Time-Dependent Hartree-Fock Approach to Nuclear Pasta at Finite Temperature

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Abstract. We present simulations of neutron-rich matter at subnuclear densities, like supernova matter, with the time-dependent Hartree-Fock approximation at temperatures of several MeV. The initial state consists of α particles randomly distributed in space that have a Maxwell-Boltzmann distribution in momentum space. Adding a neutron background initialized with Fermi distributed plane waves the calculations reflect a reasonable approximation of astrophysical matter. This matter evolves into spherical, rod-like, and slab-like shapes and mixtures thereof. The simulations employ a full Skyrme interaction in a periodic three-dimensional grid. By an improved morphological analysis based on Minkowski functionals, all eight pasta shapes can be uniquely identified by the sign of only two valuations, namely the Euler characteristic and the integral mean curvature.

1. Introduction

In systems at densities just below normal nuclear density, the spherical shape for nuclear matter is no longer favorable and the system tends to lower the total surface area by elongating the nuclei and forming nuclear rods [1, 2]. Seminal liquid-drop calculations [3, 4] predicted that with further increase in density, the shapes of inhomogeneous nuclear matter change from rods to slabs, tubes, and bubbles until the system melts into uniform matter. For a more realistic description of these so-called pasta nuclei, multi-dimensional calculations were performed in various models (e.g. [5, 6, 7]) which showed more complex structures.

Recently, a time-dependent Hartree-Fock (TDHF) approach has been utilized to describe pasta nuclei in zero-temperature supernova matter [8, 9]. In this work we perform such calculations at finite temperature. The TDHF simulations produce a great variety of three-dimensional structures. A very general and powerful means to quantify such complex structures is provided by the Minkowski functionals, from integral geometry [10, 11, 12]. They were already introduced for structure analysis of galaxy clusters in Ref. [13] and later used for cosmological problems (see e.g. [14]). They provide an optimal technique to classify the different pasta shapes as already exploited in [15, 16, 17].

2. TDHF description

In this framework, we want to describe the pasta structure with the time-dependent Hartree-Fock (TDHF) approximation proposed by Dirac [18]. In general, the TDHF equations are
Figure 1. Typical pasta shapes at $T = 7$ MeV. Bubble shape illustrations show gas phase indicated by the color-scale.

Figure 2. Map of pasta shapes achieved in TDHF calculations. Each dot represents two calculations. The solid black line shows a phase separation line discussed in Sec. 4.

derived from a time-dependent variational principle with the variational space restricted to one single, time dependent Slater determinant. In nuclear applications, TDHF usually employs an effective interaction as, e.g., the Skyrme force, for a review see [19]. With the advance of computational power, it is now possible to perform full 3D calculations without any symmetry restrictions (e.g. [20, 21]).

The TDHF calculations are performed on an 3D grid in coordinate space with 16 grid points in each direction with a grid spacing of 1 fm. We simulate infinite matter using periodic boundary conditions. The Coulomb problem is solved in the jellium approximation. The kinetic energy operator is evaluated in Fourier space and time evolution is performed using a Taylor expansion of the mean-field propagator. For the present calculations we choose Skyrme parametrization SLy6 which was developed with an emphasis on describing neutron rich matter [22].

3. Map of regimes

We initialize the calculations by distributing a number $N_{\alpha}$ of $\alpha$ particles randomly over the grid and in momentum space following a Maxwell-Boltzmann distribution with a given initialization temperature $T_{\text{init}}$. To that end, we use ground-state wave functions for the $\alpha$ particles from a stationary HF calculation. Further neutrons are introduced in plane wave states using a Fermi distribution with the same temperature to get a proton fraction of 1/3. Spin up and spin down states are occupied simultaneously to avoid a large spin excitation. The number $N_{\alpha}$ is varied to produce systems with different densities.

The excitation state of matter is characterized by its actual temperature $T$. Because it is difficult to measure temperature in the quantum simulation of a micro-canonical ensemble we introduce as a rough measure $T$ estimated by the excitation energy $E^*$ through the relation $E^* = (\pi^2 A)(2\varepsilon_F) T^2$ where $A$ is the total number of nucleons and $\varepsilon_F$ the Fermi energy of the system [23]. This excitation temperature $T$ is to be distinguished from the “initial temperature” $T_{\text{init}}$ which we use to boost stochastically the initial ensemble of $\alpha$ particles and background neutrons. Calculating the excitation temperature $T$ for the different values of the initial temperature $T_{\text{init}}$, we find empirically $T \approx 7\ \text{MeV} + \sqrt{T_{\text{init}}(T_{\text{init}} + 100\ \text{MeV})}/6$. This is taken henceforth for a rough calibration of $T$.

Each setup is evolved in time for 1500 fm/c. After that time, the system goes over into a pasta...
Table 1. Signs of the integral mean curvature and Euler characteristic for each observed shape.

| shape | sph | rod | rod(2) | rod(3) | slab | rod(2) | b | rod | b | sph | b |
|-------|-----|-----|--------|--------|------|--------|---|-----|---|-----|---|
| $W_2$ | > 0 | > 0 | > 0 | - to + | ≈ 0 | < 0   | < 0 | < 0 | < 0 | < 0 | < 0 |
| $W_3$ | > 0 | = 0 | < 0 | < 0 | = 0 | < 0 | = 0 | > 0 | < 0 | < 0 | < 0 |

state where some type of equilibrium is achieved and shapes are satisfyingly stable. Depending on the temperature differently strong fluctuations can be observed.

In Fig. 1 many different pasta shapes are classified. Among the structures found are rod and slab structures discovered, e.g., by QMD calculations [17]. Rod(2) corresponds to rods forming a two-dimensional layer. The shape rod(3) describes three rods in x-, y- and z-direction crossing in one point. Similar shapes were seen in [8, 24] and the rod(3) structure was also found in [6].

Fig. 2 shows for which density and temperature the different shapes appear. Note that two calculations for each point in the map were performed. As we have random initial conditions, the final shapes may differ although the same values for temperature and mean density are assumed. The hatched areas with a mixture of colors indicate the different final states reached in these cases. At higher densities, bubble structures can be seen (the gas phase has a pasta like shape). Many shapes can coexist here in one point of the map.

For slab and rod(3) structures, the final state seems to highly depend on the initial condition. The similarity of these two structures is, that liquid and gas phase have the same shapes, symmetrically complementing each other and filling out almost the same volume.

4. Minkowski Functionals and structure classification

There are four Minkowski functionals $W_\nu$ defined for a spatial domain $K$ in three dimensions: they are proportional to its volume $W_0 \propto V$, its surface-area $W_1 \propto A$, the integral mean curvature $W_2 \propto \int_{\partial K} dA (\kappa_1 + \kappa_2)/2$, and the topological Euler–Poincaré characteristic $W_3 \propto \chi$, equal to the integrated Gaussian curvature $\int_{\partial K} dA \kappa_1 \cdot \kappa_2$. Here, $\kappa_1$ and $\kappa_2$ are the principle curvatures on $\partial K$, the bounding surface of $K$. The Euler characteristic is a topological constant.

These shape indices form a complete basis of all functionals defined on unions of convex sets which are translational and rotational invariant, additive, and at least continuous on convex sets [25], providing a complete scalar morphological characterization of the pasta shapes.

The TDHF results for pasta matter are given as gray-scale data with a density $\rho_i$ assigned to each voxel $i$ (= grid point). In order to compute the Minkowski functionals of a domain $K$, the density field is turned into binary data via thresholding at the threshold density $\rho_{th}$. The Minkowski functionals of the union of all black voxels (each voxel $i$ with $\rho_i > \rho_{th}$), interpreted as a polygon $K$, can quantify the shape of the pasta matter in dependence of $\rho_{th}$. Beforehand the marching cube algorithm [26] is applied, in order to reduce voxelization errors. The Minkowski functionals of the polygon are evaluated, e.g., using the linear-time algorithm [27, 28] 1.

The threshold density can take on values $\rho_{th} \in [0, \rho_{max}]$. But for small thresholds $\rho_{th} \approx 0$ and for high thresholds $\rho_{th} \approx \rho_{max}$, the Minkowski functionals show erratic behavior; thus, the structure values for these thresholds are ignored [27, 29].

Calculating the values of the Minkowski scalars for all shapes as a function of threshold density (Fig. 3), we see that we can uniquely classify the different shapes in simple fashion: only the signs of integral mean curvature and Euler characteristic are needed (see TAB. 1).

The central regime with solid lines in Fig. 3 indicates the physical values for the threshold density which yield reliably stable values of $W_2$ and $W_3$ for lowest value of temperature are

1 Implementations can be found at www.theorie1.physik.fau.de
$W_2$, proportional to the integral mean curvature, and $W_3$, proportional to the Euler characteristic as function of threshold density for the samples shown in Fig. 1.

$\rho_{th} \in [0.03 \text{ fm}^{-3}, 0.08 \text{ fm}^{-3}]$. For low $\rho_{th}$ only few dots are below $\rho_{th}$ due to quantum fluctuations in the gas phase, and for high $\rho_{th}$ there are fluctuations in the liquid phase respectively.

Rod(2), rod(2) bubble, and rod(3) consist in channels and tunnels; thus, the domain has a negative Euler characteristic $\chi < 0$ [30]. The bubble shapes are the complements of the according sphere, rod, or rod(2) shapes. As the sign of both main curvatures $\kappa_1$ and $\kappa_2$ changes, $W_2$ also changes sign but the Euler characteristic remain constant.

For the slab and rod(3) shapes, which are symmetric in gas and liquid phase, the integral mean curvature as a function of the threshold $\rho_{th}$ is point symmetric w.r.t. a mid value for the threshold density, trivially true for the slab with $W_2 \approx 0$, but holds also for the rod(3) shape.

Especially at higher temperatures and mean densities mixtures of phases can appear, in a sense that at different threshold densities the pasta matter can take on different shapes (cf. [9]). With increasing threshold densities the shapes can change to shapes which appear usually at lower mean densities. For these cases we take the pasta phase with the bigger range in $\rho_{th}$.

To show the fraction of liquid and gas phase and the transition to uniform matter, we plotted the threshold density profiles for various calculations in Fig. 4 as an additional observable. For $T = 7 \text{ MeV}$ and low mean density, there is a big peak at small densities and a long tail to high densities. With increasing mean density a peak at high density develops. At the densities where rod(3) and slab shapes appear the peaks for low and high densities have nearly the same width and height. At higher mean densities the peak for low densities disappears and only a tail remains. With increasing temperature the double peak structure vanishes and finally a single peak around the mean density is forming which moves successively to central density with ever higher $T$.

As the pasta structures vanish with higher density, the variance from the mean value of the calculation of these plots decreases. Going through the systematics of the results, we found as a reasonable value for a limit of the variance to observe pasta structures $10^{-4} \text{ fm}^{-6}$. The phase separation line computed with this observable is displayed in Fig. 2 as a bold line.
5. Conclusion
In this work we have studied the nuclear composition of supernova matter at sub-nuclear densities using time-dependent Hartree-Fock with the Skyrme energy functional. The initial state is prepared by placing $N_\alpha$ $\alpha$ particles stochastically over the simulation box with periodic boundary conditions and adding $2N_\alpha$ neutrons in plane waves. We have varied the excitation state by initializing the $\alpha$ particles and the neutrons with a certain amount of kinetic energy. As a measure for the actual excitation, we introduce a rough estimate for the resulting temperature based on the excitation energy. The thus given initial states evolve to a topologically stable state of pasta matter within about 1000 fm/c. This allows us to deduce a map of pasta shapes in the plane of temperature and density. Those TDHF results agree qualitatively with the phase diagram calculated in QMD [17]. In realm of “rod” structure, we include further sub-structures, coined rod(2) and rod(3), which appeared in earlier Hartree-Fock calculations [6, 8].

To characterize these structures, we use Minkowski functionals which allows us to characterize the various shapes in terms of a few key numbers. By taking the variance of the density profile as a further observable, we can define a phase border between uniform matter and pasta shapes.

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