SHELL CORRECTION AND PARTICLE–PHONON COUPLING *

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The shell energies of spherical nuclei obtained by folding in the particlenumber space and in the energies of individual nucleons are compared. The effect of coupling of the single-particle motion with the shape vibration on the magnitude of the both types of the shell corrections is discussed.

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Already in the 60's Myers and Świątecki have proposed the macroscopicmicroscopic method of evaluating the binding energy of deformed nuclei [1]. This method with modifications proposed by Strutinsky [2], provides the most accurate mass formulae [3,4]. The original Strutinsky prescription for the evaluation of the shell energy by smoothing the single-particle energy spectra (*e*-folding) was improved in 1969 by Nilsson *et al.* [5]. In this approach the microscopic energy correction consists of shell and pairing parts which are added to the binding energy evaluated within one of the macroscopic models, *e.g.* the Lublin–Strasbourg drop [4]. Despite of the known problems arising when dealing with finite-depth nuclear mean-field potentials, the Strutinsky method is widely used up to the present.

A revised version of the shell-correction method, based on a new way of evaluating the smooth part of the total single-particle energy was recently proposed in Ref. [6]. The new estimate of the smooth energy bases on the folding in the particle number space (\mathcal{N} -folding). It properly fulfils the plateau condition, which is not always true in the Strutinsky approach, and it is more stable with respect to the energy cut-off in the single particle spectrum — important when dealing with nuclei far from stability.

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In the new approach, the spherical nuclei are more bound (by a couple of MeV) than it is predicted by the traditional Strutinsky method, while the deformed isotopes have almost the same energy in both models. It raises a question: what does it mean? Is the new approach able to reproduce the measured masses and details of the potential energy surface of nuclei? The answer is yes — if one takes into account the coupling between the collective and individual particle motions.

Following the ideas of Ref. [7] we have shown in [8] that the coupling of the shape vibrations with the single particle motion, completely neglected in all previous calculations of the Strutinsky type, decreases the magnitude of the shell energy for spherical nuclei by a couple of MeV.

The consideration which follows will explain the influence of the particlephonon coupling on the magnitude of the shell effects. Let us consider a deformed single-particle potential $V(\vec{r}; \{\alpha_k\})$. Around spherical shapes $(\alpha_{\nu} = 0)$ the potential can be written as:

$$V(\vec{r}; \{\alpha_{\nu}\}) \approx V(\vec{r}; 0) + \sum_{\nu} \left[\frac{\partial V(\vec{r}; \{\alpha_{\nu}\})}{\partial \alpha_{\nu}} \right]_{\alpha_{\nu}=0} \alpha_{\nu} = V(\vec{r}; 0) + \hat{H}' .$$
(1)

The deformation parameters α_{ν} in the above expansion can be expressed by the boson creation (\widehat{B}_{ν}^{+}) and annihilation operators (\widehat{B}_{ν}) representing the surface vibrations. In the 2nd quantization the linear in α_{ν} term which couples the single-particle Hamiltonian with the shape vibrations is

$$\widehat{H}' \equiv \sum_{i,j;\nu} \left[\langle j | \frac{\partial V}{\partial \alpha_{\nu}} | i \rangle \, \widehat{c}_{j}^{+} \widehat{c}_{i} \, \widehat{B}_{\nu}^{+} + \langle i | \frac{\partial V}{\partial \alpha_{\nu}} | j \rangle \, \widehat{c}_{i}^{+} \widehat{c}_{j} \, \widehat{B}_{\nu} \right] \,. \tag{2}$$

Here c_i^+ and c_i are the fermion creation and annihilation operators, respectively.

The perturbed single-particle energies e'_i are given by

$$e'_{i} = e_{i} + \Delta e_{i} = e_{i} - \sum_{i,j;\nu} \frac{\langle i; 0_{\nu} | \hat{H}' | j; 1_{\nu} \rangle \langle j; 1_{\nu} | \hat{H}' | i; 0_{\nu} \rangle}{(e_{j} + \hbar \Omega_{\nu}) - (e_{i} + 0)} , \qquad (3)$$

where e_i and $|i\rangle$ are energies and wave-functions of the unperturbed Hamiltonian and $\hbar\Omega_{\nu}$ is the energy of the surface phonon of the polarity ν .

Let us remind that the shell energy is given by

$$E_{\text{shell}} = \sum_{i} e'_{i}(n_{i} - \tilde{n}_{i}) , \qquad (4)$$

where n_i and \tilde{n}_i are the occupation probabilities in a nucleus with and without shell structure, respectively. The perturbed E_{shell} and unperturbed $E_{\rm shell}^{(0)}$ shell energy differs by

$$\Delta E_{\text{shell}} = E_{\text{shell}} - E_{\text{shell}}^{(0)} \approx \sum_{i} \Delta e_i (n_i - \bar{n}_i) \ . \tag{5}$$

According to Ref. [7] this difference is of the order 5 MeV for spherical ²⁰⁸Pb, because Δe_i has the same sign as $n_i - \bar{n}_i$ both for the hole and particle states. In case of deformed nuclei, where the high degeneracy of the single-particle levels is absent, the shell energy is almost unchanged.

This effect can be easily explained by the study of the influence of the collective shape vibration on the single particle motion within the Born–Oppenheimer approximation. Let us consider the spherical Bohr Hamiltonian for quadrupole oscillations

$$\widehat{H}_{\text{coll}} = -\frac{\hbar^2}{2D} \left(\beta^{-4} \frac{\partial}{\partial \beta} \beta^4 \frac{\partial}{\partial \beta} + \beta^{-2} (\sin 3\gamma)^{-1} \frac{\partial}{\partial \gamma} \sin 3\gamma \frac{\partial}{\partial \gamma} \right) + \frac{1}{2} C \beta^2 , \quad (6)$$

where D and C are the mass and stiffness parameters and β and γ are the quadrupole axial and nonaxial deformation, respectively. The ground-state wave-function of \hat{H}_{coll} reads:

$$\Psi_0 = (8\pi^2)^{-1/2} (2\pi)^{-1/4} b^{-5/2} \exp(-\beta^2/4b^2) , \qquad (7)$$

where $b = (\hbar^2/4CD)^{1/4}$. The mass and stiffness parameters can be estimated from the experimental data using the following relations:

$$\sqrt{\frac{C}{B}} = E_{2^+}; \qquad \sqrt{C \cdot B} = \frac{1}{2} \left(\frac{3}{4\pi} Z e R_{\circ}^2\right)^2 / B(E2; 2^+ \to 0^+) , \qquad (8)$$

which are valid in harmonic approximation.

The effective shell energy reduction can be obtained as the expectation value between the ground state collective wave functions:

$$\langle E_{\rm shell} \rangle = 8\pi^2 \int_0^\infty d\beta \int_{\gamma=0}^{60^\circ} |\Psi_0|^2 E_{\rm shell}(\beta,\gamma) \beta^4 |\sin 3\gamma| \, d\gamma \,. \tag{9}$$

The shell energy of 90 Zr evaluated by \mathcal{N} -folding method [6] for the singleparticle spectrum of the Yukawa-folded Hamiltonian as in Ref. [3] is plotted in Fig. 1 (solid line and squares) as function of the quadrupole deformation β . Similar as it was already predicted by Myers and Świątecki [1] the shell correction for this double-magic nucleus is negative and its magnitude decreases with deformation. The dashed line represents the probability $|\Psi_0|^2\beta^5$ which

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stays in the integral (9) after performing the integration over γ . It is seen in Fig. 1 that the probability is picked up at non-zero β deformation which corresponds to a significantly smaller than for the spherical shape ($\beta = 0$) magnitude of the shell correction. The effective shell energy $\langle E_{\text{shell}} \rangle$ obtained by Eq. (9) is by 3.7 MeV smaller than $E_{\text{shell}}^{(0)}=8.7$ MeV.



Similar effect may be observed for other spherical nuclei. Using the experimental data on energies E_{2^+} and $B(E2; 2^+ \to 0^+)$ transitions (NUDAT data base) and two types of folding: the traditional Strutinsky *e*-folding (circles) and the new \mathcal{N} -folding method (squares), we have evaluated the effective shell energies (filled symbols) and compared them with their static values (open symbols) in Fig. 2. It is visible that the coupling with the shape vibrations diminishes the magnitude of the shell corrections by a few MeV. Due to this effect the shell energies obtained by \mathcal{N} -folding would be closer to their experimental values while the Strutinsky type estimates would become too small.

These results give a hope that the macroscopic-microscopic model with the new shell energy could reproduce the binding energies of the known isotopes, if the effect of particle-phonon coupling is taken into account.



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