PHYSICAL REVIEW LETTERS

VOLUME 71 | 4 OCTOBER 1993 | NUMBER 14

Prebifurcation Periodic Ghost Orbits in Semiclassical Quantization

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(Received 26 May 1993)

Classical periodic orbits are stationary-phase points in path integral representations of quantum propagators. We show that complex solutions of the stationary-phase equation, not corresponding to real classical periodic orbits, give additional contributions to the propagator which can be important, especially near bifurcations. We reveal the existence and relevance of such periodic ghost orbits for a kicked top.

PACS numbers: 03.65.Sq, 05.45.+b

For a time-independent Hamiltonian system, the quantum propagator can be represented by a Feynman path integral [1]. Its semiclassical version arises from a stationary-phase approximation. The path integral is then dominated by contributions from classical orbits since these render the phase of the integrand stationary. In particular, classical periodic orbits determine, as $\hbar \to 0$, the trace of the propagator and the energy spectrum [2]. Similarly, for periodically driven systems, the spectrum of quasienergies is accessible through the traces $\mathrm{Tr}F^n$ where F, the so-called Floquet operator, is the single-period propagator and n an integer counting the number of periods of the driving. In the limit $\hbar \to 0$, the nth such trace is determined by classical orbits of period n [3].

The stationary-phase equation for the path integral may have nonphysical solutions not corresponding to real classical orbits. The ghost solutions we have in mind do not live in the classical phase space, but rather in a space arising from the latter by complexification of coordinates [4]. Such complex periodic orbits have complex actions $S = S' + iS''$. Their contributions to the path integral involve the factors $\exp[i(S' + iS'')/\hbar]$ which for $S'' > 0$ become negligibly small in the semiclassical limit $\hbar \to 0$. It is precisely due to their asymptotic loftiness that these ghosts usually do not even deserve mention. However, for not too small $\hbar$, their contributions to the quantum propagator may become important. Furthermore, in any situation where a ghost orbit has a small imaginary part of the action, its contribution becomes lofty only for rather small values of $\hbar$. On the other hand, observe that the vanishing of the imaginary part of the action of such a complex orbit would lead to a nonvanishing contribution to the propagator even in the limit $\hbar \to \infty$ which invalidates standard semiclassical quantization involving only real orbits.

Imagine, for example, a system undergoing a bifurcation when a control parameter k is varied: below some critical value k_c, a periodic orbit ceases to exist. The lost orbit might survive as a complex ghost for $k < k_c$, whose imaginary part of the action S'' tends to zero as the ghost approaches reality with $k \to k_c$ from below. As a precursor of a classical orbit, the ghost then makes a contribution to the propagator not contained in the standard semiclassical approximation. Such a phenomenon is particularly important close to a tangent bifurcation where two periodic orbits bifurcate from no periodic orbit at all.

The complex actions of our ghosts are reminiscent of semiclassical treatments of tunneling phenomena—which also give "exponentially small" corrections to the standard semiclassical approximation as $\hbar \to 0$—and of the complex free energies encountered in first-order phase transitions [5]. Classically forbidden orbits are also encountered in semiclassical collision theory [6], especially in the context of the so-called rainbow scattering [7]. We should mention the "generalized Gaussian wave packets" which have proven convenient for describing semiclassical dynamics [8].

We have been led to contemplate complex precursors of real periodic orbits following a semiclassical analysis of a kicked top which we must briefly recapitulate [3,9]. The dynamical variables of that top are the components of an angular momentum $\mathbf{J}$ which obey the commutation rules $[J_x, J_y] = iJ_z$, etc. The squared angular momentum $\mathbf{J}^2 = j(j+1)$ is conserved. The quantum number j fixes the dimension of the Hilbert space as $2j+1$. The semiclassical limit is obtained with $j \to \infty$ and $1/j$ can be considered as our effective $\hbar$. The stroboscopic quantum dynamics of the top is generated by the Floquet operator

$$F = e^{-i\frac{k}{2j}J_z^2}\, e^{-i\frac{\pi}{2}J_y}. \tag{1}$$

This accounts for a rotation by $\pi/2$ about the y axis followed by a nonlinear torsion about the z axis with strength k. The classical version of the kicked top has the sphere $\lim_{j\to\infty} \mathbf{J}^2/j(j+1) = 1$ as its phase space.

We specify the classical stroboscopic dynamics using a pair of stereographic projection coordinates x, y related to the spherical coordinates θ, φ by $x + iy = e^{i\varphi}\tan(\theta/2)$. The classical stroboscopic dynamics then takes the form of a map $x, y \to X, Y$,

$$\begin{aligned} X &= f(x,y)\cos ka(x,y) + g(x,y)\sin ka(x,y), \\ Y &= g(x,y)\cos ka(x,y) - f(x,y)\sin ka(x,y), \end{aligned} \tag{2}$$

with

$$f = \frac{1-x^2-y^2}{(1-x)^2+y^2},\quad g = \frac{2y}{(1-x)^2+y^2},\quad a = \frac{2x}{1+x^2+y^2}.$$

For $k \gg 1$, the classical dynamics is globally chaotic.

By using coherent states and the standard semiclassical technique ($j = 1/\hbar \gg 1$), one can express the traces $\mathrm{Tr}F^n$ in terms of periodic orbits of period n of the map (2). As pointed out above, these periodic orbits appear as solutions of a stationary-phase equation. The resulting semiclassical structure is, as usual,

$$(\mathrm{Tr}F^n)_{\mathrm{sc}} = \sum_{\text{periodic orbits}} A^{(n)} e^{ijS^{(n)}}, \tag{3}$$

where the $S^{(n)}$ and the $A^{(n)}$ are, respectively, the actions and amplitudes (related to stability properties) of the periodic orbits, independent of j. It is to be stressed that the map (2) being real leads to real values of actions $S(n)$ for real solutions of the fixed-point equations, as is shown in Ref. [10]. Clearly, the Fourier transform of $\mathrm{Tr}F^n$ with respect to $j = 1/\hbar$,

$$T_n(\omega; j_0, M) = \frac{1}{M}\sum_{j=j_0}^{j_0+M-1} e^{-ij\omega}\,\mathrm{Tr}F^n, \tag{4}$$

will exhibit peaks of location $\omega = S^{(n)} (\mathrm{mod}\ 2\pi)$, height $A^{(n)}$, and width of order $1/M$. To check on the accuracy of the semiclassical approximation for the traces $\mathrm{Tr}F^n$ and the T_n, one may compare it with the exact quantum result obtained by representing the Floquet operator as a $(2j+1)\times(2j+1)$ matrix. Any discrepancies between the quantum and the semiclassical T_n are expected to disappear as j_0 increases.

The following surprise arises, as was first realized but not conclusively explained in [10]. In some ranges of the control parameter k, the (Fourier transformed) traces $T_n(\omega; j_0, M)$ come out practically identical from the semiclassical and quantum calculations, even for j_0 down to unity. However, in other ranges of k, some quantum $T_n(\omega; j_0, M)$ differ significantly from their semiclassical approximants by exhibiting one or several additional peaks not corresponding to any real classical periodic orbit [see Fig. 1(a)]. In contrast to the peaks associated with real orbits, the additional "quantum peaks" have

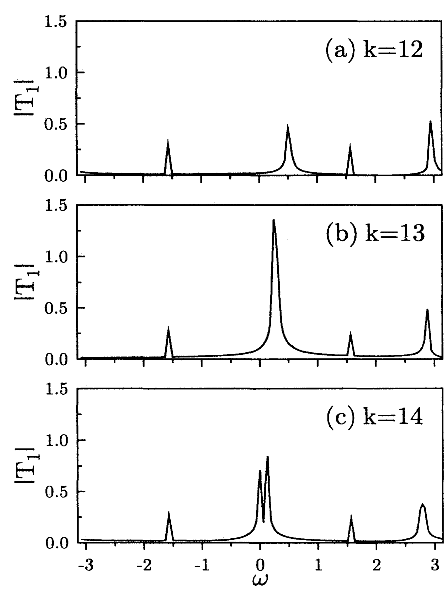

FIG. 1. Fourier transformed trace $T_1(\omega; j_0 = 1, M = 100)$ of the Floquet operator of the kicked top for various values of the control parameter k: (a) below $k_c = 12.73$ with a ghost peak at $\omega = 0.51$ and three peaks corresponding to real periodic orbits; (b) slightly above k_c where the highest peak corresponds to an unresolved doublet due to two real periodic orbits; and (c) sufficiently far above k_c where the doublet is resolved.

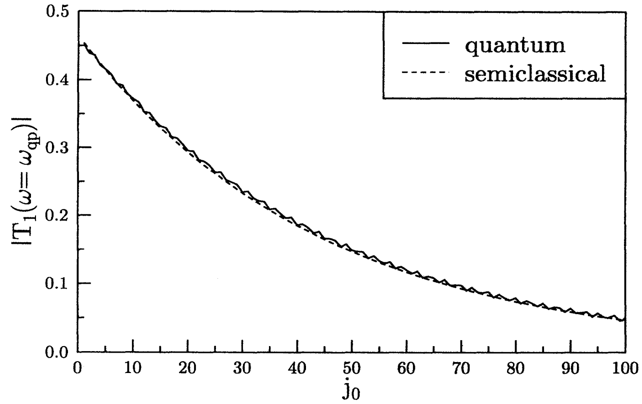

FIG. 2. Exponential decay with j_0 (with $M = 100$ fixed) of the height of the ghost peak at $\omega = 0.51$ in Fig. 1(a).

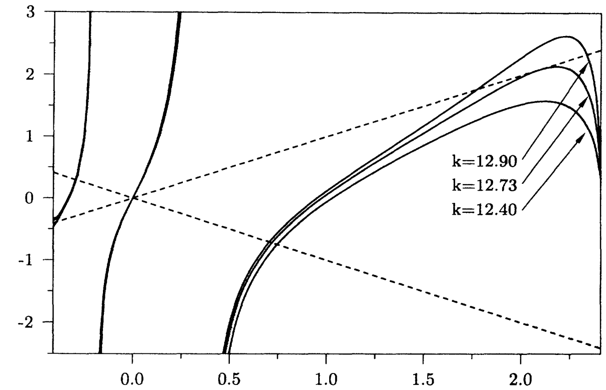

FIG. 3. Graph of the fixed-point equation (5) for $k = k_c = 12.73, k > k_c, k < k_c$; in the latter case (5) still allows for complex ghost solutions.

a height decreasing exponentially with increasing j_0 (see Fig. 2). Part of the surprise, in fact the better one, lies in the persistence of the quantum peaks up to fairly large values of j_0. Figure 2 reveals that the quantum peak in $T_1(\omega; j_0, M)$ for $k = 12$ has split into two separate peaks at $k = 14$, both associated with real classical fixed points.

We could formally reproduce quantum peaks by assuming a term in the periodic-orbit sum (3) with a complex action $S = S' + iS''$. For the case in Figs. 1 and 2 we would need $S = 0.51 + 0.02i$. This is why we found ourselves pushed to search for ghosts, fixed points ($n = 1$) of the complexified version of the map (2). These can be shown to obey

$$G(x,k) = \sqrt{1+2x-x^2}\tan\frac{kx}{2(1+x)} = \pm x, \qquad y = \pm\sqrt{1+2x-x^2}. \tag{5}$$

Figure 3 depicts graphs of $G(x,k)$ and $\pm x$ versus x. A tangent bifurcation arises when one of the straight lines touches the curve $G(x,k)$ tangentially, i.e., for $\partial G(x,k)/\partial x = 1$. Such is the case for $k_c = 12.73, x_c = 2.09, y_c = 0.90$. As is obvious from Fig. 3, the degenerate fixed point found for $k = k_c$ splits into two real ones for $k > k_c$ but has fled reality for $k < k_c$. Instead, for $k = 12$ we incur two pairs of complex (ghost) solutions $x = 2.24 \pm i0.78$, $y = 1.28 \mp i0.75$ and $x = -0.42 \pm i0.02$, $y = 0.18 \pm i0.19$. In order to find the ghosts' complex actions, we invoke the action $S(x,y,k)$ of the kicked top from [10],

$$S = 2k\left(\frac{v}{1+v}\right)^2 + 2i\ln\frac{\sqrt{2}(1+x^2+y^2)}{(1+v)(1-x-iy)} - \frac{k}{2}, \tag{6}$$

where the auxiliary function $v(x,y,k)$ is defined implicitly by

$$v\exp\left\{-ik\frac{1-v}{1+v}\right\} = \frac{(x-iy)(1+x+iy)}{1-x-iy}. \tag{7}$$

This gives $S = 0.51 \pm 0.02i$ for both pairs of ghost solutions, the degeneracy being due to a symmetry of the kicked top [9]. Of physical relevance are the ghosts with positive imaginary parts of their action. It is quite satisfactory to recover in the real part $S' = 0.51$ the location of the quantum peak of Fig. 1(a) and in the imaginary part $S'' = 0.02$ the decay rate of the height of the quantum peak with j_0 from Fig. 2. In fact, if we admit these ghosts to the periodic orbit sum (3) we gain a nearly perfect reproduction of Fig. 1(a) for $k = 12$. Moreover, expanding the fixed-point equations (5) and the action (6) in powers of $k - k_c, x - x_c, y - y_c$ we find the ghosts to imply $\mathrm{Im}(x - x_c) \propto (k_c - k)^{1/2}$ and $S'' \propto (k_c - k)^{3/2}$. It is the exponent 3/2 in the latter power law that renders the ghost visible in quantum features like $T_1(\omega)$ still rather far from the bifurcation and for rather large values of $j = 1/\hbar$.

When k approaches the critical value k_c from either above or below, the contribution of the real fixed points (above) and the ghosts (below) to $T_1(\omega)$ blows up, as is visualized in Fig. 4. Clearly, this failure of the saddle-point integration is due to its restriction to quadratic fluctuations around the saddle point in the Feynman type integral representing $\mathrm{Tr}F$.

It is well known [11] how an improved semiclassical approximation can be constructed close to a tangent bifurcation. One must look more closely at the Feynman type integral,

$$\mathrm{Tr}F = j\iint dx\, dy\, A(x,y)\, e^{ijS(x,y)}, \tag{8}$$

with the action (6); the prefactor $A(x,y)$, independent of j, has been given in [10]. At the critical point (x_c, y_c, k_c) of a tangent bifurcation, the matrix of second derivatives of $S(x,y)$ has one vanishing eigenvalue and thus implies divergence of the integral in (8) unless (at least) cubic terms in the expansion of S in $x - x_c, y - y_c$ are kept.

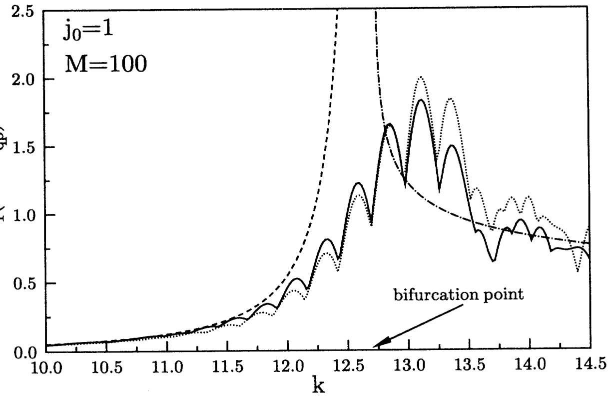

FIG. 4. Height of the quantum peak versus k near k_c. Full curve: exact quantum mechanics; dotted: semiclassics of Airy type, Eq. (10); dashed: ghost approximation ($k < k_c$); dash-dotted: standard Gutzwiller approximation ($k > k_c$).

After a suitable coordinate change $x - x_c, y - y_c \to q, p$ the action in (8) takes a certain normal form. In one of the new integration variables, say p, the action retains a finite quadratic piece even at $k = k_c$. Upon doing the usual saddle-point integral over p, we are left with

$$\mathrm{Tr}F = \sqrt{j}\int dq\ \tilde{A}(q)\ e^{i\tilde{S}(q)},\qquad \tilde{S}(q) = S_0(k) + (k - k_c)S_1 q + \tfrac{1}{3}S_3 q^3, \tag{9}$$

where S_1 and S_3 can be expressed in terms of derivatives of $S(x, y)$ with respect to x, y, k up to order 3. The saddle points of the remaining q integral, $\hat{q} = \pm\sqrt{(k_c - k)S_1/S_3}$, reproduce the fixed points (real for $k > k_c$, ghosts for $k < k_c$) close to the bifurcation. In constructing the above normal form $\tilde{S}(q)$ one keeps all terms of weights up to $(k - k_c)^{3/2}$, counting q as of order $(k - k_c)^{1/2}$. By this self-consistent procedure, a quadratic term $(k - k_c)S_2 q^2$ in $\tilde{S}(q)$ can be dropped since it is outweighed by the cubic term $S_3 q^3/3$. The new prefactor $\tilde{A}(q)$ then results from $A(x, y)$ as a power series in q and $(k - k_c)$, independent of j. If we replace $\tilde{A}(q)$ by its value at $q = 0, k = k_c$, our trace takes the form of an Airy function,

$$\mathrm{Tr}F = 2\pi\tilde{A}(0)S_3^{-1/3}j^{1/6}\mathrm{Ai}[S_1 S_3^{-1/3}(k - k_c)j^{2/3}]. \tag{10}$$

This regularizes the divergence of the naive saddle-point integral. By Fourier transforming according to (4) we have obtained the dotted curve in Fig. 4 which nicely fits the exact quantum result for $k \approx k_c$ and thus interpolates between the ghost contribution below and the periodic-orbit one above the bifurcation. This interpolation could be improved by retaining the power series for $\tilde{A}(q)$ which yields additive corrections to (10) involving derivatives of the Airy function. From (10) or Fig. 4, we can estimate the interval Δk around k_c within which one must use the Airy type of approximation rather than the standard Gutzwiller or ghost ones, as $\Delta k \approx S_3^{1/3}S_1^{-1}j^{-2/3}$. For larger values of $|k - k_c|$ the standard Gutzwiller or ghost formulas give equally good approximations to the exact result as the Airy type one, which can be also formally proved using the well known asymptotic form of the Airy function as it is known from the pioneering works of Berry and Upstill and later of Ozorio de Almeida and Hannay [11] on catastrophe diffraction integrals.

Let us sum up. Complex periodic ghost orbits with small imaginary parts of their actions show up when control parameters are steered close to bifurcation values. They are observable as quantum peaks in (Fourier transformed with respect to $1/\hbar$) traces of propagators. For all bifurcations except those of tangent type, real periodic orbits whose action is very close to the one of the ghosts exist on both sides of the bifurcation. The corresponding peaks will then generally hide the ghost contributions. This is why the tangent bifurcation is the easiest one to observe ghosts. Nevertheless, a quantum peak has recently been *experimentally* observed in high-resolution spectra of the He atom in a magnetic field [12]; we now understand this peak as due to a ghost related to a 1:5 resonance bifurcation.

When complex ghosts visit, conventional semiclassical quantization is in jeopardy. Fortunately, by simply including the ghosts in all stationary-phase integrations, the validity of semiclassical approximations can be improved, i.e., extended to larger effective $\hbar$.

Many questions are raised by the finding reported here. The frequency of appearance of ghosts must be investigated: one might argue that when dealing with long periodic orbits, one is always close to a bifurcation. The inclusion of ghosts might improve chances to obtain, say for the kicked top, reasonable approximations for the quasienergy spectrum at not too large values of j.

Laboratoire de Spectroscopie Hertzienne de l'ENS et de l'Université Pierre et Marie Curie is unité associée 18 du CNRS. M.K. and F.H. thank the Sonderforschungsbereich No. 237 "Unordnung und grosse Fluktuationen" der Deutschen Forschungsgemeinschaft. F.H. thanks the Ecole Normale Supérieure for support and hospitality. M.K. was partially supported by Polish KBN Grant No. 200799101.

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