Semiclassical Spectra from Periodic-Orbit Clusters in a Mixed Phase Space

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We calculate complete quasienergy spectra (rather than partial information thereon) from classical periodic orbits for the kicked top, throughout the transition from integrability to well-developed chaos. The standard error incurred for the quasienergies is a small percentage of their mean spacing, even though the effective Planck constant is not pushed to small values. The price paid is the inclusion of collective contributions of clusters of periodic orbits near bifurcations into Gutzwiller's trace formula. [S0031-9007(97)03790-3]

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Since Gutzwiller's seminal work [1,2], it is known that the level density of autonomous hyperbolic systems can be semiclassically approximated by a sum of individual contributions from periodic orbits. Similarly, the spectrum of integrable systems may be calculated semiclassically by Einstein-Brillouin-Keller (EBK) quantization. Gutzwiller's result was later extended to periodically driven systems [3,4] whose stroboscopic period-to-period evolution is generated by a unitary Floquet operator F with unimodular eigenvalues $e^{-i\varphi_i}$. The quasienergies φ_i are encoded in the traces $\operatorname{tr} F^n$, $n = 1, 2, \ldots,$ which are approximated as

$$\operatorname{tr} F^n = \sum_{\text{p.o.}}^{\text{period } n} \frac{n_0}{|2 - \operatorname{tr} M|^{1/2}} \exp\left(i\frac{S}{\hbar} - i\frac{\pi}{2}\nu\right) \quad (1)$$

for systems with a single classical degree of freedom. Each period-n orbit provides a summand determined by its primitive period n_0, the action S, the Maslov index ν, and the trace of the linearized map M.

The Gutzwiller type result (1), as well as its corrections to be discussed presently, can be derived from the integral representation

$$\operatorname{tr} F^n = \int \frac{dq'dp}{2\pi\hbar} |S_{q'p}|^{1/2} e^{i/\hbar[S(q',p;n)-q'p]-i(\pi/2)\mu} \quad (2)$$

which involves, besides the Morse index μ, the action $S(q', p; n)$; the latter generates the n-step map $(q, p) \to (q', p')$ through $S_p = q$, $S_{q'} = p'$, where indices on S denote partial derivatives. The stationary-phase approximation leading from the integral (2) to the periodic-orbit sum (1) is sensible if all stationary points are well separated.

Generic systems, however, come with a mixed phase space, where stability islands reside inside a chaotic sea. Upon varying a suitable control parameter, one may observe the transition from regular to predominantly chaotic behavior. We are here concerned with semiclassically evaluating *complete* quasienergy spectra (rather than parts or modulations of such) for such a transition, a goal not previously attained.

The transition in question proceeds as periodic orbits arise, disappear, or coalesce at bifurcations. Meyer [5] has classified the codimension-one variants of such catastrophes, i.e., the ones generically encountered upon varying a single parameter. The simplest type is the tangent bifurcation at which a pair of periodic orbits is born (or disappears for the opposite sense of change of the control parameter). The general cases are period-m bifurcations where a "central" orbit of period l coalesces with satellites of m-fold period $n = ml$. At the bifurcation the nth iterate of the linearized map M is the identity close to the coalescing orbits and gives, for one degree of freedom, the condition $\operatorname{tr} M^n = 2$. Clearly, a tangent bifurcation may be seen as the special case $m = 1$.

As a dynamical system is driven through a sequence of bifurcations towards globally chaotic behavior, the simple Gutzwiller type trace formula (1) ceases to reasonably approximate the integral (2), mostly since different periodic orbits approach one another so closely as to no longer yield independent additive stationary-phase contributions to the integral (2). Right at a bifurcation, individual contributions to $\operatorname{tr} F^n$ even diverge. To construct a "collective" contribution [6] in the neighborhood of a bifurcation, one must approximate the action function S in (2) by a suitable normal form whose stationary points yield the cluster of classical periodic points related to the bifurcation; the ensuing "diffraction catastrophe integral" then constitutes a cluster contribution to the trace $\operatorname{tr} F^n$ in question. For some recent progress with several diffraction integrals relevant for our present study, refer to Refs. [7–10]. Even the breakup of rational tori into chains of intertwined elliptic and hyperbolic periodic orbits in the near integrable case entails a collective correction to the trace formula [11]. Applications of diffraction integrals have previously been restricted to revealing the impact of individual orbit clusters on the quantum propagator, for instance, by "inverse-$\hbar$ spectroscopy" [8,9,11,12], or on modulations of a (weighted) density of states [10].

When periodic orbits disappear as a control parameter passes through a critical value the nonlinear classical map loses a number of real solutions in favor of complex ones. A complex "ghost" orbit has no classical significance but does yield a saddle-point contribution [12] to the integral (2). In the immediate neighborhood of the said bifurcation the ghosts again form (part of) a cluster which

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must be treated by an appropriate diffraction integral; then one obtains a uniform interpolation between the asymptotic behaviors on both sides of the bifurcation, due to saddles for ghosts on one side and stationary phases for real orbits on the other. The best known such case arises for a tangent bifurcation; the diffraction integral there takes the familiar Airy function form [6,12].

A ghost orbit often makes itself felt surprisingly far away from the bifurcation from which it originates, since the imaginary part of its action [which, in principle, entails exponential suppression through the factor $\exp(-\mathrm{Im}\, S/\hbar)$] may decay slowly as one steers the dynamics away from the bifurcation. We, in fact, find that a ghost frequently loses its weight through another mechanism, i.e., the so-called Stokes transition, after which the corresponding saddle of the integrand in (2) can no longer be reached by deforming the original contour of integration to one of steepest descent without crossing a singularity. The transition is encountered when the real parts of the action are identical for a ghost $(-)$ and another "dominant" orbit in its vicinity $(+)$, with $\mathrm{Im}\, S_+ < \mathrm{Im}\, S_-$. The phenomenon has been investigated in [13,14], where a uniform approximation of the suppression factor is given. Incidentally, the Stokes phenomenon also implies that only ghosts with $\mathrm{Im}\, S > 0$ are relevant.

Another surprise will be incurred below, in our search for reliable semiclassical approximations to the traces $\mathrm{tr}\, F^n$: Classically nongeneric bifurcations become important. These have codimension two, i.e., could be located only by controlling two parameters. Even though we shall be concerned with varying but a single parameter and never actually hit such a bifurcation, we do get sufficiently close for collective treatments of all participating orbits to become necessary.

Leaving generalities for the moment we now turn to pursuing our goal for a periodically kicked angular momentum, often referred to as kicked top [15,16]. The angular momentum $\mathbf{J}$ involved has components obeying the usual commutation rules $[J_x, J_y] = iJ_z$, etc. The squared angular momentum $\mathbf{J}^2 = j(j+1)$ is conserved and, with the quantum number $j = \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$ fixed, the Hilbert space is assigned the dimension $2j+1$. That dimension also plays the role of the inverse of Planck's constant such that classical behavior is attained in the limit $j \to \infty$. We shall work here with the particular top whose dynamics is a sequence of rotations by angles p_i alternating with torsions of strength k_i as described by the Floquet operator,

$$F = \exp\left(-ik_z \frac{J_z^2}{2j+1} - ip_z J_z\right)\exp(-ip_y J_y) \times \exp\left(-ik_x \frac{J_x^2}{2j+1} - ip_x J_x\right). \tag{3}$$

The corresponding classical map may be obtained by writing out the stroboscopic dynamics of the rescaled angular momentum vector $\mathbf{X} = \mathbf{J}/(j + 1/2)$ in the Heisenberg picture and then, with the limit $j \to \infty$ in mind, degrading

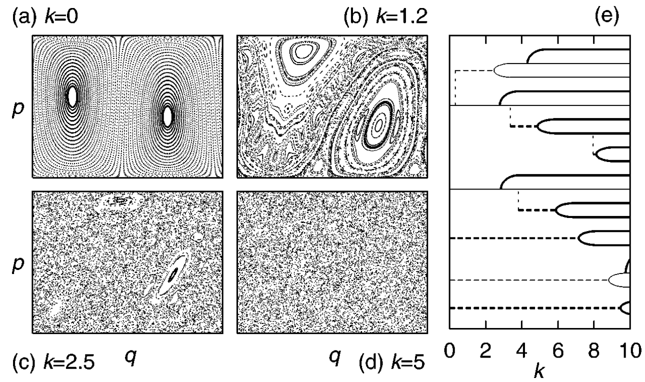

FIG. 1. (a)–(d) phase-space portraits for the kicked top. The spherical phase space is parametrized by the azimuthal angle $\varphi \equiv q$ and the Cartesian coordinate $z \equiv p$. Varying the control parameter k from 0 to 5, the system undergoes the transition from integrability through mixed phase space to well-developed chaos. (e) Bifurcation tree including periodic orbits of period one (thin lines) and two (thick lines). Solid lines are real orbits, dashed lines are ghost solutions with $\mathrm{Im}\, S > 0$. Ghost lines end at Stokes transitions, where vertical lines connect them to the dominant orbit. This is not indicated for strongly suppressed ghosts with large $\mathrm{Im}\, S$.

$\mathbf{X}$ to a c-number vector. The classical phase space is thus revealed as the unit sphere $\mathbf{X}^2 = 1$. The classical stroboscopic map is easily written as the sequence of three rotations, one about the x axis by the angle $p_x + k_x x$, the second by p_y about the y axis, and the last one by $p_z + k_z z$ about the z axis.

We perform a one-parameter study of the top, holding the p_i fixed ($p_x = 0.3$, $p_y = 1.0$, $p_z = 0.8$) while varying the control parameter $k \equiv k_z = 10k_x$ in the range $0 \le k \lesssim 10$. For $k = 0$ we incur a pure linear rotation, and thus classical integrability. Only two primitive periodic orbits then arise, i.e., fixed points located at the intersections of the rotation axis with the unit sphere. For $k = 5$ the phase-space portrait in Fig. 1 displays well-developed chaos.

Bifurcations are found numerically by solving the equation $\mathrm{tr}\, M^m = 2$ simultaneously with $p = p'$, $q = q'$ for the triple (q, p, k). All periodic orbits can be picked up by going through the sequence of bifurcations as k is swept up from zero to its current value. Figure 1(e) displays the bifurcation tree thus obtained, showing twenty orbits of length one and two subsequently used in the evaluation of $\mathrm{tr}\, F^2$ for $0 \le k < 10$.

The divergence of individual contributions at bifurcations is illustrated in Fig. 2(a), which displays the quantum-mechanically exact $\mathrm{tr}\, F^2(k)$ for $j = 3$ together with the sum of individual contributions from real periodic orbits and ghosts, Eq. (1). Stokes transitions are taken into account for those ghosts that are not sufficiently suppressed by having a large imaginary part of the action.

We proceed further to include collective contributions regularizing the behavior close to bifurcations. The broken line in Fig. 2(b) results when one groups the orbits according to the codimension-one bifurcations in which they participate (tangent bifurcations of orbits with primitive period one and two, and period-doubling bifurcations of orbits with period one) and employs the closed formulas from [8].

A typical codimension-one cluster is that of the two period-one orbits that come into existence via the tangent bifurcation at $k = 2.44$. One of the orbits is unstable while the other, initially stable, becomes unstable in a period-doubling bifurcation at $k = 4.30$; as it does, a stable period-two orbit shows up as a satellite. Close to this bifurcation one has thus another cluster, formed by the satellite and the period-one orbit that changes its stability. Somewhere in between these two bifurcations one clearly has to rearrange the clusters. Unfortunately, the regrouping allows for ambiguities when an orbit is involved in several subsequent bifurcations. Whenever a regrouping is found necessary we choose its location along k so as to minimize the discontinuity in the approximated trace, taken as a function of k. In most cases, as in the example under discussion, the remaining discontinuity is tiny. In three situations, however, we have to avoid such patchwork and to enlarge our clusters to include orbits that are involved in subsequent bifurcations. In two cases the clusters stem from bifurcations of codimension two, where one would have to control two parameters to let all participating orbits coalesce.

In one of the codimension-two situations, endangering the semiclassical approximation of $\mathrm{tr}\, F^2$ around $k \approx 8$, a third orbit of equal length is found in close neighborhood to a pair of orbits that participate in a tangent bifurcation at $k = 8.12$, and the Stokes transition rendering the ghost orbits irrelevant occurs at $k = 7.98$. This type of cluster formed by three orbits of equal period is also frequently encountered for $\mathrm{tr}\, F^3$. It can be described by the normal form,

$$S^{(1)}(q', p) = q'p - \varepsilon q' - aq'^3 - bq'^4 - \frac{\sigma}{2} p^2, \quad (4)$$

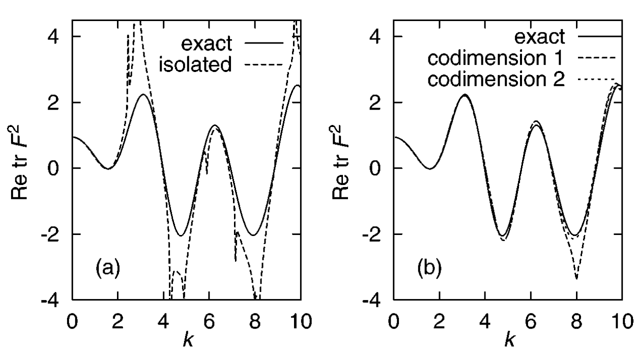

FIG. 2. The real part of the quantum mechanically exact $\mathrm{tr}\, F^2(k)$ for $j = 3$ is compared with various levels of semiclassical approximations. In (a), individual contributions from all real orbits and ghosts are summed up and Stokes transitions taken into account. In (b), collective contributions of orbit clusters are used to regularize the behavior close to bifurcations. Clusters connected to codimension-one bifurcations are found to be insufficient at $k \approx 8$. Enlarging the clusters further gives an accurate approximation.

with $\sigma = \pm 1$. This describes three orbits, two of which bifurcate at $\varepsilon = 0$. A uniform approximation is obtained by introducing $S^{(1)}$ into the exponent of Eq. (2) and expanding $|S_{q'p}|^{1/2} = 1 + Aq' + Bq'^2$. Here A and B are determined by requiring that the resulting contribution,

$$C^{(\mathrm{cluster})} = \frac{1}{\sqrt{2\pi\hbar}} \int dx (1 + Ax + Bx^2) \times \exp\left[\frac{i}{\hbar}(-\varepsilon x - ax^3 - bx^4) - i\frac{\pi}{2}\left(\mu + \frac{\sigma}{2}\right)\right], \quad (5)$$

has the right stationary-phase limit as $\hbar \to 0$, which gives three individual contributions of the type encountered in Eq. (1). The integral can be expressed by Pearcey's function and its derivatives [17]. It turns out that this expression also correctly treats the Stokes transition of the complex saddles.

Upon treating the codimension-two event as discussed, we obtain the dotted line in Fig. 2(b) for the second trace, $\mathrm{tr}\, F^2$. This ultimate level of approximation reproduces the exact result quite nicely.

The other codimension-two case encountered is that of a tripling bifurcation close to a tangent bifurcation of the satellite period-three orbit. This involves another satellite of period three that can be taken into account by an extended normal form, as is discussed in greater detail in [9], where a uniform approximation is given. It becomes relevant in the evaluation of $\mathrm{tr}\, F^3$, as does also the third scenario of higher codimension, where a tangent bifurcation of period-three orbits takes place on a broken torus formed by another pair of period-three orbits. The result for $\mathrm{tr}\, F^3$ is considerably improved by treating all four orbits collectively, using the contribution

$$C^{(\mathrm{cluster})} = \int_0^{2\pi} \frac{d\varphi}{\sqrt{2\pi\hbar}} (A + B\cos(\varphi + \varphi_0) + C\cos 2\varphi) \times \exp\left[\frac{i}{\hbar}(a\cos(\varphi + \varphi_1) + b\cos 2\varphi) - i\frac{\pi}{2}\left(\mu + \frac{\sigma}{2}\right)\right],$$

where all coefficients are determined to yield the correct stationary-phase limit.

With the help of these collective contributions, the traces $\mathrm{tr}\, F$ and $\mathrm{tr}\, F^3$ come out with a quality comparable to that of $\mathrm{tr}\, F^2$.

In general, the Floquet operator F acts as an $N \times N$ matrix with $N = 2j + 1$ whose eigenvalues $e^{-i\varphi_i}$ are determined by the set of traces with, for integral j, $n = 1, \ldots, j$. For $j = 3$ the first three traces thus provide sufficient information to retrieve all seven quasienergies. Indeed, from these traces one obtains the first half of the coefficients in the secular polynomial $\det(F - z) = \sum_{n=0}^{N} a_{N-n}(-z)^n = 0$ using Newton's formulas [18]; the second half follows from the unitarity of F which entails

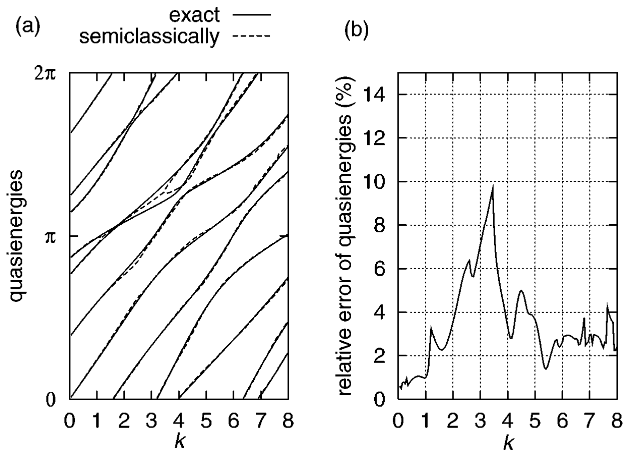

FIG. 3. (a) Exact and semiclassical level curves as a function of k. (b) Relative error $\frac{\Delta\varphi}{2\pi/(2j+1)}$ of the quasienergies.

the so-called self-inversiveness [19,20], $a_{N-n} = a_n^* a_N$. We benefit from the fact that $a_N = \det F$, needed to exploit the self-inversiveness of the polynomial, is accessible semiclassically: For the top, $\det F$ factorizes into a product of determinants of pure rotations and torsions, and each integrable factor can be treated individually by EBK quantization which even gives the exact result, $\det F = \exp[-\frac{i}{3} j(j+1)(k_x + k_z)]$.

The quasienergies $\varphi_i(k)$ from the semiclassically approximated secular polynomial are plotted together with the exact ones in Fig. 3(a). Noteworthy is the coalescence of two semiclassical phases mimicking a close avoided crossing of exact ones. The corresponding eigenvalues cease to be unimodular there. Self-inverse polynomials are capable of such behavior; to impose unitarity on them certain additional restrictions have to be fulfilled by the set of traces which are not automatically respected by the semiclassically approximated ones. As a quantitative measure of accuracy we employ the standard deviation between exact and semiclassical quasienergies,

$$\Delta\varphi = \sqrt{\frac{1}{2j+1}\sum_{i=1}^{2j+1}(\varphi_i^{(\mathrm{sc})} - \varphi_i^{(\mathrm{qm})})^2}\,, \tag{6}$$

which is shown in Fig. 3(b). The error is a small single-digit percentage of the mean spacing $2\pi/(2j+1)$, a little higher only in the short k interval where the two semiclassical phases mentioned are degenerate.

Similarly small is the error we have incurred for $j = 2$ and even $j = 1$. Semiclassical behavior of the spectrum begins to prevail for surprisingly small values of j indeed, fortunately so before with increasing j the infamous exponential proliferation of periodic orbits would render semiclassical work cumbersome. Our accuracy is comparable to the one previously found with different semiclassical strategies that avoid periodic orbits [16].

To summarize, we have demonstrated that complete spectra for the kicked top can be calculated from periodic classical orbits, provided one improves in several ways upon the trace formula for hyperbolic systems, Eq. (1): Contributions from isolated periodic orbits must be complemented by accounting for isolated ghosts as well as clusters of orbits associated with bifurcations of codimension $1, 2, \ldots$. New questions are opened up, for classical and quantum dynamics: Will the case improve for independent periodic orbits as the effective Planck constant $1/j$ is diminished? Or will the exponential proliferation of periodic orbits (and thus bifurcations) overrun the improving phase-space resolution ($\propto 1/j$)?

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