Tata Institute of Fundamental Research
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Internal Seminar

Entropy-driven phase transition in lattice gas models in three dimensions

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There are a class of phase transitions, primarily driven by entropy, unlike temperature like in normal transitions. These transitions are manifested in different experimental systems like freezing in hard-spheres of PMMA colloids, nematic transitions in liquid crystals, etc. The minimal models for studying these transitions are volume exclusion models. In such systems, all allowed configurations have equal energy, and therefore any phase transitions are driven purely by gain in entropy. The corresponding models studied on lattices are called hard-core lattice gas (HCLG) models. These models serve as nice abstraction for actual experimental systems and understanding their phase diagram on lattice is helpful in general understanding of entropy-driven phase transitions. Various shapes have been studied on many two-dimensional lattices using approximate theories and numerical simulations. In three-dimensions, it is more complicated to study them because of the lack of efficient algorithms to simulate such systems at high densities or large exclusion volumes. Here we study two problems on a cubic lattice: (1) hard rods of length k and (2) hard cubes of size $2 \times 2 \times 2$. We obtain the detailed phase diagram and characterize the nature of the phase transitions for both these models.

Wednesday, Sep 25th 2019

11:30 AM (Tea/Coffee at 11:00 AM)

Seminar Hall, TIFR-H