

SEMICLASSICAL SHELL STRUCTURE
AND NUCLEAR DOUBLE-HUMPED FISSION BARRIERS*To the memory of V. M. Strutinsky*

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Institute for Nuclear Research, National Academy of Sciences of Ukraine, Kyiv

We derived the semiclassical trace formulas for the level density as sums over periodic-orbit families and isolated orbits within the improved stationary phase method. Averaged level-density shell corrections and shell-structure energies are continuous through all symmetry-breaking (bifurcation) points with the correct asymptotics of the standard stationary phase approach accounting for continuous symmetries. We found enhancement of the nuclear shell structure near bifurcations in the superdeformed region. Our semiclassical results for the averaged level densities with the gross-shell and more thin-shell structures and the energy shell corrections for critical deformations are in good agreement with the quantum calculations for several single-particle Hamiltonians, in particular for the potentials with a sharp spheroidal shape. Enhancement of the shell structure owing to bifurcations of the shortest 3-dimensional orbits from equatorial orbits is responsible for the second well of fission barrier in a superdeformation region.

Keywords: nuclear shell structure, fission barriers, nuclear deformations, energy shell corrections, semiclassical periodic orbit theory, quantum and classical chaos.

Introduction

Many remarkable phenomena like the nuclear fission, stability of deformed nuclei and superheavy element production were described within the shell-correction method (SCM) suggested originally by Vilen Mitrofanovich Strutinsky [1, 2]. The shell structure of nuclei within this macroscopic-microscopic model is measured by the energy shell-structure component δE for a given deformed nuclear shape, see also [3, 4]. It is associated with a non-homogeneity of the single-particle (s.p.) energy-level distribution near the Fermi surface. According to the SCM, nuclei are stable at a deformation for which the Fermi energy corresponds to the minimum of the s.p. level density and therefore, approximately to the energy shell correction δE .

The periodic orbit (PO) theory (POT) is a nice tool for studying analytically within the SCM the correspondence between classical and quantum mechanics and, in particular, the interplay of deterministic chaos and quantum-mechanical behavior [5 - 12]. But also for systems with the integrable or mixed classical dynamics, the POT leads to a deeper understanding of the origin of shell structure in finite fermionic systems from such different areas as the nuclear, metallic cluster or mesoscopic-semiconductor physics [5 - 17]. The POT is the analytical background of the SCM, in particular, for explanation of the famous double-humped fission barriers and isomer states in the superdeformed region. For any potential well, the s.p. level-density and energy shell corrections can be related to an existence of POs by the POT, and near the Fermi surface, they are responsible, in particular, for double-humped structure of fission barriers.

Bifurcations of POs may have significant effects, e.g., in connection with the so called "superdeformations" of atomic nuclei [8 - 16]. In the semiclassical trace formulae that connect the quantum-mechanical density of states with a sum over the POs (or their families) in the classical system, divergences arise at critical points where bifurcations of POs occur or where symmetry breaking (or restoring) transitions take place. At these points the standard stationary-phase approximation, used in the semiclassical evaluation of the trace integrals, breaks down. Various ways of avoiding these divergences have been studied with employing the uniform approximations [12 - 16]. Here we discuss the so called improved stationary-phase method (improved SPM, or shortly ISPM) for the evaluation of the trace integrals in the phase-space representation, based on the studies in [14 - 16]. Away from the critical points, our results reduce asymptotically to the extended Gutzwiller trace formula [6, 7, 12]. For instance, they become identical to those of Berry and Tabor approach for the leading-order families of POs in the case of integrable systems [12].

The main purpose of the present talk devoted to the memory of V. M. Strutinsky is to report on the extension of the semiclassical approach suggested in [6, 7] to the spheroidal cavity, which may be taken as a simple and realistic enough model for a deformed strongly nucleus [8], and to specify the role of orbit bifurcations in the shell structure responsible for the superdeformation [8, 14, 15]. The enhancement of the shell structure owing to the bifurcations of the three-dimensional (3D) POs from equatorial (EQ) ones by using the spheroidal cavity model was predicted in [8]. We applied the ISPM

[14 - 16] for the bifurcating orbits and succeeded quantitatively in reproducing the superdeformed shell structure within the POT, hereby observing this considerable enhancement of the shell-structure amplitude near the bifurcation points. Therefore, following Ref. [8], in [14, 15] we confirm the original idea of V. M. Strutinsky. The ISPM answers approximately within the POT to Strutinsky's questions [8 - 11]: Why are nuclei deformed and what is the deep reason of the double-humped

barrier of fission, first of all the existence of its second potential well?

The phase space trace formula and ISPM

The level density $g(\varepsilon)$ is obtained from the semiclassical Green's function by taking the imaginary part of its trace in phase space variables, see [16], also for references therein,

$$g(\varepsilon) = \sum_i \delta(\varepsilon - \varepsilon_i) \approx \sum_{CT} \int \frac{d\mathbf{r}' d\mathbf{p}''}{(2\pi\hbar)^3} \delta(\varepsilon - H(\mathbf{r}'', \mathbf{p}'')) |\mathfrak{I}_{CT}(\mathbf{p}'_{\perp}, \mathbf{p}''_{\perp})|^{1/2} \exp\left(\frac{i}{\hbar} \Phi_{CT} - \frac{i\pi}{2} \mu_{CT}\right), \quad (1)$$

where δ -function describes the energy conservation, Φ_{CT} is the action phase,

$$\Phi_{CT} = S_{CT}(\mathbf{r}', \mathbf{r}'', \varepsilon) - \mathbf{p}''(\mathbf{r}'' - \mathbf{r}'),$$

$$S_{CT} = \int_{\mathbf{r}'}^{\mathbf{r}''} d\mathbf{r} \mathbf{p}(\mathbf{r}) \quad (2)$$

is the action along the classical trajectory CT in the potential well of the Hamiltonian $H(\mathbf{r}, \mathbf{p})$. μ_{CT} is the Maslov phase associated with the number of caustic and turning points of the catastrophe theory by Maslov & Fedoryuk [16]. In Eq. (1), $\mathfrak{I}_{CT}(\mathbf{p}'_{\perp}, \mathbf{p}''_{\perp})$ is the Jacobian of transformation from the perpendicular, \mathbf{p}'_{\perp} , at the initial Cartesian coordinate \mathbf{r}' to the final, \mathbf{p}''_{\perp} , momentum at \mathbf{r}'' of a CT. Separating a short trajectory without reflections from the potential boundary one may present approximately the level density $g(\varepsilon)$ (1) in terms of the sum of smooth part $g_{ETF}(\varepsilon)$ of the extended Thomas - Fermi model [12] and its oscillating component $\delta g_{scl}(\varepsilon)$,

$$g(\varepsilon) \approx g_{ETF}(\varepsilon) + \delta g_{scl}(\varepsilon). \quad (3)$$

The second term can be calculated by using the stationary phase method (SPM) for the asymptotical ($k_F R \gg 1$) evaluation of the integrals through the SPM conditions,

$$\left(\frac{\partial}{\partial \mathbf{p}''} \Phi_{CT}\right)^* \equiv (\mathbf{r}' - \mathbf{r}'')^* = 0,$$

$$\left(\frac{\partial}{\partial \mathbf{r}'} \Phi_{CT}\right)^* \equiv (\mathbf{p}'' - \mathbf{p}')^* = 0, \quad (4)$$

which are just the definition of POs (k_F is the Fermi momentum in units of \hbar , R is a size of the nucleus).

Now, we describe the reason for divergences and discontinuities of the oscillation density amplitudes in the standard SPM (or SSPM) at the bifurcation potential parameter where a PO transfers into the same and a newborn of the isolated PO or the PO family. These singularities occur owing to the *second-order* expansion of the action phase Φ_{CT} as function of the phase-space integration variable $\xi = \{\mathbf{r}', \mathbf{p}''\}$ in Eq. (1) near the stationary phase-space point $\xi = \xi^*$ with an extension of the integration limits in ξ of Eq. (1) to the $\pm\infty$. In order to solve these problems, we found that the bifurcation point is similar to the caustic singularity considered by Fedoryuk within a catastrophe theory, see for instance Appendix A in [16]. Therefore, we use the ISPM [14 - 16], i.e. the exact integrations within the finite limits bounded by the physically accessible region of a classical motion and the expansion of action phases and amplitudes in Eq. (1) to higher order terms if necessary.

Enhancement of shell structure at bifurcations

Following the ideas of [8], by using the spheroid cavity model in semiclassical POT calculations of the oscillating part of the level density $\delta g_{scl}(\varepsilon)$ one finally arrives at [14, 15]

$$\delta g_{scl}(\varepsilon) \approx \delta g_{3D}(\varepsilon) + \delta g_{2D}(\varepsilon) + \delta g_{EQ}(\varepsilon) = \text{Re} \sum_{po} \delta g_{po}^{scl}(\varepsilon),$$

$$\delta g_{po}^{scl}(\varepsilon) = A_{po} \exp\left(ikL_{po} - i\frac{\pi}{2}\sigma_{po}\right). \quad (5)$$

The sum runs the leading families of POs, $\delta g_{po}^{scl}(\varepsilon)$ is their contribution of twice degenerated families of the 3D and meridian 2D families of Pos and one-parametric EQ orbits, $k = \sqrt{2m\varepsilon/\hbar}$ is the wave number of the particle, L_{po} is the length of PO, σ_{po} is the Maslov phase determined through the

turning and caustic points along the PO, i.e. to the Maslov index [12, 16]. For the oscillating 3D and 2D PO amplitudes $A_{3D/2D}$ in Eq. (5) one obtains

$$A_{3D/2D} \propto L_{po} \operatorname{erf}(Z_1^-, Z_1^+) \operatorname{erf}(Z_2^-, Z_2^+) \left[(Mn_v)^2 \sqrt{\det K_{po}} \right]^{-1}. \quad (6)$$

The finite limits Z_n^\pm ($n=1, 2$) for the integrations in Eq. (1) are given by

$$Z_1^\pm = \sqrt{-i\pi Mn_v K_{po}^{11} / \hbar} \left[\sigma_1^\pm(\sigma_2^*) - \sigma_1^* \right],$$

$$Z_2^\pm = \sqrt{-i\pi Mn_v (\det K_{po} / K_{po}^{11}) / \hbar} \left[\sigma_2^\pm - \sigma_2^* \right] \quad (7)$$

for the case of a non-zero element K_{po}^{11} of the matrix K_{po} of curvatures of the energy surface, and similar expressions for vanishing K_{po}^{11} can be found in [15]. The primitive integers (n_v, n_u, n_φ) and the repetition number M determine the PO, $M(n_v, n_u, n_\varphi)$, through the frequency (resonance) relations $\omega_v : \omega_u : \omega_\varphi = n_v : n_u : n_\varphi$, $\omega_\kappa = \partial H / \partial I_\kappa$ ($\kappa = v, u, \varphi$) with the Hamiltonian $H(I_v, I_u, I_\varphi)$ depending only on the partial actions I_v, I_u, I_φ in the cylindric

coordinates v, u, φ ,

$$I_v \propto \int_{v_{\min}}^{v_{\max}} dv \sqrt{\cosh^2 v - \sigma_1 - \sigma_2 / \sinh^2 v},$$

$$I_u \propto \int_{-u_{\max}}^{u_{\max}} du \sqrt{\sigma_1 - \sin^2 u - \sigma_2 / \cos^2 u}, \quad I_\varphi \propto \sqrt{\sigma_2}. \quad (8)$$

The integration boundaries are determined by the accessible classically tori region through the deformation parameter $\eta = b/a$ (b and a are semiaxes of the spheroid with the usual volume conservation condition, $a^2 b = R^3$, R the radius of the equivalent sphere). The tensor K_{po}^{nm} of the energy surface curvatures (with the diagonal terms K_{po}^{11} and K_{po}^{22}) in Eqs. (5) and (6) is defined with respect to new action variables σ_1 and σ_2 introduced instead of I_u and I_φ for a given particle energy ε , according to Eq. (8), see details for all explicit analytical expressions, including the specific Maslov phases, in [15]. For the contribution of one-parametric families of EQ POs, one finds Eq. (5) (po is EQ in this case) with the amplitude

$$A_{EQ} \propto \sqrt{\frac{\sin^3 \phi}{Mn_v k R \eta F_{EQ}}} \operatorname{erf}[Z_1^-, Z_1^+] \operatorname{erf}[Z_2^-, Z_2^+] \operatorname{erf}[Z_\perp^-, Z_\perp^+], \quad (9)$$

where $\phi = \pi n_v / n_u$. The Gutzwiller stability factor F_{EQ} and the additional integration limits Z_\perp^\pm in the last error function are given by

$$F_{EQ} = 4 \sin^2 \left[Mn_v \arccos(1 - 2\eta^{-2} \sin^2 \phi) / 2 \right] \text{ and}$$

$$Z_\perp^\pm \propto \sqrt{F_{EQ} / Mn_v \sin \phi \det K_{EQ}}, \quad (10)$$

K_{EQ} is the EQ-orbit curvature. For the semiclassical shell correction energy δE one then obtains [6 - 16]

$$\delta E = \sum_{po} \left(\hbar / t_{po} \right)^2 \delta g_{po}^{scl}(\varepsilon_F),$$

$$N = \int_0^{\varepsilon_F} d\varepsilon g(\varepsilon), \quad t_{po} = M T_{po}, \quad (11)$$

where N is the particle number (the protons or the neutrons) in nucleus, ε_F is the Fermi energy, T_{po} is the primitive (for the repetition number $M=1$) period of motion of particle along the PO at the energy $\varepsilon = \varepsilon_F$.

Fig. 1 shows the enhancement of shell structure amplitudes $|A_{3D}|$ and $|A_{EQ}|$ of a typical bifurcation scenario, see Eq. (6). At a critical point $\eta = 1.618\dots$ the EQ “star” PO (5, 2) undergoes a bifurcation at which the 3D orbit (5, 2, 1) is born; the latter does not exist below $\eta = 1.618\dots$. In the SSPM (dashed lines) the amplitude of the (5, 2) orbit diverges at this deformation, whereas that of the bifurcated orbit (5, 2, 1) is finite but discontinuous. As seen in Fig. 1, the ISPM (solid lines) leads to the finite amplitude $A_{(5,2)}$ for the (5, 2) orbit. 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_{po} in $\hbar^{-1/2}$ (or in $(k_F L_{po})^{1/2}$) near the bifurcation point and surface energy $\varepsilon \approx \varepsilon_F$ can be understood through the local increase of the number of parameters of the PO family with the same action from one of EQ POs to the two parameters of 3D POs, and the corresponding one more exact integration than within the SSPM.

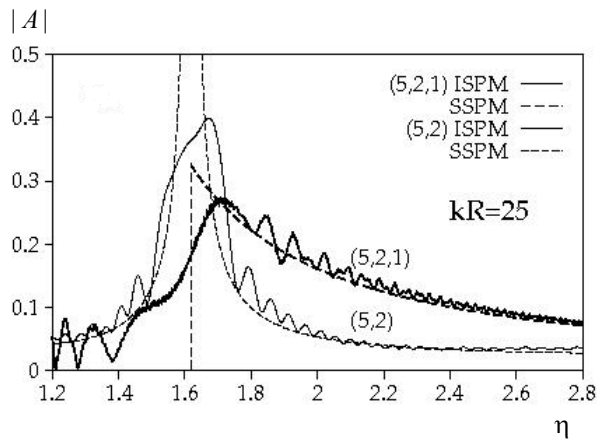


Fig. 1. Moduli of amplitudes $|A_{po}|$ vs deformation $\eta = b/a$. Solid and dashed: using the ISPM and SSPM for the star-like EQ (5, 2) and 3D (5, 2, 1) POs as examples.

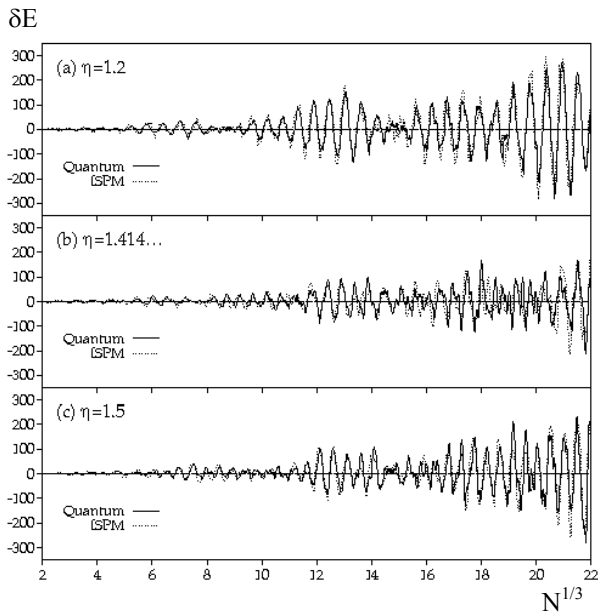


Fig. 2. Shell-correction energy δE ($2mR^2/\hbar^2$) vs cube root of particle number $N^{1/3}$ at the critical deformations $\eta = 1.2, \sqrt{2}, 1.5$.

Similarly, the dominant POs near $\eta = \sqrt{3} = 1.732 \dots$ are also the bifurcating 3D (6, 2, 1) and twice ($M = 2$) repeated EQ triangles 2(3, 1). For $\eta = 2.0$ the short 3D (5, 2, 1), (6, 2, 1), (7, 2, 1) and (8, 2, 1) POs determine the major pattern of the shell energy. Thus, we emphasize that the amplitude enhancement owing to the bifurcations of these POs is responsible for the formation of the shell structure at large deformations around the superdeformed shape where the second well of the double-humped barrier

Comparison with quantum numerical results

In Figs. 2 and 3, we present the semiclassical shell-correction energies δE , see Eq. (11), versus the particle number parameter $N^{1/3}$ for various critical deformations (ISPM, dotted lines) as compared with the corresponding quantum-mechanical (“Quantum”) results (solid lines). We observe a very good agreement of the shell (and super) shell structure at all deformations. Close examination of different PO contributions shows that for the deformation $\eta = 1.2$ in upper panel of Fig. 2, a good convergence is obtained by including only the shortest elliptic 2D and EQ POs. For $\eta = \sqrt{2}$ the bifurcation of double-repeated short diameters in the equatorial plane into that and meridian butterflies becomes also important. In the superdeformation region near $\eta = 1.618 \dots$ (see Fig. 3) the bifurcations of the EQ star (5, 2) and the simplest 3D (5, 2, 1) POs, and the hyperbolic 2D PO (4, 2, 1) become dominating.

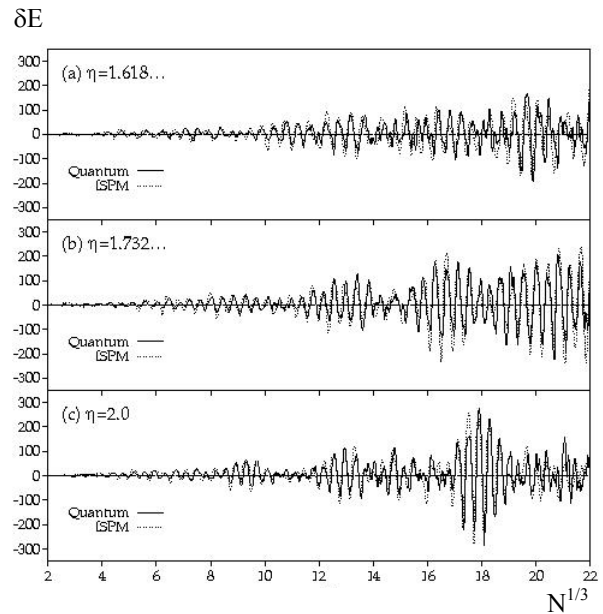


Fig. 3. The same at other bifurcations $\eta = 1.618 \dots, 1.732 \dots, 2.0$.

occurs, as it was earlier predicted in [8]. This is in good agreement with the ISPM vs QM comparison of the level-density shell corrections at the critical deformations as well with the quantum Fourier transformation of the level density $g(k)$ as function of the wave number k to the PO length variable L in the so called Fourier spectra [15]. Therefore, the shell-structure amplitude enhancement owing to the PO bifurcations is the physical phenomenon observed in quantum calculations of the shell corrections and can be interpreted as the reason for

the second well of the Strutinsky double-humped fission barrier at large deformations within the spheroid nuclear model.

For perspectives, it would be worth to apply the general points of this semiclassical theory to the shell corrections of the moment of inertia [17] for rotating nuclei as well as for the transport coefficients (e.g., inertia parameter) of the low-lying collective excitations [18] in the nuclear collective dynamics of fission processes.

Conclusions

1. We derived the semiclassical *ISPM* trace formulas as sums over contributions of *families and isolated* POs which are *continuous* through *all symmetry-breaking and bifurcation* points.

2. We found *enhancement* of the shell structure near *bifurcations* in the *superdeformed* region.

3. Our *ISPM* results for the level densities averaged with the gross-shell and more *thin-shell* structures and shell-structure energies for critical deformations are in good agreement with quantum SCM calculations.

4. Bifurcations of the shortest 3D POs from EQ orbits can be interpreted as responsible mainly for the superdeformed second well of the double-humped fission barrier, in line of earlier predictions in [6].

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**КВАЗИКЛАСИЧНА ОБОЛОНКОВА СТРУКТУРА
ТА ЯДЕРНІ ДВОГОРБИ БАР'ЄРИ***Пам'яті В. М. Струтинського***О. Г. Магнер**

За допомогою поліпшеного методу стаціонарної фази отримано квазікласичні густини рівнів як суми по ізольованих періодичних орбітах та їхніх сімействах. Установлено, що оболонкові поправки до енергій та до усередненої густини рівнів є неперервними функціями в точках порушення симетрії (біфуркацій) з правильною асимптотикою стандартного методу стаціонарної фази. Показано посилення ядерної оболонкової структури поблизу точок біфуркацій у супердеформованій області. Квазікласичні результати для усереднених компонент густини рівнів як у випадку великих оболонок, так і більш тонкої структури, а також для оболонкових поправок до енергії при критичних деформаціях добре узгоджуються з квантовими розрахунками для різних одночастинкових гамільтоніанів, зокрема з потенціалами, що мають різку стінку сфероїдальної форми. Підсилення оболонкової структури через біфуркації найкоротших екваторіальних орбіт у тривимірні приводить до появи другої ями в бар'єрі поділу ядер у супердеформованій області.

Ключові слова: ядерна оболонкова структура, бар'єри поділу, ядерні деформації, оболонкові поправки до енергії, квазікласична теорія періодичних орбіт, квантовий та класичний хаос.

**КВАЗИКЛАСИЧЕСКАЯ ОБОЛОЧЕЧНАЯ СТРУКТУРА
И ЯДЕРНЫЕ ДВУГОРБЫЕ БАРЬЕРЫ***Памяти В. М. Струтинского***А. Г. Магнер**

С помощью улучшенного метода стационарной фазы получены квазиклассические плотности уровней как суммы по изолированным периодическим орбитам и их семействам. Установлено, что оболочечные поправки к энергиям и к усредненной плотности уровней являются непрерывными функциями в точках нарушения симметрии (бифуркаций) с правильной асимптотикой стандартного метода стационарной фазы. Показано усиление ядерной оболочечной структуры вблизи точек бифуркаций в супердеформированной области. Квазиклассические результаты для усредненных компонент плотности уровней, как в случае больших оболочек, так и более тонкой оболочечной структуры, а также для оболочечных поправок к энергии при критических деформациях хорошо согласуются с квантовыми расчетами для различных одночастичных гамильтонианов, в частности с потенциалами, имеющими резкую стенку сфероидальной формы. Усиление оболочечной структуры из-за бифуркаций кратчайших экваториальных орбит в трехмерные приводит к появлению второй ямы в барьере деления ядер в супердеформированной области.

Ключевые слова: ядерная оболочечная структура, барьеры деления, ядерные деформации, оболочечные поправки к энергии, квазиклассическая теория периодических орбит, квантовый и классический хаос.

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