# Two Phase Transitions in system of hard rods on two dimensional lattices

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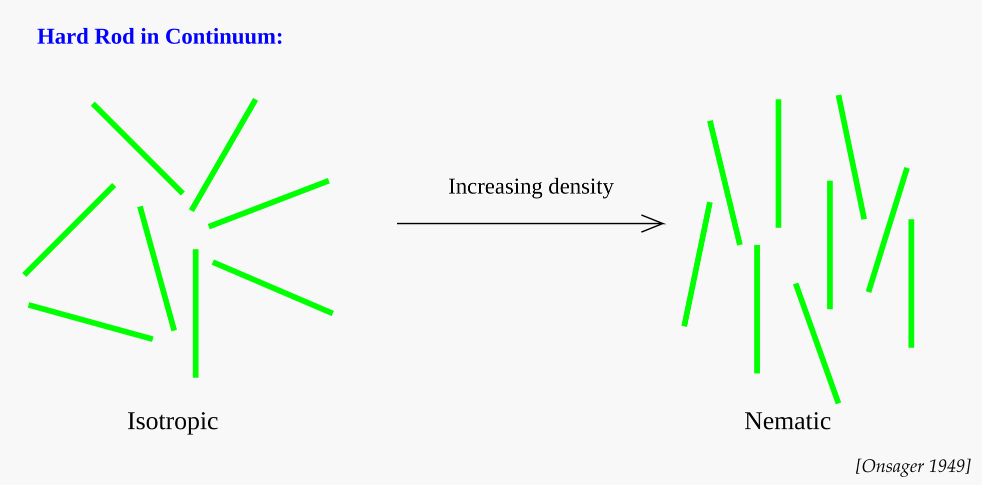
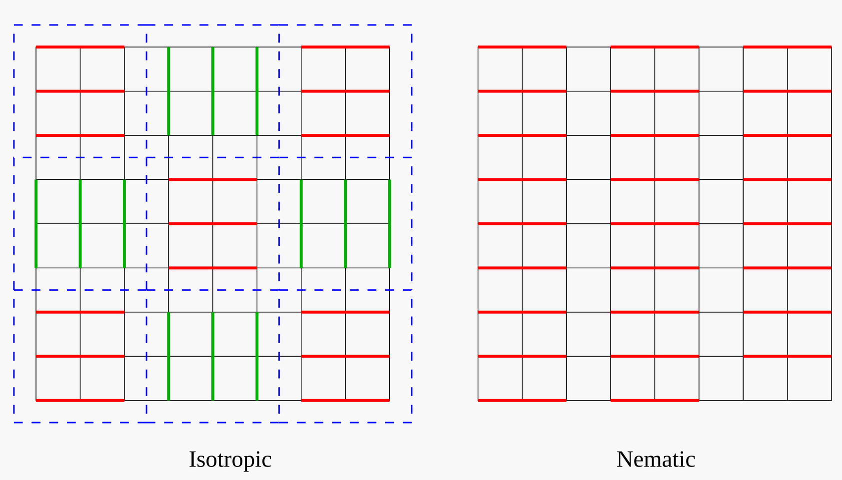
## INTRODUCTION AND THE MODEL

- Hard Rods in continuum undergo isotropic-nematic transition with increasing density.

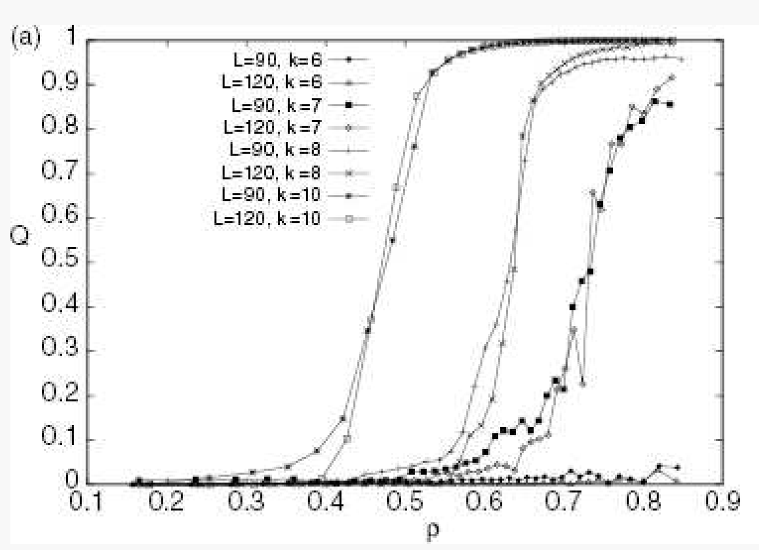



What happens on lattices?

- Square lattice of dimensions $L \times L$.
- $k$-mers: Rods occupying $k$ consecutive lattice sites either in horizontal or vertical direction having excluded volume interaction.
- $\rho \to 0$ : Isotropic,
  $\rho \to 1$ : Isotropic.




- Entropy per site: $S_{dis}(\rho = 1) \geq \log 2/k^2$ and $S_{nem}(\rho = 1) = 0$



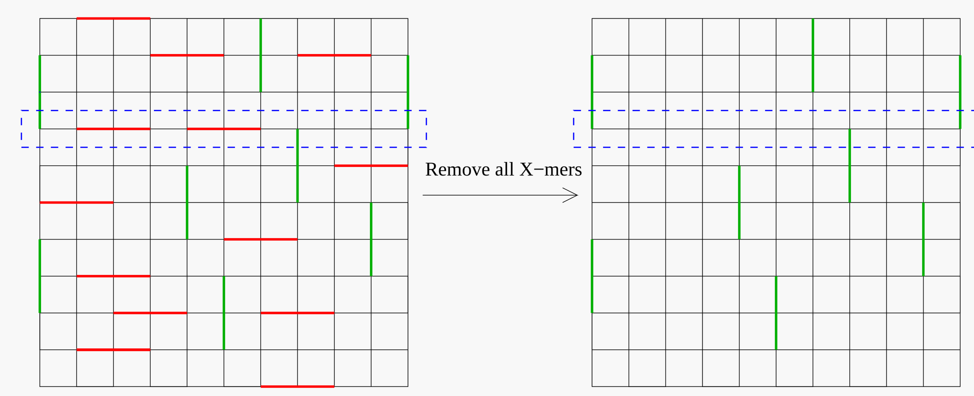

- Existence of an intermediate nematic phase for $k \geq 7 \implies$ two phase transitions [Ghosh and Dhar 2007].
- Isotropic-nematic transition : 2D Ising (square lattice), 2D $q = 3$ Potts (triangular lattice).
- Is there an efficient algorithm to study the high density?

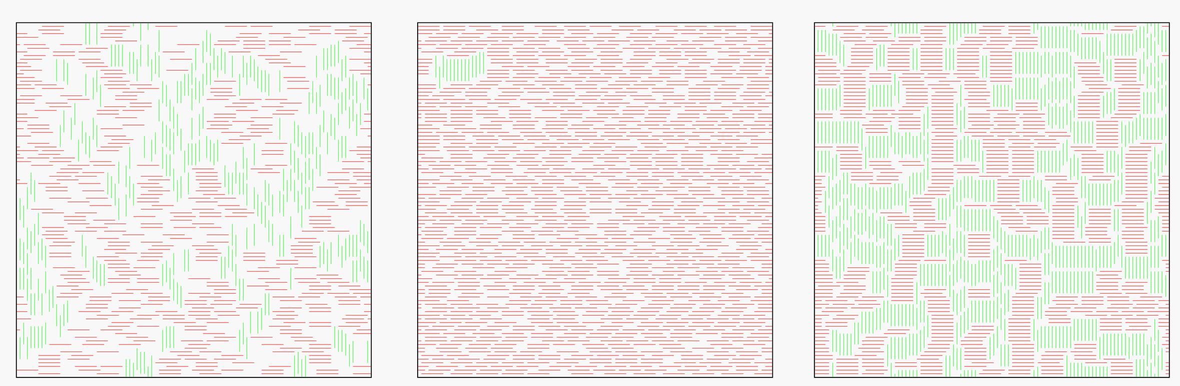
- What is the nature of the second transition from nematic to isotropic phase at high density?
- Is the high density disordered (HDD) phase, a reentrant low-density disordered phase or a qualitatively distinct phase?

## THE MONTE CARLO ALGORITHM

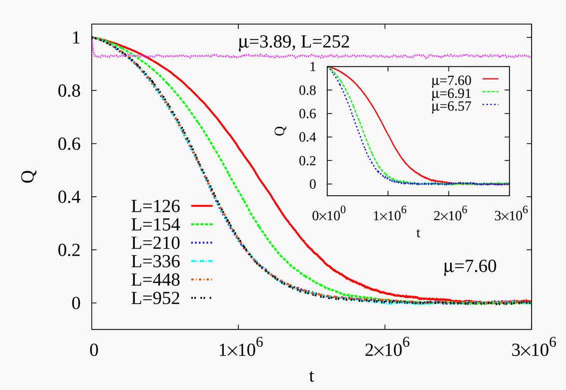
The Monte Carlo algorithm is as follows:

- Remove all the $X$-mers, reoccupy all the rows with $X$-mers, keeping $Y$-mers unmoved.
- Repeat the same procedure for $Y$-mers along the columns.



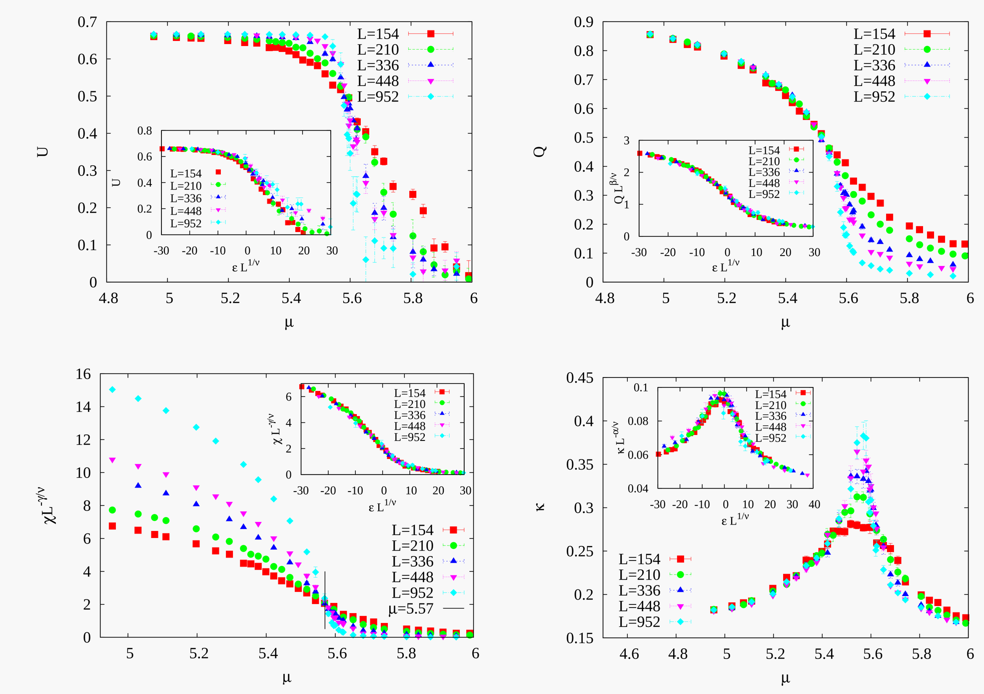
Low density — Intermediate density — High density




Order parameter vs time: System equilibrates at high density

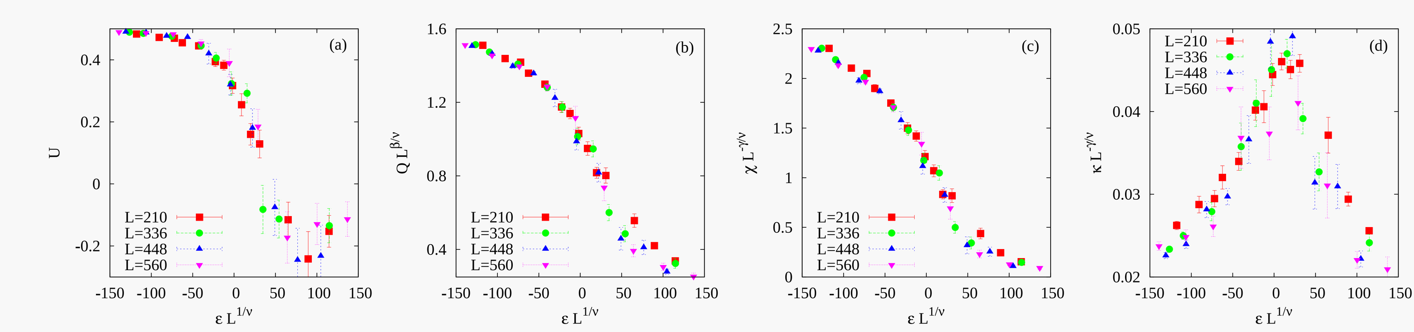
## SIMULATION RESULTS

- Quantities of interest:
  $\rho = k(n_v + n_h)/L^2$, $m = k(n_v - n_h)/L^2$, $Q = \frac{\langle |m| \rangle}{\langle \rho \rangle}$, $\chi = \frac{L^2 \langle m^2 \rangle}{\langle \rho \rangle^2}$, $\kappa = L^2 \left[ \langle \rho^2 \rangle - \langle \rho \rangle^2 \right]$, and $U = 1 - \frac{\langle m^4 \rangle}{3 \langle m^2 \rangle^2}$.
- The second transition is demonstrated on both square and triangular lattice for $k = 7$.
- Transition is continuous.
- Critical exponents for square lattice : $\nu = 0.90 \pm 0.05$, $\alpha/\nu = 0.22 \pm 0.07$, $\beta/\nu = 0.22 \pm 0.07$, $\gamma/\nu = 1.56 \pm 0.07$.



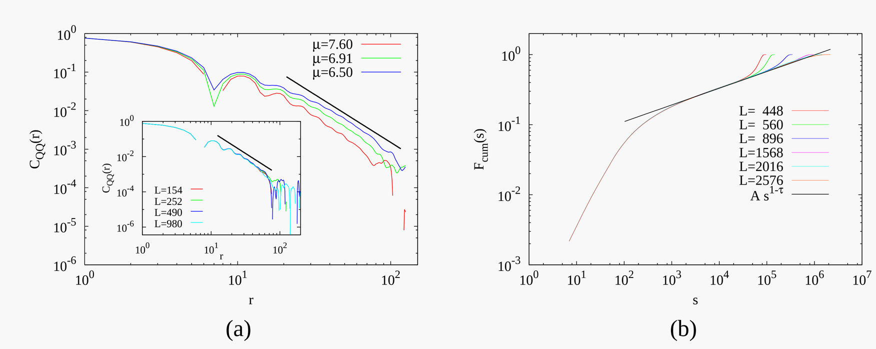
Data collapse of Binder cumulant, Order parameter, its second moment, and compressibility for different system sizes of the square lattice

- Critical exponents for triangular lattice are same as those of $q = 3$ Potts model in two dimensions.



Data collapse of Binder cumulant, Order parameter, its second moment, and compressibility for different system sizes of the triangular lattice.

- Existence of a crossover length scale $\geq 1400$, beyond which nature of correlations changes.
- Correlations decay as a power law, up to the given length scale.



(a) Deacy of the Order parameter correlation with distance for square lattice, (b) Cumulative probability distribution of clusters for square lattice

## DISCUSSION

- An efficient Monte Carlo algorithm for studying the problem of hard, rigid rods on lattices is demonstrated.
- Numerical evidence for the existence of the second phase transition from nematic to disordered phase is presented.
- Nature of the second transition and the critical exponents are determined for both square and triangular lattices.
- Evidence of a crossover over length scale $\geq 1400$ is found.
- It is expected that the nature of the transition will be independent of the rod length $k$.

[a]

[a]Ref: http://arxiv.org/abs/1211.2536