Nuclear “pasta” phases by Quantum Molecular Dynamics

Katsuhiko Sato
The Univ. of Tokyo

Collaboration: G. Watanabe (Univ. Trent)
H. Sonoda (Univ. Tokyo)
K. Yasuoka (Keio Univ.),
T. Ebisuzaki (RIKEN)
T. Maruyama (JAERI)
With increasing matter density, the shape of nuclei changes from sphere to cylinder, slab, cylindrical bubble and spherical bubble, successively, and eventually becomes homogeneous nuclear matter. (Ravenhall et al., 83, Hashimoto et al., 84,)

Essentially this change is described by the surface energy

\[ g \equiv \frac{\text{surface area}}{(\text{volume})^{2/3}} \]

minimum principle.

Meatball
Spaghetti
Lasagna
Anti-spaghetti
Anti-meatball

”Pasta” Phases
Nuclear Pasta Structure

- **Liquid drop model**
  Ravenhall et al., 83, Hashimoto et al., 84, Oyamatsu et al., 84, ....
  Watanabe et al., 00, and 01, Iida et al., 01, .... Oyamatsu & Iida (06,)
  stability and fluctuations analysis with the analogy of liquid crystal
  Pethick, Potekhin, 98, Watanabe et al., 00, ....

- **QMD (Quantum Molecular Dynamics) method**
  Maruyama, 98, Watanabe et al., 01, .... 06, Sonoda et al. 07
  Conventional MD  Horowitz et al. 04, .............., 05
  complementary, large volume and large particles simulations are possible.

We improved Maruyama method and succeeded to construct the pasta structure by QMD.

QMD is very suitable method for studying Nuclear Pasta Structure.

- No assumptions on nuclear shapes, since nuclear system is treated in degrees of freedom of nucleons.
- Thermal fluctuations are necessarily included.

\[ \mathcal{H} = \sum_i \frac{p_i^2}{2m_i} + V_{\text{Pauli}} + V_{\text{Skyrme}} + V_{\text{sym}} + V_{\text{surface}} + V_{\text{MD}} + V_{\text{Coulomb}} \]

The surface term, which depends on the density gradient, is added to the original Maruyama model in order to make the surface of nuclei smooth. In the original model, the surface of large nuclei are slightly bumpy.


The original model without the surface term.
Equations of Model Hamiltonian

\[ \mathcal{H} = \sum_i \frac{P_i^2}{2m_i} + V_{\text{Pauli}} + V_{\text{Skyrme}} + V_{\text{sym}} + V_{\text{surface}} + V_{\text{MD}} + V_{\text{Coulomb}} \]


Definition of densities

\[
\langle \rho_i \rangle = \sum_{j(\neq i)} \rho_{ij} = \sum_{j(\neq i)} \int d^3 r \rho_i(r) \rho_j(r)
\]

\[
\langle \bar{\rho}_i \rangle = \sum_{j(\neq i)} \bar{\rho}_{ij} = \sum_{j(\neq i)} \int d^3 r \bar{\rho}_i(r) \bar{\rho}_j(r)
\]

\[
\rho_i(r) = \frac{1}{(2\pi L)^{3/2}} \exp \left\{ -\frac{1}{2L} (r - R_i)^2 \right\}
\]

\[
\bar{\rho}_i = \frac{1}{(2\bar{L})^{3/2}} \exp \left\{ -\frac{1}{2\bar{L}} (r - R_i)^2 \right\}
\]

\[
L = 1.95\text{fm}^2, \quad \tau = 1.33333, \quad \bar{L} = \frac{(1 + \tau)^{1/\tau}}{2} L
\]

Pauli potential

\[
V_{\text{Pauli}} = \frac{C_p}{2(q_0 p_0 / \hbar c)^3} \sum_{i,j(\neq i)} \exp \left[ -\frac{|R_i - R_j|^2}{2q_0^2} - \frac{|P_i - P_j|^2}{2p_0^2} \right] \delta_{\tau_i \tau_j} \delta_{\sigma_i \sigma_j}
\]

\[
C_p = 115.0\text{MeV}, \quad p_0 = 120.0\text{MeV}, \quad q_0 = 2.5\text{fm}
\]

\( \tau_i \) : isospin, \( \sigma_i \) : spin
Skyrme potential

\[
V_{\text{Skyrme}} = \frac{\alpha}{2\rho_0} \sum_i <\rho_i> + \frac{\beta}{(1 + \tau)\rho_0} \sum_i <\tilde{\rho}_i>^\tau
\]
\[
\alpha = -121.9\text{MeV}, \quad \beta = 197.3\text{MeV}
\]

Symmetry potential

\[
V_{\text{Sym}} = \frac{C_{s0}}{2\rho_0} \sum_{i,j(\neq i)} (1 - 2|c_i - c_j|)\rho_{ij}
\]
\[
C_{s0} = 25.0\text{MeV}, \quad c_i : \text{isospin}
\]

Surface potential

\[
V_{\text{Surface}} = \frac{V_{SF}}{2\rho_0} \frac{5/3}{2\rho_0} \sum_{i,j(\neq i)} \int d^3r \nabla \rho_i(r) \nabla \rho_j(r)
\]
\[
V_{SF} = 20.68\text{MeV}
\]

Momentum dependent potential

\[
V_{\text{MD}} = C_{ex}^{(1)} \sum_{i,j(\neq i)} \frac{1}{1 + \left(\frac{|P_i - P_j|}{\mu_1 n_i}\right)^2} + C_{ex}^{(2)} \sum_{i,j(\neq i)} \frac{1}{1 + \left(\frac{|P_i - P_j|}{\mu_2 n_i}\right)^2}
\]
\[
C_{ex}^{(1)} = -258.5\text{MeV}, \quad C_{ex}^{(2)} = 375.6\text{MeV},
\]
\[
\mu_1 = 2.35\text{MeV}, \quad \mu_2 = 0.4\text{MeV}
\]

Coulomb potential

\[
V_{\text{Coulomb}} = \frac{e^2}{2} \sum_{i,j(\neq i)} \left(\tau_i + \frac{1}{2}\right) \left(\tau_j + \frac{1}{2}\right) \frac{1}{|r - r'|} \rho_i(r) \rho_j(r')
\]
These Hamiltonians include free parameters, 14 in Model 1, and 13 in Model 2.

The values of these parameters are determined to reproduce the saturation properties of symmetric nuclear matter, and the binding energy and rms radius of stable nuclei.
Simulation settings

Eq. Motion of nucleons in QMD

\[
\dot{R}_i = \frac{\partial H}{\partial P_i} - \xi_R \frac{\partial H}{\partial R_i}, \\
\dot{P}_i = -\frac{\partial H}{\partial R_i} - \xi_P \frac{\partial H}{\partial P_i}.
\]

Ground state is obtained by cooling of hot matter by frictional relaxation, the time scale of the cooling

\~O(1,000—10,000) fm/c,

much larger than

\[ \tau_{\text{relax}} \equiv \frac{\text{length scale of inhomogeneity}}{\text{sound velocity}} \]

\[ \sim \frac{10 \text{fm}}{0.1 c} \sim 100 \text{fm/c} \]

Simulation Settings

2,048 or 10,976 nucleons in simulation box. Periodic boundary condition. Proton fraction \( x = n/(p+n) = 0.3. \)

Computation: RSCC (RIKEN Super Combined Cluster) with MD GRAPE (the pipeline processing module for calculating the forces between particles, originally developed for the gravitational N-body problem)

CPU time to get one model; 2 ~ 3 weeks for spherical cases (lower density cases)

1. ~ 1.5 months for Spaghetti and Lasagna phases (higher cases).
Pasta at zero temperature

Cooling of hot nuclear matter (~10 MeV) below 0.1 MeV

Model 1

- **Sphere**: $0.100 \, \xi_0$
- **Cylinder**: $0.200 \, \xi_0$
- **Slab**: $0.393 \, \xi_0$
- **Cylinder-like Holes**: $0.490 \, \xi_0$
- **Spherical Holes**: $0.575 \, \xi_0$

Red: Protons
Blue: Neutrons

$\xi_0 = 0.168 \, \text{fm}^{-3}$

(Nuclear density)
Sponge-like Structure

Between cylinder and slab, slab and cylinder-like holes
Multiply connected “Sponge-like” structure appears

Between cylinder and slab

Between slab and cylinder holes

10976 nucleons at 0.3 $\rho_0$
10976 nucleons at 0.45 $\rho_0$

These intermediate phases at least meta-stable
Minkowski Functionals

A powerful tool for morphological analysis

Euler characteristic

\[ \chi = \frac{1}{2\pi} \int_{\partial} G dA \]

\( \Delta = \) (number of isolated regions) - (number of tunnels) + (number of cavities)

About a surface of a body \( K \) in 3D space

mean curvature \( H = (\kappa_1 + \kappa_2)/2 \)

Gaussian curvature \( G = \kappa_1 \kappa_2 \)

\( \kappa_1, \kappa_2 \) : principal curvatures

\[ \chi = 9 \]

\( \chi = 3 - 3 = 0 \)

\( \chi = 1 - 5 = -4 \)

Figures from a Hikage slide
Pasta phases are discriminated by H and □.

SP: H > 0, □ > 0

C: H > 0, □ = 0

S: H = 0, □ = 0

CH: H < 0, □ = 0

SH: H < 0, □ > 0

□ < 0 · · · Sponge-like Structure
Phase diagram at zero temperature

Model 1

Model 2

Melting density of the pasta in Model 1 is 0.7 nuclear density, higher than that of Model 2, 0.65 nuclear density by the effect of surface term.
Pasta at finite temperatures

Model 1

0.393 $\bar{h}_0$ (Slab nuclei at zero temperature)

$T=0$ MeV

$T=1$ MeV

$T=2$ MeV

Slab Nuclei → Evaporated Neutrons → Connected Slab

dripped neutrons Increases
nuclear surfaces become more diffusive
Pasta at finite temperature

- **T=3MeV**: Cylindrical hole-like structure
- **T=5MeV**: Cannot identify nuclear surface
- **T=6MeV**: Phase separation disappears

Phase transition, Melting surface, Dripped protons, Disappearance of phase separation occur successively.
Phase diagram at finite temperatures

Thermal fluctuation increases volume fraction of nuclei. Above T = 4 ~ 6 MeV, cannot identify surface. At T = 6 ~ 10 MeV, Liquid-gas phase separation.
Comparison of Phase diagrams between two models

Model 1

Nuclear pasta remains in higher temperature in Model 1:
limit for identification of nuclear surface: T = 4 ~ 6 MeV (Model 1), 2 ~ 3 MeV (Model 2)
Phase separation line: T = 6 ~ 10 MeV, 3 ~ 5 MeV
Case of $X = p / (p + n) = 0.1$, Model 2
(deep side of inner crust of neutron stars)

The proton distribution of cylinder phase at $\rho = 0.2 \rho_0$ and $T = 0.1 \text{MeV}$.

Neutrons which spread over the whole space are not depicted in this figure.

Phase diagram

Spherical and cylindrical phase are only observed in $0.18 - 0.53 \rho_0$.
No pasta phases are observed in densities higher than $0.53 \rho_0$.

More systematic survey of the nuclear pasta phases of $x = 0.1$ is under progress.
Neutrino Opacity of Pasta Phases

Neutrino transport
--- a key element for success of supernovae

● Neutrinos are trapped in collapsing phase by coherent scattering with nuclei (K. Sato, 75)
Lepton fraction, $Y_{lep}$, affects EOS.

How pasta phases change neutrino transport in collapsing cores?
Pioneering investigation were done by Horowitz group (04, ...).
Neutrino cross section of neutrino-Pasta

Cross section of neutrino-nucleon system due to coherent scattering

\[
\frac{1}{N} \frac{d\sigma}{d\Omega} (q) = \frac{G_F^2 E_{\nu}^2}{4\pi^2} (1 + \cos \theta) \cdot c_v^{(n)} \cdot \bar{S}(q)
\]

Neutrino-neutron cross section

Because collapsing cores are poly-crystalline, the opacity would be well characterized by the angle-average of \( \bar{S}(q) \).

Total transport cross section:

\[
\sigma_t = \langle \bar{S}(E_{\nu}) \rangle \sigma_t^0
\]

\( \langle \bar{S}(E_{\nu}) \rangle \) \hspace{1em} \text{Angle-averaged amplification factor by pasta structure}

\[
\sigma_t^0 = \frac{2G_F^2 E_{\nu}^2}{3\pi} c_v^{(n)2}
\]
QMD results: change of the amplification factors with increasing density

\(Y_e=0.3, \ T=1\ \text{MeV}\)

Compared with the Lattimer-Swesty model (LS-EOS),

- the energy of peaks are lower, and
- the width of peaks are wider,

due to lattice disorder and irregularity of nuclei.
QMD results: change of the amplification factors with increasing density

\[ Y_e = 0.3, \ \Box = 0.0660 \text{fm}^{-3} \ (\text{Slab at } T=0) \]

- Peak is lowered and broader by increasing temperature due to lattice disorder and irregularity of nuclei.
- Transition from slab (2 MeV) to rod-like bubbles (3 MeV) dramatically changes peak energy lower, and peak height higher.

Difficult to discuss the effects on supernova explosion at present stage.
Summery

• Vivid pictures of nuclear pasta structure were obtained by QMD simulations.
• Difference of phase diagrams of two models available at present was investigated, but ambiguity on the dependence on nuclear potentials still remains.
• Neutrino opacity of the pasta phases described well by QMD were calculated.
• More systematic survey is under progress.