INSTITUTO DE FÍSICA
Universidade Federal Fluminense

Isotropic-nematic phase transition for rigid rods on lattices

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Outline

- Introduction, simulational results for model on a lattice.

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- Solution of the model on a four-coordinated Bethe lattice

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- Final discussion and comments

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Situation less clear for rigid k-mers on lattices. Only analytically soluble case: dimers ($k=2$): orientational correlations decay exponentially for $\rho<1$ and with power law for $\rho=1$ (Heilmann and Lieb (1972)).

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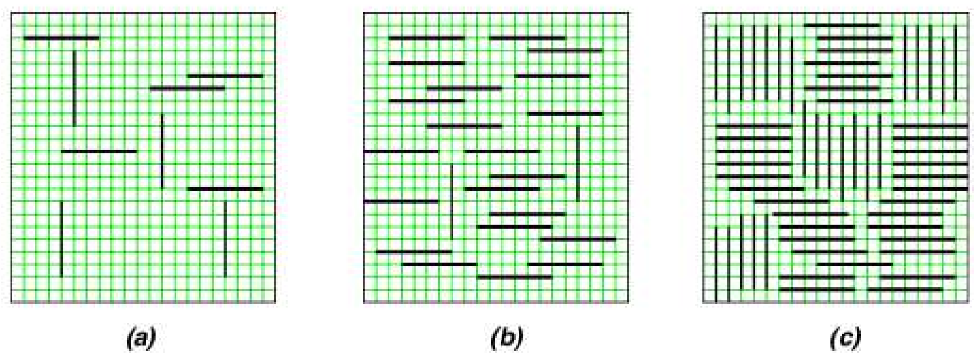

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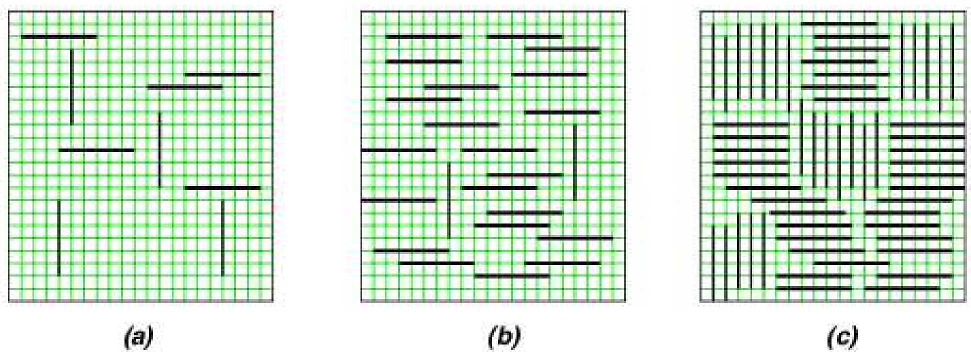

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Difficulties with simulations at high densities. Second transition is studied comparing approximate entropies of the states.

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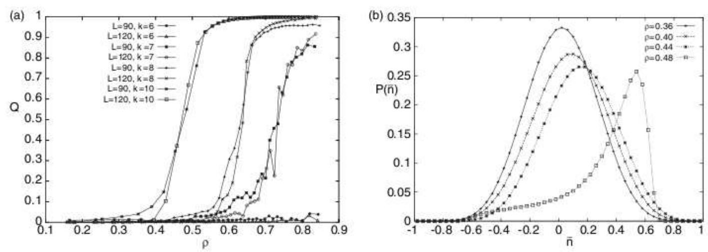

Fig. 3: (a) The order parameter Q as a function of densities ρ is shown for different k and L. (b) Distribution of normalized $n_v - n_h$, $\bar{n}$, for $k = 10$, $L = 120$ is shown for different values of densities.

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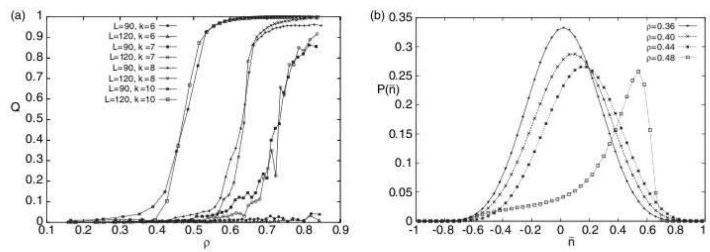

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Second transition is studied comparing approximate entropies of the states close to full lattice ($\rho = 1 - \epsilon$):

A. Ghosh and D. Dhar

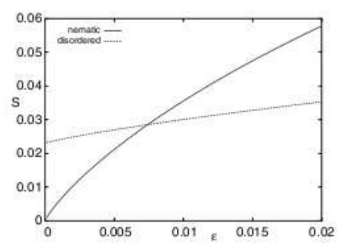

Fig. 4: Entropy per site for nematic and disordered states as a function of ϵ for $k = 8$.

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Cayley tree with coordination $q = 4$. Directions 1 (horizontal) and 2 (vertical).

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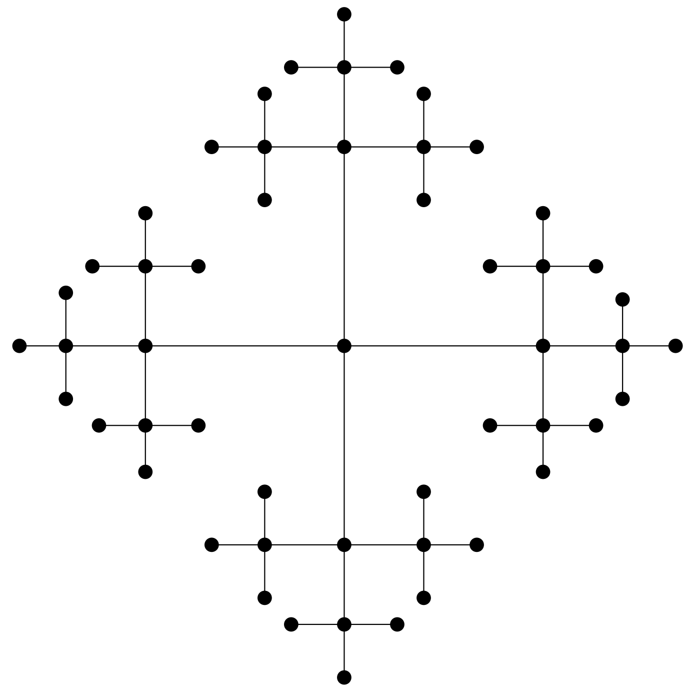

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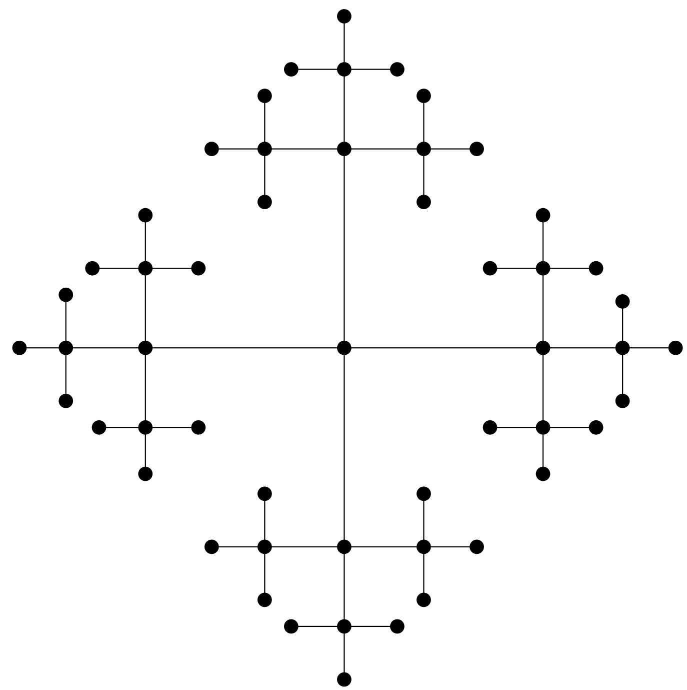

Grand-canonical formalism: activity of monomer in rod in direction i: z_i.

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Partial partition functions (ppf) for rooted sub-trees: $g_{i,j}$, with $i = 1, 2$ and $j = 1, 2, \ldots, k-1$:

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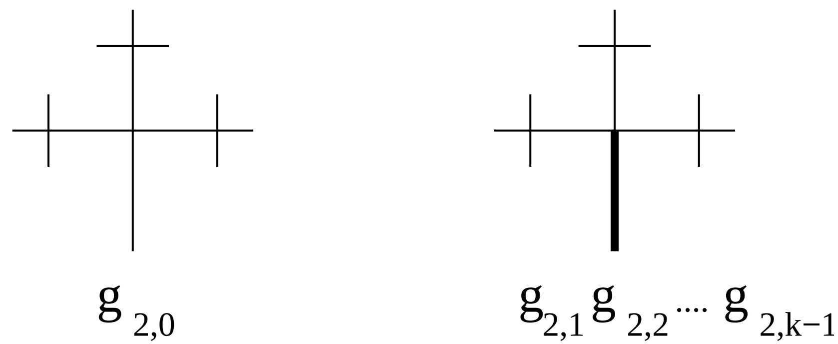

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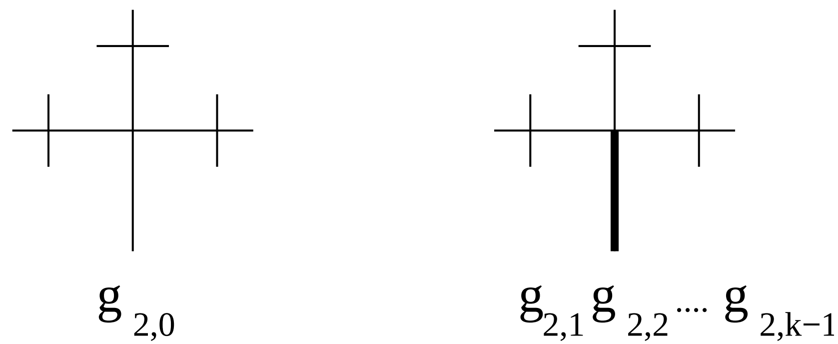

Recursion relations for ppf: build a subtree with $m + 1$ generations connecting 3 subtrees with m generations to new root bond and site.

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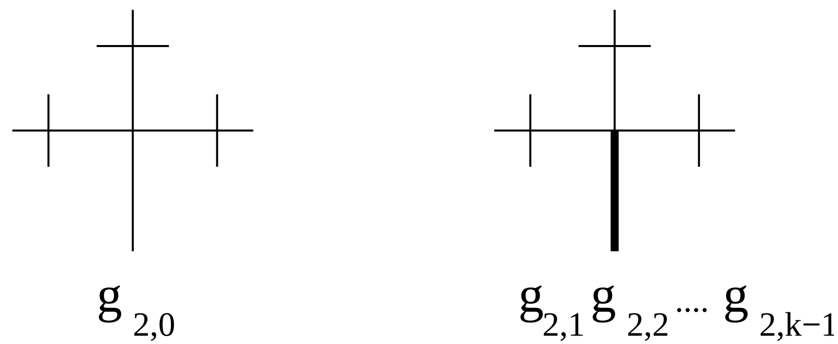

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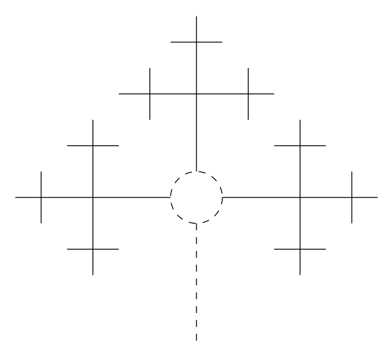

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Recursion relations:

$$g'_{1,0} = (g_{1,0} + z_1 g_{1,k-1}) g_{2,0}^2 + z_2 g_{1,0} \sum_{j=0}^{k-1} g_{2,j} g_{2,k-j-1},$$

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Ratios of ppf:

$$R_{i,j} = \frac{g_{i,j}}{g_{i,0}},$$

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In general, recursion relations converge to a simple fixed point upon iteration (thermodynamic limit). At fixed point $R_{i,j} = \alpha_i^j$, where:

$$\alpha_1[1 + z_1\alpha_1^{k-1} + kz_2\alpha_2^{k-1}] = z_1,$$

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Attaching 4 subtrees to the central site of the tree, we obtain the partition function of the model on the Cayley tree:

$$\Xi = g_{1,0}^2 g_{2,0}^2 + 2z_1 g_{1,k-1} g_{1,0} g_{2,0}^2 + 2z_2 g_{2,k-1} g_{2,0} g_{1,0}^2$$

$$z_1 g_{2,0}^2 \sum_{j=1}^{k-2} g_{1,j} g_{1,k-j-1} + z_2 g_{1,0}^2 \sum_{j=1}^{k-2} g_{2,j} g_{2,k-j-1}.$$

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We may then obtain the densities of monomers in horizontal and vertical rods at the central site at the fixed point:

$$\rho_1 = \frac{kz_1\alpha_1^{k-1}}{1 + kz_1\alpha_1^{k-1} + kz_2\alpha_2^{k-1}},$$

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The bulk free energy is obtained using an ansatz proposed by Gujrati (1995). The result is:

$$\phi_b = \ln(1 + kz_1\alpha_1^{k-1} + kz_2\alpha_2^{k-1}) - \ln(1 + z_1\alpha_1^{k-1} + kz_2\alpha_2^{k-1}) -$$

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$$(k+1)\alpha^{k+1} - \frac{1}{\alpha} + \frac{1}{z} = 0.$$

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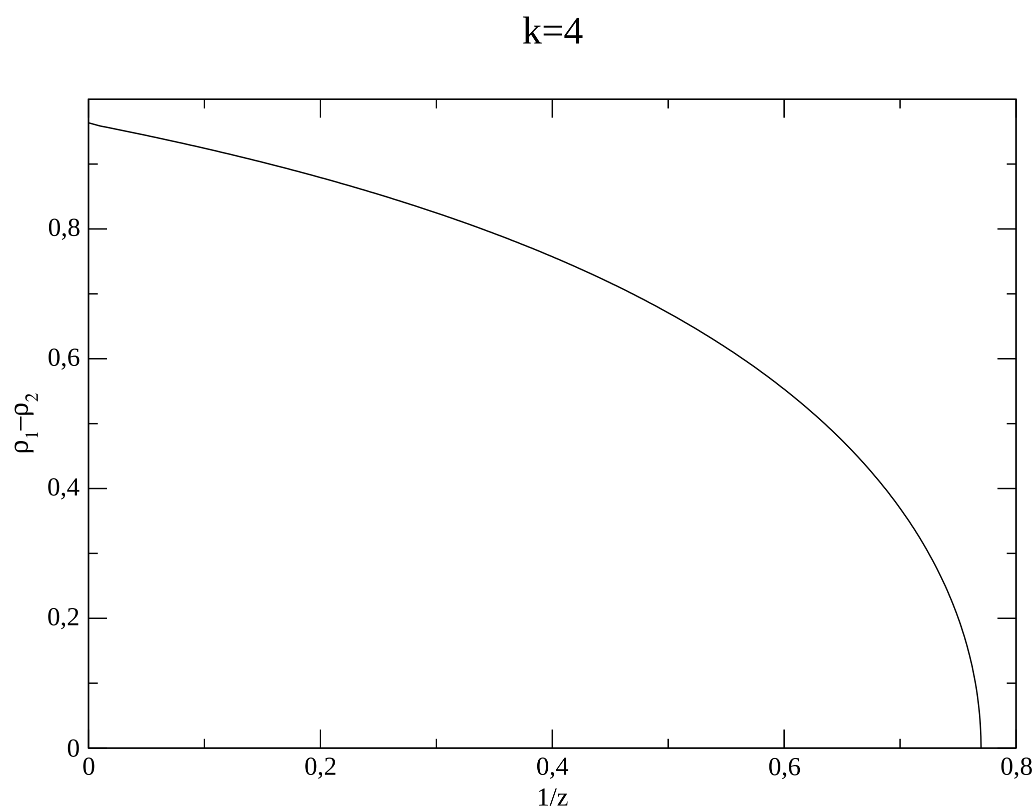
Nematic order parameter as a function of the activity for tetramers:



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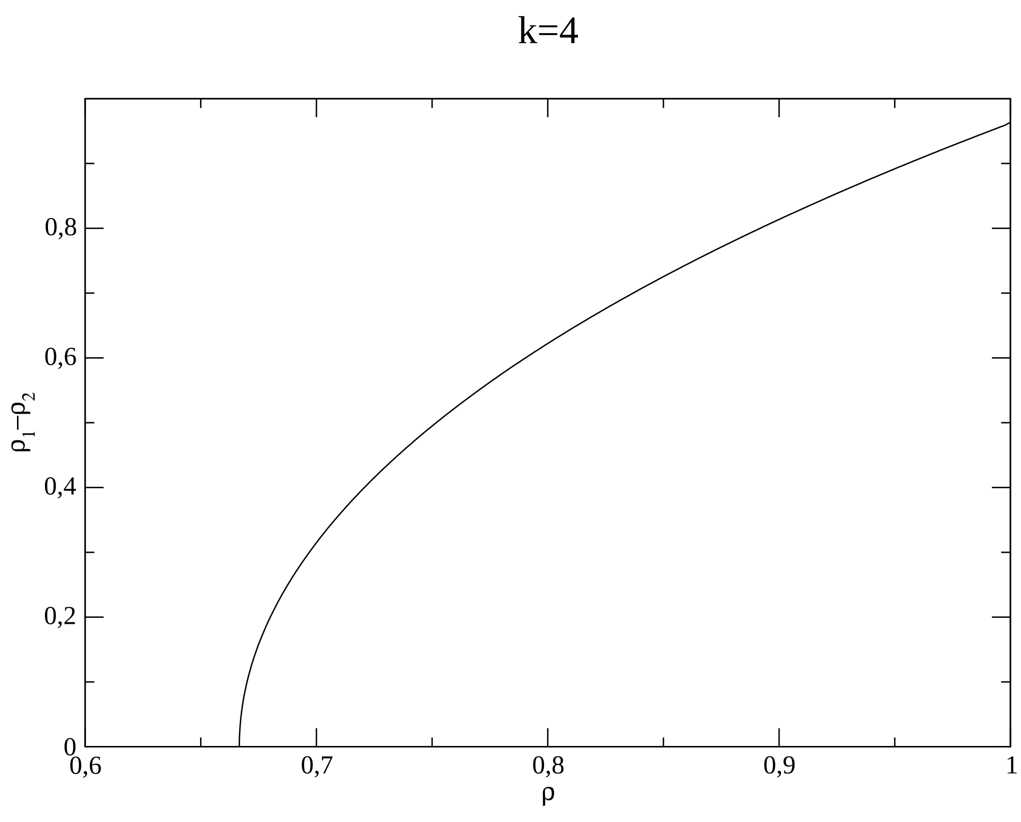
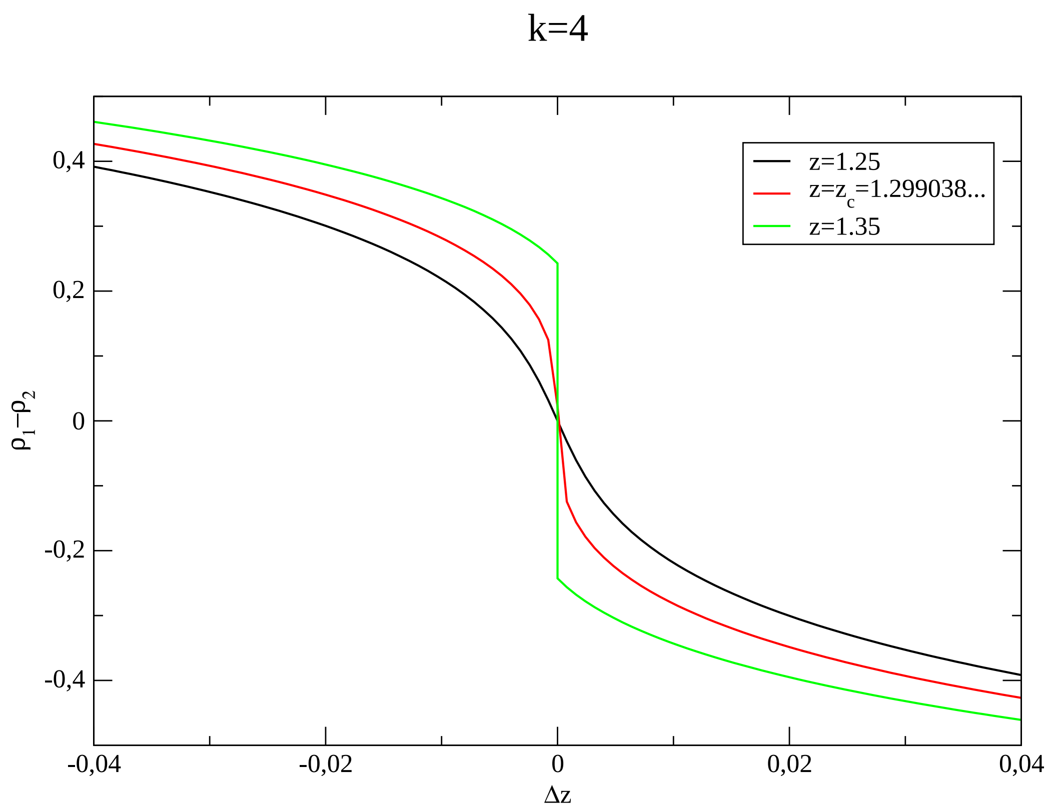
Nematic order parameter as a function of the monomer density $\rho = \rho_1 + \rho_2$ for tetramers:



Solution on BL

Nematic order parameter as a function of $\Delta z = z_1 - z_2$ for fixed values of $z = (z_1 + z_2)/2$:



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- Second transition not found. May be present on a Husimi lattice solution.
- Lowest value of k for which there is a transition still an open question.
- At $z \to \infty$ ($\rho \to 1$) eigenvalue of the Jacobian associated to fixed point becomes equal to 1. Limiting cycle (period 2) is stable.