## Research Interest

Nucleation in simple models

Nucleation is ubiquitous in nature and the presence of impurities is observed in almost every real and experimental systems showing nucleation. In Ref [1], we have studied the impact of static/dynamic impurities on nucleation properties, e.g., free energy barrier, nucleation rate, etc., on two dimensional Ising lattice-gas. We have shown that both free energy barrier height and critical cluster size decreases monotonically with increasing static impurity density when impurities react neutrally with both solute (+1 spin) and solvent (-1 spin) particles. Dynamic impurities preferentially occupy the boundary positions of the growing cluster when the temperature is low. This reduces the surface tension and therefore the free energy barrier height.

The natural question that comes in mind is, what would happen if we vary the impurity-solute and impurity-solvent interaction energy. Is it possible to determine, numerically, the regime for which the impurities prefer to sit at the boundaries of the cluster? Are there any other interesting phases? We address such questions and study the nucleation properties at different regimes of the behaviour map in the ongoing work.

Most of the simulation methods used to study crystallisation consider the system as closed, in which total number of particles is conserved, which is in contrary with most of the experimental and natural process of nucleation. The variation of free energy barrier in the presence of such absolute confinement would be interesting to study. In Ref [2], the authors have mathematically calculated the confinement free energy assuming the presence of single big cluster in the system. It would be interesting to verify the proposed free energy expression against numerical simulations.

Spin flip dynamics or random transformation of solute into solvent and vice versa may not be appropriate dynamics to model the nucleation phenomena. In spin flip dynamics, we assume instantaneous transport of particles ignoring the diffusive properties of the solution. More realistic nucleation model might be obtained if we replace the spin flip dynamics by Kawasaki dynamics in which particles move to the nearest neighbouring sites. Building a framework for studying the nucleation properties of open system with pure Kawasaki/ particle exchange dynamics is still lacking.

Polymorphism is the existence of a solid material in more than one crystalline structure. Finding out the existence of polymorphism for simple lattice models is a potential area of future research. If the lattice-polymorphism exists, analysing the stability of polymorphs is also necessary. In a recent work [3], we studied the kinetic control of competing nucleation in dimer lattice-gas model of two types of particles, showing that the nucleation rate of the stable cluster can be decreased by tuning the mobility of the particles. Role of particle mobility in the context of polymorphism needs better understanding.

Phase transition in hard core lattice gas models

Entropy driven phase transition is an example of athermal phase transition which only depends on the shape and the symmetries of the constituent particles. Examples include freezing transition in the system of hard spherical particles, nematic transition in the system of hard rods, etc. These are also realized in experimental systems, e.g., disordered to nematic transition in tobacco mosaic virus, ordering transitions in the adsorbed layer of gas on metallic surface, etc. Hard core lattice gas models are the minimal models to study such entropy driven phase transitions.

During my PhD, I studied the phase transitions in the system of hard particles with various geometrical shapes, e.g., hard $2 \times 2$ square on square lattice [4], mixture of hard $2 \times 2$ squares and dimers on square lattice [5], hard Y-shaped particles on triangular lattice [6], hard rectangular plates on cubic lattice [7] and hard cubes on cubic lattice [8]. Various high-density phases, e.g., sublattice, columnar, layered, etc. are observed. Both analytical techniques and large-scale Monte Carlo simulations are used to study the phase transitions and critical properties of such systems. The conventional algorithms, using local update of particles, often suffer from slowing down at high densities, near full packing. Developing new algorithms, like cluster update Wang-Landau algorithm [9], which could overcome this problem is both challenging and interesting.

Active random walk

System of self-propelled particles exhibit non-equilibrium phases which are observed in real world as in flock of birds, sheep, school of fish, etc. Self-propelled particle can be modelled as active Brownian motion which propels at a fixed speed and rotates its direction gradually with rotational diffusion. We study, in Ref [10], exact probability distribution and first passage properties of single active run and tumble particle on square lattice using different analytical techniques. Validation of the obtained results are done using kinetic Monte Carlo simulations. We are interested in studying the motility induced phase separation, if exists, in the system of multiple active particles obeying hard-core constrain.

References

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