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TEMPERATURE DEPENDENCE OF THE NUCLEAR SHELL ENERGIES*

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The $\mathcal{N}$-averaging Strutinsky shell-correction method is used to obtain the change with temperature of shell effects as well as of the macroscopic part of nuclear energy in a relativistic mean-field approach with the NL3 parameter set for even–even spherical nuclei.

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Selfconsistent calculations were performed within the relativistic mean-field theory (RMFT) with the NL3 parameters set [1] which reproduced the ground-state properties of nuclei with a good accuracy. Our RMFT approach is based on the Dirac equation for neutrons and protons, the Klein–Gordon equations for mesons and Maxwell equations for photons.

The temperature dependent macroscopic part of the nuclear energy can be obtained as [2]

$$E_{\rm macr}(Z,A;T) = E_{\rm RMFT}(Z,A;T) - \delta E^{(n)}_{\rm shell}(A-Z;T) - \delta E^{(p)}_{\rm shell}(Z;T)\,, \quad (1)$$

where E_{RMFT} is the selfconsistent RMFT energy evaluated without taking into account the pairing correlations and $\delta E^{(q)}_{\rm shell}$ are the shell-correction energies of protons ($q=p$) and neutrons ($q=n$). At $T=0$ the shell energy is a difference between the sum of single-particle energies $e^{(q)}_\nu$ and the

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corresponding energy in which the shell structure is washed out:

$$\delta E^{(q)}_{\rm shell}(\mathcal{N};0) = 2\sum_{\nu>0}^{\mathcal{N}/2} e^{(q)}_{\nu} - \widetilde{E}^{(q)}(\mathcal{N};0)\,. \tag{2}$$

We have used two methods to evaluate the energy $\widetilde{E}^{(q)}$. The traditional Strutinsky approach in which one performs the smoothing in the single-particle energy space (e-averaging) and a new prescription, [4], in which $\widetilde{E}^{(q)}$ is obtained by averaging in the particle number space ($\mathcal{N}$-averaging).

In the both above cases the smoothed energy is subtracted from the RMFT mean-field single particle energies sum in order to obtain the shell correction.

The absolute value of shell-correction energy is known to decrease with increasing temperature. The temperature dependence of the shell energy is often approximated by the phenomenological function [6]

$$E^{(q)}_{\rm shell}(\mathcal{N};T) = \delta E^{(q)}_{\rm shell}(\mathcal{N};0)\,\frac{\tau}{\sinh\tau}\,, \tag{3}$$

where $\tau = \frac{2\pi^2 T}{\hbar\omega_0}$ and $\hbar\omega_0 = 41 {\rm MeV}/A^{1/3}$ represents the average spacing between the two harmonic oscillator shells.

Here the above prescription serves only as the reference for two new effects: the $\mathcal{N}$-averaging shell correction method used to evaluate the shell energy and once more to smooth it's dependence on temperature. In the new shell-correction method of Ref. [4] one replaces this phenomenological function by the shell correction obtained by the $\mathcal{N}$-averaging [4] at given temperature.

The new prescription for the temperature dependence is then following: For each nucleon-number N in the interval $\mathcal{N}_{\rm min} \le N \le \mathcal{N}_{\rm max}$ one calculates the energies of N particles assuming single-particle occupation numbers in the form of Fermi functions

$$E(N;T) = \sum_{i=1}^{\infty} \frac{e_i}{1+\exp\left[(e_i-\lambda)/kT\right]}\,, \tag{4}$$

where the Fermi energy λ is estimated from the particle-number condition. Then using the values of $E(N;T)$ for $\mathcal{N}_{\rm min} \le N \le \mathcal{N}_{\rm max}$ one evaluates the smooth energy $\widetilde{E}(\mathcal{N};T)$ by performing the averaging in the particle-number

$$\widetilde{E}(\mathcal{N};T) = \sum_{N=\mathcal{N}_{\rm min}}^{\mathcal{N}_{\rm max}} \frac{2}{3\,N^{2/3}}\,E(N;T)\; j\left(\frac{\mathcal{N}^{1/3}-N^{1/3}}{\gamma}\right)\,, \tag{5}$$

where

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

is the normalized Strutinsky weight function of the 6th order and $\gamma = 0.78$ is the smearing width. The limits in the sum (5) are taken as $\left(\mathcal{N}^{1/3} \pm 3\gamma\right)^3$. These limits were tested in order to include the sufficient part of single particle level scheme and evaluate the shell energy with the accuracy of the order 0.01 MeV. The temperature dependent shell correction for the $\mathcal{N}$ nucleon system is then given by the difference of (4) and (5)

$$E_{\mathrm{shell}}(\mathcal{N}; T) = E(\mathcal{N}; T) - \widetilde{E}(\mathcal{N}; T) \,. \tag{7}$$

The variation of the macroscopic energy, (Eq. (1)), with temperature can be approximated by a parabola

$$E_{\mathrm{macr}}(Z, A; T) \approx E_{\mathrm{macr}}(Z, A; 0) + a\, T^2 \,, \tag{8}$$

where a is an average level-density parameter which is very important in several fields of nuclear physics *e.g.* in the analysis of fission dynamics and decay of compound nuclei [5]. The other applications can be found in the textbooks *e.g.* in Ref. [6]. Frequently a is assumed to be proportional to the mass number $a \approx A/10$ MeV^{-1} which is of course a very crude approximation. It can be much better approximated by a liquid-drop like formula where, for the newest approach, one obtains ($I = (N - Z)/A$)

$$a_{\mathrm{LD}}/\mathrm{MeV} = 0.356\, A^{2/3} + 1.47\, A^{2/3}\, I^2 + 0.0031\, \frac{Z^2}{A^{1/3}} \,. \tag{9}$$

In Fig. 1 the comparison of the total shell corrections (left) as well as the macroscopic energy (right) obtained for ^{216}Th in the traditional Strutinsky's procedure (old) and its improved version (new) is shown. These calculations are performed either (old, new) with a temperature smoothing using the phenomenological function in Eq. (3) or (new$T$) with the $\mathcal{N}$-averaging procedure, adopted once more to smooth the shell energy with temperature as described in Eq. (7). It clearly appears that the shell corrections obtained with the phenomenological function (3) practically vanish at $T = 2$ MeV whereas those (new$T$) produced by the exact temperature smoothing seem to survive, for this nucleus, up to $T \simeq 4$MeV. The right part of Fig. 1 illustrates the parabolic dependence on temperature of the macroscopic energy of ^{216}Th obtained in the newest method. It is similar in all the three cases.

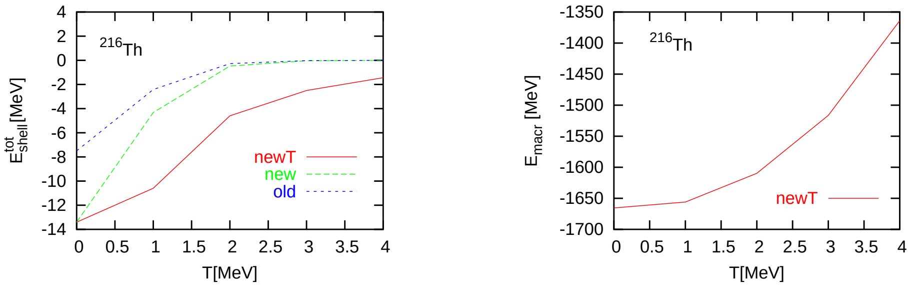

Fig. 1. Total shell corrections (left) for ^{216}Th estimated with the new approach with the two methods: Eqs. (3) (new) and (7) (new$T$) compared to the traditional Strutinsky method (old). The macroscopic energy in the newest case (new$T$) is shown in the right panel.

We have performed our calculations for 171 spherical (or nearly spherical) even–even nuclei from ^{16}O to ^{224}Cf at temperatures from T=0 to T=4 MeV. The dependence of the level density parameter a estimatd from Eq. (8) on temperature, isospin and mass number for most of nuclei is shown in Fig. 2. The results were obtained with the $\mathcal{N}$-averaging shell-correction method also in smoothing the single-particle energies with temperature, *i.e.* through Eq. (7) (new$T$) for several isotopic and isotonic chains.

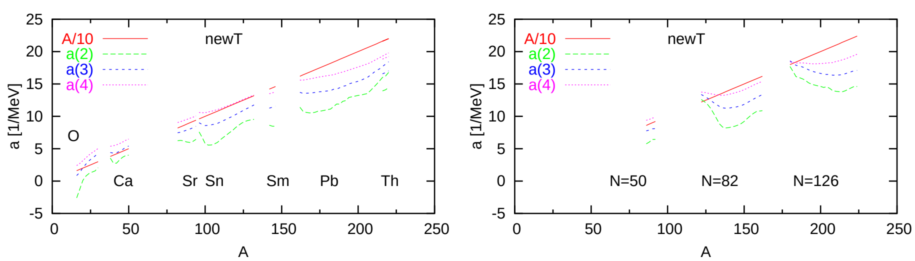

Fig. 2. Level-density parameters $a(T)$ at T=2 to 4 MeV estimated from Eq. (8) $a = (E_{\rm macr}(Z,A;T) - E_{\rm macr}(Z,A;0))/T^2$ with the new temperature smoothing method (new$T$). As a reference the commonly used rough approximation $A/(10 \text{ MeV})$ is also given.

The following conclusions can be drawn from our investigation: (a) the traditional Strutinsky method predicts shell-correction energies a couple MeV larger for spherical nuclei than the new procedure, (b) the phenomenological formula (3) of Ref. [6] predicts a faster decrease of the absolute value of shell energy with temperature than the one estimated with the full $\mathcal{N}$-averaging method for even–even spherical nuclei, (c) the shell structure in the level-density parameters a is visible up to a temperature of $T \simeq 2$ MeV.

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