Semiclassical shell-structure moment of inertia within the phase-space approach

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Abstract
The moment of inertia for nuclear collective rotations was derived within the semiclassical approach based on the cranking model and the Strutinsky shell-correction method by using the non-perturbative periodic-orbit theory in the phase space variables. This moment of inertia for adiabatic (statistical-equilibrium) rotations can be approximated by the generalized rigid-body moment of inertia accounting for the shell corrections of the particle density. A semiclassical phase-space trace formula allows to express quite accurately the shell components of the moment of inertia in terms of the free-energy shell corrections for integrable and partially chaotic Fermi systems, in good agreement with the quantum calculations.

Keywords: Nuclear collective rotations, cranking model, shell corrections, periodic orbit theory.

1. Introduction
Many significant phenomena deduced from experimental data on nuclear rotations were explained within theoretical approaches based mainly on the cranking model [1, 2, 3, 4] and the Strutinsky shell-correction method [5, 6] extended by Pashkevich and Frauendorf [7, 8]. For a deeper understanding of the correspondence between classical and quantum physics of the shell components of the moment of inertia (MI), it is worth to analyze them within the semiclassical periodic-orbit theory (POT) [9, 10, 11, 12, 13, 14, 15]. See also Refs. [16, 17] for the semiclassical description of the so called “classical rotation” as an alignment of the particle angular momenta along the symmetry axis, but also the magnetic susceptibilities in metallic clusters and quantum dots [18]. The semiclassical perturbation expansion of Creagh [15] was used in the POT calculations [19] of the MI shell corrections for a spheroidal cavity mean field. The non-perturbative Gutzwiller POT extended to the bifurcation phenomena [20, 21, 22, 23] was applied in [25] within the cranking model for the adiabatic collective rotations (around an axis perpendicular to the symmetry axis) in the case of the harmonic-oscillator mean field. The MI Θ for the collective adiabatic (statistical-equilibrium) rotations was described as a sum of the Extended Thomas-Fermi (ETF) MI Θ_{ETF} [24] and shell corrections δΘ [25, 26]).

In the present work, we obtain a semiclassical phase-space trace formula for the MI shell components δΘ in terms of the free-energy shell corrections δF for integrable Hamiltonians, including those of the harmonic-oscillator mean field [25, 27] and a spheroidal cavity [21, 23], as well as for partially chaotic Fermi systems [26].

2. Cranking model for nuclear rotations
Within the cranking model, the nuclear collective rotation of the independent-particle Fermi system is associated with a many-body Hamiltonian (Routhian)
\[ H_\omega = H - \omega \ell_x, \]
and its eigenvalue equation is given by
\[ H_\omega \psi_\omega^i = \varepsilon_\omega^i \psi_\omega^i. \]
The frequency (Lagrange multiplier) ω is determined by the angular momentum projection I_x onto the x axis (perpendicular to the symmetry z axis) through the constraint for ω = ω(I_x),
\[ \langle \ell_x \rangle_\omega \equiv d_s \sum_i n_i^x \int d\mathbf{r} \psi_\omega^i(\mathbf{r}) \ell_x \bar{\psi}_\omega^i(\mathbf{r}) = I_x, \]
where \( \ell_x \) and \( n_i^x \) are respectively the particle angular-momentum projection onto the x axis and the occupation...
numbers,
\[ n_i^\omega = \left[ 1 + \exp \left( \frac{\varepsilon_i^\omega - \lambda^\omega}{T} \right) \right]^{-1}, \]  
(4)

\( T \) is the temperature. In the following \( \lambda^\omega \) is the chemical potential, and \( d_\omega \) the spin (spin-isospin) degeneracy. Brackets, like in \( \langle \ell_x \rangle \) indicate a quantum average and a bar above the functions the complex conjugation. For simplicity, the spin degree of freedom is included here only through the degeneracy factor \( d_\omega \), and then, the moment of inertia \( \Theta_x \) can be considered as the following susceptibility:
\[ \Theta_x(\omega) = \frac{\partial \langle \ell_x \rangle \omega}{\partial \omega} = \frac{\partial^2 E(\omega)}{\partial \omega^2}, \]  
(5)
where
\[ E(\omega) = \langle H \rangle_\omega = d_\omega \sum_i n_i^\omega \int d\psi_i^\omega(\mathbf{r}) \ H \overline{\psi_i^\omega}(\mathbf{r}) \]  
(6)
is the energy \( E(I_x) \) of the yrast line due to the constraint (3). For the particle number conservation, one has
\[ N = d_\omega \sum_i n_i^\omega \int d\psi_i^\omega \overline{\psi_i^\omega} = d_\omega \sum_i n_i. \]  
(7)

In the coordinate representation, Eq. (5) can be re-written for the adiabatic rotations through the one-body Green’s function \( G \):
\[ \Theta_x = \frac{2d_\omega}{\pi} \int_0^\infty d\varepsilon \ n(\varepsilon) \int d\mathbf{r}_1 \int d\mathbf{r}_2 \ell_x(\mathbf{r}_1) \ell_x(\mathbf{r}_2) \times \text{Re}[G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)] \text{Im}[G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)]. \]  
(8)
This representation is useful within the semiclassical POT, weakening the criterium of the quantum perturbation approximation: The rotation excitation energy \( h\omega \) becomes smaller than the distance between major shells \( h\Omega \) \( (h\Omega \approx \varepsilon_F/\sqrt{N^{1/3}} \) with the Fermi energy \( \varepsilon_F \)). This is in contrast to the quantum criterium of smallness of the excitation energies with respect to the nearest neighbor single-particle (s.p.) level spacing around the Fermi surface.

3. Semiclassical Green’s function and particle density

For the s.p. Green’s function \( G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) \), we shall use the semiclassical Gutzwiller trajectory expansion [10],
\[ G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) \approx G_{\text{sc}l}(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) = \sum_{\text{CT}} G_{\text{CT}}, \]
\[ G_{\text{CT}} = A_{\text{CT}} \exp \left[ i \frac{S_{\text{CT}}(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) - i\pi}{2} \mu_{\text{CT}} \right], \]  
(9)
where the sum runs over the classical trajectories (CT) from point \( \mathbf{r}_1 \) to point \( \mathbf{r}_2 \) with the particle energy \( \varepsilon \) (see Fig. 1). \( A_{\text{CT}}(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) \) is the amplitude depending on the

CTs degeneracy (in the case \( \mathbf{r}_1 = \mathbf{r}_2 \)) and their stability propagator, \( S_{\text{CT}}(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) \) is the particle action, \( \mu_{\text{CT}} \) the Maslov phase determined by the caustic and turning catastrophe points along the CT [10, 11, 12, 15, 22].

There are several reasons leading to oscillations of the MI in Eq. (8), local and non-local, where only the local part is related to the shell effects, whereas non-local contributions could have their origin in reflections of the particle from the boundary. The nearly local approximation \( (|\mathbf{s}_{12}| = |\mathbf{r}_2 - \mathbf{r}_1| \ll R) \) is valid after a statistical averaging over many microscopic quantum states. Then, the small parameter, which is the product of the two dimensionless quantities \( \omega/\Omega \) and \( S/\hbar \), used in [19] for applying the perturbation approach of Creagh to the classical dynamics [15] becomes in our approach more weak, \( (\omega/\Omega) S/\hbar \gg 1 \), under the usual semiclassical condition \( S/\hbar \sim k_F R \sim N^{1/3} \gg 1 \), where \( k_F = p_F/\hbar \) is the Fermi momentum in \( \hbar \) units and \( R \) is the mean nuclear radius. According to (9), one can split the Green’s function \( G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) \) into a contribution \( G_{\text{CT}0} \) coming from the direct path between the two points and a contribution \( G_{\text{CT}1} \) that contains the contributions from all other trajectories involving reflections
\[ G_{\text{sc}l} = G_{\text{CT}0} + G_{\text{CT}1}, \]  
(10)
where \( G_{\text{CT}0} \) is the component related to the trajectory \( \mathbf{r}_2 \) for which the action \( S_{\text{CT}0} \) disappears in the limit \( \mathbf{r}_2 \rightarrow \mathbf{r}_1 \). One obtains
\[ G_{\text{CT}0} = - \frac{m}{2\pi \hbar^2 s_{12}} \exp \left[ i \frac{S_{12}(\mathbf{r})}{\hbar} \right], \]  
(11)
with the nucleon mass \( m \), the particle momentum \( p(\mathbf{r}) = \sqrt{2m[\varepsilon - V(\mathbf{r})]} \), \( \mathbf{r} = (\mathbf{r}_1 + \mathbf{r}_2)/2 \), and the potential \( V(\mathbf{r}) \).

For a semiclassical statistical equilibrium rotation with constant frequency \( \omega \), one finds [25, 26] according to (8),
\[ \Theta \approx \Theta_{\text{GRB}} = m \int d\mathbf{r} r_2^2 \rho_{\text{sc}l}(\mathbf{r}) = \Theta_{\text{ETF}} + \delta\Theta_{\text{sc}l}, \]  
(12)
where $ \Theta_{\text{GRB}} = \Theta_{\text{GRB}}^{\text{ETF}} + \delta \Theta_{\text{GRB}}^\text{cl}$ is the generalized rigid-body (GRB) MI, with [24, 26]

$$\Theta_{\text{ETF}} \approx \Theta_{\text{GRB}}^{\text{ETF}} = m \int dr_1^2 \rho_{\text{ETF}}(r) \tag{13}$$

and $\delta \Theta_{\text{cl}}$ its shell correction [25, 26],

$$\delta \Theta_{\text{cl}} \approx \delta \Theta_{\text{GRB}}^{\text{cl}} = m \int dr_1^2 \delta \rho_{\text{cl}}(r) \tag{14}$$

with $r_1^2 = y_1^2 + z_1^2$. Such a splitting (12) is associated with that of the spatial particle density $\rho(r)$,

$$\rho(r) = -\frac{1}{\pi} \text{Im} \int d\varepsilon \ n(\varepsilon) [G(r_1, r_2; \varepsilon)]_{r_1 = r_2 = r} , \tag{15}$$

and the one of equation (10) in terms of its ETF particle density $\rho_{\text{ETF}}$ and its shell correction $\delta \rho_{\text{cl}}(r)$,

$$\rho_{\text{cl}}(r) = \rho_{\text{ETF}} + \delta \rho_{\text{cl}}(r), \tag{16}$$

where

$$\rho_{\text{ETF}}(r) = -\frac{1}{\pi} \text{Im} \int d\varepsilon \ \bar{n}(\varepsilon)[G_{\text{CT}_0}(r_1, r_2; \varepsilon)]_{r_1 = r_2 = r} \tag{17}$$

and

$$\delta \rho_{\text{cl}}(r) = -\frac{1}{\pi} \text{Im} \int d\varepsilon \ \delta n(\varepsilon)[G_{\text{CT}}(r_1, r_2; \varepsilon)]_{r_1 = r_2 = r} \tag{18}$$

The standard decomposition of the occupation numbers $n = \bar{n} + \delta n$ into the smooth and fluctuating parts is used as usually in the shell correction method [6].

4. Phase space trace formulas

Substituting (15) and (9) into the integrand (12), for the total semiclassical MI $\Theta_x$, one obtains the phase-space trace formula:

$$\Theta_{\text{cl}} \approx d_s m \int d\varepsilon \ n(\varepsilon) \frac{dr_1^2 dp_1}{(2\pi\hbar)^3} \frac{r_1^2}{\varepsilon} f_{\text{cl}}(r_2, p_1, \varepsilon) \tag{19}$$

$$\approx \Theta_{\text{ETF}} + \delta \Theta_{\text{cl}},$$

where

$$f_{\text{cl}}(r_2, p_1, \varepsilon) = G_{\text{cl}}(r_2, p_1, \varepsilon) \exp \left[ i \frac{1}{\hbar} \frac{r_2^2}{\varepsilon} \right] \tag{20}$$

and where now $r_2^2 = y_2^2 + z_2^2$. Here $G_{\text{cl}}(r_2, p_1, \varepsilon)$ is a semiclassical Green’s function in the mixed phase-space representation obtained by the Fourier transformation of the Green’s function $G_{\text{cl}}(r_1, r_2, \varepsilon)$, Eq. (9),

$$G_{\text{cl}}(r_2, p_1, \varepsilon) = \text{Re} \sum_{CT} \left| J_{\text{CT}}(p_1^\perp, p_2^\perp) \right|^{1/2} \left[ \delta[\varepsilon - H(r_2, p_2)] \right] \times \exp \left\{ \frac{i}{\hbar} S_{\text{CT}}(r_1, r_2, \varepsilon) - i\frac{\pi}{2} \mu_{\text{CT}} \right\} \tag{21},$$

where $J_{\text{CT}}(p_1^\perp, p_2^\perp)$ is the Jacobian for the transformation from the perpendicular-to-CT momentum $p_1^\perp$ to the $p_2^\perp$ one. We inserted formally the additional integral over $r_1$ with the $\delta(r_2 - r_1)$ function in (12) and transformed the spacial coordinates $r_1$ and $r_2$ to the phase-space variables $r_2$ and $p_1$ [22, 26]. Using then the Fourier transformation of this $\delta$ function from the coordinate difference $r_2 - r_1$ to a new momentum $\tilde{p}$ and integrating the MI in such a phase space representation over perpendicular-to-CT components of $\tilde{p}$ by the stationary phase method, one arrives at (19). Note that the ETF component of the Green’s function $CT_0$ (10) under the nearly local approximation $(r_1 \rightarrow r_2 \rightarrow r$ and $p_1 \rightarrow p_2 \rightarrow r)$ is related to the Thomas-Fermi spectral function (20)

$$f_{\text{cl}}(r, p, \varepsilon) \rightarrow f_{\text{TF}}(r, p, \varepsilon) = \delta(\varepsilon - H(r, p)). \tag{22}$$

Equation (19) looks similar (the same besides of the factor $m r_1^2/\varepsilon$) to the semiclassical s.p. energy $E_{\text{cl}}$,

$$E_{\text{cl}} = d_s \int d\varepsilon \ n(\varepsilon) g_{\text{cl}}(\varepsilon) = d_s \int d\varepsilon \ n(\varepsilon) \int \frac{dr_2 dp_1}{(2\pi\hbar)^3} \times \ f_{\text{cl}}(r_2, p_1, \varepsilon) \approx E_{\text{ETF}} + \delta E_{\text{cl}}, \tag{23}$$

where $E_{\text{ETF}}$ is the ETF energy and $\delta E_{\text{cl}}$ the energy shell correction. We used also the phase-space trace formula for the semiclassical level density $g_{\text{cl}}(\varepsilon)$ [10, 11, 12, 15, 22, 23] with a similar decomposition,

$$g_{\text{cl}}(\varepsilon) = \int \frac{dr_2 dp_1}{(2\pi\hbar)^3} f_{\text{cl}}(r_2, p_1, \varepsilon) \tag{24}$$

$$\approx \delta g_{\text{TF}}(\varepsilon) + \delta g_{\text{cl}}(\varepsilon). \tag{25}$$

Therefore, multiplying and dividing identically (19) by the energy $E_{\text{cl}}$ (23), one finally arrives at

$$\Theta_{\text{cl}} \approx m \left( \frac{r_2^2}{\varepsilon} \right) E_{\text{cl}}, \tag{26}$$

where the brackets mean the average over the phase space variables $r_2, p_1$ and energy $\varepsilon$ with a weight $\varepsilon$,

$$\langle \frac{r_2^2}{\varepsilon} \rangle = \frac{\int d\varepsilon \ v \int \frac{dr_2 dp_1}{(2\pi\hbar)^3} f_{\text{cl}}}{\int d\varepsilon \ v \int \frac{dr_2 dp_1}{(2\pi\hbar)^3}}. \tag{27}$$

Using now the same subdivision in terms of the ETF and shell components for the MI (19) and s.p. energy (23), after the statistical averaging for a finite temperature $T$ one finds

$$\delta \Theta_{\text{cl}} \approx m \left( \frac{r_2^2}{\varepsilon} \right) \delta F, \tag{28}$$

where $\delta F$ is the free-energy shell correction. Here we used the stationary phase (periodic orbit (PO)) conditions for the evaluation of integrals over the phase-space variables $r_2$ and $p_1$ [22]. Within the POT, at a given temperature $T$, one has the PO sum [11, 12, 16, 18, 25, 26]

$$\delta F = \sum_{PO} \frac{\pi t_{PO} T/\hbar}{\sinh(\pi t_{PO} T/\hbar)} \delta E_{\text{PO}}, \tag{29}$$
where $\delta E_{\text{PO}}$ is the PO component of the energy shell-correction,

$$
\delta E \approx \delta E_{\text{scl}} = \sum_{\text{PO}} \delta E_{\text{PO}} \quad \text{with}
$$

$$
\delta E_{\text{PO}} = \frac{\hbar^2}{m t_{\text{PO}}} \delta g_{\text{PO}}(\lambda).
$$

Here $t_{\text{PO}}$ and $\delta g_{\text{PO}}(\varepsilon)$ are the period of the particle motion along the PO (accounting for its repetition number) and the PO component of the oscillating (shell) correction to the level density, taken both at the chemical potential $\varepsilon = \lambda$ for $\omega = 0$, which, at zero temperature, is equal to the Fermi energy $\varepsilon_f$. This PO component can be represented as

$$
\delta g_{\text{PO}}(\varepsilon) = \sum_{\text{PO}} \delta g_{\text{PO}}(\varepsilon),
$$

where

$$
\delta g_{\text{PO}}(\varepsilon) = \text{Re} \left\{ B_{\text{PO}} \exp \left[ \frac{i}{\hbar} S_{\text{PO}}(\varepsilon) - \frac{i \pi}{2} \mu_{\text{PO}} \right] \right\},
$$

with $B_{\text{PO}}$ the amplitude of the density oscillations depending on the PO classical degeneracy and stability, and $S_{\text{PO}}(\varepsilon)$ the action along the PO [10, 11, 12, 15, 26, 23]. In (25), $g_{\text{ETF}}(\varepsilon)$ is the smooth ETF component and $\delta g_{\text{scl}}(\varepsilon)$ the semiclassical oscillating contribution [15] where the latter can be expressed in terms of the PO sum, Eqs. (31) and (32). The POs appear through the stationary phase (PO) condition for the calculation of the integrals over $r_2$ and $p_1$ in (24) by the improved stationary phase method [21, 22, 23] as mentioned above. For the phase space average $\langle r_1^2 / \varepsilon \rangle$, Eq. (27), one again obtains approximately, through the Green’s function (21), a decomposition into an ETF and a shell-correction contributions:

$$
\langle r_1^2 / \varepsilon \rangle \approx \langle r_1^2 / \varepsilon \rangle_{\text{ETF}} + \delta \langle r_1^2 / \varepsilon \rangle.
$$

5. Comparison with quantum calculations

In Figs. 2 and 3, we show the quantum and semiclassical energy shell corrections $\delta E$ for the spheroidal cavity at small (almost no contributions from PO bifurcations) and large deformations (important contributions of PO bifurcations). At zero temperature, the energy shell correction $\delta E$ corresponds to the free-energy shell correction $\delta F$. With increasing temperature $T$, one observes an exponential decrease of the free-energy shell corrections $\delta F \sim \exp(-\pi t_{\text{PO}} T / \hbar)$ [16, 18, 25, 26]. Minima of the energy shell corrections $\delta E$ are related to magic particle numbers.

Evaluating the factor $\langle r_1^2 / \varepsilon \rangle$ of Eq. (27) in (28) within the simplest TF approximation for the level density $g_{\text{scl}}(\varepsilon) \approx g_{\text{TF}}(\varepsilon)$ (25) and the TF spectral function $f_{\text{scl}} \approx f_{\text{TF}}$ (22) corresponding to the CTM component of the Green’s function (21) in the nearly local approximation, one can simply neglect $\hbar$ corrections (surface and curvature terms) and shell effects. For the spheroidal cavity potential, one obtains from (27) and (22)

$$
\langle r_1^2 / \varepsilon \rangle \approx \langle r_1^2 / \varepsilon \rangle_{\text{TF}} = \frac{a^2 + b^2}{3\lambda},
$$

where $a$ and $b$ are the semi-axes of the spheroidal cavity, $a^2 b = R^3$, $R$ is the radius of the equivalent sphere. Using this estimate, one may evaluate the MI shell correction for two selected deformations $\eta = b/a$ (see Fig. 4 and 5).

One notices that there is a large supershell effect in both $\delta E$ and $\delta \Theta_x$. The shell structure is much enhanced by the bifurcations of the shorter 3-dimensional (3D) orbits from the parent equatorial (EQ) orbits [21] at $\eta = 2$. Both kinds of PO families yield the essential contributions through $\delta F$, in contrast to the classical perturbation results of [19].

Fig. 2: Semiclassical (SCL ISPM, i.e. using the improved stationary phase method) and quantum (QM) shell corrections $\delta E$ versus the particle number variable $N^{1/3}$ for the spheroidal cavity potential (in units of $\varepsilon_0 = \hbar^2/2mR^2$) for the deformation $\eta = b/a = 1.2$ (after [21]).

Fig. 3: The same as in Fig. 2 but for a large deformation $\eta = 2.0$ (after [21]).
Fig. 4: Comparison of quantum (QM) and semiclassical (SCL ISPM) moment of inertia shell corrections $\delta \Theta_x^{(2)}$ (in single-particle units $mR^2$) in the case of the perpendicular collective rotation at zero temperature as function of $N^{1/3}$ at the same deformation as in Fig. 2.

Fig. 5: Same as Fig. 4 but for a deformation $\eta = 2.0$.

where the EQ orbits do not contribute and 3D PO contributions are not considered. Our non-perturbation results for the MI shell corrections can be applied for larger rotational frequencies and larger deformations ($\eta \sim 1.5 - 2.0$) where the bifurcations play the dominating role like in the case of the deformed harmonic oscillator [25].

6. Conclusions

We derived the shell components $\delta \Theta$ of the moment of inertia in terms of the free-energy shell correction $\delta F$ within the non-perturbative extended Gutzwiller POT for any effective mean-field potential using the phase-space variables. For the deformed spheroidal cavity and the harmonic oscillator potentials, we found a good agreement between the semiclassical POT and quantum results for $\delta F$ and $\delta \Theta$ using the Thomas-Fermi approximation for $\langle r^2 / \varepsilon \rangle$ at several critical deformations and temperatures. For smaller temperatures a remarkable interference of the dominant short three-dimensional and parent equatorial orbits and their bifurcations in the superdeformed region are shown. For larger temperatures, the shorter EQ orbits are dominant in this comparison. An exponential decrease of the shell corrections with increasing temperature is analytically demonstrated.

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