Nuclear statistical equilibrium equation of state with a parametrized Dirac–Brückner Hartree–Fock calculation

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1. Introduction

The equation of state (EOS) for dense matter is essential in research into high-energy astrophysical phenomena such as core-collapse supernovae and compact star mergers (see, e.g., Refs. [1–6]). Uncertainties, however, still exist in modeling the EOS, which may be resolved in the case of neutron star matter at zero temperature and in beta equilibrium, via observations of binary neutron star mergers [7–9]. Some phenomenological EOSs may satisfy such constraints of the neutron star observations and nuclear saturation properties [10], but high-energy astrophysical phenomena encounter thermodynamic conditions that vary over wide ranges of density, temperature, and charge fraction. To reliably extrapolate EOS and to address the extreme values that are unobtainable in terrestrial experiments and in neutron star matter, we require a sophisticated approach, such as the variational method (VM) [11] or the chiral effective field theory [12]. These theories are based on fundamental nuclear
forces and determined through nucleon–nucleon scattering data, using a few artificial parametrizations. Relativistic many-body theories, such as Dirac–Brückner Hartree–Fock (DBHF) [13–21] in the current study, are yet other approaches starting from nucleon–nucleon scattering data.

In addition to the theoretical framework for homogeneous nuclear matter, the calculations for inhomogeneous nuclear matter also affect high-energy astrophysical phenomena, especially in core-collapse supernovae. A modern approach to describe inhomogeneous nuclear matter for the supernova EOSs adopts the extended nuclear statistical equilibrium (NSE) models, which are used to obtain the number densities of all nuclei and nucleons [22–27]. A variation in the extended NSE models stems from the choice of theory of homogeneous nuclear matter and the nuclear mass data, as well as from the differing descriptions of the in-medium effects on nuclei, such as nuclear excitations and nuclear pasta phases, under hot and dense conditions [28,29]. In contrast, classic EOSs such as the Lattimer and Swesty EOS [30] and the Shen, Toki, Oyamatsu, and Sumiyoshi EOS [31–33] adopt a single-nucleus approximation to optimize some of the parameters for a representative nucleus. These EOSs cannot be used to precisely evaluate weak interaction rates of inhomogeneous matter in astrophysical simulations or to obtain exact values of the total mass fraction and the average mass and proton numbers of heavy nuclei [34,35]. Although some hybrid approaches have been developed to self-consistently describe both the ensemble of various nuclei and individual nuclear properties [36,37], they require high computational resources and are not suitable for constructing data tables covering a wide range of thermodynamic conditions.

We have constructed two EOSs with the same approach for inhomogeneous nuclear matter, the extended NSE model, but based on different theories for homogeneous nuclear matter. One is a phenomenological theory [38–40], and the other is a sophisticated theory [41]. The former was originally used in the STOS EOS and it is derived using the relativistic mean field (RMF) theory with the TM1 parameter set [42]. The latter was originally developed for the Togashi EOS [43] by the variational method [11] to treat the AV18 two-body potential [44] and the UIX three-body potential [45,46]. The theory of homogeneous nuclear matter determines not only the EOS above the density of nuclear saturation but also the EOS of inhomogeneous nuclear matter at sub-nuclear densities, such as the free energy of dripped nucleons and the bulk energies of heavy nuclei.

In this paper, we construct a new NSE EOS by using the parametrized results of the Dirac–Brückner Hartree–Fock (DBHF) approach [21] as an alternative to the VM EOS. The DBHF theory employs the bare nuclear interaction adjusted to account for the nucleon–nucleon scattering data. In contrast to non-relativistic many-body theories such as the VM EOS with the three-body potential adjusted to reproduce the nuclear saturation properties, the DBHF theory is able to reproduce the nuclear saturation properties starting from two-body forces. The calculations of the DBHF theory, however, are technically difficult due to handling a self-consistent solution of three integral equations: the Bethe–Salpeter equation, the single-particle self-energy, and Dyson’s equation. In order to overcome these complications, we employ analytical formulae of the interaction energy for homogeneous nuclear matter and the effective masses of nucleons that are fitted to the DBHF calculation in the zero-temperature limit [21]. The temperature dependence has only been considered in the kinetic energy part to obtain the free energy at finite temperature. In their DBHF calculation, the authors utilize the Bonn A potential for two-body interactions [16] and the subtracted T-matrix representation [18]. We note that several DBHF calculations have already been done, producing results that are somewhat dependent on the nucleon–nucleon potential and the formulation of self-energy [14–21].

There are pros and cons in the many-body approaches used to calculate EOSs. In the VM EOS, the speed of sound for neutron star matter becomes superluminal at densities higher than 0.90 fm$^{-3}$,
which is below the central density of the maximum mass neutron star (see Fig. 2). By contrast, the DBHF EOS in this work does not violate the causality at least below the central density of the maximum mass neutron star, $0.91 \text{ fm}^{-3}$. The disadvantage of the DBHF is the ladder approximation in the Bethe–Salpeter equation [47]. Some effects ignored by the approximation may be addressed using the VM EOS [11,48]. We note that different two-body potentials are used in the two approaches; the VM adopts the AV18 potential [44], the DBHF EOSs the Bonn A potential [16].

In non-relativistic Brückner Hartree–Fock (BHF) [49], the kinetic and interaction energies of nucleons are separately calculated (see Eq. (4) of Ref. [50]) and three-body interaction is introduced to reproduce the nuclear saturation properties as in the VM EOS. In general, BHF theories lead to softer EOSs or lower sound velocities than DBHF theories [50]. The RMF theory and the Hartree approximation are effective theories of DBHF theory by using coupling constants as parameters, in which the Fock terms for nucleon self-energy and the higher-order diagrams in the Bethe–Salpeter equation are disregarded. The RMF theory ensures that the upper limit of sound velocity is the speed of light at high densities because of the dominant vector potential term [51]. The RMF with the TM1 parameter set used for the STOS [33] and one of our EOSs [40] is developed to describe the behaviors of the DBHF theory [42].

Our DBHF model and its properties for homogeneous nuclear matter are described in Sect. 2. In Sect. 3, we present the calculations for inhomogeneous nuclear matter in a framework similar to that used in our previous models. In Sect. 4, we compare the new EOS with the VM EOS calculated in the same framework for inhomogeneous nuclear matter, but using a different theory for homogeneous matter [11]. Section 5 is devoted to the summary and conclusion.

2. Homogeneous nuclear matter

The properties of homogeneous nuclear matter determine not only the EOS above the density of nuclear saturation, $n_{s0}$, but also that for the inhomogeneous nuclear matter below $n_{s0}$, through the free energy of the nuclei and the dripped nucleons, as noted in the following section. The free energy of a baryon of homogeneous matter consists of kinetic and interaction parts,

$$\omega(n_B, x, T) = \omega_\text{kin}(n_B, x, T) + \omega_\text{int}(n_B, x),$$

where $n_B$, $x$, and $T$ are the number density, the charge fraction (the proton-to-baryon ratio), and temperature, respectively. In this work, we utilize the fitting formulae for the total energies and vector and scalar potentials at zero temperature, as detailed in the DBHF theory [21].

The kinetic part of the energy and entropy per baryon at a finite temperature are expressed as

$$\omega_\text{kin}(n_B, x, T) = \frac{2}{2\pi^2 n_B} \sum_{i=p,n} \int_0^\infty dk k^2 (f_i + \bar{f}_i)$$

$$\times \left[ E_i^*(k) + (M_i - M_i^*) \frac{M_i^*}{E_i^*(k)} \right] - ST,$$

$$S = \frac{2}{2\pi^2 n_B} \sum_{i=p,n} \int_0^\infty dk k^2 \left[ -f_i \ln f_i - (1 - f_i) \ln(1 - f_i) 
- f_i \ln f_i - (1 - f_i) \ln(1 - f_i) 
\right]$$

where $M_i^*$ denotes the effective masses, $E_i^*(k) = \sqrt{k^2 + M_i^{*2}}$ the effective energies of protons and neutrons, $f_i(v_i) = \{1 + \exp(\frac{E_i^* - v_i}{T})\}^{-1}$ the Fermi distribution, and $f_i = f_i(-v_i)$. We refer to
Table 1. Bulk properties of nuclear matter obtained using the EOSs for homogeneous nuclear matter, which are based on the relativistic mean field theory using the TM1 parameter set [33,42], the variational method [11,43], and the DBHF based on the Bonn A potential [21].

| Model | $n_{00}$ (fm$^{-3}$) | $E_0$ (MeV) | $K_0$ (MeV) | $J_0$ (MeV) | $L_0$ (MeV) |
|-------|------------------|---------|---------|---------|---------|
| TM1   | 0.145            | -16.3   | 281     | 36.9    | 110.8   |
| VM    | 0.160            | -16.0   | 245     | 30.0    | 35.0    |
| DBHF  | 0.179            | -16.6   | 232     | 34.5    | 66.8    |

The kinetic energy at zero temperature [14] and the finite-temperature extension [52]. The number densities of nucleons, $x n_B$ and $(1 - x) n_B$, lead to the corresponding kinetic chemical potentials, $v_p$ and $v_n$, respectively. The effective masses are evaluated in the zero-temperature limit using the fitting formulae for scalar and vector potentials (Eqs. (15), (16), (19), and (20) in Ref. [21]), $\Sigma^S_i (k_{Fn}, k_{FP}, k)$ and $\Sigma^V_i (k_{Fn}, k_{FP}, k)$, as functions of kinetic momentum and the Fermi momenta for protons and neutrons. These formulae can accurately reproduce the results of the DBHF calculation up to a density high enough to correspond to simulations of compact stars, $n_B \approx 1.2$ fm$^{-3}$. The effective mass is given by

$$M_i^* = \frac{M_i + \Sigma^S_i (k_{Fn}, k_{FP}, k_F)}{1 + \Sigma^V_i (k_{Fn}, k_{FP}, k_F)} (i = p \text{ or } n).$$

(4)

The Fermi momenta are directly determined by the number densities of the nucleons. In this work, we do not consider the finite-temperature effects on the effective masses, as their temperature dependence is weak at temperatures typical for supernova simulations ($T \lesssim 30$ MeV) [15].

The interaction term is obtained by subtracting the kinetic term from the total energy per baryon at zero temperature. The fitting formulae, presented in Eqs. (21) and (22) in Ref. [21], precisely provide the total energy densities as a function of $n_B$, for both symmetric nuclear matter, $\epsilon_{snm}$, and neutron matter, $\epsilon_{nm}$. The interaction energy in our model is defined as

$$\omega_{int}(n_B, x) = \frac{4x(1 - x)\epsilon_{snm}(n_B) + (1 - 2x)^2\epsilon_{nm}(n_B)}{n_B} \omega_{kin}(n_B, x, T = 0).$$

(5)

Although this parabolic expression is approximate, the obtained results reproduce well the exact calculation for asymmetric nuclear matter. In fact, the differences in radii of neutron stars obtained by the parametrized and the exact EOSs are at most equal to 0.2 km for the same mass of neutron stars, whereas the maximum masses of neutron stars almost coincide (see Fig. 6 in Ref. [21]).

The nuclear saturation properties of our model are summarized and compared with those of the VM EOS [11,43] and the RMF EOS with the TM1 parameter set in Table 1 [33,42]. Figure 1 displays the free energy per baryon of homogeneous nuclear matter as a function of density for the DBHF [21] and VM EOSs at different temperatures and charge fractions. As the figure shows, the DBHF fitting formula provides a larger nuclear saturation density of symmetric nuclear matter, $n_{00}$, a smaller compressibility, $K_0$, and a lower internal energy per baryon of symmetric matter at the saturation point $E_0$, which implies that the symmetric matter of the DBHF fitting formula is softer than that of the VM EOS. In contrast, the values of the symmetry energy, $J_0$, and its slope parameter in the density dependence, $L_0$, which characterize the property of asymmetric nuclear matter, are larger than those of the VM EOS. The neutron-rich matter in the DBHF EOS tends to have a larger free energy than in the VM EOS, especially at high densities. These differences between the VM and
Fig. 1. Free energies of homogeneous nuclear matter per baryon as a function of density for the DBHF calculation (solid red lines) and the VM calculation (dashed black lines) at $x = 0.0$ (thin lines), 0.1, 0.2, 0.3, 0.4 (medium lines), and 0.5 (thick lines), at $T = 0$ MeV (top left), 3 MeV (top right), 10 MeV (bottom left), and 30 MeV (bottom right).

DBHF EOSs come from not only the theory but also the nuclear potentials (the AV18 two-body potential [44] or the Bonn A potential [16]).

At $T = 30$ MeV and below $n_B \sim 0.2$ fm$^{-3}$, the DBHF EOS gives smaller free energies than the VM EOS even for neutron matter. This is due to the differences in the effective mass and in the formulation of the single-particle energy. At high temperatures, the ratio of kinetic energies to nucleon mass energies is not negligible. The relativistic effect of the single-particle energy at high temperatures is taken into account in the DBHF EOS but not in the VM EOS. The DBHF EOS, however, also lacks some finite-temperature effects such as temperature dependences in the effective mass and interaction energies.

Figure 2 illustrates the mass–radius relations for the three EOSs. The VM EOS results in the smallest radii for neutron stars, whereas the RMF EOS with the TM1 parameter set results in the largest radii. The DBHF EOS results in intermediate radii compared with those of the other EOSs, and larger maximum mass, $2.3 M_\odot$, than those of the other EOSs, $2.2 M_\odot$. The crust EOSs at sub-nuclear densities are calculated using the formulation explained in the following section, but neutron star structures can be mainly determined by the EOSs at supra-nuclear densities. All the EOSs satisfy the maximum mass limit $M_{\text{max}} \geq 2.14^{+1.1}_{-1.0} M_\odot$, which is determined by the mass of the heaviest observed pulsar [53]. On the other hand, the RMF EOS is excluded by the gravitational wave observation of the neutron star merger, GW170817 [7]. From some analysis of the observed tidal deformability, radii of neutron stars are tuned to be relatively small. The LIGO and Virgo observations [9] revealed
Fig. 2. Mass–radius relations of neutron stars for the DBHF EOS (solid red line), the VM EOS (dashed black line), and the RMF EOS using the TM1 parameter set (dash-dotted blue line).

that the radii in the event would be $R = 11.9^{+1.4}_{-1.4}$ km at the 90% credible level if they assume that the equation of state supports neutron stars with masses larger than 1.97 $M_{\odot}$. An analysis [54] also showed that the radius of a neutron star with 1.4 $M_{\odot}$ would be $R_{1.4} \lesssim 13.4$ km. The DBHF EOS is also excluded by a narrow margin from the other constraint by the LIGO and Virgo observations, $R \lesssim 12.8$ km, which is based on an analysis of the tidal deformability without the assumption about the maximum mass of neutron stars [9].

3. Inhomogeneous nuclear matter

We perform the calculation for inhomogeneous nuclear matter in almost the same manner as in the previously developed models [40,41]. In the current model, to ensure a smooth transition from inhomogeneous to homogeneous nuclear matter, we modify the treatment of nuclear pasta phases and the excluded volume effects for translational energies. These modifications do not affect the EOS at low and at supra-nuclear densities, only making a difference at the narrow density range just below nuclear saturation, $0.1 \leq n_{n,0} \lesssim n_n \lesssim n_{n,0}$. The shell energy and the surface tension of heavy nuclei are determined from the updated experimental and theoretical mass data, as presented in Refs. [55,56]. These values affect the average mass number and the mass fraction of heavy nuclei, but changes in these values due to the choice of the theoretical mass data are quite small [29]. The total free energy density is given by

$$f = f_{p,n} + \sum_{N,Z} n(N, Z)(F_m(N, Z) + F_t(N, Z)),$$  (6)

where $f_{p,n}$ is the free energy density of the free nucleons outside of the nuclei, $n(N, Z)$ is the number density of individual nuclei with the proton number $1 \leq Z \leq 1000$ and neutron number $1 \leq N \leq 1000$, $F$ is the mass energy, and $F_t$ is translational energy. The free energy density of the free nucleons is expressed as

$$f_{p,n} = \eta(n'_p + n'_n)\omega(n'_p + n'_n, \frac{n'_p}{n'_p + n'_n}, T),$$  (7)

where $\eta = 1 - V_{ex}/V$, $V$ is the total volume, $V_{ex}$ is the excluded volume that is occupied by nuclei and expressed as $V_{ex} = \sum_{N,Z} V_N(N, Z)$, $V_N$ is the nuclear volume (defined later), $n'_{p/n}$ is the local number density of protons and neutrons in the unoccupied volume $(V - V_{ex})$ for nucleons and is
defined as \( n'_{p/n} = (N'_{p/n})/(V - V_{ex}) \). \( N'_{p/n} \) is the number of free protons and neutrons, and \( \omega \) is the free energy per baryon of homogeneous matter of nucleons.

The mass energy of heavy nuclei with \( 6 \leq Z \leq 1000 \) consists of the bulk, Coulomb, surface and shell energies, as \( F_p(N, Z) = F_{bulk}(N, Z) + F_{coul}(N, Z) + F_{surf}(N, Z) + F_{shell}(N, Z) \). The nuclear bulk energies are evaluated using the same model for dripped nucleons and homogeneous nuclear matter in the previous section. They are given by \( F_{bulk}(N, Z) = A(\omega(n_e, Z/A, T)) \), where \( A = N + Z \) and \( n_s(T, N, Z) \) is defined as the density at which the free energy per baryon, \( \omega(n_B, Z/A, T) \), reaches its local minimum value around \( n_{so} \). For the nuclei whenever experimental or theoretical mass data are available [55,56]. The shell energies are defined as the deviation of the mass data from the gross part of the liquid-drop mass model, \( F_{0shell}(N, Z) = M_{data}(N, Z) - [F_{bulk}(N, Z) + F_{surf}(N, Z) + F_{coul}(N, Z)]_{n_B=0, T=0} \). They are assumed to be positive to avoid negative entropy production with the formula for temperature dependence, \( F_{shell}(T) = F_{0shell} \tau \sinh \tau \) with \( \tau = 2\pi^2 T/(41A^{-1/3}) \) [29].

The Coulomb and surface energies are calculated using the liquid-drop model in the Wigner–Seitz cell that contains dripped nucleons and uniformly distributed electrons. The number density of electrons is expressed as \( n_e = Y_p n_B \). The sum of the cell volumes \( V_C \) for all nuclei is equal to the total volume of the system, \( V \). We assume that the nuclear shape changes from a droplet to a bubble, as it is dependent on the filling factor in each cell, \( u(N, Z) \). The filling factor is defined as \( u(N, Z) = V_N/V_C \), where the nuclear volume is set as \( V_N = A/n_s \) and the cell volume as \( V_C = (Z - n'_p V_N)/(n_e - n'_n) \).

The smooth function for the Coulomb energy used in our model can be found in Refs. [30,57]. In the previous models, the maximum filling factor for droplets is assumed to be \( u = 0.3 \) and the minimum filling factor for bubbles is assumed to be \( u = 0.7 \). The simple interpolation used for intermediate phases, \( 0.3 < u < 0.7 \), is a cubic function of \( u \).

The Coulomb energy is represented as:

\[
F_{coul}(N, Z) = \frac{(36\pi)^{1/3}}{5} e^2 n_s^2 \left( \frac{Z/A - n'_p/n_s}{Z/A - n'_n/n_s} \right)^2 V_C^{5/3} D_C(u), \tag{8}
\]

\[
D_C(u) = \frac{u^{5/3} (1 - u)^2 D(u) + u^2 (1 - u)^5/3 D(1 - u)}{u^2 + (1 - u)^2 + C_{cp} u^2 (1 - u)^2}, \tag{9}
\]

where \( D(u) = 1 - u^{1/3} + \frac{1}{2} u \). The surface energy is often determined by the size condition, which states that \( F_{sur} = 2F_{coul} \) in the single-nucleus approximation [26,30]. In the NSE description, however, the mixture contains also nuclei that do not satisfy the size condition. The surface energies are expressed as the product of the nuclear surface area and the surface tension:

\[
F_{surf}(N, Z) = 4\pi \left( \frac{3V_N}{4\pi} \right)^{2/3} \sigma(T, n'_n, n'_p) D_S(u), \tag{10}
\]

\[
D_S(u) = \frac{u^2 (1 - u)^2/3 + u^{2/3} (1 - u)^2}{u^2 + (1 - u)^2 + C_{sp} u^2 (1 - u)^2}, \tag{11}
\]

\[
\sigma(T, n'_n, n'_p) = \sigma_0 \left\{ \frac{16 + C_{st}}{(1 - Z/A)^{-3} + (Z/A)^{-3} + C_{st}} \right\} \left( \frac{T_{coul}^2 - T^2}{T_{coul}^2 + T^2} \right)^{5/4} \left( 1 - \frac{n'_p + n'_n}{n_s} \right)^2.
\]

The expressions for \( D_C \) and \( D_S \) asymptotically approach the factors for the nuclear droplet phase as \( \lim_{u \to 0} D_C = u^{5/3} D(u) \) and \( \lim_{u \to 0} D_S = u^{2/3} \), and for the nuclear bubble phase as \( \lim_{u \to 1} D_C = (1 - u)^{5/3} D(1 - u) \) and \( \lim_{u \to 1} D_S = (1 - u)^{2/3} \). Therefore, the new evaluations are almost equal to
those obtained by the previous model at low densities \((n_B \lesssim 0.1 n_{s0})\). The coefficients \(C_{cp} = -0.863\) and \(C_{sp} = 4.19\) are set to reproduce the Coulomb and surface energies of the nuclear slab phase at \(u = 0.5\). The values of \(\sigma_0 = 1.11\) MeV/fm\(^2\) and \(C_{st} = 23.5\) MeV are optimized to minimize the sum of the shell energies per baryon, in other words, the deviation of the gross terms of the mass formula (bulk, Coulomb, and surface energies) per baryon, using the mass data [29], \(\sum_{Z \geq 6} F_{\text{shell}}(N,Z)/A\).

The values of surface tensions for the VM EOS are \(\sigma_0 = 1.01\) MeV/fm\(^2\) and \(C_{st} = 42.5\) MeV. Figure 3 shows the surface tensions for the two EOSs. The larger values of \(n_{s0}\) of the DBHF EOS lead to greater surface tensions for the nuclei with \(0.32 \lesssim Z/A\). We define the critical temperature, \(T_c(N,Z)\), as the temperature at which both \((\partial P_{\text{bulk}}/\partial n_B)|_{x=Z/(Z+N)} = 0\) and \((\partial^2 P_{\text{bulk}}/\partial n_B^2)|_{x=Z/(Z+N)} = 0\), where the bulk pressure is equal to \(P_{\text{bulk}} = n_B^2 \partial \omega(n_B,x,T)/\partial n_B\) [37]. In our previous models [40,41], we adopted a different \(Z/A\) dependence and fixed values for \(\sigma_0 = 1.15\) MeV/fm\(^2\) [30] and \(T_c(N,Z) = 18\) MeV, for different calculations dealing with homogeneous nuclear matter, i.e., the RMF or the VM.

The translational energies of heavy nuclei are expressed as Boltzmann gases with excluded volume effects,

\[
F_t(N,Z) = \kappa_1 T \left\{ \log \left( \frac{n(N,Z)/\kappa_2}{g^0(N,Z)(M(N,Z)T/2\pi\hbar^2)^{3/2}} \right) - 1 \right\},
\]

where \(\kappa_1 = 1, \kappa_2 = 1 - n_B/n_{s0}\), and the spin degeneracy factor of the ground state is denoted as \(g^0(N,Z)\). In previous models, we had assumed that the excluded volume suppresses the translational motions and the translational energy becomes zero with \(\kappa_1 = 1 - n_B/n_{s0}\) and \(\kappa_2 = 1\), as described in Ref. [30]. The reduction of \(\kappa_2\) in the new model is introduced so that the number densities of the nuclei can be excluded, which is a principle that has become widely used [22,58–60]. It must be noted that the transition to homogeneous nuclear matter is a quite uncertain procedure, and it has not yet been settled which excluded volume expression is more realistic. The differences arising from this treatment are influential for a density range that is much narrower than one step of the density mesh for the supernova EOS data. The free energy densities for light nuclei \((Z \leq 5)\) are described in the same way as in the older model (see Refs. [40,41]), which is based on a quantum approach for light clusters as quasiparticles.
4. Results

We compare some quantities of the new EOSs based on the DBHF [21] and VM [11] for $T = 1$ MeV, 3 MeV, and 10 MeV and $Y_p = 0.2$ and 0.4, which are typical values used in supernova simulations. The VM EOS is calculated using the same approach that was explained in Sect. 3, only with a slight difference from the multi-nucleus EOS constructed in Ref. [41]. The differences from the previously constructed VM EOS are the surface tensions, shell energies, and treatment of nuclear pasta phases and excluded volume effects.

Figure 4 shows the mass number distributions and average charge fractions as functions of mass number for heavy nuclei at $n_B = 9.5 \times 10^{-4}$ fm$^{-3}$, which are defined as

$$X_A = \frac{\sum_{Z+N=A} An(N,Z)}{n_B},$$

(13)

$$<Z/A> = \frac{\sum_{Z+N=A} Z/An(N,Z)}{\sum_{Z+N=A} n(N,Z)}.$$  

(14)

Overall, because of the larger values of $n_s$, $J_0$, and $\sigma (Z/A \gtrsim 0.32)$ and the smaller value of $E_0$, the nuclei with medium mass numbers, $40 \lesssim A \lesssim 90$, are more abundant in the DBHF EOS than in the VM EOS. These nuclei in the DBHF EOS have lower mass and bulk energies, $F_m$ and $F_{\text{bulk}}$, and larger surface and Coulomb energies, $F_{\text{surf}}$ and $F_{\text{Coul}}$, than those in the VM EOS. For $A \gtrsim 100$, the large saturation densities for the DBHF EOS, $n_s$, lead to larger Coulomb energies and reduce...
the mass fraction of nuclei, even though the bulk energies are lower than those in the VM EOS. The large symmetry energy for the DBHF EOS, \(J_0\), also causes the increase of the mass energies of the neutron-rich, heavy-mass nuclei with low values of the charge fraction \(Z/A\), although the impact on the mass fractions is weaker than that of Coulomb energies. As the bottom panels of Fig. 4 show, the charge fraction decreases as \(A\) increases and, as a result, the bulk energies of nuclei with \(A \gtrsim 100\) increase more in the DBHF EOS than in the VM EOS. As for \(A \lesssim 40\), the larger surface tensions for the nuclei with \(Z/A \gtrsim 0.32\), which are shown in Fig. 3, make the mass energies of nuclei with small mass numbers larger in the DBHF EOS even with low bulk energies. Hence, the mass fractions of nuclei for \(A \lesssim 40\) in the DBHF EOS tend to be less than those in the VM EOS at \(T = 3\) MeV. The shell effects disappear around \(T \approx 2–3\) MeV and the mass distributions are smooth at \(T = 3\) MeV.

Figure 5 shows the average mass numbers of heavy nuclei \((Z \geq 6)\) as a function of density. The DBHF EOS tends to give smaller average mass numbers, because there are fewer heavy-mass nuclei than in the VM EOS at \(n_B \gtrsim 10^{-3}\) fm\(^{-3}\). At \(T \gtrsim 3\) MeV and at \(n_B \lesssim 10^{-3}\) fm\(^{-3}\), the DBHF EOS provides slightly larger average mass numbers than the VM EOS due to the large populations of medium-mass nuclei as discussed in the previous paragraph.

Figure 6 presents the mass fractions of free nucleons, light nuclei \((Z \leq 5)\), and heavy nuclei \((Z \geq 6)\). Because of the lower bulk energies of medium-mass nuclei, the mass fraction of heavy

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Fig. 5. Average mass number of heavy nuclei with \(Z \geq 6\) as a function of density for the DBHF EOS (thick red line) and the VM EOS (thin black line), at \(Y_p = 0.2\) (left) and 0.4 (right), and at \(T = 1\) MeV (dashed lines), 3 MeV (dash-dotted lines), and 10 MeV (solid lines).

Fig. 6. Mass fractions of nucleons (dashed lines), light nuclei with \(Z \leq 6\) (dash-dotted lines), and heavy nuclei with \(Z \geq 6\) (solid lines) as a function of density for the DBHF EOS (thick red line) and the VM EOS (thin black line) at \(Y_p = 0.2\) (left) and 0.4 (right) and at \(T = 1\) MeV.
Fig. 7. Critical lines at which the mass fractions of light nuclei (dashed lines) and heavy nuclei (solid lines) become $X_a > 10^{-4}$ and $X_A > 10^{-4}$, shown for the DBHF EOS (thick red lines) and the VM EOS (thin black lines) at $Y_p = 0.2$ (left) and 0.4 (right).

Fig. 8. Entropy per baryon as a function of density for the DBHF EOS (thick red line) and the VM EOS (thin black line), at $Y_p = 0.2$ (left) and 0.4 (top right) and at $T = 1$ MeV (dashed lines), 3 MeV (dash-dotted lines), 10 MeV (dashed double-dotted lines), and 30 MeV (solid lines).

The mass fraction of heavy nuclei is larger than that of the VM EOS at lower densities ($\lesssim 10^{-6}$ fm$^{-3}$). At $Y_p = 0.2$ and $n_B \gtrsim 10^{-4}$ fm$^{-3}$, the DBHF EOS gives a smaller mass fraction of heavy nuclei and more dripped neutrons than the VM EOS because of the larger value of the symmetry energy for the DBHF EOS, $J_0$. Figure 7 shows the critical lines at which the mass fraction of heavy nuclei, $X_A = \sum_{Z \geq 6} A n(N,Z)/n_B$, and that of light nuclei, $X_a = \sum_{Z \leq 5} A n(N,Z)/n_B$, become $10^{-4}$ fm$^{-3}$. Heavy nuclei show up at lower densities in the DBHF EOS than in the VM EOS, but both EOSs have similar critical densities at which light nuclei appear. The DBHF EOS has larger saturation densities; hence, the transitions occur from nuclei to nucleons at larger densities.

Figures 8, 9, and 10 display the relevant thermodynamic quantities. On the whole, there are few differences between the two EOSs at sub-nuclear densities and at $T = 1, 3, 10$ MeV, since the same NSE model is applied. The slight differences primarily stem from the nuclear compositions. The smaller entropy at $n_B \sim 10^{-6}$ fm$^{-3}$ and $T = 1$ MeV in the DBHF EOS is due to the appearance of heavier nuclei at lower densities. As for the behavior of pressure, when mass fractions of heavy nuclei with large Coulomb energies become large at low $T$ and high $Y_p$, negative Coulomb pressures overcome positive thermal pressures and, the total pressure becomes negative (see Refs. [38,61] for details). As shown in Figs. 6 and 7, the different composition of inhomogeneous nuclear matter basically leads to the pressure difference between the two EOSs at sub-nuclear density and $T = 1, 3, 10$ MeV. The positive pressure of leptons and photons, however, is considerably larger than the
Fig. 9. Baryonic pressure as a function of density for the DBHF EOS (thick red line) and the VM EOS (thin black line), at $Y_p = 0.2$ (left) and 0.4 (right) and at $T = 1$ MeV (dashed lines), 3 MeV (dash-dotted lines), 10 MeV (dashed double-dotted lines), and 30 MeV (solid lines).

Fig. 10. Neutron chemical potential subtracted from the proton one, $\mu_n - \mu_p$, as a function of density for the DBHF EOS (thick red line) and the VM EOS (thin black line), at $Y_p = 0.2$ (left) and 0.4 (right) and at $T = 1$ MeV (dashed lines), 3 MeV (dash-dotted lines), 10 MeV (dashed double-dotted lines), and 30 MeV (solid lines).

baryonic one normally and the total pressure never becomes negative. The relevant quantities around the nuclear density and above depend on the nuclear bulk properties. The DBHF EOS at supra-nuclear density leads to larger pressures than the VM EOS, which leads to larger radii of neutron stars, as shown in Fig. 2. The sound velocity of the VM EOS exceeds speed of light around $n_B = 0.90 \text{ fm}^{-3}$ [43], whereas the DBHF EOS does not. The larger values of $J_0$ and $L_0$ in the DBHF EOS make the chemical potential difference between neutrons and protons, $\mu_n - \mu_p$, larger at supra-nuclear densities, which may affect charge current weak interactions in proto-neutron stars [62].

5. Summary and conclusion

We constructed a new EOS for astrophysical simulations based on the extended model of nuclear statistical equilibrium for inhomogeneous nuclear matter. For the homogeneous one, the parametrized DBHF calculations at zero temperature are utilized, in which the self-energies of nucleons and the energy densities for symmetric and neutron matter are obtained based on the Bonn A potential for nucleon–nucleon interaction. The behavior of the DBHF EOS at higher densities is different from that in non-relativistic many-body frameworks such as the VM EOS [11]. These microscopic
approaches, DBHF and VM EOSs, also provide different properties to effective many-body theories, Skyrme Hartree–Fock or RMF EOSs [22–24,30–32,40].

We utilized an extended NSE model [40,41] to calculate the EOS at sub-nuclear densities. We made some modifications by introducing smooth functions of the filling factor for the Coulomb and surface energies of nuclear pasta phases and the surface tensions that were optimized to reproduce the nuclear experimental and theoretical mass data. The DBHF and VM EOSs exhibit some differences in nuclear compositions and thermodynamic quantities at sub-nuclear densities due to the softer properties of symmetric nuclear matter and stiffer properties of asymmetric nuclear matter in the DBHF EOS. On the whole, the DBHF tends to give larger mass fractions than the VM EOS for the nuclei with $40 \lesssim A \lesssim 90$ and smaller ones for the other nuclei, because of its larger values of $n_{s0}, J_0,$ and $\sigma (Z/A \gtrsim 0.32)$ and smaller value of $E_0$. The pressures at supra-nuclear densities and neutron star radii are larger in the DBHF EOS due to the stiffer properties of asymmetric nuclear matter in the DBHF EOS.

Our EOS tables for the DBHF EOS and the VM EOS, the latter of which has been updated from the previous model [41] as for the extended NSE calculation, will be available online, at http://user.numazu-ct.ac.jp/~sumi/eos/. In the near future, we will report on the comparison of astrophysical simulations [63] using the modern EOSs, the DBHF and the VM EOSs.

In this work, we compared the two modern theories of homogeneous nuclear matter. There are, however, still many uncertainties both in the nucleon–nucleon potentials and in the many-body calculations [64]. The model of inhomogeneous nuclear matter also requires further improvements. One example is the evaluation of free energies for medium-mass neutron-rich nuclei, which have a considerable effect on the neutrino luminosities of neutronization bursts and the masses of proto-neutron stars [65]. The modeling of nuclear excitations is the most relevant problem when it comes to determining the nuclei that show up during the core collapse of supernovae [29].

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