Semiclassical and quantum shell-structure calculations of the moment of inertia

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Shell corrections to the moment of inertia (MI) are calculated for a Woods-Saxon potential of spheroidal shape. For the statistical equilibrium collective rotations under consideration, the MI is obtained within the cranking model in an approach which goes beyond the quantum perturbation approximation based on the non-perturbative energy spectrum. For the calculation of the MI shell corrections, the Strutinsky smoothing procedure is used to obtain the average occupation numbers of the particle density using the solutions of the Woods-Saxon eigenvalue problem. We found that these shell components are practically proportional to those of the energy shell corrections, in qualitative agreement with the semiclassical results obtained analytically for the spheroidal cavity within the periodic orbit theory.

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I. INTRODUCTION

Many significant phenomena in nuclear rotations can be explained within the theoretical approaches based on the cranking model [1–5], and the Strutinsky shell-correction method (SCM) [6, 7]. This approach was extended by Pashkevich and Frauendorf [8, 9] to the description of collective rotational bands. For a deeper understanding of the correspondence between the classical and the quantum approach and their applications to high-spin physics, it is worthwhile to analyze the shell components of the moment of inertia (MI) within the semiclassical periodic-orbit theory (POT) [10–20]. The cranking model is, to some extent, of semiclassical nature because the collective rotation of the nuclear many-body systems is described as a classical transformation from the laboratory to the body-fixed coordinate system, rotating around the former with fixed angular velocity [4, 5]. Using this semiclassical picture, one can reduce the complex problem of the rotation of a many-body system to a much simpler diagonalization of an effective mean-field (one-body) Hamiltonian in the rotating frame. Its spectrum can be considered as quasi-continuous, since the rotational excitations are not small as compared with the distances between non-perturbative neighboring levels, thus violating the condition of applicability of the quantum perturbation expansion. One could, however, consider another perturbation approach based on the concept of a statistical equilibrium rotation with a generalized rigid-body (GRB) moment of inertia \( \Theta_{\text{GRB}} \) [21] (see Refs. [19, 22–26]),

\[
\Theta \approx \Theta_{\text{GRB}} = m \int \, d\mathbf{r} \, r_\perp^2 \rho(\mathbf{r}) ,
\]

where \( m \) is the nucleon mass, \( r_\perp \) the distance between a given point \( \mathbf{r} \) of the nucleus and the rotation axis, and \( \rho(\mathbf{r}) = \bar{\rho} + \delta \rho(\mathbf{r}) \) the one-body quantum particle-number density. According to the SCM [6, 7], \( \bar{\rho} \) is a smooth density and \( \delta \rho(\mathbf{r}) \) its shell correction. It is obviously this shell component \( \delta \rho(\mathbf{r}) \) which determines the MI shell correction \( \delta \Theta \approx \delta \Theta_{\text{GRB}} \).

The semiclassical perturbation expansion [16, 27] by Greagh has been used in the POT calculations of the MI shell corrections for a spheroidal cavity mean field [28]. The nonperturbative Gutzwiller POT, extended to the bifurcation phenomena at large deformations [20, 29–31], on the other hand, was applied [25] within the cranking model and a harmonic-oscillator mean field to describe collective rotations (around an axis perpendicular to the symmetry axis). For adiabatic collective rotations (rotations at statistical equilibrium) the MI is then described as the sum of a smooth Extended Thomas-Fermi (ETF) MI \( \Theta_{\text{ETF}} \) [22, 32] and shell corrections \( \delta \Theta \) [19, 22–24]. In a more realistic description of the MI for collective rotations, the ETF approach has already been successful, as in the case of the nuclear energy [33], by including self-consistency and spin effects into the calculations [22, 32].

As shown in Refs. [19, 22–24], one can obtain, through a semiclassical phase-space trace formula, with a good approximation, analytical expressions for MI shell components \( \delta \Theta \) in terms of the energy shell corrections \( \delta E \), for an arbitrary potential well,

\[
\delta \Theta \propto \delta E ,
\]

a relation which has been worked out for integrable Hamiltonians, such as for a harmonic oscillator [22, 25] or a spheroidal-cavity [19, 23, 24] mean field. Corrections accounting for a finite surface diffuseness and finite temperature effects of the nuclear system can also been taken into account as demonstrated in Refs. [24] and [19], respectively. The exponential decrease of the MI shell corrections \( \delta \Theta \) with increasing temperature and the possibility to express \( \delta \Theta \) through the free-energy shell corrections \( \delta F \) have in particular been discussed in Ref. [19]. For the deformed Woods-Saxon (WS) potential well (of

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spheroidal type) with large depth and small surface diffuseness, as in Refs. [14, 31], we are going, in the present study, to compare the quantum MI shell corrections \( \delta \Theta \) with the energy shell corrections calculated both by the SCM, which will allow us to assess the validity of the semiclassical POT relationship (2) [19, 22, 24, 25].

II. MI SHELL CORRECTIONS

A. The cranking model

Collective rotations of a Fermi system associated with a many-body Hamiltonian can be described in the independent-particle approximation by the cranking model. The complex problem of a rotating many-body Fermi system can then be reduced, in the restricted subspace of Slater determinants, to a much simpler eigenvalue problem of a single-particle (s.p.) Hamiltonian

\[
\hat{H}^\omega = \hat{H} - \omega \cdot \hat{\ell} = \hat{H} - \omega \cdot \hat{\ell}_x ,
\]

where \( \hat{\ell}_x \) is the s.p. angular-momentum operator with component \( \hat{\ell}_x \), having defined \( 0x \) as rotation axis perpendicular to the symmetry \( 0z \) axis. The Hamiltonian (3) is usually referred to as the Routhian. For simplicity, we shall discard the spin and isospin degrees of freedom, in particular the spin-orbit and asymmetry interactions. The rotation frequency \( \omega \) of the body-fixed coordinate system with respect to the laboratory frame is the Lagrange multiplier of our problem, associated with the constraint on the nuclear angular momentum \( I_x \). The angular velocity \( \omega \) needs to be adjusted in such a way that the quantum average \( \langle \hat{\ell}_x \rangle^\omega \) of the s.p. angular-momentum operator \( \hat{\ell}_x \) yields the required angular momentum \( I_x \). This quantum average is obtained in a similar way as the expectation value of the many-body Routhian in the subspace of Slater determinants,

\[
\langle \hat{\ell}_x \rangle^\omega \equiv d_s \sum_i n_i^\omega \int d\mathbf{r} \psi_i^\omega (\mathbf{r}) \hat{\ell}_x \overline{\psi}_i^\omega (\mathbf{r}) = I_x ,
\]

where, \( d_s \) is the spin (spin-isospin) degeneracy of the s.p. states, \( n_i^\omega \) their occupation numbers, with corresponding eigenvalues \( \varepsilon_i^\omega \) and eigenfunctions \( \psi_i^\omega (\mathbf{r}) \) of \( \hat{H}^\omega \), Eq. (3), and \( \overline{\psi}_i (\mathbf{r}) \) their complex conjugate. For relatively small angular velocities \( \omega \) and at zero nuclear temperature, the chemical potential \( \lambda^\omega \) is, to a good approximation, equal to the Fermi energy: \( \lambda^\omega \approx \varepsilon_F = \hbar^2 k_F^2 / 2m \), where \( \hbar k_F \) is the Fermi momentum. Within the same approach, one approximately has for the particle number

\[
N = d_s \sum_i n_i^\omega \int d\mathbf{r} \psi_i^\omega (\mathbf{r}) \overline{\psi}_i (\mathbf{r}) \approx d_s \int_0^{\infty} d\varepsilon \ n^\omega (\varepsilon) .
\]

This equation determines the chemical potential \( \lambda^\omega \) for a given number \( N \) of nucleons.

B. MI as a collective response

Since the continuous parameter \( \omega \) is introduced and the uncertainty relation between the angular momentum and the rotation angles of the body-fixed coordinate system is neglected, the cranking model is semiclassical in nature [5, 19, 23, 24]. One may thus consider the collective MI \( \Theta_x \), for a rotation around the \( x \) axis, as the response of the quantum average \( \delta \langle \hat{\ell}_x \rangle^\omega \) to the external cranking field \( -\omega \hat{\ell}_x \), Eq. (3) [18, 19, 22–25, 34–36],

\[
\delta \langle \hat{\ell}_x \rangle^\omega = \Theta_x \delta \omega ,
\]

where

\[
\Theta_x = \partial \langle \hat{\ell}_x \rangle^\omega / \partial \omega = \partial^2 E(\omega) / \partial \omega^2 ,
\]

with \( E(\omega) = \langle \hat{H} \rangle^\omega \approx E(0) + I_x^2 / (2\Theta_x) \). For a nuclear rotation around the \( x \) axis, one can treat, as shown in Refs. [1, 3, 4, 8, 9], the term \( -\omega \hat{\ell}_x \) as a small perturbation. With the constraint (4) and the MI, Eq. (7), if treated in second-order quantum perturbation theory, one obtains the well-known Inglis cranking formula [1, 4, 5].

For the derivation of the MI shell corrections within the SCM [6, 8, 9], beyond the quantum perturbation approach, it turns out to be helpful to use the coordinate representation of the MI through the s.p. Green’s functions \( G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) \) as this was done for the other transport coefficients in Ref. [19, 25, 34, 36]. Taking advantage of the analogy of our problem of a rotating many-body system with magnetism, where the magnetization \( M \) is proportional to the field strength \( B \) with the magnetic susceptibility \( \chi \) as the proportionality constant, the MI \( \Theta_x \), Eq. (7), can be expressed in a coordinate representation, as a kind of susceptibility, or as the response function for collective vibrations [19], in terms of the Green’s function \( G \) (see also Refs. [22–24, 34]). For adiabatic rotations, one then has

\[
\Theta_x = \frac{2d_s}{\pi} \int_0^{\infty} d\varepsilon \ n(\varepsilon) \int d\mathbf{r}_1 \int d\mathbf{r}_2 \hat{\ell}_x (\mathbf{r}_1) \hat{\ell}_x (\mathbf{r}_2) \times \text{Re} \ [G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)] \ \text{Im} \ [G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)] ,
\]

where \( \ell = |\mathbf{r} \times \mathbf{p}| \) is the particle angular momentum. Formally, with the help of the spectral representation of the Green’s function \( G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) \), one can also obtain from Eq. (8) the famous Inglis formula for the MI [4, 5].

Within the semiclassical POT, the coordinate representation (8) is extremely useful, since it allows to weaken the applicability criterion of the quantum perturbation approximation, because the maximal rotational excitation energy \( \hbar \Omega \) for which the approximation is valid becomes now significantly larger than the nearest-neighbor s.p. level spacing around the Fermi surface \( \varepsilon_F \). At the same time, \( \hbar \Omega \) still remains somewhat smaller than the energy distance between major shells \( \hbar \Omega \approx \varepsilon_F / N^{1/3} \) as shown by Migdal [37]. These two conditions are in contrast to the quantum perturbation approach where, in the derivation of the standard Inglis cranking formula the
excitation energies are required to be small with respect to the s.p. level spacing. This more severe restriction obviously comes about when using the spectral representation of the Green’s function $G$ in Eq. (8).

C. Statistically equilibrium rotation

For a semiclassical statistical-equilibrium rotation with constant frequency $\omega$, one approximately obtains [19, 22, 25] Eq. (1) for the MI $\Theta_x$ in terms of the GRB MI (to simplify the notation, the sub-script $x$ will be omitted in what follows),

$$\Theta \approx m \int \mathrm{d}r \, r_\perp^2 \rho(r) = \bar{\Theta} + \delta \Theta ,$$  \hspace{1cm} (9)

with $r_\perp^2 = y^2 + z^2$ and the smooth part $\bar{\Theta} = m \int \mathrm{d}r \, r_\perp^2 \bar{\rho}(r)$ of the MI [19, 22, 23, 25, 32], while the shell correction is given by [19, 22, 23, 25],

$$\delta \Theta = m \int \mathrm{d}r \, r_\perp^2 \delta \rho(r) .$$ \hspace{1cm} (10)

Eq. (9) is a local approximation (valid for the statistically averaged rotation [21, 22, 25]) to the general equation (8).

The separation in (9) of the MI into a smooth (average) part and a shell correction has, of course, its origin in the corresponding subdivision of the spatial particle density

$$\rho(r) = -\frac{1}{\pi} \mathrm{Im} \int \mathrm{d}\varepsilon \, n(\varepsilon) \left[ G(r, r_2; \varepsilon) \right]_{r_1 = r_2 = r} = \bar{\rho} + \delta \bar{\rho}$$ \hspace{1cm} (11)

into a smooth part $\bar{\rho}$ and a shell correction given by

$$\delta \rho(r) = -\frac{1}{\pi} \mathrm{Im} \int \mathrm{d}\varepsilon \, \delta n(\varepsilon) \left[ G(r, r_2; \varepsilon) \right]_{r_1 = r_2 = r} .$$

Eq. (11) is stemming originally from the standard decomposition of the occupation numbers into smooth and fluctuating (shell) parts as usual in the SCM [7]

$$n = \bar{n} + \delta n .$$ \hspace{1cm} (12)

III. QUANTUM CALCULATIONS

In this section, we will describe a system of independent fermions (nucleons) moving in a deformed mean field of the form of a Woods-Saxon (WS) of spheroidal shape with $\Omega$ as symmetry axis.

One then has to solve the Schrödinger equation with a potential

$$V(r, \theta) = \frac{V_0}{1 + \exp \left\{ \left[ r - R(\theta) \right] / \alpha \right\} ,} \hspace{1cm} (13)$$

where $R(\theta)$ denotes the radius of the spheroidal surface [19, 40, 41] in spherical coordinates $\{r, \theta, \varphi\}$ and $\alpha$ the surface diffuseness. Introducing semi-axes $a$ and $b$ through the equation

$$(x^2 + y^2)/a^2 + z^2/b^2 = 1 ,$$ \hspace{1cm} (14)

where, because of volume conservation, one must require that $a^2b = R_0^3$, with $R_0$ the radius of the corresponding spherical shape, one can define through

$$\eta = \frac{b}{a}$$ \hspace{1cm} (15)

a deformation parameter that will be larger one for prolate ($b > a$) and smaller one for oblate ($a > b$) shapes.

To solve the Schrödinger (eigenvalue) equation with the potential (13) one can conveniently use the expansion of the WS eigenfunctions in terms of the well-known deformed axially-symmetric harmonic-oscillator (HO) basis [38], as explained in the appendix. The particle density $\rho(q, z)$ can then be written in cylindrical coordinates $\{q, z, \varphi\}$, where $q = \sqrt{x^2 + y^2}$, in the standard form:

$$\rho(q, z) = \sum_i n_i |\psi_i(q, z, \varphi)|^2 ,$$ \hspace{1cm} (16)

where the WS eigenfunctions $\psi_i(q, z, \varphi)$ are given in terms of the HO eigenfunctions $\Phi_i$ [Eq. (A.2)]. For the MI of statistical equilibrium rotation one has $\Theta \approx \Theta_{\text{GRB}}$, where

$$\Theta_{\text{GRB}} = m \int \mathrm{d}r \, r_\perp^2 \rho(q, z) = \sum_i n_i \Theta_i$$ \hspace{1cm} (17)

with

$$\Theta_i = m \sum_{j, k} A_{ij} A_{ik} \left( J_j^y + J_k^z \right) .$$ \hspace{1cm} (18)

Here $A_{ij}$ are the expansion coefficients of the WS eigenfunctions in the HO basis (see Appendix). In Eq. (18) we also introduced

$$J_j^y = \int \mathrm{d}r \, y^2 \Phi_j^y(r) \Phi_k(r) = \frac{\hbar}{2m \omega_z} \delta_{n_j, n_k} Q_{n_j, n_k}^{(y)} ,$$ \hspace{1cm} (19)

and

$$J_j^z = \int \mathrm{d}r \, z^2 \Phi_j^z(r) \Phi_k(r) = \frac{\hbar}{m \omega_z} \delta_{n_j, n_k} Q_{n_j, n_k}^{(z)} ,$$ \hspace{1cm} (20)

with

$$Q_n^{(y)} = \int_0^\infty \xi \mathrm{d}\xi \, \exp(-\xi) \mathcal{L}_{n_z}(\xi) \mathcal{L}^{(A)}_{n_z}(\xi) ,$$ \hspace{1cm} (21)

and

$$Q_n^{(z)} = \int_{-\infty}^\infty \xi^2 \mathrm{d}\xi \, \exp(-\xi^2) \mathcal{H}_{n_z}(\xi) \mathcal{H}^{(A)}_{n_z}(\xi) .$$ \hspace{1cm} (22)

Finally, these functions are expressed in terms of the standard Hermite $\mathcal{H}_{n_z}(\xi)$ and associated Laguerre polynomials $\mathcal{L}^{(A)}_{n_z}(\xi)$ [see Eqs. (A.7) and (A.8) defined in the
new dimensionless variables $\xi$ and $\zeta$, Eq. (A.6). The calculation of the $\Theta_i$ in Eq. (18) is thus reduced to the determination of the transformation matrices $A_{jk}$ and the calculation of the simple integrals (21) and (22) which can be solved analytically through the orthogonality relations of the orthogonal polynomials $M(a, b, z)$ [39].

To study the correspondence between quantum and classical description we will carry our study with a WS potential (13) having a relatively sharp edge (small diffuseness) and a large depth, in order to simulate in this way the classical motion of particles inside a box of spheroidal shape.

IV. SEMICLASSICAL APPROACH

Within the POT, both the s.p. energy of the system and the MI can be subdivided into an average part and a semiclassical shell correction, as this has been done in Eq. (9). It is then possible [19, 23] to express these shell components through one another

$$\delta \Theta_{\text{scl}} \approx m \left( \frac{r^2}{\varepsilon} \right)_{\text{ETF}} \delta E_{\text{scl}} ,$$

(23)

where $\delta E_{\text{scl}}$ is the semiclassical energy shell correction, with a proportionality coefficient given by

$$\left( \frac{r^2}{\varepsilon} \right)_{\text{ETF}} = \frac{\int \frac{d\varepsilon}{\varepsilon} \int dr dp \left( \frac{r^2}{\varepsilon} \right) g_{\text{ETF}}(r, p; \varepsilon)}{\int \frac{d\varepsilon}{\varepsilon} \int dr dp g_{\text{ETF}}(r, p; \varepsilon)} ,$$

(24)

where $g_{\text{ETF}}(r, p; \varepsilon)$ is the ETF approximation to the semiclassical level-density distribution $g_{\text{scl}}(r, p; \varepsilon) = \frac{\partial f_{\text{scl}}(r, p)}{\partial \varepsilon}$ and $f_{\text{scl}}(r, p)$ is the Fermi distribution in phase-space [19, 24]. For the simple TF approach, one has

$$g_{\text{scl}}(r, p; \varepsilon) \approx g_{\text{TF}}(r, p; \varepsilon) = \delta(\varepsilon - H(r, p)) ,$$

(25)

with $H(r, p)$ being the classical Hamiltonian. Notice that the relationship $H(r, p) = \varepsilon$ appears in Eq. (24) after integration over the momentum $p$ due to the $\delta$ functions of $H(r, p) - \varepsilon$ and their derivatives with respect to $\varepsilon$ (see Ref. [24]). In the derivation of Eq. (23) for the MI shell correction $\delta \Theta_{\text{scl}}$, the improved stationary phase (periodic orbit) conditions for the evaluation of integrals over the phase space variables $r$ and $p$ has been used [19, 20, 22–24, 30, 31]. Within the POT, the PO sum for the energy shell corrections $\delta E_{\text{scl}}$ writes [12–14, 16, 19, 20, 22, 29–31]

$$\delta E_{\text{scl}} = d_s \sum_{\text{PO}} \frac{\hbar^2}{t_{\text{PO}}} \delta g_{\text{PO}}(\varepsilon_F) ,$$

(26)

where $t_{\text{PO}} = M_{\text{PO}}^{-1}(\varepsilon_F)$ is the period of particle motion along the PO (taking into account its repetition number $M$) and $t_{\text{PO}}^{-1}$ is the period of the particle motion along the primitive ($M = 1$) PO, taken at the Fermi energy $\varepsilon = \varepsilon_F$. For the shell correction to the semiclassical level density, one can write

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

(27)

where

$$\delta g_{\text{PO}}(\varepsilon) = A_{\text{PO}}(\varepsilon) \cos \left( \frac{S_{\text{PO}}(\varepsilon)}{\hbar} - \frac{\pi}{2} \mu_{\text{PO}} - \phi \right) ,$$

(28)

with $A_{\text{PO}}$ being the density amplitude. In the argument of the cosine function the phase $S_{\text{PO}}$ corresponds to the action for the PO (or the family of POs), $\mu_{\text{PO}}$ is the Maslov index (see Ref. [42]) and $\phi$ is an additional phase that depends on the dimension of the problem and the degeneracy of the considered orbits [16, 19, 20, 31]. The Fermi energy $\varepsilon_F$ is determined by the particle-number conservation condition (5), that can be written in the form

$$N = d_s \int_0^{\varepsilon_F} d\varepsilon \ g(\varepsilon) ,$$

(29)

where $g(\varepsilon)$ is the total level density. One now needs to solve this equation to determine the Fermi energy as function of the particle number, since $\varepsilon_F$ is needed in (26) to obtain the energy shell correction $\delta E_{\text{scl}}$. If one were to use the exact level density $g(\varepsilon)$ in (29), one would obtain a step function for the Fermi energy as function of the particle number. Using the semiclassical level density

$$g(\varepsilon) \approx g_{\text{ETF}}(\varepsilon) + \delta g(\varepsilon)$$

(30)

with $\delta g(\varepsilon)$ given by (27) with (28), similar discontinuities would appear. To avoid such a behaviour, one can apply some kind of Gauss averaging on the level density $g(\varepsilon)$ in Eq. (29), or, what amounts to the same, on the quantum level density, with, however, a width parameter $\gamma$ that would be much smaller than in the case of a shell-correction calculation by the Strutinsky smoothing, namely with $\gamma \ll \hbar \Omega$, i.e. much smaller than the distance between mayor shells, but still larger than the energy distance between s.p. levels. Because of the slow convergence of the PO sum in Eq. (27), it is, however, more convenient to use in (29) the exact level density $g(\varepsilon)$, averaged as just explained above, to determine the Fermi energy $\varepsilon_F(N)$ as function of the particle number $N$.

The rapid convergence of the PO sum in (26) is ensured by the factor in front of the density component $\delta g_{\text{PO}}$, a factor which is inversely proportional to the time $t_{\text{PO}}$ squared along the PO. Therefore, only POs with reasonably short periods which occupy a large enough phase-space volume will contribute. Let us mention at this point, that the energy shell correction $\delta E$ in Eq. (23) is, of course, through Eq. (29), function of the particle number $N$. For the ETF average $(r^2/\varepsilon)_{\text{ETF}}$, Eq. (24), one can simply use its TF approximation, which gives for the
spheroidal cavity its expression through the semi-axes $a$ and $b$ [19, 23, 24]:

$$\langle r^2 \rangle_{\text{ETF}} \approx \frac{a^2 + b^2}{3\epsilon_F}.$$  \hspace{1cm} (31)

Expressed in units of the classical (TF), i.e. the rigid-body MI,

$$\Theta_{\text{TF}} = m \left( a^2 + b^2 \right) \frac{N}{5},$$  \hspace{1cm} (32)

one obtains for the MI shell correction, Eq. (23),

$$\frac{\delta \Theta_{\text{scl}}}{\Theta_{\text{TF}}} = \frac{5 \delta E_{\text{scl}}}{3N\epsilon_F}.$$  \hspace{1cm} (33)

V. DISCUSSIONS OF SHELL EFFECTS

When calculating the energy shell corrections $\delta E$ for a system of $N$ particles in a cavity of spheroidal deformation one obtains, when plotted as function of $N^{1/3}$, some regular oscillations which are presented in Fig. 1. This calculation has been carried out for a spheroidal cavity at deformation $\eta = 1.2$, i.e. for a rather small deformation, using both the quantum-mechanical (QM) and a semiclassical (scl) resolution of the problem. A solid agreement is obtained between both these methods over a very large range of particle numbers as shown in the figure, where the energy shell correction is displayed in units of the Fermi energy $\epsilon_F$. It is not astonishing that this agreement is less pronounced for small particle numbers $N$ where the number of s.p. states becomes gradually too small to carry out the Strutinsky smoothing procedure with some reasonable accuracy. The deep minima (large negative shell corrections) that appear in Fig. 1 correspond to major closed shells that are present in nuclei and metallic clusters and that are, for the here considered potential, well reproduced in both the quantum and the semiclassical calculations.

Figs. 2 and 3 show a comparison of the shell corrections to the energy and the MI as functions of the particle number variable, $N^{1/3}$, for the spheroidal cavity, as in Fig. 1, and for a spheroidal WS potential, respectively. For the WS potential, we take a constant radius $R_0 = r_0 A^{1/3}$ with $r_0 = 1.14$ fm, for a given particle number $A = 250$ (corresponding approximately to the center of the Fermium (Z=100) isotopic chain), which means that the radius $R_0$ is fixed in our calculations to a constant $R_0 = 7.18$ fm. Since in the case of the spheroidal cavity, the spectrum is calculated in the dimensionless variable $k_i R_0$, where $k_i = \sqrt{2m\epsilon_i}$ with $\epsilon_i$ being the energy spectrum, this dimensionless variable is independent of the specific value of the radius $R_0$, one could, for a comparison of Figs. 2 and 3, formally consider both systems to have the same fixed radius $R_0$. Note also that the plateau condition of the Strutinsky smoothing procedure
for the spheroidal cavity is obtained in the dimensionless
$k_i R_0$ spectrum, in contrast to the WS problem where
this condition has to be satisfied by averaging over the
energy spectrum $\varepsilon_i$ with a Gaussian of width param-
eter $\gamma \approx 12 - 14$ MeV and a correction polynomial of
the order of degree $M = 6$ in the energy shell-correction
calculation.

For the WS case (Fig. 3), the shell components $\delta E$ and
$\delta \Theta$ of the energy and the MI are calculated as functions
of the nucleon number, $N^{1/3}$, in a WS potential well with
a depth $V_0 = -300$ MeV, a diffuseness $\alpha = 0.2$ fm and
a radius $R_0 = 7.18$ fm (for a fixed s.p. spectrum) by
the standard SCM. We have chosen a small diffuseness $\alpha$
and a large depth $V_0$ for the WS-type potential in order
to verify the quantum relationship (2) for this potential,
now close to a spheroidal cavity, by comparing it with the
semiclassical relationship derived analytically [19, 22–24]
for the spheroidal cavity. We have found that one is not
able to chose $\alpha$ smaller than $\alpha \approx 0.2$ fm because then
the expansion of the WS eigenfunctions in the HO ba-
sis states becomes badly convergent, and would require
a prohibitive number of major shells $n_0$ in the HO spec-
trum to be taken into account. Moreover, we would like
to dispose of a rather large interval of particle numbers
$N^{1/3}$ to see several (as much as possible) major shells
in order to test the correspondence (2) between maxima
and minima of the shell structure in the MI $\delta \Theta$ and the
energy $\delta E$ shell corrections as functions of $N^{1/3}$. Note
also that there is a difference in the plateau conditions for
the calculation of the MI shell corrections $\delta \Theta$ found from
the s.p. sum in Eq. (17) as compared to the energy shell
correction calculation. The reason is that the quantities
$\Theta_i$, Eq. (18), which take the role of a “s.p. spectrum”
in Eq. (17), differ from the real energy spectrum $\varepsilon_i$ by
the coefficients $A_{ij}$ from the expansion (A.1) of the WS
eigenfunctions in the deformed HO basis. This leads to
somewhat different values of the Strutinsky smoothing
parameters $\Theta_i$, Eq. (18), which take the role of a “s.p. spectrum”
in Eq. (17), differ from the real energy spectrum $\varepsilon_i$ by
the coefficients $A_{ij}$ from the expansion (A.1) of the WS
eigenfunctions in the deformed HO basis. This leads to
somewhat different values of the Strutinsky smoothing
parameters $\gamma = 12 - 16$ MeV and $M = 6 - 8$ needed
to obtain a plateau in the averaging procedure for the
calculation of $\delta \Theta$, and thus significantly increases the
number $n_0$ of shells in the HO basis to be taken into
account, like $n_0 \approx 20 - 30$ for a HO basis deformation
parameter $q = 1.2$ and a number of about 60 Gaussian
integration points, as compared with a much more stable
energy shell-correction calculations where even $n_0 = 10$
and $q = 1.0 - 1.2$ can be used. These Strutinsky aver-
aging parameters are found about the same for a whole
region of particle numbers $N^{1/3}$ shown in Figs. 2 and 3.
Another problem is that there is no reasonable plateau
condition for “billiard” (cavity) potentials, even for en-
FIG. 3. Quantum-mechanical energy and MI shell corrections, presented as in Fig. 2 (case of the spheroidal cavity), but obtained here in the same units as in Fig. 2, and at the same deformation ($\eta = 1.2$), for a WS potential of depth $V_0 = -300$ MeV, radius $R_0 = 7.18$ fm and diffuseness $\alpha = 0.2$ fm.

ergy shell correction calculations by averaging over the energy spectrum $\varepsilon_i$. As well known and mentioned above, one needs rather to consider the wave numbers $k_i$ as a “spectrum” for the spheroidal cavity to obtain a well pronounced plateau. For the opposite limit of the HO potential, the energy spectrum $\varepsilon_i$ is used for the averaging procedure. If we decrease now the diffuseness $\alpha$ of the WS potential from a value of $\alpha \approx 0.6$ fm, realistic for a nuclear mean-field, to a value of $\alpha \approx 0.2$ fm, to make that potential resemble a spheroidal cavity, to be able to compare our quantum WS results with the result of the semiclassical calculation for that cavity, we need to find some reasonable choice for $\alpha$ in order to be able to still satisfy the Strutinsky plateau condition for the average over the energies $\varepsilon_i$ spectrum. Such a compromise is achieved for the parameters of the WS potential well as indicated in the caption of Fig. 3.

In the POT calculations presented in Fig. 2 for the spheroidal cavity, the Fermi energy $\varepsilon_F(N)$ changes of course with the particle number $N$ through Eq. (29). The MI shell corrections, on the other hand, are divided by the constant TF MI (32) at $N = A$ and multiplied by a factor $A$ to use units for the MI that are independent of the particle number $A$. Here one should take into account that, because using a constant radius $R_0$, this TF MI $\Theta_{TF}$ is proportional to the particle number $A$. Thus when displaying the ratio $\delta\Theta/\Theta_{TF}, A$ as function of $N^{1/3}$, as we do in Figs. 2 and 3, one obtains a result that has practically a constant amplitude. For the spheroidal cavity this scale in particle numbers $A$ can be explained by (33) taking into account that the amplitude of $\delta E_{scl}/\varepsilon_F$ as function of $N^{1/3}$ is almost constant with an almost constant period.

The very “non professional” looking behavior of the shell corrections in Fig. 1 calls for some explanation. When plotting the energy shell correction $\delta E_{scl}/\varepsilon_F$ as function of the Fermi energy $\varepsilon_F$, deduced from Eq. (26), one obtains a smooth curve without any sharp peaks, peaks which, however, appear as soon as one substitutes the function $\varepsilon_F(N)$ which is found as explained in detail in section IV. The same behavior is, of course, and for the same reasons, also observed for the MI shell corrections. One can therefore conclude that the spikes observed in Figs. 1 do not have any profound physical meaning, but have their origin simply in the quantum structure of our s.p. spectrum. For obvious reasons, we have therefore used a slightly larger Gaussian width parameter for the averaging of the level density $g(\varepsilon)$ in Eq. (29), to make appear more clearly in Fig. 2 the proportionality between $\delta\Theta$ and $\delta E$ as derived in the semiclassical approximation.
in Eq. (33).

The agreement between the variation of both these quantities \(\delta E_{\text{sc}}/\varepsilon_f\) and \(\delta \Theta/\Theta_{\text{TF}}\) with \(N^{1/3}\) in Fig. 2 is striking and, thus, confirms our relations Eqs. (23) and (33). Notice that the factor \(1/f_{\text{PO}}^2\) in Eq. (26), with the time period \(t_{\text{PO}}\) of the particle motion along the PO, enhances, for the rather small deformation presented in the example of Figs. 1 and 2, shorter meridian and equatorial POs in the spheroidal cavity. The contributions of longer orbits \([29, 31]\). They are, however, expected to be more important at larger deformations. All these properties differ significantly from the results of classical perturbation theory of Ref. [28], where equatorial orbits, e.g., do not contribute at all.

One notices the presence of several major shell closures in the range of \(N^{1/3}\) values between 2 and 7 for which a close correspondence between the energy and the MI shell correction is observed, thus constituting a qualitative confirmation of our semiclassical relationship (23). For large particle numbers, i.e. in the limit when \(k_F R \sim N^{1/3} \gg 1\), semiclassical methods are particularly well adapted, but we encounter problems with the Strutinsky shell-correction method beyond \(N^{1/3} \gtrsim 6\), because, for the mean-field potential that we have been gradually filling, the Fermi energy comes close to the continuum of the s.p. spectrum, which is always difficult to handle. For smaller particle numbers, in particular below \(N^{1/3} \approx 3\), on the other hand, shell corrections \(\delta E\) or \(\delta \Theta\) are not well defined because then the number of s.p. states becomes too small to carry out the Strutinsky smoothing procedure with a good accuracy, as already pointed out at the beginning of the present section.

One has to note that the family of periodic orbits that gives the main contribution to the semiclassical shell-correction amplitude for the case of the spheroidal cavity is enhanced as compared to the case of the WS potential. Due to the integrability of the spheroidal cavity, the symmetry parameter\(^1\) \(K\) is larger there, for the orbits with highest degeneracy \((K = 2)\), as compared to those in the axially-symmetric WS potential, where the orbits with highest degeneracy only have \(K = 1\) for the same deformation. Therefore, the shell-correction amplitudes, Eq. (33), of both the energy and the MI are expected to be enhanced by a factor \(N^{1/6}\) for the spheroidal square-well as compared to those for the WS potential \([20, 31]\). Note that in the comparison of the quantum shell correction \(\delta E\) for a smooth-edge WS potential (Fig. 3) with the semiclassical result for an infinitely deep spheroidal square-well potential (Fig. 2) one needs to take into account different boundary conditions. Indeed, these lead to an additional shift of the Maslov phase in \(\delta E\), Eq. (26), for the spheroidal cavity, Eq. (28), as compared with the case of the WS potential \([42]\).

The shell correction \(\delta \Theta_{\text{sc}}\), Eq. (23), of the MI turns out to be much smaller than the classical TF (rigid-body) component, similar to the energy shell-correction \(\delta E\) compared to the corresponding TF term. Many important physical phenomena, such as fission isomerism or high-spin physics depend, however, dramatically on these shell effects. On the other hand, shell effects are expected to play a major role for the magnetic susceptibility, as a reaction of a system of charged particles to a magnetic field, which are expressed by exactly the same type of equations as we have for the MI, as mentioned above. There, the oscillating (shell) components are going to be largely enhanced as compared to the case of the MI, studied here (see, e.g., Ref. [18]). Our nonperturbative approach for the MI shell corrections can, of course, be applied for larger rotational frequencies and larger deformations (e.g. for \(\eta \sim 2.0\)) where bifurcations will play a dominant role, like in the case of a deformed harmonic oscillator \([22, 25, 26]\).

As becomes evident from Fig. 2 for the deformed spheroidal cavity, and Fig. 3 for an almost sharp-edged WS potential, a qualitative agreement is observed between the semiclassical POT and the quantum results, thus confirming our relation (23), which establishes the correspondence between \(\delta \Theta\) and \(\delta E\), as this was already observed for the harmonic oscillator potential \([22, 25]\).

VI. CONCLUSIONS

The shell corrections to the moment of inertia are determined through the generalized rigid-body MI for equilibrium rotations beyond the quantum perturbation expansion. We have shown that, for a WS potential of spheroidal deformation, the semiclassical relation (23) between energy and moment-of-inertia shell corrections holds and is in qualitative agreement with the quantum result. This correspondence between \(\delta E\) and \(\delta \Theta\) is also observed for a spheroidal cavity. A more systematic investigation of the relationship between these two shell corrections and a comparison between semiclassical and quantum results is on our agenda. It will be of particular interest to carry out this study at a large range of deformations, since at larger deformations the bifurcation phenomenon is expected to play an important role \([14, 20, 22, 29, 31, 42]\).

As for further perspectives, on could think of applying our semiclassical theory to the shell corrections of other transport coefficients, such as the inertia and friction parameters, that play e.g. an important role in the description of the fission process \([49, 50]\). We also plan to apply our approach to nuclear systems with a more realistic surface diffuseness \([20, 43]\) within the nuclear collective dynamics, in particular involving magic nuclei.

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\(^1\) The symmetry (or degeneracy) parameter \(K\) of a family of POs is the number of single-valued integrals of a particle motion of fixed energy, which determine in a unique way the action integral of the family along the PO for the whole family.
where the above discussed effects should be strongest. Using a more realistic Hamiltonians with more generally deformed mean-field potentials and diffused edges, one could, in addition, study the bridge bifurcations due to an unlocal symmetry restoration [43], as explained in our review [20]. In this connection it is obvious that our POT results could be extremely interesting for calculations of shell effects in the magnetic susceptibilities in quantum dots [18, 35].

One of the most attractive applications of the semi-classical periodic-orbit theory, however, seems to us its extension to the spin-orbit and pairing interactions [44–47], and the study of their influence on the collective vibrational and rotational excitations in heavy deformed neutron-rich nuclei (see e.g. Ref. [48]). To compare our vibrational and rotational excitations in heavy deformed 47], and the study of their influence on the collective vibrational and rotational excitations in heavy deformed neutron-rich nuclei (see e.g. Ref. [48]). To compare our theoretical predictions for the moment of inertia with the experimental data on rotational bands in well deformed nuclei, one could think of combining the smooth ETF MI with the corresponding PO shell corrections.

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Appendix A: Harmonic oscillator basis

For the quantum calculations of the MI and the energy shell corrections in the spheroidal WS potential (13), one can perform the diagonalization procedure through an expansion of the WS eigenfunctions \( \psi_i(r) \) in the basis of a deformed harmonic oscillator:

\[
\psi_i(r) = \sum_j A_{ij} \Phi_j(r) .
\]  
(A.1)

The HO basis states \( \Phi_j \) are defined in cylindrical coordinates \( \{ \varrho, \varphi, z \} \) as

\[
\Phi_j(r) = |n_z n_\varpi \Lambda \rangle = R_{n_z}^{(\Lambda)}(\varrho) Z_{n_z}(z) \phi_\Lambda(\varphi) ,
\]  
(A.2)

where \( n_z, n_\varpi, \) and \( \Lambda \) are the quantum numbers of the state

\[
R_{n_z}^{(\Lambda)}(\varrho) = \left( \frac{2m_\varpi}{\hbar} \right)^{1/2} \exp(-\xi/2) L_{n_z}^{(\Lambda)}(\xi) ,
\]  
(A.3)

\[
Z_{n_z}(z) = \left( \frac{m_\varpi}{\hbar} \right)^{1/4} \exp(-\zeta/2) H_{n_z}(\zeta) ,
\]  
(A.4)

\[
\phi_\Lambda(\varphi) = (2\pi)^{-1/2} \exp(i \Lambda \varphi) ,
\]  
(A.5)

with

\[
\xi^{1/2} = (m_\varpi/\hbar)^{1/2} \varrho = b_\perp \varrho , \quad \zeta = (m_\varpi/\hbar)^{1/2} z = b_z z .
\]  
(A.6)

The frequencies \( \omega_\perp \) and \( \omega_z \) of the axially-symmetric HO basis are connected, as usual, by the volume conservation condition \( \omega_\perp^2 \omega_z = \omega_0^3 \), with \( \omega_0 \) being the deformation parameter of the basis, i.e. \( \omega_\perp = \omega_0 q^{1/3} \) and \( \omega_z = \omega_0 q^{-2/3} \). It is convenient to use dimensionless variables as we have done through Eqs. (A.6) by introducing an inverse length \( b_0 = \sqrt{m_\varpi/\hbar} \) as a parameter of the HO basis (for nuclear systems with \( A \approx 200 – 300 \) considered in our study, one obtains together with \( \hbar \omega_0 \approx 50 \text{ MeV}/A^{1/3} \) a value of \( b_0 \approx 0.45 \text{ fm}^{-1} \)) and consequently corresponding inverse lengths \( b_\perp = b_0 q^{1/6} \) and \( b_z = b_0 q^{-1/3} \).

The functions \( L_n^{(\Lambda)}(x) \) and \( H_n(x) \) in Eqs. (A.3) and (A.4) are related to the standard generalized Laguerre \( L_n^{(\Lambda)}(x) \), and Hermite \( H_n(x) \) polynomials by

\[
L_n^{(\Lambda)}(x) = \left( \frac{n!}{(n+\Lambda)!} \right)^{1/2} x^{\Lambda/2} L_n^{(\Lambda)}(x) ,
\]  
(A.7)

and

\[
H_n(x) = (2^n n! \pi^{1/2})^{-1/2} H_n(x) .
\]  
(A.8)

The functions \( L_n^{(\Lambda)}(x) \) and \( H_n(x) \) obey orthogonality relations similar, up to constants, to those of the Laguerre, \( L_n^{(\Lambda)}(x) \), and Hermite, \( H_n(x) \), polynomials themselves [38]. One thus obtains the following relation for the transformation coefficients \( A_{ij} \) in Eq. (A.1):

\[
\sum_j A_{ij} A_{ji} = 1 .
\]  
(A.9)

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