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Finite size effects in neutron star and nuclear matter simulations

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Abstract

In this work we study molecular dynamics simulations of symmetric nuclear and neutron star matter using a semi-classical nucleon interaction model. Our aim is to gain insight on the nature of the so-called "finite size effects", unavoidable in this kind of simulations, and to understand what they actually affect. To do so, we explore different geometries for the periodic boundary conditions imposed on the simulation cell: cube, hexagonal prism and truncated octahedron. For nuclear matter simulations we show that, at sub-saturation densities and low temperatures, the solutions are non-homogeneous structures reminiscent of the "nuclear pasta" phases expected in neutron star matter simulations, but only one structure per cell and shaped by specific artificial aspects of the simulations—for the same physical conditions (i.e. number density and temperature) different cells yield different solutions. The particular shape of the solution at low enough temperature and a given density can be predicted analytically by surface minimization. We also show that even if this behavior is due to the imposition of periodic boundary conditions on finite systems, this does not mean that it vanishes for very large systems, and it is actually independent of the system size. We conclude that, for nuclear matter simulations, the cells' size sets the only characteristic length scale for the inhomogeneities, and the geometry of the periodic cell determines the shape of those inhomogeneities.

To model neutron star matter we add a screened Coulomb interaction between protons, and perform simulations in the three cell geometries. Our simulations indeed produce the well known nuclear pasta, with (in most cases) several structures per cell. However, we find that for systems not too large results are affected by finite size in different ways depending on the geometry of the cell. In particular, at the same certain physical conditions and system size, the hexagonal prism yields a single structure per cell while the cubic and truncated octahedron show consistent results, with more than one structure per cell. For systems of the size studied in this work these effects are still noticeable, but we find evidence to support

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that the dependence of the results on the cell geometry becomes smaller as the system size is increased. When the Coulomb interaction is present, the competition between opposing interactions of different range results in a proper, physically meaningful length scale that is independent of the system size and periodic cell of choice. Only under these conditions "finite size effects" will vanish for large enough systems (i.e. cells much larger than this characteristic length). Larger simulations are in order, but our computational capabilities forbid it for the time being.

Keywords: Nuclear astrophysics; Nuclear matter phase transition; Molecular dynamics simulations; Finite size effects

1. Introduction

In the inner crust of neutron stars, nucleons (protons and neutrons) exist at low temperatures and densities. They are also embedded in a (charge neutralizing) degenerate electron gas. Under those conditions, instead of forming the usual quasi-spherical nuclei found in Earth ("normal" nuclei), nucleons behave like a complex fluid called Neutron Star Matter (NSM). In NSM, nucleons attract each other through the short-ranged nuclear interaction while protons, in addition, repel each other through the Coulomb interaction screened by the electron gas. Studies of low density NSM have found that the attractive-repulsive interplay of nuclear and Coulomb forces may drive nucleons to take non-uniform configurations which are collectively known as "nuclear pasta" [1].

1.1. Non-homogeneous phases of neutron star matter

In the context of nuclear systems, the existence of nuclear pasta was early proposed in a pioneering work by Ravenhall et al. [1]. There the authors argued that the interplay between surface and Coulomb self-energies, which at low densities produce the almost spherical normal nuclei, is modified when those nuclei form a dense lattice:

> (...) ordinary nuclei are more or less spherical. While not disputing this fact, we observe that in the density range we have cited, where the fraction of space filled by dense matter, u, ranges from 0.1 to 1, the contribution to the Coulomb energy of the system coming from neighboring nuclei (the so-called Coulomb lattice energy) rivals in importance the nuclear Coulomb self-energy.

To analyze the effect of the long range Coulomb interaction at sub-saturation densities they used a static compressible liquid drop model in the Wigner–Seitz approximation. The Wigner–Seitz approximation was devised to simplify calculations in a charge neutral lattice of arbitrary shape. It consists in replacing the charge neutral unit cell with another cell of a simple geometry, adequate for the chosen lattice dimensionality: a sphere in $3D$, a cylinder in $2D$ or a slab in $1D$. Lattice Coulomb energy is included implicitly by making the electrostatic potential vanish at the cell's boundary.

The calculations from [1] were made at zero temperature with a proton fraction $x = 0.3$. Authors assumed nucleons to be arranged in dense matter regions at saturation density ρ_0 but filling only a fraction of space. With this model they found that for a rather wide range of densities, NSM arranged in these idealized lattice geometries is more stable than uniform matter or