eq. (4)] computed for $k\in(7.3380,7.4380)$ using $N_+=10^8$ two-particle periodic orbits. The dash-dotted line uses standard length truncation of Eq. (5) ($N_S=3.9601\times10^8$) and the solid line uses amplitude truncation $\mathcal{A}(v_a,w_a,v_b,w_b)>\varepsilon=0.000\,139\,746\,08$ ($N_A=3.914\,883\,65\times10^8$). $\oplus$ symbols indicate the positions of two-particle levels obtained from torus quantization.

As before, specifying ε determines the maximum winding numbers. In this case, the combined winding numbers of each single-particle periodic orbit to be used must satisfy the condition $w_a^2+w_b^2\leqslant[1/4\varepsilon^{4/3}]$. Then, for given winding numbers (w_a,w_b) which satisfy this condition, one sweeps through the allowed values of v_a and v_b until the two-particle amplitude (6) becomes less than ε.

As an example, we consider $N_+=10^8$ two-particle orbits in Eq. (5) for $k\in(7.3380,7.4380)$. In this interval, there should be two multiplets [4], a quartet $\{|0\ 1,\ \pm1\ 2\rangle, |\pm1\ 2,\ 0\ 1\rangle\}$ at $k=7.3831$ and an octet $\{|\pm1\ 1,\ \pm3\ 1\rangle, |\pm3\ 1,\ \pm1\ 1\rangle\}$ at $k=7.3932$. As shown in Fig. 3, ST ($w_{a_{\max}}=w_{b_{\max}}=100, v_{a_{\max}}=v_{b_{\max}}=200$) does not resolve these two multiplets, but AT ($\varepsilon=0.000\,139\,746\,08$) does partially resolve them. We further checked that the two peaks have the correct degeneracies consistent with a quartet and an octet by numerically computing the area under each peak. We find these areas to be 3.91 and 8.6 which have relative errors of 2% and 7%, respectively. This error arises since the two peaks are not fully resolved and decreases as more orbits are included. The area under the large unresolved peak is 12.25 which also has an error of about 2% relative to an unresolved 12-fold degenerate multiplet. We also performed a similar analysis for the other set of unresolved peaks [4] and found comparable results.

We have not mentioned the cross term in Eq. (4). Amplitude truncation of the cross term is not necessary since this contribution involves only a summation over single-particle periodic orbits and hence the computational difficulties associated with the numerical evaluation of the dynamical term Eq. (5) do not arise. Thus, standard length truncation of the cross term suffices. Nonetheless, one has to be very careful to truncate the cross term so that its length cutoff matches that of the dynamical term. For example, a standard truncation of the dynamical term such that ($w_{a_{\max}}=w_{b_{\max}}=50$, $v_{a_{\max}}=v_{b_{\max}}=100$) requires the cross term to be truncated at ($w_{\max}=70$, $v_{\max}=141$) since

$$L_{\max}^{(\mathrm{cross})}=L_{\max}^{(\mathrm{dyn})}\Rightarrow v_{\max}^{(\mathrm{cross})}=\sqrt{2}v_{\max}^{(\mathrm{dyn})}=\sqrt{2}(100)\approx 141.$$

(This point was overlooked in our previous analysis of the disk in Ref. [4]. This has been corrected in the current analysis and does not affect our previous results. We mention it here to emphasize that the two oscillatory terms must be truncated consistently.) The corresponding amplitude truncation of the dynamical term requires the cross term to be truncated at ($w_{\max}=92$, $v_{\max}=184$) since the length of the longest two-particle orbit used by this method is $369R$. The same principle applies to higher dimensions. For example, for the three-particle density of states

$$\rho_3^{\mathrm{sc}}(k)=(\overline{\rho}_1*\overline{\rho}_1*\overline{\rho}_1)(k)+3(\overline{\rho}_1*\overline{\rho}_1*\widetilde{\rho}_1(k)+3(\overline{\rho}_1*\widetilde{\rho}_1*\widetilde{\rho}_1)(k)+(\widetilde{\rho}_1*\widetilde{\rho}_1*\widetilde{\rho}_1)(k), \tag{7}$$

one would use AT for the last two terms and ST for the second term, but all three oscillatory terms must be truncated consistently and the threshold constants for the last two terms must be chosen accordingly.

To summarize, we have shown that amplitude truncation of the trace formula for the disk billiard is more effective than standard length truncation for the quantization of low angular momentum states ($m\leqslant 5$). It is inappropriate for the higher-m states when the radial quantum number $n\leqslant 2$, but quickly improves with increasing energy. The reason for this is the direct correspondence between the classical and quantum angular momenta. This correspondence is useful for the multiparticle problem where it will be more productive to use this tactic to resolve all the low-energy levels since they will arise from the situation where all the particles have small azimuthal quantum numbers. An important result of the analysis is that longer orbits generally possess larger amplitudes, unlike many systems where the shortest orbits play the dominant role [2].

One could also do an analogous study of the three-dimensional spherical billiard [10,2] which has the same periodic orbits. While the amplitudes of the orbits are different for the spherical cavity, they do seem to have the same behavior as in the disk. In Fig. 4 of Ref. [11], one can clearly see that for a given winding w the amplitude decays with v, the number of vertices. However, it is interesting to note that an orbit with an arbitrary large value of v becomes more important as the winding number is increased. We observe the same nontrivial behavior in the disk.

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