Machine learning Minkowski functionals of neutron star crusts

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Abstract. We study the structures attained by neutron star matter with proton to neutron ratios ranging from \( x = 0.05 \) to 0.5, densities in the range of \( 0.04 \text{ fm}^{-3} < \rho < 0.08 \text{ fm}^{-3} \), and temperatures \( T < 4 \text{ MeV} \). In particular, since the Minkoswki functionals are related to the morphology of the pasta shapes, we study their variation at those densities, temperatures and proton contents using machine learning technology.

1. Introduction
The structure of neutron star crusts are expected to be of relevance for the neutrino flow [1] and to the synthesis of heavy nuclei in neutron star mergers [2]. Recently, the structure of a conglomerate of protons and neutrons (known as nuclear matter, NM) and of a similar system embedded in an electron cloud (known as neutron star matter, NSM) were studied, respectively, in [3] and [4]. Such studies found that both NM and NSM attain “pasta” structures which vary as functions of proton content, density and temperature, and that they exhibit crystal-to-solid and solid-to-liquid phase transitions similar to those found before for isospin-symmetric NM [5].

In this work, the Minkowski functionals obtained in [4] to characterize the morphology of the NSM pasta, are studied using machine learning technology.

2. Nuclear Pasta
Nuclear pastas are arrangements of protons and neutrons theorized to exist in neutron star crusts [6]. The pastas at zero temperature have been studied since the 1980s using static methods such as the liquid drop model [6, 7], mean field theories [8] and Thomas-Fermi models [9]. At higher temperatures the pastas have been investigated dynamically using quantum molecular dynamics [10, 11, 12] and classical potential models [13, 14, 15]. More recently models that can identify local minima by cooling, such as the classical molecular dynamics model (CMD) have been used to study non-traditional phases [5].

CMD has been used, for instance, to calculate \( E_{\text{sym}} \) in clustered media [16], to study pasta structures, phase transitions, and the symmetry energy in the different pasta structures [5]. In recent works NM and NSM have been studied to determine their pasta-like structures, their
Table 1. Parameter set for the CMD computations.

| Parameter | Value      | Parameter | Value |
|-----------|------------|-----------|-------|
| $V_r$     | 3097.0 MeV | $\mu_r$  | 1.648 fm$^{-1}$ |
| $V_a$     | 2696.0 MeV | $\mu_a$  | 1.528 fm$^{-1}$ |
| $V_0$     | 379.5 MeV  | $\mu_0$  | 1.628 fm$^{-1}$ |
| $r_c$     | 5.4/20 fm  |           |       |

$E_{\text{sym}}$ and their phase changes at saturation and sub-saturation densities, low temperatures, and proton fractions in the range of 10% to 50% [1, 2, 3, 4, 17].

3. Classical Molecular Dynamics

The model used, classical molecular dynamics, is a well-established computational technique that has been successful in determining the pasta structures in NM and NSM [14, 15, 5, 18, 1]. In CMD nucleons are classical particles interacting through pair potentials with their dynamics dictated by their equations of motion; the details and main advantages of CMD have been presented elsewhere [14, 15, 5]; in particular, the model adapted to NSM was described in [4]. Briefly, CMD treats NSM as composed of protons, neutrons and electrons with $pp$, $nn$ and $np$ potentials, and with a screening potential to mimic the effect of the electron gas. In the CMD model nucleons interact through the Pandharipande potentials (modified to yield a binding energy $E(\rho_0) = -16$ MeV/nucleon and a compressibility of about 250 MeV), given by

$$V_{np}(r) = \frac{V_r}{r} e^{-\mu_r r} - \frac{V_r}{r_c} e^{-\mu_r r_c} - \frac{V_a}{r} e^{-\mu_a r} + \frac{V_a}{r_c} e^{-\mu_a r_c}$$

$$V_{nn}(r) = \frac{V_0}{r} e^{-\mu_0 r} - \frac{V_0}{r_c} e^{-\mu_0 r_c}$$

(1)

with the cutoff radius $r_c$ after which the potentials are set to zero. The values of $\mu_r$, $\mu_a$, $\mu_0$ and $V_r$, $V_a$, $V_0$ were first set by Pandharipande for cold nuclear matter [19], and improved by [2] to reproduce cold NM binding energies more accurately. The corresponding values are summarized in Table 1. The Coulomb effect of the electron gas is introduced through the Thomas-Fermi expression [14, 13, 10]

$$V_{TF} = \frac{q^2}{r} e^{-r/\lambda},$$

(2)

with a screening length of $\lambda = 10$ fm, and a cutoff distance for $V_{TF}$ of 20 fm, values which ensure that the properties of the resulting pasta remain essentially constant (see [20]).

3.1. Minkowski functionals

The pasta can be characterized with the Minkowski functionals which quantify the shape and connectivity of the spatial structures formed by the nucleons. Here a brief description of the Minkowski functionals will be presented, a more thorough description can be found in [15, 3].

The Minkowski functionals [21] have been used in pasta studies (see e.g. [15, 22, 23, 24]), and correspond to the volume ($V$), surface area ($S$), Euler characteristic ($\chi$), and integral mean curvature ($B$). In particular, the Euler characteristic can be interpreted as

$$\chi = \text{isolated regions} + \text{cavities} - \text{tunnels},$$

(3)
Table 2. Relationship between pasta shapes and the curvature and Euler characteristic.

| $\chi > 0$ | $\chi \sim 0$ | $\chi < 0$ |
|------------|---------------|-----------|
| B < 0      | Anti-Gnocchi  | Gnocchi   |
|            | Anti-Spaghetti| Lasagna   |
|            | Anti-Jungle Gym| Jungle Gym|

while $B$ is a measure of the mean curvature of the surface of a given structure. It is now known [15] that the pasta structures can be classified according to Table 2, connecting the different structures with the curvature ($B$) and the Euler characteristic. Notice that the “anti” prefix means the inverted situation between occupied and empty regions, the “jungle gym” stands for a 3D rectangular trellis, and the signs of these functionals are also correlated with the pasta phases [25].

3.2. Road map

Before closing this section, it is instructive to summarize the path to be taken i) to obtain the pastas, ii) calculate the Minkowski functionals, and iii) use neural networks to interpolate the value of the Minkowski functionals for arbitrary values of temperature and density.

(i) Molecular dynamics simulation of neutron star matter. To simulate the NSM, the LAMMPS code [26] was used with the potentials described above. Systems with $A = 4000$ nucleons in a cubic cell under periodic boundary conditions were prepared with isospin contents of $x = z/A = 0.1, 0.2, 0.3, 0.4,$ and $0.5,$ at densities varying between $0.02 \text{ fm}^{-3} < \rho < 0.085 \text{ fm}^{-3},$ and temperatures varying from $T = 4 \text{ MeV}$ down to $0.2 \text{ MeV}$ ($\Delta T < 0.1\%$). With the nucleons placed initially at random separated by at least $0.01 \text{ fm},$ and endowed with velocities according to a Maxwell-Boltzmann distribution to correspond to a desired temperature, the equations of motion were solved to mimic the evolution of the system. The nucleon positions, momenta, energy per nucleon, pressure, temperature, and density, were stored at fixed time-steps. The end product of this step were pasta structures at various values of $x, \rho$ and $T$.

(ii) Minkowski functionals. To calculate the Minkowski functionals of the pasta structures produced by CMD, the structures had to be “voxelized”, i.e., represented by “voxels”, or regular units of volume; the appendix of [3] presents the procedure used. Here the cubic voxels used were of $d = 2.35 \text{ fm}$ per side, and $\chi$ was computed according to Eq. (3).

(iii) Neural network interpolation of the Minkowski functionals. Steps (i) and (ii) are both computationally-demanding and labor-intensive, but provide values for the Minkowski functionals in a dense grid of temperature and density that can be used to train interpolating neural networks. That is, the values of the proton content, density and temperature (at which the final configurations were obtained through CMD for the 4000 particles) and the respective values of the corresponding Minkowski functionals (obtained from the voxelization of the final configurations) were used to train a neural network which would then serve to estimate the values of the Minkowski functionals for any value of $x, \rho$ and $T$.

4. Neural network interpolation of the Minkowski functionals

CMD was used to produce 9600 configurations of the nucleons at the values of $x, \rho$ and $T$ specified in (i) in section 3.2. The configurations were obtained from a Markov chain each separated from the previous one by 10,000 time steps to avoid correlations between the positions of the nucleons. The Minkowski functionals were then obtained for each configuration as described in section 3.1.
Table 3. Neural network interpolations of the integral mean curvature $B$ and Euler characteristic $\chi$ as a function of neutron ratio $x$, density $\rho$ and temperature $T$.

| $x = z/A$ | Curvature (a.u.) | Euler number |
|-----------|------------------|--------------|
| 0.05      | ![3D plot](image) | ![3D plot](image) |
| 0.20      | ![3D plot](image) | ![3D plot](image) |
| 0.35      | ![3D plot](image) | ![3D plot](image) |
| 0.50      | ![3D plot](image) | ![3D plot](image) |

Finally, a dataset composed of the values of $x$, $\rho$ and $T$ and their respective values of the four Minkowski functionals ($V$, $S$, $B$ and $\chi$) was used to train a neural network.

Fully-connected feed-forward neural network were used (as implemented in the software scikit-learn [27]) for each functional, although with a common architecture that consisted of 4 hidden layers with 50 neurons in each layer and rectifier activation function. The stochastic gradient-based optimization method Adam [28] was used to determine the weights of the network. The ranges of the independent variables $x$, $\rho$ and $T$ were given in section 3.2. A Monte Carlo cross-validation scheme was used for model selection, with 80% of the data randomly selected to train the network and the remaining 20% used to test the performance of the model. The results are shown in the figures of Tables 3 and 4. Notice that the values of $x$, $\rho$, $T$ do not need to be the same as those used to train the network.

Table 3 shows the behavior of the curvature $B$ and Euler characteristic $\chi$ for several values of $x$ and as a function of temperatures (horizontal) between 0 and 4 MeV, and densities (depth)
Table 4. Neural network interpolations of the volume $V$ and surface area $S$ as a function of neutron ratio $x$, density $\rho$ and temperature $T$.

| $x = z/A$ | Surface (a.u.) | Volume (a.u.) |
|-----------|----------------|---------------|
| 0.05      | ![Surface](image1) | ![Volume](image2) |
| 0.20      | ![Surface](image3) | ![Volume](image4) |
| 0.35      | ![Surface](image5) | ![Volume](image6) |
| 0.50      | ![Surface](image7) | ![Volume](image8) |

ranging from 0.04 to 0.08 fm$^{-3}$. While a smooth evolution is is seen for both $B$ and $\chi$ at low temperatures, not much change is observed at higher $T$ and $\rho$. Less variations are observed for the surface and volume functionals in Table 4. These results, along with the connection of $B$ and $\chi$ with the pasta morphology listed in Table 2, one can expect that a pasta-structure diagram can be produced as a function of $x$, $T$ and $\rho$ with the use of the trained neural networks.
5. Conclusions
The figures of Tables 3 and 4 show that it is possible to use machine learning techniques to estimate the Minkowski functionals for any value of \( x \), \( T \), and \( \rho \). The three-dimensional representation of the functionals also indicate that their variations can be linked to the evolution of the pasta structures as a function of \( x \), \( T \) and \( \rho \), e.g. from pasta to anti-pasta as \( \chi \) goes from positive to negative, etc. Such connection of these functionals to the pasta structures will be established in a forthcoming article for both nuclear matter and neutron star matter.

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