Columnar Order in the Hard Square Lattice Gas

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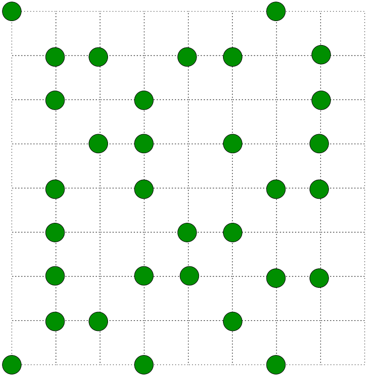
Introduction

- Real gases display a **complex and rich phase diagram**
- To model the **behaviour of a large collection of molecules** represents a theoretical challenge
- Real gases display **significant deviations from ideal behaviour** at high densities
- Lattice gas models, in which **particles are constrained to be on the sites of a lattice**, serve as the simplest models of complex physical systems.

Lattice Gases

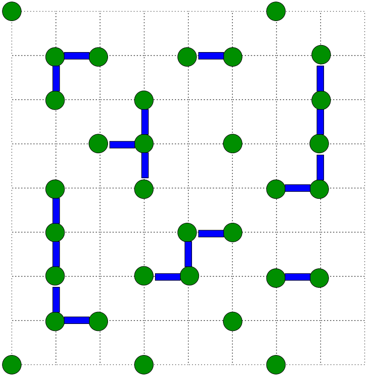


- On-site exclusion lattice gas: Two particles **cannot be at the same lattice site**.
- Each particle has a fugacity $z = \exp(\mu)$ associated with it.
- The partition function of this model **can be evaluated explicitly**.

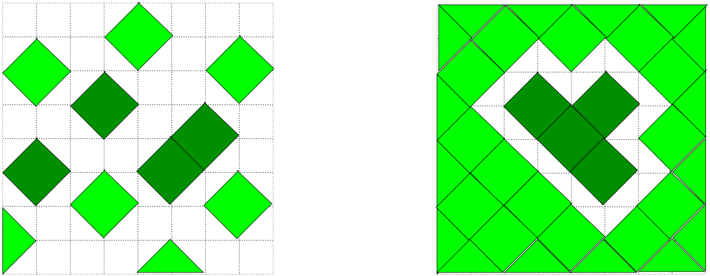
We have:

$$\Omega = 1 + \binom{N}{1} z + \binom{N}{2} z^2 + \ldots = (1+z)^N \quad (1)$$

Lattice Gases



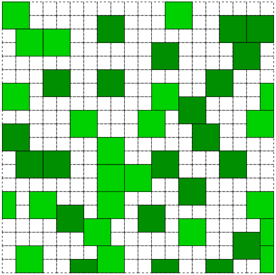
- Turn on an **interaction energy** between nearest neighbour particles.
- This is known as the Lee-Yang lattice gas.
- This model reduces to the **Ising model in a finite magnetic field**.

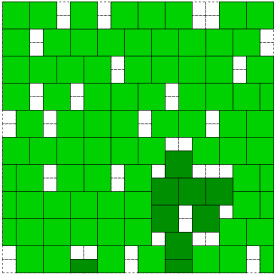


- A good first approximation is when the interaction is **purely of the exclusion type**
- The system is disordered at low density and **sublattice ordered** at high density.
- The stability of the ordered phase **can be proved using Peierls arguments**.

The Hard Square Lattice Gas

- We study the lattice gas of particles where each particle is a 2×2 **square that occupies** 4 **elementary plaquettes** of the square lattice.





The system is disordered at low density and **columnar ordered** at high density.

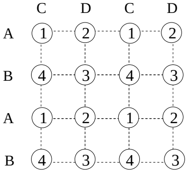
Activity Expansions

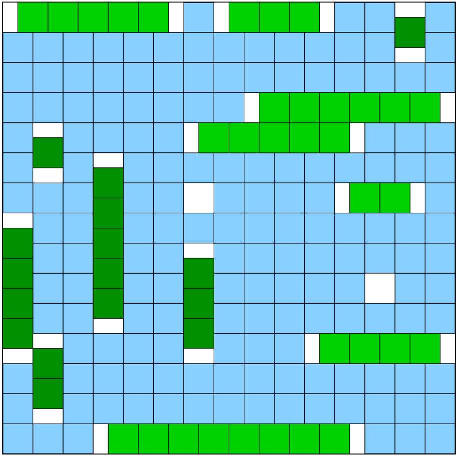
- The **low-activity** series of this model can be computed easily

$$-f(z) = z - \frac{9}{2!}z^2 + \frac{194}{3!}z^3 - \frac{6798}{4!}z^4 + \ldots \qquad (2)$$

- This expansion has a **finite radius of convergence**.
- At high densities the **sublattice ordered state is unstable** because a **single square vacancy can break up into half-vacancies** and can be moved arbitrarily far apart.
- For this model the **standard high-activity cumulant expansion breaks down**.

Columnar Order





A **configuration near full packing** consisting only of horizontal and vertical rod defects.

Columnar Order

- In the columnar ordered state the **even (odd) rows or columns are preferentially occupied** over the others.
- The leading order correction to the high-activity expansion is thus of **order** $1/\sqrt{z}$.
- There is as yet **no rigorous proof** of the existence of this type of order in this system.

Order Parameters

- The **row order parameter** of the system is defined to be

$$O_{\mathrm{r}} = 4[(\rho_1 + \rho_2) - (\rho_3 + \rho_4)], \tag{3}$$

- The **column order parameter** is

$$O_{\mathrm{c}} = 4[(\rho_1 + \rho_4) - (\rho_2 + \rho_3)]. \tag{4}$$

- Equivalently, we can also define a single $\mathbb{Z}_4$ **complex order parameter**

$$O_{Z4} = 4\sqrt{2}[(\rho_1 - \rho_3) + i(\rho_2 - \rho_4)]. \tag{5}$$

- The **phase of the complex order parameter** O_{Z4} takes the values $\pi/4, -3\pi/4, -\pi/4$ and $3\pi/4$ in the A, B, C, and D phases respectively.

High-Activity Expansion

- We **introduce explicit symmetry breaking** by assigning different fugacities to the A (even) and B (odd) rows.
- The partition function $\Omega(z_A, z_B)$ can be written as an **expansion in terms of the fugacities of the particles on the B-rows (defects)** and the corresponding partition functions of the A-rows.

$$\frac{\Omega(z_A, z_B)}{\Omega(z_A, 0)} = 1 + z_B W_1(z_A) + \frac{{z_B}^2}{2!} W_2(z_A) + \ldots \qquad (6)$$

- Taking the logarithm we arrive at the **cumulant expansion**

$$\frac{1}{N} \log \frac{\Omega(z_A, z_B)}{\Omega(z_A, 0)} = z_B \kappa_1(z_A) + \frac{{z_B}^2}{2!} \kappa_2(z_A) + \ldots \qquad (7)$$

High-Activity Expansion

- When there are no B-particles in the lattice, the partition function of the system **breaks up into a product of 1-d partition functions** of particles on the A-rows.
- The A-particles behave as a **1-d lattice gas with nearest neighbour exclusion**.
- The terms in the series can be computed using the **properties of the 1-d lattice gas**.

High-Activity Expansion

- It is possible to **explicitly evaluate the first few terms** in this series. We have

$$\kappa_1(z_A) = \frac{1}{2}\left(\frac{\rho_{1d}(z_A)}{z_A}\right)^2 = \frac{1}{8}\left(\frac{1}{{z_A}^2}\right) - \frac{1}{8}\left(\frac{1}{{z_A}^{5/2}}\right) + \mathcal{O}\left(\frac{1}{{z_A}^3}\right)$$

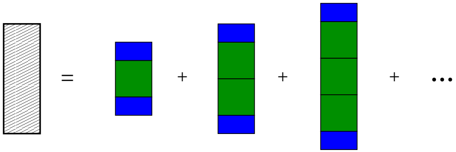
and

$$\frac{\kappa_2(z_A)}{2!} = \frac{1}{16}\left(\frac{1}{{z_A}^3}\right) + \frac{3}{64}\left(\frac{1}{{z_A}^{7/2}}\right) - \frac{21}{64}\left(\frac{1}{{z_A}^4}\right) + \mathcal{O}\left(\frac{1}{{z_A}^{9/2}}\right) \quad (8)$$

- At the point $z_A = z_B = z$ terms involving an **arbitrary number of defects contribute at all orders**.

High-Activity Expansion: Order $1/z$

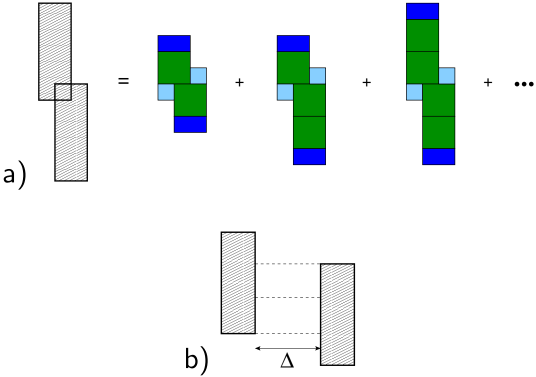
- We **regroup the terms** of the series in powers of $\sqrt{z}$.
- At order $1/z$ the contributing objects are **defects aligned in the vertical direction (rods of arbitrary length)**.



- The term of **order** $1/z^{\frac{n+1}{2}}$ **involves at most** n **rods.**

High-Activity Expansion: Order $1/z^{3/2}$

- At Order $1/z^{3/2}$ we have contributions from terms involving **two rods**.



(the distance Δ between the rods is summed over)

High-Activity Expansion

- We can thus generate the **exact series expansion for the free energy and the density** of the hard square lattice gas up to order $1/z^{3/2}$.
- We have

$$-f(z) = \frac{1}{4}\log z + \frac{1}{4z^{1/2}} + \frac{1}{4z} + \frac{\left(3\log\left(\frac{9}{8}\right) + \frac{11}{96}\right)}{z^{3/2}} + \mathcal{O}\left(\frac{1}{z^2}\right)$$

and

$$\rho(z) = \frac{1}{4} - \frac{1}{8z^{1/2}} - \frac{1}{4z} - \frac{\left(\frac{9}{2}\log\left(\frac{9}{8}\right) + \frac{11}{64}\right)}{z^{3/2}} + \mathcal{O}\left(\frac{1}{z^2}\right) \tag{9}$$

Phase Transition in the Hard Square Lattice Gas

- At high densities the system can order in any one of **four columnar ordered states**.

- This model posseses $\mathbb{Z}_4$ symmetry and hence the transition is expected to lie in the **universality class of a model with $\mathbb{Z}_4$ symmetry**.

- There are several well studied models that exhibit a transition that break a $\mathbb{Z}_4$ symmetry in two dimensions such as the **Eight-Vertex model and the Ashkin-Teller-Potts model**.

The Ashkin-Teller-Potts Model

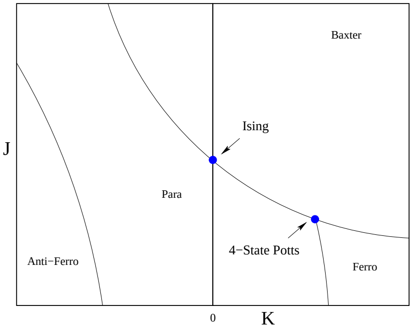
- Two Ising degrees of freedom at every site with a **four spin coupling** term.

- The Hamiltonian of the **isotropic square lattice Ashkin-Teller model** is given by

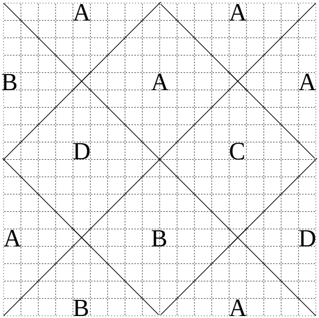
$$H = -\left[\sum_{\langle i,j\rangle} J_2\sigma_i\sigma_j + J_2\tau_i\tau_j + J_4\sigma_i\sigma_j\tau_i\tau_j\right] \tag{10}$$

- This model has several phases, separated by **lines of critical points**.

The Ashkin-Teller-Potts Model



- When $K = \beta J_4$ **is large** and $J = \beta J_2$ **is small** we have **ferromagnetic order**.
- In the **paramagnetic phase** $\langle \sigma\tau \rangle$, $\langle \sigma \rangle$ and $\langle \tau \rangle$ are all zero.
- When both J and K are large $\langle \sigma \rangle$, $\langle \tau \rangle$ and $\langle \sigma\tau \rangle$ **all acquire a nonzero expectation value**.



- We **coarse grain the system** using a grid at an angle $\frac{\pi}{4}$ with respect to the lattice axes.

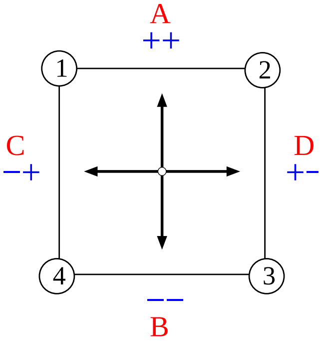
- From symmetry, there are **two types of surface tensions** in this high density phase. $\sigma_{AB} = \sigma_{CD}$ and $\sigma_{AC} = \sigma_{CB} = \sigma_{BD} = \sigma_{DA}$.

- We map this 4-state model to the **Ashkin-Teller model** with surface tension energies K and $2J - K$.

Ising Energy Densities

- We ascribe **Ising labels to the phases** in the hard square lattice gas.
- The four phases in the Ashkin-Teller model can be described by a **complex valued "clock" variable** Θ with the following definition

$$\Theta_{AT} = \exp\left(\frac{i\pi}{4}\right)\frac{(\sigma + i\tau)}{\sqrt{2}} \tag{11}$$



We obtain:

$$\begin{aligned} E(\sigma) &\cong (\rho_1 + \rho_3) \\ E(\tau) &\cong (\rho_2 + \rho_4) \end{aligned} \tag{12}$$

Monte Carlo Simulations

- Simulations of exclusion gases are **inefficient because of "jamming"** (the number of available local moves become very small at high density).

- We use the following algorithm that avoids this problem:

  - We **evaporate all particles that lie on a 1D line** (horizontal or vertical) of the system.

  - We then reoccupy the empty line using a **configuration chosen from an ensemble of a 1D lattice gas** with nearest neighbour exclusion.

- Using this algorithm, we are able to obtain reliable estimates of thermodynamic quantities from **lattices upto size 1600 X 1600**.

Monte Carlo Simulations: Results

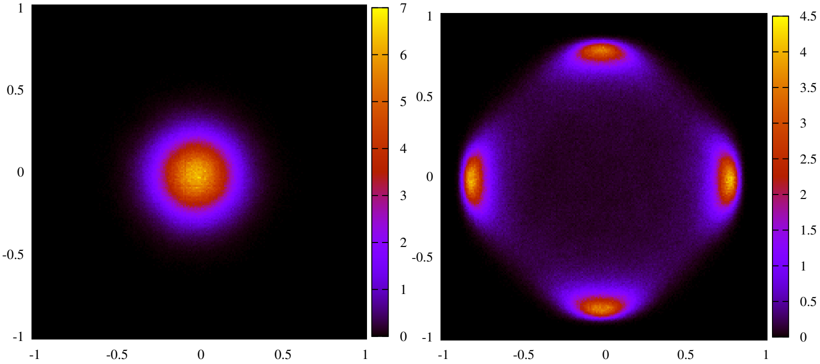


Figure: A histogram of the complex order parameter $O_r + iO_c$ at z = 50 (Left) and z = 100 (Right)

Monte Carlo Simulations: Results

- We **estimate of the critical point of the system to be** $z_c = 97.5 \pm 0.5$.

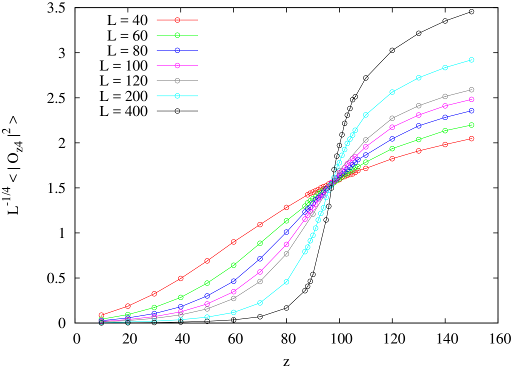
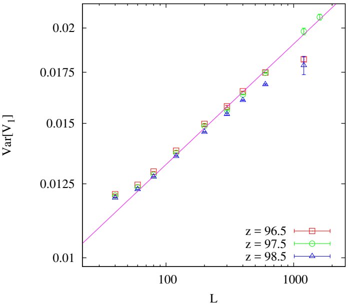
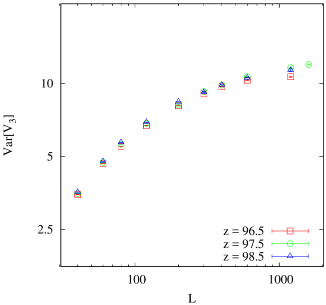


Figure: Plot of $L^{-7/4}\langle |O_{Z4}|^2 \rangle$ with respect to z, showing a critical crossing at the value $z_c = 97.5$.

Monte Carlo Simulations: Results

- We monitor the **variance of** $V_i = \rho_1 + \omega_i \rho_2 + {\omega_i}^2 \rho_3 + {\omega_i}^3 \rho_4$, where ω_i with $i = 1$ to 4 are the fourth roots of unity.

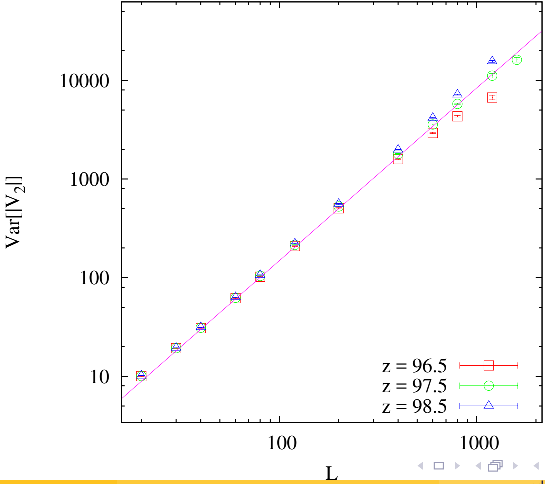




The Variance of V_1 rises with a **detectable power** **(**$\simeq 0.16$**)** with increasing system size whereas that of V_3 **saturates to a finite value**.

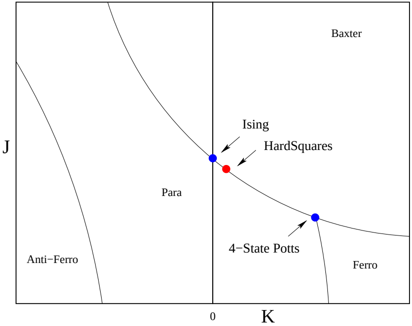
Monte Carlo Simulations: Results

- We verify that the scaling exponent γ/ν is equal to $7/4$ **consistent with the critical behaviour of the Ashkin-Teller model**.



Monte Carlo Simulations: Results

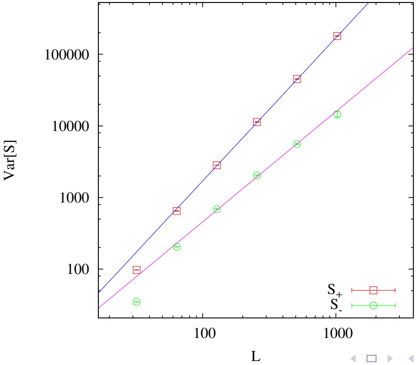
- We place the critical point of this model **slightly to the ferromagnetic side of the Ising point** of the Ashkin-Teller model.



The **phase diagram of the Ashkin-Teller model**.

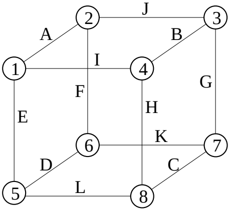
Slidability

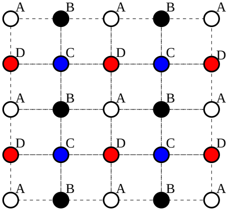
- The columnar ordered phases are characterised by the **deconfinement of half vacancies** along stacks of particles that can be slid to the left or right.
- We monitor the **number of horizontal and vertical slidable stacks** in the system.



Hard Cubes on the Cubic Lattice

- The series expansion developed here can be extended to **three dimensional systems that exhibit columnar order**.
- The extended objects that contribute to order $1/z$ in the $z_A = z_B = z$ series in this case turn out to be **rigid rods along the** x- **or** y- **directions**.





Summary

- We developed a **high-activity expansion** for the hard square lattice gas.
- We placed the phase transition in this model in the **Ashkin-Teller universality class**.

References:

Kabir Ramola, Deepak Dhar, *High-Activity Perturbation Expansion for the Hard Square Lattice Gas*, Phys. Rev. E **86**, 031135, (2012).

Kabir Ramola, Kedar Damle, Deepak Dhar, *Columnar Order and Ashkin-Teller Criticality in Mixtures of Hard-Squares and Dimers* (in preparation).

Thank You.