Study of low-density nuclear matter by QMD simulations: Role of symmetry energy

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Introduction

At subnuclear densities, where nuclei are about to melt into uniform matter, various exotic structures collectively known as "nuclear pasta" may appear.
The study of pasta phase is important for both neutron stars and core-collapse supernova. For example:

- neutrino-pasta scattering is important for neutrino transport in core-collapse supernova (Horowitz et al, PRC69, 045804(2004))
- e^--pasta scattering is important to determine the transport properties: shear viscosity, thermal conductivity and electrical conductivity (Horowitz et al, PRC78, 035806(2008))
- the electrical conductivity of the pasta is relevant for the decay of neutron star magnetic fields (Pons et al, Nature 9, 431(2013))
- also important for crustal oscillations, pulsar glitches, neutron star cooling etc.

- The properties of pasta phase has been studied mostly using static methods such as the liquid-drop model, the Thomas-Fermi method and the Hartree-Fock method
- All these models assume few specific shapes and obtain the favorable shape by minimizing the free energy.
- Their phase diagrams possess a universal basic feature that, 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.
- But for better understanding of the pasta phase physics it is important to adopt a dynamical approach which allows arbitrary nuclear structures.
- Only few groups used dynamical approach so far: Horowitz et al (CMD), Maruyama et al (QMD) and Dorso et al (CMD)

Symmetry energy

- The density dependence of nuclear symmetry energy is very important to understand many aspects of nuclear physics and astrophysics
- Experiments constrain the symmetry energy (E_{sy})at saturation density to be around ~ 32 MeV but the slope of symmetry energy L is still very uncertain and lies in the range $\sim 20 - 120$ MeV
- Recent static calculations (Grill et al, PRC 85, 055808 (2012), Bao et al PRC89, 045807 (2014)) showed that L could have dramatic effects on the pasta structures. For some models pasta phase doesn't appear at all if L is high.
- This motivates us to study the effect of symmetry energy and its slope on the pasta phase within a dynamical model.
- We adopt here the Quantum molecular dynamics (QMD) model developed by Maruyama et al (PRC 57, 655 (1998), PRC 68, 035806 (2003)).

QMD

The single-nucleon state is represented by a Gaussian wave packet:

$$\phi_i(\mathbf{r}) = \langle \mathbf{r}|\phi_i\rangle = \frac{1}{(2\pi L)^{3/4}} \exp\left[-\frac{(\mathbf{r}-\mathbf{R}_i)^2}{4L} + \frac{i}{\hbar}\,\mathbf{r}\cdot\mathbf{P}_i\right] ,$$

The N-nucleon wave function:

$$|\Phi\rangle = |\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots \otimes |\phi_N\rangle \ .$$

The Hamiltonian

$$\mathcal{H} = T + V_{Pauli} + V_{local} + V_{sym} + V_{MD} + V_{Coul}$$

$$T = \sum_i \frac{\mathbf{P}_i^2}{2m_i} ,$$

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

$$V_{\rm local} = \frac{\alpha}{2\rho_0} \sum_{i,j(\neq i)} \rho_{ij} + \frac{\beta}{(1+\tau)\ \rho_0^\tau} \sum_i \left[\sum_{j(\neq i)} \int d^3\mathbf{r}\ \tilde{\rho}_i(\mathbf{r})\ \tilde{\rho}_j(\mathbf{r})\right]^\tau ,$$

ρ_i and $\tilde{\rho}_i$ are single-nucleon densities and ρ_{ij} gives the overlap between nucleons

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

$$\tilde{\rho}_i(\mathbf{r}) = \frac{1}{(2\pi \tilde{L})^{3/2}} \exp\left[-\frac{(\mathbf{r} - \mathbf{R}_i)^2}{2\tilde{L}}\right], \quad \rho_{ij} = \int d^3\mathbf{r}\rho_i(\mathbf{r})\rho_j(\mathbf{r}), \quad \tilde{L} = \frac{(1+\tau)^{1/\tau}}{2} L$$

$$
\begin{aligned}
V_{\rm sym} &= \frac{C_{\rm s}^{(1)}}{2\rho_0}\sum_{i,j(\neq i)}\left(1-2|c_i-c_j|\right)\,\rho_{ij} + \frac{C_{\rm s}^{(2)}}{(1+\gamma)\rho_0}\sum_i\left[\sum_{j(\neq i)}\left(1-2|c_i-c_j|\right)\,\tilde{\rho}_{ij}\right]^{\gamma}\,, \\
V_{\rm MD} &= V_{\rm MD}^{(1)} + V_{\rm MD}^{(2)} \\
&= \frac{C_{\rm ex}^{(1)}}{2\rho_0}\sum_{i,j(\neq i)}\frac{1}{1+\left[\frac{\mathbf{P}_i-\mathbf{P}_j}{\hbar\mu_1}\right]^2}\,\rho_{ij} + \frac{C_{\rm ex}^{(2)}}{2\rho_0}\sum_{i,j(\neq i)}\frac{1}{1+\left[\frac{\mathbf{P}_i-\mathbf{P}_j}{\hbar\mu_2}\right]^2}\,\rho_{ij}\,, \\
V_{\rm Coulomb} &= \frac{e^2}{2}\sum_{i,j(\neq i)}\left(\tau_i+\frac{1}{2}\right)\left(\tau_j+\frac{1}{2}\right)\iint d^3\mathbf{r}\,d^3\mathbf{r}'\,\frac{1}{|\mathbf{r}-\mathbf{r}'|}\,\rho_i(\mathbf{r})\rho_j(\mathbf{r}')\,,
\end{aligned}
$$

$$
c_i = 1 \quad \text{and} \quad \tau_i = \frac{1}{2} \quad \text{for protons}
$$

$$
c_i = 0 \quad \text{and} \quad \tau_i = -\frac{1}{2} \quad \textit{forneutrons}
$$

Parameter set

C_{P} (MeV)	207
p_0 (MeV/c)	120
q_0 (fm)	1.644
α (MeV)	-92.86
β (MeV)	169.28
τ	1.33333
$C_{\mathrm{ex}}^{(1)}$ (MeV)	-258.54
$C_{\mathrm{ex}}^{(2)}$ (MeV)	375.6
μ_1 (fm^{-1})	2.35
μ_2 (fm^{-1})	0.4
L (fm^2)	2.1

Equations of motion

To simulate the dynamical relaxation we use QMD equations of motion with frictional terms:

$$\dot{\mathbf{R}}_i = \frac{\partial \mathcal{H}}{\partial \mathbf{P}_i} - \mu_R \frac{\partial \mathcal{H}}{\partial \mathbf{R}_i} \ ,$$

$$\dot{\mathbf{P}}_i = -\frac{\partial \mathcal{H}}{\partial \mathbf{R}_i} - \mu_P \frac{\partial \mathcal{H}}{\partial \mathbf{P}_i} \ ,$$

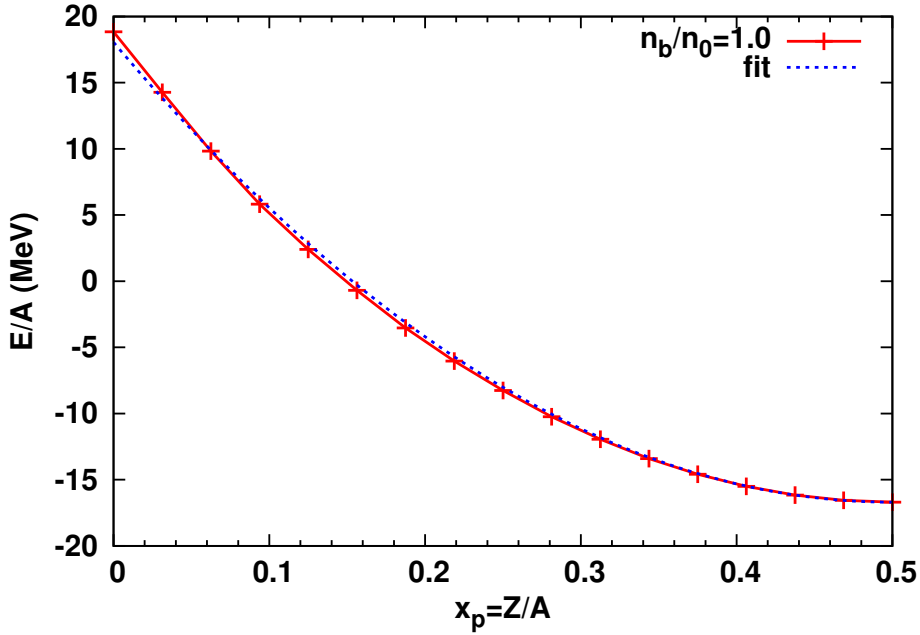
$$\mu_R, \mu_P > 0 \, \text{and} \ll 1$$

where μ_R and μ_P are friction coefficients

Implementation

- We perform QMD simulations for various densities keeping proton fraction fixed to $x_p = 0.5$ and 0.3 at $T = 0$
- We take 2048 nucleons in a cubic box and impose the periodic boundary conditions (PBC)
- Electrons are considered as uniform background and make the system charge neutral
- Coulomb interaction is calculated by using the Ewald method which is efficient to sum up contributions of long-range interactions in a system with PBC

- As an initial condition we first prepare a uniform hot nuclear gas at $k_B T \sim 20$ MeV
- Then we cool the system down with the frictional relaxation method until the temperature drops to $\lesssim 0.1$ MeV
- For speeding up the simulation to practical wall-times we have ported the QMD code to a GPU version. All the calculations are done in LOEWE-CSC cluster of Frankfurt



$$E/A = E/A|_{\rm sat} + E_{sy}(1-2x_p)^2$$

$$L = 3\rho_0 \frac{dE_{sy}}{d\rho}\Big|_{\rm sat} = 3\rho_0 \frac{E_{sy}(1.1\rho_0) - E_{sy}(0.9\rho_0)}{1.1\rho_0 - 0.9\rho_0}$$

$C_s^{(1)}$	$C_s^{(2)}$	γ	$E_{sy}(MeV)$	$L(MeV)$
30.0	-15.0	3.0	34.7	79.0
25.0	0.0	0.0	34.6	94.3
18.0	22.5	3.0	34.7	117.9
25.0	-15.0	3.0	32.2	71.1

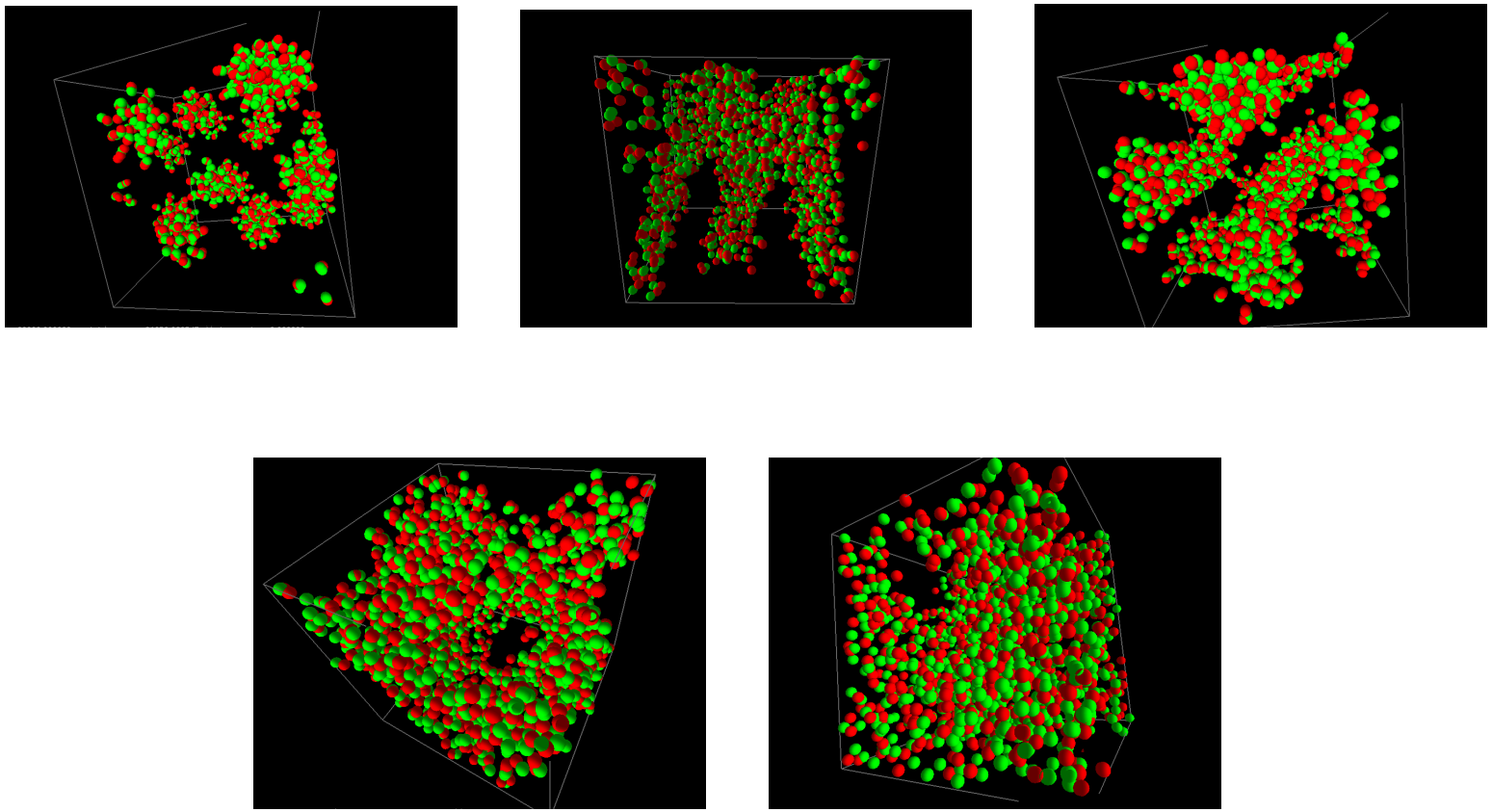


Figure : The nucleon distribution of typical phases with simple structures of cold matter at densities $0.1\rho_0$, $0.25\rho_0$, $0.4\rho_0$,$0.45\rho_0$ and $0.55\rho_0$ respectively

Minkowski Functionals

- According to integral geometry the morphological properties of d-dimensional objects can be completely described by only $d+1$ independent functionals known as Minkowski functionals
- For 3d, these are related to the volume (V), the surface area (A), the integral mean curvature (H) and the Euler characteristic (χ)
- The Euler characteristic can also be written as

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

- We use the normalized quantities $< H >= (1/A) \int H \, dA$ and χ/V

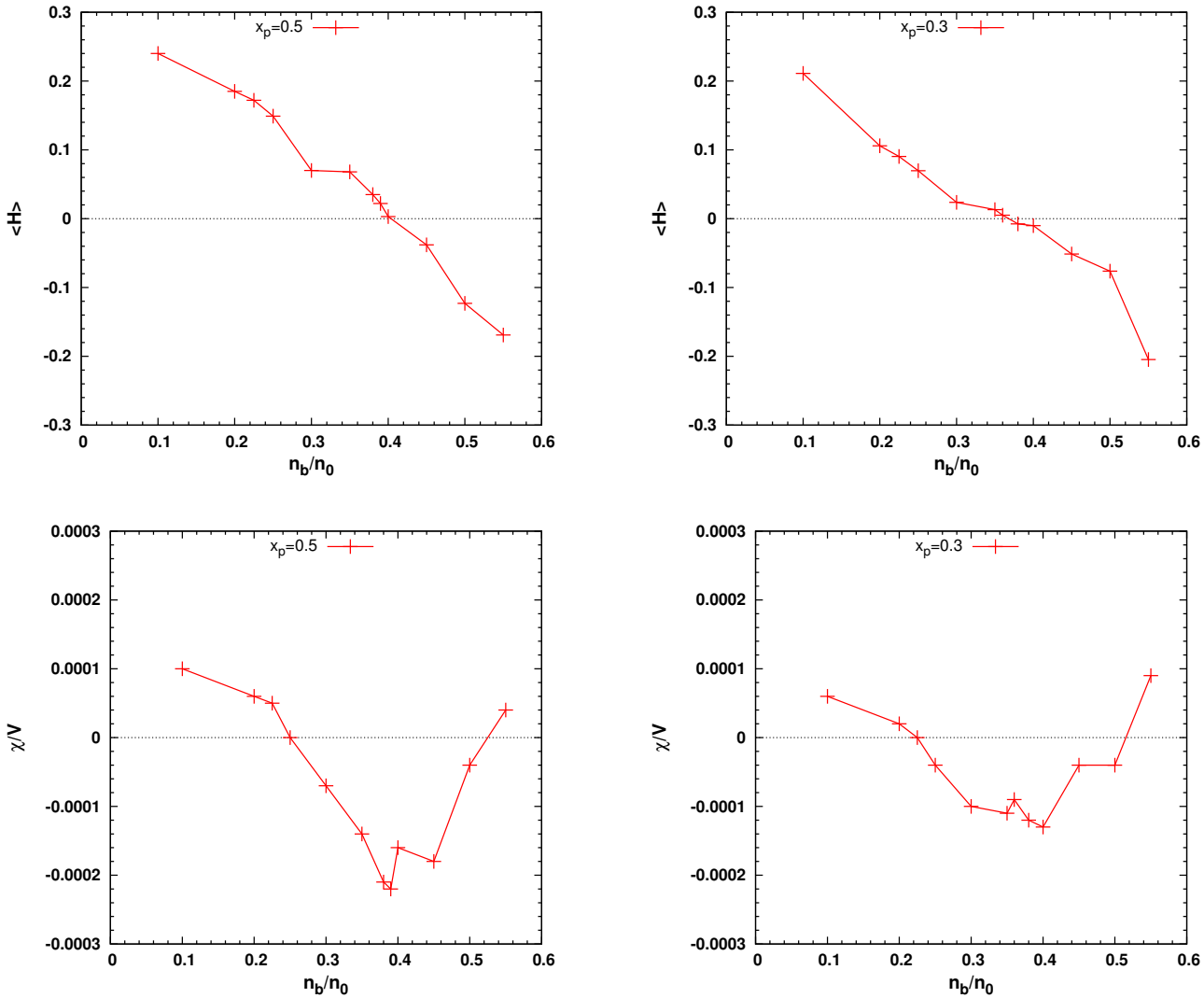


Figure : Minkowski functional for $x_p = 0.5$ (left) and 0.3 (right) respectively

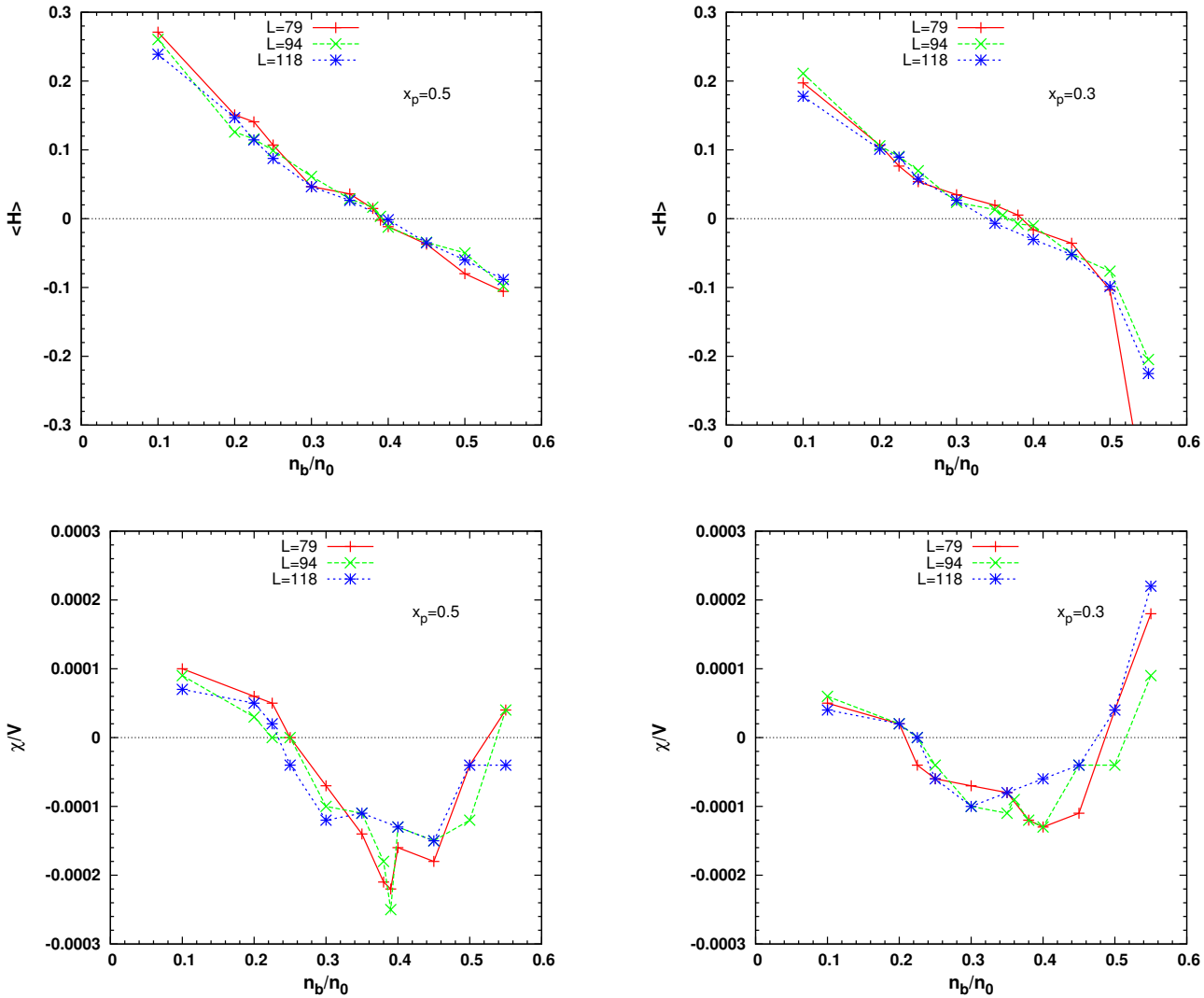


Figure : Comparison of Minkowski functional for different L

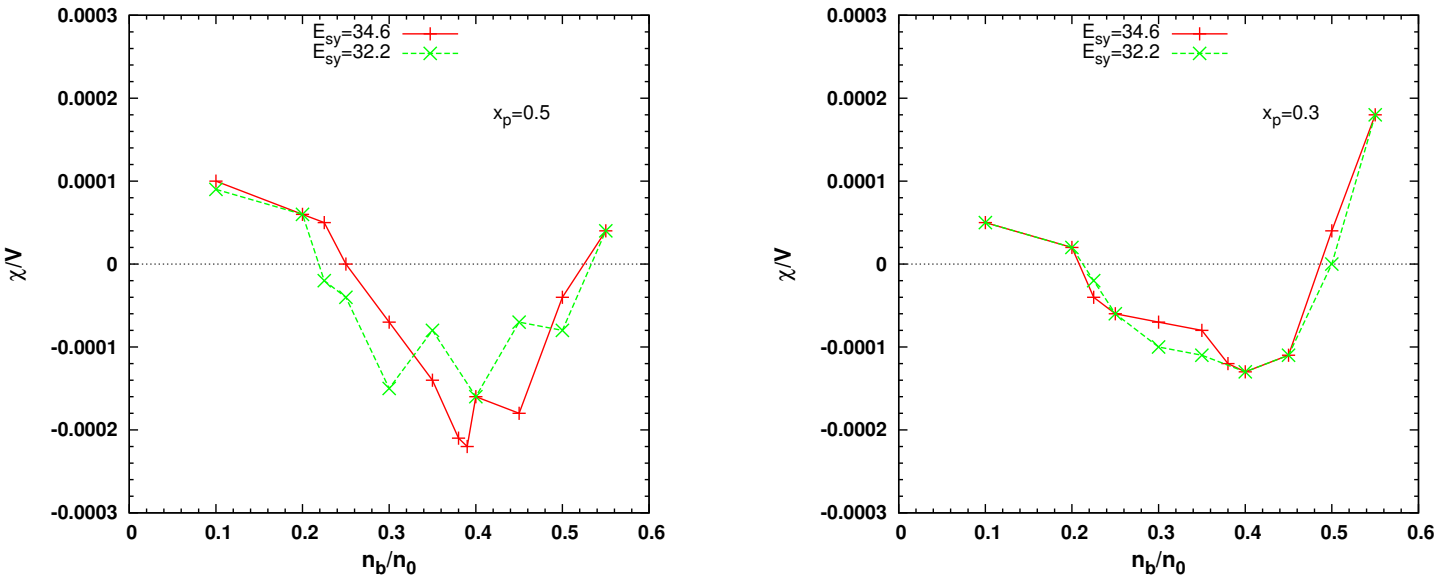


Figure : Comparison of Minkowski functional for two different E_{sy}

- We have investigated the effect of symmetry energy and its slope on the pasta phase and obtained some preliminary results
- It seems that value of L is important for pasta phase properties, high L could eliminate some of the regular pasta shapes as in static calculations but need better statistics to confirm and we are currently working on that
- For neutron stars more realistic x_p is < 0.1. For that we need a larger system ($\gtrsim 10000$ nucleons) to have enough number of protons in the simulation box. With the GPU version of our code it is not difficult to achieve.
- It is also very straight forward to study the pasta phase for finite temperatures within this set up.
- Next we plan to calculate some of the transport properties using this model