FISSION BARRIER AND LDM PARAMETERS IN THE THOMAS–FERMI APPROXIMATION

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1. Introduction

In 1967 STRUTINSKY proposed the shell correction method [1]. Since the first succesful applications of this theory there has always been a high interest in justifying this phenomenological theory by microscopical methods.

According to the shell correction method the energy of a deformed nucleus can be written as

$$E = E_{LD} + \delta E_1 + \delta E_2 \tag{1}$$

where E_{LD} is the average energy calculated within the framework of the liquid drop (LDM) model [2], the shell correction δE_1 is calculated in a given deformed shell model potential. The parameters of this potential have to be consistent with the deformation parameters of the LDM energy. δE_2 is the second order correction term.

Recently BRACK and QUENTIN have verified [3] the validity of the shell correction method within the framework of the Hartree–Fock approximation.

The problem of relating the shell correction theory to the statistical theory (the first approximation of which is the Thomas–Fermi (TF) theory) was discussed by TYAPIN [4], and since then it has been investigated in many papers (see e.g. [5]). For carrying out this program one has to substitute the smooth part (E_{LD}) of energy (1) by the energy calculated on the basis of the statistical theory, and the shell correction δE_1 has to be calculated from the single particle potential obtained from the statistical theory. For practical applications it would be desirable, if the smooth energy of the statistical theory reproduced the experimental data (fission barriers, average energy of the nucleus, etc.) as well, as the LDM energy does. This problem will be discussed in this paper, the problem of the potential has been discussed in [6].

2. The Thomas–Fermi energy of the nucleus

The energy of the nucleus can be written as

$$E = E_{kin} + E_{pot} + E_{coul}\,, \tag{2}$$

where the kinetic energy is in the TF approximation:

$$E_{kin} = \varkappa \int \mathrm{d}\vec{r}\,[\varrho_n^{5/3} + \varrho_p^{5/3}] + c \int \mathrm{d}\vec{r}\left[\frac{(\nabla \varrho_n)^2}{\varrho_n} + \frac{(\nabla \varrho_p)^2}{\varrho_p}\right]. \tag{3}$$

Here $\varrho_{n(p)}$ is the neutron (proton) density, $\varkappa = 119.06$ MeVfm^2 and $c = \hbar^2/72\,M$ (where M is the mass of a nucleon) according to [7]. For the potential energy E_{pot} the usual decomposition is applied (e.g. [8]):

$$E_{pot} = E_{NM} + E_{LR} \tag{4}$$

with terms arising from the short-range and long-range components (E_{NM} and E_{LR}, respectively) of the nuclear forces.

In the local density approximation (e.g. [8]) E_{NM} has the form

$$E_{NM} = \int \mathrm{d}\vec{r}\, w(\varrho_n, \varrho_p)\,, \tag{5}$$

where $w(\varrho_n, \varrho_p)$ is assumed to reproduce the results of nuclear matter calculations [9, 12]. The expression for E_{LR} is

$$\begin{aligned} E_{LR} = \frac{1}{2} \sum_{\tau\tau'} \int \mathrm{d}\vec{r}_1 \mathrm{d}\vec{r}_2\, v_{\tau\tau'}(|\,\vec{r}_1 - \vec{r}_2\,|_1\, \varrho) \cdot \varrho_\tau(\vec{r}_1) * \\ * [\varrho_\tau(\vec{r}_2) - \varrho_\tau(\vec{r}_1)]\,. \quad \tau, \tau' = p, n \end{aligned} \tag{6}$$

This energy vanishes for constant density. The density-dependent effective interaction in Eq. (6) is

$$\begin{aligned} v_{\tau\tau'} = v_{\tau'\tau} = \sum_{i=1}^{5} (a_i^{\tau\tau'} + b_i^{\tau\tau'} k_F^{\tau\tau'}) \exp\,[-(\vec{r}_1 - \vec{r}_2)^2/\lambda_i^2]\,, \\ v_{\tau\tau} = v_{\tau'\tau'},\ k_F^{\tau\tau'} = \left[\frac{\varrho_\tau + \varrho_{\tau'}}{2}\right]^{1/3},\ \tau, \tau' = p, n \end{aligned} \tag{7}$$

taken from [10]. The values of the constants of this expression are found in [10].

The Coulomb energy is calculated in the usual way:

$$E_{coul} = \frac{e^2}{2} \int \mathrm{d}\vec{r}_1 \mathrm{d}\vec{r}_2\, \frac{\varrho_p(\vec{r}_1)\varrho_p(\vec{r}_2)}{|\,\vec{r}_1 - \vec{r}_2|}\,. \tag{8}$$

The Coulomb exchange energy is neglected.

The next step is to minimize the energy with respect to the densities ϱ_n and ϱ_p. The constraints

$$\int \mathrm{d}\vec{r}\, \varrho_\tau(\vec{r}) = N_\tau, \quad \tau = p, n \tag{9}$$

have to be taken into account, where N_p is the charge number and N_n the neutron number of the nucleus.

There are two different methods to minimize the energy. Solution of the coupled integro-differential TF equations is very time consuming. Hence the second method will be chosen, assuming an approximate analytical expression for the nuclear densities. These expressions (see item 3) depend on some set of deformation parameters (i.e. for given deformation) and varying the variational parameters the minimal energy in the TF approximation is obtained.

3. Parametrization of the density

Instead of the more general form suggested in [6] the following expression will be used for the description of densities:

$$\varrho_\tau = \varrho_{0\tau} \frac{1 + b_{1\tau}\left(\frac{l(r,z)}{R_\tau}\right)^2 + b_{2\tau}\left(\frac{l(r,z)}{R_\tau}\right)^4}{1 + \exp\left[l(r,z)/a_\tau\right]} \qquad \tau = p, n \tag{10}$$

where $\varrho_{0\tau}$ is the scale factor (determined by the constraint (9)); R_τ is the radius of a sphere with a volume equal to that of the region inside the nucleus; a_τ is the diffuseness parameter, $l(r, z)$ is the distance from the point with cylindrical co-ordinates r and z to the surface of the nucleus (see [6]); $b_{1\tau}$ and $b_{2\tau}$ are the parameters defining the radial dependence of the density. The parameters characterizing the deformation are incorporated in $l(r, z)$ (see [11]). If $b_{1\tau} = b_{2\tau} = 0$, we obtain the Fermi distribution.

4. Results

The minimum energy of the nucleus ^{240}Pu at several deformations was calculated. As a first approximation the nuclear densities were described by the Fermi distribution. The variational parameters R_τ and a_τ were varied simultaneously for both the protons and neutrons.

The long-range energy was calculated as in Eqs (6) and (7). The energy density function $w(\varrho_n, \varrho_p)$ for the short-range energy was taken from [12].

The results are shown in Fig. 1. The fission barrier obtained by us are seen not to agree with the experimental value (~6 MeV). The binding energy of the spherical shape is overestimated.

Using the same effective nuclear interaction, but approximating the nuclear densities with the "wine-bottle" shape ($b_{1\tau} \neq 0$, $b_{2\tau} \neq 0$), it was tried to improve the results. Neither in this way was any essential improvement achieved.

The dependence on deformation of both the Coulomb and surface energy is in good agreement with the results of standard calculations [13] (see Figs 2, 3). The slight difference is due to the fact that in the standard calculations sharp surface densities were assumed. On the other hand, the effective nuclear interactions used in our calculation are fitted to the results of nuclear matter calculations and to the binding energies of spherical nuclei. Hence, one can assume that the discrepancies of our results could be overcome by the slight re-adjustment of the effective interaction used in this paper. Investigating the statistical potential, which is necessary for obtaining the shell-correction δE_1, the same conclusions were obtained [6].

To prove this assumption the following investigation was carried out. The binding energy of fictive spherical nuclei was calculated with relative neutron excess $x = (N-z)/(N+z) = 0$ and 0,2, and for mass number $A = 40\,(20)\,300$. Following DWORZECKA and MOSZKOWSKI's proposal [14] the constants of the semi-empirical mass formula were determined by the least square method. The results of this calculation are shown in Table I. These results suggest that after re-adjusting the effective nuclear interaction (the test of this procedure may be the fit to the LDM parameters) there is a hope to improve our results.

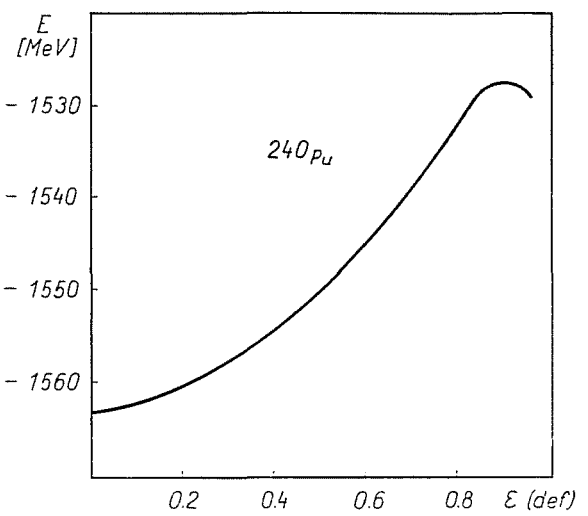

Fig. 1. Deformation energy curve of ^{240}Pu. The deformation parameter ε is defined in [11]

Table I

Volume, surface and curvature energies, and the corresponding asymmetry energies in the semi-empirical mass formula of Ref. [14], i.e. $E = (W_{vol} + W_{Avol}X^2)A + (W_{sur} + W_{Asur}X^2)A_+^{2/3} + (W_{cur} + W_{Acur}X^2)A^{1/3}$. Our results are given in the first row, the second row shows the results of Ref. [15], which can be considered as test values (see the text)

W_{vol}	W_{Avol}	W_{sur}	W_{Asur}	W_{cur}	W_{Acur}
—15,1	16,69	20,71	41,20	0,97	—143,9
—16,43	31,54	18,34	—75,92	13,1	53,71

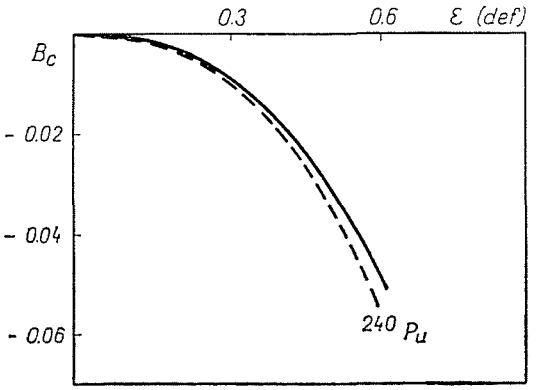

Fig. 2. Dependence of the Coulomb energy on the deformation. The quantity $B_c = [E_{coul}(\varepsilon) - E_{coul}(0)]/E_{coul}(0)$ is shown. The solid line refers to the results of standard calculation [13], the dashed line shows the result of the present work

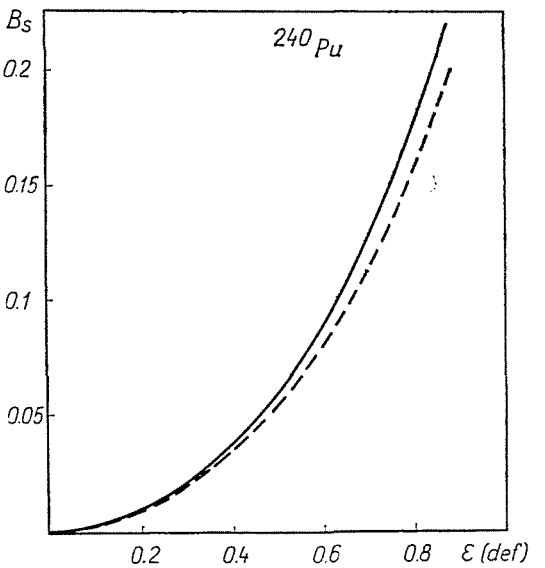

Fig. 3. Dependence of the surface energy on the deformation. The quantity $B_s = [E_s(\varepsilon) - E_s(0)]/E_s(0)$ is shown. The solid line refers to the results of standard calculation [13], the dashed line shows the result of the present work

Chu and others [15] determined the constants of the semi-empirical mass formula for various types of the Skyrme interaction using the least squares method. The good results obtained in this paper prove our assumption that the application of any re-adjusted interaction will give the requested numerical test for the approximation of the smooth energy term in the shell correction method within the framework of the TF theory.

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Summary

The fission barrier of ^{240}Pu was calculated in the Thomas–Fermi approximation. The discrepancies between the obtained results and known data demand the re-adjustment of the effective interaction used in the present work. The fit to the LDM parameters gives a good test for the re-adjusting procedure.

References

1. STRUTINSKY, V. M.: Shell Effects in Nuclear Masses and Deformation Energies, Nucl. Phys. **A95** (1967) pp. 420—442
2. MYERS, W. D.—SWIATECKI, W. J.: Nuclear Masses and Deformations, Nucl. Phys. **81** (1960) pp. 1—60
3. BRACK, M.—QUENTIN, P.: Self-consistent Average Density Matrices and the Strutinsky's Energy Theorem, Phys. Lett. **56B** (1975) p. 421
4. TYAPIN, A. S.: Method obolochechnoy popravki, Yadernaya fisica **11** (1970) pp. 98—104
5. BHADURI, R. K.—ROSS, C. K.: Shell Correction in the Independent Particle Model, Phys. Rev. Lett. **27** (1971) pp. 606—609
6. BALÁZS, E.—PASHKEVICH, V. V.: The Radial Dependence of the Shell-Model Potential, Preprint of JINR, Dubna E4—10588 (1977) pp. 1—19
7. KIRZHNITS, D. A.: Field Theoretical Methods in Many-Body Systems, Pergamon Press Oxford, 1967
8. BRUECKNER, K. A.—GAMMEL, J. L.—WEITZNER, H.: Theory of Finite Nuclei, Phys. Rev. **110** (1958) pp. 431—445
9. LOMBARD, R. J.: The Energy-Density Formalism in Nuclei, Ann. of Phys. **77** (1973) pp. 380—413
10. SPRUNG, D. W. L.: A Density-Dependent Local Effective Interaction between Nucleons in Nuclear Matter, Nucl. Phys. **A168** (1973) pp. 273—307
11. PASHKEVICH, V. V.: On the Asymmetric Deformation of Fissioning Nuclei, Nucl. Phys. **A169** (1971) pp. 275—293
12. FÁI, G.—NÉMETH, J.: Density-Dependent Effective Interaction in Finite Nuclei II, Nucl. Phys. **A208** (1973) pp. 463—476
13. PASHKEVICH, V. V.: Private communication.
14. DWORZECKA, M.—MOSZKOWSKI, S.: Comparison of Hartree—Fock and Energy-Density Formalism Calculations for Some Spherical Nuclei, Phys. Rev. **C12** (1975) pp. 619—627
15. CHU, Y. H.—JENNINGS, B. K.—BRACK, M.: Nuclear Binding Energies and Liquid Drop Parameters in the Extended Thomas–Fermi Approximation, Phys. Lett. **68B** (1977) pp. 407—410

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