Nuclear mass formula with shell energies obtained by a new method and its application to superheavy elements

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A nuclear mass formula is constructed which is composed of two parts, one describing the general trend of the masses as a function of Z and N and the other representing deviations of individual masses from this general trend. These deviations, referred to as shell energies, are calculated by a new method for spherical as well as deformed nuclei only with use of spherical single-particle potentials. The root-mean-square deviation from experimentally known masses is 0.68 MeV. The obtained mass formula is applicable to any nucleus with $Z \geq 2$ and $N \geq 2$. By this mass formula α-decay energies are calculated, and α-decay half-lives of superheavy elements are estimated.

1 Introduction

Our group has been investigating for years the mass formula which is composed of two parts, one representing the general trend of the masses as a function of proton and neutron numbers (Z, N) and the other representing the deviations from this general trend [1, 2, 3]. The latter may be called shell energies in a broad sense; it is caused by the shell structure and, if any, the deformation of the nucleus. The mass formula in Ref. [4], which we obtained previously and is referred to as TUYY formula in the following, was fairly successful in estimating the nuclear masses. However, it includes many adjustable parameters, and cannot be extrapolated to the region of superheavy nuclei where no empirical data to determine the necessary parameter values are available. Recently, we have solved this problem [5]. In this report we briefly explain a new method of treating deformed nuclei in which only spherical single-particle potentials are used. The mass formula obtained by this new method is capable of predicting the masses of nuclei far from stability such as very neutron- or proton-rich nuclei and superheavy nuclei. In section 2, we outline the calculation of the spherical shell energies. In section 3, we explain how to take into account the deformation effect. In section 4, we construct a mass formula. Finally, we apply our mass formula to superheavy nuclei in section 5.

2 Crude and refined spherical shell energies

We first calculate shell energies for neutron groups and for proton groups in spherical nuclei using an extreme single-particle model; we refer to them as crude shell energies. We use a spherical single-particle potential recently proposed [6, 7]. This potential reproduces fairly well the single-particle levels of 15 double-magic or magic-submagic nuclei in a wide nuclidic region ranging from ^{4}He, ^{8}He to ^{208}Pb. The potential parameters are assumed to be smooth functions of Z and N with due consideration of the charge symmetry; several parameter sets were obtained in Refs. [6, 7], and we adopt the set HD.

Once the single-particle potential of the nucleus (Z, N) is prepared, we put n neutrons or n protons in it from its bottom. Then the sum of the single-particle energies, which is denote by $E_{\mathrm{nsp}}(n; Z, N)$ (or $E_{\mathrm{psp}}(n; Z, N)$), is a function of n, Z and N. For the purpose of extracting the deviations from a general tendency in this sum, we construct a smooth function $\overline{E}_{\rm nsp}(n;Z,N)$ (or $\overline{E}_{\rm psp}(n;Z,N)$) to represent the general tendency of $E_{\rm nsp}(n;Z,N)$ (or $E_{\rm psp}(n;Z,N)$). Then, the deviations are given as

$$E_{i{\rm fl}}(n;Z,N)=E_{i{\rm sp}}(n;Z,N)-\overline{E}_{i{\rm sp}}(n;Z,N),\ \ (i={\rm n,p}). \tag{1}$$

With these deviations, we obtain the crude shell energies as

$$E_{\rm ncr}(Z,N)=E_{\rm nfl}(N;Z,N),\ \ E_{\rm pcr}(Z,N)=E_{\rm pfl}(Z;Z,N). \tag{2}$$

The subtraction of the smooth function $\overline{E}_{i{\rm sp}}(n;Z,N)$ as in Eq. (1) is made in two steps. In the first step we subtract the Thomas-Fermi energy $E_{i{\rm TF}}(n;Z,N)$. Although this first step subtracts a large part of the smooth energy, a considerable amount still remains. In the second step, we further subtract a smooth function $\Delta E_{i{\rm av}}(n;Z,N)$ (i=n, p), which should be an approximation to $\overline{E}_{i{\rm sp}}(n;Z,N)-E_{i{\rm TF}}(n;Z,N)$ (i=n, p). For details see Ref. [5].

Next, we modify these crude shell energies by taking into account the BCS-type pairing, and also make some phenomenological reduction of the shell energies; we refer to the neutron and proton shell energies thus obtained as refined spherical shell energies. In order to include the pairing effect, we take a weighted average of the crude shell energies of neighboring nuclei with the weights related to the occupation probabilities of the BCS theory. It is likely that the simple single-particle plus pairing model is not sufficient to take full account of the configuration mixing. The remaining configuration mixing will probably reduce the magnitudes of the shell energies. This effect is simply represented by a multiplication of the shell energies by a reduction factor μ (a smooth function of $N+Z$ and $N-Z$). Then we obtain the refined spherical neutron and proton shell energies $E_{\rm ns}(Z,N)$ and $E_{\rm ps}(Z,N)$.

For a spherical nucleus the nuclear shell energy is simply the sum of the refined spherical neutron and proton shell energies:

$$E_{0{\rm s}}(Z,N)=E_{\rm ns}(Z,N)+E_{\rm ps}(Z,N). \tag{3}$$

3 Deformation

The shell energy of a deformed nucleus is expressed as the sum of two parts: the intrinsic shell energy and the average deformation energy. As our method was already explained in a previous report [2], we only give a sketch of it.

3.1 Intrinsic shell energy

We first assume that the intrinsic shell energy of a deformed nucleus is expressed as a superposition of the proton and neutron shell energies of some spherical nuclei with certain mixing weights:

$$E_{\rm in}(Z,N)=\sum_{Z'}W_{\rm p}(Z';Z,N)E_{\rm ps}(Z',N'')+\sum_{N'}W_{\rm n}(N';Z,N)E_{\rm ns}(Z'',N'), \tag{4}$$

where N'' and Z'' are integers closest to NZ'/Z and ZN'/N, respectively. In this equation, the mixing weights $W_{\rm p}(Z';Z,N)$ and $W_{\rm n}(N';Z,N)$ are obtained as

$$W_{\rm n}(N';Z,N)=-\frac{1}{4\pi}\frac{d\Omega_{\rm oc}(r(N'))}{dN'}, \tag{5}$$

where $\Omega_{\rm oc}(r(N'))$ is the occupied solid angle for the radial coordinate $r(N')$. This shows that the mixing weight is related to the rate of the decrease of the occupied solid angle as r increases.

In the actual calculation, some modification is made in this procedure to get a reasonably large deformation. We use an intermediary coordinate $r_{\rm im}$ and an intermediary shape $\Omega_{\rm im}(r_{\rm im})$ defined by

$$\begin{aligned} dr_{\rm im}&=\{1-h[1-\Omega_{\rm oc}(r)/4\pi]\}dr, \quad \text{with } h=0.46,\\ \Omega_{\rm im}(r_{\rm im}){r_{\rm im}}^2dr_{\rm im}&=\Omega_{\rm oc}(r)r^2dr, \end{aligned} \tag{6}$$

and with $r_{\rm im}$ and $\Omega_{\rm im}(r_{\rm im})$ we proceed as above.

3.2 Average deformation energy

We limit the deformation to axially and reflectionally symmetric shapes and assume the same shape for the neutron group and proton group. We use uniform neutron and proton distributions with a sharp-cut surface. Then the nuclear shape is described by the following radii as a function of the polar angle θ:

$$R(\theta) = \frac{R_0}{\lambda}\left[1 + \alpha_2 \mathrm{P}_2(\cos\theta) + \alpha_4 \mathrm{P}_4(\cos\theta) + \alpha_6 \mathrm{P}_6(\cos\theta) + \cdots\right], \tag{7}$$

where $\mathrm{P}_{2i}(\cos\theta)$ $(i = 1, 2, \ldots)$ are the Legendre polynomials and α_{2i} are parameters to specify the shape. Furthermore, R_0 is the radius of the sphere whose volume is equal to that of the deformed nucleus under consideration, and this volume conservation is guaranteed by the denominator λ. We take the expansion in Eq. (7) down to the $\mathrm{P}_6(\cos\theta)$ term.

As the contributions to the average deformation energy, we consider three kinds, the changes of the surface energy ΔE_{s} and the Coulomb energy ΔE_{C}, and an energy to favor prolate shapes. The third energy is usually not considered explicitly. In the present study, however, the experimentally observed dominance of the prolate deformation is not obtained without such an energy. We assume the energy to favor prolate shapes as

$$\Delta E_{\mathrm{prl}} = -C_{\mathrm{prl1}} \alpha_2 A^{2/3} \exp\left[-C_{\mathrm{prl2}} {\alpha_2}^2\right],\ C_{\mathrm{prl1}} = 0.28,\ C_{\mathrm{prl2}} = 5, \tag{8}$$

where the factor $A^{2/3}$ is introduced since this energy is a surface effect. The average deformation energy is given as the sum of the above three energies:

$$\overline{E_{\mathrm{def}}} = \Delta E_{\mathrm{s}} + \Delta E_{\mathrm{C}} + \Delta E_{\mathrm{prl}}. \tag{9}$$

3.3 Shell energies of deformed nuclei

Once the parameter values are fixed, the shell energy of the nucleus (Z, N) is obtained by minimizing the sum of the intrinsic shell energy and the average deformation energy:

$$E_{\mathrm{sh}}(Z, N) = \min_{\alpha_2, \alpha_4, \alpha_6} \left[E_{\mathrm{in}}(Z, N) + \overline{E_{\mathrm{def}}}(Z, N)\right]. \tag{10}$$

The deformation parameters α_2, α_4 and α_6 giving the minimum energy specify the shape of the ground state.

4 Mass formula

The functional form of our mass formula is similar to the TUYY formula [4]. It consists of three parts as

$$M(Z, N) = M_{\mathrm{g}}(Z, N) + M_{\mathrm{eo}}(Z, N) + M_{\mathrm{sh}}(Z, N), \tag{11}$$

where $M_{\mathrm{g}}(Z, N)$ is the term representing the gross feature of the nuclear mass surface, $M_{\mathrm{eo}}(Z, N)$ is the even-odd term, and $M_{\mathrm{sh}}(Z, N)$ is the shell term for which we use the shell energies obtained in the last section. The functional form of the gross term and even-odd term are given in Ref. [5]. The gross term is the same as Eq. (2) of Ref. [4], but we make small modifications on the constants and coefficients.

In order to determine the values of the parameters in the gross and even-odd terms we compare the calculated masses with the Audi-Wapstra95 [8] excluding the systematics values and also excluding the nuclides with $Z = 0, 1$ and/or $N = 0, 1$. Then, 1835 masses are available. We first determine the parameters in the even-odd term by inspecting the trend of the even-odd mass differences. The parameters in the gross term are determined by the least-squares method in which we take the weight for each nuclide as $1/(\Delta_i + 0.7\ \mathrm{MeV})^2$ where Δ_i is the error in the mass of that nuclide. If the absolute magnitude of a parameter becomes too large in this least-squares method, we constrain it to a reasonable magnitude not to cause a drastic variation in light nuclei. The root-mean-square (RMS) deviation of our formula from experimental data is 680.2 keV. In Fig. 1, deviations of calculated masses from experimental data are roughly shown.

5 Application to superheavy elements (SHE)

Responding to the recent increasing interest in superheavy elements we give some results based on the new mass formula. To compare our predicted quantities with, we take two recent mass formulas, the Finite Range Droplet Model (FRDM) [9] and the Extended Thomas-Fermi Strutinsky Integral (ETFSI) [10].

5.1 Nuclear shell energies of SHE

For the mass formulas other than ours we tentatively define the shell energies as follows:

$$E_{\rm sh}(Z,N)c^2 \equiv M_{\rm th}(Z,N) - (M_{\rm g}(Z,N) + M_{\rm eo}(Z,N)). \tag{12}$$

where $M_{\rm th}(Z,N)$ are their theoretical mass values and $M_{\rm g}(Z,N)$ and $M_{\rm eo}(Z,N)$ are ours.

We show these shell energies in Figs. 2, 3 and 4. These Figures show that the three kinds of shell energies are similar to each other in the region of $Z = 90 - 110$ and $N = 136 - 160$, and slightly different in the region $Z = 110 - 130$ and $N = 180 - 190$. According to our shell energies, the alleged magicity at $Z = 114$ is not so remarkable, while the nucleus $^{310}126$ is doubly-magic although its double-magicity is not so strong as ^{132}Sn and ^{208}Pb.

5.2 Q_α and T_α of SHE

The main decay mode for the known heaviest elements is α-decay. We compare the calculated α-decay Q-values, Q_α, with other formulas. We also estimate the α-decay half-lives T_α: we use the phenomenological formula by Viola and Seaborg [11],

$$\log T_\alpha(Z,N) = (aZ + b)/\sqrt{Q_\alpha} + (cZ + d), \tag{13}$$

with

$$a = 1.66175, b = -8.5166, c = -0.20228, d = -33.9069 \text{ [12]}. \tag{14}$$

We show Q_α and T_α in Figs. 5, 6 and 7. In Fig. 5(a), our α-decay Q-values present a feature of magicity at $Z = 114$ and at $Z = 126$ as relatively wide gaps between isotope lines, while those of FRDM have a large gap only at $Z = 114$, and those of ETFSI show no gap. Our α-decay half-lives T_α depend on nuclides rather moderately compared with other predictions.

References

[1] H. Koura, T. Tachibana, M. Uno and M. Yamada, JAERI-Conf **95-008** (1995) 250.
[2] H. Koura, T. Tachibana, M. Uno and M. Yamada, JAERI-Conf **96-008** (1996) 284.
[3] H. Koura, M. Uno, T. Tachibana and M. Yamada, Int. Conf. on Exotic Nuclei and Atomic Masses (ENAM98), Bellaire, Michigan, 1998, ed. B.M. Sherill, D.J. Morrissey, and C.N. Davids, (The American Institute of Physics, 1998) p. 114.
[4] T. Tachibana, M. Uno, M. Yamada and S. Yamada, Atomic Data and Nuclear Data Tables **39** (1988) 251.
[5] H. Koura, M. Uno, T. Tachibana and M. Yamada, Nucl. Phys., submitted for publication.
[6] H. Koura and M. Yamada, Nucl. Phys., to be published.
[7] H. Koura and M. Yamada, Technical Report of Advanced Research Institute for Science and Engineering, Waseda University, **No.99-14** (1999) 1.
[8] G. Audi and A.H. Wapstra, Nucl. Phys. **A 595** (1995) 409.
[9] P. Möller, J.R. Nix, W.D. Myers and J. Swiatecki, Atomic Data and Nuclear Data Tables **59**, (1995) 185.
[10] Y. Aboussir, J.M. Pearson, A.K. Dutta and F. Tondeur, Atomic Data and Nuclear Data Tables **61**, (1995) 127.
[11] V.E. Viola, Jr. and G.T. Seaborg, J. Inorg. Nucl. Chem. **28** (1966) 741.
[12] Z. Patyk, J. Skalski, A. Sobiczewski and S. Ćwiok, Nucl. Phys. **A 502** (1989) 591c.

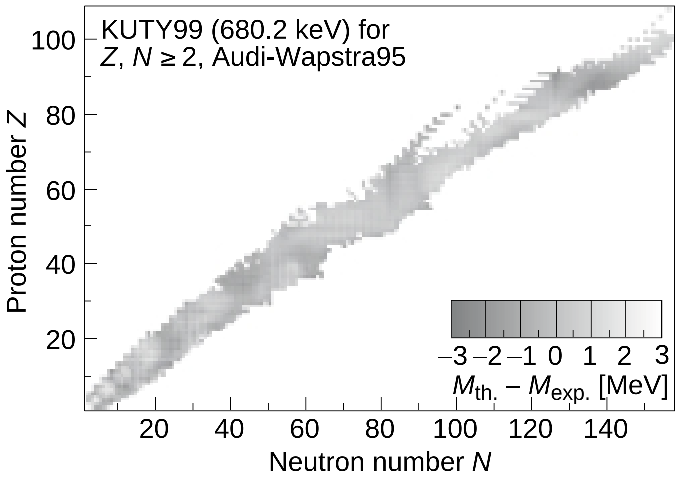


Figure 1: Calculated masses minus experimental masses.

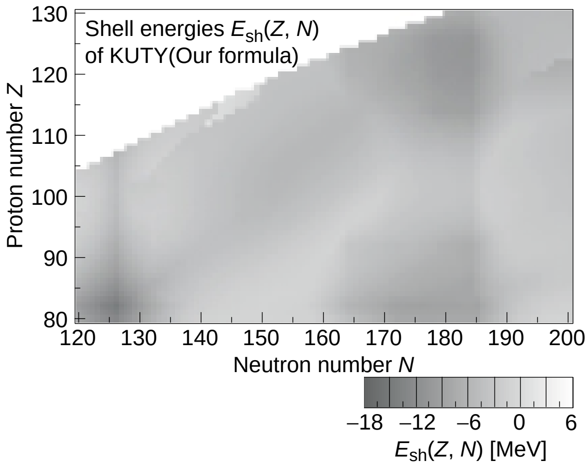


Figure 2: Shell energy of KUTY formula [5].

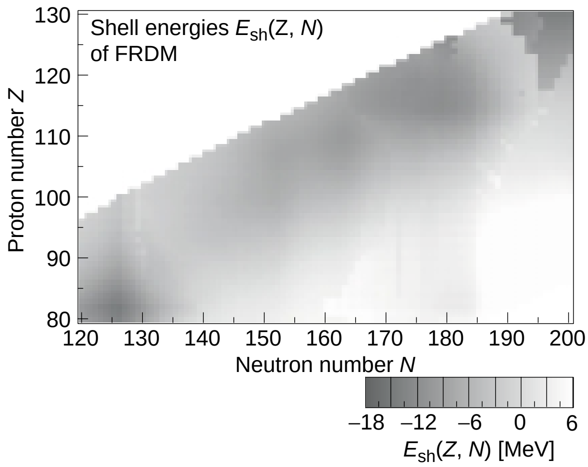


Figure 3: Shell energy of FRDM formula [9] defined by Eq. (12).

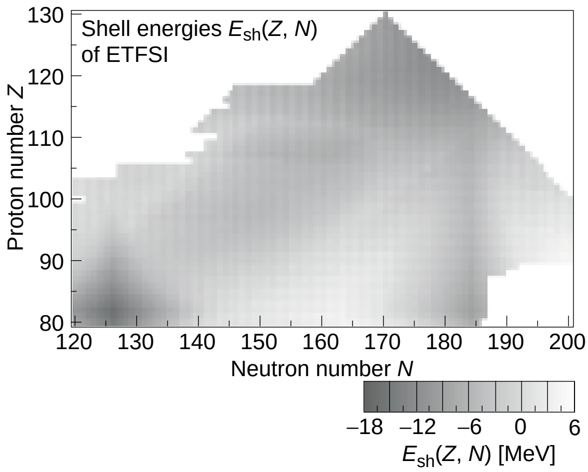
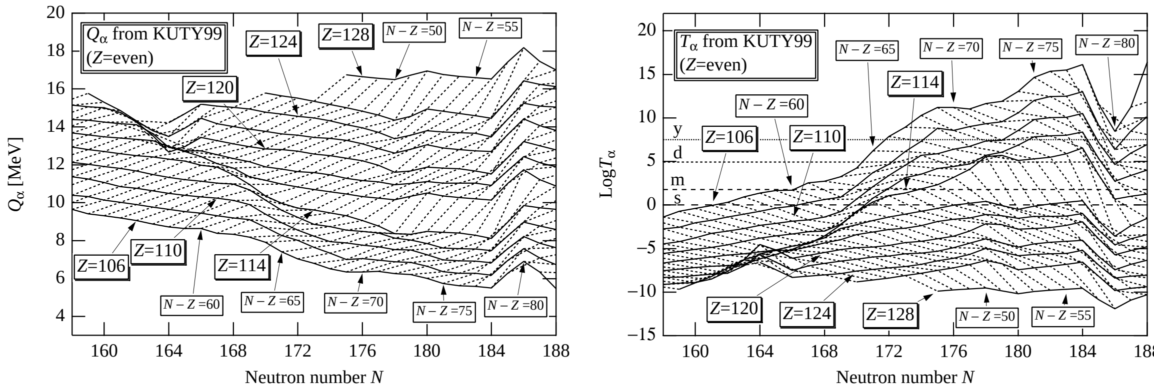
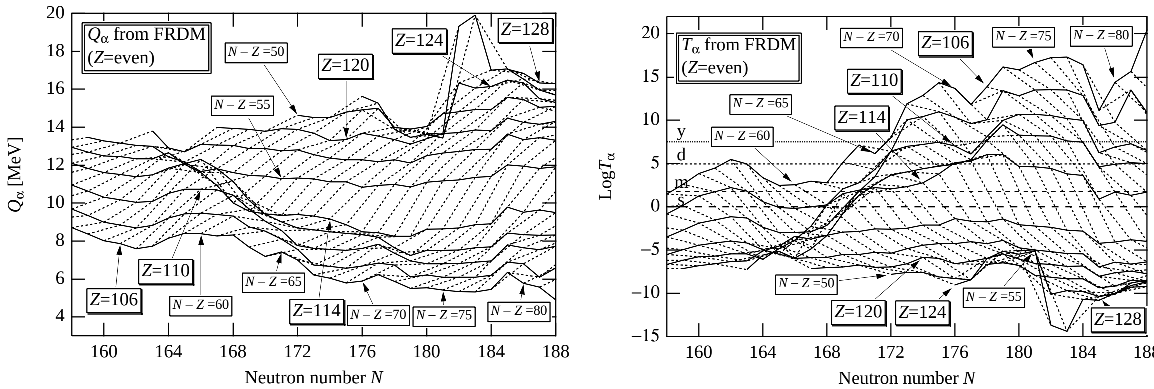


Figure 4: Shell energy of ETFSI formula [10] defined by Eq. (12).



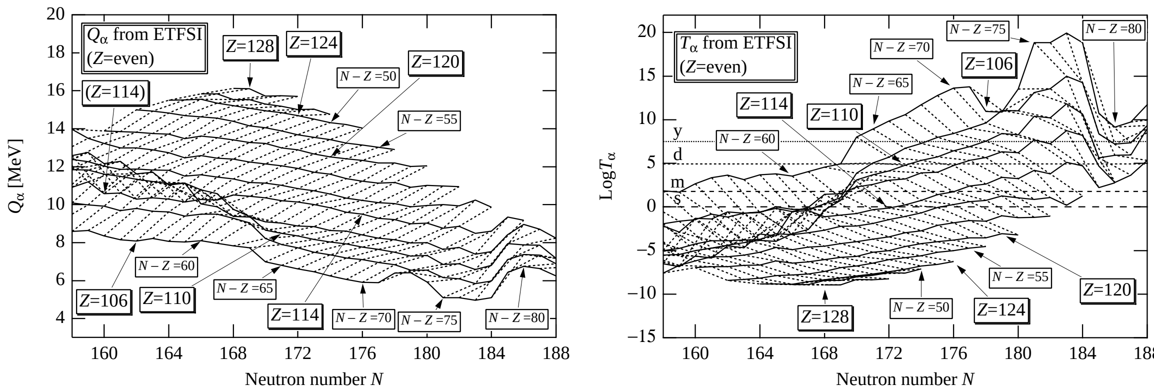
(a) (b)

Figure 5: Q_α (a) and T_α (b) of superheavy elements from KUTY formula [5] for even Z. The solid lines connect isotopes and dashed lines connect α-decay chains.



(a) (b)

Figure 6: Q_α (a) and T_α (b) of superheavy elements from FRDM formula [9] for even Z. Same notation as in Fig. 5.



(a) (b)

Figure 7: Q_α (a) and T_α (b) of superheavy elements from ETFSI formula [10] for even Z. Same notation as in Fig. 5.