Studies of the neutron star crust

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Abstract. The physics of the neutron star crust is highly relevant for many observable phenomena like the temperature evolution of accreting neutron stars or the evolution of supernovae. In order to investigate the structure and dynamics of the crust we perform extensive molecular-dynamics-type simulations of the nucleons in the crust including the neutralizing effect of the electron background. Simulations for a range of densities, temperatures and proton-to-neutron ratios have been performed. Results for the isospin dependence of the energy per particle and nucleonic correlation functions as obtained from the simulation runs are discussed.

1. Introduction
The structure of neutron stars is highly complex, encompassing a high-density homogeneous core of leptons, nucleons and potentially more exotic particles like hyperons and quarks in the center, followed by a solid crust of exotic nuclear structures and nuclei, finally surrounded by an atmosphere of light nuclei. The crust itself can be divided into an outer region with nuclei arranged in a crystal structure embedded in an electron plasma and the inner crust beyond the neutron drip, which includes a gas of free neutrons. The structure and properties of the crust region are important for many aspects in neutron star and supernova physics like heat transport and neutrino opacities. In order to study the inner crust we developed an efficient code that can be used for large-scale quantum molecular dynamics simulations of the system. In particular we study the development of the pasta phase in the transition region between crust and core. We investigate the sensitivity of the specific pasta structures and the density range of the transition on the isospin dependence of the nuclear interaction. In addition we compute correlation functions that can be used to derive basic transport coefficients of the crustal matter.

The actual composition of the outer crust of the neutron star is still quite uncertain (see [1]). It depends very strongly on the isospin dependence of the nuclear interactions, which is still not very well understood. As a consequence the position of the neutron drip line, beyond which additional neutrons are no longer bound, is quite unclear, in particular in the case of heavier elements. This has been demonstrated, e.g. in [2], where it was shown that the drip point for the example of uranium isotopes varies by more than 70 neutrons, looking at a range of standard Skyrme and relativistic mean field (RMF) approaches. Fig. 1 shows the least bound neutron states in uranium in a specific calculation. It demonstrates a distinct shell closure for a neutron number of 258, stabilizing isotopes up to this value, compared to other calculations that yield a drip point of $N = 184$. This uncertainty, related to the strength of the various shell closures, continues in the inner crust, where nuclei are immersed in a gas of dripped neutrons and where
the system becomes more and more isospin asymmetric. A modeling approach of this region is discussed in the following section.

2. Modeling Approach

The model description of the nuclear crust used in our simulations is based on the so-called Quantum Molecular Dynamics (QMD) - approach that was pioneered a long time ago in [3]. Within this approach the single-nucleon wave function is described by a Gaussian function

$$\psi(r_i) = \frac{1}{(2\pi C_W)^{3/4}} \exp \left[ -\frac{(r_i - R_i)^2}{4C_W} + i r_i \cdot P_i \right],$$

(1)

with center-of-mass position $R_i$ and momentum $P_i$. The main (very significant) approximations employed are that the width parameter $C_W$ is chosen to be constant in time and the total wave function of the system is taken as product of the single-particle wave functions. This in the end leads to classical equations of motion of the particle positions and momenta $R_i, P_i$, where the densities involved in determining the forces are given by the overlap densities of the Gaussian wave functions. For an extensive discussion of the formalism see [4]. The dynamics of the system is governed by a Skyrme-type Hamiltonian. The overall structure of the Hamiltonian is given by

$$H = T + V_{\text{Pauli}} + V_{\text{Skyrme}} + V_{\text{sym}} + V_{\text{MD}} + V_{\text{Coul}}.$$

(2)

$T$ is the kinetic energy and $V_{\text{Pauli}}$ is a phenomenological Pauli potential which approximates the effect of the fully antisymmetrized many-body wavefunction [5]. $V_{\text{Skyrme}}$ is the nucleon-nucleon Skyrme-like interaction with a momentum-dependent part $V_{\text{MD}}$ and $V_{\text{Coul}}$ contains the Coulomb interaction. $V_{\text{sym}}$ is the isospin-dependent part of the potential. In this work we follow closely the formulation developed in [6], extending this treatment by non-linear isospin-dependent interactions in order to study isospin effects in more detail. All terms are explicitly discussed in [7].

Figure 1. Single-particle energies of the least bound neutron states in the uranium isotope chain. The results are obtained in an RMF calculation using the NL-Z2 parameter set. The line shows the Fermi energy. A clear shell closure for $N=258$ can be observed.
3. Results of the Simulations

Comprehensive numerical studies of the inner crust of neutron stars require extensive long-time simulations for a variety of conditions, including scans of relevant densities, proton-to-neutron ratios, and temperatures, as well as repeating such scans for different interaction parameters.

After establishing that the properties of saturated nuclear matter and nuclear binding energies have reasonable values (see [7]), a closer study of isospin-asymmetric matter follows. In order to test this aspect we calculate the isospin dependence of the energy density around nuclear saturation $\rho_0 \approx 0.165\text{fm}^{-3}$. In the numerical runs this is simply done by changing the relative number of protons and neutrons in the simulation box. The results are shown in Fig. 2. In the left panel one can clearly observe significant deviations from a simple parametrization of the density-dependent energy per particle $\epsilon$ as quadratic function like

$$\epsilon(\rho, \delta) = \epsilon_0(\rho) + \epsilon_{\text{sym}}(\rho)\delta^2$$

where $\delta$ is defined as $\delta = (\rho_n - \rho_p)/(\rho_n + \rho_p)$ and is related to the proton over nucleon ratio $Y_p$ via $\delta = 1 - 2Y_p$. Adding a further term to the parametrization as $\epsilon_{\text{sym},4}(\rho)\delta^4$ [8] leads to a very good fit of the numerical results as shown in the right panel of the figure. This demonstrates that one has to take into account higher order terms in describing the isospin dependence of nuclear matter energies if one wants to describe a larger range of isospin values beyond symmetric nuclear matter.

In a range of densities of the inner crust close to the transition to the core, the transition from the regular lattice structure to the homogeneous core might give rise to unusual shapes of nuclei as was pointed out originally in [9, 10], generating the so-called nuclear phasta phase. The typical sequence of structures expected, starting from spherical clusters/nuclei, are rod-like nuclei and then slabs, followed by the inverted configurations as rod-like and spherical holes in nuclear matter. In order to quantitatively assess what types of structures are present at some given density in the simulated nucleonic configurations, one can calculate the so-called Minkowski functionals that can be used to characterize the shape of a 3D object [11].

Figure 2. Energy per particle as function of $Y_p$. The simulation results are shown as symbols for three different densities $0.9\rho_0$, $\rho_0$, and $1.1\rho_0$, respectively. The left panel displays the result of a quadratic fit to the numerical values, whereas the right panel shows the corresponding result for a fit up to quartic terms in the asymmetry.
The four independent functionals are the volume and surface of the object as well as the mean integral curvature $H$ and Euler characteristic $\chi$ defined as

\begin{align}
H &= \frac{1}{2} \int_{\partial K} (\kappa_1 + \kappa_2) dA \\
\chi &= \frac{1}{2\pi} \int_{\partial K} \kappa_1 \cdot \kappa_2 dA.
\end{align}

(4)

implying an integral over the surface $\partial K$ of the object. $\kappa_1$ and $\kappa_2$ are the principal curvatures at the various surface points. As for rods and slabs at least one of the curvatures vanishes, the corresponding value of $\chi$ is zero as well. On the other hand, entering the phase with hole-like structures, switches the sign of $H$ from positive to negative values. In practice, given a simulation-generated configuration, numerical calculations using the formula (4) first require the actual determination of the surface. In practice this can be done by defining a density threshold which divides clustered regions from the outside. Fig. 3 shows such a calculation of the values of $H$ and $\chi$ averaged over the simulation box for different baryon densities as a function of this threshold $\rho_{th}$. The figure shows that there is a range of densities, where the values of the functionals are reasonably constant allowing for a reliable determination of their value. Using this procedures the averaged values of $H$ and $\chi$ are shown in Fig. 4. The different curves show results for changing the isospin-related interaction parameters leading to distinct slope parameters $L$ as indicated in the figure. Overall the isospin dependence turns out to be rather weak. As argued before, one can clearly observe the sign-change of $H$ as function of density. In the right panel it can be observed that the Euler characteristic attains negative values in the intermediate range of densities. This comes about as one can also express the value of $\chi$ the as number of connected regions plus the number of cavities minus the number of connecting tunnels [11]. Thus the figure shows the development of tunnels between nuclear slabs [7]. This result stresses the complexity of the pasta region as there are many competing nearly degenerate states of matter, therefore even for low temperatures the system might consist of a superposition of various structures.

One important aspect of studying the pasta phase of the neutron star crust is to investigate the transition from the pasta to the homogeneous matter of the stellar core. This can be done
by calculating the two-nucleon correlation function defined as [7]

\[ \xi_{NN} = \langle \Delta_N(x) \Delta_N(x+r) \rangle. \]  

(5)

The average is taken over the position \( x \) and the direction of \( r \). \( \Delta_N(x) \) denotes the deviation of the nucleon density field \( \rho_N(x) \) from the average:

\[ \Delta_N = \frac{\rho_N(x) - \rho_{av}}{\rho_{av}}. \]  

(6)

where \( \rho_{av} = N/V \) is the average density of nucleons. In Fig. 5 the simulation results of the correlation is shown for densities around the transition point of around \( \rho \approx 0.65 \rho_0 \) to the core, comparing different isospin parameters characterized by the indicated values of the slope parameter \( L \) given as the change of nuclear symmetry energy with density

\[ L = 3\rho_0 \left. \frac{\partial e_{sym}(\rho)}{\partial \rho} \right|_{\rho=\rho_0}. \]  

(7)

There is a rather clear and rapid transition for which the correlation changes significantly within a small density window, indicating that in the case of infinite systems the crust-core transition is of first-order type. The two sets of isospin parameters result in slightly different results, but do not affect the overall conclusion.

Correlation functions are important input for determining a variety of transport properties of the matter. In particular correlations in momentum space enter the expressions for electrical and heat conductance as well as shear viscosity [12]. The corresponding structure factor \( S_i(q) \) for protons and neutrons (\( i = p, n \)) is given by

\[ S_i(q) = < \rho_i^*(q) \rho_i(q) > \]  

(8)

with the Fourier-transformed densities \( \rho_i(q) \). Determining this value for different temperatures gives the results presented in Fig. 6. In this case the numerical runs were performed for a baryon
density of $0.1 \rho_0$, below the onset of the pasta phase, again for a proton fraction $Y_p = 0.3$. The two panels show results for different temperatures $T = 1$ and 4 MeV. Thus, the parameters correspond to values that are relevant during the evolution of the matter in supernova explosions. The structure factor exhibits clear peaks that correspond to the cluster sizes in the system. Note that these structures survive somewhat reduced also for higher temperatures. This can have significant consequences for the heat transport and the supernova evolution, which needs to be investigated in more detail. Work along this line is in progress.

Figure 5. Nucleon-nucleon correlation function for different densities and slope parameters $L$. The results were obtained for a proton to nucleon ratio of 0.3.

Figure 6. Snapshots of structures obtained in the QMD simulation for various densities for a proton-to-neutron ratio of 0.3. The green and red symbols correspond to neutrons and protons, respectively.
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References
[1] Rüster S B, Hempel M and Schaffner-Bielich J 2006 Physical Review C 73 035804 ISSN 0556-2813
[2] Schramm S, Gridnev D, Tarasov D V, Tarasov V N and Greiner W 2012 International Journal of Modern Physics E 21 1250047 ISSN 0218-3013
[3] Aichelin J and Stöcker H 1986 Physics Letters B 176 14–19 ISSN 03702693
[4] Aichelin J 1991 Physics Reports 202 233–360 ISSN 03701573
[5] Dorso C, Duarte S and Randrup J 1987 Physics Letters B 188 287–294 ISSN 03702693
[6] Maruyama T, Niita K, Oyamatsu K, Maruyama T, Chiba S and Iwamoto A 1998 Physical Review C 57 655–665 ISSN 0556-2813
[7] Nandi R and Schramm S 2016 Physical Review C 94 025806 ISSN 2469-9985
[8] Chen L W, Cai B J, Ko C M, Li B A, Shen C and Xu J 2009 Physical Review C 80 014322 ISSN 0556-2813
[9] Ravenhall D, Pethick C and Wilson J 1983 Physical Review Letters 50 2066–2069 ISSN 0031-9007
[10] Hashimoto M a, Seki H and Yamada M 1984 Progress of Theoretical Physics 71 320–326 ISSN 0033-068X
[11] Michielsen K and De Raedt H 2001 Physics Reports 347 461–538 ISSN 03701573
[12] Horowitz C J and Berry D K 2008 Physical Review C 78 035806 ISSN 0556-2813