Shell energy and the level-density parameter of hot nuclei

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Macroscopic-microscopic calculations have been performed with the Yukawa folded mean field for 134 spherical even-even nuclei and 6 deformed ones at temperatures $0 \leqslant T \leqslant 5$ MeV and elongations ranging from oblate shapes to the scission configuration of fissioning nuclei. The Strutinsky type free-energy shell corrections for this sample of nuclei and their temperature and deformation dependence are found by a folding procedure in particle-number space. The average dependence of the single-particle level-density parameter on mass number A and isospin I is determined and compared with previous estimates obtained using the relativistic mean-field theory, the Hartree-Fock approximation with the Skyrme effective interaction, and the phenomenological Thomas-Fermi approach adjusted to experimental data. The estimates for the level-density parameter obtained for different deformations are fitted by a liquid-drop type expression.

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I. INTRODUCTION

The nuclear single-particle (s.p.) level-density parameter plays a crucial role in transport theories dealing with the fission dynamics or the decay of compound nuclei (confer, e.g., Refs. [1–3]). The aim of the present article is to determine this quantity as well as the temperature dependence of the shell energy for high excited nuclei ($T \leqslant 5$ MeV). The macroscopic-microscopic method [4] with the Yukawa folded mean-field potential [5] and the Lublin-Strasbourg Drop (LSD) model [6] as well as the new Strutinsky shell-correction method [7] has been used in the present study. In Ref. [8] we have already studied the mass-number and isospin dependence of the s.p. level-density parameter obtained for spherical nuclei in the relativistic mean-field theory (RMFT) [9] with the NL3 parameter set [10] and in Ref. [11] with the Skyrme SkM* effective interaction [12].

In these previous studies [8,13], to which the present investigation represents a substantial improvement and extension, the traditional Strutinsky shell-correction method [14] was used to extract the shell effects from the RMFT self-consistent energies in a way similar to Refs. [15–17] for the Gogny Hamiltonian with the D1S force [18]. To obtain the shell-correction energy at finite temperature the phenomenological expression of Refs. [19,20] for its variation with temperature was used rather than to evaluate the Strutinsky shell-correction energy at finite temperatures [21]. Similarly as in Ref. [22], the s.p. level-density parameter was approximated in Refs. [23,24], where the investigation was based on the RMFT-NL3 model by a liquid-drop type expression. In Ref. [25] the latest version of the Strutinsky smoothing method based on the $\mathcal{N}$-folding method [7] was used to evaluate the smoothed s.p. free energy at finite temperatures. The same method was also applied in Ref. [11] to extract the level-density parameter from self-consistent Hartree-Fock calculation with the Skyrme SkM* force. All these results were restricted to spherical even-even nuclei and the dependence of the single-particle level-density parameter on deformation was not investigated. One has also to realize that the self-consistent models have systematically underestimated the s.p. level density as compared to the phenomenological Thomas-Fermi approach [26], which was adjusted to the experimental data, as shown in Fig. 3 below. That is why, in the present investigation, we decided to apply our method to the s.p. level scheme obtained with a Yukawa folded [5] (YF) mean-field potential. The same sample of spherical even-even nuclei was used and it turns out that the level-density parameter obtained in this way is, indeed, much closer to the phenomenological data (Fig. 3) than all previous self-consistent estimates. Encouraged by these results we have performed an additional study of the deformation dependence of the level-density parameter obtained with the YF model.

II. NUCLEAR ENERGY

In the macroscopic-microscopic method [4] the nuclear energy consists of the macroscopic part, e.g., of liquid drop type and the shell and pairing corrections. It is well known that the pairing correlations disappear at temperature of the order of $T \approx 1$ MeV. That is why we have decided not to include them in our investigation as we are rather interested in hot nuclei. The microscopic corrections are then simply given by

$$E_{\mathrm{micr}} = E^{(p)}_{\mathrm{shell}} + E^{(n)}_{\mathrm{shell}}. \tag{1}$$

This shell-correction energy is obtained as the difference between the sum of occupied s.p. energies and the corresponding sum obtained by a *smoothing* procedure [14]. Until quite recently this smoothing was always accomplished by applying the traditional Strutinsky method in which one performs a Gauss-Hermite folding in the space of the single-particle energies (the so-called e-folding) [14] using the s.p. spectra obtained within one of the phenomenological mean-field potentials, as, e.g., of Nilsson [27], Woods-Saxon [28], or Yukawa-folded [5] type. The new method consists in a folding in the particle-number space (the so-called $\mathcal{N}$-folding) [7] and allows, in fact, smoothing of any quantity that fluctuates with

the number of particles, as, e.g., the free energy at different temperatures. In the ground state (i.e., for zero temperature) the shell energy is defined by the following expression

$$E^{(q)}_{\rm shell} = \sum_{\nu_{\rm occ}} \varepsilon^{(q)}_{\nu} - \tilde{E}^{(q)}, \qquad q = \{n, p\}, \tag{2}$$

where $\tilde{E}^{(q)}$ is the smoothed sum of s.p. energies obtained, e.g., by the $\mathcal{N}$-smoothing approach of Ref. [7] applied to the Yukawa folded single-particle levels.

III. YUKAWA-FOLDED POTENTIAL

The Yukawa-folded [5] single-particle potential $V_{\rm sp}$ contains the central mean-field $V_{\rm cent}$, as well as a spin-orbit potential $V_{\rm so}$ and, in the case of protons, a Coulomb field $V_{\rm Coul}$

$$V^{(q)}_{\rm sp}(\vec{r}\,) = V^{(q)}_{\rm cent}(\vec{r}\,) + V^{(q)}_{\rm so}(\vec{r}\,) + V_{\rm Coul}(\vec{r}\,)\delta_{pq}, \tag{3}$$

where $q = \{n, p\}$. The central potential is given by the volume integral

$$V_{\rm cent}(\vec{r}_1) = \int V(r_{12}) \frac{\rho(\vec{r}_2)}{\rho_0}\, d^3r_2, \tag{4}$$

where $r_{12} = |\vec{r}_1 - \vec{r}_2|$, ρ is the diffuse density of the nucleus, and $V(r_{12})$ is the folding potential, which is [5]

$$V(r_{12}) = V^{(q)}_0\, g_\lambda(\vec{r}_1, \vec{r}_2). \tag{5}$$

Here $V^{(q)}_0$ is the strength of the interaction that can be chosen differently for protons and neutrons and the Yukawa folding function

$$g_\lambda(\vec{r}_1, \vec{r}_2) = \frac{1}{4\pi\lambda^2} \frac{e^{-|\vec{r}_1 - \vec{r}_2|/\lambda}}{|\vec{r}_1 - \vec{r}_2|} \tag{6}$$

of width λ is normalized to unity

$$\int g_\lambda(\vec{r}_1, \vec{r}_2) d^3r_2 = 1. \tag{7}$$

The diffuse density $\rho(\vec{r}_2)$ is again obtained by a folding procedure using the same Yukawa function but with a slightly different width parameter d:

$$\rho(\vec{r}_2) = \int \rho_0(\vec{r}_1) g_d(\vec{r}_1, \vec{r}_2) d^3r_1, \tag{8}$$

where the uniform density of the nucleus ρ_0 is given by

$$\rho_0(\vec{r}\,) = \begin{cases} \rho_0 = 3A/4\pi R_0^3 & \text{for } r \leqslant R_0 \\ 0 & \text{for } r > R_0 \end{cases} \tag{9}$$

and R_0 is the radius of the corresponding spherical nucleus.

The Coulomb potential $V_{\rm Coul}$ is calculated assuming a uniform charge distribution in the nucleus

$$V_{\rm Coul}(\vec{r}_1) = \frac{3eZ}{4\pi R_0} \int_V \frac{d^3r_2}{|\vec{r}_1 - \vec{r}_2|}\,, \tag{10}$$

whereas the spin-orbit term is obtained from the central potential $V_{\rm cent}$ using the standard prescription

$$V_{\rm so} = i\Lambda^{(q)} \vec{\nabla} V_{\rm cen} \cdot [\vec{\sigma} \times \vec{\nabla}\,], \qquad q = \{n, p\}, \tag{11}$$

where $\vec{\sigma}$ is the vector of 2×2 Pauli matrices.

TABLE I. Constants used in the Yukawa-folding procedure.

Constant	Value	Unit	Constant	Value	Unit
λ	0.8	fm	d	0.7	fm
V_s	52.5	MeV	V_a	48.7	MeV
C_{1p}	2.76×10^{-4}	MeV	C_{2p}	0.3092	MeV
C_{1n}	2.07×10^{-4}	MeV	C_{2n}	0.3479	MeV
D_1	1.117×10^{-2}		D_2	3.15	

The following parameters of the single-particle potentials for protons and neutrons [31] were used:

$$V^{(p)}_{\rm o} = V_s + V_a\,\bar{\delta} \qquad \text{and} \qquad V^{(n)}_{\rm o} = V_s - V_a\,\bar{\delta}\,, \tag{12}$$

where

$$\bar{\delta} = \frac{I + D_1 Z^2/A^{5/3}}{1 + D_2/A^{1/3}}, \qquad I = \frac{N - Z}{A} \tag{13}$$

and

$$\Lambda^{(p)} = C_{1p}A + C_{2p} \qquad \text{and} \qquad \Lambda^{(n)} = C_{1n}A + C_{2n} \tag{14}$$

with the appropriate constants listed in Table I above.

IV. THE PARTICLE-NUMBER CONSERVING SHELL-CORRECTION METHOD

The shell energy is the difference between the sum of occupied single-particle energies and its smoothed value $\tilde{E}^{(q)}(\mathcal{N}_q)$ corresponding to the number $\mathcal{N}_q$ of particles of species $q(q = \{n, p\})$, which is obtained by a folding procedure in the particle number space ($\mathcal{N}$ space). To perform the smearing procedure one has to define a set of quantities S_n corresponding to different particle numbers n but built on the same single-particle energy spectrum

$$S_n = \sum_{\nu=1}^{n} \varepsilon_\nu - bn^{4/3} - V'n, \tag{15}$$

from which the harmonic oscillator *background* is subtracted to keep the quantities S_n small. The parameters b and V' in the above expression are obtained by minimizing the mean-square deviations:

$$\sum_{n=\mathcal{N}_{\rm min}}^{\mathcal{N}_{\rm max}} {S_n}^2 = \min, \tag{16}$$

where the limits $\mathcal{N}_{\rm min}$ and $\mathcal{N}_{\rm max}$ of the sum are equal to $(\mathcal{N}^{1/3} \mp 3\gamma)^3$, respectively, and $\gamma = 0.78$ is the smearing width used in the folding [7].

To obtain the smoothed sum of s.p. energies $\tilde{E}^{(q)}$ in Eq. (2) one has now to perform a Gauss-Hermite folding of the set S_n to obtain

$$\tilde{S}_{\mathcal{N}} = \sum_{n=\mathcal{N}_{\rm min}}^{\mathcal{N}_{\rm max}} \frac{2}{3\,n^{2/3}}\, S_n\, j\!\left(\frac{\mathcal{N}^{1/3} - n^{1/3}}{\gamma}\right), \tag{17}$$

where $j(u)$ is a normalized weight function that is given by a Gaussian multiplied by a sixth-order correction polynomial [7]

$$j(u) = \frac{1}{\gamma\sqrt{\pi}} e^{-u^2} \left(\frac{35}{16} - \frac{35}{8}u^2 + \frac{7}{4}u^4 - \frac{1}{6}u^6 \right). \quad (18)$$

Having obtained the folded value $\tilde{S}_{\mathcal{N}}$, where shell effects have already been washed out, we can now get an estimate of the smooth energy $\tilde{E}^{(q)}(\mathcal{N})$ by restoring the harmonic oscillator background that was subtracted in Eq. (15):

$$\tilde{E}^{(q)}(\mathcal{N}) = \tilde{S}_{\mathcal{N}} + b\mathcal{N}^{4/3} + V'\mathcal{N}. \quad (19)$$

V. FREE-ENERGY SHELL CORRECTION

A mean-field Hamiltonian with a Yukawa-folded single-particle potential [Eq. (3)] was used to obtain the double degenerate single-particle levels $\varepsilon_\nu^{(q)}$ of protons and neutrons of 134 spherical even-even and 6 deformed nuclei. The s.p. energy sums for these nuclei (disregarding pairing correlations) were evaluated as well as their deformation dependence parametrized through the elongation parameter c of the so-called *Funny Hills* shape parametrization [29]. Assuming that the single-particle spectrum does not change with temperature (see Ref. [30]), similar sums but at different temperatures ($T = 0, 1, 2, 3, 4, 5$ MeV) are determined as

$$E_{sp}(\mathcal{N}; T) = \sum_{\nu=1}^{\infty} 2\,\varepsilon_\nu n_\nu, \quad (20)$$

where the single-particle occupation numbers are given by

$$n_\nu = \frac{1}{1 + \exp[(\varepsilon_\nu - \mu)/T]} \quad (21)$$

and μ is the chemical potential obtained from the particle number equation

$$\mathcal{N} = \sum_{\nu=1}^{\infty} 2n_\nu\,, \quad \mathcal{N} = \{Z, N\}. \quad (22)$$

The Helmholtz free-energy is then obtained according to

$$F(\mathcal{N}; T) = E(\mathcal{N}; T) - S(\mathcal{N}; T)T, \quad (23)$$

where S is the entropy given by

$$S = -\sum_{\nu=1}^{\infty} [n_\nu \ln(n_\nu) + (1 - n_\nu)\ln(1 - n_\nu)]\,. \quad (24)$$

It is a well-known fact that with increasing temperature the shell effects are gradually washed out to disappear completely at temperatures around T = 3 MeV. The free shell-correction energy is defined as the difference between the free energy $F(\mathcal{N}; T)$, Eq. (23), at that temperature and its smooth part $\tilde{F}(T)$ obtained here by the same $\mathcal{N}$-folding method as was described in the previous section.

The frequently used phenomenological approximation of Refs. [19,20] gives the temperature dependence of the free shell-correction energy in the form

$$F_{\text{shell}}(\mathcal{N}; T) = F_{\text{shell}}(\mathcal{N}; 0)\,\frac{\tau}{\sinh\tau}, \quad (25)$$

where $F_{\text{shell}}(\mathcal{N}; 0)$ is the shell-correction energy at zero temperature and $\tau = 2\pi^2 T/\hbar\omega$ with $\hbar\omega = 40A^{-1/3}$ MeV.

Supposing a quadratic temperature dependence of the smooth free energy

$$\tilde{F}(\mathcal{N}; T) = \tilde{F}(\mathcal{N}; 0) - aT^2 \quad (26)$$

allows us to obtain the level-density parameter that determines the smooth entropy as

$$\tilde{S} = 2aT. \quad (27)$$

The level-density parameter a enters the definition of the Helmholtz free energy, so its proper value is crucial for, e.g., evaluating the adiabatic fission barriers at finite temperatures.

The level-density parameter a has often been approximated in the form

$$a = \frac{A}{n}\text{MeV}^{-1}, \quad (28)$$

where A is the mass number and $n \approx 10$. In Ref. [8] the variation of the level-density parameter a with Z and A was investigated. This dependence shall be confirmed by our present study of the level-density parameter obtained in the framework of the Yukawa-folded single-particle potential and the new averaging method in particle number space. The smoothed value of the free energy at given temperature T for $\mathcal{N}$ nucleons is obtained as

$$\tilde{F}(\mathcal{N}; T) = \sum_{N=\mathcal{N}_{\min}}^{\mathcal{N}_{\max}} \frac{2}{3\,N^{2/3}}\; F(N; T)\; j\left(\frac{\mathcal{N}^{1/3} - N^{1/3}}{\gamma}\right), \quad (29)$$

where the normalized Strutinsky weight function $j(u)$ is the sixth-order polynomial given in Eq. (18). The lower and upper limits in Eq. (29) given as $\left(\mathcal{N}^{1/3} \mp 3\gamma\right)^3$ are such that a large-enough number of single-particle levels are included to ensure the accuracy of the estimate of the smooth energy of the order of 0.01 MeV. The free shell energy for the $\mathcal{N}$ nucleon system at temperature T is given by the difference

$$F_{\text{shell}}(\mathcal{N}; T) = F(\mathcal{N}; T) - \tilde{F}(\mathcal{N}; T). \quad (30)$$

The levels-density parameter a is then obtained from Eq. (26)

$$a = [\tilde{F}(\mathcal{N}; 0) - \tilde{F}(\mathcal{N}; T)]/T^2. \quad (31)$$

VI. RESULTS

We first show the results of calculations performed as described above for 134 nearly spherical nuclei between the proton and neutron drip lines, having, according to Ref. [31], almost vanishing quadrupole moments. In Fig. 1 the free shell-correction energy for protons and neutrons, evaluated according to Eq. (30), is plotted for temperatures $T = 0, 1, 2, 3, 4$, and 5 MeV as a function of the mass number A of these nuclei. One notices the rapid decrease of these shell-correction energies with temperature leading essentially

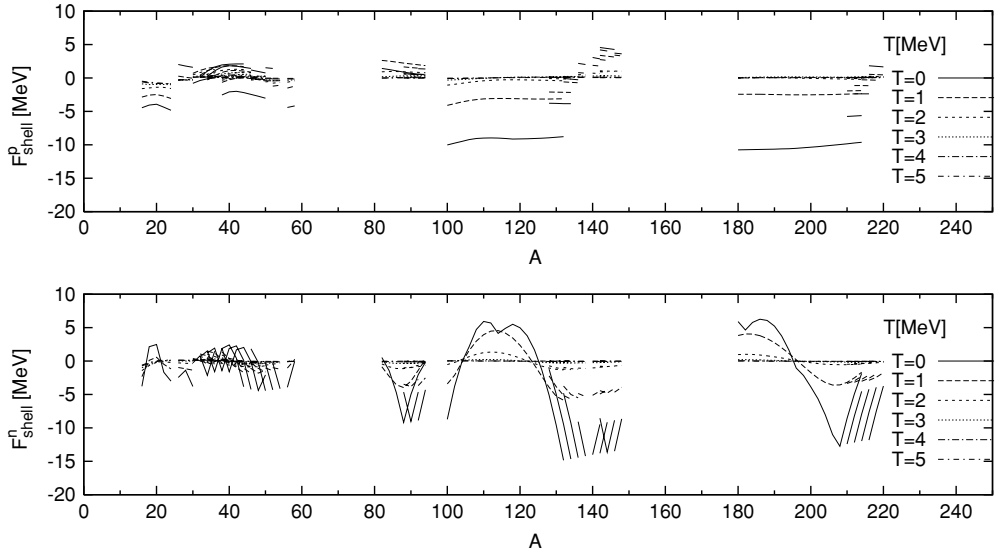

FIG. 1. Free shell-correction energy for protons (upper part) and neutrons (lower part) for a sample of 134 nearly spherical nuclei evaluated at various temperatures T with the Yukawa-folded potential as function of mass number A.

to their disappearance beyond $T \approx 2$–3 MeV. It appears from the figure that the proton shell-correction energies remain essentially constant as function of A along a given isotopic chain (a weak A dependence remains through the radius constant R_0 and the mass and isospin dependence of the depth parameter $V_0^{(q)}$), whereas the parallel lines appearing for the neutron shell-correction energies correspond to different neighboring isotopic chains.

In Fig. 2 the difference of the average total (neutron + proton) free energy $\tilde{F}$ at zero and finite temperature is shown as a function of the mass number A, as well as the corresponding factor n obtained from it through Eq. (28). One can notice that this quantity varies with mass number being substantially smaller than the commonly used value of 10 for nuclei with mass number smaller then 180.

In Fig. 3 the results of our calculation are compared to the values obtained with the self-consistent (RMFT and Skyrme Hartree-Fock) approaches and the phenomenological Thomas-Fermi estimates that are the closest to the experimental values of the level-density parameter [37]. We find that our YF values are much closer to the phenomenological estimate than those obtained in a self-consistent mean-field approach that are close to each other but are found to underestimate the level-density parameter significantly. The fact that our approach gives a fair

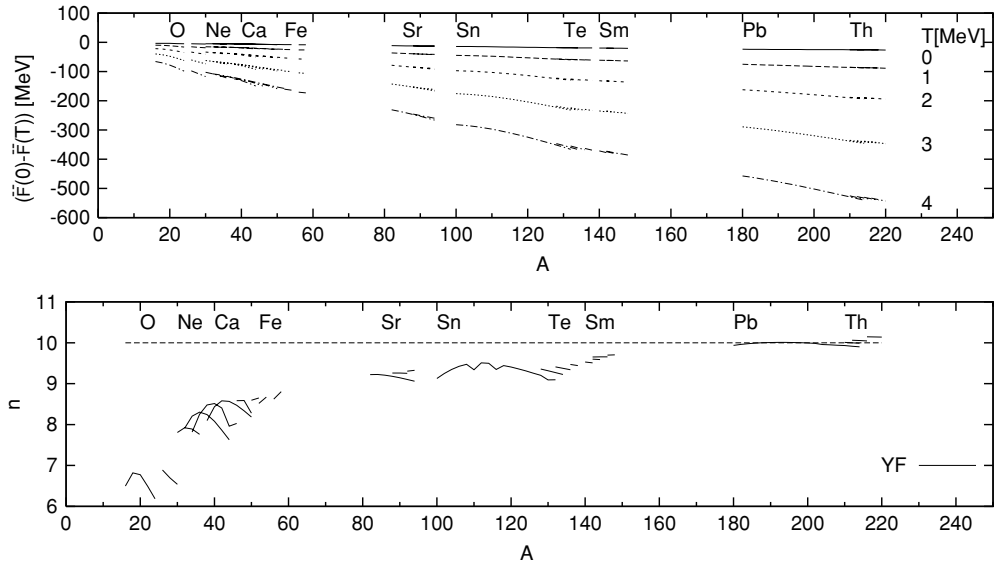

FIG. 2. Differences between the averaged total free energies at $T = 0$ and $T = 1, 2, 3, 4$ MeV for spherical even-even nuclei as function of the mass number A (upper part) obtained within the Yukawa-folded approach. The corresponding factor $n = A/a$ of Eq. (28) is also shown (lower part). The frequently used heuristic value $n = 10$ is given as a dashed line.

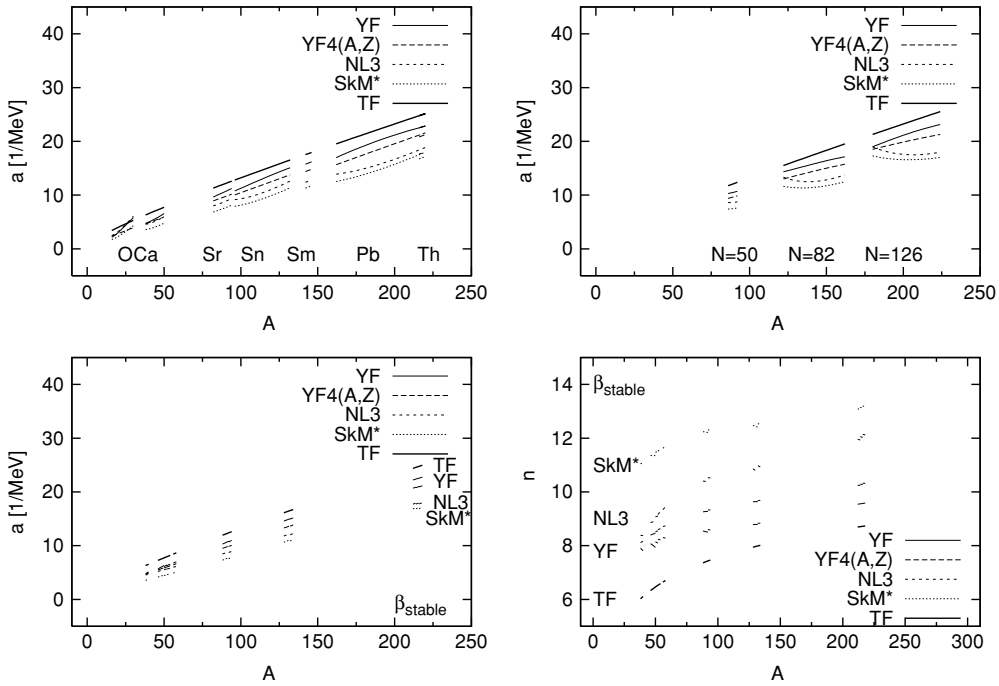

FIG. 3. Level-density parameter obtained with the Yukawa-folded mean-field approach (YF) and their liquid-drop type fit, Eq. (32), [YF4(A, Z)] to spherical and deformed nuclei as compared to the self-consistent results of RMFT [25], Skyrme Hartree-Fock [11] calculations, and Thomas Fermi estimates (TF) [26] for spherical even-even isotopes (upper left), isotones (upper right), and β-stable nuclei (lower left). The corresponding factor $n = A/a$ is also shown (lower right).

reproduction of the experimental level-density parameter does not really come as a surprise, considering that the Hamiltonian of our approach with the Yukawa folded mean-field potential has an unity effective mass. It is, indeed, well known that effective interactions like the Skyrme or Gogny forces, which mostly have an isoscalar effective mass of the order of 0.7 (needed for the description of giant vibrations), yield a level density that is too low, at least in spherical nuclei. It is only

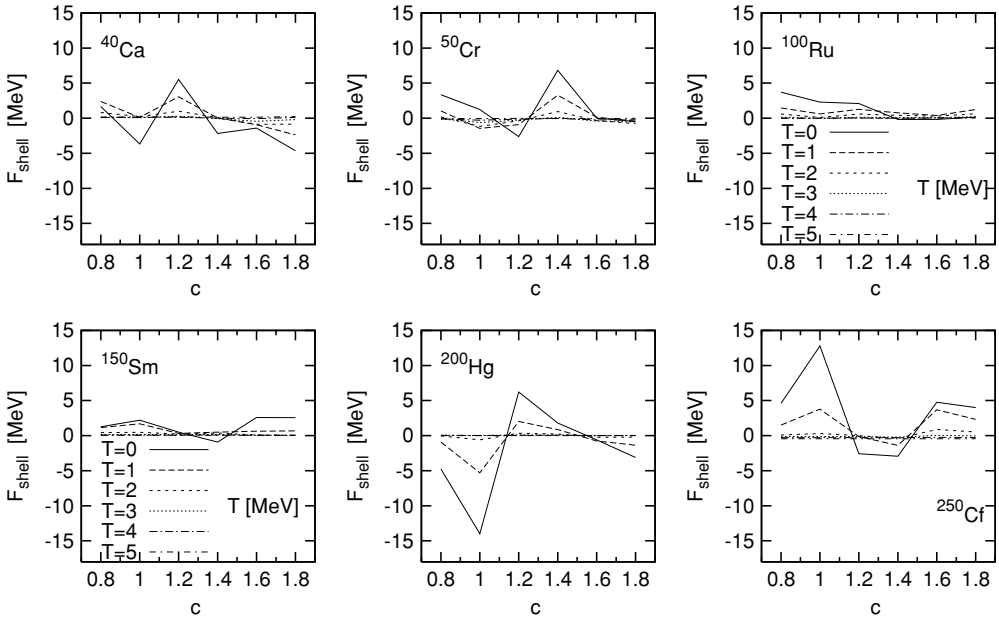

FIG. 4. Deformation dependence of the total (neutron + proton) shell correction energy as function of the *Funny-Hills* elongation parameter c (see text) for different temperatures T.

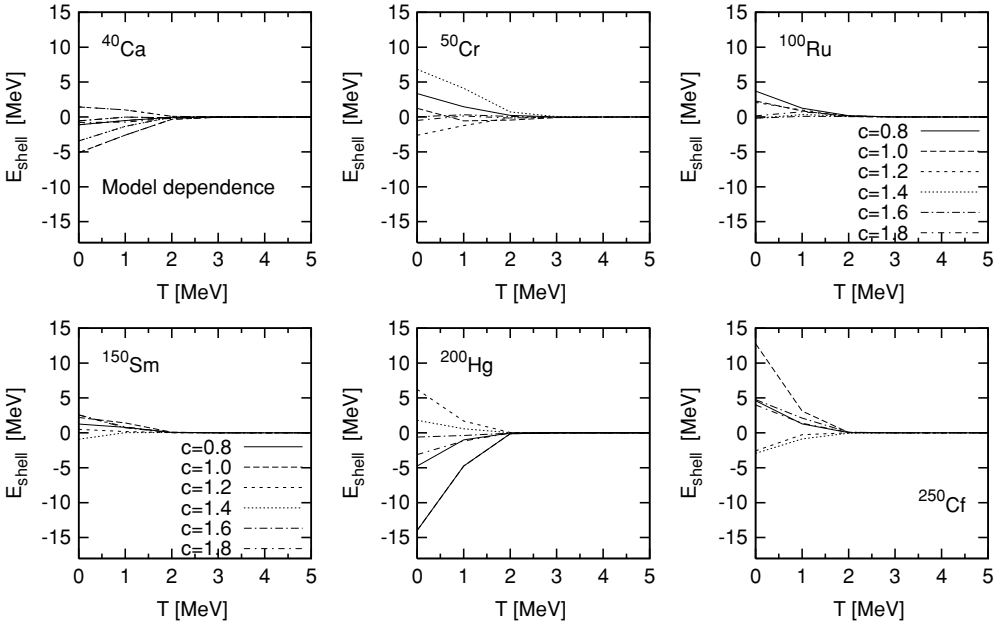

FIG. 5. Temperature dependence of the total shell-correction energy for different values of c as obtained with the approximation of Eq. (25).

through considering correlations that go beyond the mean-field approach that level densities close to the experimental data are obtained [33]. However, the work of Tondeur and Pearson (see, e.g., Ref. [34,35]) have shown that a reasonable level density can be obtained at the level of the Hartree-Fock approximation when a density functional with an effective mass close to $m^*/m = 1$ is chosen.

As the Yukawa-folded level-density parameters turn out to be the closest to the phenomenological estimates, their dependence on deformation has been investigated for a few even-even nuclei: ^{40}Ca, ^{50}Cr, ^{100}Ru, ^{150}Sm, ^{200}Hg, ^{250}Cf.

Figure 4 shows the deformation dependence of the shell-correction free energy at different temperatures. These shell corrections plotted here for different selected nuclei as function of the Funny-Hills [29] elongation parameter c are seen to oscillate around zero up to $T \approx 3$ MeV, essentially vanishing above this temperature.

It is now interesting to compare the decrease with temperature of these shell-correction energies between the predictions of the phenomenological function [Eq. (25)] presented in Fig. 5 and the exact result obtained by the above described folding procedure in $\mathcal{N}$ space shown in Fig. 6. It is interesting

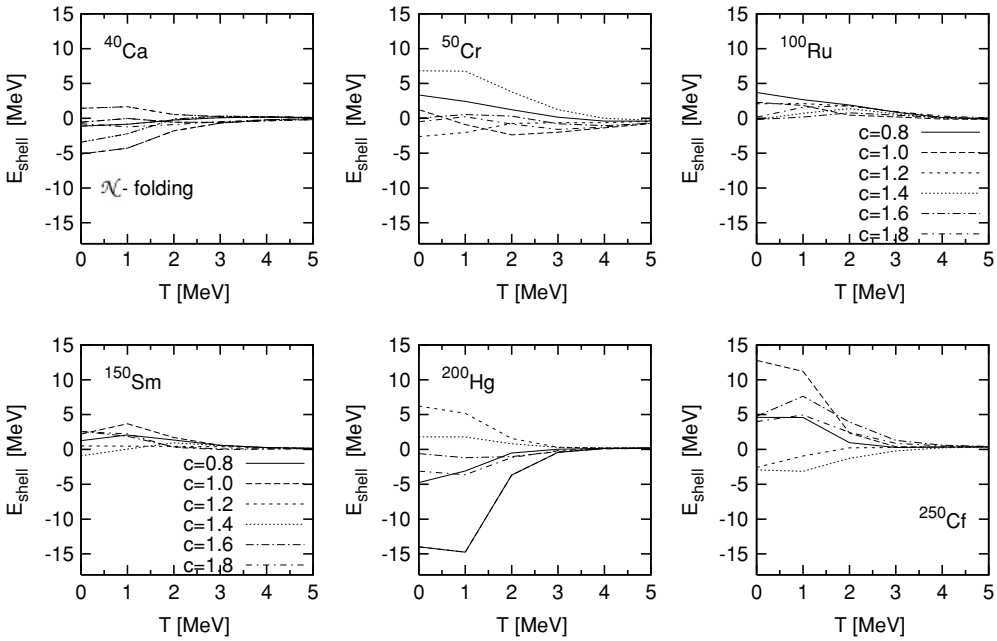

FIG. 6. Same as Fig. 5 but with the temperature dependence obtained by a folding procedure in $\mathcal{N}$ space (see text).

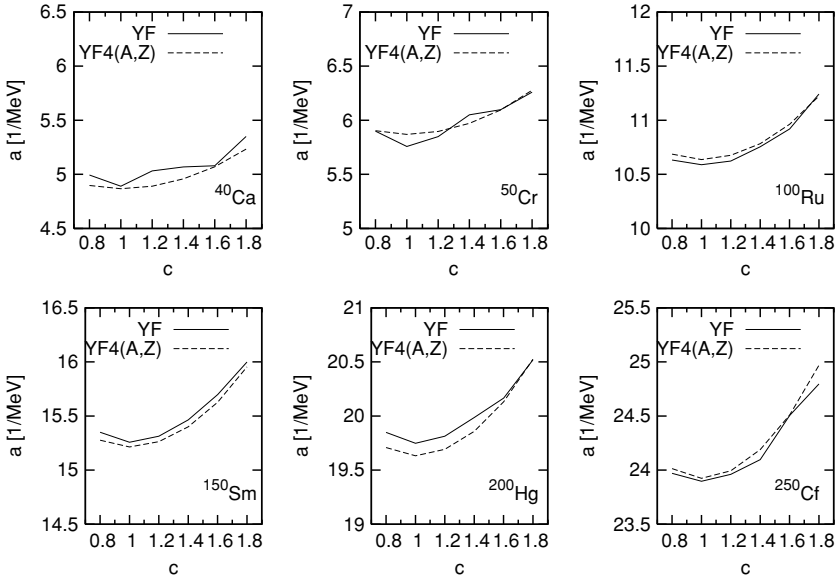

FIG. 7. Level-density parameter as function of c obtained by folding in $\mathcal{N}$ space (YF, solid lines) as compared to the four-parameter fit, Eq. (32) (YF4, dashed lines).

to notice that the evaluation of the temperature dependence obtained by folding in particle number space produces results quite similar to those obtained by the approximate treatment of Eq. (25), but with a somewhat higher critical temperature at which the shell-correction energy disappears, as can be clearly seen by a comparison of both figures. This is in particular the case for light nuclei where these shell effects survive up to $T = 4$ to 5 MeV.

Because of the the unnatural increase of a for the spherical case $c = 1$, caused by the omitting in our averaging the zero-point vibrations [36], we decided to use for the cases $T = 0$ and $c = 1$ the value of a obtained by the traditional Strutinsky folding in the e space. For the rest of points (i.e., $T \neq 0$ and $c \neq 1$) we used the $\mathcal{N}$-folding. We have found that sample of the a parameter data for the 134 spherical and 6 deformed nuclei is well approximated by the following formula [YF4(A, Z)]:

$$a/\mathrm{MeV} = 0.092A + 0.036A^{2/3}B_{\mathrm{surf}}(\mathrm{def}) + 0.275A^{1/3} \times B_{\mathrm{curv}}(\mathrm{def}) - 0.00146Z^2/A^{1/3}B_{\mathrm{Coul}}(\mathrm{def}), \quad (32)$$

where B_{surf}, B_{curv}, and B_{Coul} are the ratios of surface, curvature, and Coulomb energy of a deformed as compared to the corresponding spherical nucleus [38]. We did not include any isospin dependence here because it leads only to a marginal improvement of the quality of the fit. The level-density parameter grows with increasing nuclear deformation, as shown in Fig. 7, which shows the level-density parameter a for six different nuclei in different regions of the periodic table as obtained by our folding procedure and by the fit of Eq. (32) [denoted by YF4(A, Z)]. The quality of the fit is quite satisfactory (watch for the scale). It should just be treated here as a rough estimate and starting point to a broader investigation of a much larger amount of nuclei.

VII. CONCLUSIONS

The following conclusions can be drawn from our analysis:

(i) The free energy evaluated using the energy spectra obtained in a Yukawa-folded mean field exhibits a parabolic temperature dependence.

(ii) The level-density parameter a varies substantially with the mass and deformation (elongation) of a nucleus and can be well approximated by a liquid-drop type expression even in the absence of isospin-dependent terms but with the inclusion of a curvature term.

(iii) The self-consistent RMFT and Skyrme Hartree-Fock approaches produce very similar predictions for the single-particle level densities, but they are consistently too small in comparison with the phenomenological Thomas-Fermi estimates of Ref. [26] adjusted to the experimental data.

(iv) The Yukawa-folded mean-field approach predicts single-particle level densities in much closer agreement with the Thomas-Fermi estimates of Ref. [26] than the self-consistent models.

(v) The shell corrections obtained with the Yukawa-folded mean field and folding in particle number space $\mathcal{N}$ survive up to $T \approx 5$ MeV for lighter nuclei, whereas the phenomenological temperature smoothing predicts its disappearance already at $T \approx 3$ MeV.

The level-density parameter obtained by the described above method can be applied to high excited nuclei only. In our model the enhancement of the level density around the Fermi energy due to the nonlocality of the single-particle potential is missed. This effect is important at low excitations [39,40] and this is the reason why at zero temperature our estimates of the a parameter are too small.

In the next step we are going to perform dynamical calculations like in Ref. [3] of the decay of hot compound

nuclei to confront the theoretical predictions for light-particle multiplicities and fission rates with the experimental data and to test the quality of the single-particle level-density parameter derived in the present article.

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