

## Phase diagram of nuclear “pasta” and its uncertainties in supernova cores

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We examine the model dependence of the phase diagram of inhomogeneous nuclear matter in supernova cores using the quantum molecular dynamics (QMD). Inhomogeneous matter includes crystallized matter with nonspherical nuclei—“pasta” phases—and the liquid-gas phase-separating nuclear matter. Major differences between the phase diagrams of the QMD models can be explained by the energy of pure neutron matter at low densities and the saturation density of asymmetric nuclear matter. We show the density dependence of the symmetry energy is also useful to understand uncertainties of the phase diagram. We point out that, for typical nuclear models, the mass fraction of the pasta phases in the later stage of the collapsing cores is higher than 10–20%.

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### I. INTRODUCTION

Terrestrial matter basically consists of spherical nuclei. However, such an ordinary picture, that is, “nuclei are spherical,” might not be true in collapsing supernova cores just before bounce and in the deepest region of inner crusts of neutron stars. In dense matter close to the normal nuclear density  $\rho_0 \simeq 0.16 \text{ fm}^{-3}$ , nuclei would adopt nonspherical shapes, including rod and slab. Phases with these exotic nuclei are called “pasta” phases [1,2].

The pasta phases attract the attention of many researchers in the fields of nuclear physics [3] and astrophysics [4–6]. Pasta phases have important astrophysical effects on, e.g., neutrino opacity in supernova cores [7,8], neutrino emissivity in neutron star cooling [9–12], etc. Moreover, it has been shown in our previous work [8] that the pasta phases would occupy 10–20% of the mass of collapsing stellar core. In such a case, the pasta phases could have a remarkable impact on neutrino transport in the core and hence success of supernova explosion.

Equilibrium states of the pasta phases have been investigated in many earlier works (e.g., Refs. [9,13–19]). These works have confirmed that, with increasing density, nuclear shape basically changes in the sequence sphere, rod, slab, rodlike bubbles, spherical bubbles, and, finally, uniform nuclear matter (in some nuclear models, however, all of the above pasta phases do not appear [9,16–18,20,21]). Although these earlier works have studied the phase diagram of the pasta phases using various nuclear models, the following two points are worth consideration. First, in these works (except for Ref. [13]) authors consider the above-mentioned specific nuclear structures and determine the equilibrium state by comparing the free energy among them. It is hardly possible to know in advance whether these assumed phases include the true equilibrium state or there are other more stable states. Thus, we have to examine how the phase diagram is changed

by relaxing this assumption. Second, in collapsing supernova cores, where the pasta phases would appear, temperature reaches typically a few MeV. Thermal fluctuations on the nucleon distribution are not completely negligible considering that the nucleon Fermi energy and the nuclear binding energy are from several to tens MeV. However, thermal fluctuations cannot be properly incorporated by the framework employed in the earlier works such as a liquid-drop model and the Thomas-Fermi approximation.

To overcome the above problems, we use quantum molecular dynamics (QMD) [22–25]. In these works, we have confirmed the pasta phases appear at zero and nonzero temperatures and the sequence of nuclear structures with increasing density is the same as that in the earlier works. There we have also obtained spongelike “intermediate” phases. However, we have studied the pasta phases using only one specific nuclear force. We note that uncertainties of nuclear force, especially those of the surface energy and the symmetry energy, have large effects on the phase diagram at subnuclear densities [16–18,26]. Thus, in the present work, we shall reveal the influence on the phase diagram by uncertainties of nuclear force in the framework of QMD.

In the followings, we set the Boltzmann constant  $k_B = 1$ .

### II. FRAMEWORK OF QUANTUM MOLECULAR DYNAMICS

#### A. Models

In our previous studies [22–24,27], we used nuclear force developed by Maruyama *et al.* (Model 1) [28] with medium equation-of-state (EOS) parameter set. In the present work, we also use another model by Chikazumi *et al.* (Model 2) [29] to investigate the model dependence of phase diagram.

The Hamiltonian of both the models is written as,

$$\mathcal{H} = K + V_{\text{Pauli}} + V_{\text{Skyrme}} + V_{\text{sym}} + V_{\text{surface}} + V_{\text{MD}} + V_{\text{Coulomb}}, \quad (1)$$

where  $K$  is the kinetic energy;  $V_{\text{Pauli}}$  is the Pauli potential, which is introduced to reproduce effects of the Pauli exclusion principle;  $V_{\text{Skyrme}}$  is the Skyrme-type interactions;  $V_{\text{sym}}$  is the symmetry energy;  $V_{\text{surface}}$  is the potential dependent on the density gradient;  $V_{\text{MD}}$  is the momentum-dependent potential in the form of the exchange term of the Yukawa interaction; and  $V_{\text{Coulomb}}$  is the Coulomb potential. Each term is expressed as follows [30]:

$$K = \sum_i \frac{\mathbf{P}_i^2}{2m_i}, \quad (2)$$

$$V_{\text{Pauli}} = \frac{1}{2} C_P \left( \frac{\hbar}{q_0 p_0} \right) \sum_{i,j(\neq i)} \exp \left[ -\frac{(\mathbf{R}_i - \mathbf{R}_j)^2}{2q_0^2} - \frac{(\mathbf{P}_i - \mathbf{P}_j)^2}{2p_0^2} \right] \delta_{c_i c_j} \delta_{\sigma_i \sigma_j}, \quad (3)$$

$$V_{\text{Skyrme}} = \frac{\alpha}{2\rho_0} \sum_{i,j(\neq i)} \rho_{ij} + \frac{\beta}{(1+\tau)\rho_0^\tau} \sum_i \left[ \sum_{j(\neq i)} \int d\mathbf{r} \tilde{\rho}_i(\mathbf{r}) \tilde{\rho}_j(\mathbf{r}) \right]^\tau, \quad (4)$$

$$V_{\text{sym}} = \frac{C_s}{2\rho_0} \sum_{i,j(\neq i)} (1 - 2|c_i - c_j|) \rho_{ij}, \quad (5)$$

$$V_{\text{surface}} = \frac{V_{\text{SF}}}{2\rho_0^{5/3}} \sum_{i,j(\neq i)} \int d\mathbf{r} \nabla \rho_i(\mathbf{r}) \cdot \nabla \rho_j(\mathbf{r}), \quad (6)$$

$$V_{\text{MD}} = \frac{C_{\text{ex}}^{(1)}}{2\rho_0} \sum_{i,j(\neq i)} \frac{1}{1 + \left[ \frac{|\mathbf{P}_i - \mathbf{P}_j|}{\hbar \mu_1} \right]^2} \rho_{ij} + \frac{C_{\text{ex}}^{(2)}}{2\rho_0} \times \sum_{i,j(\neq i)} \frac{1}{1 + \left[ \frac{|\mathbf{P}_i - \mathbf{P}_j|}{\hbar \mu_2} \right]^2} \rho_{ij}, \quad (7)$$

$$V_{\text{Coulomb}} = \frac{e^2}{2} \sum_{i,j(\neq i)} c_i c_j \iint d\mathbf{r} d\mathbf{r}' \frac{1}{|\mathbf{r} - \mathbf{r}'|} \rho_i(\mathbf{r}) \rho_j(\mathbf{r}'), \quad (8)$$

where  $\mathbf{R}_i$  and  $\mathbf{P}_i$  are the centers of position and momentum of the wave packet of  $i$ th nucleon and  $m_i$ ,  $\sigma_i$ , and  $c_i$  ( $c_i = 1$  for protons and  $c_i = 0$  for neutrons) denote the mass, the spin, and the electric charge (in units of  $e$ ) of  $i$ th nucleon. Here  $\rho_{ij}$  means the overlap between the densities of  $i$ th and  $j$ th nucleons,

$$\rho_{ij} = \int d\mathbf{r} \rho_i(\mathbf{r}) \rho_j(\mathbf{r}), \quad (9)$$

and the single-nucleon densities  $\rho_i(\mathbf{r})$  and  $\tilde{\rho}_i(\mathbf{r})$  are given by

$$\rho_i(\mathbf{r}) = \frac{1}{(2\pi L_w^2)^{3/2}} \exp \left[ -\frac{(\mathbf{r} - \mathbf{R}_i)^2}{2L_w^2} \right], \quad (10)$$

$$\tilde{\rho}_i(\mathbf{r}) = \frac{1}{(2\pi \tilde{L}_w^2)^{3/2}} \exp \left[ -\frac{(\mathbf{r} - \mathbf{R}_i)^2}{2\tilde{L}_w^2} \right], \quad (11)$$

TABLE I. Parameter sets for model 1 [28] and model 2 [29].

	Model 1	Model 2
$C_P$ (MeV)	207	115
$p_0$ (MeV/c)	120	120
$q_0$ (fm)	1.644	2.5
$\alpha$ (MeV)	-92.86	-121.9
$\beta$ (MeV)	169.28	197.3
$\tau$	1.33333	1.33333
$C_s$ (MeV)	25.0	25.0
$V_{\text{SF}}$ (MeV)	0	20.68
$C_{\text{ex}}^{(1)}$ (MeV)	-258.54	-258.54
$C_{\text{ex}}^{(2)}$ (MeV)	375.6	375.6
$\mu_1$ (fm $^{-1}$ )	2.35	2.35
$\mu_2$ (fm $^{-1}$ )	0.4	0.4
$L_w^2$ (fm $^2$ )	2.1	1.95
$\rho_0$ (fm $^{-3}$ )	0.165	0.168

with the normal width  $L_w$  and the modified width  $\tilde{L}_w$  of the wave packet,

$$\tilde{L}_w^2 = \frac{(1+\tau)^{1/\tau}}{2} L_w^2. \quad (12)$$

(The squared widths  $L_w^2$  and  $\tilde{L}_w^2$  correspond to  $L$  and  $\tilde{L}$ , respectively, in the notation of Refs. [28,29].)

Parameters for the models are shown in Table I. Note that  $V_{\text{SF}} = 0$  for model 1, i.e., model 1 does not include  $V_{\text{surface}}$ . Model parameters  $q_0$ ,  $p_0$ , and  $C_P$  in the Pauli potential are determined by fitting the kinetic energy of free Fermi gas at zero temperature. The other model parameters are determined to reproduce the saturation properties of symmetric nuclear matter [i.e., the saturation density ( $\simeq 0.16$  fm $^{-3}$ ), saturation energy ( $-16$  MeV per baryon), and incompressibility (280 MeV)], and the binding energy and rms radius of the ground state of stable nuclei. Especially these properties of heavy nuclei are better reproduced by model 2 than by model 1 due to the term  $V_{\text{surface}}$  [31]. Note that  $V_{\text{surface}}$  is just a potential depending on the density gradient and is different from the surface energy. The surface energy comes from an energy loss due to the deficiency of nucleons interacting with each other in the region of the nuclear surface.

## B. Equations of motion

We show equations of motion of QMD, which we employ to simulate the equilibrium states at zero and nonzero temperatures. The Hamiltonian form of the QMD equations of motion is written as

$$\begin{aligned} \dot{\mathbf{R}}_i &= \frac{\partial \mathcal{H}}{\partial \mathbf{P}_i}, \\ \dot{\mathbf{P}}_i &= -\frac{\partial \mathcal{H}}{\partial \mathbf{R}_i}. \end{aligned} \quad (13)$$

We cool down the system using the following equations of motion in which we introduce extra friction terms to the above

equations [28]:

$$\begin{aligned}\dot{\mathbf{R}}_i &= \frac{\partial \mathcal{H}}{\partial \mathbf{P}_i} - \xi_R \frac{\partial \mathcal{H}}{\partial \mathbf{R}_i}, \\ \dot{\mathbf{P}}_i &= -\frac{\partial \mathcal{H}}{\partial \mathbf{R}_i} - \xi_P \frac{\partial \mathcal{H}}{\partial \mathbf{P}_i}.\end{aligned}\quad (14)$$

Here, the friction coefficients  $\xi_R$  and  $\xi_P$  are positive definite, which determine the relaxation time scale and lead to a monotonic decrease of the total energy.

Instead of the normal kinetic temperature, which loses its physical meaning for the system with momentum-dependent potentials, we use effective temperature  $T_{\text{eff}}$  proposed by Ref. [29]:

$$\frac{3}{2}T_{\text{eff}} = \frac{1}{\mathcal{N}} \sum_i \frac{1}{2} \mathbf{P}_i \cdot \frac{d\mathbf{R}_i}{dt}, \quad (15)$$

where  $\mathcal{N}$  is the total number of particles. If we perform Metropolis Monte Carlo simulations with the setting temperature  $T_{\text{set}}$ , the long-time average of the effective temperature coincides with  $T_{\text{set}}$  quite well [24]. This shows  $T_{\text{eff}}$  is consistent with the temperature in the Boltzmann statistics.

To obtain the equilibrium state at finite temperatures, we use the Nosé-Hoover thermostat [32–34] modified for momentum-dependent potentials [24,35]. The Hamiltonian of the system with this thermostat is

$$\mathcal{H}_{\text{Nosé}} = \sum_i \frac{\mathbf{P}_i^2}{2m_i} + \mathcal{U}(\{\mathbf{R}_i, \mathbf{P}_i\}) + \frac{sp_s^2}{2Q} + g \frac{\ln s}{\beta}. \quad (16)$$

Here  $\mathcal{U}$  is the momentum-dependent potential,  $s$  is the additional dynamical variable for time scaling,  $p_s$  is the momentum conjugate to  $s$ ,  $Q$  is the thermal inertial parameter corresponding to a coupling constant between the system and the thermostat,  $g$  is a parameter to be determined as  $3N$  by the condition for generating the canonical ensemble in the classical molecular dynamic simulations, and  $\beta$  is the reciprocal of  $T_{\text{set}}$  of the thermostat. Then equations of motion are

$$\begin{aligned}\frac{d\mathbf{R}_i}{dt} &= \frac{\mathbf{P}_i}{m_i} + \frac{\partial \mathcal{U}}{\partial \mathbf{P}_i}, \\ \frac{d\mathbf{P}_i}{dt} &= -\frac{\partial \mathcal{U}}{\partial \mathbf{R}_i} - \xi \mathbf{P}_i, \\ \frac{1}{s} \frac{ds}{dt} &= \xi, \\ \frac{d\xi}{dt} &= \frac{1}{Q} \left[ \sum_i \left( \frac{\mathbf{P}_i^2}{m_i} + \mathbf{P}_i \cdot \frac{\partial \mathcal{U}}{\partial \mathbf{P}_i} \right) - \frac{g}{\beta} \right],\end{aligned}\quad (17)$$

with

$$\xi \equiv \frac{sp_s}{Q}, \quad (18)$$

where  $\xi$  means the thermodynamic friction coefficient. During the time evolution described by the above equations,  $\mathcal{H}_{\text{Nosé}}$  is conserved and  $T_{\text{eff}}$  fluctuates around  $T_{\text{set}}$ .

### III. PURE NEUTRON MATTER AND STABLE NUCLEI

To understand the properties of our QMD models, we first calculate the energy and the proton chemical potential of pure neutron matter at zero temperature. In addition, we investigate the surface diffuseness and the surface tension of stable nuclei. These are one of the key uncertainties that affects the phase diagram at subnuclear densities [16–18,26]. To obtain pure neutron matter at zero temperature, we use the frictional relaxation method [Eq. (14)] with the cooling time scale of  $\mathcal{O}(10^3)$  fm/c. We calculate the proton chemical potential at zero temperature from the change of the energy by inserting a proton into the pure neutron matter. Here we relax the position and momentum of the proton with fixing those of neutrons (for more details about the procedures, see Ref. [23]). To obtain the ground state of finite nuclei, we use the conjugate gradient method [36].

Energy  $E_n$  per baryon of pure neutron matter is shown in the left panel of Fig. 1. At subnuclear densities,  $E_n$  of both the QMD models exhibits reasonable values compared with those of other nuclear models. At lower densities of  $\rho_n \lesssim 0.1$  fm $^{-3}$ , model 1 gives relatively small energy but close to SkM, which gives the lowest energy among the other models. At densities below 0.12 fm $^{-3}$ , the energy of pure neutron matter for model 2 is larger than that for model 1. This tends to prevent neutrons from dripping out of nuclei. As we will see later, the number density of dripped neutrons for model 2 is indeed smaller than that for model 1.

According to Ref. [26], parameter  $L$  of the density-dependent symmetry energy coefficient also plays an important role in determining the density region of the pasta phases. This parameter is directly related to the derivative of the energy of pure neutron matter with respect to  $\rho_n$  at the normal nuclear density [see Eq. (4) in Ref. [26]]:

$$L = 3\rho_0 \frac{\partial}{\partial \rho_n} \left( \frac{\epsilon_n}{\rho_n} \right)_{\rho_0}, \quad (19)$$

where  $\epsilon_n$  is the energy density of pure neutron matter. The left panel of Fig. 1 shows a larger slope of the energy for model 1 than model 2, which leads to a larger value of  $L$  for

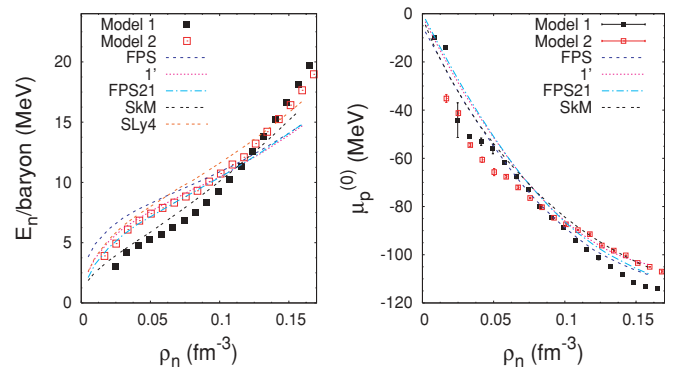


FIG. 1. (Color online) Energy per baryon (left panel) and proton chemical potential  $\mu_p^{(0)}$  (right panel) in pure neutron matter calculated by the QMD models and several other nuclear forces. The line denoted by SLy4 is from Ref. [21]. The other lines (FPS, 1', FPS21, and SkM) are from Ref. [37].

TABLE II. Several quantities of typical heavy nuclei calculated by each QMD model.  $E_B/A$  is the empirical binding energy from Ref. [39].  $E/A$  is the binding energy calculated by QMD.  $\rho_{\text{in}}$  is the central nucleon density of the nucleus.  $b_p$  and  $b_n$  are the surface diffuseness parameter for protons and neutrons, respectively, defined as Eq. (20).  $W$  is the binding energy defined as Eq. (22) evaluated for the central density and a proton fraction of the nucleus.  $\sigma$  is the surface tension defined as Eq. (21).

	$^{56}\text{Fe}$		$^{90}\text{Zr}$		$^{208}_{82}\text{Pb}$		$^{238}_{92}\text{U}$	
$E_B/A$ (MeV)	-8.79		-8.71		-7.87		-7.57	
Model	1	2	1	2	1	2	1	2
$E/A$ (MeV)	-9.09	-8.77	-9.25	-8.68	-8.66	-7.65	-8.31	-7.38
$\rho_{\text{in}}$ ( $\text{fm}^{-3}$ )	0.226	0.215	0.213	0.211	0.193	0.163	0.173	0.160
$b_p$ (fm)	4.0	3.2	4.2	3.2	3.4	3.1	3.3	3.0
$b_n$ (fm)	4.1	3.3	4.0	3.5	3.8	3.4	3.8	3.4
$W(\rho_{\text{in}}, x_p)$ (MeV)	-14.11	-14.80	-14.47	-14.72	-14.05	-14.51	-14.18	-14.26
$\sigma$ ( $\text{MeV fm}^{-2}$ )	0.66	1.13	1.03	1.09	0.62	1.07	0.73	1.03

model 1. From Eq. (19), we obtain  $L = 93$  MeV for model 1 and  $L = 80$  MeV for model 2. This difference affects the density at which matter becomes uniform, as we will discuss in the next section.

In the right panel of Fig. 1, we show the proton chemical potential  $\mu_p^{(0)}$  in pure neutron matter at zero temperature calculated by the QMD models together with those by other nuclear models. This result shows QMD model 1 gives slightly lower values of  $\mu_p^{(0)}$  at high densities compared with other nuclear models, whereas model 2 gives lower values at low densities. As discussed in Refs. [17,18], uncertainty of  $\mu_p^{(0)}$  little affects the phase diagram of supernova matter because the number density of dripped neutrons is very small [38].

In Table II we show several quantities related to the surface diffuseness and the surface energy of typical heavy nuclei,  $^{56}\text{Fe}$ ,  $^{90}\text{Zr}$ ,  $^{208}\text{Pb}$ , and  $^{238}\text{U}$ , calculated for each QMD model. We calculate the surface diffuseness parameter, which, following the spirit of Ref. [40], we define as

$$b_i \equiv \frac{\rho_{i,\text{in}}}{|d\rho_i/dr|_{\text{max}}}, \quad (i = p, n). \quad (20)$$

Here we have replaced  $\rho_0$  in the definition of Ref. [40], which is employed for the semi-infinite system, by the central density  $\rho_{i,\text{in}}$  of the finite nucleus.

We estimate the surface energy  $\sigma$  within the framework of QMD by subtracting the contributions of the bulk and the Coulomb energies from the total binding energy  $E$ :

$$\sigma = \frac{E - E_{\text{coul}} - AW(\rho_{\text{in}}, x_p)}{4\pi R^2}. \quad (21)$$

Here  $A$  and  $x_p$  are the mass number and the proton fraction of the nucleus,  $E_{\text{coul}}$  is the Coulomb energy of the nucleus, and  $W(\rho_{\text{in}}, x_p)$  is the bulk energy evaluated for the central density  $\rho_{\text{in}}$  of the nucleus. For  $W(\rho_{\text{in}}, x_p)$ , we assume the following form,

$$W(\rho_{\text{in}}, x_p) \equiv W_V + \frac{1}{2}K_0 \left(1 - \frac{k_{\text{in}}}{k_0}\right)^2 + 4S_V \left(x_p - \frac{1}{2}\right)^2, \quad (22)$$

where  $W_V$  is the binding energy of symmetric nuclear matter at  $\rho_0$ ,  $K_0$  is the incompressibility, and  $k_{\text{in}} \equiv (3\pi^2\rho_{\text{in}}/2)^{1/3}$  and  $k_0 \equiv (3\pi^2\rho_0/2)^{1/3}$  are the wave numbers of nucleon at  $\rho = \rho_{\text{in}}$  and  $\rho_0$ , respectively. We set  $W_V = -16$  MeV,  $K_0 = 280$  MeV,  $S_V = 34.6$  MeV, and  $\rho_0 = 0.165 \text{ fm}^{-3}$  for model 1 [28] and  $W_V = -16$  MeV,  $K_0 = 280$  MeV,  $S_V = 33$  MeV, and  $\rho_0 = 0.168 \text{ fm}^{-3}$  for model 2 [29,31]. The nuclear radius  $R$  in Eq. (21) is defined as

$$R \equiv \left(\frac{3}{4\pi} \frac{A}{\rho_{\text{in}}}\right)^{1/3}. \quad (23)$$

Table II shows that the surface energy  $\sigma$  estimated for model 2 is systematically higher than that for model 1. We also see that the surface diffuseness parameters  $b_i$  of both neutrons and protons are smaller for model 2 than model 1, which means model 2 yields steeper density profile of the nuclear surface. Both of these two facts consistently indicate that the nuclear surface energy for model 2 is greater than that for model 1.

## IV. NUCLEAR MATTER AT SUBNUCLEAR DENSITIES

### A. Simulations and snapshots

We studied the  $(n, p, e)$  system of the proton fraction  $x_p = 0.3$  at zero and nonzero temperatures. The value of  $x_p = 0.3$  is typical for matter in collapsing supernova cores. For this purpose, we use 2048 nucleons (614 protons and 1434 neutrons) in a cubic simulation box with periodic boundary condition [41]. We assume that the system is not magnetically polarized, i.e., it contains equal numbers of protons (and neutrons) with spin up and spin down. The relativistic degenerate electrons can be well approximated as a uniform background in our situations [42–44]. The Coulomb interaction is calculated by the Ewald sum (expressions used in our simulations are given in Ref. [23]). To obtain equilibrium states both at zero and nonzero temperatures, we perform simulations in the following procedure. We first prepare nuclear matter at  $T = 10$  MeV by equilibrating the system for about 3000 fm/c using the Nosé-Hoover thermostat. To reproduce the ground state, we cool down the system with the

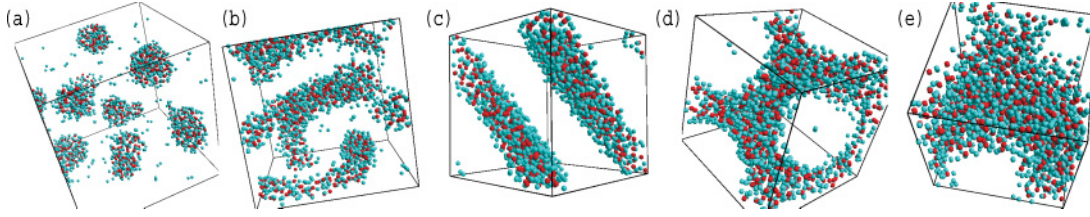


FIG. 2. (Color online) Nucleon distribution of the pasta phases at zero temperature for QMD model 2. Simulations are performed with 2048 nucleons at a proton fraction  $x_p = 0.3$ . Each red (blue) particle corresponds to a proton (neutron). Each picture shows the pasta phase with (a) spherical nuclei ( $0.1\rho_0 = 0.0168 \text{ fm}^{-3}$ ), (b) cylindrical nuclei ( $0.2\rho_0 = 0.0336 \text{ fm}^{-3}$ ), (c) slablike nuclei ( $0.393\rho_0 = 0.0660 \text{ fm}^{-3}$ ), (d) cylindrical holes ( $0.49\rho_0 = 0.0823 \text{ fm}^{-3}$ ), and (e) spherical holes ( $0.575\rho_0 = 0.0966 \text{ fm}^{-3}$ ). Box sizes are (a) 49.58 fm, (b) 39.35 fm, (c) 31.42 fm, (d) 29.19 fm, and (e) 27.67 fm.

frictional relaxation (14) for the time scale of  $\mathcal{O}(10^{3-4}) \text{ fm}/c$ . This time scale is sufficiently larger than the relaxation time scale of the system  $\mathcal{O}(10^2) \text{ fm}/c$ , which is determined by the typical length scale of the structure  $\mathcal{O}(10) \text{ fm}$  and the sound velocity  $\mathcal{O}(10^{-1})c$ . To obtain nuclear matter at some fixed nonzero temperature of  $T_{\text{set}}$ , we start from a snapshot with the effective temperature  $T_{\text{eff}} \simeq T_{\text{set}}$  obtained in the above cooling process. We then equilibrate it with the Nosé-Hoover thermostat for at least 5000 fm/c.

In Fig. 2, we show nucleon distributions of the pasta phases at zero temperature obtained by the simulations for model 2. Compared with those for model 1 (see, e.g., Fig. 2 in Ref. [22]), less dripped neutrons are observed. Especially, dripped neutrons almost disappear when nuclei become planar. This would be due to the higher energy  $E_n$  of pure neutron matter at low densities as shown in Fig. 1. As stated later in Sec. IV C, this relative lack of dripped neutrons decreases the density at which the fission instability of spherical nuclei occurs.

In Fig. 3 we show how slablike nuclei melt to be uniform nuclear matter with increasing temperature. We can see a basic picture of phase transitions at nonzero temperatures for fixed densities from this figure. Suppose we increase the temperature from zero. At  $T \simeq 1 \text{ MeV}$ , neutrons start to evaporate from nuclei. At  $T = 2-3 \text{ MeV}$ , increase of the volume fraction of nuclear matter region due to its thermal expansion triggers a transition of the nuclear structure: slablike nuclei start to connect with each other to form cylindrical bubbles. At  $T \simeq 4 \text{ MeV}$ , protons cannot be completely confined in nuclei and start to evaporate. In this situation, nuclear surface can no longer be identified, but in many cases there remains clustering of protons and neutrons, i.e., nuclear matter does not completely become uniform. Finally, the clustering inside nuclear matter completely disappears and matter becomes

uniform. We observe this transition at  $T = 6-7 \text{ MeV}$  in the case of Fig. 3.

**B. Identification of phases**

As can be seen from the snapshots of the nucleon distribution in the previous section, especially at nonzero temperatures, nuclei have complicated shapes and moreover nuclear surface becomes diffuse. We thus need to quantitatively identify the nuclear shape from nucleon distributions obtained by the simulations. For this purpose, we use the two-point correlation function and the Minkowski functionals, especially the area-averaged integral mean curvature  $\langle H \rangle$  and the Euler characteristic density  $\chi/V$ . The Euler characteristic  $\chi$  is a purely topological quantity and is expressed as

$$\chi = (\text{number of isolated regions}) - (\text{number of tunnels}) + (\text{number of cavities}). \tag{24}$$

For detailed procedures of calculating the Minkowski functionals, see Ref. [23] (see also Refs. [45–47] for the algorithm of the calculation).

With these quantities, we can completely classify the following typical pasta phases:

$$\begin{cases} \langle H \rangle > 0 & \text{and} & \chi/V > 0 & \text{for spherical nuclei (SP)} \\ \langle H \rangle > 0 & \text{and} & \chi/V = 0 & \text{for cylindrical nuclei (C)} \\ \langle H \rangle = 0 & \text{and} & \chi/V = 0 & \text{for slablike nuclei (S)} \\ \langle H \rangle < 0 & \text{and} & \chi/V = 0 & \text{for cylindrical holes (CH)} \\ \langle H \rangle < 0 & \text{and} & \chi/V > 0 & \text{for spherical holes (SH)}. \end{cases} \tag{25}$$

As shown above,  $\chi/V$  is always positive or zero for these phases. However, in our previous studies [23,24], and also in the present study, we obtain “spongelike” phases with multiply connected structures characterized by  $\chi/V < 0$ . We call the phases with  $\chi/V < 0$  intermediate phases, which

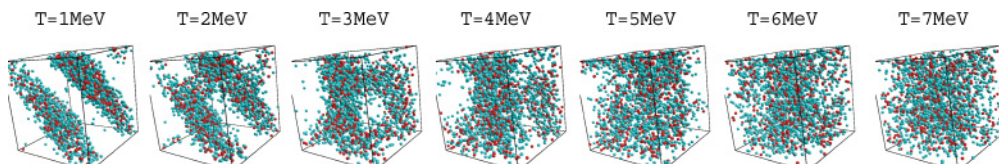


FIG. 3. (Color online) Nucleon distribution at  $T = 1-7 \text{ MeV}$  and a fixed density for model 2. Simulations are performed with 2048 nucleons at  $x_p = 0.3$  and  $\rho = 0.393 \rho_0 = 0.0660 \text{ fm}^{-3}$  (the box size is 31.42 fm), where the phase with slablike nuclei is obtained at zero temperature. Each red (blue) particle corresponds to a proton (neutron).

appear in the density region between those of the phases with rodlike nuclei and slablike nuclei [here we denote as (C,S)] and between slablike nuclei and rodlike bubbles [denote as (S,CH)]. The former phase (C,S) gives  $\langle H \rangle > 0$  and  $\chi/V < 0$  and the latter one, (S,CH), gives  $\langle H \rangle < 0$  and  $\chi/V < 0$ . Considering similarity of exotic structures observed in nuclear matter and diblock copolymers, several authors pointed out a possibility of more complex structures than ordinary pasta structures, i.e., rods or slabs [25,43,48]. In diblock copolymer melts, one experimentally finds complicated structures, e.g., so-called gyroid (G) structure and the ordered bicontinuous double diamond (OBDD) structure. Although the intermediate phases obtained in our studies are different from G and OBDD phases, it is possible that some complicated structure other than one-dimensional lattice of slablike nuclei, hexagonal lattice of rodlike ones, and BCC lattice of spherical ones appears [25,43].

The quantities  $\langle H \rangle$  and  $\chi/V$  can be calculated only if nuclear surface can be identified. Suppose we increase the temperature, nuclei start to melt and nuclear surface cannot be necessarily identified. In this situation, the density inhomogeneity of long wavelength starts to be smoothed out but still remains. Further increasing temperature and exceeding some critical point, matter becomes uniform. To determine the boundary where inhomogeneity disappears, we use the two-point correlation function defined as

$$\xi_{ii}(r) = \frac{1}{4\pi} \int d\Omega_{\mathbf{r}} \frac{1}{V} \int d\mathbf{x} \delta_i(\mathbf{x}) \delta_i(\mathbf{x} + \mathbf{r}) \quad (26)$$

$$\equiv \langle \delta_i(\mathbf{x}) \delta_i(\mathbf{x} + \mathbf{r}) \rangle_{\mathbf{x}, \Omega_{\mathbf{r}}} \quad (27)$$

Here  $i$  specifies the species of particles (proton or neutron, or both collectively),  $\langle \cdots \rangle_{\mathbf{x}, \Omega_{\mathbf{r}}}$  denotes an average over the position  $\mathbf{x}$  and the direction of  $\mathbf{r}$ , and  $\delta_i(\mathbf{x})$  is the fluctuation of the density field  $\rho^{(i)}(\mathbf{x})$  given by

$$\delta_i(\mathbf{x}) \equiv \frac{\rho^{(i)}(\mathbf{x}) - \overline{\rho^{(i)}}}{\overline{\rho^{(i)}}}, \quad (28)$$

with the average density of protons or neutrons or both collectively:

$$\overline{\rho^{(i)}} \equiv \frac{N_i}{V}. \quad (29)$$

If the system of nuclear matter is separated into liquid and gas phases, the two-point correlation function  $\xi_{NN}(r)$  of nucleons oscillates around zero even at long distances. Otherwise,  $\xi_{NN}(r)$  is almost zero (for  $r \gtrsim 7$  fm in our cases) without oscillating. In this case we judge the system is uniform (see Ref. [24] for more details).

### C. Phase diagrams

In Fig. 4 we show the phase diagram of the pasta phases at zero temperature calculated by QMD. The upper and the lower panels of Fig. 4 are the phase diagram for model 1 and 2, respectively. The sequence of nuclear shapes with increasing density is the same as that predicted by all the previous works including those by QMD. The density region of the phases with nonspherical nuclei for model 2 is larger than that for

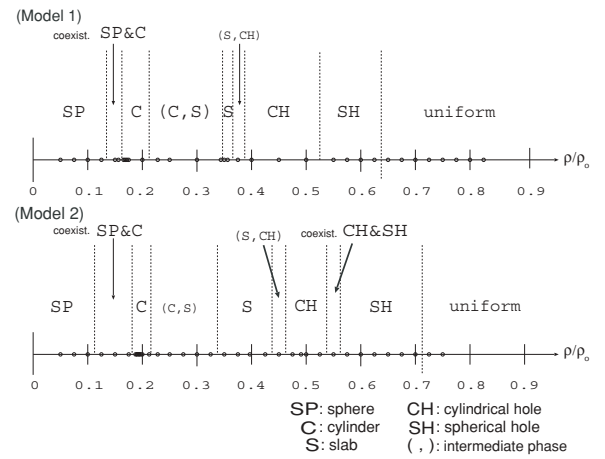


FIG. 4. Phase diagram of the pasta phases at zero temperature for model 1 (upper panel) and model 2 (lower panel). Proton fraction is  $x_p = 0.3$ . Horizontal axis is normalized in units of the normal nuclear density  $\rho_0$  for each model. Abbreviations SP, C, S, CH, and SH mean phases with spherical nuclei, cylindrical nuclei, slablike nuclei, cylindrical holes, and spherical holes, respectively. The parentheses (A,B) show an intermediate phase between A and B phases.

model 1: spherical nuclei begin to elongate at a lower density and spherical bubbles remain until a higher density for model 2.

The decrease of the density at which nuclei start to be deformed would be due to the smaller number density of dripped neutrons for model 2 compared with model 1, which is originated from the larger energy of pure neutron matter at low densities shown in Fig. 1. Nuclei are more neutron rich due to the smaller number density of dripped neutrons. The nucleon number density inside the nuclei is relatively small because of the smaller saturation density of nuclear matter at the lower proton fraction. Thus the volume fraction of the nuclei increases, which decreases the fission instability of spherical nuclei [43]. Furthermore, the decrease of the number density of dripped neutrons increases the mass number of nuclei, which also increases their volume fraction. As a result, although the saturation density of asymmetric nuclear matter of  $x_p = 0.3$  for model 2 is higher (see below), the volume fraction of nuclei for model 2 is about 10% higher than that for model 1 at  $\rho = 0.1\rho_0$ . Thus the density at which the fission instability occurs for model 2 should be  $\sim 0.01\rho_0$  lower than that for model 1. This value is consistent with our present results, which indicate the difference between the two models is smaller than  $0.05\rho_0$ .

As to the boundary between the regions of the phase with spherical holes and of the uniform phase, however, the increase of the density  $\rho_m$  at which matter becomes uniform would be due to higher saturation density at a proton fraction  $x_p = 0.3$  for model 2. The saturation density and the saturation energy per baryon at  $x_p = 0.3$  are  $0.136 \text{ fm}^{-3}$  and  $-12.01 \text{ MeV}$  for model 1 and  $0.147 \text{ fm}^{-3}$  and  $-9.86 \text{ MeV}$  for model 2 [49]. The saturation density directly affects  $\rho_m$  and, consequently, the  $\rho_m$  of model 2 is higher than that of model 1. Here one should keep in mind an effect of the surface energy. In Sec. III, we show that model 2 gives a larger surface tension compared with model 1. The larger surface tension of model 2

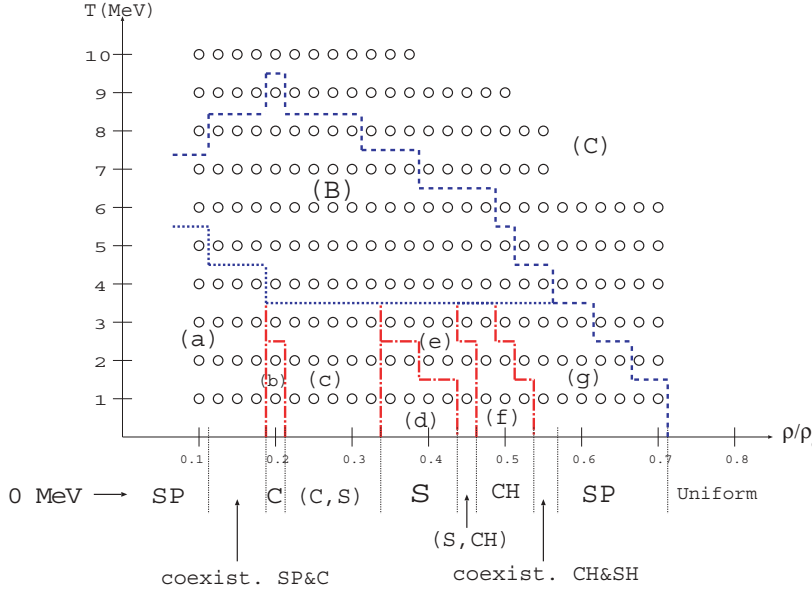


FIG. 5. (Color online) Phase diagram of nuclear matter of  $x_p = 0.3$  at subnuclear densities by QMD model 2 plotted in the  $\rho$ - $T$  plane. The horizontal axis is normalized in unit of the nuclear saturation density. The dashed lines correspond to phase separation lines. The dotted lines show the boundary above which nuclear surface cannot be identified. The dash-dotted lines show boundaries between different phases. Abbreviations are the same as described in the caption to Fig. 4. The meanings of regions (a)–(g), (B), and (C) are explained in the text. Simulations have been carried out at the points denoted by circles.

favors the uniform phase without bubbles and acts to decrease  $\rho_m$ . However, this effect should be small compared to the contribution of the saturation density, which can be understood by taking account of the incompressible property of nuclear matter; in the incompressible limit,  $\rho_m = \rho_s$  and the surface tension does not affect  $\rho_m$  at all.

The result that the model 2 yields a wider density region of the pasta phases compared with model 1 can be also understood in terms of the density-dependence parameter  $L$  of the symmetry energy. Within a macroscopic model employed in Ref. [26] see Eq. (1) and Eq. (4) of that reference], the saturation density at a fixed value of  $x_p$  is given by [26]

$$\rho_s(x_p) = \rho_0 [1 - 3L(1 - 2x_p)^2 / K_0], \quad (30)$$

where  $K_0$  is the incompressibility. This equation means smaller  $L$  yields higher  $\rho_s(x_p)$  of asymmetric nuclear matter. The above higher  $\rho_s(x_p = 0.3)$  of model 2 than that of model 1 shows a smaller  $L$  of model 2, which is consistent with the results of  $L$  obtained from the energy of pure neutron matter in Sec. III. According to a result of a comprehensive analysis of Ref. [26], there is a systematic trend that nuclear models with smaller  $L$  yields a wider density region of the pasta phases.

Phase diagram of model 2 for  $x_p = 0.3$  at nonzero temperatures is shown in Fig. 5. Each region of this phase diagram is defined as follows: (a) SP, (b) C, (c) (C,S), (d) S, (e) (S,CH), (f) CH, (g) SH, (B) phase-separating region, and (C) uniform matter. Abbreviations SP, C, S, CH, SH, and (A,B) are the same as in Fig. 4. Compared with the phase diagram of model 1 (see Fig. 19 in Ref. [24]), both the pasta phases and the liquid-gas phase-separating region survive until higher temperatures: in the case of model 1, the nuclear surface cannot be identified above 2–3 MeV and the critical temperature  $T_c$  of the phase separation is at  $T \gtrsim 6$  MeV, whereas for model 2, the surface melting temperature is at 3–4 MeV and  $T_c$  is at  $T \gtrsim 9$  MeV. The increase of the surface melting temperature can be explained by higher energy of pure neutron matter, which prevents neutrons from dripping out of nuclei. In addition, as described

in Sec. III, the surface diffuseness for model 2 is smaller than that for model 1. These properties keep the high density contrast between the inside and the outside of nuclei, and hence the nuclear surface remains to be identified at higher temperatures. However, the increase of the critical temperature of the phase separation for model 2 may be explained by the smaller value of  $L$ , which increases the density where the proton clustering instability takes place [26]. Phase separation at high temperatures would be also induced by the proton clustering. Thus the same expectation may be possible for this situation, i.e., higher symmetry energy due to the smaller value of  $L$  destabilizes uniform matter against the phase separation. As a result, the phase separation occurs at relatively higher temperatures for model 2.

## V. DISCUSSION AND CONCLUSION

We investigated the phase diagram of the pasta phases both at zero and nonzero temperatures by QMD with two different models. Properties of these two models are compared by calculating the energy and the proton chemical potential of pure neutron matter, the surface diffuseness, and the surface energy of several typical heavy nuclei. Differences in the phase diagram, especially the expansion of the density and temperature region of the nonuniform phases, can be explained by these properties of pure neutron matter. The sequence of the nuclear shape with increasing density and the qualitative feature of thermal fluctuation on the nucleon distribution with increasing temperature are the same as observed in our previous study [24]. The general picture of the change of the nucleon distribution at a fixed density with increasing temperature is as follows.

At low temperatures,  $T = 1$ –1.5 MeV for model 1 and  $T = 1$ –2 MeV for model 2; the number density of evaporated neutrons increases with temperature. However, the structure of nuclei does not largely change from that at  $T = 0$ . The

nuclear surface becomes diffuse and the volume fraction of nuclei increases by thermal expansion.

At intermediate temperatures,  $T = 1.5\text{--}2.5$  MeV for model 1 and  $T = 2\text{--}3$  MeV for model 2; the nuclear shape is significantly deformed and in some cases phase transition between different nuclear structures is triggered by the increase of the volume fraction of nuclei. Thus the density of the phase boundary between the different nuclear shapes decreases with increasing temperature.

At high temperatures,  $T \simeq 2.5\text{--}3$  MeV for model 1 and  $T \simeq 3\text{--}4$  MeV for model 2; evaporated nucleons are dominant and the nuclear surface can no longer be identified. However, the long-range correlations between nucleons due to the liquid-gas phase separation remain until a higher temperature  $T \simeq 6$  MeV for model 1 and  $T \simeq 9$  MeV for model 2. Above these temperatures, inhomogeneity disappears at any density.

The density-dependence parameter  $L$  of the symmetry energy is the key to understand the uncertainties of the density region of the pasta phases in cold neutron stars [26]. This parameter is also helpful to understand the present results and to predict the general tendency of phase diagram of the pasta phases in supernova cores. From the energy of cold neutron matter, we obtain  $L = 93$  MeV for QMD model 1 and  $L = 80$  MeV for model 2. The larger critical temperature  $T_c$  for the phase separation of model 2 would be due to the smaller value of  $L$ . In addition, the smaller  $L$  also yields a higher saturation density of asymmetric nuclear matter [see Eq. (30)], which in turn increases the density at which the system becomes uniform nuclear matter. If one uses a nuclear force with a smaller value of  $L$ , the density and temperature region of nonuniform nuclear matter would broaden.

Let us now discuss the abundance of nonuniform phases of nuclear matter in supernova cores. Here we take an EOS by Shen *et al.* [50] as an example, which is one of the widely used EOSs in supernova simulations. For the nuclear model employed in this EOS, we estimate  $L \simeq 120$  MeV, which is

rather high in the range of uncertainty of nuclear forces (see, e.g., Fig. 1 of Ref. [26]). In our previous work [8], using EOS by Shen *et al.*, we have estimated the mass fraction of the pasta phases just before bounce and have obtained  $\sim 10\text{--}20\%$ . Because we can expect values of  $L$  for other typical EOSs are smaller than  $L = 120$  MeV for EOS by Shen *et al.*, our previous estimate of the mass fraction using Shen's EOS would be very conservative. It is reasonable to conclude that the mass fraction of the pasta phases would be larger than  $10\text{--}20\%$  in the later stage of the collapse.

As we have shown in Ref. [8], neutrino opacity via weak neutral current in the pasta phases can be significantly different from that without taking account of the pasta phases. Furthermore, even if nuclear surface melts, the neutrino opacity of the vector current contribution in the liquid-gas phase-separating system is still larger than that of the completely uniform gas phase. Our present result also indicates expansion of the phase-separating region for smaller values of  $L$ . Although the influence of the phase-separating region on the mechanism of the supernova explosion has yet to be revealed completely, it could exist not only during collapsing phase but also after bounce. Depending on the location of the neutrino photosphere and the temperature profile in the late stage, these region can affect the success of supernova explosions [51].

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