Formation of Nuclear “Pasta” in Supernovae

Gentaro Watanabe,1,2 Hidetaka Sonoda,3,2 Toshiki Maruyama,4 Katsuhiko Sato,3,5 Kenji Yasuoka,6 and Toshikazu Ebisuzaki2

1CNR INFM-BEC and Department of Physics, University of Trento, 38050 Povo, Italy
2RIKEN, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan
3Department of Physics, University of Tokyo, Tokyo 113-0033, Japan
4ASRC, Japan Atomic Energy Agency, Tokai, Ibaraki 319-1195, Japan
5IPMU, University of Tokyo, Kashiwa, Chiba, 277-8568 Japan
6Department of Mechanical Engineering, Keio University, Yokohama, 223-8522, Japan

(Dated: August 27, 2009)

In supernova cores, nuclear “pasta” phases such as triangular lattice of rod-like nuclei and layered structure of slab-like nuclei are considered to exist. However, it is still unclear whether or not they are actually formed in collapsing supernova cores. Using ab-initio numerical simulations called the Quantum Molecular Dynamics (QMD), we here solve this problem by demonstrating that a lattice of rod-like nuclei is formed from a bcc lattice by compression. We also find that, in the transition process, the system undergoes zigzag configuration of elongated nuclei, which are formed by a fusion of two original spherical nuclei.

PACS numbers: 26.50.+x, 21.65.-f, 02.70.Ns, 97.60.Bw

The mechanism of collapse driven supernova explosions has been a long-standing mystery. Matter in supernova cores is also yet to be understood and these issues are closely connected. In the initial stage of the explosions, the collapsing iron core experiences an adiabatic compression, which leads to an increase of the central density from $\sim 10^8$ g cm$^{-3}$ to around the normal nuclear density $\sim 3 \times 10^{14}$ g cm$^{-3}$ (corresponding to the nucleon number density $\rho_0 = 0.165$ fm$^{-3}$) just before the star rebounds. Thereby, the Coulomb repulsion between protons in nuclei, which tends to make a nucleus deform, becomes comparable to the surface tension of the nuclei, which favors a spherical nucleus. The pasta phases (phases consisting of “spaghetti”-like columnar nuclei and of “lasagna”-like planar nuclei, etc.) are thus expected to be formed in the inner cores during the collapse of stars and amount to more than 20% of the total mass of the cores just before the bounce. Since the coherent scattering of neutrons is very different between pasta nuclei and spherical ones, pasta phases can have a significant influence on the dynamics of explosions. Thus there is a growing interest in pasta phases.

However, the above speculation that the pasta phases are formed in collapsing cores is based on phase diagrams of the equilibrium state (e.g., Refs. [10, 11, 12, 13, 14] for non-zero temperatures) or static and perturbative calculations [15, 16]. Since formation of the pasta phases from a bcc lattice of spherical nuclei is accompanied by dynamical and drastic changes of the nuclear structure, the fundamental question whether or not the pasta phases are formed in supernova cores is still open, and an ab-initio approach is called for. In the present work, we answer this question using the Quantum Molecular Dynamics (QMD) [17, 18]. QMD can properly incorporate the thermal fluctuations and is a powerful and suitable approach [19] to describe the deformation of nuclei in the present problem as has been exploited for studying the equilibrium phase diagram [12, 20] and the transition dynamics between the pasta phases [21].

We use the QMD Hamiltonian of Ref. [18] with the standard medium-equation-of-state parameter set [22]. In our simulations, we consider a system with protons, neutrons, and charge-neutralizing electrons in a cubic box with periodic boundary condition. The electrons are relativistic and degenerate, and can be well approximated as a uniform background [13, 29]. We calculate the Coulomb interaction by the Ewald sum. Our simulations are carried out for the proton fraction $x \simeq 0.39$ and 0.49 using different initial conditions of the bcc lattice. In the following, we focus on the results for $x \simeq 0.39$ (the qualitative results are the same for $x \simeq 0.49$).

The initial condition of $x \simeq 0.39$ is obtained in the following way. We first prepare an isolated nucleus of $^{208}$Pb at zero temperature and make a unit cell of the bcc lattice by setting two copies of the nuclei in a box with the periodic boundary condition. Using the Nosé-Hoover thermostat for momentum-dependent potentials [12], we then equilibrate this sample at the temperature $T = 1$ MeV. We combine eight replica of this bcc unit cell to make a sample of the total number of nucleons $N = 3328$ (with 1312 protons and 2016 neutrons) at the nucleon number density $\rho = 0.15\rho_0$ (the box size $L = 51.23$ fm) and equilibrate at $T = 1$ MeV for $\simeq 7800$ fm/c using the Nosé-Hoover thermostat and further relax for $\simeq 4100$ fm/c without the thermostat. Equilibrating this sample at different temperatures, we also prepare initial conditions for various temperatures.

We simulate the compression of the bcc phase of spherical nuclei in the collapse. Starting from the above ini-
tial conditions, we increase the density by changing the box size $L$ (the particle positions are rescaled at the same time). Here the average rate of the compression is $\lesssim O(10^{-6}) \rho_0/(fm/c)$ yielding the time scale of $\gtrsim 10^5$ fm/$c$ to reach the typical density range of the phase with rod-like nuclei. This is much larger than the time scale of the change of nuclear shape (e.g., $\sim 1000$ fm/$c$ for nuclear fission) and thus the dynamics observed in our simulation would be determined by the intrinsic physical properties of the system, not by the density change applied externally. We perform adiabatic compression and isothermal compression at various temperatures [26]. In all the cases, we observe the formation of rod-like nuclei; here we show some typical examples in which we obtain a clear lattice structure of the rod-like nuclei.

Figure 1 shows the snapshots of the formation process of the pasta phase in adiabatic compression. Here, we start from the initial condition of $x = 0.39$ and $T = 0.25$ MeV ($t = 0$ fm/$c$). At $t \approx 57080$ fm/$c$ and $\rho \simeq 0.243\rho_0$ [Fig. 1(c)], the first pair of two nearest-neighbor nuclei start to touch and fuse (dotted circle), and then form an elongated nucleus [see, e.g., Fig. 1(d)]. After multiple pairs of nuclei become such elongated nuclei, we observe zigzag structure as shown in Fig. 1(d). These elongated nuclei start to stick together at $t \approx 59000$ fm/$c$ and $\rho = 0.246\rho_0$, and all the nuclei fuse to form rod-like nuclei at $t \lesssim 72700$ fm/$c$ and $\rho \lesssim 0.267\rho_0$. At $t = 76570$ fm/$c$ and $\rho = 0.275\rho_0$, we stop the compression ($T \approx 0.5$ MeV in this stage). We then relax the system microcanonically for $65510$ fm/$c$ and further relax at $T = 1$ MeV for $\approx 10000$ fm/$c$ (after that we take back the temperature to $\approx 0.5$ MeV and relax for $\approx 20000$ fm/$c$; for the increase and decrease of the temperature between 0.5 and 1 MeV, we take $\approx 5000$ and $\approx 15000$ fm/$c$, respectively). Finally, we obtain a triangular lattice of rod-like nuclei [Figs. 1(h-1) and (h-2)]. Remarkable point is that, in the middle of the transition process, pair of spherical nuclei get closer to fuse in a way such that the resulting elongated nuclei take a zigzag configuration (hereafter, we call it “zigzag pairing”) and they further connect to form wavy rod-like nuclei. This feature is observed in all the other cases in which we obtain a clear lattice structure of rod-like nuclei (among them, the highest temperature case is the adiabatic compression from $T = 1.5$ MeV), and the above scenario of the transition process is qualitatively the same also for those cases. It is very different from a generally accepted picture (see, e.g., p. 462 of Ref. [12]) that all the nuclei elongate in the same direction along the global axis of the resulting rod-like nuclei and they join up to form straight rod-like nuclei.

It has been regarded so far that the formation of the pasta phases in supernova cores is triggered by the fission instability with respect to the quadrupolar deformation of spherical nuclei [12]. To examine this point, we investigate the variance of the radius of each nuclei over the solid angle and the area-averaged mean curvature of the nuclear surface; neither of these quantities show a significant increase throughout the compression process until the nuclei start to touch [see also Fig. 1(h)]. This means that, before nuclei deform to be elongated due to the fission instability, they stick together keeping their spherical shape. This is consistent with the result of Ref. [28] (see also Ref. [20]), which shows that, within an incompressible liquid-drop model, the condition for the fission instability is not satisfied if one takes account of the background electrons.

To understand the mechanism which triggers the formation of the pasta phases, we calculate the distance $r_{nn}$ between centers of mass (for protons) of nearest-neighbor nuclei in the compression process of our simulations [27]. Figure 2 shows the mean value $\langle r_{nn} \rangle$ and the standard deviation $\Delta r_{nn}$ of $r_{nn}$ calculated for 16 nuclei in the simulation box. Let us first focus on the result obtained for

\begin{align*}
\text{FIG. 1: (Color online) Snapshots (two-dimensional projection) of the transition process from the bcc lattice of spherical nuclei to the pasta phase with rod-like nuclei. The red particles show protons and the green ones neutrons. In panels (a)-(g) and (h-1), nucleons in a limited region relevant for the two rod-like nuclei in the final state (h) [surrounded by the dotted lines in panel (h-2)] corresponding to eight nuclei in the initial condition (a) are shown for visibility. The vertices of the dashed lines in panels (a) and (d) show the equilibrium positions of nuclei in the bcc lattice and their positions in the direction of the line of sight are indicated by the size of the circles: vertices with a large circle, with a small circle, and those without a circle are in the first, second, and third lattice plane, respectively. The dotted circle in panel (c) show the first pair of nuclei start to touch. The solid lines in panel (d) represent the direction of the two elongated nuclei: they take zigzag configuration. In the final state [(h-1) and (h-2)], almost perfect triangular lattice of rod-like nuclei is obtained.}
\end{align*}
FIG. 2: (Color online) Distance $r_{nn}$ between centers of mass of nearest-neighbor nuclei in the compression process. The blue line shows the mean value ($r_{nn}$) and the blue filled region shows the standard deviation $\Delta r_{nn}$ of $r_{nn}$ normalized by $r_{nn}^{(0)}$ (a value of $r_{nn}$ for a perfect bcc lattice without displacement of nuclei). Panel (a) is for the isothermal compression at $T = 0$ MeV and panel (b) is for the adiabatic compression starting from $T = 0.25$ MeV. The first pair of nuclei touch at a density in the red filled region (corresponding to $r_{nn}^{(0)} \simeq 18.9$ fm for both cases) whose width shows its uncertainty.

the isothermal compression at $T = 0$ MeV [Fig. 2(a)], where we can see a clear signature due to the absence of thermal fluctuations. We note that there is a significant increase of $\Delta r_{nn}$ just before the nuclei start to connect. This shows that, before pairs of nuclei touch, nuclei displace from the equilibrium position of the bcc lattice and the bcc structure is spontaneously broken. As a result, each pair of nuclei approach to fuse and then form an elongated nuclei arranged in a zigzag configuration. At non-zero temperatures, thermal fluctuation smears the above signature and it would also assist triggering the formation of the pasta phases; however even in the case of the adiabatic compression starting at $T = 0.25$ MeV, we can still see a significant increase of $\Delta r_{nn}$ just before the nuclei touch and fuse [Fig. 2(b)].

Using a simplified model, we now examine our results of the QMD simulations. When nearest neighbor nuclei are so close that the tails of their density profile overlap with each other, net attractive interaction between these nuclei starts to act due to the interaction between nucleons in different nuclei in the overlapping surface region. We consider that this attraction between nuclei leads to the spontaneous breaking of the bcc structure. In order to examine this hypothesis, we consider a minimal model in which each nucleus is treated as a point charged particle interacting through the Coulomb potential and the potential of the Woods-Saxon form: $V(r) = V_0 \{ 1 + \exp [(r - R)/a] \}^{-1}$, which describes the finite size of nuclei and models the internuclear attraction when the nearest neighbor nuclei start to touch. Since nuclei start to connect before they are deformed, it is reasonable to treat a nucleus as a sphere and incorporate only its center-of-mass degree of freedom. Parameters $R$ and $a$ represent the interaction radius of a nucleus and range of the effective nuclear forces, respectively and we take $V_0 = -11.5$ MeV, $R = 17$ fm, and $a = 0.5$ fm [30]. With this model, we carry out the isothermal (keeping the system cool at $T < 0.01$ MeV by the frictional relaxation method throughout the simulation; this small but non-zero temperature is sufficient for symmetry breaking) compression of the bcc lattice of 128 nuclei of $^{208}$Pb, which corresponds to 8 times larger system than that of the QMD simulations. In Fig. 3 we show the snapshots of this simulation. Here we compress from 0.221$\rho_0$ ($L = 90.00$ fm) at a rate of $\dot{\rho} < O(10^{-6}) \rho_0/(fm/c)$. At 0.246$\rho_0$ ($L = 86.91$ fm) the first pair of nuclei starts to get closer [Fig. 3(b)] and then we stop the compression and relax the system. We observe zigzag pairing around the first pair [Fig. 3(c)] and finally we obtain a zigzag structure [Fig. 3(d)]. This supports that the zigzag structures observed in the QMD simulations are not caused by a finite size effect of the simulation box.

In conclusion, we have shown that an ordered structure of rod-like nuclei can be formed by compressing a
bcc lattice of spherical nuclei. Our result establishes that the pasta phases can be formed in collapsing supernova cores. Unlike a generally accepted conjecture, we have observed that nuclei start to connect before they deform due to the fission instability. This spontaneous breaking of the bcc structure is due to an attraction between nuclei caused by the overlap of the tails of nucleon distribution of neighboring nuclei. We have also discovered that, in the transition process, the system takes a zigzag configuration of elongated nuclei, which are formed by a fusion of original two spherical nuclei. Since a drastic change of the qualitative behavior of the potential between two nuclei of $Z = 82$ and $A = 208$ estimated by using the experimentally determined nucleon density distribution and mean-field potential of the Woods-Saxon form.

We are grateful to Chris Pethick and K. Iida for helpful discussions and comments. We used MDGRAPE-2 and -3 of the RIKEN Super Combined Cluster System. This work was supported in part by the JSPS and by the MEXT through Research Grants No. 19104006.

* These two authors contributed equally.

[1] H. A. Bethe, Rev. Mod. Phys. **62**, 801 (1990).
[2] S. A. Colgate and R. H. White, Astrophys. J. **143**, 626 (1966).
[3] G. Baym, H. A. Bethe, and C. J. Pethick, Nucl. Phys. A**175**, 225 (1971).
[4] D. G. Ravenhall, C. J. Pethick and J. R. Wilson, Phys. Rev. Lett. **50**, 2066 (1983).
[5] M. Hashimoto, H. Seki, and M. Yamada, Prog. Theor. Phys. **71**, 320 (1984).
[6] H. Sonoda et al., Phys. Rev. C **75**, 042801(R) (2007)
[7] G. Watanabe, K. Iida, and K. Sato, Nucl. Phys. A**687**, 512 (2001).
[8] C. J. Horowitz, M. A. Pérez-García, and J. Piekarewicz, Phys. Rev. C **69**, 045804 (2004); C. J. Horowitz et al., ibid. **70**, 065806 (2004).
[9] B. K. Jennings and A. Schwenk, [nucl-th/0512013](http://arxiv.org/abs/nucl-th/0512013) A. Burrows, S. Reddy, and T. A. Thompson, Nucl. Phys. A**777**, 356 (2006); C. J. Horowitz, Eur. Phys. J. A **30**, 303 (2006); H.-T. Janka et al., Phys. Rev. **442**, 38 (2007); M. Liebendorfer et al., New Astro. Rev. **52**, 373 (2008); N. Chamel and P. Haensel, Living Rev. Relativ. **11**, 10 (2008).
[10] P. Bonche and D. Vautherin, Nucl. Phys. A**372**, 496 (1981).
[11] M. Lassaut et al., Astron. Astrophys. **183**, L3 (1987).
[12] G. Watanabe et al., Phys. Rev. C **69**, 055805 (2004).
[13] W. G. Newton, Phys. Part. Nucl. **39**, 1173 (2008); W. G. Newton and J. R. Stone, Phys. Rev. C **79**, 055805 (2009).
[14] S. S. Avancini et al., Phys. Rev. C **79**, 035804 (2009).
[15] C. J. Pethick and D. G. Ravenhall, Annu. Rev. Nucl. Part. Sci. **45**, 429 (1995).
[16] K. Iida, G. Watanabe, and K. Sato, Prog. Theor. Phys. **106**, 551 (2001).
[17] J. Aichelin, Phys. Rep. **202**, 233 (1991).
[18] T. Maruyama et al., Phys. Rev. C **57**, 655 (1998).
[19] Shell effects, which are not incorporated in QMD, are less important since they are washed out by thermal fluctuations at several MeV at subnuclear densities [12].
[20] G. Watanabe et al., Phys. Rev. C **66**, 012801(R) (2002); ibid., **68**, 035806 (2003).
[21] G. Watanabe et al., Phys. Rev. Lett. **94**, 031101 (2005).
[22] Parameters of this Hamiltonian are determined to reproduce the saturation properties of nuclear matter, and the binding energy and the rms radius of finite nuclei, especially of heavier ones relevant to the present study [13, 23] [see also H. Sonoda et al., Phys. Rev. C **77**, 035806 (2008) for model dependence of the phase diagram within QMD]. It is also confirmed that a QMD Hamiltonian close to the present model provides a good description of nuclear reactions including the low energy region (several MeV per nucleon) [24], which would be important for the present case.
[23] T. Kido et al., Nucl. Phys. A**663**, 877c (2000).
[24] K. Niita, JAERI-conf. **96-009**, 22 (1996).
[25] G. Watanabe and K. Iida, Phys. Rev. C **68**, 045801 (2003); T. Maruyama et al., ibid. **72**, 015802 (2005).
[26] For $x = 0.39$, we perform isothermal compression at $T = 0, 0.1$, and $0.25$ MeV, and adiabatic compression starting from $T = 0.25$, $0.5$, $0.75$, and $1$ MeV. (For $x = 0.49$, we carry out adiabatic compression starting from $T = 0.25$, $0.5$, $0.75$, 1, and $1.5$ MeV.) In the isothermal compression at $T = 0$ MeV, we keep the system cool by frictional relaxation method (see, e.g., Refs. [18, 20]) throughout the compression process (as a result, $T < 0.01 – 0.04$ MeV). In the isothermal compression at non-zero temperatures, we keep the temperature using the Nosé-Hoover thermostat. (In the adiabatic compression, we compress the system without any thermostat.)
[27] Here, we employ the clustering algorithm: we identify protons which are within the threshold distance $r_{th}$ from at least one of them are in the same nucleus. We take $r_{th} = 3.5 – 4$ fm and have checked that the results do not change by varying $r_{th}$ around this value. In calculating $\langle r_{nn} \rangle$ and $\Delta r_{nn}$, nuclei which connect to the other ones are excluded. The sudden reduction of $\Delta r_{nn}$ when the first pair of nuclei touch is due to this treatment.
[28] S. Brandt, Master thesis, Copenhagen Univ. (1985).
[29] T. J. Büvernich, I. N. Mishustin, and W. Greiner, Phys. Rev. C **76**, 034310 (2007).
[30] In the relevant range of $r_{nn} \gtrsim 16$ fm [cf. $r_{nn}^{(0)} = 18.82$ fm at the highest density in this simulation corresponding to Figs. 3(b)-(d)], this parameter set well reproduces the qualitative behavior of the potential between two nuclei of $Z = 82$ and $A = 208$ estimated by using the experimentally determined nucleon density distribution and mean-field potential of the Woods-Saxon form.