

## SEMICLASSICAL SHELL-STRUCTURE MOMENT OF INERTIA FOR EQUILIBRIUM ROTATION OF A SIMPLE FERMI SYSTEM

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Semiclassical shell-structure components of the collective moment of inertia are derived within the mean-field cranking model in the adiabatic approximation in terms of the free-energy shell corrections through those of a rigid body for the statistically equilibrium rotation of a Fermi system at finite temperature by using the nonperturbative extended Gutzwiller periodic-orbit theory. Their analytical structure in terms of the equatorial and 3-dimensional periodic orbits for the axially symmetric harmonic oscillator potential is in perfect agreement with the quantum results for different critical bifurcation deformations and different temperatures.

### 1. INTRODUCTION

The collective rotations of nuclei were successfully described within several theoretical approaches, in particular, the cranking model [1–5]. It was shown [4, 5] that the moments of inertia (MI) can be presented as a sum of the smooth classical rigid-body term with  $\hbar$  corrections of the Extended Thomas–Fermi approach (ETF) [6–8] and shell corrections [4] given by the shell-correction method (SCM) [9, 10] adjusted to the rotational problem. Exact analytical solutions for any rotational frequency were derived for the harmonic oscillator potential [11], and extended to finite temperatures in [12]. It is worth to apply [12–16] the semiclassical periodic-orbit theory (POT) [6, 17, 18] as one of the powerful and fruitful theoretical tools for a deeper understanding and analytical analysis of the main features of the shell structure in a finite rotating Fermion system. For the collective rotations of deformed nuclei this structure was considered semiclassically in [16] by using the perturbation theory of Creagh [6, 19] within the spheroid cavity model.

In the present work the shell-structure corrections to the MI for the collective rotation are derived within the cranking model in terms of the free-energy shell corrections in the adiabatic approximation by using the nonperturbative POT based on the semiclassical Gutzwiller expansion for the Green’s function [17], but extended here to systems of higher symmetries [6, 18]. Explicit analytical results are obtained for the deformed harmonic oscillator potential.

### 2. NUCLEAR-ROTATION CRANKING MODEL

Within the cranking model, the nuclear rotation around the  $x$  axis perpendicular to the symmetry  $z$  axis of the axially symmetric mean-field potential  $V(\mathbf{r})$  can be described by solving the eigenvalue problem for the single-particle (s.p.) Hamiltonian in the body-fixed rotating coordinate system, which is usually called the *Routhian* [3–5],

$$H_\omega = H - \omega \ell_x, \quad (1)$$

$$\langle \ell_x \rangle_\omega \equiv d_s \sum_i n_i \langle \ell_x \rangle_i^\omega = I_x.$$

Here,  $\ell_x$  is the operator of the angular momentum projection onto the  $x$  axis, and  $d_s$  is the spin (spin–isospin) degeneracy. The Lagrangian multiplier  $\omega$  (rotation frequency of the body-fixed coordinate system) is defined through the constraint on the nuclear angular momentum  $I_x$  evaluated as the quantum average of the operator  $\ell_x$ , as done in Eq. (1) yielding  $\omega = \omega(I_x)$ .

The particle number conservation determines the chemical potential  $\lambda$  through the Fermi occupation numbers  $n_i$  in the s.p. state  $i$ ,  $N = d_s \sum_i n_i$ , where  $n_i \equiv n(\varepsilon_i) = \{1 + \exp[(\varepsilon_i - \lambda)/T]\}^{-1}$ , with the eigenvalues  $\varepsilon_i$  of Hamiltonian  $H$  and the temperature  $T$ . For the MI  $\Theta_x$  one has [14, 15, 20, 21],

$$\Theta_x = (\partial \langle \ell_x \rangle_\omega / \partial \omega)_{\omega=0} = (\partial^2 E(\omega) / \partial \omega^2)_{\omega=0}, \quad (2)$$

where  $E(\omega) = \langle H_\omega \rangle + \omega I_x$  is the energy of the rotating Fermi system. The yrast line  $E(I_x)$  can be determined by eliminating the frequency  $\omega$  through the definition of the kinematical MI  $\Theta_x = I_x / \omega$  (equivalent to the dynamical MI, Eq. (2), in the adiabatic approximation) yielding at zero temperature  $E(I_x) = E(0) + I_x^2 / 2\Theta_x$ . In the case of the

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deformed harmonic oscillator (HO) potential the spectrum of the Hamiltonian of Eq. (1) is given by  $\varepsilon_i = \hbar\omega_\perp (N_{\perp i} + 1) + \hbar\omega_z (N_{zi} + 1/2)$ , where  $N_{\perp i} = N_{xi} + N_{yi}$ , with  $N_{\kappa i}$  and  $\omega_\kappa$  ( $\kappa = x, y, z$ ) are the HO quantum numbers and partial frequencies, respectively. In this case one finds [2, 3] for the MI (see also [11, 12])

$$\Theta_x = \frac{d_s \hbar}{2\omega_\perp \omega_z} \left[ \frac{(\omega_z - \omega_\perp)^2}{\omega_\perp + \omega_z} (\aleph_y + \aleph_z) + \frac{(\omega_z + \omega_\perp)^2}{\omega_\perp - \omega_z} (\aleph_z - \aleph_y) \right], \quad (3)$$

$$\aleph_\kappa = \sum_i n_i (N_{\kappa i} + 1/2).$$

In the case of a statistically equilibrium rotation

$$\omega_x \aleph_x = \omega_y \aleph_y = \omega_z \aleph_z, \quad (4)$$

the moment of inertia (3) equals the rigid-body value given by

$$\Theta_x^{\text{rig}} = m \int d\mathbf{r} \rho(\mathbf{r}) (y^2 + z^2) = d_s \hbar (\aleph_y / \omega_\perp + \aleph_z / \omega_z), \quad (5)$$

where  $\rho(\mathbf{r})$  is the particle density and  $m$  is the nucleon mass. The second term for  $\Theta_x$  in Eq. (3) corresponds to transitions between s.p. levels inside a major  $N$  shell,  $\Delta N = 0$ , in contrast to the first component related to the coupling of s.p. levels through shells,  $\Delta N = 2$  [3]. In the spherical limit, this term is reduced identically to the diagonal alignment moment of inertia  $\Theta_z$ ,  $\Theta_x \rightarrow \Theta_z \rightarrow -d_s \sum_i (dn_i/d\varepsilon_i) |\langle i | \ell_x | i \rangle|^2$  [12].

For the shell correction calculations, it is convenient to re-write the MI  $\Theta_x$ , Eq. (3), for the inertia  $\Theta_x$  in terms of the free energy  $F$  of the HO system at finite temperature  $T$  and the rigid-body inertia  $\Theta_x^{\text{rig}}$ , Eq. (5) by eliminating the quantum numbers  $\aleph_y$  and  $\aleph_z$ . Finally, from Eq. (3), one obtains the explicit expressions of  $\delta\Theta_x$  and  $\delta\Theta_z$  in terms of the SCM free-energy shell corrections  $\delta F$  [12],

$$\delta\Theta_x = [(1 + \eta^2) / 3\omega_\perp^2] \delta F, \quad (6)$$

$$\delta\Theta_z = (2/3\omega_\perp^2) \delta F, \quad \eta = \omega_\perp / \omega_z$$

with  $\omega_\perp^2 \omega_z = \omega_0^3$  and the obvious spherical limit  $\delta\Theta_x \rightarrow \delta\Theta_z$  at  $\eta \rightarrow 1$ .

### 3. SEMICLASSICAL SHELL-STRUCTURE APPROACH

For the derivations of shell effects within the POT, it turns out to be helpful to use the coordinate

representation through the Green's functions  $G$  [12, 21],

$$\Theta_x = (2d_s/\pi) \int_0^\infty d\varepsilon n(\varepsilon) \times \int d\mathbf{r}_1 \int d\mathbf{r}_2 \ell_x(\mathbf{r}_1) \ell_x(\mathbf{r}_2) \text{Re} [G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)] \times \text{Im} [G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)], \quad (7)$$

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, one obtains from (7) the well-known second-order perturbation result of the cranking model [3–5] including the diagonal terms. For the Green's function  $G$  we shall use in (7) the semiclassical Gutzwiller trajectory expansion [17] extended to the symmetries of Hamiltonian [6, 18, 22],

$$G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) = \sum_\alpha G_\alpha = \quad (8)$$

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

The summation index  $\alpha$  runs over all classical isolated paths that, for a given energy  $\varepsilon$ , connect the two spatial points  $\mathbf{r}_1$  and  $\mathbf{r}_2$  inside the potential well  $V(\mathbf{r})$ . Here,  $S_\alpha$  is the classical action along such a trajectory  $\alpha$ , and  $\mu_\alpha$  denotes the phase associated with the Maslov index determined by the number of caustic and turning points along the path  $\alpha$  [6, 18]. The amplitudes  $\mathcal{A}_\alpha$  of the Green's function depend on the classical stability factors and trajectory degeneracy, due to the symmetries of that potential [6, 17, 18, 22].

Among all classical trajectories  $\alpha$  in Eq. (8), we may single out one  $\alpha_0$  which connects directly  $\mathbf{r}_1$  and  $\mathbf{r}_2$  without intermediate turning points. Thus, for the Green's function  $G$ , Eq. (8), one has a separation,

$$G = G_{\alpha_0} + G_1 \approx G_0 + G_1, \quad (9)$$

where  $G_{\alpha_0}$  is associated with the  $\alpha_0$  component of sum (8),

$$G_{\alpha_0} \approx G_0 = -\frac{m}{2\pi\hbar^2 s} \exp \left[ \frac{i}{\hbar} s p(\mathbf{r}) \right], \quad (10)$$

$$s = |\mathbf{r}_2 - \mathbf{r}_1|, \quad p(\mathbf{r}) = \sqrt{2m[\varepsilon - V(\mathbf{r})]}$$

for points that are spatially close  $\mathbf{r}_1 \rightarrow \mathbf{r}_2 \rightarrow \mathbf{r}$  in the nearly local approximation [21, 23, 24].

The second fluctuating term  $G_1$  in Eq. (9) is determined by all other trajectories  $\alpha$  in (8) besides

of  $\alpha_0$  [18, 20, 22]. According to the approximate separation (9) one obtains from (7)

$$\Theta_x = \Theta_x^{00} + \Theta_x^{01} + \Theta_x^{10} + \Theta_x^{11}, \quad (11)$$

with

$$\begin{aligned} \Theta_x^{\nu\nu'} &= (2d_s/\pi) \int d\varepsilon n(\varepsilon) \times \\ &\times \int d\mathbf{r}_1 \int d\mathbf{r}_2 \ell_x(\mathbf{r}_1) \ell_x(\mathbf{r}_2) \operatorname{Re} [G_\nu(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)] \times \\ &\times \operatorname{Im} [G_{\nu'}(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)]. \end{aligned} \quad (12)$$

As shown in [21], the first component of Eq. (11),  $\Theta_x^{00}$ , averaged over the phase-space variables in the local approximation, leads to the Thomas–Fermi rigid-body moment of inertia because such an averaging removes not only nonlocal oscillating terms, but also the  $\hbar$  corrections of the ETF approach [7, 8]. The shell-structure component  $\delta\Theta_x^{01}$  of  $\Theta_x^{01}$  in (12) for the MI can be related semiclassically to the shell correction  $\delta\rho(\mathbf{r})$  of the particle density  $\rho(\mathbf{r})$  through that of the rigid body MI  $\delta\Theta_x^{\text{rig}}$ . Indeed, calculating  $\Theta_x^{01}$ , Eq. (12), through using the nearly local approximation  $G_0$  ( $\nu = 0$ ) for  $G_{\alpha 0}$ , Eq. (10), and  $G_1$  ( $\nu' = 1$ ) we select the shell component  $\delta\Theta_x^{01}$  of  $\Theta_x^{01}$  just like the free energy shell corrections  $\delta F$ . Using the transformation of  $\mathbf{r}_1$  and  $\mathbf{r}_2$  to the center-of-mass and relative coordinates,  $\mathbf{r} = (\mathbf{r}_1 + \mathbf{r}_2)/2$  and  $\mathbf{s} = \mathbf{r}_2 - \mathbf{r}_1$ , as well as the spherical system of coordinates for  $\mathbf{s}$ ,  $d\mathbf{s} = s^2 ds \sin\theta_s d\theta_s d\varphi_s$  one obtains for an almost equilibrium rotation

$$\begin{aligned} \delta\Theta_x^{01} &= - [d_s m / (\pi \hbar)^2] \int d\varepsilon \delta n(\varepsilon) \times \\ &\times \int d\mathbf{r} \int ds \int \sin\theta_s d\theta_s d\varphi_s \ell_x(\mathbf{r} - \mathbf{s}/2) \times \\ &\times \ell_x(\mathbf{r} + \mathbf{s}/2) \cos [p(\mathbf{r})s/\hbar] \times \\ &\times \operatorname{Im} [G_1(\mathbf{r} - \mathbf{s}/2, \mathbf{r} + \mathbf{s}/2; \varepsilon)] \approx \delta\Theta_x^{\text{rig}} = \\ &= m \int d\mathbf{r} (y^2 + z^2) \delta\rho(\mathbf{r}). \end{aligned} \quad (13)$$

For the classical angular-momentum projection in the integrand of the first equation we used the approximation  $\ell_x(\mathbf{r} - \mathbf{s}/2)\ell_x(\mathbf{r} + \mathbf{s}/2) \approx \ell_x^2(\mathbf{r}) = (y^2 + z^2)p^2(\mathbf{r})$ . The classical angular-momentum projection  $\ell_x(\mathbf{r})$  in the rotating frame is caused in the adiabatic approach [3, 12] by the global rotation rather than by the motion of particles along the trajectories  $\alpha$  inside the nucleus. We then integrated in Eq. (13) explicitly over  $s$  and found sine squared in the integrand over  $\varepsilon$  and  $\mathbf{r}$  with mean value 1/2 for the averaging over energies  $\varepsilon$ . Adding and subtracting

identically this value 1/2 from the sine squared we first integrate over spherical angles  $\theta_s$  and  $\varphi_s$  in the term related to this 1/2, writing simply  $4\pi$  because of independence of this integrand of angles of the vector  $\mathbf{s}$ . Performing then first the integration over  $\varepsilon$  in this term and taking smooth quantities in front of the sharply peaked  $\delta n(\varepsilon)$  at the energy  $\varepsilon = \lambda$  in the integrand (see [10, 20]), one obtains the rigid-body shell correction  $\delta\Theta_x^{\text{rig}}$ , as shown in Eq. (13). The cranking model for nuclear rotations implies that the correlation corrections in (10) should be small enough, with respect to the main rigid-body component  $\delta\Theta_x^{\text{rig}}$ , to be neglected. Other contributions  $\Theta_x^{10}$  and  $\Theta_x^{11}$  to  $\Theta_x$  in Eq. (11) can also be referred to as a fluctuation correction to the rigid-body MI at leading order in  $\hbar^{1/2}$  (see Appendixes A and B).

As shown in Appendix B, we finally arrive at the semiclassical MI shell corrections for the perpendicular (collective) and parallel (alignment) rotations for the deformed HO

$$\begin{aligned} \delta\Theta_{x,\text{scl}} &\approx \delta\Theta_{x,\text{scl}}^{\text{rig}} = [(1 + \eta^2) / 3\omega_\perp^2] \delta F_{\text{scl}}, \\ \delta\Theta_{z,\text{scl}} &\approx \delta\Theta_{z,\text{scl}}^{\text{rig}} = (2/3\omega_\perp^2) \delta F_{\text{scl}}. \end{aligned} \quad (14)$$

It turns out that these expressions are the same as the ones found in Eq. (6) but avoiding the equilibrium rotation condition (4). Here,  $\delta F_{\text{scl}}$  is the semiclassical periodic-orbit (p.o.) sum for the free-energy shell correction,

$$\delta F_{\text{scl}}(T, N) = \sum_{\text{p.o.}} \delta U_{\text{p.o.}} Q(\mathcal{Z}_{\text{p.o.}}), \quad (15)$$

$$Q(\mathcal{Z}) = \pi \mathcal{Z} / \sinh(\pi \mathcal{Z}), \quad \mathcal{Z}_{\text{p.o.}} = t_{\text{p.o.}} T / \hbar,$$

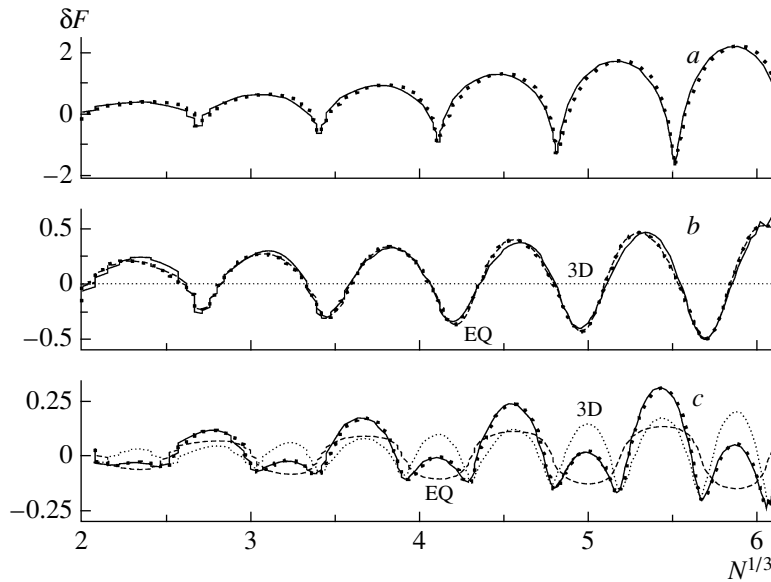
where  $\delta U_{\text{p.o.}}$  is the p.o. component of the semiclassical energy shell correction at zero temperature,  $\delta U_{\text{scl}} = \sum_{\text{p.o.}} \delta U_{\text{p.o.}}$ , and  $t_{\text{p.o.}}$  is the time of particle motion along the p.o. [6, 13–16, 18]. The sums over p.o. run, in case of a classical degeneracy, over families of periodic orbits.

For the deformed HO potential, one has to consider the two cases of rational and irrational ratios of the frequencies  $\omega_\perp$  and  $\omega_z$  ( $\omega_x = \omega_y = \omega_\perp$ ).

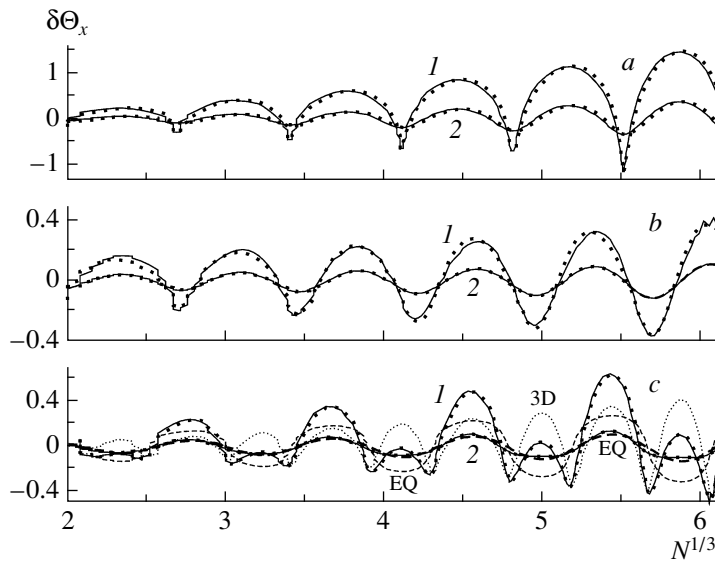
Following basically [18, 22], one notes that the well-known p.o. families (Lissajous figures) have mainly classical degeneracies  $\mathcal{K} = 4$  and 2 depending on the commensurable and incommensurable frequency relations.

### 3.1. Incommensurable Frequencies

We shall consider first the case of the incommensurable frequencies of the axially-symmetric HO, corresponding to an irrational value of  $\eta$ , Eq. (6). In



**Fig. 1.** The semiclassical shell-structure free-energy corrections  $\delta F$  (15)–(17) (wide dotted line) and corresponding quantum calculations (solid line) as function of the particle number variable,  $N^{1/3}$ , for the critical deformations  $\eta = 1.0$  (a), 1.2 (b), and 2.0 (c) at a temperature  $T = 0.1$  in HO units  $\hbar\omega_0$ . The SCM smoothing parameters are  $\gamma = (1.5-2.5)\hbar\omega_0$ , and  $M = 4-8$ . Narrow dots (3D) in Figs. 1b and 1c show the contributions coming from 3D orbits, the thin dashed line (EQ) those of EQ orbits.



**Fig. 2.** The semiclassical shell correction  $\delta\Theta_x$  to the moment of inertia, Eq. (14), in units  $\hbar/\omega_0$  (wide dotted line) and the corresponding quantum calculations as function of the particle number variable,  $N^{1/3}$ , for temperature (in HO units  $\hbar/\omega_0$ ) of  $T = 0.1$  (solid line 1) and  $T = 0.2$  (solid line 2). Contributions of 3D orbits are shown in part c (narrow dots 3D) together with EQ orbits at  $T = 0.1$  (thin dashed line EQ) and  $T = 0.2$  (thick dashed line EQ).

this case, there are no 3-dimensional (3D) families  $\mathcal{K} = 4$ . However, the 2D equatorial (EQ) families of p.o.s of smaller degeneracy  $\mathcal{K} = 2$  exist with a given period number  $n$  in the  $(x, y)$  plane ( $z = 0$ ), perpendicular to the symmetry  $z$  axis. They give dominant contributions to the energy shell corrections  $\delta U_{\text{scI}}$  as

compared with the remaining isolated ( $\mathcal{K} = 0$ ) p.o.s along the symmetry  $z$  axis [22]. The time of motion along the EQ p.o.s,  $t_n = n\mathcal{T}_{\text{EQ}}$ , is determined by the main period  $\mathcal{T}_{\text{EQ}} = 2\pi/\omega_{\text{EQ}} = 2\pi n_{\perp}/\omega_{\perp} = 2\pi n_z/\omega_z$  (frequency  $\omega_{\text{EQ}}$ ) of the primitive ( $n = 1$ ) p.o. in this  $(x, y)$  plane.

For the contribution of the EQ ( $\mathcal{K} = 2$ ) orbits to the energy shell correction  $\delta U_{\text{scl}}$  one writes [6, 22]

$$\delta U_{\text{EQ}} = \sum_n \delta U_n^{\text{EQ}}, \quad (16)$$

$$\text{with } \delta U_n^{\text{EQ}} = \frac{2d_s \lambda \omega_{\text{EQ}}^2 \sin(2\pi n \lambda / \hbar \omega_{\text{EQ}})}{(2\pi \omega_{\perp} n)^2 |\sin(\pi n \omega_z / \omega_{\text{EQ}})|}.$$

### 3.2. Commensurable Frequencies

For the case of rational ratios of frequencies,  $\omega_{\perp} : \omega_z = n_{\perp} : n_z$ , where  $n_{\perp}$  and  $n_z$  are primitive integers, one finds the time of particle motion,  $t_n = n \mathcal{T}_{3\text{D}}$ , with the period  $\mathcal{T}_{3\text{D}} = 2\pi / \omega_{3\text{D}} = 2\pi n_{\perp} / \omega_{\perp} = 2\pi n_z / \omega_z$  for its motion along the 3D p.o.s ( $\mathcal{K} = 4$ ). For the commensurable case at deformations  $\eta > 1$ , the EQ orbits yield contributions  $\delta U_{\text{EQ}}$  (16) to  $\delta U_{\text{scl}}$  together with 3D orbits  $\delta U_{3\text{D}}$  (17):  $\delta U_{\text{scl}} \approx \delta U_{3\text{D}} + \delta U_{\text{EQ}}$ , where

$$\delta U_{3\text{D}} = (d_s \lambda^2 \omega_{3\text{D}}^2 / 4\pi^2 \hbar \omega_0^3) \times \sum_n \cos[2\pi n \lambda / \hbar \omega_{3\text{D}} - \pi n (2n_{\perp} + n_z)] / n^2. \quad (17)$$

## 4. COMPARISON WITH QUANTUM CALCULATIONS

The semiclassical free-energy shell correction  $\delta F_{\text{scl}}$ , Eq. (15), is displayed in Fig. 1 as function of the particle-number variable,  $N^{1/3}$ , and compared at a temperature of  $T = 0.1 \hbar \omega_0$  for different critical bifurcation deformations  $\eta = 1, 6/5$ , and 2 with the corresponding quantum SCM results. This comparison shows practically a perfect agreement between the semiclassical and quantum results. For the spherical case ( $\eta = 1$ ) one has only contributions of the families of 3D orbits (with degeneracy  $\mathcal{K} = 4$ ). At the bifurcation points  $\eta = 6/5$  and 2 the relatively simple families of 3D p.o.s (of highest degeneracy  $\mathcal{K} = 4$ ) appear along with EQ trajectories of smaller degeneracy. For  $\eta = 6/5$  one mainly has contributions from EQ p.o.s because all 3D orbits are too long here. For the bifurcation point  $\eta = 2$  one finds an interference of the two comparably large contributions of 3D, Eq. (17), and EQ, Eq. (16), orbits with different periods,  $\mathcal{T}_{3\text{D}} = 2\mathcal{T}_{\text{EQ}}$ , as clearly seen from the bottom part of Fig. 1. A similar comparison is made in Fig. 2 for the shell corrections to the moment of inertia  $\delta \Theta_x$ . Again a perfect agreement is observed between semiclassical and quantum results which is not really astonishing because of the proportionality of these two quantities (see Eqs. (6) and (14)). In particular, one finds the same clear interference of contributions of 3D and

EQ orbits in the shell corrections to the MI at  $\eta = 2$ . The exponential decrease of shell oscillations with increasing temperature, due to the temperature factor  $Q(t_n T / \hbar)$ , Eq. (15), is clearly seen. The critical temperature for a disappearance of shell effects in the MI is found, for prolate deformations ( $\eta > 1$ ) and particle numbers  $N \sim 100-200$ , approximately at  $T_{\text{cr}} = \hbar \omega_{\text{EQ}} / \pi \sim \hbar \omega_0 / \pi \approx 2-3$  MeV just as for  $\delta F$  [6, 18]. The particle-number dependence of the shell corrections to  $\delta \Theta_z$  (alignment) in Eqs. (6) and (14) is similar to that of  $\delta \Theta_x$  because of their relations,  $\delta \Theta_z \propto \delta \Theta_x \propto \delta F$ , as explained above.

## 5. CONCLUSIONS

For a Fermi system we found, within a semiclassical approach based on the extended Gutzwiller POT, a relation between the shell components of the collective MI and the free energy. This relation is obtained via the shell correction to the rigid-body MI for a statistically equilibrium rotation. This relation is proven to be exact for the HO potential and, in this sense, such an equilibrium rotation which leads to the rigid-body moment of inertia can be considered as a selfconsistent condition. The semiclassical shell components of the MI are obtained as a sum over periodic orbits in a potential well. For the deformed HO potential we have shown the perfect agreement between the semiclassical POT and quantum results for all these shell corrections at several critical bifurcation deformations and temperatures. The moment of inertia has the spherical limit of alignment of the s.p. angular momenta along the symmetry axis. The exponential decrease of all shell corrections with increasing temperature clearly appears.

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*Appendix A*

## JACOBIAN CALCULATIONS AND CLASSICAL HO DYNAMICS

The solutions of the classical Newtonian dynamical equations for a phase-space trajectory  $\alpha$  in a HO potential, going from an initial point  $\mathbf{r}_1$  at initial time  $t = 0$  to a final point  $\mathbf{r}_2$  at time  $t = t_{\alpha}$ , can be written analytically in the explicit form [22]

$$x_{\kappa}(t) = x_{\kappa 1} \frac{\sin(\omega_{\kappa} t + \phi_{\kappa})}{\sin \phi_{\kappa}}, \quad (\text{A.1})$$

$$p_\kappa(t) = m\dot{x}_\kappa(t) = m\omega_\kappa x_{\kappa 1} \frac{\cos(\omega_\kappa t + \phi_\kappa)}{\sin \phi_\kappa},$$

$$\kappa = 1, 2, 3,$$

with  $x_1, x_2$ , and  $x_3$  being, respectively,  $x, y$ , and  $z$  and the corresponding phases  $\phi_1, \phi_2$ , and  $\phi_3$  that are determined through the coordinates of the initial point  $\mathbf{r}_1 = \mathbf{r}$ , for an energy,

$$\varepsilon = \frac{m}{2} \left( \frac{x_1^2 \omega_1^2}{\sin^2 \phi_1} + \frac{x_2^2 \omega_2^2}{\sin^2 \phi_2} + \frac{x_3^2 \omega_3^2}{\sin^2 \phi_3} \right), \quad (\text{A.2})$$

which allows to express one of the phases through  $\varepsilon$  and the two others, e.g.,  $\phi_3(\varepsilon, \phi_1, \phi_2)$ .

In the case (i) of incommensurable frequencies (irrational  $\eta$ ) all closed classical trajectories in the axially symmetric HO potential are EQ orbits with degeneracy  $\mathcal{K} = 2$  and 3D trajectories with a non-periodic motion in  $z$  direction. In the case (ii) of commensurable frequencies (rational  $\eta$ ) 3D and EQ p.o.s both contribute with the degeneracies  $\mathcal{K} = 4$  and 2, respectively. Closed HO trajectories are p.o.s (or parts of p.o.s) and nonclosed ones are isolated ( $\mathcal{K} = 0$ ).

For the case of isolated nonclosed classical trajectories in Eq. (8) one may apply the Gutzwiller approximation [6, 17, 18] for the Green's function  $G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)$  (8) with amplitude

$$\mathcal{A}_\alpha(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) = -\frac{1}{2\pi\hbar^2} \left| \mathcal{J}_\alpha(\mathbf{p}_1, t_\alpha; \mathbf{r}_2, \varepsilon) \right|^{1/2}. \quad (\text{A.3})$$

For calculation of the Jacobian  $\mathcal{J}_\alpha(\mathbf{p}_1, t_\alpha; \mathbf{r}_2, \varepsilon)$  for the transformation of initial momentum  $\mathbf{p}_1$  and time of motion  $t_\alpha$  to the final coordinate  $\mathbf{r}_2$  and energy  $\varepsilon$ , we need to express the variations  $\delta\mathbf{p}_1$  and  $\delta\mathbf{r}_2$  of initial momentum  $\mathbf{p}_1$  (at point  $\mathbf{r}_1$ ) and final coordinate  $\mathbf{r}_2$  through  $\delta\phi_\kappa$

$$\delta p_{\kappa 1} = -\frac{m\omega_\kappa x_{\kappa 1}}{\sin^2 \phi_\kappa} \delta\phi_\kappa, \quad (\text{A.4})$$

$$\delta x_{\kappa 2} = -x_{\kappa 1} \frac{\sin(\omega_\kappa t_\alpha)}{\sin^2 \phi_\kappa} \delta\phi_\kappa.$$

Using locally along the trajectory between  $\mathbf{r}_1$  and  $\mathbf{r}_2$  a transformation to Cartesian coordinates  $\{x', y', z'\}$ , where  $x'$  is locally along, and  $y', z'$  perpendicular to the trajectory, one obtains [17, 18], owing to invariance properties of the Jacobian, for any  $\mathbf{r}_1 \neq \mathbf{r}_2$

$$\mathcal{J}_\alpha(\mathbf{p}_1, t_\alpha; \mathbf{r}_2, \varepsilon) = \quad (\text{A.5})$$

$$= -\frac{m^2}{p_1 p_2} \left( \frac{\partial p_{y1}}{\partial y_2} \frac{\partial p_{z1}}{\partial z_2} - \frac{\partial p_{z1}}{\partial y_2} \frac{\partial p_{y1}}{\partial z_2} \right) = 0,$$

where we have used the Hamilton–Jacobi equation of classical motion. For closed orbits ( $\mathbf{r}_1 = \mathbf{r}_2$ ) an enhancement of the amplitudes  $\mathcal{A}_{\text{p.o.}}$  in (8) is observed [18, 22] due to increased degeneracy (see main text).

CALCULATION OF THE p.o. COMPONENTS OF  $\delta\Theta_x$

To obtain the component  $\Theta_x^{01}$  of the MI one has, according to Eqs. (7) and (8), to evaluate

$$\int_0^{s_{\max}} ds \cos [sp(\mathbf{r})/\hbar] = -[\hbar^2/2p^2(\mathbf{r})] \times \quad (\text{B.1})$$

$$\times \sin^2 [s_{\max}p(\mathbf{r})/2\hbar] + (\hbar s_{\max}/p) \sin (s_{\max}p/\hbar),$$

whereas for  $\Theta_x^{10}$  one needs

$$\int_0^{s_{\max}} ds \sin [sp(\mathbf{r})/\hbar] = [\hbar^2/p^2(\mathbf{r})] \times \quad (\text{B.2})$$

$$\times \sin [s_{\max}p(\mathbf{r})/\hbar] - [\hbar s_{\max}/p(\mathbf{r})] \cos [s_{\max}p(\mathbf{r})/\hbar].$$

The local average over phase-space variables in (B.2) yields zero, whereas the  $\sin^2$  term in (B.1) contributes a factor 1/2 yielding the finite value  $-\hbar^2/4p^2$  for the integral. Thus  $\Theta_x^{10}$  is contributing to the nonlocal correlation part of  $\Theta_x$ .

For the shell correction to  $\Theta_x^{11}$  one substitutes (see Eq. (12)) the  $G_1$  for contributions of trajectories  $\alpha \neq \alpha_0$  and one can write  $\delta\Theta_x^{11} = \delta\Theta_{x,+1}^{11} + \delta\Theta_{x,-1}^{11}$  where, according to (8),

$$\delta\Theta_{x,\epsilon}^{11} = \frac{d_s}{2} \text{Im} \sum_{\alpha, \alpha' \neq \alpha_0} \int d\varepsilon \delta n(\varepsilon) \int d\mathbf{r}_1 \times \quad (\text{B.3})$$

$$\times \int d\mathbf{r}_2 \ell_x(\mathbf{r}_1) \ell_x(\mathbf{r}_2) \mathcal{A}_\alpha(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) \mathcal{A}_{\alpha'}(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) \times$$

$$\times \exp \left[ \frac{i}{\hbar} (S_{\alpha'} + \epsilon S_\alpha) - i \frac{\pi}{2} (\mu_{\alpha'} + \epsilon \mu_\alpha) \right],$$

$$\epsilon = \pm 1.$$

The stationary phase method (SPM) condition for the integrations over  $\mathbf{r}_1$  and  $\mathbf{r}_2$  writes [20]

$$\left[ \frac{\partial}{\partial \mathbf{r}_1} (S_{\alpha'} + \epsilon S_\alpha) \right]^* = 0, \quad (\text{B.4})$$

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

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  $\alpha'$  and  $\alpha$  at the given initial  $\mathbf{r}_1$  and final  $\mathbf{r}_2$  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 in (B.3) is trivially zero. There is no such a contribution to  $\delta\Theta_{x,-1}^{11}$  because the integral in (B.3) then is over a function  $\delta n(\varepsilon)$  which is strongly fluctuating near the Fermi surface where the rest of the integrand is approximately constant, just like for the particle number conservation we have  $\int d\varepsilon \delta n(\varepsilon) = 0$  [10, 20, 23]. In what follows we shall investigate in more detail case (ii) of commensurable frequencies. In that case other solutions for  $\alpha'$  must be considered corresponding to a particle motion along path  $\alpha$  from initial point  $\mathbf{r}_1$  with momentum  $\mathbf{p}_{1\alpha'}^* = -\epsilon\mathbf{p}_{1\alpha}^*$ , but performing an arbitrary number of additional p.o. 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 (B.3) as function of  $\mathbf{r}_1$  and  $\mathbf{r}_2$  around the stationary points  $\mathbf{r}_1^*$  and  $\mathbf{r}_2^*$ , we may use the amplitudes of the Gutzwiller expression (A.3) for isolated paths [18, 20, 22]. According to Eq. (A.5), 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 zero) for the isolated trajectories and  $\Theta_x^{11}$  results to zero. For commensurable frequencies, assuming  $x_{\kappa 1}^* = x_{\kappa 2}^*$  for any  $\kappa$ , automatically implies  $x_{\kappa 1}^* = x_{\kappa 2}^*$  for all  $\kappa$ , corresponding to closed p.o.s. In this case, the contribution of these orbits is small (of the relative order  $\hbar^{1/2}$  for 3D orbits or of order  $\hbar$  for EQ orbits) as compared to the leading  $\delta\Theta_x^{01}$  term in Eq. (13). The appearance of the factor  $\hbar^{1/2}$  is due to the SPM integration over one of the variables  $x_{\kappa 1} = x_{\kappa 2}$ , leading to a closed trajectory in the commensurable case. For the case  $\epsilon = 1$ , one can simply exchange  $\alpha'$  and  $\alpha$ , and  $\mathbf{r}_1$  and  $\mathbf{r}_2$ , and the direction of motion along  $\alpha'$  with respect to the trajectory  $\alpha$ . In the case of incommensurable frequencies, trajectories in 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 (B.3) generates a factor  $\hbar^{1/2}$  which results in  $\delta\Theta_x^{11}$  being small and eventually negligible as compared to  $\delta\Theta_x^{01}$ .

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# КВАЗИКЛАССИЧЕСКАЯ ОБОЛОЧЕЧНАЯ СТРУКТУРА МОМЕНТА ИНЕРЦИИ ПРИ РАВНОВЕСНОМ ВРАЩЕНИИ ФЕРМИ-СИСТЕМЫ

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Оболочечные компоненты коллективного момента инерции в квазиклассическом адиабатическом приближении выражены через оболочечные поправки к свободной энергии в рамках модели принудительного вращения ферми-системы. С помощью общей квазиклассической теории Гуцвиллера, в которой не используется классическая теория возмущений, показано, что эти компоненты описываются как оболочечные поправки к твердотельному моменту инерции, отвечающему статистически равновесному вращению при конечных температурах. Их аналитическая структура, выраженная через характеристики экваториальных и трехмерных периодических орбит в потенциальной яме гармонического осциллятора, находится в хорошем согласии с квантовыми расчетами при различных критических деформациях и различных температурах.