ASYMMETRY AND SPIN-ORBIT EFFECTS IN BINDING ENERGY IN THE EFFECTIVE NUCLEAR SURFACE APPROXIMATION

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Abstract

Isoscalar and isovector particle densities are derived analytically by using the approximation of a sharp edged nucleus within the local energy density approach with the proton-neutron asymmetry and spin-orbit effects. Equations for the effective nuclear-surface shapes as collective variables are derived up to the higher order corrections in the form of the macroscopic boundary conditions. The analytical expressions for the isoscalar and isovector tension coefficients of the nuclear surface binding energy and the finite-size corrections to the β stability line are obtained.

1 Introduction

The simple and accurate solution of some problems involving the particle density distributions uses the nuclear effective surface (ES) approximation[1, 2, 3, 4]. It exploits the property of saturation of the nuclear matter and a narrow diffuse-edge region in finite nuclei. The ES is defined as the location of points of the density gradient maximum. The coordinate system related locally to the ES is specified by a distance ξ from the given point to the surface and tangent coordinate η (see Fig. 1). The variational condition of the nuclear energy minimum at fixed other integrals of motion within the local energy density theory, in particular, the extended Thomas-Fermi (ETF) approach[5, 6] is simplified much in the ξ, η coordinates for any deformations by using expansion in small parameter a/R ∼ A^{-1/3} ≪ 1 for heavy enough nuclei (a is the diffuse edge thickness of the nucleus, and R its mean curvature radius). The accuracy of the ES approximation in the ETF approach was checked[4] by comparing results of the Hartree-Fock (HF) and ETF theories based on Skyrme forces[5, 7] without spin-orbit and asymmetry terms. Within the ES approximation a rather reasonable agreement of the calculations with the experimental data on a mean particle-number dependence on the excitation energies and reduced transition probabilities of the low-lying collective states of non-magic nuclei was found[8]. In the present work, we extend the ES approach[4] taking into account the spin-orbit and the asymmetry effects in nuclei.

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2 LOCAL ENERGY DENSITY AND CONSTRAINTS

We begin with the nuclear energy $E$ within a local energy functional approach\cite{5, 7}:

$$E = \int dr \mathcal{E}[\rho_+(r), \rho_-(r)], \quad \mathcal{E}(\rho_+, \rho_-) \approx -b_v \rho_+ \rho_- + \frac{b_{\text{sym}}}{2} \mathcal{X}^2 \rho_+ + \frac{e}{4} (1 - \mathcal{X}) \Phi \rho_+$$

$$+ \rho_+ [\varepsilon_+(\rho_+) - \varepsilon_-] + \left( A + B \rho_+ + \frac{\Gamma}{4 \rho_+} \right) (\nabla \rho_+)^2 + A_- (\nabla \rho_-)^2,$$

(1)

where $\mathcal{E}[\rho_+(r), \rho_-(r)]$ is the energy density as a function of the isoscalar $\rho_+$ and isovector $\rho_-$ particle densities. It overlaps approximately most of the realistic Skyrme forces\cite{7}. $\rho_{\pm} = \rho_n \pm \rho_p$, $\mathcal{X} = (N - Z)/A$, $N = \int dr \rho_n$, $Z = \int dr \rho_p$, $A = N + Z$, $\Phi$ is the Coulomb potential and $\overline{\Phi}$ is its average up to a small exchange component \cite{1, 2, 10}. As usually, $\mathcal{E}$ of (1) contains the volume, and the surface terms without and with the gradient density terms \cite{1, 3, 4}, $b_v = 16$ MeV is the separation energy per particle and $b_{\text{sym}} = 60$ MeV is the symmetry energy constant of the nuclear matter. The semiclassical $\hbar$ corrections appear through $\Gamma = \hbar^2/18m$ in the ETF kinetic energy density\cite{5, 6}, $m$ is the nucleon mass. In (1), we have neglected relatively small isovector (spin-orbit and semiclassical) corrections. The isoscalar surface energy density part, independent of the density gradient terms, is determined by the function $\varepsilon_+(\rho_+)$ which satisfies the saturation condition:

$$\varepsilon_+(\overline{\rho}) = 0, \quad \frac{d\varepsilon_+(\overline{\rho})}{d\rho_+} = 0,$$

(2)

where $\overline{\rho} = 3/4\pi r_0^3 \approx 0.16$ fm$^{-3}$ is the density of the infinite nuclear matter, $r_0 = R/A^{1/3}$ is constant independent of $A$. For the isovector component one has

$$\varepsilon_- = \frac{b_{\text{sym}}}{2} \left( \mathcal{X}^2 - \rho_+^2 / \rho_+^2 \right) - \frac{e}{4} \left[ (1 - \rho_- / \rho_+) \Phi - (1 - \mathcal{X}) \overline{\Phi} \right].$$

(3)

The spin-orbit gradient terms in (1) are defined with a constant: $B = -9mW_0^2/16\hbar^2$, $W_0 = 100 - 130$ MeV fm$^3$ (see refs. 5, 7).

From the condition of the energy $E$ (1) minimum together with the constraints for the fixed particle number $A$, neutron excess $N - Z$, and deformation $Q$ of the nucleus\cite{1, 2, 9}:

$$A = \int dr \rho_+(r), \quad N - Z = \int dr \rho_-(r), \quad Q = \int dr \rho_+(r) q(r),$$

(4)
one arrives at the variational Lagrange equations:
\[
\frac{\delta E}{\delta \rho_+} - \lambda_+ - \lambda_Q q = 0, \quad \frac{\delta E}{\delta \rho_-} - \lambda_- = 0.
\] (5)

Here, \( \lambda_+ \), \( \lambda_- \) and \( \lambda_Q \) are the corresponding Lagrange multipliers where \( \lambda_+ \) and \( \lambda_- \) are the isoscalar and isovector chemical potentials, respectively.

### 3 ISOSCALAR AND ISOVECTOR PARTICLE DENSITIES

*In the nuclear volume*, up to the second order in \( \rho_+ - \overline{\rho} \) one gets\cite{1, 3, 4}:
\[
\varepsilon_+ (\rho_+) = \frac{K}{18 \overline{\rho}^2} (\rho_+ - \overline{\rho})^2, \quad \varepsilon(w) = \frac{\varepsilon_+}{b_v} = (1 - w)^2, \quad w = \frac{\rho_+}{\overline{\rho}}.
\] (6)

where \( K \) is the incompressibility of the infinite nuclear matter. From the Lagrange equations (5) one finds for the volume densities \( \rho_\pm^{(v)} \):
\[
\rho_+^{(v)} \approx \overline{\rho} \left( 1 + \frac{9 \Lambda_{\text{tot}}^{(+)} K}{b_v} \right), \quad \rho_-^{(v)} \approx \overline{\rho} \left( \chi + \frac{\Lambda_{\text{tot}}^{(-)} b_{\text{sym}}}{b_v} \right).
\] (7)

Small finite-size corrections of the order of \( a/R \sim aH \) (\( H \) is a mean ES curvature) are determined by the surface components of the corresponding chemical potentials:
\[
\Lambda_{\text{tot}}^{(+)} = \lambda_+ + b_v - \frac{b_{\text{sym}}}{2} \chi^2 - \frac{c}{4} \overline{\Phi} + \lambda_Q q(r) \sim aH \sim a/R \sim A^{-1/3},
\]
\[
\Lambda_{\text{tot}}^{(-)} = \lambda_- - b_{\text{sym}} \chi + \frac{c}{4} \overline{\Phi} \sim aH.
\] (8)

*For the dimensionless isoscalar density \( w(x) \) (6), from the first equation (5), up to the leading order in \( a/R \) one obtains the ordinary first-order differential equation:*
\[
\frac{dw}{dx} = -w \sqrt{\frac{\varepsilon(w)}{w + \beta w^2 + \gamma}}, \quad x = \frac{\xi}{a}, \quad a = \sqrt{\frac{A}{18 \overline{\rho}^2} \frac{K}{b_v^2}},
\] (9)

where \( \beta = \overline{\Phi} \frac{\Lambda}{A}, \ \gamma = \Gamma / 4 \overline{\Phi} A \). By differentiating equation (9) one finds the boundary condition from the definition of the ES: \( \partial^2 w / \partial x^2 = 0 \) at \( x = 0 \) (\( \xi = 0 \)),
\[
(w_0 - \beta w_0^2 - \gamma) \varepsilon(w_0) + w_0 (w_0 + \beta w_0^2 + \gamma) \left( \frac{dx(w)}{dw} \right)_{w=w_0} = 0,
\] (10)

together with the condition of the exponentially vanishing the density outside the nucleus: \( w \sim \exp(-x) = \exp(-\xi/a) \). Solving the problem (9), (10), one arrives at the solution in the inverse form \( x(w) \):
\[
x = - \int_{w_0}^w \frac{d\tau}{\tau} \sqrt{\frac{\tau + \beta \tau^2 + \gamma}{\varepsilon(\tau)}}.
\] (11)
With the quadratic approximation (6) for $\epsilon(w)$ one gets the analytical solutions in terms of the algebraic, trigonometric and logarithmic functions. For $\beta = \gamma = 0$ it simplifies to $w(x) = \tanh^2 \left( (x - x_0)/2 \right)$ for $x \leq x_0 = 2 \arctanh \left( 1/\sqrt{3} \right)$ and zero for $x$ outside the nucleus[4]. In Fig. 2 (left) the influence of the semiclassical correction to $w(x)$ is shown by comparing the $\gamma = 0$ (dashed line) and the “exact” (thin solid line) cases. This correction is small everywhere, besides the quantum tail outside the nucleus for $x \geq 1$. Almost the same results one obtains for the SkM* and SLy7 forces[7]. One should also notice a rather big effect of the spin-orbit interaction as compared to the simplest analytical solution at $\beta = \gamma = 0$.

We found also a good convergence of the expansion of the $\epsilon(w)$ in powers of $1 - w$ in the density solution (11) by comparing the exact numerical function[7] $\epsilon(w)$ to its approximate solution (6). The agreement is within a precision of the line thickness. Fig. 2 (right) presents a weak sensitivity of the isoscalar solution $w(x)$ (11) on the different Skyrme forces with (6) for $\epsilon(w)$.

\[ w(x) = \tanh^2 \left( (x - x_0)/2 \right) \quad \text{for} \quad x \leq x_0 = 2 \arctanh \left( 1/\sqrt{3} \right) \quad \text{and zero for} \quad x \text{outside the nucleus}[4]. \]

For the isovector density up to the leading order in $a/R$, after simple transformations one finds the equation and the boundary condition in the form

\[ \frac{dw_-}{dw} = c_{\text{sym}} \sqrt{\frac{1 + \beta w}{\epsilon(w)}} \sqrt{1 - \frac{w^2}{w'_2}}, \quad w_-(1) = 1, \quad w_- = \frac{\rho_-}{\rho'_-} \approx \frac{\rho_-}{\rho'_-}, \quad (12) \]

where $c_{\text{sym}} = a \sqrt{-b_{\text{sym}}/2p A_-}$. Up to the leading order of the ES approximation in $a/R$, one obtains the analytical solution through the expansion in powers of $1 - w$,

\[ w_- = w \cos \left[ u(w) \right], \quad u(w) = \frac{1 - w}{c_{\text{sym}} \sqrt{1 + \beta}} \left[ 1 + \frac{1 - w}{c_{\text{sym}} (1 + \beta) + \beta/2} \right]. \quad (13) \]

The dependence of the dimensionless isovector density $w_-(x)$ (13) on the semiclassical and spin-orbit effects versus the corresponding results for the density $w(x)$ (11) are shown in Fig. 3 (left). A weak sensitivity of the dimensionless isovector density $w_-$ on the choice of the Skyrme forces is seen in Fig. 3 (right).

Fig. 2: Density $w(x)$ (11) (left) as a function of $x = \xi/a$ and its comparison (right) for several Skyrme forces[7] ($n = 5-7, 230a$ and 230b in SLyn) for $\epsilon(w)$ (6).
4 ES EQUATIONS AND LDM BOUNDARY CONDITIONS

For more exact isoscalar particle density we calculate the main terms of higher order in the parameter $a/R$ in the first equation (5). Integrating this equation over the ES in normal-to-surface $\xi$ direction and using the equation (9) up to the leading order in $a/R$, one arrives at the differential equation

$$P_+|_{ES} = P_s^{(+)} + \mathcal{P} A_{tot}^{(+)} = \left\{ \frac{K}{2p^2} (\rho_- - p) \left[ 1 + \frac{3}{2p^2} (\rho_- - p) \right] + \frac{b_{\text{sym}}}{2p^2} (\rho_-)^2 \right. $$

$$ - \left. \frac{e^2}{4} \left[ \frac{d}{d\rho_+} ((\rho_+ - \rho_-)\Phi) - \Phi \right] \right\}^{(v)}, \quad P_s^{(+)} = 2\sigma_+ H. \tag{14}$$

This equation can be considered with respect to the unknown sought profile shape $y = Y(\eta)$ of the ES in the cylindrical coordinates $y, z$ with the symmetry axis $z$ (see Fig. 1) through the curvature $H = (1/R_1 + 1/R_2)/2$ in terms of the main ES curvature radii\[1, 3\]

$$R_1 = LY(\eta), \quad R_2 = -L^2 / (\partial^2 Y / \partial \eta^2), \quad L = \left[ 1 + (\partial Y(\eta) / \partial \eta)^2 \right]^{1/2}. \tag{15}$$

Fig. 3: Isovector density $w_-(x)$ (13) compared to the isoscalar one $w(x)$ (11) as a function of $x = \xi/a$ within the approximation (6) to $\epsilon(w)$ calculated for the same SLy7 forces (left) and $w_-(x)$ for several Skyrme forces\[7\] (right).

Eq. (14) is associated with the macroscopic boundary condition\[10, 11, 12\] with the isoscalar capillary surface pressure $P_s^{(+)}$ which is proportional to the surface tension coefficient $\sigma_+$:

$$\sigma_+ \approx 2 \int_{-\infty}^{\infty} d\xi \left( A + B \rho_+ + \frac{\Gamma}{4\rho_+} \right) \left( \frac{\partial \rho_+}{\partial \xi} \right)^2. \tag{16}$$

For more exact isovector particle density similarly one obtains the isovector macroscopic boundary condition\[12\],

$$P_\pm|_{ES} = P_s^{(-)}, \quad P_+ = \mathcal{P} A_{tot}^{(-)} = \mathcal{X} \left[ b_{\text{sym}} (\rho_- - p - \mathcal{X}) - \frac{e}{4} \left( \Phi - \mathcal{X} \right) \right]^{(v)}, \tag{17}$$
with the isovector surface pressure

\[ P_s^{(-)} = 2\sigma_- H, \quad \sigma_- \approx 2A - \int_{-\infty}^{\infty} d\xi \left( \frac{\partial \rho}{\partial \xi} \right)^2, \quad (18) \]

where \( \sigma_- \) is the isovector tension coefficient.

### 5 SURFACE ENERGY

The nuclear energy \( E = E_v + E_s \) (1) in the ES approximation is split into the volume, \( E_v = -b_v A + b_{sym}(N - Z)^2/2A + \epsilon Z\Phi/4 \), and the surface terms:

\[ E_s = \sigma S = \left( b_s^{(+)} + b_s^{(-)} \right) S/4\pi r_0^2, \quad \sigma = \sigma_+ + \sigma_-, \quad b_s^{(\pm)} = 4\pi r_0^2 \sigma_\pm, \quad (19) \]

where \( S \) is the surface area of the ES. The energy \( E_s \) (19) is determined by the sum of the isoscalar \( b_s^{(+)} \) and isovector \( b_s^{(-)} \) surface energy constants. These constants are proportional to the same tension coefficients \( \sigma_\pm \) which appear in (16) and (18) and expressed through the surface pressures in (14) and (18), respectively,

\[ b_s^{(+)} = \frac{54ab_v^2}{Kr_0} \int_0^1 dw \sqrt{(w + \beta w^2 + \gamma)\epsilon(w)}, \quad (20) \]

\[ b_s^{(-)} = 108\alpha_\Lambda A^2 ab_w^2 \frac{1}{Kr_0} \int_0^1 dw \frac{\sqrt{w(1-w)}}{\sqrt{1+\beta w}} \{ \cos[u(w)] - w \sin[u(w)] u'(w) \}^2, \quad (21) \]

where \( \alpha_\Lambda = A_- / A \) and see (13) for \( u(w) \). Simple expressions for constants (20) and (21) in terms of the algebraic and trigonometric functions can be easily obtained by calculating explicitly the integrals over \( w \) in the above equations with \( \epsilon(w) \) taken from eq.(6). Neglecting relatively small spin-orbit terms and semiclassical corrections one finds the approximate relationship between the isovector and the isoscalar energy constants, \( b_s^\approx = \alpha_\Lambda \Lambda^2 b_s^\approx \).

In Table 1 the analytical, \( b_{s,an} \) with the approximated (6) for \( \epsilon(w) \), the numerical, \( b_{s,num} \) with the exact \( \epsilon(w) \), and \( b_s^{(+)} \) from ref.7 are shown for all Skyrme forces. One can see a very good agreement between all these calculations, besides of SIII. Modula of the isovector constants for the Lyon Skyrme forces SLyn[7] are much larger than for other ones. The precision of the spin-orbit and semiclassical terms of the isovector energy density part (1) is not enough accurate for all considered Skyrme interactions as the isovector surface tension \( \sigma_- \) which appears in the surface energy (19) becomes inconsistent with that of the capillary isovector pressure (17), (18). These terms can be improved by fitting to more detailed experimental information.

The \( \beta \)-stability line is determined by the equivalence of the neutron and proton chemical potentials, \( \lambda_- = \lambda_n - \lambda_p = 0 \), and \( \Lambda_{tot}^{(-)} = 2b_s^{(-)} H/4\pi r_0^2 \Phi \), according to (8), (17) and (18). With the finite-size correction, one obtains \( \Lambda \approx \Lambda_0 \left( 1 - 2b_s^{(-)} r_0 H/3b_{sym} \Lambda_0^2 \right) \), where \( \Lambda_0 \approx 3A^{2/3}e^2/10r_0 b_{sym} \) is the leading term[10].

### 6 CONCLUSIONS

The asymmetry and spin-orbit terms of the energy density within the ETF with Skyrme forces were taken into account analytically by using expansion in \( a/R \ll 1 \) of the ES at any deformation. We
Table 1: The isoscalar (20) and isovector (21) energy surface constants \( b^\pm \) with Skyrme parameters [7].

|          | SkM  | SIII | SGII | SLy230a | SLy230b | SLy4  | SLy6  | SLy7  |
|----------|------|------|------|---------|---------|-------|-------|-------|
| \( b^+_\text{an} \) | 17.1 | 11.8 | 15.3 | 17.3    | 17.5    | 17.5  | 17.5  | 15.9  |
| \( b^+_\text{num} \) | 18.5 | 11.6 | 16.5 | 18.5    | 18.7    | 18.7  | 18.7  | 17.0  |
| \( b^+_\text{sym} \)  | 16.0 | 17.0 | 14.8 | 16.9    | 16.7    | 18.1  | 17.4  | 17.0  |
| \( b^-/A^2 \)        | -3.23| -3.72| -1.08| -7.61   | -26.3   | -26.3 | -15.7 | -10.5 |

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