



6. Microscopic Study of Nuclear “Pasta” by Quantum Molecular Dynamics 量子分子動力学法による核物質「パスタ」の微視的研究

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Structure of cold dense matter at subnuclear densities is investigated by quantum molecular dynamics (QMD) simulations. We succeeded in showing that the phases with slab-like and rod-like nuclei etc. can be formed dynamically from hot uniform nuclear matter without any assumptions on nuclear shape. We also observe intermediate phases, which has complicated nuclear shapes. Geometrical structures of matter are analyzed with Minkowski functionals, and it is found out that intermediate phases can be characterized as ones with negative Euler characteristic. Our result suggests the existence of these kinds of phases in addition to the simple “pasta” phases in neutron star crusts.

Collapse-driven supernovae (SNe) and the following formation of neutron stars (NSs) are the most dramatic processes during the stellar evolution. These objects provide not only astrophysically significant phenomena but also interesting material phases inside them; both are strongly connected with each other. Investigating the properties of nuclear matter under extreme condition is one of the essential subjects to clarify the mechanism of collapse-driven SNe [1] and the structure of NS crusts [2]. This subject is also interesting in terms of the fundamental problem of the complex fluids of nucleons.

At subnuclear densities, nuclear matter exhibits the coexistence of a liquid phase with a gas phase due to the internucleon interaction which has long-range attractive part. At sufficiently low temperatures and low densities, which are relevant to NS interiors, long-range Coulomb interactions make the system separate periodically into gas and spherical liquid drops, adding a crystalline property to the liquid-gas coexistence.

In the density region where nuclei are about to melt into uniform matter, it is expected that the energetically favorable configuration of the mixed phase possesses interesting spatial structures such as rod-like and slab-like nuclei and rod-like and spherical bubbles etc., which are referred to as nuclear “pasta”. This picture was first proposed by Ravenhall et al. [3] and Hashimoto et al. [4] independently. Their predictions both based on free energy calculations with liquid drop models assuming some specific nuclear shapes. These works clarify that the most energetically stable nuclear shape is determined by a subtle balance between nuclear surface and Coulomb energies. Although detailed

aspects of equilibrium phase diagrams vary with nuclear models [5], the realization of the “pasta” phases as energy minimum states can be seen in a wide range of nuclear models and basic feature of phase diagrams is universal [9, 10], i.e. with increasing density, the shape of the nuclear matter region changes like sphere \rightarrow cylinder \rightarrow slab \rightarrow cylindrical hole \rightarrow spherical hole \rightarrow uniform. This feature is also reproduced by the Thomas-Fermi calculations by several groups [6–8].

The phases with these exotic nuclear structures, if they are realized in NS crusts or SN cores, bring about many astrophysical consequences. As for those to NS phenomena, it is interesting to note the relevance of nonspherical nuclei in neutron star matter (NSM) to pulsar glitches [15] and cooling of NSs [5]. On the other hand, “pasta” phases in supernova matter (SNM) are expected to affect the neutrino transport [3, 10] and hydrodynamics in SN cores [7].

Though the properties of “pasta” phases in equilibrium state have been investigated actively, the formation and the melting processes of these phases have not been discussed except for some limited cases which are based on perturbative approaches [2, 11]. It is important to adopt a microscopic and dynamical approach which allows arbitrary nuclear structures in order to understand these processes of nonspherical nuclei. At finite temperatures, it is considered that not only nuclear surface becomes obscure but also nuclei of various shapes may coexist. Therefore, it is necessary to incorporate density fluctuations without any assumptions on nuclear shape to investigate the properties of “pasta” phases at finite temperatures. Although the works done by Williams and Koonin [6] and Lassaut et al. [7]

do not assume nuclear structure, they can not incorporate fluctuations of nucleon distributions in a satisfying level because they are based on the Thomas-Fermi calculation which is one-body approximation. In addition, only one structure is contained in the simulation box in these works, there are thus possibilities that nuclear shape is strongly affected by boundary effect and some structures are prohibited implicitly.

We have started studying dense matter at sub-nuclear densities by quantum molecular dynamics (QMD) [13] which is one of the molecular dynamics (MD) approaches for nucleon many body systems (see, e.g., Ref. [14] for review). MD for nucleons including QMD, which is a microscopic and dynamical method without any assumptions on nuclear structure, is suitable for incorporating fluctuations of particle distributions. The final aim of our study is to understand the above mentioned formation and melting processes of non-spherical nuclei and to investigate the properties of matter consists of nonspherical nuclei at finite temperatures. For the first step, the question posed in this paper is as follows: *Can the phases with nonspherical nuclei be formed dynamically?*

There is a pioneering work by Maruyama et al. [12] which attempts to investigate the structure of matter at subnuclear densities by QMD. Unfortunately, they did not treat the Coulomb interaction consistently and could not anneal the system successfully. As a result, they could not reproduce the phases with nonspherical nuclei of simple structures. In the present work, we improve the above shortcomings and obtain phase diagrams for cold dense matter of the proton fraction $x = 0.3$ and 0.5 at subnuclear densities. We also discuss nuclear shape changes with a topological quantity, i.e. the Euler characteristic.

While there are a lot of versions of MD for fermions, we choose QMD among them based on trade-off between calculational amounts and accuracies. The typical length scale l of inter-structure is $l \sim 10$ fm and the density region of interest is just below the normal nuclear density $\rho_0 = 0.165 \text{ fm}^{-3}$. The required nucleon number N in order to reproduce n structures in the simulation box is about $N \sim \rho_0 (nl)^3$ (for slabs), it is thus desirable that we prepare nucleons of order 10000 if we try to reduce boundary effects. While it is very hard task to treat such a large system by, for example, FMD and AMD (see, e.g., Ref. [14] and references therein) whose calculational amounts scale as $\sim N^4$, it is feasible to do it by QMD whose calculational amounts scale

as $\sim N^2$. It is also noted that we mainly focus on macroscopic structures; the exchange effect would not be so important for them. Therefore, QMD, which is less elaborate in treating the exchange effect, has the advantage of other models.

We have performed QMD simulations of infinite (n,p,e) system with fixed proton fraction $x = 0.3$ and 0.5 for various nucleon densities ρ (the density region is $0.05 - 1.0 \rho_0$). We set a cubic box which is imposed periodic boundary conditions in which 2048 nucleons (1372 nucleons in some cases) are contained. The relativistic degenerate electrons which ensure the charge neutrality are treated as a uniform background and the Coulomb interaction is calculated by the Ewald method. For nuclear interaction, we use an effective Hamiltonian developed by Maruyama et al. (medium EOS model) [12] which reproduce the bulk properties of nuclear matter and the properties of stable nuclei, especially heavier ones, i.e. binding energy and root-mean-square radius.

We first prepare an uniform hot nucleon gas at $k_B T \sim 20$ MeV as an initial condition which is equilibrated for $\sim 500 - 2000$ fm/c in advance. In order to realize the ground state of matter, we then cool it down slowly for $O(10^3 - 10^4)$ fm/c keeping the nucleon density constant by frictional relaxation method etc. until the temperature gets ~ 0.1 MeV or less. Note that any artificial fluctuations are not given during the simulation.

The QMD equations of motion with friction terms are solved using the fourth-order Gear predictor-corrector method in conjunction with multiple time step algorithm [16]. Integration time steps Δt are set to be adaptive in the range of $\Delta t < 0.1 - 0.2$ fm/c depending on the degree of convergence. At each step, the correcting operation is iterated until the error of position Δr and the relative error of momentum $\Delta p/p$ get smaller than 10^{-6} , where Δr and $\Delta p/p$ are estimated as the maximum values of correction among all particles. Computer systems which we use are equipped with MD-GRAPE II.

Shown in Figs. 1 and 2 are the resultant nucleon distributions of cold matter at $x = 0.5$ and 0.3 , respectively. We can see from these figures that the phases with rod-like and slab-like nuclei, cylindrical and spherical bubbles, in addition to the one with spherical nuclei are reproduced in the both cases of $x = 0.5$ and 0.3 . We here would like to mention some reasons of discrepancies between the present result and the result obtained by Maruyama et al. which says "the nuclear shape may not have these simple sym-

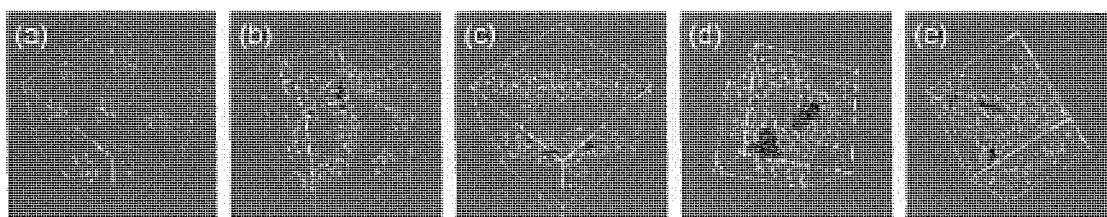


FIG. 1: The nucleon distributions of typical phases with simple structures of cold matter at $x = 0.5$; (a) sphere phase, $0.1\rho_0$; (b) cylinder phase, $0.18\rho_0$; (c) slab phase, $0.4\rho_0$; (d) cylindrical hole phase, $0.5\rho_0$ and (e) spherical hole phase, $0.6\rho_0$. The darker particles represent protons and the brighter ones represent neutrons.

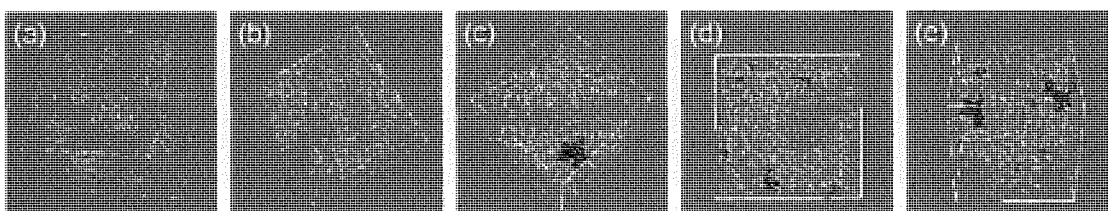


FIG. 2: Same as Fig. 1 at $x = 0.3$; (a) sphere phase, $0.1\rho_0$; (b) cylinder phase, $0.18\rho_0$; (c) slab phase, $0.35\rho_0$; (d) cylindrical hole phase, $0.5\rho_0$ and (e) spherical hole phase, $0.55\rho_0$. The darker particles represent protons and the brighter ones represent neutrons.

metries" [12]. The most crucial reason seems to be the difference in treatment of the Coulomb interaction. In the present simulation, we calculate the long range Coulomb interaction in a consistent way using the Ewald method. For the system of interest where the Thomas-Fermi screening length is comparable to or larger than the size of nuclei, this treatment is more adequate than that with introducing an artificial cutoff distance as in Ref. [12]. The second reason would be the difference in the relaxation time scales τ . In our simulation, we can reproduce the bubble-phases (cylindrical and spherical bubbles) with $\tau \sim 10^3$ fm/c and the nucleus-phases (cylindrical and planar nuclei) with $\tau \sim O(10^4)$ fm/c. However, the matter in the density region corresponding to a nucleus-phase is quenched in an amorphous state when $\tau \lesssim 10^3$ fm/c. In the present work, we take τ much larger than typical time scale $\tau_{th} \sim O(100)$ fm/c for nucleons to thermally diffuse the distance of $l \sim 10$ fm at $\rho \simeq \rho_0$ and $k_B T \simeq 1$ MeV. This temperature is below the typical value of the liquid-gas phase transition temperature in the density region of interest, it is thus considered that our results are thermally relaxed in a satisfying level.

Phase diagrams of matter in the ground state are shown in Figs. 3 (a) and (b) for $x = 0.5$ and 0.3 , respectively. As can be seen from these fig-

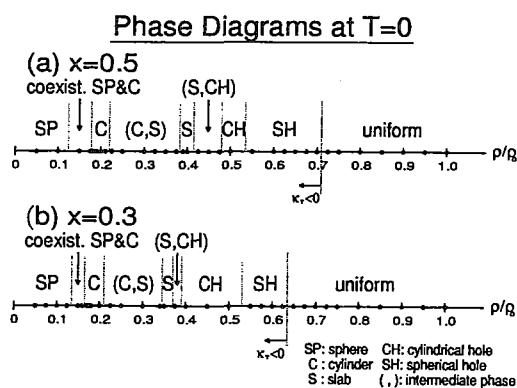


FIG. 3: Phase diagrams of cold matter at $x = 0.5$ (a) and $x = 0.3$ (b). Matter is unstable against phase separation in the density region shown as $\kappa_T < 0$, where κ_T is the isothermal compressibility. The symbols SP, C, S, CH and SH stand for nuclear shapes, i.e. sphere, cylinder, slab, cylindrical hole and spherical hole, respectively. The parentheses (A,B) show intermediate phases between A-phase and B-phase suggested in this work. They have complicated structures different from those of both A-phase and B-phase. Simulations have been carried out at densities denoted by small circles.

ures, the obtained phase diagrams basically reproduce the sequence of the energetically favored nuclear shapes predicted by simple discussions [4] which only take account of the Coulomb and

surface effects; this prediction is that the nuclear shape changes like sphere \rightarrow cylinder \rightarrow slab \rightarrow cylindrical hole \rightarrow spherical hole \rightarrow uniform, with increasing density. Comparing Figs. 3 (a) and (b), we can see that the phase diagram shifts towards the lower density side with decreasing x , which is due to the tendency that as the nuclear matter at larger nucleon excess, the saturation density is lowered. It is remarkable that the density dependence of the nuclear shape, except for cylindrical bubbles (just in the case of $x = 0.3$) and spherical nuclei and bubbles, is quite sensitive and phases with intermediate nuclear shapes which are not simple as shown in Figs. 1 and 2 are observed in two density regions: one is between the cylinder phase and the slab phase, the other is between the slab phase and the cylindrical hole phase. We note that these phases are different from coexistence phases with nuclei of simple shapes and we will refer to them as “intermediate phases”.

To extract the morphological characteristics of the nuclear shape changes and the intermediate phases, we introduce the Minkowski functionals (see, e.g., Ref. [17] and references therein) as geometrical and topological measures of the nuclear surface. Let us consider a homogeneous body $K \in \mathcal{R}$ in the d -dimensional Euclidian space, where \mathcal{R} is the class of such bodies. Morphological measures are defined as functionals $\varphi : \mathcal{R} \rightarrow \mathbb{R}$ which satisfy the following three general properties: (1) *Motion invariance*, i.e. $\varphi(K) = \varphi(gK)$, where g denotes any translations and rotations. (2) *Additivity*, i.e. $\varphi(K_1 \cup K_2) = \varphi(K_1) + \varphi(K_2) - \varphi(K_1 \cap K_2)$, where $K_1, K_2 \in \mathcal{R}$. (3) *Continuity*, i.e. $\lim_{n \rightarrow \infty} \varphi(K_n) = \varphi(K)$ if $\lim_{n \rightarrow \infty} K_n = K$, where K is a convex body and $\{K_n\}$ is a sequence of convex bodies. Hadwiger’s theorem in integral geometry states that there are just $d+1$ independent functionals which satisfy the above properties; they are known as Minkowski functionals. In three dimensional space, four Minkowski functionals are related to the volume, the surface area, the integral mean curvature and the Euler characteristic.

Here, we particularly focus on the integral mean curvature and the Euler characteristic; the results of other quantities will be discussed elsewhere. Both are described by surface integrals of the following local quantities, the mean curvature $H = (\kappa_1 + \kappa_2)/2$ and the Gaussian curvature $G = \kappa_1 \kappa_2$, i.e. $\int_{\partial K} H dA$ and $\chi \equiv \frac{1}{2\pi} \int_{\partial K} G dA$, where κ_1 and κ_2 are the principal curvatures and dA is the area element of the surface of the body

K . The Euler characteristic χ is a purely topological quantity and

$$\begin{aligned} \chi = & \text{(number of isolated regions)} \\ & - \text{(number of tunnels)} \\ & + \text{(number of cavities)}. \end{aligned} \quad (1)$$

Thus $\chi > 0$ for the sphere and the spherical hole phases and the coexistence phase of spheres and cylinders, and $\chi = 0$ for the other ideal “pasta” phases, i.e. the cylinder, the slab and the cylindrical hole phases. We introduce the area-averaged mean curvature, $\langle H \rangle \equiv \frac{1}{A} \int H dA$, and the Euler characteristic density, χ/V , as normalized quantities, where V is the volume of the whole space.

We calculate these quantities by the following procedure. We first construct proton and nucleon density distributions $\rho_p(\mathbf{r}) = |\Phi_p(\mathbf{r})|^2$ and $\rho(\mathbf{r}) = |\Phi(\mathbf{r})|^2$ from data of the centers of position of the nucleons through a QMD trial wave function (see Ref. [12]), where $\Phi_p(\mathbf{r})$ and $\Phi(\mathbf{r})$ are the total proton and nucleon wave functions. We set a threshold proton density $\rho_{p,th}$ and then calculate $f(\rho_{p,th}) \equiv V(\rho_{p,th})/A(\rho_{p,th})$, where $V(\rho_{p,th})$ and $A(\rho_{p,th})$ are the volume and the surface area of the regions in which $\rho_p(\mathbf{r}) \geq \rho_{p,th}$. We find out the value $\rho_{p,th} = \rho_{p,th}^*$ where $\frac{d^2}{d\rho_{p,th}^2} f(\rho_{p,th}^*) = 0$ and define the regions in which $\rho_p(\mathbf{r}) \geq \rho_{p,th}^*$ as nuclear regions. For spherical nuclei, for example, $\rho_{p,th}^*$ corresponds to a point of inflection of a radial density distribution. In the almost whole phase-separating region, the values of $\rho_{p,th}^*$ distribute in the range of about $0.7 - 0.9\rho_0$ in the both cases of $x = 0.5$ and 0.3 , where $\rho_{p,th}^*$ is the threshold nucleon density corresponds to $\rho_{p,th}^*$. We then calculate A , $\int H dA$ and χ for the determined nuclear surface. We evaluate A by the triangle decomposition method, $\int H dA$ by the algorithm shown in Ref. [17] in conjunction with a calibration by correction of surface area, and χ by the algorithm of Ref. [17] and by that of counting deficit angles [18] which are confirmed that both of them give the same results.

We have plotted the obtained ρ dependence of $\langle H \rangle$ and of χ/V for the surface of $\rho_{th} = \rho_{th}^*$ at $x = 0.5$ in Figs. 4(a) and 4(b), respectively. In addition to the values of $\langle H \rangle$ for the surface of $\rho_{th} = \rho_{th}^*$, we have also investigated those for the surface of $\rho_{th} = \rho_{th}^* \pm 0.05\rho_0$ to examine the extent of the uncertainties of this quantity which stem from the arbitrariness in the definition of the nuclear surface, but we could not observe any remarkable differences in $\langle H \rangle$ from the values for

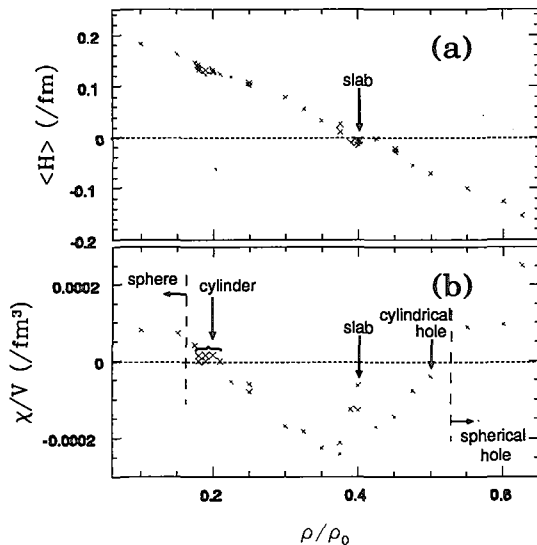


FIG. 4: Density dependence of the area-averaged mean curvature $\langle H \rangle$ (a) and the Euler characteristic density χ/V (b) of cold matter at $x = 0.5$.

$\rho_{th} = \rho_{th}^*$ (they were smaller than $0.015/\text{fm}$). We could not see these kinds of uncertainties in χ/V except for the densities near below the density at which matter turns into uniform.

The behavior of $\langle H \rangle$ shows that it decreases almost monotonously from positive to negative with increasing ρ until the matter turns into uniform. The densities correspond to $\langle H \rangle \simeq 0$ are about $0.4\rho_0$ for $x = 0.5$; these values are consistent with the density regions of the phase with slab-like nuclei (see Fig. 3). As mentioned previously, χ/V is actually positive in the density regions corresponding to the phases with spherical nuclei, coexistence of spherical and cylindrical nuclei, and spherical holes because of the existence of isolated regions. As for those corresponding to the phases with cylindrical nuclei, planar nuclei and cylindrical holes, $\chi/V \simeq 0$. The fact that the values of χ/V are not exactly zero for nucleon distributions shown as slab phases in Fig. 1 reflects the imperfection of these “slabs”, which is due to the small nuclear parts which connect the neighboring slabs. However, we can say that the behavior of χ/V depicted in Fig. 4(b) shows that χ/V is negative in the density regions of the intermediate phases, even if we take account of the imperfection of the obtained nuclear shapes and the uncertainties of the definition of the nuclear surface. This means that the intermediate phases consist of nuclear surfaces which are saddle-like at each point on average and they consist of each highly connected

nuclear and gas regions due to a lot of tunnels (see Eq. (1)).

Let us now refer to discrepancies from the results of previous works which do not assume nuclear structure [6, 7]; the intermediate phases can not be seen in these works. We can give following two reasons for the discrepancies: (1) These previous calculations are based on the Thomas-Fermi approximation which can not sufficiently incorporate fluctuations of nucleon distributions. This shortcoming may result in favoring nuclei of smoothed simple shapes than in the real situation. (2) There is a large possibility that some highly connected structures which have two or more substructures in a period are neglected in these works because only one structure is contained in a simulation box.

If the phases with highly connected nuclear and bubble regions are realized as the most energetically stable state, we can say that it is not unnatural thing [19]. It is considered that, for example, a phase with perforated slab-like nuclei, which has negative χ/V , could be more energetically stable than that with extremely thin slab-like nuclei. The thin planar nucleus costs surface-surface energy which stems from the fact that nucleons in it feel surfaces of both sides. We have to examine the existence of the intermediate phases by more extensive simulations with larger nucleon numbers and with longer relaxation time scales in the future.

Here we would like to discuss astrophysical consequences of our results. Pethick and Potekhin have pointed out that “pasta” phases with rod-like and slab-like nuclei are analogous to the liquid crystals according to the similarity of the geometrical structures [15]. It can also be said that the intermediate phases observed in the present work are “sponge”-like phases because they have both highly connected nuclear and bubble regions shown as $\chi/V < 0$. The elastic properties of the sponge-like intermediate phases are qualitatively different from those of the liquid crystal-like “pasta” phases because the former ones do not have any directions in which restoring force does not act, on the other hand the latter ones have. Our results suggest that the intermediate phases occupy a large fraction of the density region in which nonspherical nuclei can be seen (see Fig. 3). If this is also true for more neutron-rich case as $x \sim 0.1$, it leads to increasing of the maximum elastic energy that can be stored in the NS crust than that in the case of the all nonspherical nuclei have simple

structures. Besides, the cylinder and the slab phases which are liquid crystal-like lie between the sponge-like intermediate phases or the crystalline solid-like phase, and the releasing of the strain energy would, in consequence, concentrate in the domain of these liquid crystal-like phases. The above mentioned effects of the intermediate phases should be taken into account in considering the crust dynamics of starquakes etc. if these phases exist in NSM. In the context of pulsar glitch phenomena, the effects of the sponge-like nuclei on pinning rate of superfluid neutron vortices also have yet to be investigated.

For neutrino cooling of NSs, some version of the direct URCA process which is suggested by Lorenz et al. [5] that this might be allowed in the “pasta” phases would be suppressed in the intermediate phases. This is due to the fact that the proton spectrum is no longer continuous in the sponge-like nuclei. The last point which we would like to mention is about the effects of the intermediate phases on neutrino trapping in SN cores. The nuclear parts connect over a wide region which is much larger than that characterized by the typical neutrino wave length ~ 20 fm. Thus the neutrino scattering processes are no longer coherent in contrast to the case of the spherical nuclei, and this may, in consequence, reduce the diffusion time scale of neutrinos as in the case of “pasta” phases with simple structures. This reduction softens the SNM and would thus act to enhance the amount of the released gravitational energy.

The last point to be discussed is validity of the QMD model. It is considered that the contribution of the exchange effect is not so large for macroscopic scale. This can be seen by comparing the typical values of the exchange energy for this scale and of the energy difference between two successive phases of nonspherical nuclei. Suppose there are two identical nucleons bound in different nuclei each other. The exchange energy between these particles is calculated as exchange integral $K = \int U(\mathbf{r}_1 - \mathbf{r}_2) \varphi_1(\mathbf{r}_1) \varphi_1^*(\mathbf{r}_2) \varphi_2(\mathbf{r}_2) \varphi_2^*(\mathbf{r}_1) d\mathbf{r}_1 d\mathbf{r}_2$, where U is the potential energy. Asymptotic form of the wave function is $\varphi_i \sim \exp(-\kappa_i r)$, with $r = |\mathbf{r}_1 - \mathbf{r}_2|$ and $\kappa_i = \frac{1}{\hbar} \sqrt{2mE_i}$, ($i = 1, 2$), where E_i is the binding energy and m is the nucleon mass. The exchange integral reads $K \sim \exp[-(\kappa_1 + \kappa_2)R] \sim 5 \times 10^{-6}$ MeV for the internuclear distance $R \simeq 10$ fm and $E_i \simeq 8$ MeV, which is extremely smaller than the typical energy difference per nucleon between the “pasta”

phases of order 0.1 keV (NSM) - 10 keV (SNM). In the future, we further have to confirm the validity of our results by another model which is more elaborate in treating the exchange effect.

Our calculations demonstrate that the “pasta” phases can be formed dynamically from hot uniform matter in the proton-rich cases of $x = 0.5$ and 0.3 without any assumptions on nuclear shape. This suggests that the existence of these phases in NS crusts because they cool down keeping the local thermal equilibrium after proto-NSs are formed and their cooling time scale is much larger than the relaxation time scale of our simulations. This conclusion has to be confirmed in more neutron-rich cases of $x \sim 0.1$ in the future. Our results also suggest that the existence of the highly connected intermediate phases which are characterized as $\chi/V < 0$. This provides a vivid picture that NS inner crusts which consist of dense matter at subnuclear densities may be rich in properties due to the possibilities of a variety of material phases.

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