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SEMICLASSICAL SHELL-STRUCTURE MOMENTS OF INERTIA IN HEATED FERMI SYSTEMS

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The moment of inertia for collective rotation is derived analytically for the harmonic-oscillator Hamiltonian within the cranking model for any rotation frequency and at finite temperature. Semiclassical shell-structure moments of the inertia are obtained in terms of the free-energy shell corrections through the rigid-body inertia of the statistically equilibrium rotation of a heated Fermi system by using the 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 quantum results for critical deformations and temperatures.

Keywords: cranking model, nuclear rotations, moment of inertia, periodic orbit theory, shell-correction energy, harmonic oscillator potential.

Introduction

Several theoretical approaches, in particular the cranking model, were used for the description of many remarkable properties of collective nuclear rotations [1 - 7]. It was shown [4, 6] that the moments of inertia can be presented as a sum of a smooth classical rigid-body term with the $\hbar$ corrections of the Extended Thomas-Fermi approach (ETF) [8 - 10] and their shell corrections [4]. Such shell-nanostructure phenomena were successfully described on the basic of the mean-field approach within the shell correction method (SCM) [11, 12] adapted to the rotational problem in [4]. The independent particle model near the Fermi surface is used for calculations of the shell corrections to the free energy and moment of inertia. However, the total free energy and moment of inertia in the SCM are beyond this model. In particular, the smooth ETF parts can be associated with a leptodermic expansion in which the basic ingradient is the nuclear surface formed by a nuclear many-body interacton. For the shell correction calculations, it is worth to apply for solving this problem the semiclassical periodic orbit theory (POT) as one of the powerful and fruitful theoretical tools for the analytical understanding of the main features of shell structure in finite Fermion systems [8, 13 - 18]. The semiclassical shell corrections to the moments of inertia for rotations around the symmetry axis like alignment of the individual-particle angular momenta (the so called "classical rotation") were derived within the POT at finite temperatures in terms of periodic orbits in [13] (see also [16, 17] for similar derivations of the magnetic susceptibilities). For collective rotations of deformed nuclei this periodic-orbit structure was considered semiclassically in Ref. [18] by applying the classical perturbation theory of Creagh [8, 19] to the spheroid cavity model.

In the present work the shell components of the moments of inertia for the collective rotations within the nonperturbative POT based on the mean-field cranking model are derived asymptotically for large semiclassical parameter $k_F R \sim N^{1/3} \gg 1$ in terms of the free-energy shell corrections for nucleus with large enough particle numbers N, Fermi momentum k_F in $\hbar$ units and a spatial size R. Explicit analytical results are obtained for the deformed harmonic oscillator potential. One of the main purposes is to use this simple completely analytical example as a test in order to find a general relation of the shell components of the moment of inertia to those of the rigid body through the free-energy shell corrections valid for any mean-field potential well within the cranking model.

Cranking model for nuclear rotations

Within the cranking model, the collective nuclear rotation of an axially symmetric mean-field potential around the x axis, perpendicular to the symmetry z axis, can be described by solving the eigenvalue problem for the single-particle (s.p.) Hamiltonian (Routhian) in the framework of a rotating coordinate system [3, 4, 6],

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

Here, H is the unperturbed Hamiltonian, ℓ_x the projection on to the x axis of the angular-momentum operator, and d_s the spin (spin-isospin) degeneracy. The Lagrangian multiplier ω is the rotation frequency of the body-fixed coordinate system. Its value $\omega = \omega(I_x)$ can be found from Eq. (1) for each given value of the constraint angular

momentum I_x. The particle number conservation determines the chemical potential λ_ω through the occupation numbers n_i^ω for a system of independent nucleons in the s.p. state i,

$$N = d_s \sum_i n_i^\omega,$$

$$n_i^\omega \equiv n\left(\varepsilon_i^\omega\right) = \{1+\exp\left[(\varepsilon_i^\omega - \lambda_\omega)/T\right]\}^{-1}, \qquad (2)$$

with the eigenvalues ε_i^ω of the Routhian H_ω, $\lambda_\omega = \lambda \approx \varepsilon_F$ at $\omega = 0$, where ε_F is the Fermi energy, $\varepsilon_F = \hbar^2 k_F^2/2m$, k_F the Fermi momentum in units of $\hbar$, m the nucleon mass, and T the temperature. The moment of inertia $\Theta_x(\omega)$ is defined similarly to the magnetic or isolated susceptibilities [16, 17, 21],

$$\Theta_x(\omega) = \frac{\partial \langle \ell_x \rangle_\omega}{\partial \omega} = \frac{\partial^2 E(\omega)}{\partial \omega^2}, \qquad (3)$$

where $E(\omega) = \langle H \rangle_\omega + \omega I_x$ is the energy of a Fermi system. The yrast line $E(I_x)$ can be obtained by elimination of the frequency ω from the constraint of (1) at zero temperature T.

For the case of the harmonic oscillator (HO) Hamiltonian the direct diagonalization (without using a perturbation expansion) of the Routhian, Eq. (1), yields for any frequencies ω analytical expressions for the single-particle energies ε_i^ω and the moments of inertia $\Theta_x(\omega)$ [5]. We extended these results to finite temperatures T through the oscillator occupation numbers (see Appendix A for a detailed derivation based on Refs. [22, 23]). In the small rotation-frequency limit $\omega \to 0$ (adiabatic case) one uses the s.p. spectrum independent of ω,

$$\varepsilon_i = \hbar\omega_\perp \left(N_{\perp i} + 1\right) + \hbar\omega_z \left(N_{zi} + 1/2\right),$$

$$N_{\perp i} = N_{xi} + N_{yi}, \qquad (4)$$

where N_{xi}, N_{yi} and N_{zi} are the HO quantum numbers related to the partial HO frequencies ω_x, ω_y and ω_z, $\omega_x = \omega_y = \omega_\perp$.

From Eq. (A15) for the moment of inertia $\Theta_x(\omega)$ one finds [2, 3, 5] in the adiabatic limit $\omega \to 0$

$$\Theta_x = \frac{d_s\,\hbar}{2\omega_\perp\omega_z}\left[\frac{\left(\omega_z-\omega_\perp\right)^2}{\omega_\perp+\omega_z}\left(\aleph_y+\aleph_z\right)+\frac{\left(\omega_z+\omega_\perp\right)^2}{\omega_\perp-\omega_z}\left(\aleph_z-\aleph_y\right)\right], \qquad \aleph_\kappa = \sum_i n_i\left(N_{i\kappa}+1/2\right), \qquad (5)$$

where $\kappa = x, y, z$, $n_i = n_i^\omega$ at $\omega = 0$, according to Eq. (2). Notice that for the HO potential one may calculate analytically the matrix elements of the angular momentum projection operator ℓ_x. Substituting these and the single-particle energies into the Inglis formula for the moment of inertia in 2nd order perturbation theory one also arrives at the expression, Eq. (5), of the nonperturbative derivation.

For the statistically equilibrium rotation (selfconsistent relation [3]),

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

the moment of inertia (5) equals the rigid-body value given by

$$\Theta_x^{rig} = m\int \mathrm{d}\mathbf{r}\ \rho(\mathbf{r})\left(y^2+z^2\right) = d_s\hbar\left(\aleph_y/\omega_\perp + \aleph_z/\omega_z\right), \qquad (7)$$

where $\rho(\mathbf{r})$ is the particle density. The first term in (5) is related to the coupling of single-particle levels through major N shells ($\Delta N = 2$, see Ref. [3]) and the second term corresponds to transitions between levels inside a shell ($\Delta N = 0$). In the spherical limit, this term reduces identically to the diagonal alignment moment of inertia,

$$\Theta_x \to \Theta_z \to -d_s \sum_i (\mathrm{d}n_i/\mathrm{d}\varepsilon_i)\,|\langle i\,|\,\ell_x\,|\,i\rangle|^2. \qquad (8)$$

For calculations of the shell corrections, it is convenient to re-write the moment of inertia Θ_x, Eq. (5), in terms of the rigid body inertia Θ_x^{rig}, Eq. (7), and the free energy $F(\omega = 0)$ of the HO system at finite temperature T,

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

where η is the deformation parameter, $\eta = \omega_\perp/\omega_z$, under the usual volume conservation condition, $\omega_\perp^2\omega_z = \omega_0^3$. Notice that in this way the oscillator quantum numbers $\aleph_y$ and $\aleph_z$ could be elliminated from Eqs. (5) and (7) through the explicit expression of the free energy F for the ideal Fermi gas.

Calculating explicitly the rigid-body inertia Θ_x^{rig} (7) for the HO and determining the shell components $\delta\Theta_x$ and $\delta\Theta_z$ by the SCM [11, 12], these are obtained in terms of the free energy shell correction δF,

$$\delta\Theta_x = \left[\left(1+\eta^2\right)/3\omega_\perp^2\right]\delta F,\ \delta\Theta_z = \left(2/3\omega_\perp^2\right)\delta F, \quad (9)$$

with the obvious spherical limit, $\delta\Theta_x \to \delta\Theta_z$ at $\eta \to 1$.

Semiclassical shell-structure approach

For the POT calculations, it turns out to be helpful to use the coordinate representation through the Green's functions G [12],

$$\Theta_x = \frac{2d_s}{\pi}\int_0^\infty \mathrm{d}\varepsilon\, n(\varepsilon)\int \mathrm{d}\mathbf{r}_1 \int \mathrm{d}\mathbf{r}_2\ \ell_x(\mathbf{r}_1)\,\ell_x(\mathbf{r}_2)\,\mathrm{Re}\left[G\left(\mathbf{r}_1,\mathbf{r}_2,\varepsilon\right)\right]\mathrm{Im}\left[G\left(\mathbf{r}_1,\mathbf{r}_2,\varepsilon\right)\right], \quad (10)$$

where $n(\varepsilon)$ are the Fermi occupation numbers $n(\varepsilon_i^\omega)$ at $\omega = 0$, Eq. (2), and $\ell_x(\mathbf{r}_1)$ and $\ell_x(\mathbf{r}_2)$ are respectively the angular-momentum projections onto the x axis for the particle at the spatial points $\mathbf{r}_1$ and $\mathbf{r}_2$. With the usual energy spectral representation for the one-body Green's function in the mean-field approximation, one has the well-known second order perturbation result of the cranking model [3, 4, 6]. However, we may also include semiclassically the diagonal terms into (10) as explained below. The Green's function in (10) can be approximated by the semiclassical Gutzwiller trajectory expansion [14] extended to continuous symmetry [8, 15, 24],

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

The index α covers all classical isolated paths inside the potential well which connect the two spatial points $\mathbf{r}_1$ and $\mathbf{r}_2$ for a given s.p. energy ε. Here S_α is the classical action along such a trajectory α, and μ_α denotes a phase related to the Maslov index through the number of caustic and turning points along the path α [8,15]. The amplitudes $\mathcal{A}_\alpha$ of the Green's function depend on the classical stability factors and trajectory degeneracy owing to the geometrical and dynamical symmetries of the given Hamiltonian (see Refs. [8, 14, 15, 24] for their specific expressions).

Among all classical trajectories α in Eq. (11), we may single out one α_0 which connects directly $\mathbf{r}_1$ and $\mathbf{r}_2$ without intermediate turning points. It is associated with the component G_{α_0} of the sum (11). Therefore, for the Green's function G, Eq. (11), one has then a separation, $G = G_{\alpha_0} + G_1$. In the nearly local approximation one finds

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

for points that are spatially close $\mathbf{r}_1 \to \mathbf{r}_2 \to \mathbf{r}$, $p\left(\mathbf{r}\right)$ is the particle momentum at $\mathbf{r} = (\mathbf{r}_1+\mathbf{r}_2)/2$ (see Refs. [15, 21, 25, 26]). The second term G_1 is the fluctuating part of the Green's function (11), $G \approx G_0 + G_1$, determined by other trajectories $\alpha_1 \neq \alpha_0$ [15, 20, 24]. With this separation one obtains from (10)

$$\Theta_x = \sum_{\nu,\nu'=0}^{1}\Theta_x^{\nu\nu'},$$

$$\Theta_x^{\nu\nu'} = \left(2d_s/\pi\right)\int \mathrm{d}\varepsilon\, n(\varepsilon)\int \mathrm{d}\mathbf{r}_1\int \mathrm{d}\mathbf{r}_2\ \ell_x\left(\mathbf{r}_1\right)\ell_x\left(\mathbf{r}_2\right)\times$$

$$\times\,\mathrm{Re}\left[G_\nu\left(\mathbf{r}_1,\mathbf{r}_2,\varepsilon\right)\right]\mathrm{Im}\left[G_{\nu'}\left(\mathbf{r}_1,\mathbf{r}_2,\varepsilon\right)\right]. \quad (12)$$

The main smooth term of this moment sum for Θ_x is the Thomas-Fermi rigid-body component associated with averaging of Θ_x^{00} over the phase-space variables which removes the non-local correlations [21]. The $\hbar$ corrections of the smooth ETF approach to this TF approximation were obtained in Refs. [9, 10].

The shell-structure component $\delta\Theta_x^{01}$ of Θ_x^{01} for the moment of inertia Θ_x, Eq. (12), 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 moment of inertia. Indeed, substituting the nearly local approximation G_0 into Eq. (12) for $\nu = 0$ and G_1 for $\nu' = 1$, we select the shell component $\delta\Theta_x^{01}$ of Θ_x^{01} just as for the free-energy shell corrections δF. Using the transformation of the coordinates $\mathbf{r}_1$ 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 coordinates for $\mathbf{s}$, $\mathrm{d}\mathbf{s} = s^2\mathrm{d}s\,\sin\theta_s\mathrm{d}\theta_s\mathrm{d}\varphi_s$ one obtains for almost equilibrium rotation

$$\delta\Theta_x^{01} = -\left(\frac{d_s m}{(\pi\hbar)^2}\right)\int \mathrm{d}\varepsilon\,\delta n(\varepsilon)\int \mathrm{d}\mathbf{r}\int \mathrm{d}s\, s\int \mathrm{d}\theta_s \mathrm{d}\varphi_s\ \sin\theta_s\ \ell_x\left(\mathbf{r}-\mathbf{s}/2\right)\ \ell_x\left(\mathbf{r}+\mathbf{s}/2\right)\times$$

$$\times\cos\left(p(\mathbf{r})s/\hbar\right)\ \mathrm{Im}\left[G_1\left(\mathbf{r}-\mathbf{s}/2,\mathbf{r}+\mathbf{s}/2,\varepsilon\right)\right] \approx \delta\Theta_x^{rig} = m\int \mathrm{d}\mathbf{r}\left(y^2+z^2\right)\delta\rho\left(\mathbf{r}\right). \qquad (13)$$

For the classical angular-momentum projection in the integrand of the first expression in Eq. (13) we approximately wrote

$$\ell_x(\mathbf{r}-\mathbf{s}/2)\ \ell_x(\mathbf{r}+\mathbf{s}/2) \approx \ell_x^2(\mathbf{r}) = (y^2+z^2)p^2(\mathbf{r}). \qquad (14)$$

Note that this classical angular-momentum projection $\ell_x(\mathbf{r})$ in the rotating coordinate system is caused by the global rotation rather than by the motion of particles along the trajectories α inside the nucleus. According to the time-reversible symmetry of the Routhian, the particles are, indeed, moving in the non-rotating ($\omega = 0$) coordinate system along these trajectories in both directions with opposite signs of ℓ_x and their contributions to the total angular momentum of the nucleus turns out to be zero. We integrated then explicitly over s and found sine squared in the integrand over ε and $\mathbf{r}$ with the mean value 1/2 for the averaging over energies ε. Adding and subtracting identically this value 1/2 from the sine squared, we first integrate over spherical angles θ_s and φ_s in the term related to this 1/2, writing simply 4π because of the independence of this integrand of angles of the vector $\mathbf{s}$. Performing then the integrations over ε in this first term and taking smooth quantities in front of the sharply peaked function $\delta n(\varepsilon)$ at the energy $\varepsilon = \lambda$ one obtains the rigid-body shell correction component $\delta\Theta_x^{rig}$, as shown in Eq. (13). The cranking model for the nuclear rotation implies that the correlation corrections in (13) should be small enough with respect to the main rigid-body component $\delta\Theta_x^{rig}$ to be neglected. Other contributions obtained by using the stationary phase method [20], except for a smooth rigid-body part coming from Θ_x^{00}, can also be referred to a fluctuation correction to the rigid-body moment of inertia. Finally, for the semiclassical shell corrections to the moments of inertia for perpendicular $\delta\Theta_{x,scl}$ and parallel $\delta\Theta_{z,scl}$ (alignment along the symmetry axis) rotation, we arrive for the deformed HO with Eq. (9) at the following expressions

$$\delta\Theta_{x,scl} \approx \delta\Theta_{x,scl}^{rig} = \left[\left(1+\eta^2\right)/3\omega_\perp^2\right]\delta F_{scl},$$

$$\delta\Theta_{z,scl} \approx \delta\Theta_{z,scl}^{rig} = \left(2/3\omega_\perp^2\right)\delta F_{scl}. \qquad (15)$$

Here, δF_{scl} is the semiclassical periodic-orbit (p.o.) sum for the free energy shell component [8, 13, 15, 16],

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

$$Q(\mathcal{Z}) = \frac{\pi\mathcal{Z}}{\sinh(\pi\mathcal{Z})}, \quad \mathcal{Z}_{p.o.} = t_{p.o.}T/\hbar, \qquad (16)$$

$\delta U_{p.o.}$ is the p.o. component of the semiclassical energy shell correction, and $t_{p.o.}$ is the time of particle motion along the p.o. [8,15]. The temperature-dependent factor $Q(t_{p.o.}T/\hbar)$ in (16) decreases exponentially with increasing the p.o. period $t_{p.o.}$ or the temperature T. As this factor tends to unity at zero temperature, the semiclassical free-energy shell component δF_{scl} (16) turns into the zero temperature shell-correction energy $\delta U_{scl} = \sum_{p.o.}\delta U_{p.o.}$. At finite temperature the free-energy shell correction δF_{scl} differs from the shell correction δE_{scl} of the internal energy E_{scl} by the entropy contribution $T\delta S_{scl}$ through the standard relationship

$$\delta E_{scl} = \delta F_{scl} + T\delta S_{scl}, \qquad (17)$$

where δS_{scl} is the corresponding entropy shell correction [15]. In the zero temperature limit, $T \to 0$, the internal-energy shell correction δE_{scl} coincides, of course, with the semiclassical energy shell component δU_{scl}. Notice also that for the HO case with the help of (15) for $\delta\Theta_{x,scl}^{rig}$ one exactly obtains (9) without refering to the statistically equilibrium condition (6).

For the deformed HO potential, one has to consider two cases concerning different (rational or irrational) ratios of the frequencies $\omega_\perp$ and ω_z ($\omega_x = \omega_y = \omega_\perp$). Following basically Ref. [24], one finds mainly the well-known p. o. families (Lissajous figures) with different classical degeneracies $\mathcal{K} = 4$ and 2 depending on the commensurable or incommensurable frequency relations [15, 24].

(i) 2D ORBITS. We shall consider first the case of the partially commensurable frequencies of the axially-symmetric HO with irrational value of η. In that case, there are no isolated 3-dimensional (3D, $\mathcal{K}=4$) families. However, the 2D equatorial (EQ) families of periodic orbits of smaller degeneracy $\mathcal{K}=2$ mainly exist with a given period number n in the (x,y) plane ($z=0$), perpendicular to the symmetry z axis. The time of motion along the p. o. of the family, $t_n = n\mathcal{T}_{EQ}$, is determined by the main period $\mathcal{T}_{EQ}$ (frequency ω_{EQ}) of the primitive ($n=1$) p.o. in this (x,y) plane, $\mathcal{T}_{EQ} = 2\pi/\omega_{EQ} = 2\pi n_\perp/\omega_\perp = 2\pi n_z/\omega_z$, where $n_\perp$ and n_z are mutually simple integer numbers. For the contribution of the EQ ($\mathcal{K}=2$) orbits into the energy shell correction δU_{scl} one writes [8, 24]

$$\delta U_{EQ} = \sum_n \delta U_n^{EQ},$$

$$\delta U_n^{EQ} = \frac{2d_s\lambda\,\omega_{EQ}^2}{\left(2\pi\omega_\perp n\right)^2\sqrt{\mathcal{F}_n}}\sin\left(2\pi n\lambda/\hbar\omega_{EQ}\right), \quad (18)$$

where $\mathcal{F}_n$ is the Gutzwiller stability factor, $\mathcal{F}_n = 4\sin^2\left(\pi n\omega_z/\omega_{EQ}\right)$.

(ii) 3D ORBITS. For the case of rational ratios of frequencies, $\omega_\perp : \omega_z = n_\perp : n_z$, one finds the time of particle motion, $t_n = n\mathcal{T}_{3D}$, through the period of its motion along the 3D p. o. of the $\mathcal{K}=4$ family,

$$\mathcal{T}_{3D} = \frac{2\pi}{\omega_{3D}} = \frac{2\pi n_\perp}{\omega_\perp} = \frac{2\pi n_z}{\omega_z} = \frac{2\pi}{\omega_0}\left(n_\perp^2 n_z\right)^{1/3}. \quad (19)$$

For the commensurable case at deformations $\eta > 1$, the EQ orbits mentioned above yield the contributions δU_{EQ} (18) of the partially commensurable case (i) to the energy shell corrections δU_{scl} together with the contribution of 3D orbits δU_{3D} which leads to their interference in the level density and energy shell corrections [24],

$$\delta U_{scl} = \delta U_{3D} + \delta U_{EQ}, \quad (20)$$

$$\delta U_{3D} = \frac{d_s\lambda^2\omega_{3D}^2}{(2\pi)^2\hbar\omega_0^3}\sum_n \frac{1}{n^2}\cos\left[\frac{2\pi n\lambda}{\hbar\omega_{3D}} - \pi n\left(2n_\perp + n_z\right)\right].$$

Comparison with quantum calculations

Fig. 1 shows a comparison of the semiclassical (SCL) free-energy shell corrections, δF_{scl} with both the internal-energy shell corrections, δE_{scl}, see Eq. (17), and the quantum (QM) results obtained by the Strutinsky shell correction method [11, 12] at a finite temperature $T = 0.1$ (in units $\hbar\omega_0$ of the HO shell spacing energy) for the critical bifurcation deformations $\eta = 1$, 6/5 and 2. For our major aim being to establish a comparison of the numerical quantum and analytical POT results for these shell-structure components, it is convenient to use the chemical potential λ as a variable, rather than its smooth counterpart $\tilde{\lambda}$, defined by the particle number $N = \sum_i \tilde{n}_i$, with the averaged occupation numbers $\tilde{n}_i$ [11, 12]. With the particle number relation $N = \sum_i n_i$ which relates λ to the particle number via the Fermi occupation numbers n_i, [Eq. (2) at $\omega = 0$], one may always re-express δF and δE as functions of the particle-number variable $N^{1/3}$. The so-called plateau condition, i.e. the independence of the shell-structure internal energy δE and free energy δF on the parameters of the Strutinsky smoothing, namely the Gaussian width γ and the degree of the correction polynomial M, is nicely satisfied for $\gamma = 1.5 - 2.5\,\hbar\omega_0$ and $M = 4 - 8$. We may therefore use any value for these parameters in our calculations of the smooth parts $\tilde{E}_{s.p.}$ and $\tilde{F}_{s.p.}$ of the single-particle internal energy $E_{s.p.}$ and free energy $F_{s.p.}$, respectively, without any noticible change of the results within the precision of lines. As seen from Fig. 1, one obtains perfect agreement of the semiclassical and quantum results. Notice that this agreement is not exact but it is associated with the leading term of the free-energy shell-correction expansion in $\hbar$ for any temperature, in contrast to the POT level density calculations which reproduce exactly the s.p. spectrum for the HO potential at zero temperature [13, 15, 17]. It is in line of the standard WKB results, based on separation variables, in the asymptotic (semiclassical) limit of a large oscillator quantum number but formulated namely for the free-energy shell corrections for which one can use the s.p. picture in the SCM. A large effect of the entropy component $T\delta\mathcal{S}_{scl}$ of the internal-energy shell corrections δE as compared to the free energy contribution δF is clearly seen in this Figure. For the spherical symmetry-breaking limit $\eta = 1$ one has the contribution of the only $\mathcal{K}=4$ degenerated families of 3D orbits (see Eqs. (16) and (20)). The relatively simple most degenerated ($\mathcal{K}=4$) families of 3D orbits appear along with the EQ orbits of smaller degeneracy at the bifurcation points 6/5 and 2. For $\eta = 1.2$ one has mainly the contribution of

EQ orbits because the 3D p.o.s are too long here. For the superdeformed $\eta = 2$ shape one finds a large-scale interference of comparably large contributions of 3D and EQ orbits (see Eqs. (20) and (18), respectively) wit
motion, $\mathcal{T}_{3D} = 2\mathcal{T}_t$

Fig. 1. One observes, indeed, a modulation of the amplitude of the 3D trajectories with smaller period (as function of λ), $\hbar\omega_{3D} = 2\pi\hbar/\mathcal{T}_{3D}$, by the contribution of EQ orbits with larger period

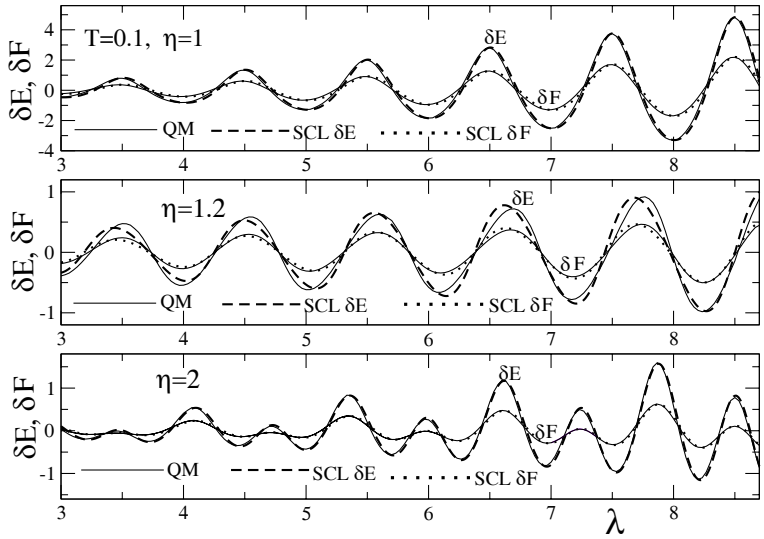

Fig. 1. Shell corr :al potential
λ for th ω_0.

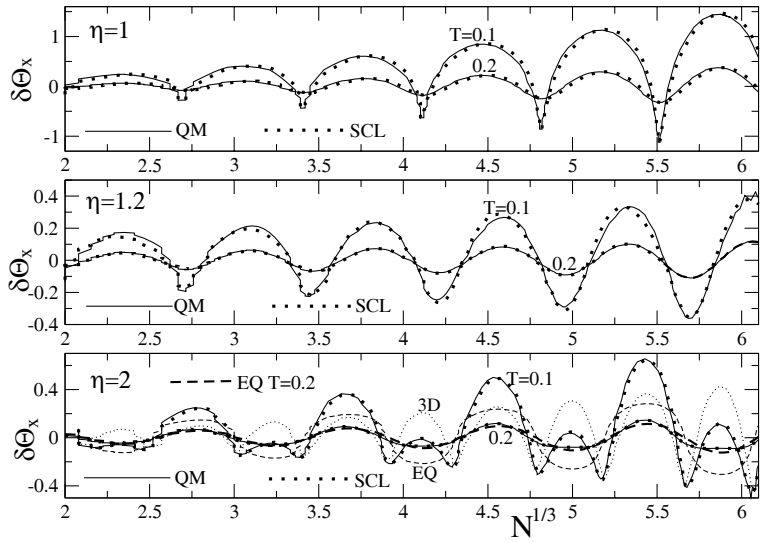

Fig. 2. Shell-structure moments of inertia $\delta\Theta_x$ (9), (16) - (20) (in units of $\hbar/\omega_0$) as functions of the particle number variable $N^{1/3}$ at temperatures $T = 0.1$ and 0.2 in units of $\hbar\omega_0$; 3D frequent dots show the contribution of 3D orbits; EQ thin dashed presents EQ orbit contribution for temperature $T = 0.1$; EQ thick dashed is the EQ orbit term for $T = 0.2$.

Fig. 2 shows a perfect agreement between the semiclassical and quantum results for the shell corrections $\delta\Theta_x$ to the moment of inertia for the same critical deformations η. From this Figure one can see a similar periodic-orbit structure for these bifurcation deformations because of $\delta\Theta_x \propto \delta F$. Again, one finds the same nice interference of the 3D and EQ orbit contributions to the shell corrections to the moment of inertia at $\eta = 2$. There is a well-known difference of the concave shape of parabolas-like minima for the λ dependence in Fig. 1 to a convex shape of maxima for the case of the particle-number variable $N^{1/3}$ in Fig. 2 because of the shell oscillations of $\lambda(N) = \tilde{\lambda} + \delta\lambda$ in the SCM, where $\tilde{\lambda}$ is the smooth chemical potential mentioned above. The exponential decrease with increasing temperature

T, owing to the temperature damping factor $Q(t_n T/\hbar)$ of Eq. (16), is clearly seen in this Figure. This corresponds approximately to the critical temperature value of the disappearance of shell effects in δF, $T_{cr} = \hbar\omega_{EQ}/\pi \sim \hbar\omega_0/\pi \approx 2-3$ MeV ($\eta > 1$) for particle numbers $N \approx 100-200$ in a heated Fermi system [8, 15] at large enough deformations η [$\hbar\omega_0 \approx (40/N^{1/3})$ MeV]. The critical temperature T_{cr} becomes slowly larger with increasing deformations η.

Conclusions

We analysed the shell-structure of the internal energy δE and free energy δF at finite temperature within the SCM by using an averaging over the chemical potential λ in terms of the shell components of both the level density and occupation numbers. These shell-structure energies are characteristic of heated Fermi systems near the Fermi surface. The POT expansions over periodic orbits of these energies are discussed for any potential well in relation with the well-known shell-structure components of the thermodynamical potential of the grand-canonical ensemble. A remarkable agreement is obtained for these POT expressions as functions of the chemical potential and particle number at critical deformations of the harmonic oscillator potential, as compared with the corresponding quantum results. We found a rather large effect in the difference of δE and δF owing to the entropy contribution $T\delta S$ even for temperatures much smaller than the distance between gross shells.

We found the relation of shell components of the collective moment of inertia to the free energy shell corrections for a Fermi system within the semiclassical approach based on the extended Gutzwiller POT. This relation was obtained via the rigid-body inertia shell corrections for statistically equilibrium rotation. For the particular case of the HO potential we have shown that it is exact, and in this sense, the condition of the statistically equilibrium rotation which leads to the rigid-body moment of inertia can be considered as a selfconsistency condition. The semiclassical shell components of the moments of inertia 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 these shell corrections at several critical bifurcation deformations and temperatures. The moment of inertia has the spherical limit of alignment of the individual-particle angular momenta along the symmetry axis. We confirmed the exponential decrease of all shell corrections with growing temperature at the same critical temperature T_{cr} as for the free-energy shell corrections.

It would be worth to apply the general ideas of this semiclassical theory to the shell corrections of the moments of inertia for the spheroid cavity and for the inertia parameter of the low-lying collective excitations in nuclear dynamics involving nuclei close to magic numbers [18, 20, 25, 26].

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Appendix A: Exact quantum solutions for harmonic oscillator

By using the standard transformation from the phase space variables κ, p_κ to the creation a_κ^+ and annihilation a_κ operators, $\kappa = x, y, z$, for the single-particle Routhian H_ω (1) one has [7]

$$H_\omega = \sum_\kappa \hbar\omega_k \left(a_\kappa^+ a_\kappa + 1/2\right) - \omega \ell_x, \qquad \text{(A1)}$$

where

$$\ell_x = \frac{\hbar}{2}\left[\frac{\omega_y + \omega_z}{\sqrt{\omega_y \omega_z}}\left(a_y a_z^+ + a_y^+ a_z\right) - \frac{\omega_y - \omega_z}{\sqrt{\omega_y \omega_z}}\left(a_y a_z + a_y^+ a_z^+\right)\right]. \qquad \text{(A2)}$$

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

$$\dot{\mathbf{A}}(\beta) = \mathcal{L}\mathbf{A}(\beta), \qquad \text{(A3)}$$

with the vector operator $\mathbf{A}(\beta)$ and a Liouville 4×4 matrix $\mathcal{L}$ (in $\hbar = 1$ units) given by

$$\mathbf{A}=\begin{pmatrix} a_y \\ a_y^+ \\ a_z \\ a_z^+ \end{pmatrix}, \qquad \mathcal{L}=\begin{pmatrix} -\omega_y & 0 & p & -q \\ 0 & \omega_y & q & -p \\ p & -q & -\omega_z & 0 \\ q & -p & 0 & \omega_z \end{pmatrix}, \qquad p=\frac{\omega}{2}\frac{\omega_y+\omega_z}{\sqrt{\omega_y\omega_z}}, \qquad q=\frac{\omega}{2}\frac{\omega_y-\omega_z}{\sqrt{\omega_y\omega_z}}. \tag{A4}$$

For the formal solution one finds

$$\mathbf{A}(\beta)=\Phi(\beta)\,\mathbf{A}(0), \quad \Phi(\beta)=e^{\beta\mathcal{L}}. \tag{A5}$$

Introducing the correlation matrix C,

$$C_{\nu\mu}=\left\langle A_\nu(\beta)A_\mu(0)\right\rangle=\left\langle A_\mu(0)A_\nu(0)\right\rangle, \tag{A6}$$

one may write the following system of equations for the $C_{\nu\mu}$:

$$\sum_\lambda\left[\Phi_{\nu\lambda}(\beta)-\delta_{\nu\lambda}\right]C_{\lambda\mu}=\mathcal{M}_{\nu\mu}, \tag{A7}$$

where $\mathcal{M}_{\nu\mu}$ is the antisymmetric matrix with $\mathcal{M}_{\nu\mu}=1$ for $\nu=2,\ \mu=1$ and $\nu=4,\ \mu=3$, and zeros otherwise in matrix $\mathcal{M}$, $\delta_{\nu\lambda}$ is the Kronecker symbol. Its formal solution for the correlation matrix C is given by

$$C=\mathcal{D}^{-1}\mathcal{M}, \qquad \mathcal{D}^{-1}=\left(\Phi(\beta)-I\right)^{-1}, \tag{A8}$$

with I being the 4×4 unit matrix. The Liouville operator $\mathcal{L}$ of (A4) has 4 eigenvalues for the Routhian H_ω (A1) [5],

$$\omega_\pm^2=\omega^2+\frac{\omega_y^2+\omega_z^2}{2}\pm\frac{\omega_y^2-\omega_z^2}{2}\sqrt{1+\frac{8\omega^2\left(\omega_y^2+\omega_z^2\right)}{\omega_y^2-\omega_z^2}}. \tag{A9}$$

According to Refs. [22, 23], as the Liouville matrix has 4 eigenvalues, the inverse matrix $\mathcal{D}^{-1}$ of (A8) can be approximated by the cubic polynomial under the conditions formulated there through its 4 unknown constants γ_ν,

$$\mathcal{D}^{-1}=\sum_{\nu=0}^{3}\gamma_\nu\mathcal{L}^\nu. \tag{A10}$$

These constants are defined by 4 linear equations:

$$\sum_{\nu=0}^{3}\gamma_\nu\ \omega_\pm^\nu=N_{\pm i}^\omega,$$

$$\sum_{\nu=0}^{3}(-1)^\nu\gamma_\nu\ \omega_\pm^\nu=-\left(N_{\pm i}^\omega+1\right),$$

$$N_{\pm i}^\omega=\left(e^{\beta\omega_\pm}-1\right)^{-1}, \tag{A11}$$

with the simple solutions

$$\gamma_0=-\frac{1}{2}, \quad \gamma_1=\frac{\left(N_{-i}^\omega+1/2\right)\omega_+^3-\left(N_{+i}^\omega+1/2\right)\omega_-^3}{\omega_-\omega_+\left(\omega_+^2-\omega_-^2\right)},$$

$$\gamma_2=0, \quad \gamma_3=\frac{\left(N_{+i}^\omega+1/2\right)\omega_--\left(N_{-i}^\omega+1/2\right)\omega_+}{\omega_-\omega_+\left(\omega_+^2-\omega_-^2\right)}. \tag{A12}$$

For instance, for relatively large β (small temperatures, $T/\hbar\omega_0\ll1$) one may use analytically the corresponding expansion in powers of a large $\beta\mathcal{L}$ and Eq. (A10) becomes the identity. Substituting (A12) into the inversed matrix $\mathcal{D}^{-1}$ (A10) we calculate explicitly the correlation matrix elements $C_{\nu\mu}$ (A8). After a lengthy derivation of the average of the single-particle angular momentum $\left\langle\ell_x\right\rangle_i$ in a state i through (A2) and

$$\omega\left\langle\ell_x\right\rangle_i=p\left(C_{14}+C_{23}\right)-q\left(C_{13}+C_{24}\right) \tag{A13}$$

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

$$\left\langle\ell_x\right\rangle_i=\omega\left[\frac{N_{-i}^\omega+1/2}{\omega_-}\left(2\frac{\omega_y^2+\omega_z^2}{\omega_+^2-\omega_-^2}-1\right)-\frac{N_{+i}^\omega+1/2}{\omega_+}\left(2\frac{\omega_y^2+\omega_z^2}{\omega_+^2-\omega_-^2}+1\right)\right], \tag{A14}$$

where $N_{\pm i}^\omega$ are the Bose temperature- and frequency-dependent distributions of (A11). By summation of (A14) over the single-particle states i one obtains a simple expression for the kinematic moment of inertia $\Theta_x(\omega)$ [5], for arbitrary frequency ω

$$\Theta_x(\omega)=\sum_i n_i^\omega\frac{\left\langle\ell_x\right\rangle_i}{\omega}=$$

$$=2\frac{\omega_y^2+\omega_z^2}{\omega_+^2-\omega_-^2}\left(\frac{\aleph_-^\omega}{\omega_-}-\frac{\aleph_+^\omega}{\omega_+}\right)-\left(\frac{\aleph_+^\omega}{\omega_+}+\frac{\aleph_-^\omega}{\omega_-}\right),$$

$$\aleph_\pm^\omega=\sum_i n_i^\omega N_{\pm i}^\omega. \tag{A15}$$

We emphasize that this expression can be, under the conditions of Refs. [22, 23], applied for finite temperatures $T = 1/\beta$ which appear through the oscillator Bose occupation numbers $N_{\pm i}^{\omega}$ in (A11). The dynamic moment of inertia of Eq. (3) is determined by the direct differentiation of (A14) with respect to ω. Both definitions of the moment of inertia lead to the same adiabatic expression, Eq. (5).

REFERENCES

1. *Inglis D.R.* Particle derivation of nuclear rotation properties associated with surface wave. // Phys. Rev. - 1954. - Vol. 96, No. 4. - P. 1059; Dynamics of nuclear deformation // Phys. Rev. - 1955. - Vol. 97, No. 3. - P. 701; Nuclear moments of inertia due to nucleon motion in a rotating well // Phys. Rev. - 1956. - Vol. 103, No. 6. - P. 1786.
2. *Bohr A., Mottelson B.R.* // Mat. Fys. Medd. Dan. Vid. Selsk. - 1955. - Vol. 30, No. 1.
3. *Bohr A., Mottelson B.R.* Nuclear Structure. Vol. II. - N.Y.: Benjamin, 1975.
4. *Pashkevich V.V., Frauendorf S.* Effect of the shell structure on the moment of inertia; Behavior of the averaged moment of inertia // Sov. J. Nucl. Phys. - 1975. - Vol. 20, No. 6. - P. 588.
5. *Zelevinsky V.G.* A simple model of a rapidly rotating nucleus // Sov. J. Nucl. Phys. - 1975. - Vol. 22, No. 6. - P. 1085.
6. *Mikhailov I.N., Neergard K., Pashkevich V.V., Frauendorf S.* Effect of rotation on the collective properties of atomic nuclei // Sov. J. Part. Nucl. - 1977. - Vol. 8. - P. 550.
7. *Afanasjev A.V., Fossan D.B., Lane G.J., Ragnarsson I.* Termination of rotation band: Disappearance of quantum many-body correlations // Phys. Rep. - 1999. - Vol. 322. - P. 1.
8. *Brack M., Bhaduri R.K.* Frontiers in Physics: Semi-classical Physics. - Boulder: Westview Press, 2003. – 458 p.
9. *Bencheikh K., Quentin P., Bartel J.* Rotations in nuclei - a semiclassical description // Nucl. Phys. A. - 1994. - Vol. 571. - P. 518.
10. *Equilibrium* deformations of rotating nuclei in a selfconsistent semiclassical approach / E. Chabanat, J. Meyer, K. Bencheikh, P. Quentin, J. Bartel // Phys. Lett. B. - 1994. - Vol. 325. - P.13.
11. *Strutinsky V.M.* Shell effects in nuclear masses and deformation energies // Nucl. Phys. A. - 1967. - Vol. 95, No. 2. - P. 420 - 442; Shells in deformed nuclei // Nucl. Phys. A. - 1968. - Vol. 122, No. 1. - P. 1.
12. *Funny* Hills: The shell-correction approach to nuclear shell effects and its application to the fission process / M. Brack, L. Damgard, A.S. Jensen., H.C. Pauli, V.M. Strutinsky, C.Y. Wong // Rev. Mod. Phys. - 1972. - Vol. 44. - P. 320.
13. *Kolomietz V.M., Magner A.G., Strutinsky V.M.* Shell effects in nuclei at large angular momenta // Sov. J. Nucl. Phys. - 1979. - Vol. 29. - P. 758.
14. *Gutzwiller M.* Chaos in Classical and Quantum Mechanics. - N.Y.: Springer-Verlag, 1990. - 432 p.
15. *Strutinsky V. M.* Semi-classical theory of nuclear shell structure // Nucleonika. - 1975. - Vol. 20, No. 7 - 8. - P. 679; *Strutinsky V.M., Magner A.G.* Semi-classical theory of nuclear shell structure // Sov. Phys. Part. Nucl. - 1976. - Vol. 7. - P. 356.
16. *Richter K., Ulmo D., Jalabert R. A.* Orbital magnetism in the ballistic regime: geometric effects // Phys. Rep. - 1996. - Vol. 276. - P. 1.
17. *Frauendorf S., Kolomietz V.M., Magner A.G., Sanzhur A.I.* Supershell structure of magnetic susceptibility // Phys. Rev. B. - 1998. - Vol. 58, No. 9. - P. 5622.
18. *Gross* shell structure at high spin in heavy nuclei / M.A. Deleplanque, S. Frauendorf, V.V. Pashkevich, S.Y. Chu, A. Unzhakova // Phys. Rev. C. - 2004. - Vol. 69. - P. 044309.
19. *Creagh S.C.* Trace formula for broken symmetry // Ann. Phys. (N.Y.). - 1996. - Vol. 248. - P. 60.
20. *Magner A.G., Vydrug-Vlasenko S.M., Hofmann H.* Gross-shell effects in nuclear response functions // Nucl. Phys. A. - 1991. - Vol. 524, No. 1. - P. 31.
21. *Gzhebinsky A.M., Magner A.G., Sitdikov A.S.* Semiclassical inertia for nuclear collective rotation // Nucl. Phys. At. Energy. - 2007. - No. 1 (19). - P. 17.
22. *Hantmaher F.P.* Theory of Matrixes. Vol. V. - Moscow: Nauka. - 1966.
23. *Smirnov V.I.* Course of the High Mathematics. Vol. III, part 2, sect. IV. - Moscow: Nauka. - 1974.
24. *Magner A.G.* Semi-classical analysis of the gross-shell structure in the deformed oscillator potential // Sov. J. Nucl. Phys. - 1978. - Vol. 28. - P. 764.
25. *Magner A.G., Gzhebinsky A.M., Fedotkin S.N.* Semiclassical inertia of nuclear collective dynamics // Phys. Atom. Nucl. - 2007. - Vol. 70, No. 4. - P. 647; Shell-structure inertia for slow collective motion // Phys. Atom. Nucl. - 2007. - Vol. 70, No. 11. - P. 1859.
26. *Gzhebinsky A.M., Magner A.G., Fedotkin S.N.* Low-lying collective excitations of nuclei as a semiclassical response // Phys. Rev. C. - 2007. - Vol. 76. - P. 064315, 16 p.

КВАЗІКЛАСИЧНА ОБОЛОНКОВА СТРУКТУРА МОМЕНТУ ІНЕРЦІЇ У НАГРІТИХ ФЕРМІ-СИСТЕМАХ

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Аналітично виведено момент інерції колективного обертання в рамках кренкінг-моделі у випадку гамільтоніана гармонічного осцилятора для будь-яких частот при скінчених температурах. За допомогою теорії періодичних орбіт отримано співвідношення квазікласичних оболонкових поправок до моменту інерції та вільної енергії через оболонковий компонент твердотільного моменту інерції статистично рівноважного

обертання нагрітих Фермі-систем. Їх аналітична структура, виражена через екваторіальні і 3-мірні періодичні орбіти в аксіально-симетричному потенціалі гармонічного осцилятора, знаходиться в доброму узгодженні з квантовими результатами при критичних деформаціях і температурах.

Ключові слова: модель примусового обертання ядер, момент інерції, теорія періодичних орбіт, оболонкові поправки до енергії, потенціал гармонічного осцилятора.

КВАЗИКЛАССИЧЕСКАЯ ОБОЛОЧЕЧНАЯ СТРУКТУРА МОМЕНТА ИНЕРЦИИ В НАГРЕТЫХ ФЕРМИ-СИСТЕМАХ

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Аналитически выведен момент инерции коллективного вращения в рамках кренкинг-модели в случае гамильтониана гармонического осциллятора для любых частот при конечных температурах. С помощью теории периодических орбит получено соотношение квазиклассических оболочечных поправок к моменту инерции и свободной энергии через оболочечный компонент твердотельного момента инерции статистически равновесного вращения нагретых Ферми-систем. Их аналитическая структура, выраженная через экваториальные и 3-мерные периодические орбиты в аксиально-симметрическом потенциале гармонического осциллятора, находится в хорошем согласии с квантовыми результатами при критических деформациях и температурах.

Ключевые слова: модель принудительного вращения ядра, момент инерции, теория периодических орбит, оболочечные поправки к энергии, потенциал гармонического осциллятора.

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