Semiclassical shell structure in rotating Fermi systems

A. G. Magner,[1,*] A. S. Sitdikov,[2] A. A. Khamzin,[2] and J. Bartel[3]
[1]*Institute for Nuclear Research, Kyiv 03680, Ukraine*
[2]*Kazan State Power-Engineering University, Kazan 420066 Russia*
[3]*Institut Pluridisciplinaire Hubert Curien, CNRS/IN2P3, Université Louis Pasteur, F-67000 Strasbourg, France*
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The collective moment of inertia is derived analytically within the cranking model for any rotational frequency of the harmonic-oscillator potential well and at a finite temperature. Semiclassical shell-structure components of the collective moment of inertia are obtained for any potential by using the periodic-orbit theory. We found semiclassically their relation to the free-energy shell corrections through the shell-structure components of the rigid-body moment of inertia of the statistically equilibrium rotation in terms of short periodic orbits. The shell effects in the moment of inertia exponentially disappear with increasing temperature. For the case of the harmonic-oscillator potential, one observes a perfect agreement of the semiclassical and quantum shell-structure components of the free energy and the moment of inertia for several critical bifurcation deformations and several temperatures.

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I. INTRODUCTION

Many significant phenomena deduced from experimental data on nuclear rotations have been explained within several theoretical approaches based mainly on the cranking model [1–9]. The rotational problem is formulated through the diagonalization of the Hamiltonian in the body-fixed rotating coordinate system. The rotation frequency of this system is determined for a given nuclear angular momentum through a constraint, as for any other integral of motion, in particular, the particle number conservation. To simplify this rather complicated problem, the Strutinsky shell correction method (SCM) [10,11] was adjusted to the collective nuclear rotations in Refs. [6] and [7]. The collective moment of inertia (MI) is expressed as function of the particle number in terms of a smooth part and an oscillating shell correction. The smooth component can be described by a suitable macroscopic model, like the extended Thomas-Fermi (ETF) approach [12–20], which has proven to be both simple and precise. For the definition of the MI shell correction, one can apply the Strutinsky averaging procedure to the single-particle (s.p.) MI, in the same way as for the well-known free-energy shell correction.

For a deeper understanding of the quantum results and the correspondence between classical and quantum physics of the MI shell components, it is worthwhile analyzing these shell components in terms of periodic orbits (POs), what is now well established as the semiclassical periodic-orbit theory (POT) [17,21–24], as well as its extension to a given angular momentum projection along with the energy of the particle [25]. Gutzwiller suggested the POT for completely chaotic Hamiltonians with only one integral of motion (the particle energy) [21]. The Gutzwiller approach of the POT extended to potentials with continuous symmetries for the description of the nuclear shell structure is given in Refs. [17,22], and [26]. The semiclassical shell-structure correction to the level density has been tested well enough versus quantum shell correction calculations for a lot of s.p. Hamiltonians in two and three dimensions (see, e.g, Refs. [17] and [27–30]). For the Fermi gas the entropy shell corrections of the POT as a sum of periodic orbits were derived in Ref. [22], and with its help, the simple analytical expression for the shell-structure energies in cold nuclei were obtained there following a general semiclassical theory [17]. These energy shell corrections are in good agreement with the quantum SCM results, for instance, for elliptic and spheroidal cavities, including the superdeformed bifurcation region [28,29]. In particular, in three dimensions, the superdeformed bifurcation nanostructure leads as a function of deformation to the double-humped shell-structure energy with the first and second potential wells in heavy enough nuclei [17,26,29], which is well known as the double-humped fission barrier in the region of actinide nuclei. At large deformations the second well can be understood semiclassically, for spheroidal-type shapes, through the bifurcation of equatorial orbits into equatorial and the shortest three-dimensional (3D) periodic orbits, because of the enhancement of the POT amplitudes of the shell correction to a level density near the Fermi surface at these bifurcation deformations.

For finite heated fermionic systems, it was also shown [4,17,31,32] within the POT that the shell structure of the thermodynamical potential and the free-energy shell corrections can be obtained by multiplying the terms of the POT expansion by a temperature-dependent factor, which decreases exponentially with temperature [31,32]. For the case of so-called *classical rotations* around the symmetry z axis of the nucleus, the MI shell correction is obtained, for any rotational frequency and at finite temperature, within the extended Gutzwiller POT through the averaging of the individual angular momenta aligned along this symmetry axis [31]. A similar POT problem, dealing with the magnetic

*magner@kinr.kiev.ua

susceptibility of fermionic systems like metallic clusters and quantum dots, was worked out in Refs. [32] and [33].

It was suggested in Ref. [35] to use the spheroidal cavity and the classical perturbation approach to the POT by Creagh [17,34] to describe the collective rotation of deformed nuclei around an axis (x axis) perpendicular to the symmetry z axis. The small parameter of the POT perturbation approximation turns out to be proportional to the rotational frequency, but also to the classical action (in units of $\hbar$), which causes an additional restriction to Fermi systems (or particle numbers) of small enough size, in contrast to the usual semiclassical POT approach.

In the present work the nonperturbative extended Gutzwiller POT is used for the calculation of MI shell corrections within the mean-field cranking model for both the collective and the alignment rotations. For the case of the harmonic-oscillator (HO) potential we extended the Zelevinsky nonadiabatic theory for any rotational frequency to finite temperature. In this case the explicit analytical MI shell correction is derived and compared with the exact quantum SCM result. In Sec. II we present the general ideas of the cranking model for calculation of the MI. In Secs. III A and III B the POT method is presented within the nonperturbative Gutzwiller approach extended to continuous symmetries for any Hamiltonian but also, in Sec. III C, for the particular case of the HO potential. The connection between the collective MI and the free-energy shell corrections through the shell-structure rigid-body MI is demonstrated in Secs. III D and III E. In Sec. IV a comparison is made between the analytical semiclassical and numerical quantum calculations for the shell-structure free energies as well as for the collective MI, and a nice agreement is found at the different critical deformations and different temperatures. Our discussion focuses mainly on the symmetry-breaking phenomena, in particular, the bifurcation, in the superdeformation region, of a given PO into the same plus a newborn PO, as well as the pecularities of the spherical limit of moments of inertia. Conclusion and perspectives are presented in Sec. V. Some details of our analytical and numerical calculations are given in Appendixes A–E. The MI for the alignment rotation and its shell corrections are derived in Appendix A. The exact quantum solutions to the MI for the HO potential are obtained for any rotation frequency at a finite temperature in Appendix B. The quantum and semiclassical shell corrections to the free energy through those of the thermodynamical potential of the grand canonical ensemble are presented in Appendix C. The smooth Thomas-Fermi component is obtained within the local approximation to the POT in Appendix D. The POT contributions to the MI shell corrections are discussed in more detail in Appendix E.

II. CRANKING MODEL FOR NUCLEAR ROTATIONS

A. General points

Within the cranking model, the nuclear rotation around the κ axis ($\kappa = x, y, z$) with the symmetry z axis of the axially symmetric mean-field potential $V(\mathbf{r})$ can be described by solving the eigenvalue problem for the s.p. Hamiltonian in the body-fixed rotating coordinate system, which is usually called the *Routhian* [4,6,7]:

$$H_\omega = H - \omega\ell_\kappa, \quad \kappa = x, y, z. \tag{1}$$

The Lagrangian multiplier ω (rotation frequency of the body-fixed coordinate system) is defined through the constraint on the nuclear angular momentum I_κ evaluated as the quantum average of the operator of the angular momentum projection ℓ_κ onto the κ axis,

$$\langle\ell_\kappa\rangle_\omega \equiv d_s \sum_i n_i^\omega \int \mathrm{d}\mathbf{r}\psi_i^\omega(\mathbf{r})\ell_\kappa\overline{\psi}_i^\omega(\mathbf{r}) = I_\kappa, \tag{2}$$

with occupation numbers n_i^ω for the Fermi system of independent nucleons,

$$n_i^\omega \equiv n\left(\varepsilon_i^\omega\right) = \left\{1 + \exp\left[\left(\varepsilon_i^\omega - \lambda^\omega\right)/T\right]\right\}^{-1}. \tag{3}$$

Here, $\psi_i^\omega(\mathbf{r})$ are the eigenfunctions and ε_i^ω the eigenvalues of the Routhian H_ω, Eq. (1), $\lambda^\omega \approx \varepsilon_F$ is the chemical potential for relatively low frequencies ω and temperatures T, ε_F is the Fermi energy, $\varepsilon_F = \hbar^2 k_F^2/2m$, k_F is the Fermi momentum in units of $\hbar$, m is the nucleon mass, and d_s is the spin (spin-isospin) degeneracy (an over bar above the quantities means complex conjugation). From Eq. (2) the rotation frequency ω can be expressed in terms of a given projection I_κ of the angular momentum of nucleus to the κ axes, $\omega = \omega(I_\kappa)$. As we introduce the continuous parameter ω and ignore the uncertainty relation between the angular momentum and the angles of the axis position, the cranking model is semiclassical in principle. Thus, we may consider the MI Θ_κ as a response of the quantum average $\delta\langle\ell_\kappa\rangle_\omega$, defined in Eq. (2), to the external cranking field $-\omega\ell_\kappa$, in Eq. (1), similarly to the magnetic or isolated susceptibilities [32,33,36,37],

$$\delta\langle\ell_\kappa\rangle_\omega = \Theta_\kappa(\omega)\delta\omega, \tag{4}$$

where

$$\Theta_\kappa(\omega) = \frac{\partial\langle\ell_\kappa\rangle_\omega}{\partial\omega} = \frac{\partial^2 E(\omega)}{\partial\omega^2}, \quad E(\omega) = \langle H\rangle_\omega$$
$$\equiv d_s \sum_i n_i^\omega \int \mathrm{d}\mathbf{r}\ \psi_i^\omega(\mathbf{r})\ H\ \overline{\psi}_i^\omega(\mathbf{r}). \tag{5}$$

Traditionally [35], we consider two different cases for the position of the rotational axis. One of them is the most important collective rotation around the x axis ($\kappa = x$) perpendicular to the symmetry z axis ($\kappa = z$) in the next subsection. Another parallel (alignment) rotation with respect to the symmetry z axis is considered in Appendix A on the basis of Refs. [15,31], and [35], and only the final results are presented in the text.

B. Collective perpendicular rotation within the perturbation approach

As shown in Refs. [1–4,6], and [7], by using the second term $-\omega\ell_x$ in the Hamiltonian H_ω, Eq. (1), for the rotation around the x axis perpendicular to the symmetry z axis as a small perturbation at second order, for the constraint (2) and

MI (5), one has the standard Inglis formulas,

$$\omega\Theta_x = I_x, \quad \Theta_x = d_s {\sum_{ij}}' \frac{(n_j - n_i)|\langle j|\ell_x|i\rangle|^2}{\varepsilon_i - \varepsilon_j}, \tag{6}$$

where the double sum over i and j is taken over all s.p. states with the occupation numbers n_i and n_j [$n_i = n_i^0$; see Eq. (3) at $\omega = 0$], except for diagonal terms with $\varepsilon_i = \varepsilon_j$, as denoted by the prime on the summation symbol, $\varepsilon_i = \varepsilon_i^0$. For particle number conservation at the same second order, one has

$$\begin{aligned} A &= d_s \sum_i n_i^\omega \int \mathrm{d}\mathbf{r}\ \psi_i^\omega(\mathbf{r})\ \overline{\psi}_i^\omega(\mathbf{r}) \\ &= d_s \sum_i n_i \int \mathrm{d}\mathbf{r}\ \psi_i(\mathbf{r})\ \overline{\psi}_i(\mathbf{r}) = d_s \sum_i n_i, \end{aligned} \tag{7}$$

because of cancellations of all corrections of the first and second order, $\psi_i(\mathbf{r}) = \psi_i^0(\mathbf{r})$. Therefore, there is no ω dependence of the chemical potential λ for the perpendicular rotation at the perturbation approach of second order.

For the energy $E(\omega)$ of Eq. (5), the yrast line $E(I_x)$ (at zero temperature, $T = 0$) can be obtained by exclusion of the frequency ω from the constraint of Eq. (6), $\omega = I_x/\Theta_x$:

$$E(I_x) = E(0) + I_x^2/2\Theta_x. \tag{8}$$

As usual, the rotation term in Eq. (8) is quantized through $I_x^2 \to I_x(I_x + 1)$ to study the rotation bands.

For the derivations of shell effects within the POT [17,21–24], it turns out to be helpful to use the coordinate representation of the MI through the Green's functions G [36–39],

$$\begin{aligned} \Theta_x = \frac{2d_s}{\pi} \int_0^\infty \mathrm{d}\varepsilon\ n(\varepsilon) \int \mathrm{d}\mathbf{r}_1 \int \mathrm{d}\mathbf{r}_2\ \ell_x(\mathbf{r}_1)\ \ell_x(\mathbf{r}_2) \\ \times \mathrm{Re}[G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)]\mathrm{Im}[G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)], \end{aligned} \tag{9}$$

where $n(\varepsilon)$ are the Fermi occupation numbers $n(\varepsilon_i)$ at $\varepsilon_i = \varepsilon$, and $\ell_x(\mathbf{r}_1)$ and $\ell_x(\mathbf{r}_2)$ are the s.p. angular-momentum projections onto the perpendicular rotation x axis at the spatial points $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively. With the usual energy-spectral representation for the one-body Green's function G in the mean-field approximation,

$$G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) = \sum_i \frac{\psi_i(\mathbf{r}_1)\ \overline{\psi}_i(\mathbf{r}_2)}{\varepsilon - \varepsilon_i + i\epsilon}, \tag{10}$$

where the sum is taken over quantum s.p. states, ε_i is eigenvalues, ψ_i eigenfunctions of the Hamiltonian H in Eq. (1), and $\epsilon \to +0$, one obtains from Eq. (9) the well-known second-order perturbation result of the cranking model [4,6,7], however, including the diagonal terms. In particular, one also has the constraint $\omega\Theta_x = I_x$ of Eq. (6) with the expression of the MI Θ_x, Eq. (9), through the Green's function for the relation of ω to a given angular momentum I_x and the corresponding yrast energy, Eq. (8). In this sense, Eq. (9) looks more general beyond the perturbation approximation, Eq. (6); see the more detailed discussion below.

C. Quantum harmonic oscillator

In the case of the deformed HO potential, the direct diagonalization of the Routhian (1) (without using a perturbation expansion) for the rotation around the perpendicular x axis yields the s.p. energies $\varepsilon_i(\omega)$ and MI $\Theta_x(\omega)$ obtained analytically for any frequencies ω [3,5]. We extended this theory to finite temperatures T through the oscillator Bose occupation numbers [39]; see Appendix B for the derivations based on Refs. [40] and [41]. For the adiabatic case of a small rotation frequency limit, $\omega \to 0$, one needs the spectrum independent of ω,

$$\varepsilon_i = \hbar\omega_\perp(N_{\perp i} + 1) + \hbar\omega_z\left(N_{zi} + \frac{1}{2}\right), \quad N_{\perp i} = N_{xi} + N_{yi}, \tag{11}$$

where $N_{\kappa i}$ and ω_κ are the HO quantum numbers and the partial frequencies, $\omega_x = \omega_y = \omega_\perp$ at the axial symmetry. From Eq. (B14), for the MI $\Theta_x(\omega)$ [5,39] in the adiabatic limit $\omega \to 0$, one finds [2,4]

$$\begin{aligned} \Theta_x = \left(\frac{\partial I_x}{\partial\omega}\right)_{\omega=0} = \frac{d_s\hbar}{2\omega_\perp\omega_z} \Bigg[\frac{(\omega_z - \omega_\perp)^2}{\omega_\perp + \omega_z}(\aleph_y + \aleph_z) \\ + \frac{(\omega_z + \omega_\perp)^2}{\omega_\perp - \omega_z}(\aleph_z - \aleph_y) \Bigg], \end{aligned} \tag{12}$$

where

$$\aleph_\kappa = \sum_i n_i \left(N_{\kappa i} + \frac{1}{2}\right). \tag{13}$$

The energy of this system $E(\omega)$ [see Eq. (5)] is then given by

$$E(\omega) = d_s\hbar(2\omega_\perp\aleph_y + \omega_z\aleph_z) + \tfrac{1}{2}\omega^2\Theta_x. \tag{14}$$

We also used in Eq. (14) the axial symmetry property $\aleph_x = \aleph_y$. Note that starting from Eq. (6) of the perturbation approach for the HO potential, one may explicitly calculate analytically the matrix elements of the angular momentum projection operator ℓ_x (see Ref. [42]). As shown in Ref. [42], using these elements and the s.p. energies (11) in Eq. (6), one arrives at the same Eq. (12) for the nonperturbative derivations. These derivations are helpful for understanding the diagonal terms in Eq. (12), in contrast to Eq. (6) of the perturbation approach. The first term in Eq. (12) is related to the coupling of the s.p. levels through a shell, $\Delta N = 2$, and the second term corresponds to the transitions between levels inside the major shell, $\Delta N = 0$ (see Ref. [4]). The shell defined by the major quantum number N_i is split into the s.p. levels $\{N_{\perp i}, N_{zi}\}$ of a gross shell, which are degenerated with the quantum degeneracy $N_{\perp i} + 1$ for the axially symmetric HO potential. The second part ($\Delta N = 0$) of Eq. (12) can be nondiagonal and diagonal in energies of $\{\aleph_\perp, \aleph_z\}$ within a major shell. Taking the spherical limit of the deformation $\omega_\perp \to \omega_z$ in Eq. (12), one may realize that the first term turns to 0 ($\aleph_y \to \aleph_z$). In the second term of Eq. (12) one has the indetermination 0 by 0 for $(\aleph_z - \aleph_y)/(\omega_z - \omega_y)$ in the spherical limit. To resolve this indetermination one may reduce it to the calculation of the derivative $\mathrm{d}\aleph_y/\mathrm{d}\omega_y$ for the spherical limit of this ratio with the help of Eq. (11). Finally, accounting also for the definition of the angular momentum in

this limit, the second ($\Delta N = 0$) term in Eq. (12) is reduced identically to the MI owing to the alignment of the individual angular momenta of particles along the symmetry z axis [see Eqs. (A6)],

$$\Theta_x \to \Theta_z \to -d_s \sum_i \frac{\mathrm{d}n_i}{\mathrm{d}\varepsilon_i} |\langle i|\ell_x|i\rangle|^2, \tag{15}$$

as shown independently without using the perturbation theory in Appendix A. Note that Eq. (6) is a nondiagonal sum over energies of the s.p. states with $\varepsilon_i \neq \varepsilon_j$, according to a quantum criterion of the perturbation approach. But the expression (9) for the MI in terms of the one-body Green's function, which interpolates analytically the perturbation approximation (6) to the correct spherical limit (15), seems to be more general as it includes the diagonal ($\varepsilon_i = \varepsilon_j$) terms beyond this approximation. Similar derivations of the rigid-body MI beyond the perturbation theory were performed within the TF model; see Appendix D.

D. Statistical equilibrium rotation

The statistical equilibrium rotation occurs under the following condition of an isotropic distribution of quanta of the energy of the HO system in the directions of all three Cartesian axes [4,5,42–44]:

$$\omega_x \aleph_x = \omega_y \aleph_y = \omega_z \aleph_z \tag{16}$$

(in fact, the last two, y and z, owe to the axial symmetry, $\aleph_x = \aleph_y$). As expected from Ref. [43] and shown explicitly in Refs. [2–5] and [42], one obtains from the general expression (12) for the MI Θ_x the rigid-body limit, Eq. (17), by using the additional statistical assumption (16):

$$\Theta_x^{\mathrm{rig}} = d_s\, m \sum_i n_i\, \langle i|y^2 + z^2|i\rangle = d_s\hbar \left(\frac{\aleph_y}{\omega_\perp} + \frac{\aleph_z}{\omega_z}\right). \tag{17}$$

Condition (16), often called a consistency between the particle density and the HO potential in Refs. [4,5], and [42], is in fact that of a statistically equilibrium rotation of the Fermi system as a whole [43], for which it is rotated as a rigid body.

For calculations of the shell corrections, it is convenient to rewrite the MI Θ_x, Eq. (12), in terms of the rigid-body MI Θ_x^{rig}, Eq. (17), and the free energy of the HO system, $F(\omega = 0)$, at finite temperature T,

$$\Theta_x = \frac{1}{\omega_\perp^2(2\eta^2-1)(\eta^2-1)}\big[\omega_\perp^2(2\eta^4+9\eta^2+1)\Theta_x^{\mathrm{rig}} - 4\eta^2(1+\eta^2)F\big], \quad \eta = \frac{\omega_\perp}{\omega_z}, \tag{18}$$

where η is the deformation parameter, under the usual volume conservation condition, $\omega_\perp^2\omega_z = \omega_0^3$. In these derivations, the oscillator quantum numbers $\aleph_y$ and $\aleph_z$ were eliminated from Eq. (12) by using Eq. (17) and the explicit expression of the free energy, $F = E(0) - T\mathcal{S}$, where $E(0)$ is given by Eq. (14) at $\omega = 0$, and $\mathcal{S}$ is the entropy of the ideal Fermi gas. Owing to the linear expression of Θ_x through the Θ_x^{rig} and F, one has the following relation for the MI shell components $\delta\Theta_x$ in terms of the $\delta\Theta_x^{\mathrm{rig}}$ and δF (see Appendix C 1 for the shell correction derivations):

$$\delta\Theta_x = \frac{1}{\omega_\perp^2(2\eta^2-1)(\eta^2-1)}\big[\omega_\perp^2(2\eta^4+9\eta^2+1)\delta\Theta_x^{\mathrm{rig}} - 4\eta^2(1+\eta^2)\delta F\big]. \tag{19}$$

As $\Theta_x = \Theta_x^{\mathrm{rig}}$ for statistically equilibrium rotation Eq. (16) from Eq. (18), under condition (16), one obtains

$$\Theta_x = \Theta_x^{\mathrm{rig}} = \frac{1+\eta^2}{3\omega_\perp^2}F. \tag{20}$$

The shell component $\delta\Theta_x^{\mathrm{rig}}$ of the rigid-body MI Θ_x^{rig} is determined by the oscillating part of the particle density $\delta\rho$ as usual in the SCM [6,7,10,11]. For the HO potential, one can find a simple relation of $\delta\Theta_x^{\mathrm{rig}}$ to the free-energy shell correction δF. Subtracting the average quantities using the Strutinsky smoothing procedure, as shown in Appendix C 1, from this relation one obtains the shell correction to the MI $\delta\Theta_x$ in terms of the free-energy shell correction δF:

$$\delta\Theta_x = \delta\Theta_x^{\mathrm{rig}} = \frac{1+\eta^2}{3\omega_\perp^2}\delta F. \tag{21}$$

As shown in Appendix A, for the MI shell corrections $\delta\Theta_z$ for a parallel (alignment) rotation around the symmetry z axis, one similarly has

$$\delta\Theta_z^{\mathrm{rig}} = \frac{2}{3\omega_\perp^2}\delta F. \tag{22}$$

From a comparison of Eqs. (21) and (22) in the spherical limit $\eta \to 1$, one obtains $\delta\Theta_x \to \delta\Theta_z$, as for the rigid-body rotation, $\delta\Theta_x^{\mathrm{rig}} \to \delta\Theta_z^{\mathrm{rig}} \to 2\delta F/3\omega_\perp^2$. Note that Eqs. (18) and (19) are helpful to find the relation of the MI Θ_x and its shell correction $\delta\Theta_x$ to the free energy F and the corresponding shell component δF as well as to show a rigid-body behavior of the cranking model rotation for the HO mean field within the semiclassical approach in the next section.

III. SEMICLASSICAL SHELL-STRUCTURE APPROACH

We first review the basic points of the POT for the semiclassical level-density and free-energy shell corrections. We then apply the POT to the rigid-body MI shell corrections for the statistical equilibrium rotation and use this theory for a general semiclassical study of the MI, taking the HO potential as the simplest analytically solved example.

A. Green's function trajectory expansion

For the Green's function (10) in Eq. (9) for the MI, one may use the semiclassical Gutzwiller trajectory expansion [21] extended to continuous symmetry [17,22,25–27] and symmetry-breaking [17,29,30] problems:

$$G(\mathbf{r}_1,\mathbf{r}_2;\varepsilon) = \sum_\alpha G_\alpha(\mathbf{r}_1,\mathbf{r}_2;\varepsilon) = \sum_\alpha \mathcal{A}_\alpha(\mathbf{r}_1,\mathbf{r}_2;\varepsilon)\exp\left[\frac{i}{\hbar}S_\alpha(\mathbf{r}_1,\mathbf{r}_2;\varepsilon) - \frac{i\pi}{2}\mu_\alpha\right]. \tag{23}$$

The summation index α runs over all isolated classical trajectories, or families of trajectories, that, for a given energy ε connect two spatial points r_1 and r_2 inside the potential well $V(r)$. Here S_α is the classical action along such a trajectory α, and μ_α denotes the phase associated with the Maslov index by the number of caustic and turning points along path α [17,22,30]. The amplitudes $\mathcal{A}_\alpha$ of the Green's function depend on the classical stability factors and trajectory degeneracy, owing to the symmetries of that potential [17,22,26,29,30]. For the case of the isolated trajectories α [17,21], one has the explicit semiclassical expression for the amplitudes through the stability characteristics of classical dynamics:

$$\mathcal{A}_\alpha(\mathbf{r}_1,\mathbf{r}_2;\varepsilon) = -\frac{1}{2\pi\hbar^2}\sqrt{|\mathcal{J}_\alpha(\mathbf{p}_1,t_\alpha;\mathbf{r}_2,\varepsilon)|}, \quad t_\alpha = \frac{\partial S_\alpha}{\partial\varepsilon}. \tag{24}$$

Here $\mathcal{J}_\alpha(\mathbf{p}_1,t_\alpha;\mathbf{r}_2,\varepsilon)$ is the Jacobian for the transformation between the two sets of variables $\mathbf{p}_1, t_\alpha$ and $\mathbf{r}_2,\varepsilon$; $\mathbf{p}_1$ and t_α are the initial momentum and time of motion of the particle along a trajectory α, and $\mathbf{r}_2$ and ε are its final coordinate and energy. In a more general case, if the mean-field Hamiltonian H obeys a higher symmetry, like that of spherical or HO potentials with rational ratios of frequencies, one has to use other expressions for the amplitude $\mathcal{A}_\alpha(\mathbf{r}_1,\mathbf{r}_2;\varepsilon)$ for close trajectories $\alpha \neq \alpha_0$, taking into account such symmetries. They account for an enhancement of the order of $\hbar$ owing to their classical degeneracy (see Refs. [17,22,27], and [30] and the discussion in section C, below). In the case of the bifurcation of POs, generated by a symmetry breaking, one may use the improved stationary-phase method (SPM) [29,30], especially for superdeformed shapes of the potential. Some examples of the specific amplitudes for degenerate families of closed POs in the HO potential are given in Appendix E; see Eqs. (E6) and (E7). We keep a general form of the amplitudes $\mathcal{A}_\alpha$ as long as possible and finally use their specific expressions (E6) and (E7) after applying the SPM for the given potential in calculations of the MI shell corrections [22,26,27,30,36]. Note that Eq. (24) can be applied to any potential wells for the contributions of nonclosed trajectories that can be considered isolated ones.

Among all classical trajectories α in Eq. (23), we may single out α_0, which directly connects $\mathbf{r}_1$ and $\mathbf{r}_2$ without intermediate turning points; see Fig. 1. It is associated with the component G_{α_0} of the sum (23) for the semiclassical Green's function. Therefore, for the Green's function G, Eqs. (23), one has then a separation:

$$G = G_{\alpha_0} + G_1 \approx G_0 + G_1. \tag{25}$$

In the nearly local approximation [38,45] for close spatial points $\mathbf{r}_1 \to \mathbf{r}_2 \to \mathbf{r}$, the first term G_{α_0} of the splitting (25) is given by

$$G_{\alpha_0} \approx G_0 = -\frac{m}{2\pi\hbar^2 s}\exp\left\{\frac{i}{\hbar}sp(\mathbf{r})\right\}, \quad s = |\mathbf{r}_2 - \mathbf{r}_1|,$$
$$p(\mathbf{r}) = \sqrt{2m[\varepsilon - V(\mathbf{r})]}. \tag{26}$$

The second term G_1 in Eq. (25) is the fluctuating part of the Green's function (23) determined by all other trajectories $\alpha \neq \alpha_0$ in the sum (23) with reflection points at the potential surface:

$$G_1(\mathbf{r}_1,\mathbf{r}_2;\varepsilon) = \sum_{\alpha\neq\alpha_0} G_\alpha(\mathbf{r}_1,\mathbf{r}_2;\varepsilon); \tag{27}$$

see one such trajectory, α_1, in Fig. 1.

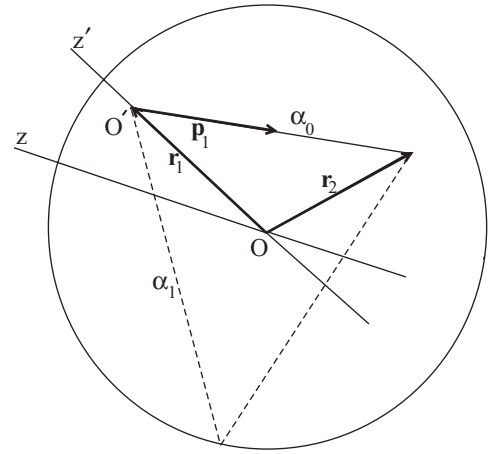

FIG. 1. Trajectories connecting points $\mathbf{r}_1$ and $\mathbf{r}_2$ without (α_0; solid line) and with (α_1; dashed line) reflection.

B. Level-density and energy shell corrections

The semiclassical level density $g(\varepsilon)$, according to Eq. (25), can be presented as the sum of the smooth and oscillating components,

$$g(\varepsilon) = -\frac{1}{\pi}\,\mathrm{Im}\int \mathrm{d}\mathbf{r}\;[G(\mathbf{r}_1,\mathbf{r}_2;\varepsilon)]_{\mathbf{r}_1=\mathbf{r}_2=\mathbf{r}}$$
$$\approx g_{\mathrm{scl}}(\varepsilon) = g_{\mathrm{ETF}}(\varepsilon) + \delta g_{\mathrm{scl}}(\varepsilon), \tag{28}$$

where $g_{\mathrm{ETF}}(\varepsilon)$ is given by the ETF approach [17,18]. The POT relates the oscillating component $\delta g_{\mathrm{scl}}(\varepsilon)$ of the level density (28) near the Fermi surface with characteristics of the classical POs [17,21–23]:

$$\delta g_{\mathrm{scl}}(\varepsilon) = \mathrm{Re}\sum_{\mathrm{po}}\delta g_{\mathrm{po}}(\varepsilon),$$
$$\delta g_{\mathrm{po}}(\varepsilon) = \mathcal{B}_{\mathrm{po}}\exp\left[\frac{i}{\hbar}S_{\mathrm{po}}(\varepsilon) - i\frac{\pi}{2}\mu_{\mathrm{po}}\right]. \tag{29}$$

This sum runs over the isolated POs and, in the case of degeneracies owing to the symmetries of a given potential well, over all families of POs. $\mathcal{B}_{\mathrm{po}}$ is the oscillation amplitude depending on the stability factors, $S_{\mathrm{po}}(\varepsilon)$ the action integral along a given PO, and μ_{po} the Maslov phase associated with the turning and caustic points along the PO; see Refs. [17] and [30] for detailed explanations (we use the same notation for the subscripts as in Ref. [17]).

The semiclassical energy shell corrections at zero temperature, $\delta E \approx \delta U_{\mathrm{scl}}$, is expressed through the PO density component $\delta g_{\mathrm{po}}(\varepsilon)$ of Eq. (28) [17,22],

$$\delta U_{\mathrm{scl}} = \mathrm{Re}\sum_{\mathrm{po}}\delta U_{\mathrm{po}}, \quad \text{with} \quad \delta U_{\mathrm{po}} = d_s\,\frac{\hbar^2}{t_{\mathrm{po}}^2}\,\delta g_{\mathrm{po}}(\lambda), \tag{30}$$

where $t_{\rm po}$ is the period of the particle motion along the considered periodic orbit and $\delta g_{\rm po}(\lambda)$ the PO component $\delta g_{\rm po}(\varepsilon)$ in the PO sum (29) at the energy ε equal to the chemical potential, $\varepsilon = \lambda$. Note that the thermodynamic derivation of Eq. (30) in Ref. [22] was presented through the POT entropy shell corrections $\delta\mathcal{S}_{\rm scl}$,

$$\delta\mathcal{S}_{\rm scl} = \frac{1}{T}{\rm Re}\sum_{\rm po}[\pi\mathcal{Z}_{\rm po}\coth(\pi\mathcal{Z}_{\rm po}) - 1]\delta\Omega_{\rm po}(T,\lambda), \qquad (31)$$

where $\delta\Omega_{\rm po}$ is the PO component of the shell correction $\delta\Omega_{\rm scl}$ to the thermodynamic potential [31,32],

$$\delta\Omega_{\rm scl}(T,\lambda) = {\rm Re}\sum_{\rm po}\delta\Omega_{\rm po}(T,\lambda),$$
$$\text{with}\quad \delta\Omega_{\rm po} = Q(\mathcal{Z}_{\rm po})\,\delta U_{\rm po}. \qquad (32)$$

The temperature-dependent factor,

$$Q(\mathcal{Z}) = \frac{\pi\mathcal{Z}}{\sinh(\pi\mathcal{Z})},\quad \text{for } \mathcal{Z} = \mathcal{Z}_{\rm po} = \frac{t_{\rm po}T}{\hbar}, \qquad (33)$$

is responsible for convergence of $\delta\Omega_{\rm scl} \to \delta U_{\rm scl}$ in the zero temperature limit $T \to 0$ [see Eq. (30)] and exponential decrease, $\sim\exp(-\pi T t_{\rm po}/\hbar)$, at higher temperatures T. The semiclassical free-energy shell correction $\delta F_{\rm scl}$ for a fixed temperature T and particle number A (protons and neutrons in the nucleus) can be calculated through the shell correction to the thermodynamical potential $\delta\Omega$ for a fixed temperature T and chemical potential λ at a given constant volume of the system [17,31,32,37,43]:

$$\delta F_{\rm scl}(T,N) = \delta\Omega_{\rm scl}(T,\lambda) = {\rm Re}\sum_{\rm po}\delta F_{\rm po},$$
$$\delta F_{\rm po} = Q(\mathcal{Z}_{\rm po})\delta U_{\rm po}. \qquad (34)$$

With these definitions from Eqs. (31), (34), and (C6), for the shell-structure internal energy δE, one obtains

$$\delta E_{\rm scl} = \delta F_{\rm scl} + T\delta\mathcal{S}_{\rm scl} = \sum_{\rm po}\cosh(\pi\mathcal{Z}_{\rm po})Q^2(\mathcal{Z}_{\rm po})\delta U_{\rm po}. \qquad (35)$$

As shown in Appendix C, the semiclassical expression (35) for δE can be obtained by using the same techniques of expansion of the amplitude $\mathcal{A}_{\rm po}(\varepsilon)$ at zero order and the action $S_{\rm po}(\varepsilon)$ at first order in powers of $\varepsilon - \lambda$ at the energy $\varepsilon = \lambda$ of the semiclassical expression of $\delta g_{\rm po}(\varepsilon)$ in Eq. (29) and integration by parts in Eq. (C7) [31]. These shell corrections are expressed through the s.p. energies near the Fermi surface, $\varepsilon = \lambda$, through $\delta g(\varepsilon)$ and $\delta n(\varepsilon)$ in the integrand of Eq. (C7).

C. Harmonic oscillator

To clarify the comparison of the quantum and semiclassical results for Fermi systems at a finite temperature, for simplicity, let us consider analytically solving example of the deformed HO potential, Eq. (E1). In this respect, one has to consider the two cases of the different [rational or irrational deformation parameter η of Eq. (18)] ratios for the frequencies ω_κ of the simplest axially symmetrical HO. As usual (with the volume conservation condition), one finds the expressions of the frequencies through ω_0 and the deformation parameter η [see Eq. (18)]:

$$\omega_\perp = \omega_0\eta^{1/3},\quad \omega_z = \omega_0\eta^{-2/3}. \qquad (36)$$

Following basically Ref. [27], we note that the analytically well-known PO families (Lissajous figures) have mainly the classical degeneracies[1] $\mathcal{K} = 4$ and 2, depending on the commensurable or incommensurable frequency relations. It indeed turns out that one-dimensional (isolated, $\mathcal{K} = 0$) trajectories yield relatively small contributions (of the relative order $\hbar$) to the shell-correction energy $\delta U_{\rm scl}$ ($\delta U_{\rm scl} \propto \hbar^{-\mathcal{K}/2}$) and may therefore be neglected [22,27]. The classical dynamics in the HO potential is considered in more detail in Appendix E 1.

1. *Incommensurable frequencies*

We consider first the case of the incommensurable frequencies of the axially symmetric HO with the irrational η. In this case, there are no isolated 3D ($\mathcal{K} = 4$) families but the 2D equatorial (EQ) ones of the POs of smaller degeneracy $\mathcal{K} = 2$ exist with a given period number n in the equatorial (x, y) plane ($z = 0$), perpendicular to the symmetry z axis. For the action S_n of the PO family specified by n, with the constant period of motion (43) linear in energy ε,

$$S_n(\varepsilon) = \varepsilon t_n,\quad t_n = n\mathcal{T}_{\rm EQ}. \qquad (37)$$

The main period $\mathcal{T}_{\rm EQ}$ (or frequency $\omega_{\rm po} = 2\pi/\mathcal{T}_{\rm po}$) of the primitive ($n = 1$) PO of a certain type in the (x, y) plane is given by

$$\mathcal{T}_{\rm EQ} = \frac{2\pi}{\omega_{\rm EQ}} = \frac{2\pi n_\perp}{\omega_\perp} = \frac{2\pi n_z}{\omega_z}. \qquad (38)$$

For the contribution of the EQ ($\mathcal{K} = 2$) orbits into the level density (29), one has [27]

$$\delta g_{\rm EQ}(\varepsilon) = \sum_n \delta g_n^{\rm EQ}(\varepsilon),$$
$$\delta g_n^{\rm EQ}(\varepsilon) = \frac{2\varepsilon}{(\hbar\omega_\perp)^2\sqrt{\mathcal{F}_n}}\sin\left[2\pi n\frac{\varepsilon}{\hbar\omega_\perp}\right], \qquad (39)$$

where $\mathcal{F}_n$ is the Gutzwiller stability factor [17,21,27],

$$\mathcal{F}_n = 4\sin^2\left(\frac{\pi n\omega_z}{\omega_{\rm EQ}}\right). \qquad (40)$$

The Maslov phase was accounted for explicitly in the argument of sine in Eq. (39). For the planar orbit contributions into the energy shell correction $\delta U_{\rm scl}$ (30), one obtains [27]

$$\delta U_{\rm EQ} = {\rm Re}\sum_n \delta U_n^{\rm EQ},$$
$$\text{with}\quad \delta U_n^{\rm EQ} = \frac{2d_s\lambda\omega_{\rm EQ}^2}{(2\pi\omega_\perp n)^2\sqrt{\mathcal{F}_n}}\sin\left(\frac{2\pi n\lambda}{\hbar\omega_{\rm EQ}}\right). \qquad (41)$$

[1]The classical degeneracy $\mathcal{K}$ is the number of independent parameters (single-valued integrals of motion besides the particle energy ε) that specify one of the orbits of the family with the same action $S_{\rm po}(\varepsilon)$.

2. *Commensurable frequencies*

3D orbits. For the case of rational ratios η of frequencies,

$$\omega_\perp : \omega_z = n_\perp : n_z, \tag{42}$$

where $n_\perp$ and n_z are primitive integers, one finds the main period of motion along the 3D PO of the $\mathcal{K} = 4$ family,

$$\mathcal{T}_{3D} = \frac{2\pi}{\omega_{3D}} = \frac{2\pi n_\perp}{\omega_\perp} = \frac{2\pi n_z}{\omega_z} = \frac{2\pi}{\omega_0}\left(n_\perp^2 n_z\right)^{1/3}, \tag{43}$$

where $\omega_{3D} = 2\pi/\mathcal{T}_{3D}$ is the main HO frequency for motion along the 3D orbit. The 3D PO action is given by Eq. (37) for $S_n(\varepsilon)$, where $t_n = n\mathcal{T}_{3D}$, $S_n^{3D}(\varepsilon) = n\varepsilon\mathcal{T}_{3D}$. For this completely degenerate case, Eq. (42), one has the subfamilies of the two-dimensional $\mathcal{K} = 2$ EQ POs along with the 3D ($\mathcal{K} = 4$) families.

For the contribution of the 3D orbits into the level-density shell correction $\delta g_{scl}(\varepsilon)$, Eq. (29), for the commensurable case, Eq. (42), one has

$$\delta g_{3D}(\varepsilon) = \sum_n \delta g_n^{3D}(\varepsilon)$$
$$\text{with} \quad \delta g_n^{3D}(\varepsilon) = \frac{\varepsilon^2}{(\hbar\omega_0)^3}\cos\left[2\pi n\frac{\varepsilon}{\hbar\omega_{3D}} - \pi n(2n_\perp + n_z)\right], \tag{44}$$

where $\omega_{3D} = 2\pi/\mathcal{T}_{3D}$ is the main HO frequency determined by the period $\mathcal{T}_{3D}$ (43).

3D and EQ orbits. For the commensurable case, Eq. (42), the EQ POs mentioned previously yield the contributions along with 3D orbits. These orbits lead to an interference of their contributions into the level-density and free-energy shell corrections. In the nonspherical $\eta > 1$ case for commensurable frequencies, the EQ orbits are isolated families that give the same contribution (39) for δg_{EQ} as in the previous incommensurable case along with Eq. (44) for δg_{3D}, according to Eq. (29):

$$\delta g_{scl}(\varepsilon) = \delta g_{3D}(\varepsilon) + \delta g_{EQ}(\varepsilon). \tag{45}$$

The smooth ETF component of the total semiclassical level density g_{scl} at leading order in $\hbar$ can be found, for instance, in Ref. [17].

For the energy shell correction δU_{scl}, Eq. (30), in this HO case, one has [27]

$$\delta U_{3D} = \mathrm{Re}\sum_n \delta U_n^{3D}$$
$$\text{with} \quad \delta U_n^{3D} = \frac{d_s\lambda^2\omega_{3D}^2}{(2\pi)^2\hbar\omega_0^3 n^2}\exp\left\{i\left[\frac{2\pi n\lambda}{\hbar\omega_{3D}} - \pi n(2n_\perp + n_z)\right]\right\}, \tag{46}$$

[see also Eq. (41) for the EQ orbit contribution]. Thus, in the case Eq. (42), the energy shell correction δU_{scl} takes approximately the form [22,27]

$$\delta U_{scl} = \delta U_{3D} + \delta U_{EQ}. \tag{47}$$

D. Particle-density and rigid-body shell corrections

The rigid-body MI Θ_κ^{rig} for rotations of any potential well around the parallel ($\kappa = z$) and perpendicular ($\kappa = x$) axes,

$$\Theta_\kappa^{rig} = m\int \mathrm{d}\mathbf{r}\, r_{\perp\kappa}^2\, \rho(\mathbf{r}),$$
$$r_{\perp z}^2 = x^2 + y^2, \quad \text{and} \quad r_{\perp x}^2 = y^2 + z^2, \tag{48}$$

respectively, is expressed through the particle density,

$$\rho(\mathbf{r}) = -\frac{d_s}{\pi}\mathrm{Im}\int \mathrm{d}\varepsilon n(\varepsilon)[G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)]_{\mathbf{r}_1=\mathbf{r}_2=\mathbf{r}}. \tag{49}$$

For the Green's function G one can apply the semiclassical expansion (23) in terms of the classical trajectories α. The integration over ε in Eq. (49) is performed over the whole s.p. energy spectrum.

Substituting the two-component splitting, Eq. (25), of the semiclassical Green's function $G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)$ (23) into Eq. (49) for the particle density $\rho(\mathbf{r})$ (49), one has approximately

$$\rho_{scl}(\mathbf{r}) = \rho_{TF}(\mathbf{r}) + \delta\rho_{scl}(\mathbf{r}), \tag{50}$$

where ρ_{TF} is given by Eq. (D2) and

$$\delta\rho_{scl}(\mathbf{r}) = -\frac{d_s}{\pi}\,\mathrm{Im}\int \mathrm{d}\varepsilon\delta n(\varepsilon)[G_1(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)]_{\mathbf{r}_1=\mathbf{r}_2=\mathbf{r}}. \tag{51}$$

In Eq. (49), we used $n = \tilde{n} + \delta n$ [see Appendix C 1 around Eq. (C10)] and neglected a small contribution of the term related to the product $\tilde{n}G_1$ owing to the particle conservation, Eq. (C4). Note that the semiclassical POT derivations of the oscillating part of the particle density, Eq. (51), were performed [46,47] in terms of the closed trajectories for various Hamiltonians. The contributions of nonperiodic closed trajectories into $\delta\rho_{scl}$ were studied in relation to the so-called Friedel oscillations of the particle density ρ_{scl} near the surface of the finite Fermi system. More precisely, we may improve the TF approximation by accounting for the $\hbar$ corrections of the ETF approach [15,17–20,46]. For simplicity, we omit both those and temperature [$\propto(T/\lambda)^2$] corrections, focusing mainly on the shell-structure components coming from G_1 of the Green's function sum, Eq. (25), and δn through those $\delta\rho_{scl}(\mathbf{r})$, Eq. (51), of the particle density $\rho_{scl}(\mathbf{r})$, Eq. (50).

Now using Eq. (50) in Eq. (48), one may similarly split the rigid-body MI Θ_κ^{rig} into the smooth and fluctuating (shell) components,

$$\Theta_{\kappa scl}^{rig} = \Theta_{\kappa TF}^{rig} + \delta\Theta_{\kappa scl}^{rig}, \tag{52}$$

where Θ_{xTF}^{rig}, according to Eq. (D1), is related to the TF approximation of the particle density $\rho_{TF}(\mathbf{r})$, Eq. (D2); see also Eq. (A12) for $\Theta_{zTF} = \Theta_{zTF}^{rig}$. As shown in Appendix D 1 by direct calculations at zero temperature, for a finite temperature T (including the entropy part $\mathcal{S}_{TF}T$), one obtains the following relation between the TF expressions for the rigid-body MI Θ_{xTF}^{rig} and free energy F_{TF},

$$\Theta_{xTF}^{rig} = \frac{1+\eta^2}{3\omega_\perp^2}F_{TF}, \quad \Theta_{zTF}^{rig} = \frac{2}{3\omega_\perp^2}F_{TF}. \tag{53}$$

Therefore, according to Eq. (18) for perpendicular and Appendix A for parallel rotations, for the HO potential within the TF approximation, without explicit use of the statistically

equilibrium rotation condition (16), one, nevertheless, obtains the same results as with Eqs. (21) and (22):

$$\Theta_{x\mathrm{TF}} = \Theta^{\mathrm{rig}}_{x\mathrm{TF}} = \frac{1+\eta^2}{3\omega_\perp^2} F_{\mathrm{TF}}, \quad \Theta_{z\mathrm{TF}} = \Theta^{\mathrm{rig}}_{z\mathrm{TF}} = \frac{2}{3\omega_\perp^2} F_{\mathrm{TF}}. \tag{54}$$

For the shell component of the sum (52), $\delta\Theta^{\mathrm{rig}}_{\kappa}$, changing the order of integrations and using the semiclassical trajectory expansion (23) for the oscillating Green's function component $G_1(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)$ of the sum (25), one finds

$$\begin{aligned}\delta\Theta^{\mathrm{rig}}_{\kappa\mathrm{scl}} &= m \int \mathrm{d}\mathbf{r}\, r^2_{\perp\kappa}\, \delta\rho_{\mathrm{scl}}(\mathbf{r}) \\ &= -\frac{m d_s}{\pi} \mathrm{Im} \sum_{\alpha\neq\alpha_0} \int \mathrm{d}\varepsilon\, \delta n(\varepsilon) \int \mathrm{d}\mathbf{r}\, r^2_{\perp\kappa} \mathcal{A}_\alpha(\mathbf{r}, \varepsilon) \\ &\quad \times \left\{ \exp\left[\frac{i}{\hbar} S_\alpha(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) - \frac{i\pi}{2} \mu_\alpha \right] \right\}_{\mathbf{r}_1 \to \mathbf{r}_2 \to \mathbf{r}}, \\ \mathcal{A}_\alpha(\mathbf{r}, \varepsilon) &\equiv \mathcal{A}_\alpha(\mathbf{r}, \mathbf{r}; \varepsilon). \end{aligned} \tag{55}$$

As usual, with the precision of the semiclassical approximation, we evaluate the spatial integral by the SPM extended to continuous symmetries [17,22,27]. The SPM condition writes

$$\begin{aligned}&\left[\frac{\partial S(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)}{\partial \mathbf{r}_1} + \frac{\partial S(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)}{\partial \mathbf{r}_2} \right]^*_{\mathbf{r}_1 = \mathbf{r}_2 = \mathbf{r}} \\ &\quad \equiv (-\mathbf{p}_1 + \mathbf{p}_2)^*_{\mathbf{r}_1 = \mathbf{r}_2 = \mathbf{r}} = 0, \end{aligned} \tag{56}$$

where an asterisk means the SPM value of the spatial coordinates and momenta, $\mathbf{r}_j = \mathbf{r}^*_j$ and $\mathbf{p}_j = \mathbf{p}^*_j$ $(j = 1, 2)$, at the closed trajectories in the phase space, $\mathbf{r}^*_1 = \mathbf{r}^*_2$ and $\mathbf{p}^*_1 = \mathbf{p}^*_2$. Thus, with the standard relations for the canonical variables, by using the action as a generating function, one arrives at the PO condition on the right-hand side of Eq. (56). Other smooth factors, $r^2_{\perp\kappa}$ and $\mathcal{A}_\alpha(\mathbf{r}, \varepsilon)$, of the integrand in Eq. (55) can be taken off the integral over $\mathbf{r}$ at these stationary points. Assuming that the quantum averages $\langle\kappa^2\rangle/\varepsilon$ are smooth enough functions of ε compared to other factors, for instance, δn, one may also take them approximately off the integral over ε at the chemical potential, $\varepsilon = \lambda$. For example, for the HO potential, they are simply exactly constants, $\langle x^2\rangle = \langle y^2\rangle \propto x_m^2 \propto \varepsilon$ and $\langle z^2\rangle \propto z_m^2 \propto \varepsilon$, where x_m, y_m, and z_m are the maximal values of coordinates x, y, and z for a classically accessible region at the given energy ε, $|x| \leqslant x_m$, $|y| \leqslant y_m$, and $|z| \leqslant z_m$, respectively:

$$x_m = y_m = \sqrt{\frac{2\varepsilon}{m\omega_\perp^2}}, \quad z_m = \sqrt{\frac{2\varepsilon}{m\omega_z^2}}. \tag{57}$$

Therefore, the main contribution to the integral in Eq. (55) comes from the PO stationary-phase points, determined by Eq. (56), as for calculations of the level-density shell corrections δg_{scl} (29) [17,22]. The SPM condition (56) is identity for any stationary point of the classically accessible spatial region for particle motion filled by PO families in the case of their high degeneracy $\mathcal{K} \geqslant 3$, for instance, for the contribution of the 3D orbits in the HO potential well with commensurable frequencies. The stationary points occupy some spatial subspace for smaller degeneracy $\mathcal{K}$. In the latter case of the EQ orbits ($\mathcal{K} = 2$) in the HO potential well, the SPM condition is identity in the equatorial plane $z = 0$.

For both parallel and perpendicular rotations, following similar derivations of the oscillating component δg_{scl}, Eq. (29), of the level density $g_{\mathrm{scl}}(\varepsilon)$ (28) and shell correction δF_{scl}, Eq. (34), after the subtraction of the heat part $T\delta\mathcal{S}_{\mathrm{scl}}$ as in Appendix C, from Eq. (55), one obtains

$$\delta\Theta^{\mathrm{rig}}_{\kappa\mathrm{scl}} = \frac{m}{\lambda} \mathrm{Re} \sum_{\mathrm{po}} \langle r^2_{\perp\kappa}\rangle_{\mathrm{po},\lambda} \delta F_{\mathrm{po}}, \tag{58}$$

where $\langle r^2_{\perp\kappa}\rangle_{\mathrm{po},\lambda}$ is the average given by

$$\langle r^2_{\perp\kappa}\rangle_{\mathrm{po},\varepsilon} = \frac{\int \mathrm{d}\mathbf{r} \mathcal{A}_{\mathrm{po}}(\mathbf{r}, \varepsilon) r^2_{\perp\kappa}}{\int \mathrm{d}\mathbf{r} \mathcal{A}_{\mathrm{po}}(\mathbf{r}, \varepsilon)} \tag{59}$$

at $\varepsilon = \lambda$, $\mathcal{A}_{\mathrm{po}}(\mathbf{r}, \varepsilon)$ are the Green's function amplitudes $\mathcal{A}_\alpha(\mathbf{r}, \varepsilon)$ for closed POs, $\alpha = \mathrm{po}$, defined specifically in Sec. III A and Appendix E. Integration over $\mathbf{r}$ is performed over the classically accessible region of the spatial coordinates. The semiclassical expression (58) is general for any potential well. Shorter POs dominate in the PO sum (58) [17,22,31]; see Eqs. (30) and (34). Therefore, according to Eq. (34) for δF_{scl}, we obtain approximately the relation

$$\delta\Theta^{\mathrm{rig}}_{\kappa\mathrm{scl}} \approx \frac{m}{\lambda} \langle r^2_{\perp\kappa}\rangle_\lambda\, \delta F_{\mathrm{scl}}, \tag{60}$$

where $\langle r^2_{\perp\kappa}\rangle_\lambda$ is an average value of the quantity (59), independent of the specific PO, at $\varepsilon = \lambda$ over short dominating POs. For the HO commensurable-frequency case the integration in Eq. (59) over $\mathbf{r}$ for the 3D contribution means over the 3D volume occupied by the 3D families of orbits, while for the EQ orbit component the integral is taken over the 2D spatial region filled by the EQ families in the equatorial ($z = 0$) plane. For the incommensurable-frequency case one has the only EQ-orbit contributions.

The average (59) can be easily calculated by using the Green's function amplitudes $\mathcal{A}_{\mathrm{po}}$, Eq. (E6) for 3D and Eq. (E7) for EQ orbits, and the scale transformation of the spatial variables, $x = x_m u_x$, $y = y_m u_y$, and $z = z_m u_z$, with the maximal values x_m, y_m, and z_m, Eq. (57), of the coordinates x, y, and z, as in Appendix D. Finally, we arrive at

$$\delta\Theta^{\mathrm{rig}}_{x\mathrm{scl}} = \frac{1+\eta^2}{3\omega_\perp^2} \delta F_{\mathrm{scl}}, \quad \delta\Theta^{\mathrm{rig}}_{z\mathrm{scl}} = \frac{2}{3\omega_\perp^2} \delta F_{\mathrm{scl}}, \tag{61}$$

where δF_{scl} is the semiclassical PO sum, Eqs. (34), (30), (41), (46), and (47) for the shell correction to the semiclassical free energy F_{scl}. The second equation is in agreement with the result (A14) obtained in Appendix A. Substituting the semiclassical approximation (61) for $\delta\Theta^{\mathrm{rig}}_{\kappa}$ into Eq. (19) for $\delta\Theta_\kappa$, one obtains

$$\delta\Theta_{x\mathrm{scl}} = \frac{1+\eta^2}{3\omega_\perp^2} \delta F_{\mathrm{scl}}, \quad \delta\Theta_{z\mathrm{scl}} = \frac{2}{3\omega_\perp^2} \delta F_{\mathrm{scl}}. \tag{62}$$

Moreover, one has the same relation (20) for the smooth TF parts in the HO case; see Appendix D 1. Thus, by using the general HO relationship (18) for the total moment Θ_x, one can prove semiclassically within the POT, up to the same $\hbar$ corrections in the smooth TF part, that Eqs. (20) and (21) are

true for the HO Hamiltonian,

$$\Theta_{x\mathrm{scl}} = \frac{1+\eta^2}{3\omega_\perp^2} F_{\mathrm{scl}}, \quad F_{\mathrm{scl}} = F_{\mathrm{TF}} + \delta F_{\mathrm{scl}}. \tag{63}$$

We emphasize that the POT expressions (62) for $\delta\Theta_{x\mathrm{scl}}$ and (63) for $\Theta_{x\mathrm{scl}}$ were derived without direct use of the statistically equilibrium rotation condition (16). However, as shown above, it is exactly the same as found by applying the POT directly to Eq. (20) under this condition.

Substituting the semiclassical PO expansion (34) for the δF_{scl} using Eq. (46) for 3D orbit families and Eq. (41) for EQ POs into Eq. (61), one arrives finally at the POT expressions for the MI shell corrections $\delta\Theta_x$ within the cranking model in terms of the POs in the HO mean field. Note that in this case the parallel, $\delta\Theta_z$, and perpendicular, $\delta\Theta_x$, MI shell components are expressed through the 3D and EQ POs through the free-energy shell correction, which contains, generally speaking, both of them for the commensurable frequencies, according to Eq. (47). The dominating contribution of one of these families or the coexistence of both together depends on the HO deformation parameter η of Eq. (18).

E. General semiclassical relation of perpendicular rigid-body rotations

Substituting (25) into Eq. (9), one has a sum of several terms,

$$\Theta_{x\mathrm{scl}} = \Theta_x^{00} + \Theta_x^{01} + \Theta_x^{10} + \Theta_x^{11}, \tag{64}$$

where

$$\Theta_x^{\nu\nu'} = \frac{2d_s}{\pi} \int \mathrm{d}\varepsilon n(\varepsilon) \int \mathrm{d}\mathbf{r}_1 \int \mathrm{d}\mathbf{r}_2\, \ell_x(\mathbf{r}_1)\, \ell_x(\mathbf{r}_2) \times \mathrm{Re}[G_\nu(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)]\mathrm{Im}[G_{\nu'}(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)], \tag{65}$$

ν and ν' run independently two integers, 0 and 1. As shown in Appendix D, the main smooth part of the semiclassical MI $\Theta_{x\mathrm{scl}}$, Eq. (64), is the TF rigid-body component related to the first term Θ_x^{00} averaged over the phase-space variables (see Ref. [38] and previous publications [12–15]). The statistical averaging over phase-space coordinates removes the nonlocal long-range correlations. The $\hbar$ corrections of the smooth ETF approach to this TF approximation were obtained in Refs. [15,19], and [20].

The shell-structure component $\delta\Theta_x^{01}$ of Θ_x^{01} [see Eq. (65) at $\nu = 0$ and $\nu' = 1$], in the total MI $\Theta_{x\mathrm{scl}}$, Eq. (64), can be related semiclassically to the shell correction $\delta\rho_{\mathrm{scl}}(\mathbf{r})$ of the particle density $\rho_{\mathrm{scl}}(\mathbf{r})$ through that of the rigid-body MI. Indeed, substituting approximation (26) for G_{α_0} and Eq. (27) for G_1 into Eq. (65) for Θ_x^{01}, we separate the shell component $\delta\Theta_x^{01}$ in the total quantity Θ_x^{01} (65) as in Appendix C 2 for the energy shell correction. Using the transformation of the coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$ to the center-of-mass and relative ones, $\mathbf{r} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ and $\mathbf{s} = \mathbf{r}_2 - \mathbf{r}_1$, with the help of Appendix E 3, by using the averaging over the phase-space variables in the local short-range approximation, $sp/\hbar \ll 1$, one arrives at

$$\delta\Theta_x^{01} = -\frac{d_s m}{\pi^2\hbar^2} \sum_{\alpha\neq\alpha_0} \mathrm{Im} \int \mathrm{d}\varepsilon \delta n(\varepsilon) \int \mathrm{d}\mathbf{r} \times \int \mathrm{d}\mathbf{s} \ell_x\left(\mathbf{r} - \frac{\mathbf{s}}{2}\right) \ell_x\left(\mathbf{r} + \frac{\mathbf{s}}{2}\right) \cos\left[\frac{s}{\hbar} p(\mathbf{r})\right] \times \mathcal{A}_\alpha\left(\mathbf{r} - \frac{\mathbf{s}}{2}, \mathbf{r} + \frac{\mathbf{s}}{2}; \varepsilon\right) \times \exp\left[\frac{i}{\hbar} S_\alpha\left(\mathbf{r} - \frac{\mathbf{s}}{2}, \mathbf{r} + \frac{\mathbf{s}}{2}; \varepsilon\right) - \frac{i\pi}{2}\mu_\alpha\right] \approx \delta\Theta_x^{\mathrm{rig}}, \tag{66}$$

where $\delta\Theta_x^{\mathrm{rig}}$ is the shell correction to the rigid-body MI in Eq. (55) related to the semiclassical particle-density shell component $\delta\rho_{\mathrm{scl}}(\mathbf{r})$, Eq. (51). Owing to averaging over phase-space variables, one survives with the local short-range approximation. In particular, for the classical angular-momentum projections in the integrand of the first expression in Eq. (66) one can use the approximation

$$\ell_x[\mathbf{r} - (\mathbf{s}/2)]\ell_x[\mathbf{r} + (\mathbf{s}/2)] \approx \ell_x^2(\mathbf{r}) = r_{\perp x}^2 p^2(\mathbf{r}), \tag{67}$$

where $r_{\perp x}^2$ is given in Eq. (48). Note that this classical angular-momentum projection in the rotating body-fixed coordinate system is caused by the global rotation rather than by the motion of particles along the trajectories inside the nucleus. According to the time-reversible symmetry of the Routhian, the particles are, indeed, moving in the nonrotating coordinate system along these trajectories in both directions with opposite signs. Their contributions to the total angular momentum of the nucleus turns out to be zero. Performing the integration over $\mathbf{s}$ in Eq. (66) in the spherical coordinate system, one obtains the rigid-body shell correction $\delta\Theta_x^{\mathrm{rig}}$ in the nearly local approximation, as explained in Appendix E 3. Note that the cranking model for the nuclear rotation implies that the correlation corrections to Eq. (66) should be small enough with respect to the main rigid-body component $\delta\Theta_x^{\mathrm{rig}}$ to be neglected within the adiabatic picture of separation of the global rotation of the Fermi system from its vibration and internal motion of the particles. Other contributions, except for a smooth rigid-body part coming from Θ_x^{00}, like Θ_x^{10} as referred to the fluctuation (nonlocal) correction to the rigid-body MI, are found semiclassically to be negligibly small owing to the averaging over phase-space variables; see Appendix E. In particular, for the HO Hamiltonian, it is shown that there is almost no contribution of the $\delta\Theta_x^{11}$ at leading order in $\hbar$. Finally, for the semiclassical shell corrections to the MI for perpendicular and parallel (alignment) rotations with respect to the symmetry z axis, we arrive, for the deformed HO with Eq. (66), at expressions (62). It turns out that these expressions are the same as those found in Eq. (21) with the semiclassical precision, but without explicit use of the equilibrium rotation condition (16). The case of the spheroid cavity requires further study and is discussed in a separate work.

IV. COMPARISON WITH QUANTUM RESULTS

Figure 2 shows the semiclassical energy shell correction δU_{scl}, Eqs. (30), (41), (46), and (47), and the corresponding

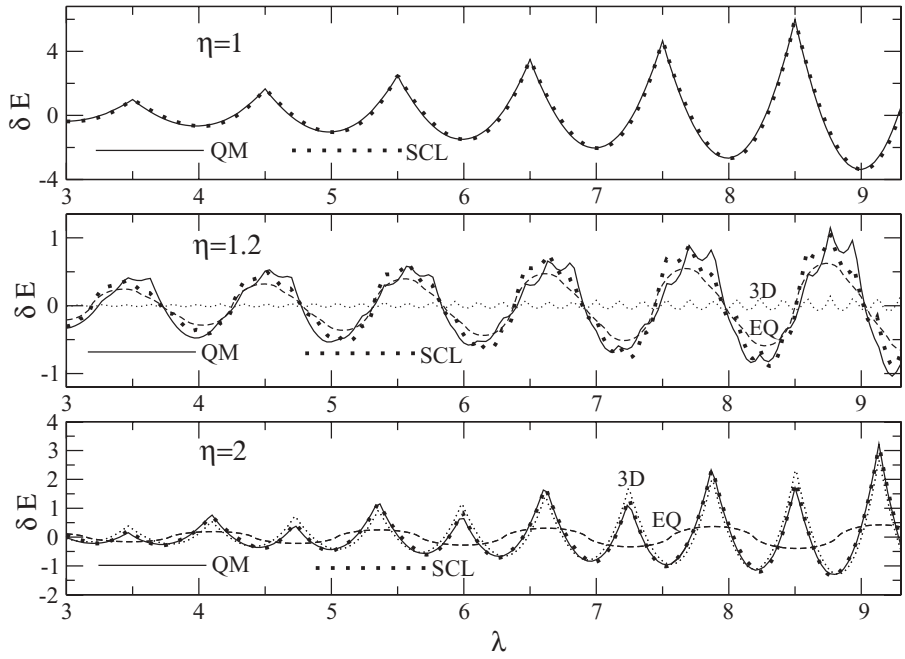

FIG. 2. Quantum (QM), Eq. (C7), and semiclassical (SCL), Eq. (47), shell-structure energies $\delta E \approx \delta U_{\rm scl}$ at zero temperature versus the chemical potential λ for the spherical HO potential (all quantities are in units of the HO shell spacing $\hbar\omega_0$) at the critical deformations $\eta = 1$, 1.2, and 2. The SCM smoothing parameters are $\gamma/\hbar\omega_0 = 1.5$–$2.5$ and $M = 4$–8. Thin dotted curves show the contribution of the 3D orbits, and thin dashed curves the EQ orbit contributions.

quantum SCM calculations of δE, Eq. (C7), as functions of the chemical potential λ at zero temperature for different critical symmetry-breaking and bifurcation deformations $\eta = 1$, 6/5, and 2 of the HO potential [17]. This comparison exhibits a practically perfect agreement between the semiclassical and the quantum results, especially for $\eta = 1$ and 2. Note that this agreement is not exact even for the semiclassical free-energy shell corrections at zero temperature because we neglected the terms of smaller order of the expansion in $\hbar^{1/2}$ after integration over the s.p. energies by parts, in contrast to the level-density calculations for the HO potential. Phases of the oscillations of the level density are linear in energy but we have to account for the energy dependence of their amplitudes. For the spherical case ($\eta = 1$), one has only contributions of the families of 3D orbits with the highest degeneracy $\mathcal{K} = 4$. At the bifurcation points $\eta = 6/5$ and 2 the relatively simple families of these 3D POs appear along with EQ trajectories of smaller degeneracy. For $\eta = 6/5$ one mainly has the contributions from EQ POs because 3D orbits are generally too long in this case. For the bifurcation point $\eta = 2$ one finds an interference of the two comparably large contributions of EQ and 3D orbits, Eqs. (41) and (46), respectively, with different periods, $\mathcal{T}_{\rm 3D} = 2\mathcal{T}_{\rm EQ}$, as shown at the bottom in Fig. 3. The semiclassical free-energy shell correction $\delta F_{\rm scl}$, Eqs. (30), (34), (41), (46), and (47), is displayed in Fig. 3 as a function of the particle number variable, $A^{1/3}$, and compared at a temperature of $T = 0.1\hbar\omega_0$

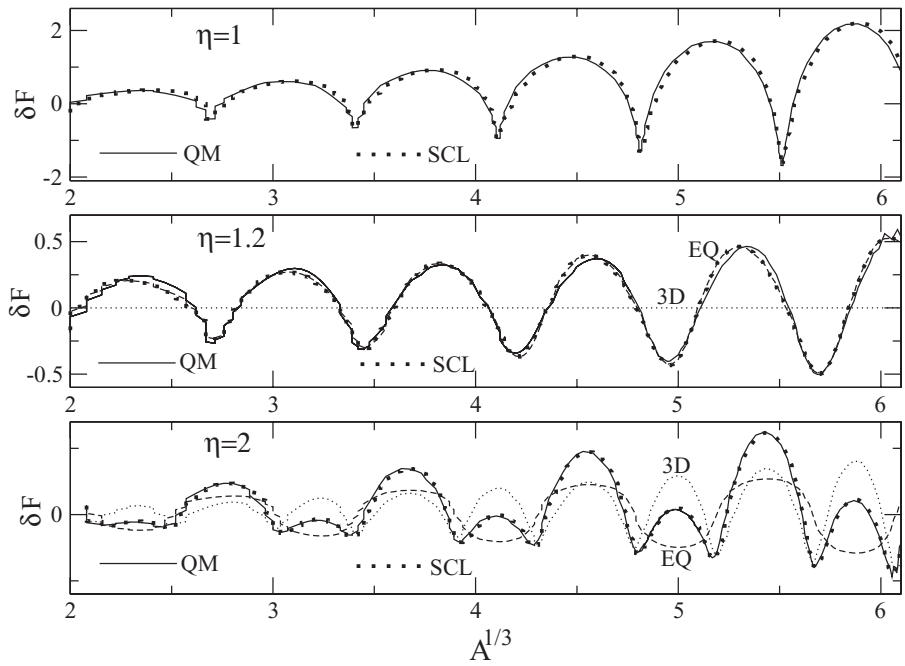

FIG. 3. Shell-structure free energy δF (in HO units, $\hbar\omega_0$) as a function of the particle number variable $A^{1/3}$ for the critical deformations $\eta = 1$, 1.2, and 2 at a temperature of $T = 0.1\hbar\omega_0$. All other parameters and notations are the same as in Fig. 2.

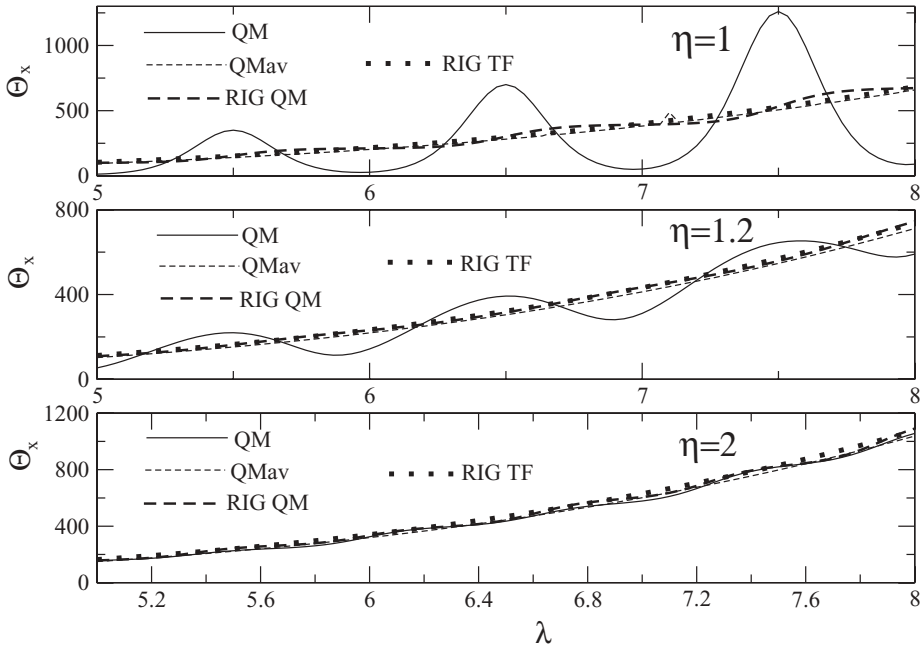

FIG. 4. Moment of inertia Θ_x, Eq. (12) (quantum; QM), its average $\tilde{\Theta}_x$ (QMav) and rigid-body value $\Theta_x^{\rm rig}$, Eq. (17), at the statistically equilibrium rotation (RIG QM) and its TF approach, Eq. (54) (RIG TF), as functions of the chemical potential λ for the same critical deformations η and temperature $T = 0.1\hbar\omega_0$ as in Fig. 3. All moments of inertia are in units of $\hbar/\omega_0$ and λ is in units of $\hbar\omega_0$.

with the corresponding quantum SCM results for the same critical deformations. This comparison also shows a practically perfect agreement between the semiclassical, Eq. (34), and the quantum, Eq. (C1), results with a similar PO structure. As shown in Figs. 2 and 3, instead of concave parabolas, depending on the chemical potential λ, we observe convex ones as functions of the particle number parameter $A^{1/3}$ owing to the oscillating component $\delta\lambda$ of $\lambda = \tilde{\lambda} + \delta\lambda$ ($\tilde{\lambda}$ is the averaged λ in the SCM).

Figures 4 and 5 show the total perpendicular and parallel MI (quantum [QM]) Θ, Eq. (12) for Θ_x and Eq. (A14) for Θ_z, depending on λ for the same critical deformations at temperature $T = 0.1\hbar\omega_o$, respectively. Large-scale oscillations are clearly shown, decreasing sharply, however, with a deformation from spherical to deformed shapes for the perpendicular rotation case. In Fig. 4 we show also the quantum rigid-body MI $\Theta_x^{\rm rig}$, Eqs. (17) and (48) (RIG QM), in the sense of the quantum particle density $\rho(\mathbf{r})$, which contains the shell correction $\delta\rho(\mathbf{r})$ owing to inhomogeneity of the energy levels near the Fermi surface. These oscillations of $\Theta^{\rm rig}(\lambda)$ are seen everywhere versus the smooth TF approach $\Theta_{\rm TF}^{\rm rig}$, Eq. (53), related to the TF particle density $\rho_{\rm TF}$, Eq. (D2), through the TF free energy $F_{\rm TF}$, but it is naturally more pronounced for the spherical shape, at the top in Fig. 4. Note that the relative scale of these oscillation amplitudes with respect to the averaged MI behavior $\tilde{\Theta}$ (QMav) is rather obviously large compared to the

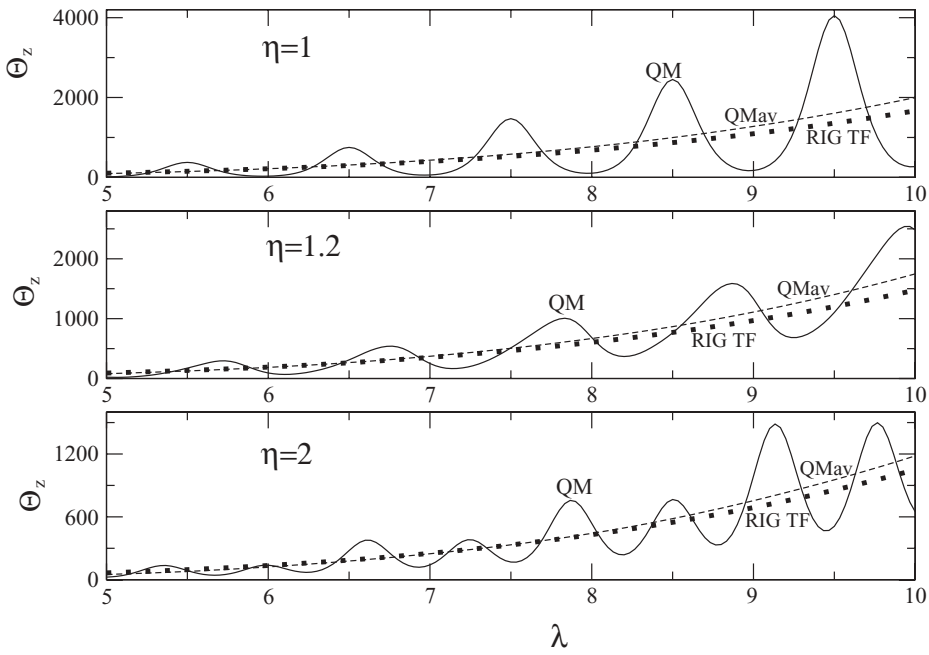

FIG. 5. Same as Fig. 4, but for the alignment moment of inertia Θ_z, Eq. (A6) (quantum; QM), its average $\tilde{\Theta}_z$ (QMav), and the rigid-body value $\Theta_{z\rm TF}^{\rm rig}$ of the TF approach, Eq. (54) (RIG TF), at statistically equilibrium rotation.

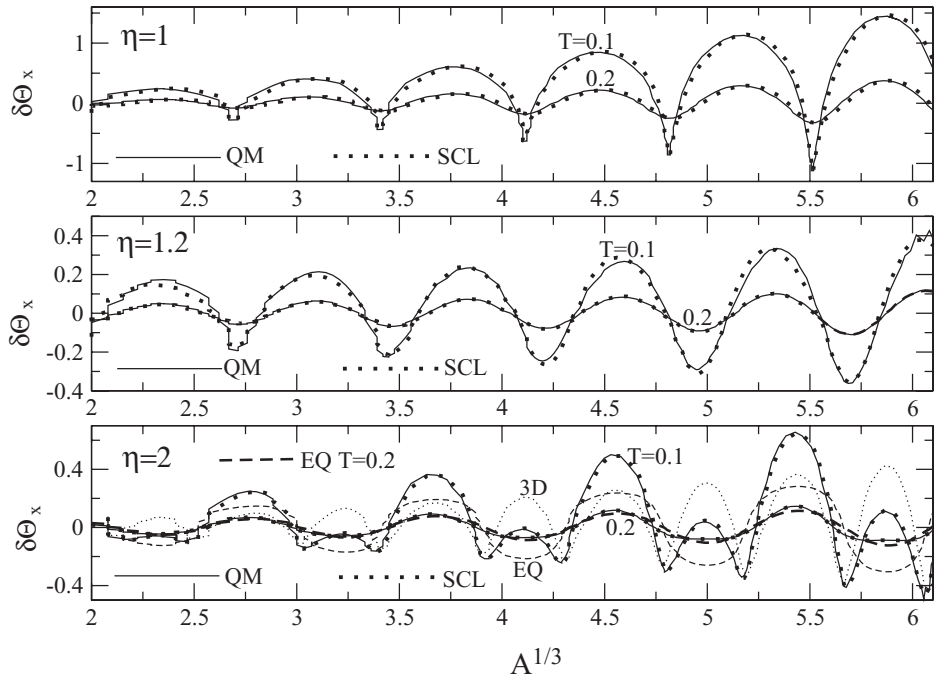

FIG. 6. Moment of inertia shell correction $\delta\Theta_x$ (in the same units as in Figs. 4 and 5) for perpendicular rotation as a function of the particle number $A^{1/3}$ at temperatures $T = 0.1$ and $0.2\hbar\omega_0$. The thin dotted line shows the contribution of 3D orbits; the thin dashed line, the contribution of EQ orbits at a temperature $T = 0.1\hbar\omega_0$; and bold dashed line, the contribution of EQ orbits at $T = 0.2\hbar\omega_0$.

rigid-body MI shell corrections $\delta\Theta_x^{\rm rig}$, while one has $\tilde{\Theta} \approx \Theta_{\rm TF}^{\rm rig}$. As shown by this comparison, we emphasize the importance of reducing oscillations of the total MI Θ_x calculations to the rigid-body MI shell correction $\delta\Theta_x^{\rm rig}$ (20) (RIG QM) of the statistical equilibrium rotation in the cranking model by its meaning itself. The quantum and semiclassical relations $\Theta \propto F$ [see Eqs. (20) and (63), respectively] seem to be important because they allow us to separate clearly the shell corrections in Θ_x by applying the standard procedure for the free-energy shell correction δF to the total free energy F (see Appendix C 1). For instance, subtraction of the constant λ from ε_i in the second of Eqs. (C7) is rather significant for obtaining the correct value of the energy shell corrections.

A comparison similar to that in Fig. 3, is presented in Fig. 6 for the quantum and semiclassical shell corrections to the MI $\delta\Theta_x$ of Eqs. (21) and (62), respectively. Again, an excellent agreement is observed between semiclassical and quantum results as for the free-energy shell components δF [see Eqs. (34) and (C1)]. It is not really astonishing because of the proportionality of $\delta\Theta_x$ to δF [Eqs. (21) and (62)]. One finds, in particular, the same clear interference of contributions of 3D and EQ POs in the shell corrections to the MI at $\eta = 2$. The exponential decrease in shell oscillations with increasing temperature, owing to the temperature factor $Q(t_n T/\hbar)$, Eq. (33) in Eqs. (34) and (32), is clearly shown in Fig. 6 too. The critical temperature for a disappearance of shell effects in the MI is found for prolate deformations ($\eta > 1$) and particle numbers $A \sim 100$–200, at approximately $T_{cr} = \hbar\omega_{\rm EQ}/\pi \sim \hbar\omega_0/\pi \approx 2$–$3$ MeV just as for δF (see Refs. [17] and [22]). By comparison of Fig. 6 with Fig. 4, one observes a huge decrease in the oscillation amplitudes of the MI for the statistically equilibrium compared to those of nonequilibrium rotations. The particle number dependence of the shell corrections $\delta\Theta_z$ to the total MI Θ_z (alignment) in Eqs. (22) and (62) is not shown because it is similar to that of $\delta\Theta_x$ through their relations, $\delta\Theta_z \propto \delta\Theta_x \propto \delta F$.

V. CONCLUSIONS

We derived the shell correction components $\delta\Theta_x$ and $\delta\Theta_z$ (perpendicular and alignment rotations) of the MI in terms of the free-energy shell correction δF within the nonperturbative extended POT through those of the rigid-body MI of the equilibrium rotations, which is exact for an HO potential. For the HO potential we extended to the finite-temperature case the Zelevinsky derivation of the nonadiabatic MI at any rotation frequency. For the deformed HO potential we found a perfect agreement between semiclassical POT and quantum results for the free-energy δF and the MI shell corrections $\delta\Theta_x$ and $\delta\Theta_z$ at several critical deformations and temperatures. For higher temperatures we show that the short EQ orbits are dominant. For low temperatures one observes a remarkable interference of the short 3D and EQ orbits in the superdeformed region. An exponential decrease in all shell corrections with increasing temperature is observed, as expected.

It would be worse to apply general points of this semiclassical theory to the shell corrections of the MI for the spheroid cavity and for the inertia parameter of the low-lying collective excitations in nuclear dynamics involving magic nuclei [35–37,45].

ACKNOWLEDGMENTS

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APPENDIX A: PARALLEL ROTATION

As related to the Routhian of the Fermi gas within the cranking model (1) for $\kappa = z$ (alignment of the angular momenta

of individual nucleons called here "parallel rotation"), for the partition function for the axially symmetric potential well, one may write [15–17,31,43]

$$\ln Z(\tau,\omega,\lambda) = d_s \sum_i \ln\{1+\exp[\tau(\lambda-\varepsilon_i+\omega\mu_i)]\}, \quad \text{(A1)}$$

where $\tau = 1/T$, ω and λ are the Lagrange multipliers, μ_i is the projection of the angular momentum in the s.p. state i. To determine these Lagrange multipliers in the case of parallel rotation, the constraints for the fixed angular momentum projection to the symmetry axis I_z and particle number A are given by

$$I_z = T\frac{\partial \ln Z}{\partial\omega} = d_s\sum_i n_i^\omega\mu_i, \quad A = T\frac{\partial \ln Z}{\partial\lambda} = d_s\sum_i n_i^\omega, \quad \text{(A2)}$$

$$E_\omega = -\frac{\partial \ln Z}{\partial\tau} = d_s\sum_i(\varepsilon_i-\omega\mu_i-\lambda)n_i^\omega,$$
$$n_i^\omega = \left\{1+\exp\left[\frac{\varepsilon_i-\omega\mu_i-\lambda}{T}\right]\right\}^{-1}, \quad \text{(A3)}$$

where n_i^ω are the ω-dependent occupation numbers (3), $\lambda^\omega = \lambda+\omega\mu_i$, E_ω is the energy corresponding to the Routhian (1) at $\kappa = z$ [counted from the constant λA, according to Eq. (A2)]. Therefore, for the actual rotation energy $E(\omega)$ of Eq. (5) in the laboratory system of coordinate, one writes

$$E(\omega) = E_\omega + \omega I_z = d_s\sum_i(\varepsilon_i-\lambda)n_i^\omega. \quad \text{(A4)}$$

It is convenient to calculate the angular momentum projection I_z by transformation of the sum over s.p. states i in the constraint relation (A2) to the integral over energy ε and angular momentum projection μ of the particle with the corresponding s.p. level density $g(\varepsilon,\mu)$,

$$I_z = d_s\int d\varepsilon\int d\mu\mu g(\varepsilon^\omega,\mu)n(\varepsilon^\omega), \quad \varepsilon^\omega = \varepsilon-\omega\mu, \quad \text{(A5)}$$

$n(\varepsilon)$ is the Fermi occupation numbers, Eq. (3), at $\omega = 0$. The MI Θ_z for alignment can be found by differentiation of the angular momentum $I_z(\omega)$, Eq. (A2) [or Eq. (A5)], in ω. With the help of Eq. (3) in the adiabatic case at $\omega\to 0$,

$$\Theta_z = \left(\frac{\partial I_z}{\partial\omega}\right)_{\omega=0} = d_s\sum_i\frac{\mu_i^2}{4T\cosh^2[(\varepsilon_i-\lambda)/2T]}$$
$$= d_s\sum_i\mu_i^2 g_{\rm Ti}(\lambda), \quad \text{(A6)}$$

where $g_{\rm Ti}(\lambda)$ is given by

$$g_{\rm Ti}(\varepsilon) = \frac{1}{4T\cosh^2[(\varepsilon-\varepsilon_i)/2T]},$$
$$g_{\rm Ti}(\lambda) = -\left(\frac{dn(\varepsilon)}{d\varepsilon}\right)_{\varepsilon=\varepsilon_i}, \quad \text{(A7)}$$

at $\varepsilon = \lambda$. It is convenient also to introduce the temperature level density $g_{\rm T}(\varepsilon)$ as the quantum level density $g(\varepsilon)$, averaged over the statistical ensemble, leading to a temperature spreading of the energy levels [17],

$$g_{\rm T}(\varepsilon) = \sum_i g_{\rm Ti}(\varepsilon) \to g(\varepsilon) = \sum_i\delta(\varepsilon-\varepsilon_i), \quad \text{(A8)}$$

in the zero temperature limit $T\to 0$.

The alignment results, Eqs. (A1)–(A6), can be applied to any axially symmetric potential, in particular, in the spherical limit where any polar axis can be considered the symmetry z axis [31]. For instance, for the HO Hamiltonian we need only to specify the spectrum ε_i, μ_i and quantum degeneracy of the levels i in summations over i. Differentiating expression (A5) for the angular momentum projection I_z of alignment of the individual angular momenta of particles along the symmetry z axis in Eq. (A6) for the adiabatic MI Θ_z (at $\omega = 0$), one has

$$\Theta_z = d_s\int d\varepsilon\int d\mu\mu\left\{\frac{\partial}{\partial\omega}[g(\varepsilon^\omega,\mu)n(\varepsilon^\omega)]\right\}_{\omega=0}$$
$$= -d_s\int d\varepsilon\int d\mu\mu^2\frac{\partial}{\partial\varepsilon}[g(\varepsilon,\mu)n(\varepsilon)]. \quad \text{(A9)}$$

For analytical calculations of the shell-structure MI $\delta\Theta_z$, we substitute the semiclassical level density,

$$g_{\rm scl}(\varepsilon,\mu) = g_{\rm ETF}(\varepsilon,\mu)+\delta g_{\rm scl}(\varepsilon,\mu),$$
$$g_{\rm scl}(\varepsilon) = \int d\mu g_{\rm scl}(\varepsilon,\mu), \quad \text{(A10)}$$

into the integrand of Eq. (A9) for $g(\varepsilon,\mu)$ with a smooth ETF component $g_{\rm ETF}(\varepsilon,\mu)$; see, for example, Ref. [25] for its main TF part. In this way, we may approximately present Eq. (A9) as a sum of the smooth and shell fluctuating parts,

$$\Theta_{z\rm scl} = \Theta_{z\rm TF}+\delta\Theta_{z\rm scl}, \quad \text{(A11)}$$

where $\Theta_{z\rm TF}$ is the TF approximation,

$$\Theta_{z\rm TF} = d_s\langle\mu^2\rangle_\lambda g_{\rm TF}(\lambda) = m\int d\mathbf{r}(x^2+y^2)\rho_{\rm TF}(\mathbf{r}), \quad \text{(A12)}$$

which is the rigid-body TF approach [25], $\Theta_{z\rm TF} = \Theta_{z\rm TF}^{\rm rig}$. By using derivations similar to those in Appendix C, we determine the shell component $\delta\Theta_{z\rm scl}$ of Eq. (A11) through the shell-structure level density $\delta g_{\rm scl}(\varepsilon,\mu)$ and fluctuations δn of the occupation numbers. The particle conservation equation (C4) is used in these derivations. For calculation of the semiclassical shell-structure component $\delta\Theta_{z\rm scl}$ of the sum (A11), one may apply the general POT for the level-density shell corrections $\delta g_{\rm scl}(\varepsilon,\mu)$ with the fixed angular momentum projection [25] for the axially symmetric HO potential [25],

$$\delta g_{\rm scl}(\varepsilon,\mu) = \frac{1}{2\mu_{\rm max}}\theta(\mu_{\rm max}-|\mu|)\delta g_{\rm scl}(\varepsilon), \quad \text{(A13)}$$

where $\delta g_{\rm scl}(\varepsilon)$ is the total semiclassical level-density shell correction, Eq. (45) [27], for the case of commensurable frequencies $\omega_\perp/\omega_z = n_\perp/n_z$, or the only $\delta g_{\rm EQ}(\varepsilon)$, Eq. (39), for the incommensurable case of an irrational ratio $\omega_\perp/\omega_z$. In Eq. (A13), $\mu_{\rm max}$ is the maximal s.p. angular momentum projection onto the symmetry z axis. By using Eqs. (A10) and (A13) for the shell-structure MI part $\delta\Theta_z$ and integrating explicitly over μ, one finds

$$\delta\Theta_{z\rm scl} = \frac{2d_s}{3}\int d\varepsilon\mu_{\rm max}(\varepsilon)\frac{d\mu_{\rm max}(\varepsilon)}{d\varepsilon}\delta g_{\rm scl}(\varepsilon)\delta n(\varepsilon). \quad \text{(A14)}$$

For the axially symmetric HO Hamiltonian $\mu_{\max} = \varepsilon/\omega_\perp$ in Eq. (A14), and according to Eq. (C7), we obtain the same rigid-body expression, Eq. (61), as in Sec. III D for alignment $\kappa = z$, after subtraction of the heat (entropy) part.

APPENDIX B: EXACT QUANTUM SOLUTIONS FOR THE HARMONIC OSCILLATOR

By using the standard transformation from the phase-space variables κ, p_κ for the creation a_κ^+ and annihilation a_κ operators ($\kappa = x, y, z$) for the s.p. Routhian H_ω, Eq. (1), one has

$$H_\omega = \sum_\kappa \hbar\omega_\kappa \left(a_\kappa^+ a_\kappa + \frac{1}{2}\right) - \omega\ell_x, \tag{B1}$$

where

$$\ell_x = \frac{\hbar}{2}\left[\frac{\omega_y + \omega_z}{\sqrt{\omega_y\omega_z}}(a_y a_z^+ + a_y^+ a_z) - \frac{\omega_y - \omega_z}{\sqrt{\omega_y\omega_z}}(a_y a_z + a_y^+ a_z^+)\right]; \tag{B2}$$

see Ref. [9]. It is convenient to use the Heisenberg representation, $a_\kappa(\tau) = e^{\tau H_\omega} a_\kappa e^{-\tau H_\omega}$, for the annihilation $a_\kappa(\tau)$ and creation $a_\kappa^+(\tau)$ operators depending formally on the imaginary time t, $\tau = it$. The Heisenberg dynamical equations for these operators can be written in the Liouville form,

$$\dot{\mathbf{A}}(\tau) = \mathcal{L}\mathbf{A}(\tau), \tag{B3}$$

for the vector operator $\mathbf{A}$ with four components, $\{a_y, a_y^+, a_z, a_z^+\}$, written in a column and Liouville 4×4 matrix $\mathcal{L}$ (in $\hbar = 1$ units) constructed one above the other in four rows, $\{-\omega_y, 0, p, -q\}$, $\{0, \omega_y, q, -p\}$, $\{p, -q, -\omega_z, 0\}$, and $\{q, -p, 0, \omega_z\}$, where p and q are given by

$$p = \frac{\omega}{2}\frac{\omega_y + \omega_z}{\sqrt{\omega_y\omega_z}}, \quad q = \frac{\omega}{2}\frac{\omega_y - \omega_z}{\sqrt{\omega_y\omega_z}}. \tag{B4}$$

For the formal solution one finds $\mathbf{A}(\tau) = \Phi(\tau)\mathbf{A}(0)$, with $\Phi(\tau) = e^{\tau\mathcal{L}}$. Introducing the correlation matrix,

$$\mathcal{C}_{\nu\mu} = \langle A_\nu(\tau)A_\mu(0)\rangle = \langle A_\mu(0)A_\nu(0)\rangle, \tag{B5}$$

for $\mathcal{C}_{\nu\mu}$ one can write the following system of equations:

$$\sum_\lambda [\Phi_{\nu\lambda}(\tau) - \delta_{\nu\lambda}]\mathcal{C}_{\lambda\mu} = -\mathcal{M}_{\nu\mu}, \tag{B6}$$

where $\mathcal{M}_{\nu\mu} = 1$ for $\nu = 1, \mu = 2$, and $\nu = 3, \mu = 4$; -1 for these exchanged indeces; and otherwise, zeros. Its formal solution for the correlation matrix $\mathcal{C}$ is given by

$$\mathcal{C} = -\mathcal{D}^{-1}\mathcal{M}, \quad \mathcal{D} = \Phi(\tau) - \mathcal{I}, \quad \Phi(\tau) = e^{\tau\mathcal{L}}, \tag{B7}$$

where $\mathcal{I}$ is the 4×4 unit matrix. The Liouville operator $\mathcal{L}$ of Eq. (B4) has four eigenvalues $\pm\omega_\pm$ for the Routhian H_ω, Eq. (B1), which are determined by [5]

$$\omega_\pm^2 = \omega^2 + \frac{\omega_y^2 + \omega_z^2}{2} \pm \frac{\omega_y^2 - \omega_z^2}{2}\sqrt{1 + \frac{8\omega^2(\omega_y^2 + \omega_z^2)}{(\omega_y^2 - \omega_z^2)^2}}. \tag{B8}$$

As the Liouville matrix has four eigenvalues, the inverse matrix $\mathcal{D}^{-1}$ of (B7) can be approximated by the cubic polynomial under the conditions formulated in Refs. [40] and [41] through its four unknown constants Υ_ν:

$$\mathcal{D}^{-1} = \sum_{\nu=0}^{3} \Upsilon_\nu \mathcal{L}^\nu. \tag{B9}$$

These constants are defined by four simple linear equations,

$$\sum_{\nu=0}^{3} \Upsilon_\nu \omega_\pm^\nu = N_{\pm i}, \quad \sum_{\nu=0}^{3} (-1)^\nu \Upsilon_\nu \omega_\pm^\nu = -(N_{\pm i} + 1),$$
$$N_{\pm i} = (e^{\tau\omega_\pm} - 1)^{-1}, \tag{B10}$$

with simple solutions,

$$\Upsilon_0 = -\frac{1}{2}, \quad \Upsilon_1 = \frac{(N_{-i} + 1/2)\omega_+^3 - (N_{+i} + 1/2)\omega_-^3}{\omega_-\omega_+(\omega_+^2 - \omega_-^2)},$$
$$\Upsilon_2 = 0, \quad \Upsilon_3 = \frac{(N_{+i} + 1/2)\,\omega_- - (N_{-i} + 1/2)\,\omega_+}{\omega_-\omega_+(\omega_+^2 - \omega_-^2)}. \tag{B11}$$

For instance, for relatively large τ [low temperatures in units of $\hbar\omega_0$, $T/\hbar\omega_0$, for $\tau = 1/T$, as in Eq. (A1)], one can use analytically the corresponding expansion in a large $\tau\mathcal{L}$ and find that Eq. (B9) becomes identity.

Substituting Eq. (B11) into the determinant of the inversed matrix $\mathcal{D}^{-1}$, Eq. (B9), we calculate the correlation matrix elements $\mathcal{C}_{\nu\mu}$, Eq. (B7). After lengthy derivations of the average of the s.p. angular momentum $\langle\ell_x\rangle_i$ in state i through Eq. (B2) and

$$\omega\langle\ell_x\rangle_i = p\,(\mathcal{C}_{14} + \mathcal{C}_{23}) - q\,(\mathcal{C}_{13} + \mathcal{C}_{24}), \tag{B12}$$

one arrives exactly at the same Zelevinsky's result [5] for arbitrary frequency ω,

$$\langle\ell_x\rangle_i = \omega\left[\frac{N_{-i} + 1/2}{\omega_-}\left(2\frac{\omega_y^2 + \omega_z^2}{\omega_+^2 - \omega_-^2} - 1\right) - \frac{N_{+i} + 1/2}{\omega_+}\left(2\frac{\omega_y^2 + \omega_z^2}{\omega_+^2 - \omega_-^2} + 1\right)\right], \tag{B13}$$

where $N_{\pm i}$ are, however, the temperature-dependent Bose quantum numbers of Eq. (B10). From this expression, by summation over the s.p. states i as in Eq. (13), one obtains the MI $\Theta_x(\omega)$ [5],

$$\Theta_x(\omega) = \sum_i n_i \frac{\langle\ell_x\rangle_i}{\omega} = 2\frac{\omega_y^2 + \omega_z^2}{\omega_+^2 - \omega_-^2}\left(\frac{\aleph_-}{\omega_-} - \frac{\aleph_+}{\omega_+}\right) - \left(\frac{\aleph_+}{\omega_+} + \frac{\aleph_-}{\omega_-}\right), \quad \aleph_\pm = \sum_i n_i\left(N_{\pm i} + \frac{1}{2}\right). \tag{B14}$$

Note that this expression, under the conditions of Refs. [40] and [41], can be applied for finite temperatures $T = 1/\tau$ that appear through the oscillator occupation numbers $N_{\pm i}$ in Eq. (B10). The dynamic MI of Eq. (5) is determined by a direct differentiation of Eq. (B14) with respect to ω. Both definitions of the MI lead to the same adiabatic expression, Eq. (12).

APPENDIX C: ENERGY SHELL CORRECTIONS

C1. Quantum calculations

For comparison of the semiclassical expression (34) of the free-energy δF and thermodynamic-potential shell corrections $\delta\Omega$ with the quantum shell components, one writes

$$\delta F = F_{\rm s.p.} - \tilde{F}_{\rm s.p.}, \quad \delta\Omega = \Omega_{\rm s.p.} - \tilde{\Omega}_{\rm s.p.}, \tag{C1}$$

where

$$F = E - T\mathcal{S} = \Omega + \lambda A, \tag{C2}$$

defined, for instance, through the thermodynamic potential of a quantum Fermi gas [43],

$$\Omega_{\rm s.p.}(T,\lambda) = d_s T \sum_i \ln\left[1 - n\left(\frac{\varepsilon_i - \lambda}{T}\right)\right]. \tag{C3}$$

The tilde in Eq. (C1) indicates the Strutinsky smoothing of the s.p. quantities [10,11,17]. For the particle number conservation, one has

$$A = d_s \sum_i n_i = d_s \sum_i \tilde{n}_i. \tag{C4}$$

In Eqs. (C3) and (C4), n_i and ε_i are the Fermi occupation numbers and energies in quantum states i for a given s.p. Hamiltonian H of Eq. (1) [see Eq. (3) at $\omega = 0$ for the occupation numbers n_i]. In Eq. (C4), $\tilde{n}_i$ are the averaged Fermi occupation numbers, determined usually by the Strutinsky smoothing procedure [10,11,17] at the averaged chemical potential $\lambda = \tilde{\lambda}$ found from the particle number conservation condition, Eq. (C4), $\tilde{\lambda} = \tilde{\lambda}(A)$:

$$\tilde{n}\left(\frac{\varepsilon - \lambda}{T}\right) = \int_{-\infty}^{\infty} {\rm d}\lambda'\, n\left(\frac{\varepsilon - \lambda'}{T}\right) \xi_M\left(\frac{\lambda' - \lambda}{\gamma}\right),$$
$$\xi_M(x) = \frac{1}{\sqrt{\pi}} \exp(-x^2) P_{2M}(x). \tag{C5}$$

Here the correction polynomial of the order of $2M$, $P_{2M}(x) = \sum_{k=0,2,\ldots}^{2M} \alpha_k H_k(x)$, is defined through the recurrence relations, $\alpha_k = -\alpha_{k-2}/2k$, $\alpha_0 = 1$, and $H_k(x)$ is the standard Hermite polynomial. The tilde in Eq. (C1) might be defined as the averaging over the chemical potential; see Eq. (C5).

According to the general thermodynamic relations, Eq. (C2) [43], one may define the shell-structure internal energy,

$$\delta E = \delta F + T\delta\mathcal{S}, \tag{C6}$$

as the internal energy shell correction δE to the total energy E of a heated system [10,11,17],

$$\delta E = E_{\rm s.p.} - \tilde{E}_{\rm s.p.} = 2\sum_i (\varepsilon_i - \lambda)\delta n_i$$
$$\approx \int {\rm d}\varepsilon\, (\varepsilon - \lambda)\, \delta g(\varepsilon) \delta n\left(\frac{\varepsilon - \lambda}{T}\right). \tag{C7}$$

The sum over spectrum ε_i in the internal energy of the heated quantum Fermi gas $E_{\rm s.p.}$ can be presented through the integral over all energies ε with the level density $g(\varepsilon)$ as

$$E_{\rm s.p.} = 2\int d\varepsilon \varepsilon g(\varepsilon) n\left(\frac{\varepsilon - \lambda}{T}\right). \tag{C8}$$

The level density $g(\varepsilon)$ [see Eq. (A8)], averaged over spectrum $g_\gamma(\varepsilon)$, with the Gaussian weight having an averaging width γ much smaller than the distance between gross shells, $\hbar\omega_0 \approx \varepsilon_F/A^{1/3} \sim$ 7–10 MeV for heavy nuclei, $A \sim$ 40–200, is expressed in terms of the smooth $\tilde{g}(\varepsilon)$ and shell-structure $\delta g(\varepsilon)$ components:

$$g_\gamma(\varepsilon) = \tilde{g}(\varepsilon) + \delta g_\gamma(\varepsilon). \tag{C9}$$

The quantum shell correction to the level density $\delta g(\varepsilon)$ in Eq. (C7) is also averaged over this γ as $\delta g_\gamma(\varepsilon)$ in Eq. (C9), and then the limit $\gamma \to 0$ is taken in the integrand of Eq. (C7). The shell correction to the Fermi occupation numbers (C4) is given by

$$\delta n(x) = n(x) - \tilde{n}(x), \quad x = (\varepsilon - \lambda)/T, \tag{C10}$$

where $\tilde{n}(x)$ is the smoothed occupation numbers, Eq. (C5), and $\delta E = \delta U$ at temperature $T = 0$. For comparison of quantum and semiclassical results for $\delta g_\gamma(\varepsilon)$, one should do the same averaging procedure for both compared quantities (the correction polynomial degree $M = 0$ in the Strutinsky SCM; see Refs. [17] and [22]). The smooth level density $\tilde{g}(\varepsilon)$ is determined by the values $\tilde{\gamma}$ and $\tilde{M}$ for the averaging parameters, the Gaussian width γ and correction polynomial degree M, on the so-called plateau in dependence of $\delta g_\gamma(\varepsilon)$ on γ for several M (usually $M =$ 4–10) at fixed characteristic energies ε. This density $\tilde{g}(\varepsilon)$ is constant independent of the averaging parameters on this plateau. The smooth density component of the level density $\tilde{g}(\varepsilon)$ can be approximated with very good precision by the ETF approach [17,18], $\tilde{g}(\varepsilon) \approx g_{\rm ETF}(\varepsilon)$. The smooth energy is given by

$$\tilde{E}_{\rm s.p.} = \int d\varepsilon \varepsilon \tilde{g}(\varepsilon) \tilde{n}\left(\frac{\varepsilon - \tilde{\lambda}}{T}\right), \tag{C11}$$

excluding any shell fluctuations in all quantities of importance, namely, in the level density $g_\gamma(\varepsilon)$, Eq. (C9), occupation numbers $n(x) = \tilde{n} + \delta n$ associated with Eq. (C10), and chemical potential $\lambda = \tilde{\lambda} + \delta\lambda$. The shell-structure occupation numbers δn are defined by the Strutinsky SCM [10,11,17] through the averaged occupation numbers $\tilde{n}_i$; see Eq. (C5). Up to small terms, of the order of $(\tilde{\gamma}/\lambda)^2$, $(\tilde{\gamma}/\lambda)\delta\lambda/\lambda$, and $(\delta\lambda/\lambda)^2$, we arrived at Eq. (C7). For convenience, writing $\tilde{\lambda} = \lambda - \delta\lambda$ from Eq. (C10), we expanded smooth quantities marked by a tilde here in $\delta\lambda$, keeping only linear terms in $\delta\lambda/\lambda$.

For calculations of the shell component $\delta\Omega$ of the thermodynamic potential Ω, one calculates first $\Omega_{\rm s.p.}(T,\lambda)$, Eq. (C3), and then, $\tilde{\Omega}_{\rm s.p.}(T,\lambda)$ by using the Strutinsky smoothing procedure over λ, as defined in Eq. (C5), directly for the sum over states in Eq. (C3). The plateau condition for $\delta\Omega$ of Eqs. (C1) is studied as a function of averaging parameters γ and M at several typical λ, and then the values $\tilde{\gamma}$ of γ's and $\tilde{M}$ of M's in Eq. (C5) at this plateau are taken for the calculations of $\delta\Omega(T,\lambda)$ as a function of λ and corresponding particle number A through $\lambda(A)$. The smoothing over λ is the same as that over spectrum ε_i because they appear in $\Omega_{\rm s.p.}$, Eq. (C3), through differences $\varepsilon_i - \lambda$. We have to keep in mind that the variable λ should be the same in quantum and semiclassical calculations for their comparison.

C2. Semiclassical derivations

For the shell-structure level density $\delta g^{\gamma}_{\rm scl}(\varepsilon)$, averaged with the same Gaussian weight and width γ (see Ref. [22]), one has

$$\delta g^{\gamma}_{\rm scl}(\varepsilon) = \sum_{\rm po} \delta g_{\rm po}(\varepsilon) \exp[-(t_{\rm po}\gamma/\hbar)^2], \quad t_{\rm po} = \frac{\partial S_{\rm po}}{\partial \varepsilon}. \tag{C12}$$

Substituting the POT expansion of this $\delta g^{\gamma}_{\rm scl}(\varepsilon)$ into Eq. (C7), we expand the smooth amplitude $\mathcal{A}_{\rm po}(\varepsilon)$ of $\delta g_{\rm po}(\varepsilon)$ (28) at zero order and its action $S_{\rm po}(\varepsilon)$ at linear order in powers of $\varepsilon - \lambda$ at an energy equal to the chemical potential, $\varepsilon = \lambda$ [17,22,31,36]. Introducing also the dimensionless energy variable x [see Eq. (C10)], in the limit $\gamma \to 0$ one finds

$$\delta E = {\rm Re} T^2 \sum_{\rm po} \delta g_{\rm po}(\lambda) \int_{-\infty}^{\infty} {\rm d}x x \delta n(x) \exp(i \mathcal{Z}_{\rm po} x), \tag{C13}$$

where $\delta g_{\rm po}(\lambda)$ is the PO component of the POT level-density shell correction, Eq. (29), at energy $\varepsilon = \lambda$, and $\mathcal{Z}_{\rm po}$ is given by Eq. (33). As usual in the Sommerfeld expansion in powers of T/λ [43], up to higher order in T/λ, the low limit is extended to $-\infty$. Integrating now by parts and using the property of 0 for $\delta n(x)$ at both integration limits, one obtains

$$\delta E = -{\rm Re} \sum_{\rm po} \delta U_{\rm po} \left[\int_{-\infty}^{\infty} {\rm d}x \frac{{\rm d}\delta n(x)}{{\rm d}x} \exp(i \mathcal{Z}_{\rm po} x) - i \mathcal{Z}_{\rm po} \int_{-\infty}^{\infty} {\rm d}x x \frac{{\rm d}\delta n(x)}{{\rm d}x} \exp(i \mathcal{Z}_{\rm po} x) \right]. \tag{C14}$$

Using the approximate relation [36],

$$\frac{{\rm d}\delta n(x)}{{\rm d}x} = -\frac{1}{4\cosh^2(x/2)}, \tag{C15}$$

one finally arrives at Eq. (35). The shell-structure components $\delta\Omega(T, \lambda)$ and δF in Eq. (C1), for the thermodynamic potential $\Omega_{\rm s.p.}(T, \lambda)$ [Eq. (C3)] and free energy $F_{\rm s.p.}$ [see Eq. (C2)], can be similarly approximated by the POT expression (34) (see Refs. [31] and [32]).

APPENDIX D: LOCAL THOMAS-FERMI MOMENT OF INERTIA

D1. The Thomas-Fermi approach

For the MI $\Theta^{\rm rig}_x$, Eqs. (17) and (48), within the TF approach, one has [12–15,17]

$$\Theta^{\rm rig}_{x{\rm TF}} = m \int {\rm d}\mathbf{r} r^2_{\perp x} \rho_{\rm TF}(\mathbf{r}) = \frac{m d_s}{6\pi^2\hbar^3} \int {\rm d}\mathbf{r} (y^2 + z^2) p_F^3, \tag{D1}$$

where $\rho_{\rm TF}$ is the TF particle density,

$$\rho_{\rm TF}(\mathbf{r}) = -\frac{d_s}{\pi} {\rm Im} \int {\rm d}\varepsilon n(\varepsilon) [G_0(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)]_{\mathbf{r}_1 = \mathbf{r}_2 = \mathbf{r}} = \frac{d_s p_F^3}{6\pi^2\hbar^3}. \tag{D2}$$

G_0 is defined in Eq. (26), $p_F(\mathbf{r}) = (2m\{\varepsilon_F - m[(x^2 + y^2)\omega_\perp^2 + \omega_z^2 z^2]\})^{1/2}$ for the HO potential. For simplicity, we put zero temperature, $T = 0$, in this section of Appendix D.

Using the "spherization" scaling transformation of the spatial coordinates x, y, z to the dimensional Cartesian coordinates u_x, u_y, u_z of vector $\mathbf{u}$, $x = x_m u_x$, $y = y_m u_y$, $z = z_m u_z$ [see Eq. (57) for maximal values of the coordinates x, y, z at the given energy $\varepsilon = \varepsilon_F$], one integrates exactly over $\mathbf{r}$ in Eq. (D1). With symmetry properties of integrals in these new coordinates, one then obtains

$$\Theta^{\rm rig}_{\kappa TF} = m\omega_\perp^2 \left(\frac{1 + \eta^2}{3\omega_\perp^2} \right) z_m x_m^4 \int {\rm d}\mathbf{u}\, u^2 \rho_0(u_x, u_y, u_z), \tag{D3}$$

where

$$\rho_0(u_x, u_y, u_z) = \rho_{\rm TF}(x, y, z) = \frac{d_s (2m\varepsilon_F)^{3/2}}{6\pi^2\hbar^3} (1 - u^2)^{3/2}, \quad u^2 = u_x^2 + u_y^2 + u_z^2. \tag{D4}$$

Taking exactly analytically the integral over the radial variable u from 0 to 1 in Eq. (D3) in the spherical coordinate system, ${\rm d}\mathbf{u} = {\rm d}u_x {\rm d}u_y {\rm d}u_z = u^2 {\rm d}u \sin\theta {\rm d}\theta {\rm d}\varphi$ and writing 4π for the angle integration, one obtains

$$\Theta^{\rm rig}_{x{\rm TF}} = \left(\frac{1 + \eta^2}{3\omega_\perp^2} \right) \frac{\varepsilon_F^4}{3(\hbar\omega_0)^3}. \tag{D5}$$

For the TF energy $E_{\rm TF}$ one has

$$E_{\rm TF} = d_s \int \frac{{\rm d}\mathbf{r}{\rm d}\mathbf{p}}{(2\pi\hbar)^3} \left\{ \frac{p^2}{2m} + \frac{m}{2} \left[\omega_\perp^2 (x^2 + y^2) + \omega_z^2 z^2 \right] \right\}. \tag{D6}$$

Using the virial theorem, according to which the average of the kinetic and HO potential parts of this integral are equivalent, and a similar "spherization" scaling transformation of the spatial coordinates and analytical integration, one obtains

$$E_{\rm TF} = m\omega_\perp^2 z_m x_m^4 \int {\rm d}\mathbf{u}\, u^2 \rho_0(u_x, u_y, u_z) = \frac{\varepsilon_F^4}{3(\hbar\omega_0)^3}. \tag{D7}$$

From a comparison of Eq. (D5) with Eq. (D7), one finds the same relation between the TF MI $\Theta^{\rm rig}_x$ and the energy $E_{\rm TF}$ at zero temperature $T = 0$,

$$\Theta^{\rm rig}_{\kappa{\rm TF}} = \left(\frac{1 + \eta^2}{3\omega_\perp^2} \right) E_{\rm TF}, \tag{D8}$$

as that obtained in the case of applying the statistically equilibrium relation (16) [see Eq. (20)]. Similarly, we may show the relation (22) between $\Theta^{\rm rig}_z$ and $E_{\rm TF}$ for the parallel rotation; see Appendix A. Note that one may obtain the mass of a Fermi particle system from the cranking model expression with a dipole kind of s.p. operator within this model for a translation invariant motion [48].

D2. From the local short-range periodic-orbit theory to the Thomas-Fermi approach

For semiclassical calculations of Θ^{00}_x from Eq. (65) of the sum (64), we have to separate the nearly local (short-range) parts from the nonlocal (long-range) contributions in the MI, Eq. (9) [38]. This is in contrast to the local POT level-density and energy shell correction calculations, where we need only closed orbits $\mathbf{r}_1 = \mathbf{r}_2 = \mathbf{r}$. This can be done by using averaging

in the phase space as in derivations of the liquid-drop model from many-body finite Fermi systems of interacting strongly particles. For calculations of the smooth MI we can apply the nearly local approximation [45], $S_\alpha(\mathbf{r}_1,\mathbf{r}_2;\varepsilon_F)/\hbar \approx k_F L_\alpha \lesssim 1$, where L_α is the length of the trajectory α in expansion (23), and k_F is the Fermi momentum in units of $\hbar$. In this almost-local case, after Strutinsky averaging [10,11,17], the most important contribution comes from the trajectory α_0, with a *short* length smaller than or of the order of the wavelength $1/k_F$ near the Fermi surface, $L_{\alpha_0} \approx s = |\mathbf{r}_2 - \mathbf{r}_1| \lesssim 1/k_F \ll R$, for a large semiclassical parameter, $k_F R \gg 1$, where R is the size of the nucleus. For simplicity of Eqs. (65) for the MI component $\tilde{\Theta}_x^{00}$, the variables $\{\mathbf{r}_1,\mathbf{r}_2\}$ can be transformed to $\{\mathbf{r},\mathbf{s}\}$, $\mathbf{r} = (\mathbf{r}_1+\mathbf{r}_2)/2$, $\mathbf{s} = \mathbf{r}_2 - \mathbf{r}_1$. The Green's function term of the sum (23), G_{α_0}, in the new variables $\mathbf{r}, \mathbf{s}$ for small enough length s of the trajectory α_0, $s/R \ll 1$, is reduced approximately to a simple well-known analytical form G_0, similar to that of a free particle motion [see Eq. (26)]. We use this approach to the Green's function to relate approximately the smooth part of the MI Θ_x^{00} of Eq. (65) with the rigid-body TF MI. With this Green's function approximation, from Eq. (65) one has

$$\begin{aligned}\Theta_x^{00} &= \frac{2d_s}{\pi}\int_0^\infty \mathrm{d}\varepsilon n(\varepsilon)\int \mathrm{d}\mathbf{r}\int \mathrm{d}\mathbf{s}\,\ell_x\left(\mathbf{r}-\frac{\mathbf{s}}{2}\right)\ell_x\left(\mathbf{r}+\frac{\mathbf{s}}{2}\right)\\ &\times \mathrm{Re}\left[G_{\alpha_0}\left(\mathbf{r}-\frac{\mathbf{s}}{2},\mathbf{r}+\frac{\mathbf{s}}{2};\varepsilon\right)\right]\\ &\times \mathrm{Im}\left[G_{\alpha_0}\left(\mathbf{r}-\frac{\mathbf{s}}{2},\mathbf{r}+\frac{\mathbf{s}}{2};\varepsilon\right)\right]\\ &\approx \frac{d_s m^2}{\pi^2\hbar^3}\int \mathrm{d}\varepsilon n(\varepsilon)\int \mathrm{d}\mathbf{r} r_{\perp x}^2 p(\mathbf{r})\\ &\times \int \sin\theta_s \mathrm{d}\theta_s \mathrm{d}\varphi_s \sin^2\left[\frac{1}{\hbar}s_{\max}p(\mathbf{r})\right]. \end{aligned} \tag{D9}$$

In the last equation, we used Eq. (67) for the classical angular momentum of the particle for the rotation around the x axis within the nearly local approximation (26). Then we transformed the integral over $\mathbf{s}$ to the spherical coordinate system, $\mathrm{d}\mathbf{s} = s^2 \mathrm{d}s\sin\theta_s \mathrm{d}\theta_s \mathrm{d}\varphi_s$, with the center at point $\mathbf{r}$ and the polar axis directed to the $\mathbf{r}$ vector, and integrated over modulus s from 0 to its maximal value $s_{\max}$, depending on angles of $\mathbf{s}$ such that the integral over angles θ_s and φ_s becomes rather complicated. However, we may note that the phase-space averaging of the sine squared in its integrand is $1/2$. Therefore, we like to separate the local part related to this mean value $1/2$ from nonlocal correlations by its identical adding and subtracting:

$$\Theta_x^{00} = \Theta_{x\mathrm{TF}} + \Delta\Theta_x^{00}, \quad \Theta_{x\mathrm{TF}} = m\int \mathrm{d}\mathbf{r} r_{\perp x}^2\,\rho_{\mathrm{TF}}(\mathbf{r}). \tag{D10}$$

Here the first local part $\Theta_{x\mathrm{TF}}$ is exactly the rigid-body MI (D1) with the TF particle density $\rho_{\mathrm{TF}}(\mathbf{r})$, Eq. (D2),

$$\rho_{\mathrm{TF}}(\mathbf{r}) = \frac{d_s m}{2\pi^2\hbar^3}\int \mathrm{d}\varepsilon n(\varepsilon) p(\mathbf{r}) \approx \frac{d_s p_F^3(\mathbf{r})}{6\pi^2\hbar^3}, \tag{D11}$$

and $\Delta\Theta_x^{00}$ includes the nonlocal long-range correlations,

$$\begin{aligned}\Delta\Theta_x^{00} &= \frac{d_s m^2}{\pi^2\hbar^3}\int \mathrm{d}\varepsilon n(\varepsilon)\int \mathrm{d}\mathbf{r} r_\perp^2 p(\mathbf{r})\int \sin\theta_s \mathrm{d}\theta_s \mathrm{d}\varphi_s\\ &\times\left\{\sin^2\left[\frac{1}{\hbar}s_{\max}p(\mathbf{r})\right]-1/2\right\}. \end{aligned} \tag{D12}$$

For simplicity, we omitted the temperature corrections, $\sim T^2/\lambda^2$, which can be easily included by using the standard Sommerfeld expansion [43]. The integral over angles θ_s, φ_s were taken within the same local approximation in the first term of the sum in Eq. (D10) as 4π. Local averaging of the nonlocal component (D12) is 0, and we arrive at the smooth TF component $\Theta_{x\mathrm{TF}}$ of Eq. (D10). The $\hbar$ corrections of a more precise ETF approach for the smooth MI can be included too (see Refs. [15,19], and [20]).

Note that we found a rigid-body inertia $\Theta_{x\mathrm{TF}}$ [see Eq. (D10)] by using essentially averaging over the phase-space variables, which removes the second nonlocal term $\Delta\Theta_x^{00}$, in particular, Strutinsky averaging over energies of the s.p. states ε_i. The result is diagonal with respect to energies ε_i of the s.p. states i, which is beyond the perturbation cranking model formula (6). Taking averaging, we ignored exclusion of the diagonal terms in Eq. (6) or (9), thinking of these formulas in a more general sense than within the perturbation approach. Thus, the averaged moment $\tilde{\Theta}_x$ can be approximated by the smooth (rigid-body) TF part $\Theta_{x\mathrm{TF}}$ of Θ_x^{00} in Eq. (D10) with $\hbar$ corrections of the ETF approach [19,20].

APPENDIX E: PERIODIC-ORBIT CONTRIBUTIONS TO $\delta\Theta_x$

E1. Classical harmonic-oscillator dynamics

The solutions of the classical Newtonian dynamical equations, $\mathbf{r} = \mathbf{r}(t)$ and $\mathbf{p} = \mathbf{p}(t)$, for a phase-space trajectory α in the HO potential,

$$H = \frac{\mathbf{p}^2}{2m} + \frac{m}{2}\left[\omega_\perp^2(x^2+y^2)+\omega_z^2 z^2\right], \tag{E1}$$

going from an initial point $\mathbf{r}_1 = \{x_1, y_1, z_1\}$ at initial time $t = 0$ to a final point $\mathbf{r}_2 = \{x_2, y_2, z_2\}$ at time $t = t_\alpha$, can be written analytically in the explicit form [27]

$$\begin{aligned}\kappa(t) &= \kappa_1\frac{\sin(\omega_\kappa t+\phi_\kappa)}{\sin\phi_\kappa},\\ p_\kappa(t) &= m\dot{\kappa}(t) = m\omega_\kappa\kappa_1\frac{\cos(\omega_\kappa t+\phi_\kappa)}{\sin\phi_\kappa}, \quad \kappa = x, y, z. \end{aligned} \tag{E2}$$

The phases ϕ_x, ϕ_y, and ϕ_z are related through the energy conservation,

$$\varepsilon = \frac{m}{2}\left(\frac{x_1^2\omega_x^2}{\sin^2\phi_x}+\frac{y_1^2\omega_y^2}{\sin^2\phi_y}+\frac{z_1^2\omega_z^2}{\sin^2\phi_z}\right), \tag{E3}$$

which allows us to express one of the phases through ε and the other two through, for example, $\phi_z(\varepsilon,\phi_x,\phi_y)$.

In the case of incommensurable frequencies (irrational η), all closed (and therefore periodic) classical trajectories in

the axially symmetric HO potential are EQ orbits with the degeneracy $\mathcal{K}=2$, and 3D trajectories appear only with a nonperiodic motion in the z direction. For commensurable frequencies (rational η), both 3D and EQ POs contribute to the degeneracies $\mathcal{K}=4$ and 2, respectively. A closed HO trajectory corresponds to a PO (or part of a PO), whereas a nonclosed trajectory is isolated ($\mathcal{K}=0$).

E2. Jacobian and amplitude calculations

For the case of isolated nonclosed classical trajectories in expansion (23), one can apply the Gutzwiller approximation [17,21,22] for the Green's function $G(\mathbf{r}_1,\mathbf{r}_2;\varepsilon)$ (see Eq. (23)] to the amplitude, Eq. (24). For calculations of the Jacobian $\mathcal{J}_\alpha(\mathbf{p}_1,t_\alpha;\mathbf{r}_2,\varepsilon)$ of transformation of the initial momentum $\mathbf{p}_1$ and time of motion t_α to the final coordinate $\mathbf{r}_2$ and energy ε, we need to express the variations $\delta\mathbf{p}_1$ and $\delta\mathbf{r}_2$ of initial momentum $\mathbf{p}_1$ (at the point $\mathbf{r}_1$) and final coordinate $\mathbf{r}_2$ through $\delta\phi_i$:

$$\delta p_{\kappa 1}=-\frac{m\omega_\kappa\kappa_1}{\sin^2\phi_\kappa}\delta\phi_\kappa,\quad \delta\kappa_2=-\kappa_1\frac{\sin(\omega_\kappa t_\alpha)}{\sin^2\phi_\kappa}\delta\phi_\kappa. \tag{E4}$$

Using also, locally along the trajectory between $\mathbf{r}_1$ and $\mathbf{r}_2$, a transformation to Cartesian coordinates $\{x',y',z'\}$, where x' is along the trajectory α, and y',z' perpendicular to it. Due to the invariance properties of the Jacobian, one then obtains [21,22] for any $\mathbf{r}_1\neq\mathbf{r}_2$:

$$\mathcal{J}_\alpha(\mathbf{p}_1,t_\alpha;\mathbf{r}_2,\varepsilon)=-\frac{m^2}{p_1p_2}\left(\frac{\partial p_{y1}}{\partial y_2}\frac{\partial p_{z1}}{\partial z_2}-\frac{\partial p_{z1}}{\partial y_2}\frac{\partial p_{y1}}{\partial z_2}\right)=0, \tag{E5}$$

where we have used the Hamilton-Jacobi equation of classical motion and Eq. (E4). Therefore, for non-closed trajectories, the amplitudes $\mathcal{A}_\alpha$, Eq. (24), vanish.

For closed ($\mathbf{r}_1=\mathbf{r}_2=\mathbf{r}$) orbits (POs) an enhancement of the amplitudes $\mathcal{A}_{\rm po}$ in Eq. (23) must be taken into account [22,27], owing to their increased degeneracy (see the text). In that particular case of the 3D family of closed (and, therefore, periodic) orbits for the amplitudes of the Green's function (23) in Eq. (59) at $\alpha\neq\alpha_0$, one finds [27]

$$\mathcal{A}_n^{\rm 3D}(\mathbf{r},\varepsilon)=-\frac{mp(\mathbf{r})}{2\pi\hbar^3},$$
$$\text{with}\quad p(\mathbf{r})=\sqrt{2m\left\{\varepsilon-\frac{m}{2}\left[\omega_\perp^2(x^2+y^2)+\omega_z^2z^2\right]\right\}}, \tag{E6}$$

independently of the period number n specifying the POs. For the EQ POs, one has [27]

$$\mathcal{A}_n^{\rm EQ}(\mathbf{r},\varepsilon)=(8\pi\hbar^5)^{-1/2}m\{|J_n(p_{z1},z_2)|^{1/2}\}_{\mathbf{r}_1\to\mathbf{r}_2\to\mathbf{r}},$$
$$J_n(p_{z1},z_2)=\left\{\frac{\partial p_{z1}}{\partial z_2}\right\}_n. \tag{E7}$$

E3. Calculations of the periodic-orbit components of $\delta\Theta_x$

To obtain the component Θ_x^{01} of the MI, according to Eq. (66), one can evaluate the integral over $\mathbf{s}$ in the spherical coordinate system, $\mathrm{d}\mathbf{s}=s^2\mathrm{d}s\sin\theta_s\mathrm{d}\theta_s\mathrm{d}\varphi_s$, with the center at the point $\mathbf{r}$ and the polar axis directed along the initial momentum $\mathbf{p}(\mathbf{r})$ for the trajectory α ($p=|\mathbf{p}(\mathbf{r})|$),

$$\frac{p^2}{\pi\hbar^2}\int_0^{s_{\max}}s\mathrm{d}s\int_0^{\pi}\sin\theta_s\mathrm{d}\theta_s\int_0^{2\pi}\mathrm{d}\varphi_s\cos\left(\frac{sp}{\hbar}\right)\times\exp\left(\frac{i}{\hbar}sp\cos\theta_s\right)=1-\cos\left(\frac{2}{\hbar}s_{\max}p\right), \tag{E8}$$

whereas for Θ_x^{10} one needs

$$\frac{p^2}{2\pi\hbar^2}\int_0^{s_{\max}}s\mathrm{d}s\int_0^{\pi}\sin\theta_s\mathrm{d}\theta_s\int_0^{2\pi}\mathrm{d}\varphi_s\sin\left(\frac{sp}{\hbar}\right)\times\exp\left(\frac{i}{\hbar}sp\cos\theta_s\right)=\frac{s_{\max}p}{\hbar}-\sin\left(\frac{2}{\hbar}s_{\max}p\right). \tag{E9}$$

The local average over phase-space variables in Eqs. (E8) and (E9) removes the oscillating terms, and in the nearly local approximation, $ps_{\max}/\hbar\ll1$, one can neglect the quantity (E9) compared to that of (E8), in which one finds the finite value 1 for the integral, as in Appendix D 2. Thus, Θ_x^{10} is contributing to the nonlocal long-range correlation part of Θ_x, whereas with Eq. (E8) one approximately obtains the rigid-body shell correction $\delta\Theta_x^{\rm rig}$ in Eq. (66). In these derivations we used the nearly local short-range approximation for the amplitude $\mathcal{A}_\alpha[\mathbf{r}-(\mathbf{s}/2),\mathbf{r}+(\mathbf{s}/2);\varepsilon]$ and action $S_\alpha[\mathbf{r}-(\mathbf{s}/2),\mathbf{r}+(\mathbf{s}/2);\varepsilon]$ in the Green's function,

$$G_1=\sum_{\alpha\neq\alpha_0}\mathcal{A}_\alpha\left(\mathbf{r}-\frac{\mathbf{s}}{2},\mathbf{r}+\frac{\mathbf{s}}{2};\varepsilon\right)\times\exp\left[\frac{i}{\hbar}S_\alpha\left(\mathbf{r}-\frac{\mathbf{s}}{2},\mathbf{r}+\frac{\mathbf{s}}{2};\varepsilon\right)-\frac{i\pi}{2}\mu_\alpha\right], \tag{E10}$$

namely,

$$\mathcal{A}_\alpha\left(\mathbf{r}-\frac{\mathbf{s}}{2},\mathbf{r}+\frac{\mathbf{s}}{2};\varepsilon\right)\approx\mathcal{A}_\alpha(\mathbf{r},\mathbf{r};\varepsilon),\quad S_\alpha\left(\mathbf{r}-\frac{\mathbf{s}}{2},\mathbf{r}+\frac{\mathbf{s}}{2};\varepsilon\right)\approx S_\alpha(\mathbf{r},\mathbf{r};\varepsilon)+\mathbf{ps}. \tag{E11}$$

By using averaging over the phase-space variables, the second nonlocal correlation term in Eq. (E8) disappears and we arrive finally at the last approximation (66) for $\delta\Theta_x^{01}$.

For the shell correction to Θ_x^{11} we substitute [see Eq. (65)] the G_1 for contributions of trajectories $\alpha\neq\alpha_0$ into the expansion (23), and one can write $\delta\Theta_x^{11}=\delta\Theta_{x,+1}^{11}+\delta\Theta_{x,-1}^{11}$, where, according to Eq. (27),

$$\delta\Theta_{x,\epsilon}^{11}=\frac{d_s}{2}\mathrm{Im}\sum_{\alpha,\alpha'\neq\alpha_0}\int\mathrm{d}\varepsilon\delta n(\varepsilon)\int\mathrm{d}\mathbf{r}_1\times\int\mathrm{d}\mathbf{r}_2\ell_x(\mathbf{r}_1)\ell_x(\mathbf{r}_2)\mathcal{A}_\alpha(\mathbf{r}_1,\mathbf{r}_2;\varepsilon)\mathcal{A}_{\alpha'}(\mathbf{r}_1,\mathbf{r}_2;\varepsilon)\times\exp\left[\frac{i}{\hbar}(S_{\alpha'}+\epsilon S_\alpha)-i\frac{\pi}{2}(\mu_{\alpha'}+\epsilon\mu_\alpha)\right],\quad\epsilon=\pm1. \tag{E12}$$

The SPM condition for the integrations over $\mathbf{r}_1$ and $\mathbf{r}_2$ is written [36]

$$\left[\frac{\partial}{\partial\mathbf{r}_1}(S_{\alpha'}+\epsilon S_\alpha)\right]^*=0,\quad\left[\frac{\partial}{\partial\mathbf{r}_2}(S_{\alpha'}+\epsilon S_\alpha)\right]^*=0, \tag{E13}$$

where asterisks mark SPM values. These conditions can be written in a more transparent form as $\mathbf{p}^*_{j\alpha'} = -\epsilon\mathbf{p}^*_{j\alpha}$, $j = 1, 2$, which implies that for $\epsilon = -1$, for instance, the particle momenta for the paths α' and α at the given initial $\mathbf{r}_1$ and final $\mathbf{r}_2$ points must be identical. One of the solutions of these SPM conditions is $\alpha' = \alpha$ for any pair of stationary points $\mathbf{r}_1 = \mathbf{r}^*_1$ and $\mathbf{r}_2 = \mathbf{r}^*_2$, and the argument in the exponential of Eq. (E12) is trivially 0. There is no such contribution to $\delta\Theta^{11}_{x,-1}$ because the integral in Eq. (E12) is then over a function $\delta n(\varepsilon)$ that is strongly fluctuating near the Fermi surface where the rest of the integrand is approximately constant, just as for the particle number conservation, we have $\int \mathrm{d}\varepsilon\delta n(\varepsilon) = 0$ [11,36,37]. In what follows we investigate in more detail the case of commensurable frequencies. In that case other solutions for α' must be considered, corresponding to a particle motion along path α from initial point $\mathbf{r}_1$ with momentum $\mathbf{p}^*_{1\alpha'} = -\epsilon\mathbf{p}^*_{1\alpha}$, but performing an arbitrary number of additional PO cycles after the spatial point $\mathbf{r}_2$ with $\mathbf{p}^*_{2\alpha'} = -\epsilon\mathbf{p}^*_{2\alpha}$. In the case $\mathbf{r}^*_1 \neq \mathbf{r}^*_2$ one has nonclosed isolated ($\mathcal{K} = 0$) stationary trajectories. In this case, expanding the phase $S_{\alpha'} + \epsilon S_\alpha$ in Eq. (E12) as a function of $\mathbf{r}_1$ and $\mathbf{r}_2$ around the stationary points $\mathbf{r}^*_1$ and $\mathbf{r}^*_2$, we can use the amplitudes of the Gutzwiller expression (24) for isolated paths [22,27,36]. According to Eq. (E5), the integrands contain the product of Jacobians $\mathcal{J}_\alpha(\mathbf{p}_1, t_\alpha; \mathbf{r}_2, \varepsilon)$ and $\mathcal{J}_{\alpha'}(\mathbf{p}_1, t_{\alpha'}; \mathbf{r}_2, \varepsilon)$ (which are 0) for the isolated trajectories, and Θ^{11}_x results in 0. For commensurable frequencies, assuming $\kappa^*_1 = \kappa^*_2$ for any $\kappa = \{x, y, z\}$ automatically implies $\kappa^*_1 = \kappa^*_2$ for all κ, corresponding to closed POs. In this case, the contribution of these orbits is small (of order $\hbar^{1/2}$ for 3D orbits or of order $\hbar$ for EQ orbits) compared to the leading $\delta\Theta^{01}_x$ term in Eq. (66). The appearance of the factor $\hbar^{1/2}$ is caused by the SPM integration over one of the variables $\kappa_1 = \kappa_2$, leading to a closed trajectory in the commensurable case. For the case $\epsilon = 1$, one can simply exchange α' and α, $\mathbf{r}_1$ and $\mathbf{r}_2$, and the direction of motion along α' with respect to trajectory α. In the case of incommensurable frequencies, trajectories in the EQ plane $z = 0$ can be considered in a similar way. For the HO potential, the SPM integration over $\mathbf{r}_1$ and $\mathbf{r}_2$ in Eq. (E12) generates a factor $\hbar^{1/2}$ that results in $\delta\Theta^{11}_x$ being small and eventually negligible compared to $\delta\Theta^{01}_x$.

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