



# Symmetry energy in the liquid–gas mixture

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## Abstract

Results from classical molecular dynamics simulations of infinite nuclear systems with varying density, temperature and isospin content are used to calculate the symmetry energy at low densities. The results show an excellent agreement with the experimental data and corroborate the claim that the formation of clusters has a strong influence on the symmetry energy in the liquid–gas coexistence region.

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## 1. Introduction

The symmetry energy,  $E_{Sym}(T, \rho)$ , is a component of the nuclear equation of state (EOS) which relates the variation of the energy per nucleon to the proton to neutron ratio. Its importance in phenomena ranging from nuclear structure to astrophysical processes has made it subject of intense investigations in recent times; see, e.g., the review of Li et al. [1] and the 2014 volume of the European Physical Journal A [2].

On the theory front,  $E_{Sym}$  has been studied mostly using mean-field approaches [1] which treat nuclear matter as a uniform fluid. At subcritical densities, however, heavy ion reactions have shown that the properties of nuclear matter are affected by the formation of clusters and, as discussed recently by Hagel et al. [3], the symmetry energy should be equally modified.

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As current EOS calculations do not produce clusterization on their own, some models have attempted to correct this deficiency by including a limited number cluster species through a number of simplifying assumptions [4–6], while others have used thermal models [7], or clever interpolations between approaches with embedded cluster correlations and mean field theories [3]. Although less elegant, numerical methods exist which yield to cluster formation without any extra additions nor adjustable parameters, and for ranges of temperature, density and isospin contents of interest.

In this work we use one such method, classical molecular dynamics (CMD), to study  $E_{Sym}$  in the low density regions, namely in the liquid–gas mixture zone. Section 2 outlines the CMD calculations used, Section 3 describes the numerical methodology used to extract  $E_{Sym}$  from the numerical data, followed in Section 4 by a comparison to other calculations, and by a summary of results in Section 5.

## 2. Classical molecular dynamics

For the sake of brevity, readers interested in learning about the virtues of CMD and its comparison to other methods are directed to a previous study [8]. Here we simply reiterate that CMD has been used since 2001 [9–16] to study reactions, critical phenomena, neutron-rich nuclei (isoscaling and neutron star crusts) and, of course, phase changes and clusterization, all without any adjustable parameters. Although lacking Pauli blocking and wave dynamics, Ref. [8] proved through two independent studies that CMD can operate safely on warm ( $T \gtrsim 1$  MeV) systems with subcritical densities. Specifically, one calculation shows the increase of the population of the energy level density at excitation energies corresponding to  $T > 1$  MeV, which renders the use of the Pauli principle unnecessary. The second one demonstrates the widening of the particle–particle distance in the liquid–gas coexistence region compared to the de Broglie wavelength, which renders the use of wave dynamics unnecessary.

The present study will use the results of CMD simulations to extract  $E_{Sym}$ . As reported elsewhere [8], the calculations used the Pandharipande potentials [17] which, among other virtues, produce cold nuclear matter with a saturation density of  $\rho_0 = 0.16 \text{ fm}^{-3}$ , a binding energy  $E(\rho_0) = -16 \text{ MeV/nucleon}$  and a compressibility of about 250 MeV.

The evolution of “infinite” systems composed of  $A = 2000$  nucleons in a cubic cell under periodic boundary conditions were studied. Simulations were carried out with isospin contents of  $x = Z/A = 0.35, 0.4$  and  $0.5$ , densities varying between  $0.01 \text{ fm}^{-3}$  and  $0.2 \text{ fm}^{-3}$ , and temperatures between  $T = 1$  and  $5$  MeV. The code used [18] had a “heat reservoir” to speed the calculations and used the Nosé–Hoover equations of motion integrated by Størmer finite differences.

For each combination of  $T$ ,  $\rho$  and  $x$  the systems were allowed to thermalize and to produce a canonical ensemble of states through a Markov chain. The average energy per nucleon, i.e. the internal energy, of each state was recorded; for robustness, each set of conditions was averaged over 200 independent configurations with a very small standard deviations (for instance, the average of all standard deviations of the 9000 runs at all densities and temperatures for the case of  $x = 0.35$  was of only 0.067 MeV). Fig. 1 shows the behavior of the energy as a function of the density at  $T = 1$  MeV and  $x = 0.35, 0.4$  and  $0.5$ . The liquid phase of the system is easily identifiable by its “U” shape, as well as the liquid saturation density by the minima of the energy curves. Furthermore, the liquid–gas coexistence region can be identified as the lower density region where the CMD data separates from the “U” curve; this is clearly noticeable for  $x = 0.4$

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