Trugilho, L. F.; Rizzi, L. G.

Microcanonical characterization of first-order phase transitions in a generalized model for aggregation. (English) \(Zbl 07491669\)


Summary: Aggregation transitions in disordered mesoscopic systems play an important role in several areas of knowledge, from materials science to biology. The lack of a thermodynamic limit in systems that are intrinsically finite makes the microcanonical thermostatistics analysis, which is based on the microcanonical entropy, a suitable alternative to study the aggregation phenomena. Although microcanonical entropies have been used in the characterization of first-order phase transitions in many non-additive systems, most of the studies are only done numerically with aid of advanced Monte Carlo simulations. Here we consider a semi-analytical approach to characterize aggregation transitions that occur in a generalized model related to the model introduced by Thirring. By considering an effective interaction energy between the particles in the aggregate, our approach allowed us to obtain scaling relations not only for the microcanonical entropies and temperatures, but also for the sizes of the aggregates and free-energy profiles. In addition, we test the approach commonly used in simulations which is based on the conformational microcanonical entropy determined from a density of states that is a function of the potential energy only. Besides the evaluation of temperature versus concentration phase diagrams, we explore this generalized model to illustrate how one can use the microcanonical thermostatistics as an analysis method to determine experimentally relevant quantities such as latent heats and free-energy barriers of aggregation transitions.

MSC:

82Bxx Equilibrium statistical mechanics
82-XX Statistical mechanics, structure of matter
82Cxx Time-dependent statistical mechanics (dynamic and nonequilibrium)

Keywords:

microcanonical thermostatistics; aggregation model; first-order phase transitions; free-energy barriers; latent heat

Full Text: DOI

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