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Simulations of cold nuclear matter at sub-saturation densities

P.A. Giménez Molinelli [a], J.I. Nichols [a], J.A. López [b], C.O. Dorso [a]

[a] *Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires and IFIBA, CONICET, Ciudad Universitaria, Buenos Aires 1428, Argentina*

[b] *Department of Physics, University of Texas at El Paso, El Paso, TX 79968, USA*

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Abstract

Ideal nuclear matter is expected to undergo a first order phase transition at the thermodynamic limit. At such phase transitions the size of density fluctuations (bubbles or droplets) scale with the size of the system. This means that simulations of nuclear matter at sub-saturation densities will inexorably suffer from what is vaguely referred to as "finite size effects". It is usually thought that these finite size effects can be diminished by imposing periodic boundary conditions and making the system large enough, but as we show in this work, that is actually not the case at sub-saturation densities. In this paper we analyze the equilibrium configurations of molecular dynamics simulations of a classical model for symmetric ideal (uncharged) nuclear matter at sub-saturation densities and low temperatures, where phase coexistence is expected at the thermodynamic limit. We show that the most stable configurations in this density range are almost completely determined by artificial aspects of the simulations (i.e. boundary conditions) and can be predicted analytically by surface minimization. This result is very general and is shown to hold true for several well known semi-classical models of nuclear interaction and even for a simple Lennard-Jones potential. Also, in the limit of very large systems, when "small size" effects can be neglected, those equilibrium configurations seem to be restricted to a few structures reminiscent to the "Pasta Phases" expected in Neutron Star matter, but arising from a completely different origin: In Neutron Star matter, the non-homogeneous structures arise from a competition between nuclear and Coulomb interactions while for ideal nuclear matter they emerge from finite (yet not "small") size effects. The role of periodic boundary conditions and finite size effects in Neutron Star matter simulations are reexamined.

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

E-mail address: pagm@df.uba.ar (P.A. Giménez Molinelli).

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1. Introduction

"Nuclear Matter" (NM), an ideal system composed of an infinite number of nucleons which interact through the nuclear potential but not Coulomb, has proved to be an useful theoretical abstraction to study and to characterize the nuclear interaction itself. At sub-saturation densities, NM presents a "liquid–vapor"-like phase transition which has been related to the multifragmentation phenomenon in heavy ion collisions [1].

On the other hand, in the inner crust of Neutron Stars nucleons are expected to exist embedded in a degenerate electron gas and at sub-saturation densities. This prompted the definition of "Neutron Star" Matter (NSM) as a charge-neutral system of nucleons and electrons (which exactly balance the charge of the protons). The study of NSM at sub-saturation densities is important for a variety of topics which include several phenomena related to heavy ion reactions, the symmetry energy term in the nuclear EOS, the structure of neutron star crusts, etc. Pioneering studies on NSM based on the compressible liquid drop model [2,3], Hartree–Fock method [4], and energy minimization techniques [5,6] showed that transitions from spherical nuclei to "nuclei" shaped as rods and slabs, which are collectively named "Pasta Phases", are to be expected in cold NSM at sub-saturation densities. For NM, however, at those same densities, coexistence between a liquid-like and a vapor-like phase is expected to exist. More recent investigations [5–17] have used dynamical methods to study such transitions in NSM. In the previous studies listed, the Coulomb interaction has been approximated either by using a Wigner–Seitz cell [5], assuming uniform electric charge densities [6], Thomas–Fermi screened Coulomb potential (see, e.g. [11]) or by an Ewald summation [19]. Dynamical simulations of NSM under periodic boundary conditions at low temperatures ($T \lesssim 1$ MeV) indeed show that nucleons self-assemble into pasta-like objects: mainly "gnocchi", "spaghetti", "lasagna" and their bubble counterparts. The issue of "finite size" effects affecting the results of NSM simulations arises occasionally, in particular when a given model yields only one structure per simulation cell (see for example [20]), but it is systematically accepted that they would disappear if the system is made large enough.

In NSM, Coulomb interaction is an essential ingredient for the formation of the pasta-like structures. Williams and Koonin [6], for instance, explained the transitions between different "nuclei" topologies in terms of a competition between a short-range nuclear surface energy, which becomes minimized through aggregation, and a long-range Coulomb energy which gets reduced by an opposite dispersion. More recent studies of Horowitz and coworkers [18] re-examine this assertion as an example of frustration, a phenomenon that emerges from the impossibility to simultaneously minimize all interactions.

However, unbeknownst to many, similar structures have been found to be stable solutions in simulations of Lennard-Jones fluids without any Coulomb interaction [39]. For the Lennard-Jones fluid, those structures occur in the density region that corresponds to phase coexistence at the thermodynamic limit, and since only one gnocchi, spaghetti or lasagna per simulation cell exists the author argues that "finite size" effects are responsible for their formation. Given the similarities between the Lennard-Jones potential and the Nuclear Interaction (short-ranged and attractive), the same situation is expected in NM simulations.

Recapitulating, when Coulomb interaction is included in a simulation, inhomogeneous solutions are explained as resulting from a competition between the short-ranged attractive nuclear part of the interaction and the long-ranged Coulomb potential. But when only short-ranged attractive interactions are present (or when a model yields only one structure per cell), the existence of equilibrium non-homogeneous structures is attributed to non-specific "finite size" (or interfacial)