Surface energy of nuclear matter above and below neutron drip with the Skyrme-type effective interactions

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Abstract. Neutron star crust consists of highly neutron excess nuclei, which are inaccessible for laboratory experiments. In the deepest region of the crust (so-called inner crust, located after the neutron drip) atomic nuclei are immersed into the sea of degenerate unbound neutrons. Study of the crust structure and equation of state in such conditions relies on the theoretical nuclear mass models. In particular, it is convenient to use the compressible liquid drop model, which contains the surface tension term. A thermodynamically consistent description must take into account adsorption of neutrons on the nucleus surface (neutron skin) and dependence of surface tension on matter properties in two-phase equilibrium. We calculate the surface tension of nuclear matter by the extended Thomas-Fermi approach. For this aim, we parametrize the number density profile of the two-phase system by Fermi-Dirac type functions, totally containing 5 parameters, and minimize the thermodynamic potential $\Omega$ to obtain equilibrium configuration. We use Skyrme-type nuclear interactions SLy4 and BSk24, fulfilling experimental data of atomic nuclei, observational constraints on the maximal neutron star mass and theoretical calculations of high-density nuclear matter. The results are presented as a function of neutron chemical potential, which is useful for compressible liquid drop models in the inner crust of a neutron star.

1. Introduction
The equation of state that couples pressure and density is a prime component of neutron star physics. Modeling the equation of state of strongly interacting nucleons in the core of the star is complicated theoretical and numerical problem, even in the zero-temperature limit which is applicable for neutron star interiors (see, for example, [1]). There are many attempts for microscopic calculations of the equation of state of the superdense matter (e.g., [2, 3, 4]) with realistic two and three-body nucleon potentials. Being combined with astrophysical data on the neutron star radii and maximal mass, the tidal deformability and other information from multi-messenger observations of neutron star mergers [5, 6], these calculations provide important constraints on the high-density equation of state and thus on the nucleon interactions.

The non-relativistic Skyrme-type effective forces have been being developed for more than 60 years [7, 8], and are widely applied in neutron star physics for constructing unified (based on the same nucleon forces in the crust and in the core) equation of states. While the usage of Skyrme functionals in the core is quite simple and straightforward due to negligible contribution of the gradient terms, in the crust of the neutron star it is not the case. The crust is inhomogeneous:
the nucleon clusters (atomic nuclei) are immersed into the gas of degenerate ultra-relativistic electrons and as well into the sea of unbound nucleons in the inner crust. As a result, the gradient terms in the Skyrme forces (related to the surface energy) play a crucial role, requiring correct implementation. The best way would be to apply quantum Hartree-Fock-Bogoliubov (HFB) calculation to obtain the properties of nuclei, the equation of state and, finally, the structure of the crust, however, it is extremely costly computationally [9]. The more feasible alternative is to use semiclassical extended Thomas-Fermi method, where kinetic energy density and spin-orbit density are described by the Wigner-Kirkwood expansion of the canonical density matrix in statistical equilibrium in powers of $\hbar$ [10]. It is less sophisticated numerically and provides good agreement with HFB results, if one includes pairing correlations [11].

The compressible liquid drop models are, probably, less accurate, but very useful because they are physically transparent and require rather modest numerical resources (see, e.g., [1, 12, 13, 14]). Here we analyse a crucial part of such model – the surface properties. We follow the formalism of the work by Douchin et al. [15] and present calculations of the surface energy within the extended Thomas-Fermi approach with parametrization of the Skyrme-like functional SLy4 [16] and BSk24 [17]. For Sly4 we reproduce results by Douchin et al. [15], while the surface energy for BSk24, up to our knowledge, was not published previously.

2. Surface energy: basic formulae

We consider a system of nucleons coexisting in the two phases, which mimics matter inside and outside the nucleus ($i$ and $o$ subscripts respectively below). The total energy of the system depends on the accurate nucleon number density profiles, which are determined by the thermodynamical equilibrium conditions. Here, for simplicity, we restrict ourselves to the system with plane boundary (for definiteness, below the $i$ phase is referred to the phase with higher baryon number density, while $o$ for low-density phase), thus neglecting the curvature effects. Following the traditional statement of the plain boundary problem, we also exclude the Coulomb terms in the energy (e.g., [20]). We apply the traditional parametrization of the neutron $\rho_n(z)$ and proton $\rho_p(z)$ number density profiles by the Fermi-Dirac type functions, suggested by Kolehmainen et al. [18]:

$$\rho_n(z) = \frac{\Delta \rho_n}{\left(1 + \exp\left(\frac{z - t_n}{a_n}\right)\right)} + \rho_{no}, \quad \rho_p(z) = \frac{\Delta \rho_p}{\left(1 + \exp\left(\frac{z}{a_p}\right)\right)} + \rho_{po},$$

(1)

where $z$ is the coordinate perpendicular to the plane interface. $\Delta \rho_n = \rho_{ni} - \rho_{no}, \Delta \rho_p = \rho_{pi} - \rho_{po}$ denote the changes of number densities while crossing the system from $z = -\infty$ to $z = \infty$. The profiles depend on five parameters $\{p_n, a_n, \rho_n, a_p, t_n\}$, combined with four parameters defining nucleons number density far from the interface between the two phases $\{\rho_{ni}, \rho_{no}, \rho_{pi}, \rho_{po}\}$. These parameters are determined by the minimization of the total energy per nucleon at fixed baryon number density [19].

The surface energy $E_{surf}$ is defined as a difference of the energy of the whole system $E_{tot}$ and the energy of the (auxiliary) reference system with a sharp interface $E_{ref}$, which depends only on the bulk terms (e.g., [18, 20, 22]):

$$E_{surf} \equiv E_{tot} - E_{ref}. \quad (2)$$

In numerical applications, instead of the energy minimization, it is convenient to minimize the thermodynamic potential $\Omega$ [20, 22] and introduce the surface tension $\sigma_s$, which is equal to the minimal value of the surface thermodynamic potential per unit area $\sigma_s = \min(\omega_s)$, where:

$$\omega_s = \int_{-\infty}^{\infty} \{\mathcal{E}(z) - \mathcal{E}_o - \mu_p [\rho_p(z) - \rho_{po}] - \mu_n [\rho_n(z) - \rho_{no}]\} dz, \quad (3)$$
$E(z)$ is the total energy density of the system, and $E_o$ corresponds to the bulk energy density of dripped particles, which describes the matter far from the surface at phase o. Finally, $\mu_n$ and $\mu_p$ denotes the neutron and proton chemical potentials respectively.

It is worth to note, that $\sigma_s$ does not depend on the choice of a reference frame (i.e. location of the sharp boundary in the reference system) [12]. In contrast, the surface energy per unit area $e_s$ depends on this choice. One can choose neutron (the boundary is localized at $z_b = z_n$), proton ($z_b = z_p$), nucleon or any other reference frame [12, 15, 20]. Here:

$$z_p = -\frac{1}{\Delta \rho_p} \int_{-\infty}^{\infty} z \frac{d\rho_p(z)}{dz} dz, \quad z_n = -\frac{1}{\Delta \rho_n} \int_{-\infty}^{\infty} z \frac{d\rho_n(z)}{dz} dz.$$

(4)

For neutron-rich nuclei in the neutron star crust, it is suitable to use the proton reference frame. It simplifies calculations of the Coulomb energy (e.g., [12, 15]). In this frame, only neutrons are adsorbed on the interface. According to the thermodynamic relations [12, 22], the surface energy per unit area $e_s$ can be written as:

$$e_s = \sigma_s + \Delta \rho_n s_n \mu_n,$$

(5)

where $s_n = z_n - z_p$ represents the neutron skin thickness.

3. Microphysical input and basic properties of two-phase boundary

The two-phase coexistence conditions can be derived by straightforward minimization of the total energy. For the plain boundary problem considered here they are especially simple. Namely, the pressure and chemical potentials of nucleons, calculated for the bulk matter far from the interface, should be the same on both sides of the interface (if neutrons or protons are absent in the o phase their chemical potential there should be larger than in i phase).

As a result, for the plain boundary the coexistence conditions lead to a one-parameter family of two-phase solutions, which is traditionally parametrized by the neutron excess in i phase $\delta = (\rho_{ni} - \rho_{pi})/(\rho_{ni} + \rho_{pi})$. In particular, for given $\delta$ one can calculate the nucleon densities far from the interface. It substantially reduces the number of parameters in the minimization procedure. Moreover, at least for a baryon number density $\rho_b \lesssim 0.06$ fm$^{-3}$ the usage of the plain boundary phase coexistence conditions provides a reasonable approximation for the number densities in i and o phases for spherical geometry, where accurate minimization with the full set of parameters is formally required (see work of Martin and Urban [21], for example).

In this paper, we implement SLy4 Skyrme functional [16], fitted to known experimental nuclear data, including five doubly magic nuclei and pure neutron matter equation of state with Urbana V14 two-body potential plus Urbana VII three-body potential of [3]. The second parametrization is Brussel-Montreal energy density functional BSk24 of Goriely et al. [17] with unconventional Skyrme forces (they include density-dependent generalizations of the usual $t_1$ and $t_2$ terms to avoid the ferromagnetic collapse of the matter), fitted to the masses of 2353 nuclei from AME 2012 table [23] and to high-density equation of state with V18 interaction of the reference [4]. For both functionals the neutron star models agree with 1-$\sigma$ mass interval for the most massive neutron star observed [24].

In the compressible liquid drop model of [14] it is more convenient to parametrize the family of two-phase solutions by $\mu_n$. The respective mapping is shown in Figure 1 which represents nucleon chemical potentials $\mu_n$ and $\mu_p$ as a function of $\delta$. The point where $\mu_n = 0$ corresponds to the neutron drip, $\delta = 0.30$ for SLy4 and $\delta = 0.33$ for BSk24. The proton drip point, where protons start to appear in both phases, takes place at $\delta = 0.87$ for SLy4 and at $\delta = 0.91$ for BSk24. At a critical value $\delta_c(SLy4) = 0.96$ and $\delta_c(BSk24) = 0.98$ two phases become the same and the interface disappears.
As it was stated in the reference [15], the crust-core boundary for the SLy4 functional occurs at $\delta_Q = 0.81$, suggesting that the two-phase equilibrium with dripped protons should not be relevant for the neutron star crust in this model. For BSk24 not $\delta$, but the baryon number density at the crust-core interface is typically quoted [19]. To calculate the respective value of $\delta$, we apply the quasineutrality and the $\beta$-equilibrium conditions [21]. It leads to the conclusion that the proton drip should not occur in the crust for BSk24. However, as shown by Pearson et al. [19], protons outside the spherical nuclear clusters appear in the bottom layers of the crust. This indicates, that the Coulomb and curvature corrections, which are neglected here, can shift proton drip point to a lower baryon number density for the realistic geometry of nuclear clusters (see also [21]).

We checked that the bulk properties (such as the saturation density $\rho^{sat} = 2\rho^{sat}_n$ and the energy of symmetric nuclear matter at saturation $\epsilon_0 = 2\mu_n(\rho^{sat}_n)$) for both parametrizations computed by our code are in agreement with the previous works (SLy4: $\mu_n(\rho^{sat}_n = 0.0798 \text{ fm}^{-3}) = -15.972 \text{ MeV}$; BSk4: $\mu_n(\rho^{sat}_n = 0.0789 \text{ fm}^{-3}) = -16.048 \text{ MeV}$). Moreover, the proton and neutron number densities in phase coexistence coincide with appropriate values from [21].

4. Results
We minimize $\omega_s$ with respect to the remaining free parameters of the Fermi-Dirac type functions (see equation [1]) within SLy4 and BSk24 functionals, thereby obtaining the surface tension and the surface energy per unit area. In our energy density functional we apply the extended Tomas-Fermi approach, employing the second-order Wigner-Kirkwood expansion, as given by Brack et al. [10] with modified coefficient $\eta_1$ as in reference [15]. For clarity, we display number density profiles for three different sets of parameters in figure 2.

The traditionally referred surface energy coefficient of symmetric matter at saturation $a_s = 4\pi r_0^2\sigma_s$ ($r_0$ determines a sphere containing one nucleon) is $a_s = 18.82 \text{ MeV}$ for SLy4 and $a_s = 18.29 \text{ MeV}$ for BSk24 Skyrme forces. We present our calculations in figure 3 as a function of neutron chemical potential. Our results for SLy4 are in agreement with Douchin et al. [15], certifying correctness of the numerical code.

The surface tension monotonically decreases with the increase of $\mu_n$, as the two phases become more and more alike; finally, it vanishes at the critical neutron chemical potential, where the
boundary disappears. The surface energy is not a monotonic function of $\mu_n$. For negative neutron chemical potential, $e_s$ decreases with the increase of $\mu_n$. At the neutron drip point ($\mu_n = 0$) it coincides with $\sigma_s$ (see equation (5)) and have a local minimum. Afterward $e_s$ increases following the growth of the neutron skin thickness. While the surface density of adsorbed neutrons $\nu_s = \Delta \rho_n s_n$ reaches a peak the after neutron drip and a local minimum near proton drip, $e_s$ attains a local maximum and then drastically falls to zero at the critical chemical potential because the boundary disappears. Both $\sigma_s$ and $e_s$ for BSk24 are typically lower than for SLy4 functional, although the more profound peak of the neutron skin thickness for BSk24 leads to a higher value of $e_s$ at the local maximum.
5. Summary and conclusions

We calculate the surface tension and the surface energy per unit area for the two phase nuclear matter with a plane interface. In these calculations we neglect the curvature effects and Coulomb term. We apply the semiclassical extended Thomas-Fermi approach along with effective Skyrme-type interactions SLy4 [16] and BSk24 [17]. For SLy4 functional we found a good agreement with [15]; the results for BSk24 are new. The explicit presentation of $\sigma$ dependence on $\mu_n$ simplifies the application of the results for the compressible liquid drop model of [14], which naturally ensures thermodynamical consistency of the surface tension terms. In subsequent work, we plan to calculate the curvature corrections for the surface properties for a set of parametrizations from the BSk family.

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