Dynamical description of exotic structures at subnuclear densities

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Abstract. The dynamics of infinite nuclear matter in the conditions of density and
temperature expected in the outermost layers of neutron stars is studied in the framework
of a microscopic time-dependent mean-field approach around zero temperature. Dynamical
processes in inhomogeneous nuclear matter are studied using a large number of nucleons in
numerical simulations without any assumptions on the morphology of nuclear matter. The
occurrence of exotic structures when varying internal conditions as densities, nuclear species
and elementary cell symmetries is investigated. The corresponding structures are studied in
terms of a phase diagram in density space evidencing some sensitivity to the isospin-dependent
part of the equation of state.

1. Introduction
Neutron stars (NS) have interested physicists and astronomers for long time insofar as they can
shed light on our understanding of fundamental properties of matter under extreme conditions.
The study of neutron stars has gained a renewed interest on the last decade by means of the
new generation of launched observatories which are enabling new observations and providing us
with a large amount of new data.

Modern nuclear physics input as well as many-body theories are valuable tools to improve
our comprehension of the physics of compact objects. Astrophysics and nuclear physics are
inextricably intermingled disciplines. Any advance in these two areas leads to a progress in the
other and this interplay enables us to deepen our knowledge of the universe. In the nuclear
domain, new experimental programs with radioactive beams are nowadays emerging (SPIRAL2,
FRIB, FAIR). Their corresponding goal is to produce those rare isotopes playing a relevant role
in astrophysical phenomena, aiming at providing answers to open questions about the nature of
NS and about nucleosynthesis processes.

In most theoretical models of NS the outermost layers have the structure of a crystal lattice
of neutron rich nuclei immersed in a degenerate electron gas and, as density increases, it is
essentially a fluid composed of dripped neutrons. In this region, where the density varies from
0.1 to 0.5 $\rho_\infty$, the saturation value of nuclear matter, the occurrence of exotic structures as rods,
slabs and other complex shapes has been predicted by theoretical approaches in the framework
of the liquid drop model [1] a few decades ago. More recently other static [2] and dynamical [3]
models have confirmed this early prediction.

The existence of these structures is assumed to be a consequence of the competition between
Coulomb and nuclear forces, this phenomenon being called ”frustration”, and to be sensitive to
the equation of state (EOS) of nuclear matter. Their presence may have important astrophysical consequences on macroscopic characteristics, as masses and radii [4], as well as on the cooling processes of the star [5]. In particular, they should affect the neutrino opacity [6] and the transport [7] and elasticity [8] properties of the crust.

Aiming at investigating the microscopic dynamics of matter in the crust, we have developed a dynamical model [10] beyond the Wigner-Seitz approximation [11]. Since these structures involve a large number of low energy configurations, a pure mean field description of the nuclear dynamics has been performed. In this approach, starting from initial crystalline lattices of nuclei, with different symmetries, non spherical structures occur as the result of microscopic self-organization processes. The survival of those meta-stable equilibrium structures has been checked over thousands fm/c. In this work, the influence of the EOS, of the isotopic composition and of the lattice symmetries on the formation of exotic structures are studied.

This paper is organized as follows, in Section 2 the essential ingredients of the model are presented. In Section 3 a selection of relevant results are shown and in Section 4 the conclusions and perspectives are given.

2. The model: Dynamical Wavelets in Nuclei for Neutron Stars (DYWAN-NS)

In the range of characteristic temperatures and densities of NS, namely \( T \ll 1 \, \text{MeV} \) and \( 10^6 \, \text{g/cm}^3 \leq \rho \leq 10^{13} \, \text{g/cm}^3 \), the stellar matter is correctly described in terms of a system of interacting nucleons in a uniform background of electrons insuring the neutrality of matter. In this context we have developed a dynamical approach which is based on the DYWAN model [12] describing heavy ion collisions.

In the present approach nuclei are initially located on the sites of a crystalline lattice with periodic boundary conditions. A static self-consistent procedure is implemented in order to solve the Hartree-Fock (HF) equation for nuclear composites, which are prepared either in their ground states or in excited states according to mechanical or thermal constraints. The HF equation is numerically solved by spanning the one-body density matrix in a convenient basis. The elements of this basis are wavelets [13], which are functions of a set of four parameters: \( \{ \langle x \rangle, \langle px \rangle, \chi, \gamma \} \) in \( x \) coordinate, with similar expressions in \( y \) and \( z \) coordinates. Here \( \chi = \langle x^2 \rangle - \langle x \rangle^2 \) and \( \gamma \) is defined as:

\[
\gamma = \frac{\sigma^2}{2\chi} \quad \text{with} \quad \sigma = \langle [x - \langle x \rangle, (p_x - \langle p_x \rangle)]_+ \rangle
\]

For this calculation a density-dependent zero-range effective interaction has been chosen with the following self-consistent field:

\[
V_q^{HF}(\rho, \xi) = \frac{t_0}{\rho_\infty} \rho + \frac{t_3}{\rho_\infty^{7/6}} \rho^{7/6} + \frac{c}{\rho_\infty^2} \xi^2 + \frac{4qc}{\rho_\infty^2} \rho \xi + \frac{\Omega}{3\rho_\infty^2} \xi^2 + \frac{4q\Omega}{3\rho_\infty^2} (\rho - \rho_\infty) \xi + V_q^C
\]

In Eq. (1) \( \rho_n \) and \( \rho_p \) stand for neutron and proton densities, \( \rho = \rho_n + \rho_p \), \( \xi = \rho_n - \rho_p \), \( q=1/2 \) for neutrons and \(-1/2 \) for protons, \( \rho_\infty=0.145 \, \text{fm}^{-3} \) is the saturation density of infinite nuclear matter and \( V_q^C \) is the Coulomb interaction. With the current values of the parameters, namely \( c=20 \, \text{MeV}, \Omega=-100 \, \text{MeV}, t_0/\rho_\infty = -356 \, \text{MeV} \, \text{fm}^3 \) and \( t_3/\rho_\infty^{7/6} = 303 \, \text{MeV} \, \text{fm}^{7/2} \), the principal static characteristics of nuclei and of infinite neutron matter are reproduced. The Coulomb term for protons is calculated using Ewald summation techniques [14], which are adapted to the calculation of long range potentials in periodic systems.

The parameters \( c \) and \( \Omega \) are related to the coefficients of the mass formula \( J \) and \( L \) corresponding to, respectively, the volume-symmetry and to the density-dependent symmetry energy as follows:

\[
c = J - \frac{\hbar^2}{6M} k_F^2 \\
L = 6c + \Omega + L_{\text{kin}}
\]
where $L_{\text{kin}}$ is the kinetic energy contribution to $L$ (see Eq. (5) below). These parameters are still uncertain because they are not completely constrained from nuclear data. It seems then worthwhile to perform a study of their influence on the overall dynamical behavior of the crust. To this end $c$ has been fixed to the value above defined but $\Omega$ was varied in the range $-120 \leq \Omega \leq -75$ MeV in order to analyze the sensitivity of the dynamics to this interaction. The density dependence of the symmetry energy has been determined here in a phenomenological way according to current estimates at the saturation value in pure neutron matter [9]. The values of the parameters reproduce the principal static characteristics of nuclei, as binding energies, radii and equilibrium densities. The associated incompressibility modulus in symmetric matter $K_{\infty} = 200$ MeV corresponds to a “soft” EOS.

The energy density per baryon $\omega_q$ is defined as:

$$\omega_q = \frac{\varepsilon}{\rho} = \frac{\int V_q^{HF} d\rho}{\rho} + \omega_{\text{kin}},$$  \hspace{1cm} (2)

where $\omega_{\text{kin}}$ corresponds to the kinetic contribution. According with Ref. [15] the isovector part of the energy density per baryon is:

$$\omega_\delta = \lim_{\delta \to 0} \frac{\partial^2 \omega_q}{\partial \delta^2}$$  \hspace{1cm} (3)

with $\delta = \xi/\rho$, and the corresponding contribution to the incompressibility modulus is:

$$K_{\text{sym}} = 9\rho^2 \frac{\partial^2 \omega_\delta}{\partial \rho^2} \bigg|_{\rho = \rho_\infty}. $$  \hspace{1cm} (4)

The kinetic contribution to the density-dependent symmetry energy is defined as:

$$L_{\text{kin}} = 3\rho \frac{\partial \omega_{\text{kin}}}{\partial \rho} \bigg|_{\rho = \rho_\infty} $$  \hspace{1cm} (5)

In Fig. 1 we have plotted the values of $L$ and of $K_{\text{sym}}$ as a function of $J$. The squares A, B and C are the results obtained with the implemented force for $\Omega = -75$, -100 and -120 MeV, respectively. The remaining symbols are extracted from Skyrme Hartree-Fock (SHF) calculations from Ref. [15] and references therein. The numbers in the figure denote the different parameter sets for SHF: 1 for SI, 2 for SIII, 3 for SIV, 4 for SVI, 5 for Skya, 6 for SkM, 7 for SkM*, 8 for SLy4, 9 for MSkA, 10 for SkI3, 11 for SkI4, 12 for SkX, 13 for SGII. In this picture the results corresponding to EOS A and B are compatible to the reference theoretical calculations, while the soft EOS C value is too low for both correlations. Nevertheless, we recall that the effective force implemented here is a simplified version of a Skyrme-like interaction. It depends on a reduced set of parameters thus providing efficient computational formula. It should be underlined here that in spite of the simplicity of the force, the global trends of the calculated physical quantities displayed in this section are in good accordance with other theoretical approaches.

The dynamical evolution of the system is governed by the time-dependent Hartree-Fock (TDHF) equation for the one body density matrix. As shown elsewhere [10] the TDHF equation is solved by a variational principle which gives the evolution of the 12 parameters of wavelets (4 for each dimension). The evolution is ruled then by the mean-field given by Eq. (1), the influence of which is felt by all nuclei belonging to the periodic box.
3. Results
Let us consider the simplest crystalline arrangement given by a simple cubic cell (SCC) box of oxygen isotopes with proton fraction \( x = \frac{\langle \rho_p \rangle}{\langle \rho \rangle} = 0.2 \), \( \langle \rho_p \rangle \) and \( \langle \rho \rangle \) being proton and total average densities, respectively. The lattice sites are located at the corners of a cube. Each nuclei at a given site is then shared equally between 8 adjacent cubes. These nuclei have been coherently excited with the same small quadrupole deformation at the initial time. In light of the lattice level density distribution it is possible to select spatial regions where the density is higher than a given threshold, called threshold density \( \rho_t \). The morphological characteristics of the selected matter distribution can be analyzed by means of Morphological Image Analysis (MIA) technics [16] in order to characterize the underlying structures. In Fig. 2 is represented the structure diagram observed for the neutron density as a function of the mean density, normalized to the saturation value, in terms of \( \rho_t \) which is represented in the vertical axis.

![Figure 2](image_url)

**Figure 2.** Neutron phase diagram in the threshold density versus the mean density plane for two values of \( \Omega \): -120 MeV (a) and -75 MeV (b), for proton fraction \( x=0.2 \). The different structures are represented in grey scale.
Two choices of the asymmetry parameter have been provided for: $\Omega = -120$ MeV (a) and $-75$ MeV (b). In both cases, for a given threshold density, the five standard types of pasta phases emerge naturally and in the same order they should appear with increasing density as predicted by static models [1] and confirmed by recent calculations. Some sensitivity to the asymmetry-dependent contribution to the effective force also emerges from Fig. (2). The stiffer force, for $\Omega = -75$ MeV, favors the occurrence of spherical and sponge-like structures, while restraining that of cylinder and slabs. This is consistent with the fact that the stiff potential is more repulsive, namely at high mean densities. The consequence is that more and more neutrons are dripped or localized at the surface of clusters. In the last case, quasi-free neutrons contribute either to build heavy spherical nuclei or to link neighboring clusters in all directions, giving rise to the so-called sponge-like structures.

As underlined by other authors [17] the inner crust of a neutron star is an extremely complex system in which the appearance of disordered phases can be favored. There is then a special interest to investigate the response of nuclear matter to the introduction of incoherent perturbations at the initial time. The behavior of the system under incoherent perturbations strongly depends on the symmetry of the crystal. It is well known from solid state physics that SCC are unstable against Coulomb interactions. In the NS context, where the nuclear field plays a preponderant role, the system is shown to loose the fingerprints of the initial lattice symmetry [18] all along the dynamical evolution.

The feasibility of those disordered phases in a different, more complex, kind of crystalline arrangement has been studied. To this end face centered cubic (FCC) lattices of symmetric oxygen nuclei have been perturbed incoherently, by shifting at random their position from the lattice sites. In addition to the 8 corner lattice sites are included here the centers of the 6 faces, giving a total of 4 lattice points per unit cell. Some snapshots of the corresponding neutron density evolution are shown in Fig. 3. In this case, the average density is $0.4 \rho_\infty$ and the threshold density for the 3-dimensional plot is $\rho_t = 0.04$ fm$^{-3}$. The stability conditions of the FCC initial lattice is such that despite of the random perturbations imposed to the location of nuclei, the system attempts to preserve symmetries exhibiting stringy or cylindrical structures. At sufficiently long times the dominant arrangement corresponds to a single infinite rod-like structure which is periodically replicated.

In order to investigate the influence of the charge and the mass of nuclear species on the onset and on the dynamical evolution of structures, iron nuclei with different isotopic compositions have been considered. In Fig. 4 the neutron phase diagram corresponding to the particular case

![Figure 3. Neutron density profiles of a perturbed supercell of 0.5 proton fraction oxygen isotopes in face centered cubic lattices at different times. The mean and threshold densities are $\langle \rho \rangle = 0.4 \rho_\infty$ and $0.04$ fm$^{-3}$, respectively.](image)
of SCC iron lattices with proton fraction $x=0.5$ is shown. The overall mean density is in this case $\langle \rho \rangle = 0.1 \rho_\infty$ and the threshold density is $\rho_t = 0.05 \text{ fm}^{-3}$. In the same way as for the system represented in Fig. 3, the positions of nuclei have been randomly shifted from the lattice sites at the initial time. In this case, the observed structures are the individual iron nuclei which undergo shape oscillations around their initial deformed states. In this case, the stability and symmetry of non-equilibrium structures seem not being substantially modified by incoherent perturbations. This behavior can be observed similarly for other kind of cells as face centered cells, not shown here, and can be interpreted as the consequence of a balance in Coulomb and nuclear forces relative weight between neighboring nuclei. For iron lattices in the symmetric $x=0.5$ case clusters are smaller than those found in perturbed oxygen systems and are stable since perturbations do not break the initial symmetries. From this result we can expect that at low densities matter could exist as a stable crystalline arrangement of iron nuclei without breaking up of symmetries as a consequence of the microscopic dynamics.

4. Conclusions
In this work we presented an overview of the microscopic DYWAN-NS model, which has been recently developed in order investigate the dynamics of matter as it should exist in the outermost layers of neutron stars. In this framework, the occurrence of self-organized structures in nuclear matter emerges as a natural consequence of the microscopic many-body dynamics. The structure of the stellar crust is self-consistently built up starting from a crystal of slightly deformed nuclei under periodic boundary conditions. The lattice is immersed in a degenerate electron gas insuring the neutrality of the system. The principal static properties of nuclear matter have been compared with other theoretical calculations. Despite the fact that a simplified effective force has been implemented, the considered macroscopic properties of nuclear matter are shown to be in close agreement with reference calculations. In the current version of the model the evolution of the system is ruled by the nuclear mean-field owing to the fact that in this work we focus the investigation on the crust at around zero temperature.

A variety of structural phases, the so-called “pasta phases”, are shown to be built self-consistently from the microscopic nuclear motion. The complex morphology of these structures has been analyzed using integral geometry techniques. Beyond spherical nuclei, rod-like structures, slabs, cylindrical bubbles, slabs with holes, connected slabs and sponges have been found. Transitions between these dynamical phases take place at constant energy.

The morphology of the dominant phases has been represented in structure diagrams on the plane defined by the threshold density $\rho_t$ and the overall mean density $\langle \rho \rangle$. A sensitivity to the
EOS has been evidenced in SCC cells with 0.2 proton fraction. The neutron diagram plots exhibit an increase of the regions corresponding to spherical and sponge-like structures at expense of slabs and cylinders with the stiffening of the effective interaction. In this case more neutrons are propelled toward the surface regions of initial clusters.

The response of the system to the effect of random perturbations on the initial lattice has been analyzed in order to investigate the possibility of the occurrence of disordered phases. The breaking of initial symmetries observed previously in oxygen SCC systems is not seen in FCC lattices, nevertheless a non-equilibrium steady cylindrical structure is formed in the particular case of oxygen isotopes with proton fraction 0.5 at $0.4\rho_\infty$.

Finally the sensitivity to the nuclear masses composition has been considered by studying the evolution of a randomly perturbed iron lattice in a SCC configuration. The corresponding proton fraction and mean density are, respectively, 0.5 and $0.1\rho_\infty$. In this case the system performs shape oscillations around the initial quasi-spherical state, which is consistent with the hypothesis of crystalline structures composed by iron nuclei at the low-density external layers.

In the present version of the model individual nucleons, either bound or unbound, evolve in a self-consistent mean-field holding in the overall box under periodic boundary conditions. The occurrence of heavy aggregates and uniform phases at low proton fraction is deeply related with the ability of the model to describe the spreading of wave functions widths, corresponding to unbound nucleons. This fact is a consequence of the time dependence of wavelet parameters.

Nevertheless, the formation and transitions between these non-equilibrium structures can be strongly modified using more sophisticated non-local effective forces and beyond a pure mean field description. These investigations are currently in progress.

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