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Periodic-orbit bifurcations and superdeformed shell structure

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We have derived a semiclassical trace formula for the level density of the three-dimensional spheroidal cavity. To overcome the divergences occurring at bifurcations and in the spherical limit, the trace integrals over the action-angle variables were performed using an improved stationary phase method. The resulting semiclassical level density oscillations and shell-correction energies are in good agreement with quantum-mechanical results. We find that the bifurcations of some dominant short periodic orbits lead to an enhancement of the shell structure for ''superdeformed'' shapes related to those known from atomic nuclei.

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I. INTRODUCTION

The periodic-orbit theory (POT) [1–7] is a nice tool for studying the correspondence between classical and quantum mechanics and, in particular, the interplay of deterministic chaos and quantum-mechanical behavior. But also for systems with integrable or mixed classical dynamics, the POT leads to a deeper understanding of the origin of shell structure in finite fermion systems from such different areas as nuclear [5,8–10], metallic cluster [11,12], or mesoscopic semiconductor physics [13,14]. Bifurcations of periodic orbits may have significant effects, e.g., in connection with the so-called ''superdeformations'' of atomic nuclei [5,6,9,15], and were recently shown to affect the quantum oscillations observed in the magneto-conductance of a mesoscopic device [14].

In the semiclassical trace formulas that connect the quantum-mechanical density of states with a sum over the periodic orbits of the classical system [1–3], divergences arise at critical points where bifurcations of periodic orbits occur or where symmetry breaking (or restoring) transitions take place. At these points the stationary-phase approximation, used in the semiclassical evaluation of the trace integrals, breaks down. Various ways of avoiding these divergences have been studied [2,4,16], some of them employing uniform approximations [17–20]. Here we employ an improved stationary-phase method (ISPM) for the evaluation of the trace integrals in the phase-space representation, based on the studies in Refs. [4,18] which we have derived for the elliptic billiard [21]. It yields a semiclassical level density that is regular at all bifurcation points of the short diameter orbit (and its repetitions) and in the circular (disk) limit. Away from the critical points, our result reduces to the extended Gutzwiller trace formula [3,5–7] and is identical to that of Berry and Tabor [4] for the leading-order families of periodic orbits.

The main purpose of the present Rapid Communication is to report on the extension of our semiclassical approach to the three-dimensional (3D) spheroidal cavity [22], which may be taken as a simple model for a large deformed nucleus [5,8] or a (highly idealized) deformed metal cluster [11,12], and to specify the role of orbit bifurcations in the shell structure responsible for the superdeformation. Although the spheroidal cavity is integrable (see, e.g., Ref. [23]), it exhibits all the difficulties mentioned above (i.e., bifurcations and symmetry breaking) and therefore gives rise to an exemplary case study of a nontrivial 3D system. We apply the ISPM for the bifurcating orbits and succeed in reproducing the superdeformed shell structure by the POT, hereby observing a considerable enhancement of the shell-structure amplitude near the bifurcation points.

II. THEORY

The level density $g(E)$ is obtained from the semiclassical Green function [1] by taking the imaginary part of its trace in $(\mathbf{I},\boldsymbol{\Theta})$ action-angle variables [6,21],

$$g(E)=\sum_i \delta(E-\varepsilon_i)\simeq \mathrm{Re}\sum_\alpha \int \frac{d\mathbf{I}'\,d\boldsymbol{\Theta}''}{(2\pi\hbar)^3}\,\delta(E-H)\times\exp\left\{\frac{i}{\hbar}[S_\alpha(\mathbf{I}',\mathbf{I}'',t_\alpha)+(\mathbf{I}''-\mathbf{I}')\cdot\boldsymbol{\Theta}'']-i\frac{\pi}{2}\mu_\alpha\right\}. \tag{1}$$

Here $\{\varepsilon_i\}$ is the single-particle energy spectrum and $H=H(\mathbf{I})$ is the classical Hamiltonian. The sum is taken over all classical trajectories α specified by the initial actions $\mathbf{I}'$ and final angles $\boldsymbol{\Theta}''$. $S_\alpha(\mathbf{I}',\mathbf{I}'',t_\alpha)=-\int_{\mathbf{I}'}^{\mathbf{I}''}\mathbf{I}\cdot d\boldsymbol{\Theta}$ is the action integral and t_α the time for the motion along the trajectory α, and μ_α is the Maslov index related to the caustic and the turning points [21,22]. In the spheroidal variables $\{u,v,\varphi\}$, the action $\mathbf{I}$ has the components

$$I_u=\frac{pc}{\pi}\int_{-u_c}^{u_c}du\,\sqrt{\sigma_1-\sin^2 u-\sigma_2/\cos^2 u},$$
$$I_v=\frac{pc}{\pi}\int_{v_c}^{v_t}dv\,\sqrt{\cosh^2 v-\sigma_1-\sigma_2/\sinh^2 u}, \tag{2}$$

$$I_\varphi = pc\sqrt{\sigma_2}.$$

Hereby $p=(2mE)^{1/2}$ is the particle's momentum and $c=(b^2-a^2)^{1/2}$ half the distance between the foci; b and a are the semiaxes (with $b>a$) of the spheroid with its volume fixed by $a^2b=R^3$ and the axis ratio $\eta=b/a$ as deformation parameter; and $\pm u_c$ (or v_c) and v_t are the caustic and turning points, respectively. In Eq. (2) we use the dimensionless ''action'' variables σ_1, σ_2 [21] in which the torus of the classical motion is given by

$$\sigma_2^- = 0 \leqslant \sigma_2 \leqslant \frac{1}{\eta^2-1} = \sigma_2^+ ,$$
$$\sigma_1^- = \sigma_2 \leqslant \sigma_1 \leqslant \frac{\eta^2}{\eta^2-1} - \sigma_2(\eta^2-1) = \sigma_1^+ . \tag{3}$$

In the ISPM, we expand the action S_α in Eq. (1) up to second-order terms around its stationary points and keep the preexponential factor at zero order, taking the integrations over the torus within the *finite* limits given by Eq. (3). For the oscillating (''shell-correction'') part of the level density $\delta g(E)=g(E)-\tilde{g}(E)$, where $\tilde{g}(E)$ is its smooth part [7,24], we obtain

$$\delta g(E) \simeq \frac{1}{E_0}\,\mathrm{Re}\sum_\beta A_\beta(E)\exp\left(ikL_\beta - i\frac{\pi}{2}\mu_\beta\right)w_\beta^\gamma, \tag{4}$$

where $k=p/\hbar$ is the wave number and $E_0=\hbar^2/2mR^2$ our energy unit. The amplitudes A_β will be specified below. The sum over β includes all two-parameter families of three-dimensional (3D) periodic orbits and elliptic and hyperbolic 2D orbits lying in a plane containing the symmetry axis (all with degeneracy parameter $\mathcal{K}=2$), the one-parameter families of (2D) equatorial orbits lying in the central plane perpendicular to the symmetry axis (with $\mathcal{K}=1$), and the (1D) isolated long diameter (with $\mathcal{K}=0$). In Eq. (4), L_β is the length of the orbit β at the stationary point (σ_1^*,σ_2^*) which for the 3D orbits lies inside the physical region of the torus (3), and is analytically continued outside this region. The $\sigma_2=0$ boundary of Eq. (3) is occupied by the 2D orbits with $\mathcal{K}=2$. The stationary points are determined by the roots of the periodicity conditions $\omega_u/\omega_v=n_u/n_v$ and $\omega_u/\omega_\varphi=n_u/n_\varphi$; hereby $\omega_\kappa=\partial H/\partial I_\kappa$ are the frequencies and n_κ are coprime integers which specify the periodic orbits $\beta=M(n_v,n_\varphi,n_u)$, where M is the repetition number. The factor $w_\beta^\gamma=\exp(-\gamma^2L_\beta^2/4R^2)$ in Eq. (4) is the result of a convolution of the level density with a Gaussian function over a range γ in the variable kR. This ensures the convergence of the POT sum (4) by suppressing the longer orbits which are not relevant for the coarse-grained gross-shell structure [6,7].

For Strutinsky's shell-correction energy δU [3,7,24], we obtain (with time reversal symmetry and a spin factor 2)

$$\delta U = 2\sum_{i=1}^{N/2}\varepsilon_i - 2\int_0^{\tilde{E}_F} E\tilde{g}(E)\,dE$$
$$\simeq 8R^2E_F\,\mathrm{Re}\sum_\beta \frac{A_\beta(E_F)}{L_\beta^2}\exp\left(ik_FL_\beta - i\frac{\pi}{2}\mu_\beta\right). \tag{5}$$

The Fermi energies E_F (and with it k_F) and $\tilde{E}_F$ are determined by the particle number conservation $N=2\int_0^{E_F}g(E)dE=2\int_0^{\tilde{E}_F}\tilde{g}(E)dE$. Due to the factor L_β^{-2}, the PO sum in Eq. (5) may converge faster for the shortest orbits than the level density (4) for small γ. Any enhancement of the amplitudes A_β of the most degenerate short periodic orbits (e.g., due to bifurcations or to symmetry restoring, as discussed below) therefore leads to an enhancement of the shell structure and hence to an increased stability of the system.

We present here only the amplitudes of the leading contributions to Eqs. (4) and (5). For further details (including, e.g., explicit expressions for the Maslov indices μ_α), we refer to a forthcoming, more extensive publication [22].

For the amplitudes A_β of the most degenerate ($\mathcal{K}=2$) families of periodic 3D and 2D orbits, we obtain

$$A_\beta^{(\mathcal{K}=2)} = \frac{icL_\beta[\partial I_u/\partial\sigma_1]_{\sigma_n^*}}{\pi(4MRn_v)^2\sqrt{K_\beta\sigma_2^*}}\prod_{n=1}^{2}\mathrm{erf}(x_n^-,x_n^+). \tag{6}$$

The quantity $K_\beta=K_\beta^{(1)}K_\beta^{(2)}$ is related to the main curvatures $K_\beta^{(n)}$ of the energy surface $E=H(\sigma_1,\sigma_2)$ in the ''action'' plane (σ_1,σ_2), given by

$$K_\beta^{(n)} = \left[\frac{\partial^2 I_v}{\partial\sigma_n^2} + \frac{\omega_u}{\omega_v}\frac{\partial^2 I_u}{\partial\sigma_n^2} + \frac{\omega_\varphi}{\omega_v}\frac{\partial^2 I_\varphi}{\partial\sigma_n^2}\right]_{\sigma_n^*}, \quad (n=1,2). \tag{7}$$

In Eq. (6), the arguments of the two-dimensional error function $\mathrm{erf}(x,y)=2\int_x^y dz e^{-z^2}/\sqrt{\pi}$ are given by the turning points in the action plane

$$x_n^\pm = \sqrt{-i\pi Mn_vK_\beta^{(n)}/\hbar}\,(\sigma_n^\pm - \sigma_n^*) \quad (n=1,2); \tag{8}$$

see Eq. (3) for the boundaries $\sigma_n^\pm$. All quantities in Eq. (6) can be expressed analytically in terms of elliptic integrals. For the 3D orbits, our result (6) is in agreement with that obtained by exact Poisson summation over the EBK spectrum (cf. Refs. [4,7]).

For the contribution of the $\mathcal{K}=1$ families of equatorial orbits to Eq. (4), we obtain the amplitudes

$$A_\beta^{(\mathcal{K}=1)} = \sqrt{\frac{i\,\sin^3\phi_\beta}{\pi Mn_vkR\eta F_\beta}}\prod_{n=1}^{3}\mathrm{erf}(x_n^-,x_n^+), \tag{9}$$

where $\phi_\beta=\pi n_\varphi/n_v$, F_β is their stability factor [1,2,6], $\sigma_1^*=\sigma_2^*=\cos^2\phi_\beta/(\eta^2-1)$, and

$$x_3^+ = kc\sqrt{\frac{-i\pi\hbar F_\beta}{64Mn_v(\sigma_2^*+1)K_\beta^{(1)}}}, \quad x_3^- = 0. \tag{10}$$

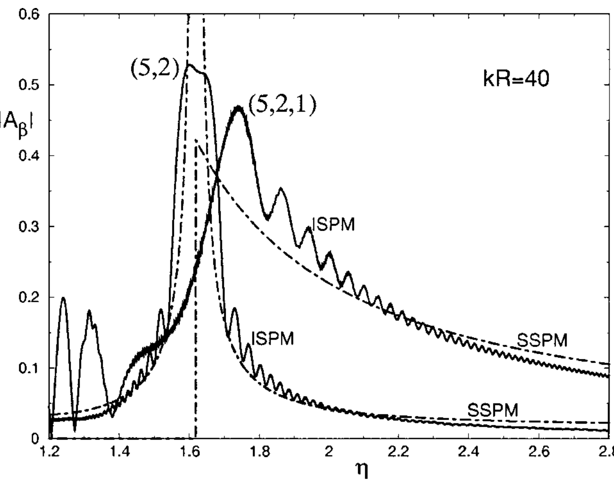

FIG. 1. Moduli of amplitudes $|A_\beta|$ vs η for the equatorial ''star'' orbit (5,2) ($\mathcal{K}=1$) and the 3D orbit (5,2,1) ($\mathcal{K}=2$) bifurcating from it at $\eta=1.618\ldots$. Solid lines: using the ISPM according to Eqs. (9) and (6), respectively; dash-dotted lines: using the standard stationary-phase approach.

The contribution of the isolated long diameter orbit, which may be expressed in terms of incomplete Airy integrals [21,22], is not important for deformations of the order $\eta\sim1.2-2$.

III. DISCUSSION OF RESULTS

In Fig. 1 we show $|A_\beta|$ versus deformation η (at $kR=40$) for a pair of orbits involved in a typical bifurcation scenario. At the critical point $\eta=1.618\ldots$ the equatorial ''star'' orbit (5,2) undergoes a bifurcation at which the 3D orbit (5,2,1) is born; the latter does not exist below $\eta=1.618\ldots$.

In the standard stationary-phase approach (SSPM; dash-dotted lines), the amplitude of the (5,2) orbit diverges at $\eta=1.618\ldots$, whereas that of the bifurcated orbit (5,2,1) is finite but discontinuous. As seen in Fig. 1, the ISPM (solid lines) leads to a finite amplitude $A_{(5,2)}^{(\mathcal{K}=1)}$ for the (5,2) orbit. This is because the factor F_β in the denominator of Eq. (9), which goes to zero at the bifurcation, is cancelled by the same factor in the numerator of x_3^+ (10) via the third error function in Eq. (9). A similar result was found for the short diameter orbit 2(2,1) in the elliptic billiard [21]. Furthermore, the ISPM softens the discontinuity for the (5,2,1) orbit, leading to a maximum amplitude slightly above the critical deformation.

The relative enhancement of these amplitudes A_β near the bifurcation point can also be understood qualitatively from the following argument. At the bifurcation of the equatorial (5,2) orbit, its degeneracy parameter $\mathcal{K}=1$ locally increases to 2, because it is there degenerate with the orbit family (5,2,1) that has $\mathcal{K}=2$ at all deformations $\eta\geqslant1.618\ldots$. This is similar to a symmetry restoring transition. An increase of the symmetry parameter $\mathcal{K}$ by one unit leads to one more exact integration compared to the SSPM, and thus the amplitudes (6) and (9) acquire an enhancement factor $\sqrt{kL_\beta}\propto\sqrt{pR/\hbar}$ (cf. Refs. [3,7]).

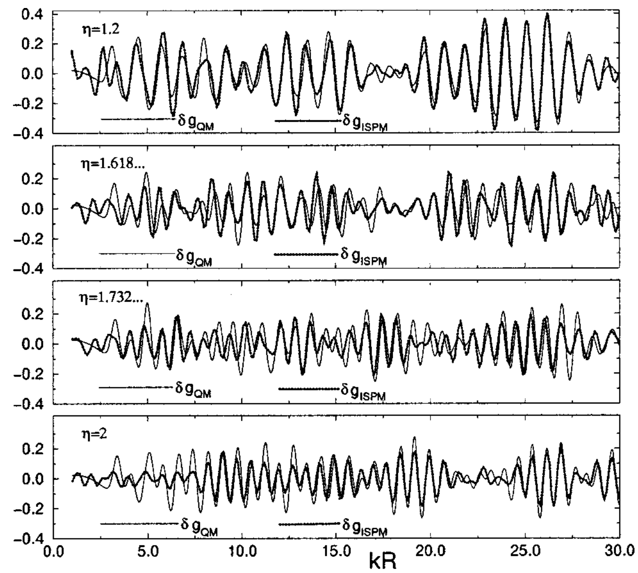

FIG. 2. Level density $\delta g(E)$ (4) (unit E_0^{-1}) vs kR for different critical deformations η. The Gaussian averaging parameter is $\gamma=0.3$. Thin solid lines: quantum-mechanical results; thick dotted lines: semiclassical results using the ISPM.

A similar enhancement of the double triangle 2(3,1) and the 3D orbit (6,2,1) is found near their bifurcation point $\eta=\sqrt{3}=1.732\ldots$. However, the curvature $K_\beta^{(1)}$ (7) for orbits like $M(3t,t,1)$ ($t=2,3,\ldots$) is identically zero and hence the SSPM is divergent for all deformations $\eta\geqslant1$, in contrast to the situation with orbits like (5,2,1) with finite $K_\beta^{(1)}$. Here we have to take into account the next nonzero third-order terms in the expansion of S_α, although the $(3t,t,1)$ ISPM amplitude (6) is finite and continuous everywhere. The amplitude can then be expressed in terms of incomplete Airy and Gairy integrals with finite limits [22]. For the equatorial orbits $t(3,1)$, like for the double triangles 2(3,1), one has a zero curvature $K_\beta^{(1)}$ only at the bifurcation point $\eta=\sqrt{3}$. Here $F_\beta/K_\beta^{(1)}\rightarrow0$, and a similar mechanism of cancellation of singularities for other orbits takes place through Eqs. (8)–(10). But the relative enhancement of the ISPM amplitudes (6,9) of such orbits at the bifurcations is of order kL_β because of a change of the degeneracy parameter $\mathcal{K}$ by *two* units (see Ref. [22] for details). In this sense we avoid here a double singularity related to a double restoring of symmetry.

In Figs. 2 and 3, we present semiclassical level densities $\delta g(E)$ (4) versus kR and shell-correction energies δU (5) versus $N^{1/3}$ for various critical deformations (thick dotted lines), and compare them to the corresponding quantum-mechanical results (thin solid lines). We observe a very good agreement of the gross-shell structure at all deformations. The most significant contributions to these results near the critical deformations are coming from bifurcating orbits with lengths smaller than about $10R$, in line with the convergence arguments for the POT sums (4) and (5) mentioned above. For the bifurcation at $\eta=1.618\ldots$, the orbits (5,2,1) and (5,2) give contributions comparable with other 2D orbits. For $\eta=\sqrt{3}$, the bifurcating orbits (6,2,1) and (6,2) are also important.

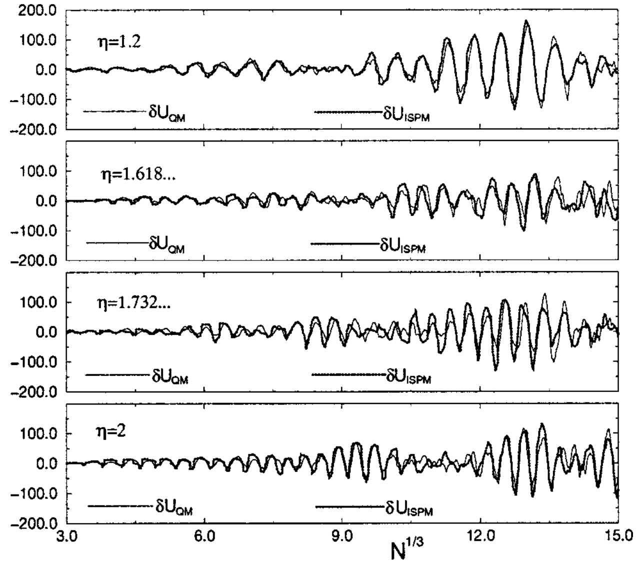

FIG. 3. Shell-correction energy δU (5) (unit E_0) vs cube root of particle number $N^{1/3}$ (same notation and same deformations as in Fig. 2).

The role of the bifurcating orbits increases for larger deformations and is dominating at the superdeformation $\eta = 2$. For this deformation, the most important orbits in the present spheroidal cavity model are the 3D orbits (5,2,1), (6,2,1), (7,2,1), and (8,2,1).

These results are in agreement with both heights and positions of the peaks in the length spectra obtained in Ref. [15] from the Fourier transforms of the quantum level densities $g(kR)$ at the same deformations.

IV. SUMMARY AND CONCLUSIONS

We have obtained an analytical trace formula for the 3D spheroidal cavity model, which is continuous through all critical deformations where bifurcations of periodic orbits occur. We find an enhancement of the amplitudes $|A_\beta|$ at deformations $\eta \sim 1.6 - 2.0$ due to bifurcations of 3D orbits from the shortest 2D orbits. We believe that this is an important mechanism which contributes to the stability of superdeformed systems. Our semiclassical analysis may therefore lead to a deeper understanding of shell structure effects in superdeformed fermionic systems, not only in nuclei or metal clusters but also, e.g., in deformed semiconductor quantum dots whose conductance and magnetic susceptibilities are significantly modified by shell effects.

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