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Surface diffuseness correction in global mass formula

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ABSTRACT

By taking into account the surface diffuseness correction for unstable nuclei, the accuracy of the macroscopic–microscopic mass formula is further improved. The rms deviation with respect to essentially all the available mass data falls to 298 keV, crossing the 0.3 MeV accuracy threshold for the first time within the mean-field framework. Considering the surface effect of the symmetry potential which plays an important role in the evolution of the "neutron skin" toward the "neutron halo" of nuclei approaching the neutron drip line, we obtain an optimal value of the symmetry energy coefficient $J = 30.16$ MeV. With an accuracy of 258 keV for all the available neutron separation energies and of 237 keV for the α-decay Q-values of super-heavy nuclei, the proposed mass formula is particularly important not only for the reliable description of the r process of nucleosynthesis but also for the study of the synthesis of super-heavy nuclei.

As one of the basic quantities in nuclear physics, the nuclear masses play a key role not only in the study of nuclear structure and reactions, but also in understanding the origin of elements in the universe. The nuclear mass formulas [1–16] are of significant importance for describing the global nuclear properties and exploring the exotic structure of the extremely neutron-rich nuclei such as the halo phenomenon, the structure of super-heavy nuclei and their decay properties [17–20], as well as the nuclear symmetry energy [21–24] which probes the isospin part of nuclear forces and intimately relates to the behavior of neutron stars. For finite nuclei, the diffuseness of the nuclear surface, which provides a measure of the thickness of the surface region and is intimately related to the nuclear surface energy [25], is an important degree-of-freedom in the calculations of nuclear masses. The notions "neutron skin" and "neutron halo" are adopted from Ref. [26] to describe the two extreme cases of two-parameter Fermi distributions of the neutron and proton peripheral density: the former refers to the case with equal diffuseness parameters for protons and neutrons and a larger half-density radius for the neutrons; the latter to the case with a much larger surface diffuseness for neutrons. For most stable nuclei, the corresponding density distribution is similar to the "neutron skin-type", with a typical value around 0.5 fm for the surface diffuseness. For nuclei near the neutron drip line, such as ^{11}Li [27], ^{22}C [28] and the giant-halo nuclei [29,30], the neutron matter extends much further, which implies the enhancement of the neutron surface diffuseness for these extremely neutron-rich nuclei. In nuclear mass calculations, all available global mass formulas, including the recent universal nuclear energy density functional (UNEDF) [31], have not yet properly considered the surface diffuseness of exotic nuclei near the drip lines. It is well known that the symmetry energy plays an important role in the structure of neutron-rich nuclei. The thickness of neutron skin of nuclei has been explored to be linearly correlated with the slope of symmetry energy and the isospin asymmetry $I = (N - Z)/A$ of nuclei [26,32]. On the other hand, the physics behind the skin and halo has been revealed as a spatial demonstration of shell effect from the relativistic continuum Hartree–Bogoliubov calculations [33]. It is therefore necessary to investigate the influence of the surface diffuseness on the nuclear symmetry energy and shell correction for nuclei approaching the drip lines.

Inspired by the Skyrme energy-density functional, a macroscopic–microscopic mass formula, Weizsäcker–Skyrme (WS) formula [13–15], was proposed with an rms deviation of 336 keV with respect to the 2149 measured masses [34] in 2003 Atomic Mass Evaluation (AME). The Duflo–Zuker formula [12] with an rms deviation of 360 keV is also successful for the mass predictions. However, both of these two successful global mass formulas can not yet cross the 0.3 MeV accuracy threshold. In the WS formula,

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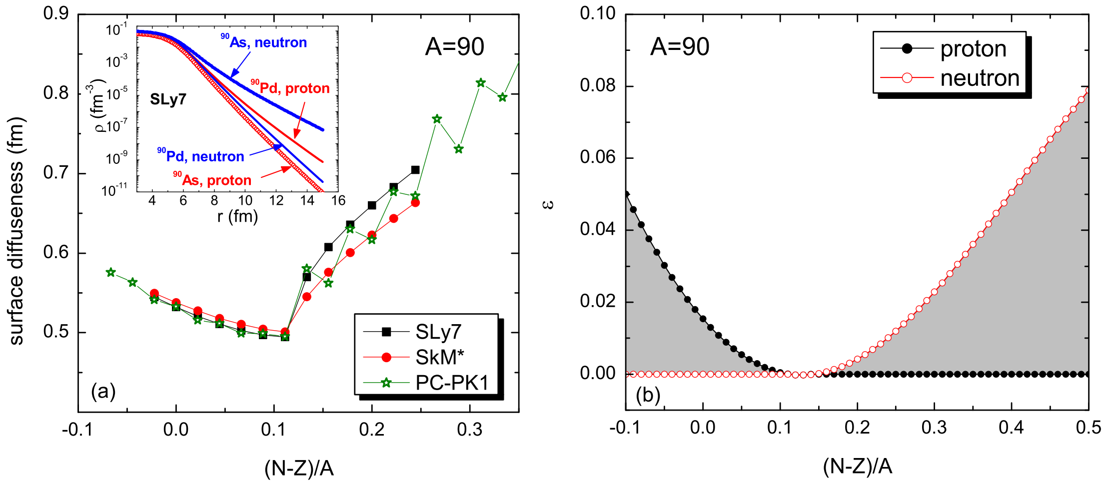

Fig. 1. (Color online.) (a) Calculated surface diffuseness of nuclei with $A = 90$. The squares and circles denote the results of the Skyrme energy density functional with SLy7 [39] and SkM* [40], respectively. The stars denote the results of the relativistic density functional calculations with PC-PK1 [7], in which the staggering is due to the influence of the pairing in the PC-PK1 calculations. The inserted figure in (a) shows the density distributions of ^{90}As and ^{90}Pd with SLy7. (b) Correction factor $\varepsilon = (I - I_0)^2 - I^4$ for the surface diffuseness in the single-particle potential with $I_0 = 0.4A/(A + 200)$. The solid and open circles denote the results for protons and neutrons, respectively.

the axially deformed Woods–Saxon potential, as a phenomenological mean-field, is adopted to obtain the single-particle levels of nuclei. With the same value for the protons and neutrons, the surface diffuseness a of the potential is set as a constant for all nuclei in the previous calculations. The obtained symmetry energy coefficient is about 29 MeV which is slightly smaller than the extracted one ($J \approx 30$–32 MeV) from some different approaches [3,5,21–24, 35–37]. The value of the symmetry coefficient can significantly affect the symmetry energy and thus the masses of nuclei near the neutron drip line. For example, the variation of the symmetry coefficient by one MeV can result in the variation of the symmetry energy by 33 MeV for the neutron-rich nuclei ^{176}Sn. For more accurate description of the masses of drip line nuclei, it is required to further constrain the coefficient of the symmetry energy based on the new measured masses of nuclei far from stability. In this work, we attempt to further improve the WS formula by considering the nuclear surface diffuseness effect together with the latest nuclear mass datasets AME2012 [38].

To explore the correlation between the isospin asymmetry and the nuclear surface diffuseness, we first study the evolution of the nuclear density distribution for a series of isobaric nuclei by using the non-relativistic SLy7 [39] and SkM* [40] and the relativistic PC-PK1 [7] density functionals. From the mean-field point of view, the properties of all the nucleons in the nuclei are determined by the mean potential provided by their interaction with the other nucleons. Therefore the study of the isospin dependence on the potential, which becomes highly diffuse near the particle drip line, is crucial to understanding unstable nuclei [41]. Fig. 1(a) shows the calculated nuclear surface diffuseness for nuclei with $A = 90$ as a function of isospin asymmetry. Here, the value of nuclear surface diffuseness is extracted from fitting the calculated total density distribution $\rho(r)$ in the range of $r \le 15$ fm with the Fermi function (under a logarithmic scale). Both the non-relativistic and relativistic density functional calculations show the enhancement of the nuclear surface diffuseness for nuclei far from stability. To illustrate this point more clearly, the sub-figure in Fig. 1(a) shows the density distributions of ^{90}As and ^{90}Pd. For the neutron-rich nucleus ^{90}As, the tail of the density distribution for the neutrons is much longer than that for the protons. For the proton-rich ^{90}Pd, in contrast, the tail for the protons is just a little longer than that for the neutrons due to the Coulomb barrier. Simultaneously, we note that the surface diffuseness for protons (neutrons) in the neutron (proton)-rich nuclei does not change appreciably with the isospin asymmetry, which was also observed in the Sn and Pb isotopic chains [42]. The enhancement of the surface diffuseness for the very neutron-rich nuclei implies that the "neutron-skin" structure tends to evolve toward the "neutron-halo" structure for nuclei approaching the neutron drip line since the repulsion of the symmetry potential will "push" the extra-neutrons to the very low density region. At the neutron-deficient side, the extra-protons will be pushed to the surface region due to the Coulomb interaction and the symmetry potential.

Although the macroscopic–microscopic approaches are found to be the most accurate ones in the description of atomic masses [43], the surface diffuseness effect for nuclei near the drip lines could affect the accuracy of the predictions. In the WS mass formula, the total energy of a nucleus is written as a sum of the liquid-drop energy, the Strutinsky shell correction and the residual correction. The liquid-drop energy of a spherical nucleus $E_{\rm LD}(A, Z)$ is described by a modified Bethe–Weizsäcker mass formula,

$$E_{\rm LD}(A,Z) = a_v A + a_s A^{2/3} + E_C + a_{\rm sym} I^2 A f_s + a_{\rm pair} A^{-1/3}\delta_{np} + \Delta_W, \quad (1)$$

with the isospin asymmetry $I = (N - Z)/A$. $E_C = a_c \frac{Z^2}{A^{1/3}}(1 - 0.76Z^{-2/3})$ and Δ_W denote the Coulomb energy term and the Wigner correction term for heavy nuclei [15], respectively. The symmetry energy coefficient of finite nuclei is expressed as $a_{\rm sym} = c_{\rm sym}[1 - \frac{\kappa}{A^{1/3}} + \xi \frac{2-|I|}{2+|I|A}]$ and the form of the correction factor f_s for the symmetry energy will be presented in Eq. (6) and Fig. 1(b). The $a_{\rm pair}$ term empirically describes the odd–even staggering effect [13]. Here, the I^2 term in the isospin dependence of δ_{np} is further introduced for a better description of the masses of even-A nuclei, with $\delta_{np} = |I| - I^2$ for the odd–odd nuclei and $\delta_{np} = (2 - |I| - I^2)17/16$ for the even–even nuclei.

To obtain the microscopic shell correction with the traditional Strutinsky procedure, the single particle levels of a nucleus are calculated by using the code WSBETA [44]. The central potential V is described by an axially deformed Woods–Saxon form

$$V(\vec{r}) = \frac{V_q}{1 + \exp[\frac{r - \mathcal{R}(\theta)}{a}]}, \quad (2)$$