Free-Energy Barriers: From Particle Condensation to Polymer Aggregation

Wolfhard Janke*[1], Johannes Zierenberg[1], and Philipp Schierz[1]

[1]Universität Leipzig, Institut für Theoretische Physik (ITP) – Postfach 100920, 04009 Leipzig, Germany

Abstract

We present a new methodology to study temperature-driven droplet formation for both particle and polymer systems [1]. In particular, this allows a shape-free determination of the free-energy barrier. Combined with rigorous results on equilibrium droplet formation of particles, this enables a well-defined finite-size scaling analysis of the free-energy barrier at fixed density. We verify our theoretical predictions using parallel multicanonical Monte Carlo simulations [2] of a Lennard-Jones particle gas and generalize this approach to aggregation in a dilute bead-spring polymer solution. Our results suggest an analogy between polymer aggregation and particle condensation, when the macromolecules are interpreted as extended particles. We will briefly comment on the role of kinetic energy on the free-energy barrier, which is commonly neglected in Monte Carlo simulation studies [3].

J. Zierenberg, P. Schierz, and W. Janke, Canonical Free-Energy Barrier of Particle and Polymer Cluster Formation, Leipzig preprint (March 2016), arXiv:1607.08355 [cond-mat.stat-mech].

J. Zierenberg, M. Marenz, and W. Janke, Scaling Properties of a Parallel Implementation of the Multicanonical Algorithm,
Comput. Phys. Commun. 184 (2013) 1155.

P. Schierz, J. Zierenberg, and W. Janke, First-Order Phase Transitions in the Real Microcanonical Ensemble (Editors'
Suggestion), Phys. Rev. E 94 (2016) 021301(R).

*Speaker