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Analytical relationship for the cranking inertia

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Abstract. The wave functions of a spheroidal harmonic oscillator without spin-orbit interaction are expressed in terms of associated Laguerre and Hermite polynomials. The pairing gap and Fermi energy are found by solving the BCS system of two equations. Analytical relationships for the matrix elements of inertia are obtained as a function of the main quantum numbers and potential derivative. They may be used to test complex computer codes developed in a realistic approach of the fission dynamics. Results given for the ^{240}Pu nucleus are compared with a hydrodynamical model. The importance of taking into account the correction term due to the variation of the occupation number is stressed.

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1 Introduction

By studying fission dynamics [1] one can estimate the value of the disintegration constant λ of the exponential decay law expressing the variation in time of the number of decaying nuclei. The partial decay half-life T is given by $T = \tau \ln 2 = 0.693147/\lambda$. The potential energy surface in a multi-dimensional hyperspace of deformation parameters $\beta_1, \beta_2, \ldots, \beta_n$ gives the generalized forces acting on the nucleus. Information concerning how the system reacts to these forces is contained in a tensor of inertial coefficients, or the effective-mass parameters $\{B_{ij}\}$. Unlike the potential energy $E = E(\beta)$ which depends on the nuclear shape, the kinetic energy is determined by the contribution of the shape change expressed by

$$E_k = \frac{1}{2}\sum_{i,j=1}^{n} B_{ij}(\beta)\frac{\mathrm{d}\beta_i}{\mathrm{d}t}\frac{\mathrm{d}\beta_j}{\mathrm{d}t}\,, \tag{1}$$

where B_{ij} is the inertia tensor. In a phenomenological approach based on incompressible irrotational flow, the value of an effective mass B^{irr} is usually close to the reduced mass $\mu = (A_1A_2/A)M$ in the exit channel of the binary system. Here M is the nucleon mass. One may use the Werner-Wheeler approximation [2].

The microscopic (cranking) model introduced by Inglis [3] leads to much larger values of the inertia. By assuming the adiabatic approximation, the shape variations are slower than the single-particle motion. According to the cranking model, after including the BCS pairing correlations [4,5], the inertia tensor is given by [6,7]

$$B_{ij} = 2\hbar^2\sum_{\nu\mu}\frac{\langle\nu|\partial H/\partial\beta_i|\mu\rangle\langle\mu|\partial H/\partial\beta_j|\nu\rangle}{(E_\nu+E_\mu)^3}(u_\nu v_\mu + u_\mu v_\nu)^2 + P_{ij}, \tag{2}$$

where H is the single-particle Hamiltonian allowing to determine the energy levels and the wave functions $|\nu\rangle$, u_ν, v_ν are the BCS occupation probabilities, E_ν is the quasiparticle energy, and P_{ij} gives the contribution of the occupation number variation when the deformation is changed (terms including variation of the gap parameter, Δ, and Fermi energy, λ, $\partial\Delta/\partial\beta_i$ and $\partial\lambda/\partial\beta_i$):

$$\begin{aligned} P_{ij} = \frac{\hbar^2}{4}\sum_{\nu}\frac{1}{E_\nu^5}\Bigg[&\Delta^2\frac{\partial\lambda}{\partial\beta_i}\frac{\partial\lambda}{\partial\beta_j} \\ &+(\epsilon_\nu-\lambda)^2\frac{\partial\Delta}{\partial\beta_i}\frac{\partial\Delta}{\partial\beta_j} + \Delta(\epsilon_\nu-\lambda)\left(\frac{\partial\lambda}{\partial\beta_i}\frac{\partial\Delta}{\partial\beta_j}+\frac{\partial\lambda}{\partial\beta_j}\frac{\partial\Delta}{\partial\beta_i}\right) \\ &-\Delta^2\left(\frac{\partial\lambda}{\partial\beta_i}\langle\nu|\partial H/\partial\beta_j|\nu\rangle + \frac{\partial\lambda}{\partial\beta_j}\langle\nu|\partial H/\partial\beta_i|\nu\rangle\right) \\ &-\Delta(\epsilon_\nu-\lambda)\left(\frac{\partial\Delta}{\partial\beta_i}\langle\nu|\partial H/\partial\beta_j|\nu\rangle + \frac{\partial\Delta}{\partial\beta_j}\langle\nu|\partial H/\partial\beta_i|\nu\rangle\right)\Bigg]. \end{aligned}$$

Similar to the shell correction energy, the total inertia is the sum of contributions given by protons and neutrons, $B = B_p + B_n$. The denominator in eq. (2) is minimum for the levels in the neighbourhood of the Fermi energy. A large value of inertia is the result of a large density of levels at the Fermi surface. As a result, in a similar way to

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the shell corrections, one can observe large fluctuations of B_{ii} when the deformation or the number of particles are changed.

In the present work we consider a single-particle model of a spheroidal harmonic oscillator without spin-orbit interaction for which the cranking approach allows to obtain analytical relationships of the nuclear inertia. Despite the limited interest of this simple single-particle model, the result of the present work may be used to test complex computer codes developed in a realistic treatment of the fission dynamics based on the deformed two-center shell model [8]. The results illustrated for the ^{240}Pu nucleus are compared with a hydrodynamical model.

2 Spheroidal harmonic oscillator

The shape of a spheroid with semiaxes a, c (c is the semiaxis along the symmetry) expressed in units of the spherical radius $R_0 = r_0 A^{1/3}$ may be determined by a single deformation coordinate which can be the quadrupolar deformation [9] $\varepsilon = 3(c-a)/(2c+a)$. The two oscillator frequencies are expressed as

$$\omega_\perp(\varepsilon) = \omega_0\left(1+\frac{\varepsilon}{3}\right), \qquad \omega_z(\varepsilon) = \omega_0\left(1-\frac{2\varepsilon}{3}\right), \tag{3}$$

and by taking into account the condition of the volume conservation $\omega_\perp^2\omega_z = (\omega_0^0)^3$, where $\hbar\omega_0^0 = 41A^{-1/3}$ MeV, the eigenvalues [1] in units of $\hbar\omega_0^0$ are given by

$$\epsilon_i = [N+3/2+\varepsilon(n_\perp-2N/3)][1-\varepsilon^2(1/3+2\varepsilon/27)]^{-1/3} \tag{4}$$

in which the quantum numbers $n_\perp$ and n_z are non-negative integers. Their summation gives the main quantum number $N = n_\perp + n_z$.

In a system of cylindrical coordinates (ρ, φ, z) the wave function [10,11] can be written as a product of the eigenfunctions

$$\psi_{n_r}^m(\rho) = \frac{\sqrt{2}}{\alpha_\perp} N_{n_r}^m \eta^{\frac{|m|}{2}} e^{-\frac{\eta}{2}} L_{n_r}^{|m|}(\eta) = \frac{\sqrt{2}}{\alpha_\perp}\psi_{n_r}^m(\eta), \tag{5}$$

$$\psi_{n_z}(z) = \frac{1}{\sqrt{\alpha_z}} N_{n_z} e^{-\frac{\xi^2}{2}} H_{n_z}(\xi) = \frac{1}{\sqrt{\alpha_z}}\psi_{n_z}(\xi), \tag{6}$$

$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}, \tag{7}$$

where $L_{n_r}^{|m|}$ are the associated (or generalized) Laguerre polynomials and H_{n_z} are the Hermite polynomials. The variables η and ξ are defined by $\eta = \rho^2/\alpha_\perp^2$, $\xi = z/\alpha_z$, where $\alpha_\perp = \sqrt{\hbar/M\omega_\perp} \approx A^{1/6}\sqrt{\omega_0^0/\omega_\perp}$, $\alpha_z = \sqrt{\hbar/M\omega_z} \approx A^{1/6}\sqrt{\omega_0^0/\omega_z}$. The normalization constants

$$(N_{n_r}^m)^2 = \frac{n_r!}{(n_r+|m|)!}, \quad (N_{n_z})^2 = \frac{1}{\sqrt{\pi}2^{n_z}n_z!} \tag{8}$$

are obtained from the orthonormalization conditions.

3 Nuclear inertia

By ignoring the spin-orbit coupling, the Hamiltonian of the harmonic spheroidal oscillator contains the kinetic energy and the potential energy term, V:

$$V = \frac{1}{2}\hbar\omega_\perp\eta + \frac{1}{2}\hbar\omega_z\xi^2 = \frac{\hbar\omega_0^0\left[(3+\varepsilon)\eta + (3-2\varepsilon)\xi^2\right]}{2[27-\varepsilon^2(9+2\varepsilon)]^{1/3}}. \tag{9}$$

Now we are making some changes in eq. (2), first of all replacing the deformation β by ε.

One may assume [6,7,10] that only the leading term of the Hamiltonian, namely the potential written above, contributes essentially to the derivative,

$$\frac{\mathrm{d}H}{\mathrm{d}\varepsilon} \simeq \frac{\mathrm{d}V}{\mathrm{d}\varepsilon}. \tag{10}$$

The contribution of P_{ij}, denoted by P_ε for a system with one deformation coordinate, sometimes assumed to be negligibly small, will be discussed in the last section.

The derivative is written as

$$\frac{1}{\hbar\omega_0^0}\frac{\mathrm{d}V}{\mathrm{d}\varepsilon} = \frac{3}{2}\left[f_1(\varepsilon)\eta + f_2(\varepsilon)\xi^2\right] \tag{11}$$

in which

$$f_1 = \frac{\varepsilon(\varepsilon+6)+9}{[27-\varepsilon^2(9+2\varepsilon)]^{4/3}}, \tag{12}$$

$$f_2 = 2\frac{\varepsilon(2\varepsilon+3)-9}{[27-\varepsilon^2(9+2\varepsilon)]^{4/3}}. \tag{13}$$

For a single deformation parameter the inertia tensor becomes a scalar B_ε whith a summation in eq. (2) performed for all states ν, μ taken into consideration in the pairing interaction.

In order to solve the problem of the pairing interaction [12], we consider the set of doubly degenerate energy levels $\{\epsilon_i\}$ expressed in units of $\hbar\omega_0^0$. Calculations for neutrons are similar to those for protons, hence for the moment we shall consider only protons.

In the absence of a pairing field, the first $Z/2$ levels are occupied, among a total number of n_t levels available. Only few levels below (n) and above (n') the Fermi energy are contributing to the pairing correlations. Usually $n' = n$. If $\tilde{g_s}$ is the density of states at Fermi energy obtained from the shell correction calculation $\tilde{g_s} = \mathrm{d}Z/\mathrm{d}\epsilon$, expressed in number of levels per $\hbar\omega_0^0$ spacing, the level density is half this quantity: $\tilde{g_n} = \tilde{g_s}/2$. We can choose as computing parameter, the cut-off energy (in units of $\hbar\omega_0^0$), $\Omega \simeq 1 \gg \tilde{\Delta}$. Let us take the integer part of $\Omega\tilde{g_s}/2 = n = n'$. When from calculation we get $n > Z/2$, we shall take $n = Z/2$ and, similarly, if $n' > n_t - Z/2$, we consider $n' = n_t - Z/2$.

The gap parameter $\Delta = |G|\sum_k u_k v_k$ and the Fermi energy with pairing correlations λ (both in units of $\hbar\omega_0^0$)

are obtained as solutions of a nonlinear system of two BCS equations:

$$n' - n = \sum_{k=k_i}^{k_f} \frac{\epsilon_k - \lambda}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}}\,, \tag{14}$$

$$\frac{2}{G} = \sum_{k=k_i}^{k_f} \frac{1}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}}\,, \tag{15}$$

with $k_i = Z/2 - n + 1$; $k_f = Z/2 + n'$.

The pairing interaction G is calculated from a continuous distribution of levels leading to $2/G \simeq 2\tilde{g}(\tilde{\lambda}) \ln 2\Omega/\tilde{\Delta}$, where $\tilde{\lambda}$ is the Fermi energy deduced from the shell correction calculations [13] and $\tilde{\Delta}$ is the gap parameter, obtained from a fit to experimental data, usually taken as $\tilde{\Delta} = 12/\sqrt{A}\hbar\omega_0^0$. The system can be solved numerically by the Newton-Raphson method. Solutions around magic numbers, when $\Delta \to 0$, have been derived by Kumar *et al.* [14].

As a consequence of the pairing correlation, the levels situated below the Fermi energy are only partially filled, while those above the Fermi energy are partially empty; there is a given probability, v_k, for each level to be occupied by a quasiparticle or by a hole, u_k, given by

$$v_k^2 = \frac{1}{2}\left[1 - \frac{\epsilon_k - \lambda}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}}\right]\,, \qquad u_k^2 = 1 - v_k^2\,. \tag{16}$$

The following relationship allows to calculate the effective mass, $\frac{\hbar\omega_0^0}{\hbar^2}B_\varepsilon$, in units of $\hbar^2/(\hbar\omega_0^0)$:

$$\frac{9}{2}\sum_{\nu\mu} \frac{\langle\nu|f_1\eta + f_2\xi^2|\mu\rangle\langle\mu|f_1\eta + f_2\xi^2|\nu\rangle}{(E_\nu + E_\mu)^3}(u_\nu v_\mu + u_\mu v_\nu)^2\,. \tag{17}$$

Matrix elements are calculated by performing some integrals,

$$\begin{aligned}
&\langle n_z' n_r' m'|f_1(\varepsilon)\eta + f_2(\varepsilon)\xi^2|n_z n_r m\rangle = \\
&\delta_{m'm} N_{n_r'}^m N_{n_r}^m N_{n_z'} N_{n_z} \\
&\quad\times\left[f_1 \int_0^\infty \mathrm{d}\eta \eta^{|m|+1} e^{-\eta} L_{n_r'}^{|m|}(\eta) L_{n_r}^{|m|}(\eta)\right. \\
&\quad\times\int_{-\infty}^\infty \mathrm{d}\xi e^{-\xi^2} H_{n_z'}(\xi) H_{n_z}(\xi) \\
&\quad+f_2 \int_0^\infty \mathrm{d}\eta \eta^{|m|} e^{-\eta} L_{n_r'}^{|m|}(\eta) L_{n_r}^{|m|}(\eta) \\
&\quad\times\left.\int_{-\infty}^\infty \mathrm{d}\xi \xi^2 e^{-\xi^2} H_{n_z'}(\xi) H_{n_z}(\xi)\right].
\end{aligned}$$

Next we can use the relationships [15] leading eventually to an important diagonal contribution $\frac{\hbar\omega_0^0}{\hbar^2}B_{\varepsilon 1}$,

$$\begin{aligned}
&\frac{9}{4}\delta_{n_r' n_r}\delta_{m'm}\sum_{\nu=k_i}^{k_f}\left[f_1(2n_r + |m| + 1)\right. \\
&\qquad\left.+f_2\left(n_z + \frac{1}{2}\right)\right]^2 \frac{(u_\nu v_\nu)^2}{E_\nu^3}\delta_{n_z' n_z}
\end{aligned} \tag{18}$$

and two nondiagonal terms, $\frac{\hbar\omega_0^0}{\hbar^2}B_{\varepsilon 2}$ and $\frac{\hbar\omega_0^0}{\hbar^2}B_{\varepsilon 3}$:

$$\begin{aligned}
&\frac{9}{4}\delta_{n_r' n_r}\delta_{m'm}\sum_{\nu\neq\mu}\frac{f_2^2}{2}(n_z + 1)(n_z + 2) \\
&\qquad\times\frac{(u_\nu v_\mu + u_\mu v_\nu)^2}{(E_\nu + E_\mu)^3}\delta_{n_z' n_z + 2}\,,
\end{aligned} \tag{19}$$

$$\frac{9}{4}\delta_{n_r' n_r}\delta_{m'm}\sum_{\nu\neq\mu}\frac{f_2^2}{2}(n_z - 1)n_z\frac{(u_\nu v_\mu + u_\mu v_\nu)^2}{(E_\nu + E_\mu)^3}\delta_{n_z' n_z - 2}\,, \tag{20}$$

where k_i and k_f have been defined above. In order to perform the summations of the nondiagonal terms for a state with a certain ν (specified quantum numbers $n_z n_r m$) one has to consider only the states with $\mu \neq \nu$ and $n_r' = n_r$; $m' = m$ for which $n_z' = n_z + 2$ or $n_z' = n_z - 2$, respectively. Finally, one arrives at the nuclear inertia in units of $\hbar^2$/MeV by adding the three terms and dividing by $\hbar\omega_0^0$.

There are several hydrodynamical formulae [16] of the mass parameters. For a spherical liquid drop with a radius $R_0 = 1.2249A^{1/3}$ fm one has

$$B^{\mathrm{irr}}(0) = \frac{2}{15}MAR_0^2 = 0.0048205A^{5/3}\ \frac{\hbar^2}{\mathrm{MeV}}\,. \tag{21}$$

When the spheroidal deformation is switched on it becomes

$$B_\varepsilon^{\mathrm{irr}}(\varepsilon) = B^{\mathrm{irr}}(0)\frac{81}{[27 - \varepsilon^2(9 + 2\varepsilon)]^{4/3}}\frac{9 + 2\varepsilon^2}{(3 - 2\varepsilon)^2}\,. \tag{22}$$

The main result of the present study is represented by eqs. (18)-(20), which could be used to test complex computer codes developed for realistic single-particle levels, for which it is not possible to obtain analytical relationships. The nuclear inertia of ^{240}Pu calculated with eq. (21) for a spherical liquid drop and with eq. (22) for spheroidal shapes is illustrated in fig. 1. One can see how $B^{\mathrm{irr}}(0)$ increases when the mass number of the nucleus is increased. The irrotational value $B_\varepsilon^{\mathrm{irr}}(\varepsilon)$ monotonously increases with the spheroidal deformation parameter ε. Due to the fact that in this single-center model the nucleus only became longer without developing a neck and never arriving at a scission configuration when the deformation is increased, the reduced mass is not reached as it should be in a two-center model [2].

The cranking inertia of the spheroidal harmonic oscillator calculated by using the analytical relationships (18)-(20) and the correction given in the next section shows very pronounced fluctuations which are correlated to the shell corrections (calculated with the macroscopic-microscopic method [13]) plotted at the bottom of fig. 1.

4 Variation of the gap parameter and Fermi energy with deformation

In fig. 2 we plotted the variation with deformation of the solutions of BCS equations for Fermi energy λ (bottom)

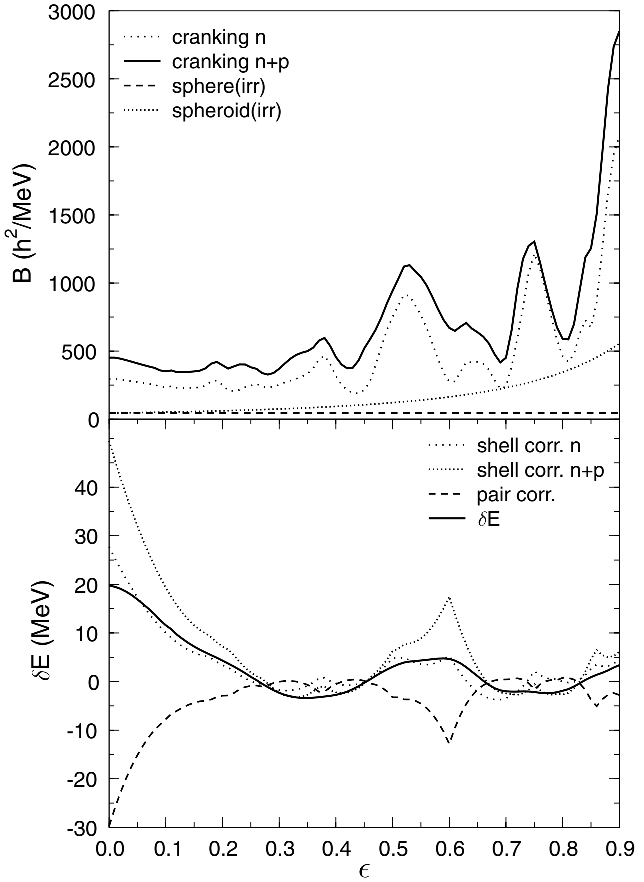

Fig. 1. Top: comparison of the effective mass (in units of $\hbar^2$/MeV) calculated by using the cranking model for the proton plus neutron level schemes, only for neutrons, as well as for the irrotational spheroidal and spherical shapes of ^{240}Pu. Bottom: shell corrections for neutrons and protons, only for neutrons, pairing corrections, and shell plus pairing corrections.

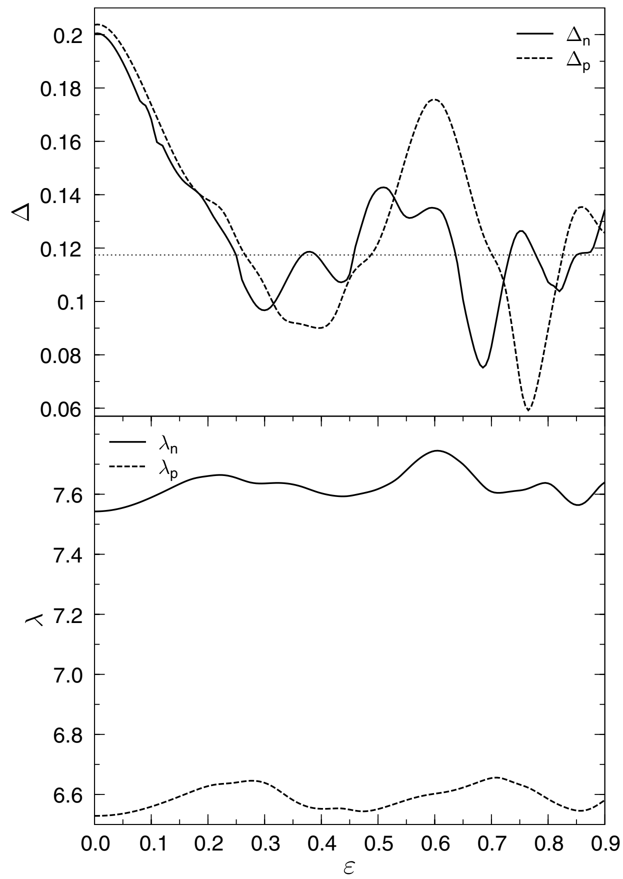

Fig. 2. The variation with deformation of the solutions of BCS equations for Fermi energy λ (bottom) and the gap parameter Δ (top) of the proton and neutron level schemes for the ^{240}Pu nucleus. The energies are expressed in units of $\hbar\omega_0^0 = 6.597$ MeV. The dotted line in the upper part corresponds to $\tilde{\Delta} = 0.117$.

and the gap parameter Δ (top) of the proton and neutron level schemes for the ^{240}Pu nucleus. The dotted line at the value 0.117 corresponds to $\tilde{\Delta}$. Their derivatives with respect to the deformation parameter are given in fig. 3. For superdeformed nuclei with $\varepsilon > 0.5$ the oscilllation amplitudes of $\mathrm{d}\lambda_n/\mathrm{d}\varepsilon$ approach their maximum values of about 2 units. In the same range of deformations the inertia is also larger as a result of the increased density of levels at the Fermi surface.

Now we can calculate the correction term as

$$P_\varepsilon = \frac{2\hbar^2}{8}\sum_\nu \frac{1}{E_\nu^5}\Bigg[\left(\Delta\frac{\mathrm{d}\lambda}{\mathrm{d}\varepsilon}\right)^2 + (\epsilon_\nu-\lambda)^2\left(\frac{\mathrm{d}\Delta}{\mathrm{d}\varepsilon}\right)^2 + 2\Delta(\epsilon_\nu-\lambda)\frac{\mathrm{d}\lambda}{\mathrm{d}\varepsilon}\frac{\mathrm{d}\Delta}{\mathrm{d}\varepsilon} - 2\Delta^2\frac{\mathrm{d}\lambda}{\mathrm{d}\varepsilon}\langle\nu|\mathrm{d}V/\mathrm{d}\varepsilon|\nu\rangle - 2\Delta(\epsilon_\nu-\lambda)\frac{\mathrm{d}\Delta}{\mathrm{d}\varepsilon}\langle\nu|\mathrm{d}V/\mathrm{d}\varepsilon|\nu\rangle\Bigg].$$

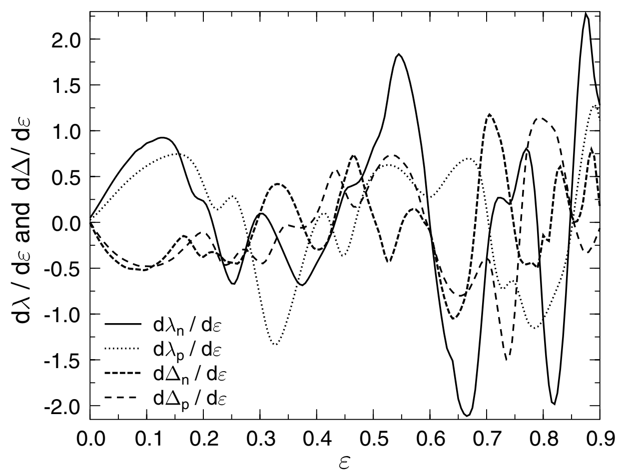

Fig. 3. The derivatives with respect to deformation of the solutions of BCS equations for Fermi energy λ and the gap parameter Δ of the proton and neutron level schemes for the ^{240}Pu nucleus. The energies are expressed in units of $\hbar\omega_0^0 = 6.597$ MeV.

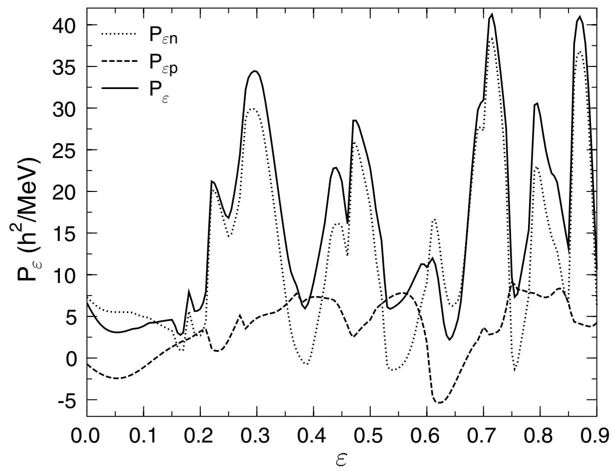

Fig. 4. Contribution, P_ε, to the mass parameter of the occupation number variation with deformation for the ^{240}Pu nucleus expressed in units of $\hbar^2$/MeV.

The result displayed in fig. 4 shows the important contribution of the neutron level scheme, $P_{\varepsilon n}$ (dotted line), reflecting the larger density of states at the Fermi energy, compared to the proton term $P_{\varepsilon p}$ (dashed line). Their sum is a positive quantity, contributing to an increase of the nuclear inertia. In a dynamical investigation using the quasiclassical WKB approximation, the quantum tunnelling penetrability depends exponentially on the action integral, in which the integral contains a square root of the product of mass parameter and deformation energy. This exponential dependence amplifies very much any variation of the inertia. Consequently, the term P_{ij} should be considered in calculations. A similar conclusion was drawn from a study of a realistic two-center shell model [17].

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