

## SEMICLASSICAL SHELL STRUCTURE OF MOMENTS OF INERTIA IN DEFORMED FERMI SYSTEMS

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The collective moment of inertia is derived analytically within the cranking model in the adiabatic mean-field approximation at finite temperature. Using the nonperturbative periodic-orbit theory the semiclassical shell-structure components of the collective moment of inertia are obtained for any potential well. Their relation to the free-energy shell corrections are found semiclassically as being given through the shell-structure components of the rigid-body moment of inertia of the statistically equilibrium rotation in terms of short periodic orbits. Shell effects in the moment of inertia disappear exponentially with increasing temperature. For the case of the harmonic-oscillator potential one observes a perfect agreement between semiclassical and quantum shell-structure components of the free energy and the moment of inertia for several critical bifurcation deformations and several temperatures.

### 1. Introduction

The collective rotations of nuclei were successfully described within several theoretical approaches, in particular, the cranking model.<sup>1–6</sup> It was shown<sup>4,5</sup> 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)<sup>7–10</sup> and shell corrections<sup>4</sup> given by the shell-correction method (SCM)<sup>11,12</sup> adjusted to the rotational problem. For the harmonic oscillator potential exact analytical solutions are obtained for any rotational frequency,<sup>13</sup> and extended to finite temperatures.<sup>14</sup> It is worth applying the semiclassical periodic-orbit theory<sup>10,15,16</sup> (POT) 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.<sup>17–21</sup> A “classical rotation” of the spherical nucleus was considered<sup>17</sup> as an alignment of the angular momenta of the particles (see also similar supershell effects in magnetic susceptibilities<sup>18,19</sup>). For collective rotations of deformed nuclei around an axis perpendicular to the symmetry axis, this structure was studied semiclassically<sup>20</sup> by using the classical perturbation theory<sup>10,22</sup> 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. Let us introduce an order parameter  $\beta = (\omega/\Omega)(S/\hbar)$  which is the product of the rotation frequency  $\omega$  in units of  $\Omega$  and the action  $S$  along short classical trajectories in units of  $\hbar$  where  $\hbar\Omega$  is the major shell spacing in an  $N$  particle system (i.e. the distance between the gross shells near the Fermi surface which is approximately given by  $\hbar\Omega = \varepsilon_F/N^{1/3}$  through the time of particle motion along dominating short periodic orbits in the potential well<sup>10,16</sup>). It turns out that, contrary to the classical perturbative results,<sup>20</sup> this order parameter can be not small in our approach ( $\beta \gtrsim 1$ ), which is largely due to the fact that the semiclassical parameter  $S/\hbar \sim k_F R \gg 1$ , where  $k_F$  is the Fermi momentum and  $R$  gives the size of the finite Fermi system,  $R = r_0 N^{1/3}$ . This approach is based on the semiclassical Gutzwiller expansion for the Green’s function,<sup>15</sup> but extended to systems of higher symmetries.<sup>10,16,23</sup> Explicit analytical results are obtained for the deformed harmonic oscillator potential, as presented in section 3 below.

## 2. Cranking Model for Nuclear Rotations

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*<sup>3–5</sup>

$$H_\omega = H - \omega \ell_x, \quad \langle \ell_x \rangle_\omega \equiv d_s \sum_i n_i \langle \ell_x \rangle_i^\omega = I_x. \quad (1)$$

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 determined through the constraint on the nuclear angular momentum  $I_x$  evaluated as the quantum average of the operator  $\ell_x$ , as in Eq. (1), i.e.  $\omega = \omega(I_x)$ . The particle number conservation determines the chemical potential  $\lambda$  through the Fermi occupation numbers  $n_i$  of 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<sup>3,18,19</sup>

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

where  $E(\omega) = E_\omega + \omega I_x$  is the energy of the rotating Fermi system, with  $E_\omega$  the eigenvalue of the Routhian  $H_\omega$  (1). The yrast line  $E(I_x)$  can be determined

(at zero temperature) by eliminating the frequency  $\omega$  through the definition of the kinematical MI  $\Theta_x = I_x/\omega$  (equivalent to the dynamical MI in the adiabatic approximation) yielding  $E(I_x) = E(0) + I_x^2/2\Theta_x$ .

For the derivation of shell effects within the POT, it turns out to be helpful to use the coordinate representation of the Green's function<sup>14,21,24,25</sup>  $G$ ,

$$\Theta_x = \frac{2d_s}{\pi} \int_0^\infty d\varepsilon n(\varepsilon) \int d\mathbf{r}_1 \int d\mathbf{r}_2 \ell_x(\mathbf{r}_1) \ell_x(\mathbf{r}_2) \text{Re}[G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)] \text{Im}[G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)], \quad (3)$$

where  $n(\varepsilon)$  are the Fermi occupation numbers  $n(\varepsilon_i)$  at  $\varepsilon_i = \varepsilon$ ;  $\ell_x(\mathbf{r}_1)$  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 (3) the well-known second-order perturbation result of the cranking model<sup>3-5</sup> including the diagonal terms. The relation between the rotation frequency  $\omega$  and the chosen angular momentum  $I_x$  is given through the constraint on the r.h.s. of Eq. (1), which can be written in the form  $I_x = \Theta_x \omega$  where the MI  $\Theta_x$  is determined through Eq. (3).

In the case of the deformed HO potential and for a rotation around the  $x$  axis, the direct diagonalization of the Routhian (1) (without using a perturbation expansion) yields the s.p. energies  $\varepsilon_i(\omega)$  and moments of inertia  $\Theta_x(\omega)$  obtained<sup>13</sup> analytically for any frequency  $\omega$ . The calculation can be easily generalized to finite temperatures by using the oscillator Bose occupation numbers.<sup>14</sup> In the small rotation-frequency limit (adiabatic case),  $\omega \rightarrow 0$ , the  $\omega$  independent s.p. spectrum can be used  $\varepsilon_i = \hbar\omega_\perp(N_{\perp i} + 1) + \hbar\omega_z(N_{zi} + \frac{1}{2})$ ,  $N_{\perp i} = N_{xi} + N_{yi}$ , where  $N_{\kappa i}$  and  $\omega_\kappa$  ( $\kappa = x, y, z$ ) are the HO quantum numbers and the partial frequencies, with, for axial symmetry,  $\omega_x = \omega_y = \omega_\perp$  and  $\omega_\perp^2 \omega_z = \omega_0^3$ . For the MI<sup>13,14</sup>  $\Theta_x(\omega)$  one finds<sup>2,3</sup> in the adiabatic limit  $\omega \rightarrow 0$

$$\Theta_x = \frac{d_s \hbar}{2\omega_\perp \omega_z} \left[ \frac{(\omega_z - \omega_\perp)^2}{\omega_\perp + \omega_z} (\aleph_y + \aleph_z) + \frac{(\omega_z + \omega_\perp)^2}{\omega_\perp - \omega_z} (\aleph_z - \aleph_y) \right], \quad (4)$$

where  $\aleph_\kappa = \sum_i n_i (N_{\kappa i} + \frac{1}{2})$ . ( $\aleph_x = \aleph_y$  for an axially symmetric potential.) The energy of this system is then given by

$$E(\omega) \equiv E_\omega + \omega I_x = d_s \hbar (2\omega_\perp \aleph_y + \omega_z \aleph_z) + \frac{1}{2} \omega^2 \Theta_x. \quad (5)$$

Notice that starting from (1) one may explicitly calculate analytically the matrix elements of the angular momentum projection operator  $\ell_x$  in the perturbation approach for the HO potential. Using these matrix elements and the s.p. eigenvalues of the Routhian Eq. (1), one also arrives at Eq. (4) as obtained in the nonperturbative derivation.

In the case of a statistically equilibrium,

$$\omega_x \aleph_x = \omega_y \aleph_y = \omega_z \aleph_z, \quad (6)$$

Eq. (4) reduces to the rigid-body MI

$$\Theta_x^{rig} \equiv m \int d\mathbf{r} \rho(\mathbf{r}) (y^2 + z^2) = d_s \sum_i n_i \langle i | y^2 + z^2 | i \rangle = d_s \hbar \left( \frac{\aleph_y}{\omega_\perp} + \frac{\aleph_z}{\omega_z} \right), \quad (7)$$

where  $\rho(\mathbf{r})$  is the particle density. The second term in Eq. (4) for  $\Theta_x$  corresponds to the transitions between s.p. levels inside ( $\Delta N = 0$ ) a major  $N$  shell,<sup>3</sup> whereas the first term is related to the coupling of s.p. levels through shells ( $\Delta N = 2$ ). In the spherical limit,<sup>14,21</sup> this term approaches identically the alignment expression for MI  $\Theta_z$  with the diagonal matrix elements of the operator  $\ell_x$ ,

$$\Theta_x \rightarrow \Theta_z \rightarrow -d_s \sum_i \frac{dn_i}{d\varepsilon_i} \left| \langle i | \ell_x | i \rangle \right|^2. \quad (8)$$

For the calculation of shell corrections it is convenient to rewrite Eq. (4), for the inertia  $\Theta_x$  in terms of the free energy  $F$  of the HO system at finite temperature  $T$  and the rigid body MI  $\Theta_x^{rig}$ , Eq. (7). By eliminating the quantum numbers  $\aleph_y$  and  $\aleph_z$  from equation (7) for  $\Theta_x^{rig}$ , and Eq. (5) for the HO energy  $E(\omega)$  at  $\omega = 0$ , one obtains

$$\Theta_x = \frac{1}{\omega_{\perp}^2 (2\eta^2 - 1) (\eta^2 - 1)} \left[ \omega_{\perp}^2 (2\eta^4 + 9\eta^2 + 1) \Theta_x^{rig} - 4\eta^2 (1 + \eta^2) F \right]. \quad (9)$$

with the deformation parameter  $\eta = \omega_{\perp}/\omega_z$ . By using the explicit definition of  $\Theta_x^{rig}$  in (7) for a HO potential, which results in  $\Theta_x^{rig} = (1 + \eta^2)F/3\omega_{\perp}^2$ , the shell component of the MI  $\delta\Theta_x$  (and  $\delta\Theta_z$ ) can thus be easily separated from its smooth part through the standard free-energy shell correction<sup>4,5,12</sup>  $\delta F$ ,

$$\delta\Theta_x = \frac{1 + \eta^2}{3\omega_{\perp}^2} \delta F \equiv \delta\Theta_x^{rig}, \quad \delta\Theta_z = \frac{2}{3\omega_{\perp}^2} \delta F \equiv \delta\Theta_z^{rig}. \quad (10)$$

The convergence (8) for the corresponding shell corrections in the spherical alignment limit  $\eta \rightarrow 1$  becomes obvious when comparing the central expressions for  $\delta\Theta_x$  and  $\delta\Theta_z$  in Eq. (10).

### 3. Semiclassical Shell-Structure Approach

For the Green's function  $G$  in (3) we shall use the semiclassical Gutzwiller trajectory expansion<sup>15</sup> extended to the Hamiltonian symmetries,<sup>10,16,23</sup>

$$G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) = \sum_{\alpha} G_{\alpha} = \sum_{\alpha} \mathcal{A}_{\alpha}(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) \exp \left[ \frac{i}{\hbar} S_{\alpha}(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) - \frac{i\pi}{2} \mu_{\alpha} \right]. \quad (11)$$

The summation index  $\alpha$  runs over all classical isolated paths inside the potential well  $V(\mathbf{r})$  which, for a given energy  $\varepsilon$ , connect two spatial points  $\mathbf{r}_1$  and  $\mathbf{r}_2$ . Here  $S_{\alpha}$  is the classical action along such a trajectory  $\alpha$ , and  $\mu_{\alpha}$  denotes the phase associated with the Maslov index<sup>10,16</sup> through the number of caustic and turning points along the path  $\alpha$ . The amplitudes  $\mathcal{A}_{\alpha}$  of the Green's function depend on the classical stability factors and trajectory degeneracy, determined by the symmetries of the potential.<sup>10,15,16,23</sup>

In our derivations, we shall use an averaging in phase-space variables, in particular, Strutinsky local averaging over the energy spectrum near the Fermi surface with a Gaussian weight function and correction polynomial. Such an averaging leads

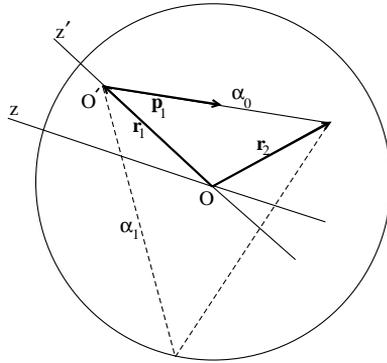


Fig. 1. Trajectories connecting points  $\mathbf{r}_1$  and  $\mathbf{r}_2$  without ( $\alpha_0$ , solid line) and with reflection ( $\alpha_1$ , dashed line).

to the dominating contribution of shorter trajectories from  $\mathbf{r}_1$  to  $\mathbf{r}_2$ . Therefore, like for the semiclassical calculations<sup>16</sup> of the averaged level density in the asymptotic limit  $S_\alpha/\hbar \gg 1$ , it is convenient to separate out in the sum (11) for the Green's function the single term  $G_{\alpha_0}$  related to the shortest trajectory  $\alpha_0$ , directly joining  $\mathbf{r}_1$  and  $\mathbf{r}_2$  (see Fig. 1) from all other terms  $G_1$  associated with longer trajectories having reflections from the potential boundary, writing

$$G = G_{\alpha_0} + \sum_{\alpha \neq \alpha_0} G_\alpha = G_{\alpha_0} + G_1, \quad (12)$$

with

$$G_{\alpha_0} \approx G_0 = -\frac{m}{2\pi\hbar^2 r_{12}} \exp \left[ \frac{i}{\hbar} r_{12} p(\mathbf{r}) \right], \quad r_{12} = |\mathbf{r}_2 - \mathbf{r}_1|, \quad (13)$$

where, in the nearly local approximation,<sup>25-27</sup>  $p(\mathbf{r}) = |\mathbf{p}(\mathbf{r})| = \sqrt{2m[\varepsilon - V(\mathbf{r})]}$ , is the particle momentum at the spatial point  $\mathbf{r} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ . The second term  $G_1$  of the Green's function trajectory expansion (12) is responsible<sup>16,23,24</sup> for the oscillating part of the level and particle densities and the MI, in particular their shell fluctuations. In the adiabatic approach<sup>3,21</sup> the classical angular-momentum projection  $\ell_x(\mathbf{r})$  in the rotating frame is essentially determined by the global rotation rather than by the motion of particles along the trajectories  $\alpha$  inside the nucleus. This picture is consistent with the separation of the intrinsic motion from vibration and rotation modes in this approach. Performing in Eq. (3) first an integration by parts over  $\varepsilon$  and then over the center of mass and relative coordinates  $\mathbf{r} = (\mathbf{r}_1 + \mathbf{r}_2)/2$  and  $\mathbf{s} = \mathbf{r}_2 - \mathbf{r}_1$  (instead of  $\mathbf{r}_1$  and  $\mathbf{r}_2$ ) one may introduce the local spherical coordinate system for the integration variable  $\mathbf{s}$  with the symmetry  $z$  axis and center at the point  $\mathbf{r}_1$ . By using the semiclassical expansion (12) we take smooth quantities in front of the sharply peaked  $\delta n(\varepsilon)$  near the Fermi energy  $\varepsilon = \lambda$  in the integrand. Averaging in phase-space variables with the energy-spectrum smoothing parameter  $\Gamma$  larger than the distance between energy levels and smaller than that

between the gross shells  $\hbar\Omega$  near the Fermi surface leads to the local approximation in terms of shorter trajectories. In this way, one approximately obtains for the MI  $\delta\Theta_x$  the shell correction  $\delta\Theta_x^{rig}$  to the rigid-body TF approach. The TF MI was derived<sup>25</sup> through Eq. (3) within the nearly local approximation (13) of the Green's function expansion (12). We applied the average in phase-space variables for convergence to the contributions to shorter trajectories in Eq. (11). The cranking model for nuclear rotations implies that the correlation corrections should be small enough, with respect to the main rigid-body component  $\delta\Theta_x^{rig}$ , to be neglected. Other contributions can also be referred to as a fluctuation correction to the rigid-body MI at leading order in  $\hbar^{1/2}$ . Finally, we arrive at the leading semiclassical MI shell correction for the perpendicular (collective) rotation for the deformed HO in the following form:

$$\delta\Theta_{x,scl} \approx \delta\Theta_x^{rig} = m \int d\mathbf{r} r_{\perp}^2 \delta\rho(\mathbf{r}), \quad r_{\perp}^2 = y^2 + z^2, \quad (14)$$

where  $\delta\rho(\mathbf{r})$  is the shell correction to the particle density

$$\rho(\mathbf{r}) = -\frac{d_s}{\pi} \text{Im} \int d\varepsilon n(\varepsilon) [G(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)]_{\mathbf{r}_1=\mathbf{r}_2=\mathbf{r}}. \quad (15)$$

A similar expression for the alignment MI shell correction  $\delta\Theta_z$  is obtained. For the particle density  $\rho(\mathbf{r})$  one has in the semiclassical approximation

$$\rho(\mathbf{r}) \approx \rho_{scl}(\mathbf{r}) = \rho_{TF}(\mathbf{r}) + \delta\rho_{scl}(\mathbf{r}), \quad (16)$$

where  $\rho_{TF}$  is for simplicity the TF approximation (more exactly ETF including the  $\hbar$  corrections),

$$\rho_{TF}(\mathbf{r}) = -\frac{d_s}{\pi} \text{Im} \int d\varepsilon n(\varepsilon) [G_0(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)]_{\mathbf{r}_1=\mathbf{r}_2=\mathbf{r}} = \frac{d_s p_F^3}{6\pi^2 \hbar^3}, \quad (17)$$

up to temperature corrections of the order of  $(T/\varepsilon_F)^2$ , and accordingly

$$\delta\rho_{scl}(\mathbf{r}) = -\frac{d_s}{\pi} \text{Im} \int d\varepsilon \delta n(\varepsilon) [G_1(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)]_{\mathbf{r}_1=\mathbf{r}_2=\mathbf{r}}. \quad (18)$$

Notice that the semiclassical POT derivations of the oscillating part of the particle density (18) were performed<sup>28</sup> in terms of the classical closed trajectories for various Hamiltonians. Thus, the semiclassical MI can be split into smooth and oscillating components,

$$\Theta_x \approx \Theta_{x\,scl}^{rig} = \Theta_{x\,TF}^{rig} + \delta\Theta_{x\,scl}^{rig}, \quad (19)$$

with the smooth TF (or ETF) part

$$\Theta_{x\,TF}^{rig} = m \int d\mathbf{r} r_{\perp}^2 \rho_{TF}(\mathbf{r}) = \frac{m d_s}{6\pi^2 \hbar^3} \int d\mathbf{r} p_F^3 r_{\perp}^2 \quad (20)$$

and the oscillating term

$$\delta\Theta_{x\ scl}^{rig} = m \int d\mathbf{r} r_{\perp}^2 \delta\rho(\mathbf{r}) = -\frac{md_s}{\pi} \text{Im} \sum_{\alpha \neq \alpha_0} \int d\varepsilon \delta n(\varepsilon) \int d\mathbf{r} r_{\perp}^2 \left\{ \mathcal{A}_{\alpha}(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) \times \exp \left[ \frac{i}{\hbar} S_{\alpha}(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) - \frac{i\pi}{2} \mu_{\alpha} \right] \right\}_{\mathbf{r}_1=\mathbf{r}_2=\mathbf{r}}. \quad (21)$$

Within a precision of the semiclassical approximation, we evaluate the spatial integral by the stationary phase method (SPM) extended to continuous symmetries<sup>10,16</sup> with the stationary phase condition,

$$\left[ \frac{\partial S_{\alpha}(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)}{\partial \mathbf{r}_1} + \frac{\partial S_{\alpha}(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)}{\partial \mathbf{r}_2} \right]_{\mathbf{r}_1=\mathbf{r}_2=\mathbf{r}}^* \equiv (-\mathbf{p}_1 + \mathbf{p}_2)_{\mathbf{r}_1=\mathbf{r}_2=\mathbf{r}} = 0. \quad (22)$$

where the 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  $\mathbf{p}_1^* = \mathbf{p}_2^*$ , i.e. the SPM equations (22) are equivalent to the periodic orbit (p.o.) conditions. Other smooth factors can be taken off the integral at these stationary points defined by Eq. (22). Assuming that quantum averages  $\langle \kappa^2 \rangle / \varepsilon$  are smooth enough functions of  $\varepsilon$  as compared to other factors, for instance  $\delta n$  or exponents with a large argument  $S_{\alpha} / \hbar$ , one may take them approximately off the integral over  $\varepsilon$  at the chemical potential,  $\varepsilon = \lambda$ . Therefore, the main contribution into the integral in Eq. (21) is coming from the p.o. stationary-phase points of Eq. (22). Similarly, like for the calculation of the level density shell corrections  $\delta g_{scl}$ , the SPM condition (22) is identity for any stationary point of the classically accessible spatial region for particle motion filled by p.o. families in the case of their high degeneracy  $\mathcal{K} \geq 3$ , for instance, for the contribution of the 3-dimensional (3D) orbits in the HO potential well. The stationary points occupy some spatial subspace for smaller degeneracy  $\mathcal{K}$ . In the latter case of the equatorial (EQ) orbits ( $\mathcal{K} = 2$ ) the SPM condition is identity in the equatorial plane  $z = 0$ . Finally, for the MI shell corrections one obtains

$$\delta\Theta_{\kappa, scl} \approx \delta\Theta_{\kappa, scl}^{rig}, \quad \delta\Theta_{\kappa, scl}^{rig} = [(1 + \eta_1^2) / 3\omega_{\perp}^2] \delta F_{scl}, \quad (23)$$

where  $\eta_1 = \eta$  for  $\kappa = x$  and  $\eta_1 = 1$  for  $\kappa = z$ .

For the Strutinsky energy shell correction at  $T = 0$  one has

$$\delta E = E_{s.p.} - \tilde{E}_{s.p.} = d_s \sum_i (\varepsilon_i - \lambda) \delta n_i \approx d_s \int d\varepsilon (\varepsilon - \lambda) \delta g(\varepsilon) \delta n(\varepsilon). \quad (24)$$

At finite temperature  $T$ , for the shell correction to the free energy,  $F = E - TS$  with  $E = d_s \sum_i \varepsilon_i n_i$ , one writes  $\delta F = \delta E - T\delta S$  where  $\delta F(T, N) = \delta\Omega(T, \lambda)$  and  $\delta\Omega$  is the shell component of the grand thermodynamical potential  $\Omega(T, \lambda)$ .

In the semiclassical approximation (POT),

$$\delta F \approx \delta F_{scl}(T, N) = \text{Re} \sum_{p.o.} \delta F_{p.o.}, \quad \delta F_{p.o.} = \delta U_{p.o.} Q(Z_{p.o.}), \quad (25)$$

with

$$\delta U_{scl} = \text{Re} \sum_{p.o.} \delta U_{p.o.}, \quad \delta U_{p.o.} = d_s \frac{\hbar^2}{t_{p.o.}^2} \delta g_{p.o.}(\lambda). \quad (26)$$

Here,

$$\delta g_{p.o.}(\varepsilon) = \mathcal{B}_{p.o.}(\varepsilon) \exp \left[ \frac{i}{\hbar} S_{p.o.}(\varepsilon) - i \frac{\pi}{2} \mu_{p.o.} \right] \quad (27)$$

is the p.o. component of the oscillating part of the level density

$$\delta g_{scl}(\varepsilon) = -\frac{1}{\pi} \text{Im} \int d\mathbf{r} [G_1(\mathbf{r}_1, \mathbf{r}_2; \varepsilon)]_{\mathbf{r}_1=\mathbf{r}_2=\mathbf{r}} \approx \text{Re} \sum_{p.o.} \delta g_{p.o.}(\varepsilon), \quad (28)$$

$S_{p.o.}(\varepsilon)$  and  $\mu_{p.o.}$  are the action and Maslov index along the p.o.,  $\mathcal{B}_{p.o.}(\varepsilon)$  is the level density amplitude depending on the p.o. stability factors and degeneracies.<sup>10,15,16,23</sup> In Eq. (25), the temperature damping factor  $Q$ , which serves the exponential convergence of the MI with increasing temperature  $T$  and time of particle motion  $t_\alpha$ , is given<sup>17-20</sup> by

$$Q(\mathcal{Z}) = \frac{\pi \mathcal{Z}}{\sinh(\pi \mathcal{Z})}, \quad \mathcal{Z}_{p.o.} = \frac{t_{p.o.} T}{\hbar}. \quad (29)$$

In the case of *incommensurable* HO frequencies one has only EQ p.o.s with the action  $S_n(\varepsilon) = \varepsilon t_n$ ,  $t_n = n \mathcal{T}_{EQ}$ , and period  $\mathcal{T}_{EQ} = 2\pi/\omega_{EQ} = 2\pi n_\perp/\omega_\perp = 2\pi n_z/\omega_z$ . For their contributions  $\delta U_{EQ}$  into the energy shell correction  $\delta U$  of the HO one finds<sup>23</sup>

$$\delta U_{EQ} = \sum_n \frac{2d_s \lambda \omega_{EQ}^2}{(2\pi\omega_\perp n)^2 \sqrt{\mathcal{F}_n}} \sin \left( \frac{2\pi n \lambda}{\hbar \omega_{EQ}} \right), \quad \mathcal{F}_n = 4 \sin^2 \left( \frac{\pi n \omega_z}{\omega_{EQ}} \right). \quad (30)$$

For the *commensurable* frequencies  $\omega_\perp : \omega_z = n_\perp : n_z$ , one has the complete degeneracy of the classical motion of particle ( $\mathcal{K} = 4$ ) along the 3D p.o.s with the period  $\mathcal{T}_{3D} = 2\pi/\omega_{3D} = 2\pi n_\perp/\omega_\perp = 2\pi n_z/\omega_z = (2\pi/\omega_0) (n_\perp^2 n_z)^{1/3}$ . The POT energy shell correction<sup>23</sup> is a sum of the contributions of the 3D and EQ p.o.s,  $\delta U_{scl} = \delta U_{3D} + \delta U_{EQ}$  where

$$\delta U_{3D} = \sum_n \frac{d_s \lambda^2 \omega_{3D}^2}{(2\pi)^2 \hbar \omega_0^3 n^2} \cos \left[ \frac{2\pi n \lambda}{\hbar \omega_{3D}} - \pi n (2n_\perp + n_z) \right]. \quad (31)$$

#### 4. Comparison with Quantum Results

Fig. 2 shows the semiclassical energy shell-correction  $\delta U_{scl}$  (26) and the corresponding quantum SCM calculations of  $\delta E$  Eq. (24) as functions of the chemical potential  $\lambda$  at zero temperature for different critical symmetry-breaking and bifurcation deformations<sup>10</sup>  $\eta = 1$  and  $6/5, 2$ . This comparison exhibits a practically perfect agreement between the semiclassical (SCL) and quantum (QM) results, especially for  $\eta = 1$  and  $2$ . Notice that this agreement is not exact even for the semiclassical free energy shell corrections at zero temperature because we neglected the terms

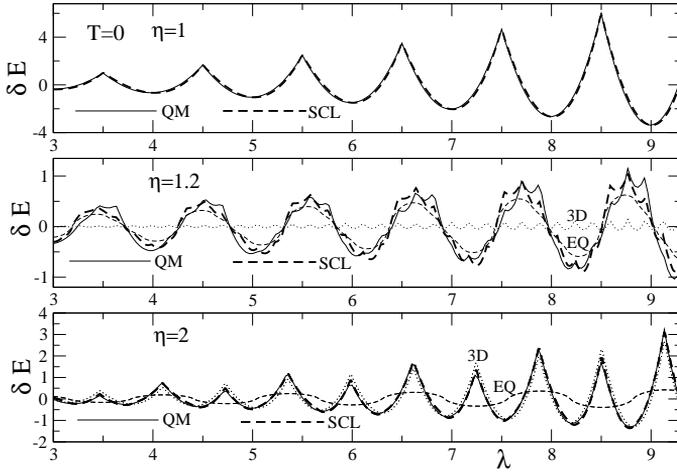


Fig. 2. The quantum (QM) Eq. (24) and semiclassical (SCL) Eq. (26) shell-structure energies,  $\delta E \approx \delta U_{scl}$ , at zero temperature  $T = 0$  vs the chemical potential  $\lambda$  for the spherical HO in units of  $\hbar\omega_0$  at critical deformations  $\eta = 1, 1.2$  and  $2$ ; 3D frequent dots show the contribution of the 3D orbits, and EQ thin dashed curves present the EQ orbit contribution.

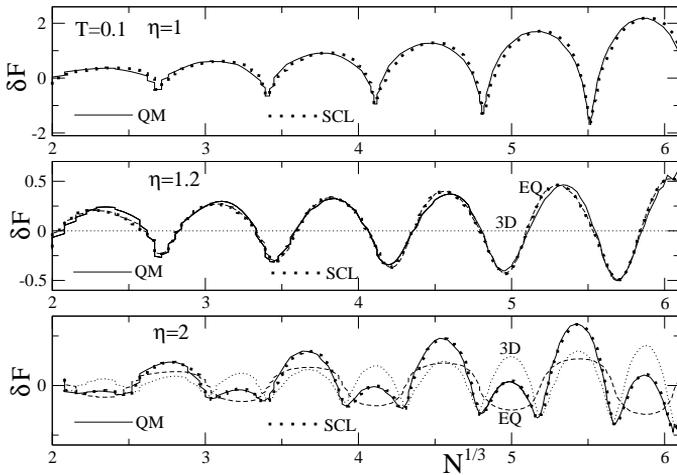


Fig. 3. The shell-structure free energy  $\delta F$  as function of particle number variable,  $N^{1/3}$  for the critical deformations  $\eta = 1, 1.2$  and  $2$  at temperature  $T = 0.1$  in HO units  $\hbar\omega_0$ ; the SCM smoothing parameters  $\gamma = 1.5 - 2.5\hbar\omega_0$ ,  $M = 4 - 8$ ; other notations are the same as in Fig. 2.

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 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 3D orbits are generally too long in this case. For the bifurcation point  $\eta = 2$  one finds an interference of two comparably large contributions of EQ and 3D orbits, Eqs. (30) and (31) respectively, with different periods,  $\mathcal{T}_{3D} = 2\mathcal{T}_{EQ}$ , as seen from the bottom part of Fig. 2. The semiclassical free-energy shell-correction  $\delta F_{scl}$ , Eq. (25), is displayed in Fig. 3 as function of the particle-number variable,  $N^{1/3}$ , and compared at a temperature of  $T = 0.1\hbar\omega_0$  with the corresponding quantum SCM results for the same critical deformations. This comparison also shows practically a perfect agreement between the semiclassical and quantum results with a similar p.o. structure. As seen from Figs. 2 and 3, instead of the concaved parabolas, depending on the chemical potential  $\lambda$ , we observe the convexed ones owing to the oscillating component  $\delta\lambda$  of  $\lambda = \tilde{\lambda} + \delta\lambda$  as functions of the particle number parameter  $N^{1/3}$  ( $\tilde{\lambda}$  is the averaged  $\lambda$  in the SCM).

A similar comparison is presented in Fig. 4 for the shell corrections to the MI  $\delta\Theta_x$ . Again, an excellent agreement is observed between semiclassical and quantum semiclassical free-energy shell-correction  $\delta F_{scl}$ , Eq. (25), is displayed in Fig. 3 as results which is not really astonishing because of the proportionality of the  $\delta\Theta_x$  to  $\delta F$  (see Eqs. (10) and (23)). One finds in particular 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. (25), is clearly seen. The critical temperature

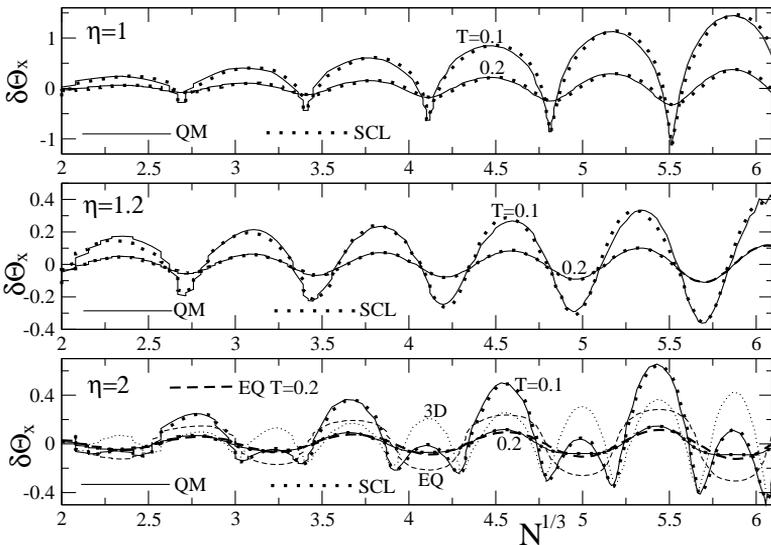


Fig. 4. Moment of inertia  $\delta\Theta_x$  (23), (25)–(31) in units  $\hbar/\omega_0$  as function of the particle number,  $N^{1/3}$ , at temperatures  $T = 0.1$  and  $0.2$  (in units  $\hbar\omega_0$ ); EQ thin dashed curves present the EQ orbit contribution for temperature  $T = 0.1$ , and EQ thick dashed is the EQ orbit term for  $T = 0.2$ ; other notations are the same as in Figs. 2 and 3.

for a disappearance of shell effects in the MI is found,<sup>10,16</sup> for prolate deformations ( $\eta > 1$ ) and particle numbers  $N \sim 100 - 200$ , approximately at  $T_{cr} = \hbar\omega_{EQ}/\pi \sim \hbar\omega_0/\pi \approx 2 - 3$  MeV just as for  $\delta F$ . The particle-number dependence of the shell corrections  $\delta\Theta_z$  to  $\Theta_z$  (alignment) in Eqs. (10) and (23) is similar to that of  $\delta\Theta_x$  because of their relations,  $\delta\Theta_z \propto \delta\Theta_x \propto \delta F$ .

## 5. Conclusion

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

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