3.30 Determination of Shell Energies — Nuclear Deformations and Fission Barriers —

Hiroyuki KOURA, Takahiro TACHIBANA*, Masahiro UNO** and Masami YAMADA*

Department of Physics and Applied Physics, Waseda University, 3-4-1 Okubo, Shinjuku-ku, Tokyo, JAPAN
*Advanced Research Center for Science and Engineering, Waseda University, 3-4-1 Okubo, Shinjuku-ku, Tokyo, JAPAN
**Ministry of Education, Science and Culture, 3-2-2 Kasumigaseki, Chiyoda-ku, Tokyo, JAPAN

e-mail address: H. Koura: *641508@cfi.waseda.ac.jp*
T. Tachibana: *tachiban@cfi.waseda.ac.jp*
M. Uno: *unom@cfi.waseda.ac.jp*
M. Yamada: *myamada@cfi.waseda.ac.jp*

We have been studying a method of determining nuclear shell energies and incorporating them into a mass formula. The main feature of this method lies in estimating shell energies of deformed nuclei from spherical shell energies. We adopt three assumptions, from which the shell energy of a deformed nucleus is deduced to be a weighted sum of spherical shell energies of its neighboring nuclei. This shell energy should be called intrinsic shell energy since the average deformation energy also acts as an effective shell energy The ground-state shell energy of a deformed nucleus and its equilibrium shape can be obtained by minimizing the sum of these two energies with respect to variation of deformation parameters. In addition, we investigate the existence of fission isomers for heavy nuclei with use of the obtained shell energies.

§1. Introduction

The nuclear ground-state energy can be expressed as a sum of a smooth function of Z (proton number) and N (neutron number) and a deviation from it (see, for example, refs. [1-3]). The deviation energy, which we may call shell energy in a broad sense, is considered to be mainly due to the nuclear shell structure and deformation. For several years we have been developing a method of calculating the shell energy. In this study we newly devised a method of expressing the shell energy of a deformed nucleus as a linear combination of the shell energies of spherical nuclei. In this report, the shell energy of a deformed nucleus is mainly treated. In section 2 we comment on the spherical shell energies, in section 3 explain how to take into account the deformation effect on them, and finally give a concluding remark in section 4.

§2. Spherical shell energy

Our method of determining shell energies starts from an extreme single-particle shell model. An extended *spherical* Woods-Saxon potential of neutron (or proton) is assumed for each nuclide. We obtain the minimum of the total energy of n neutrons (or n protons) put in this potential. These minima plotted against n show some deviations from a smooth curve, and these deviations are the origin of the shell energies. In order to extract these deviations we subtract smooth energies whose main parts are the Thomas-Fermi energies. Then, a "crude" neutron (or proton) shell energy of a nucleus with Z and N is obtained as the deviation at $n=N$ (or $n=Z$). Next, we refine these crude shell energies by taking into account the effect of pairing interactions; we take a weighted average of the crude shell energies of neighboring nuclei in which the weight is related to the occupation probability of the BCS theory. The effect of high-energy configuration mixing is simply treated by multiplying a reduction factor μ for the shell energies. The shell energies thus obtained are called "spherical shell energies" in the following. See ref. 4 for the detailed explanation.

§3. Deformation effects

The shell energy of a deformed nucleus is expressed as a sum of two parts: an intrinsic shell energy and an average deformation energy.

3. 1 *Intrinsic shell energy*

We state three important assumptions for our prescription to obtain the intrinsic shell energies of deformed nuclei.

Assumption [1]: The intrinsic shell energy comes only from the differences between the single-particle levels and their structureless positions as

$$E_{\rm in}(Z, N) = \mu \sum_{\nu} w_{{\rm p}\nu}(Z, N)\,(\varepsilon_{{\rm p}\nu} - \overline{\varepsilon_{{\rm p}\nu}}) + \mu \sum_{\nu} w_{{\rm n}\nu}(Z, N)\,(\varepsilon_{{\rm n}\nu} - \overline{\varepsilon_{{\rm n}\nu}})\ . \qquad (1)$$

Here, $\varepsilon_{j\nu}$ ($\nu=1,2,3...$) are single particle energies in the spherical potential, $\overline{\varepsilon_{j\nu}}$ are their structureless positions, and $w_{j\nu}(Z, N)$ are occupation probabilities of the ν-th spherical single-particle states in the deformed nucleus (j = n or p).

In the case of a spherical nucleus eq. (1) changes into

$$E_0(Z, N) = \mu \sum_{\nu} w_{0{\rm p}\nu}(Z, N)\,(\varepsilon_{{\rm p}\nu} - \overline{\varepsilon_{{\rm p}\nu}}) + \mu \sum_{\nu} w_{0{\rm n}\nu}(Z, N)\,(\varepsilon_{{\rm n}\nu} - \overline{\varepsilon_{{\rm n}\nu}})\ , \qquad (2)$$

where the subscript "0" indicates the spherical nucleus.

Assumption [2]: Each occupation probability in a deformed nucleus can be expressed as a linear combination of the occupation probabilities in the spherical states as

$$w_{{\rm p}\nu}(Z, N) = \sum_{Z'} W_{\rm p}(Z'; Z, N)\, w_{0{\rm p}\nu}(Z', N)\ ,$$

$$w_{n\nu}(Z, N) = \sum_{N'} W_n(N'; Z, N)\, w_{0n\nu}(Z, N'), \tag{3}$$

where $w_{0j\nu}(Z', N)$ are occupation probabilities in the selected spherical states, and $W_p(Z'; Z, N)$ and $W_n(N'; Z, N)$ are their weights.

Assumption [3]: The directionally-averaged proton and neutron radial distributions are simple weighted sums of the radial density distributions of the single-particle states,

$$\rho_j\,(r; Z, N) = \sum_{\nu} w_{j\nu}(Z, N)\sigma_{j\nu}(r), \tag{4}$$

where $\sigma_{j\nu}(r)$ are radial density distribution in ν-th single-particle states.

From these assumptions, we can deduce the following equations:

$$E_{in}(Z, N) = \sum_{N'} W_n(N'; Z, N)\, E_{0n}(Z, N') + \sum_{Z'} W_p(Z'; Z, N)\, E_{0p}(Z', N), \tag{5}$$

$$\rho_p(r; Z, N) = \sum_{Z'} W_p(Z'; Z, N)\rho_{0p}(r),$$
$$\rho_n(r; Z, N) = \sum_{N'} W_n(N'; Z, N)\rho_{0n}(r). \tag{6}$$

Equation (6) implies a possibility of determining the mixing weights $W_n(N'; Z, N)$ by comparing the directionally-averaged distributions in deformed nuclei with those in spherical nuclei. For example, in the case of uniform density with sharp-cut surface, the mixing weight $W_n(N'; Z, N)$ is obtained as

$$W_n(N'; Z, N) = -\frac{1}{4\pi}\frac{d\Omega_{occ}(r(N'))}{dN'}, \tag{7}$$

where $\Omega_{occ}(r(N'))$ is the occupied solid angle for the radial coodinate $r(N')$ (See Figs. 1 and 2). This shows that the mixing weight is related to the decrease of the occupied solid angle.

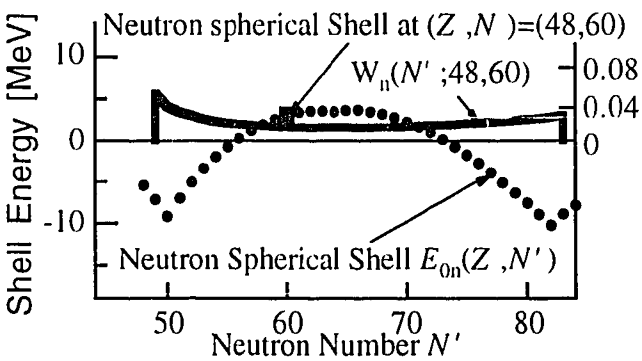

Fig. 1: Mixing weight $W_n(N'\,;Z, N)$ for the nucleus with $Z = 48$, $N = 60$ (right scale) and spherical shell energies $E_{0n}(Z,N')$ (left scale)

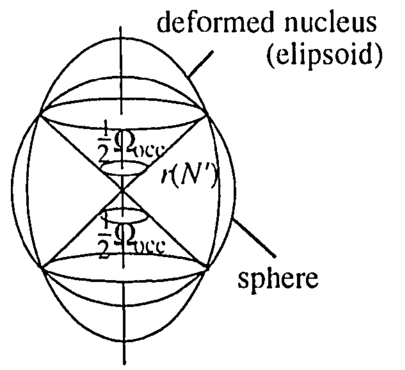

Fig. 2 : Illustration of the occupied solid angle $\Omega_{occ}(r(N'))$ in the case of prolate deformation

3. 2 *Average deformation energy*

The average deformation energy can be estimated from the liquid-drip model or its slight modification. From the liquid-drop model,

$$\Delta E_{\mathrm{DFLD}} = \Delta E_{\mathrm{surf}} + \Delta E_{\mathrm{Coul}} \ , \tag{8}$$

where ΔE_{surf} and ΔE_{Coul} are the differences of the surface and Coulomb energies of a deformed nucleus from those of the spherical nucleus.

According to experimental data, the prolate shape is dominant in most deformed nuclei. We phenomenologically use an additional term to take into account this situation as

$$\Delta E_{\mathrm{prl}}(\alpha_2, A) = -\, C_{\mathrm{prl}}\, \alpha_2\, A^{1/3} \ , \tag{9}$$

where C_{prl} is a parameter and the A-dependence is chosen somewhat arbitrarily with a conjecture that the dependence should be a little weaker than that of the surface area.

The average deformation energy is expressed as

$$\overline{E_{\mathrm{def}}} = \Delta E_{\mathrm{DFLD}} + \Delta E_{\mathrm{prl}} \ . \tag{10}$$

3. 3 *Refined shell energy*

The sum of the intrinsic shell energy and the average deformation energy is the effective shell energy of a deformed state. If we are concerned with the ground state, we should search for the minimum of the effective shell energies of various deformed states, i.e.,

$$E_{\mathrm{sh}}(Z, N) = \min_{\mathrm{deformation}} \left[E_{\mathrm{in}}(Z, N) + \overline{E_{\mathrm{def}}} \right] . \tag{11}$$

We call $E_{\mathrm{sh}}(Z, N)$ the refined shell energy. So far we have made numerical calculations for Y_2 and Y_4 deformations with deformation parameters α_2 and α_4 as

$$r(\theta) = \frac{r_0}{\lambda}\left[1 + \alpha_2\, P_2(\cos\theta) + \alpha_4\, P_4(\cos\theta) \right] , \tag{12}$$

where

$$\lambda = \left[1 + \frac{3}{4\pi}\left(\frac{4\pi}{5}\,\alpha_2^2 + \frac{4\pi}{9}\alpha_4^2 \right) \right]^{1/3} ,$$

which is introduced to stand for the condition of the volume conservation.

The shell energy of a deformed nucleus and its equilibrium shape are thus obtained. In Fig. 3 the shell energies are shown and in Fig. 4 the deformation parameters α_2 are shown.

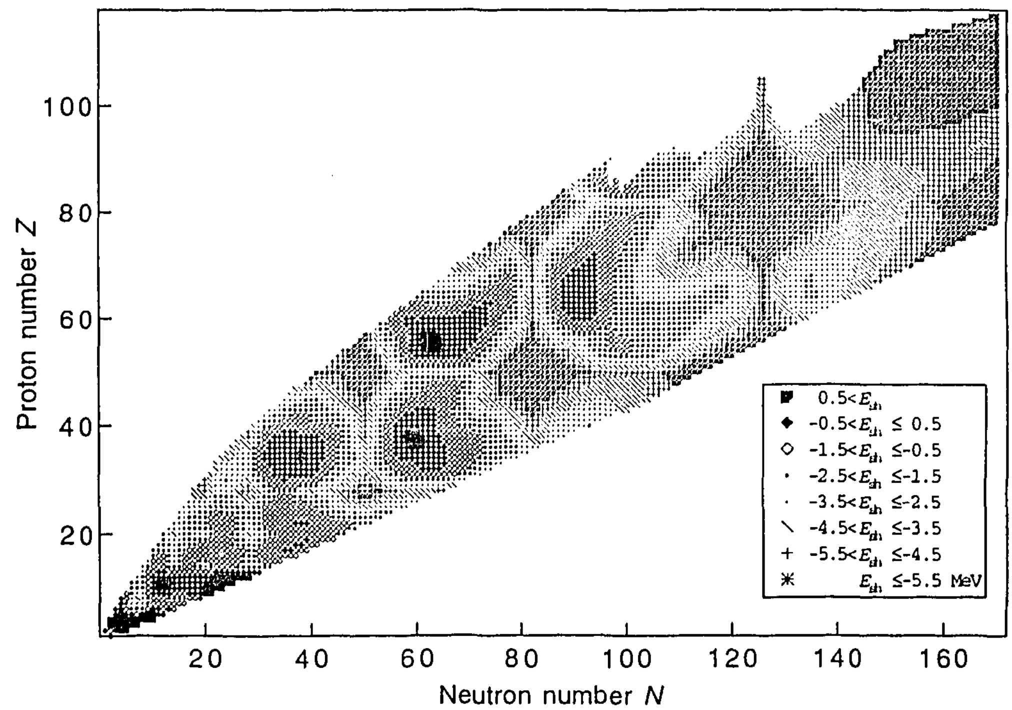

Fig. 3: Refined shell energy

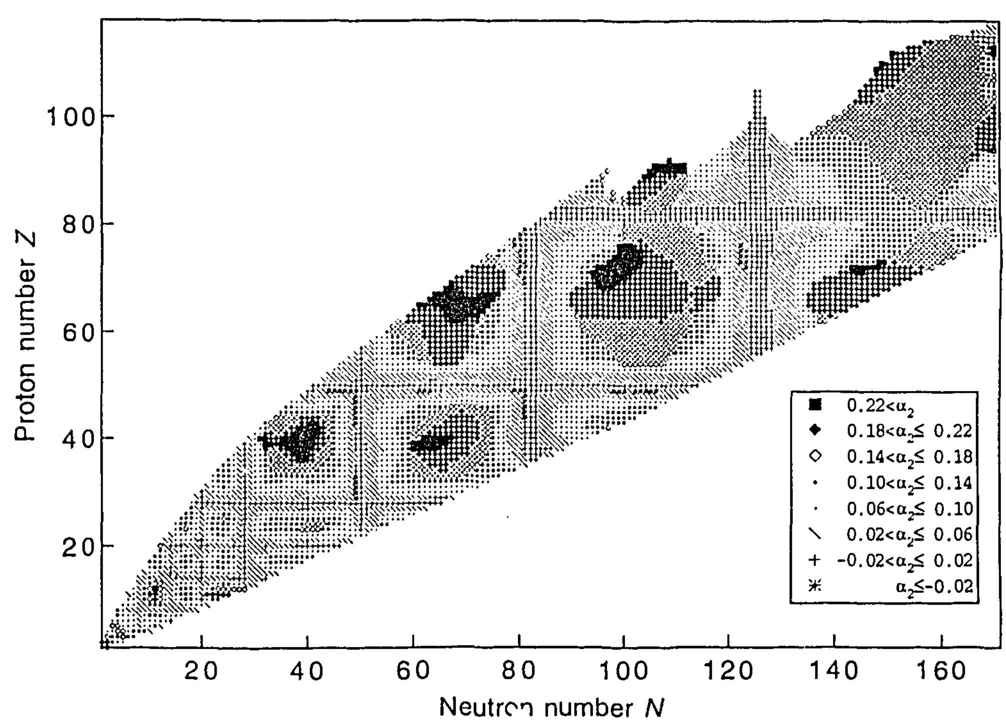

Fig. 4: Deformation parameter α_2

We can obtain the energy surface of a nucleus by mapping the effective shell energies against the deformation parameters α_2 and α_4. We, for example, show in Fig. 5 the energy surface of $^{260}106$.

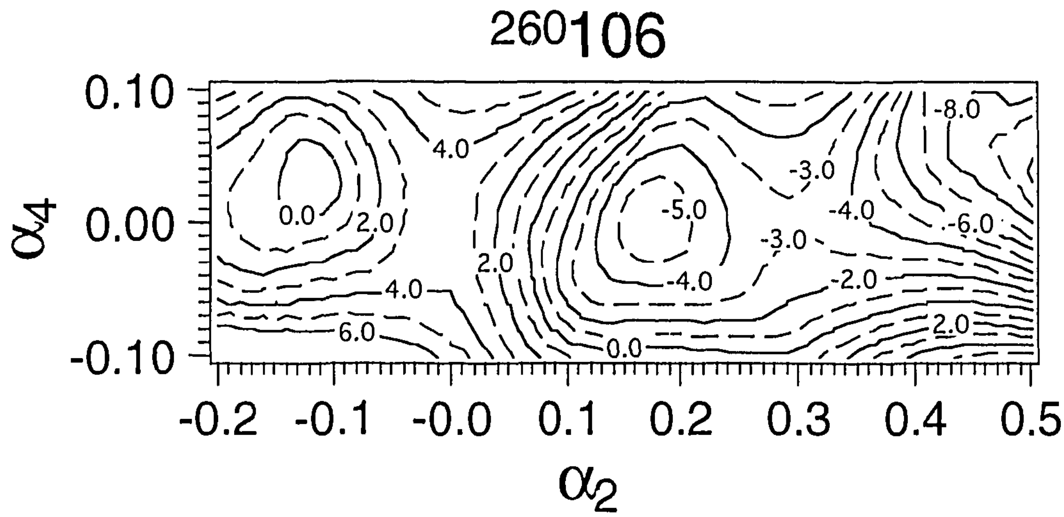

Fig. 5: Energy surface of $^{260}106$ on the deformation parameter plane (α_2, α_4)

§4. Concluding remark

The results shown in Fig. 4 can be compared with results of ref [5] in which a deformed potential is used. The ground-state deformation of $^{260}106$ calculated by our method is somewhat larger than that of ref [5], and our fission barrier is smaller.

Our previous mass formula[2] is expressed as a sum of three parts: the gross part $M^{\mathrm{TUYY}}_{\mathrm{gross}}(Z, N)$, the even-odd part $M^{\mathrm{TUYY}}_{\mathrm{even-odd}}(Z, N)$ and the shell part $M_{\mathrm{sh}}(Z, N)$. The refined shell energies $E_{\mathrm{sh}}(Z, N)$ in §3 can be adopted as $M_{\mathrm{sh}}(Z, N)$, which, at present, give the root mean square deviation of 854 keV from experimental masses. Further improvement is under way.

References

[1] M. Uno and M. Yamada, Prog. Theor. Phys., **65**, (1981), 1332

[2] T. Tachibana, M. Uno, M. Yamada and S. Yamada, Atomic Data and Nuclear Data Tables **39**, (1988), 251

[3] P. Möller and J. R. Nix, Atomic Data and Nuclear Data Tables **39**, (1988), 43

[4] H. Koura, T. Tachibana, M. Uno and M. Yamada, JAERI-Conf, 95-008, 250; M. UNO, T. Tachibana, M. Takano, H. Koura and M. Yamada, *Nuclei Far From Stability 6 / Atomic Masses and Fundamental Constants 9* (BernKastel-Kues, 1992), (IOP 132), 117

[5] R. Smolańczuk, H. V. Klapdor-Kleingrothaus and A. Sobiczewski, Acta Phys. Pol. **B24**, (1993), 457