Onset of Order in Lattice Systems:
Kitaev Model and Hard Squares

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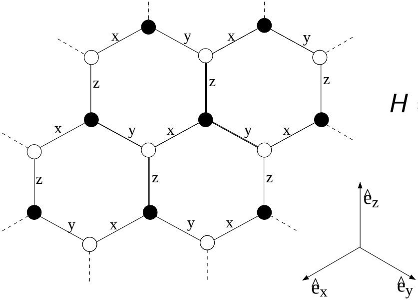
Introduction

- We discuss two models, the **Kitaev model** in the classical limit and the **Hard Square lattice gas model**.
- We investigate whether the classical analogue of the Kitaev model diplays **order-by-disorder**.
- We analyse a related **one dimensional spin model**.
- We study the **columnar ordered** phase of the hard square lattice gas and the **nature of the phase transition** to a disordered state as a function of density.

The Kitaev Model

Ref: A. Kitaev, Ann. Phys. **321**, 2 (2006)

- **Exactly soluble** two dimensional lattice model with interacting quantum spins (**spin-1/2**).



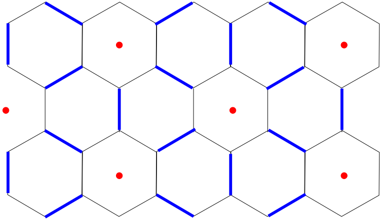
$$H = -\sum_{a \in A} \left[J_x S_a^x S_{a+e_x}^x + J_y S_a^y S_{a+e_y}^y + J_z S_a^z S_{a+e_z}^z \right] \quad (1)$$

- Can be solved as a problem of non-interacting **Majorana fermions**.
- Has been studied as a useful candidate for quantum computation because it displays **topological order**.

Spin-S Kitaev Model

Ref: G. Baskaran, D. Sen, and R. Shankar, Phys. Rev. B **78**, 115116 (2008)

- Mutually commuting $\mathbb{Z}_2$ **variables**.
- **Infinitely degenerate** classical ground states.
- Spin wave expansions about the classical ground states yield an energy minimum around an ordered state (**quantum order-by-disorder**).



Order-by-Disorder

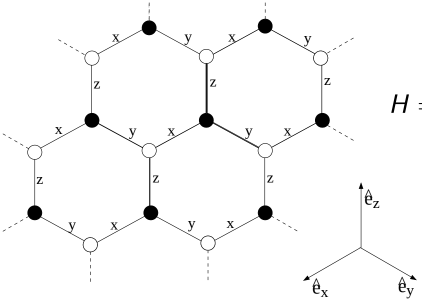
- Phenomenon where a disordered system at strictly $T = 0$ acquires a **fluctuation induced order** at temperatures just above zero.

- The relative weights of different ground states in the $T \to 0^+$ limit **differs from the actual sum over ground states** that contribute at $T = 0$.

- It is important in the study of **magnetic systems with frustration**. For example: Heisenberg spins on the **kagome lattice with antiferromagnetic couplings**.

The Kitaev Model with Classical Spins

- We consider **classical Heisenberg spins** on a hexagonal lattice with Kitaev couplings.

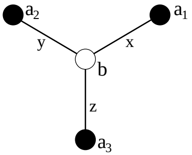


$$H = -\sum_{a \in A} [J_x S_a^x S_{a+e_x}^x + J_y S_a^y S_{a+e_y}^y + J_z S_a^z S_{a+e_z}^z] \quad (2)$$

- We consider the case when **all the couplings are equal** ($J_x = J_y = J_z$).

Finite temperature Partition Function

The **partition function** of the system is $Z[\beta] = \int \prod_s \left(\frac{d\vec{S}_s}{4\pi} \right) \exp[-\beta H]$ (3)



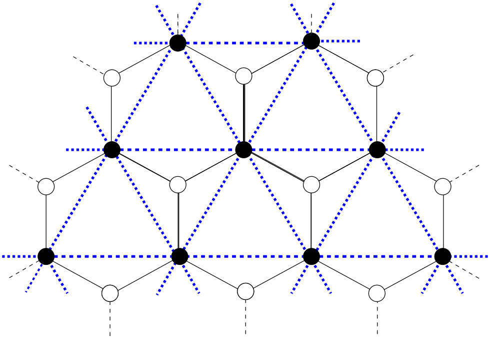
Each B-spin experiences a field $\vec{h} = (S^x_{a_1}, S^y_{a_2}, S^z_{a_3})$ due to the neighbouring A-spins

- **Integrating out the B-spins** yields an **effective Hamiltonian** for the *A*-spins.

$$H_{eff}(\{\vec{S}_a\}, \beta) = -\frac{1}{\beta} \sum_{(l,m)} F \left[\beta \left(\sqrt{{S^x_{a_1}}^2 + {S^y_{a_2}}^2 + {S^z_{a_3}}^2} \right) \right], \quad (4)$$

$$\text{where} \quad F[x] = \log \left[\frac{\sinh(x)}{x} \right]. \quad (5)$$

Finite temperature Partition Function (cont.)



- The system is thus a **triangular lattice of A-sites** interacting via H_{eff} within each down-pointing triangle.

Characterisation of the Ground State Manifold

- We note that $F(x)$ in the effective Hamiltonian is **convex**. Hence the Hamiltonian is minimised when ${S_{a_1}^{x}}^2 + {S_{a_2}^{y}}^2 + {S_{a_3}^{z}}^2 = 1$ at every B-site.

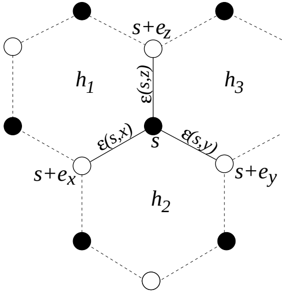
- We assign a **bond-energy vector** $\epsilon(l, m; \alpha)\vec{e}_\alpha$ at every bond $\epsilon(l, m; \alpha) = \left(S^\alpha_{a(l,m)}\right)^2 - \frac{1}{3}$, where $\alpha \equiv x, y, z$. The ground state ensemble is characterised by the constraint that the **sum of bond energies at every site is equal to** 0.

- We thus have a **divergence-free vector field** on the bonds of the lattice at zero temperature.

- We can thus parametrise the system at zero temperature using **continuously variable heights** (associated with the hexagonal plaquettes).

Mapping to a Height Model

- The bond energies can be expressed as a **difference of the height field** of the plaquettes contiguous to each bond.



$$\begin{aligned} \epsilon(s,x) &= f(h_1) - f(h_2) \\ \epsilon(s,y) &= f(h_2) - f(h_3) \\ \epsilon(s,z) &= f(h_3) - f(h_1) \end{aligned} \tag{6}$$

- For a lattice of $2N$ sites with periodic boundary conditions, the ground states form an $(N+1)$ **dimensional manifold**.

Zero temperature correlations

- The height model has the **symmetry** $f(h_i) \to f(h_i) + Const.$
- We expect the **effective Hamiltonian** to be $|\nabla f|^2$, which gives rise to the spectrum given by $\omega^2 \propto k^2$.
- Then for two sites s_1 and s_2 separated by a large distance R

$$\langle (f_{s_1} - f_{s_2})^2 \rangle \sim \log R \tag{7}$$

- This implies that

$$\langle (S_{s_1}^{\alpha})^2 (S_{s_2}^{\beta})^2 \rangle_c \sim \frac{1}{R^2}. \tag{8}$$

Finite temperature height model

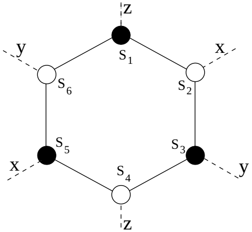
- At finite temperatures, $\nabla.\epsilon \neq 0$ **at the B-sites**.
- This is equivalent to introducing a **continuously variable charge** $Q_{b(l,m)}$ at every B-site.
- The partition function takes the form

$$Z[\beta] = (\text{Const.}) \left[\prod_{l,m} \int df_{l,m} \int dQ_{b(l,m)} \right] \left[\prod_{\text{bonds}} \left(\frac{1}{3} + \epsilon(\text{bond}) \right)^{-1/2} \right] \times \exp \left[\sum_{l,m} F \left(\beta \sqrt{1 + Q_{b(l,m)}} \right) \right]. \quad (9)$$

Zero Temperature Limit

- The linear term in Q in the above exponential vanishes due to the overall **charge neutrality of the system**.
- Hence the leading behaviour of the integral over the range of Q at large β can be determined asymptotically exactly using a **saddle point approximation**.
- Each integration to leading order is **independent of the configuration** $\{f_{l,m}\}$ and gives a factor $C\beta^{-1/2}$ where C is a constant.
- Thus the classical limit of the spin-S Kitaev model **does not display order-by-disorder**.

Finite Temperature Correlations



The plaquette-transformation:

$(S_1^x, S_1^y, S_1^z) \rightarrow (-S_1^x, -S_1^y, S_1^z)$

$(S_2^x, S_2^y, S_2^z) \rightarrow (S_2^x, -S_2^y, -S_2^z)$

$\vdots$

is a **symmetry of the Hamiltonian**

- This leads to $\langle S_{s_1}^{\alpha} S_{s_2}^{\beta} \rangle = 0$ when sites s_1 and s_2 are not nearest neighbours.
- At finite temperature, the height fluctuations are still logarithmic, but the spin-squared correlations **decay exponentially**.
- At **infinite temperature** we have

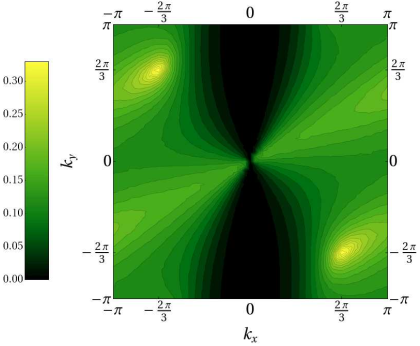
$$\langle (f_R - f_0)^2 \rangle_{\beta=0} = \frac{2\sqrt{3}}{45\pi} \log[R] + \mathcal{O}(1) \quad \text{for large R.} \qquad (10)$$

Monte Carlo Simulations

- In order to test our predictions, we **simulate the effective Hamiltonian** H_{eff}.
- For finite temperature simulations, two kinds of moves were employed:
  -**single spin moves** and
  -**6-spin cluster moves** (to efficiently thermalise the system at low temperatures).
- We looked for possible **signatures of ordering** as the temperature is decreased by measuring various correlation functions.

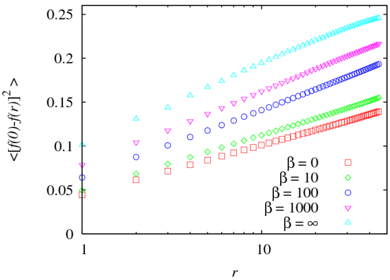
Monte Carlo Simulations: Results

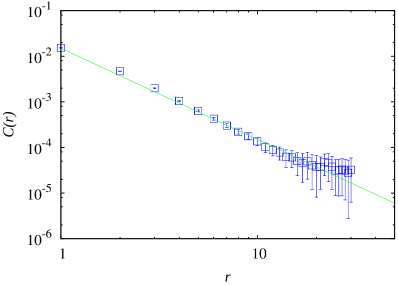
- We define the spin-squared **structure factor** as
  $S(\vec{k}) = \frac{1}{\sqrt{LM}} \sum_{\vec{r}} (\langle {s_A^z}^2(0) {s_A^z}^2(\vec{r}) \rangle - \frac{1}{9}) \exp{(i\vec{k}.\vec{r})}$



We find that the peaks in $|S(\vec{k})|^2$ **do not scale with system size**.

Monte Carlo Simulations: Results (cont.)





The height fluctuations are **logarithmic at all temperatures** (Left). The spin-squared correlation function **decays as** $1/R^2$ at zero temperature (Right).

Spin-S Kitaev Model: Lower Bounds on Energy

- We next study the **quantum spin-S Kitaev model**
- We **normalise** the Hamiltonian by the **size of the spin**

$$H = -\frac{J}{S(S+1)} \sum_{a \in A} [S_a^x S_{a+e_x}^x + S_a^y S_{a+e_y}^y + S_a^z S_{a+e_z}^z] \qquad (11)$$

- We derive an **exact lower bound for the ground state energy** of this model. We have

$$\langle \psi | H | \psi \rangle \geq -JN \sqrt{\frac{S}{S+1}}. \qquad (12)$$

Spin-S Kitaev Chain

- When the z-**coupling is set to zero** in the spin-S Kitaev model, the Hamiltonian of the resulting **spin chain** is

$$H = \sum_n \left(J_{2n-1} S^x_{2n-1} S^x_{2n} + J_{2n} S^y_{2n} S^y_{2n+1} \right) \qquad (13)$$

- There is a $\mathbb{Z}_2$ **valued conserved quantity** $W_n = \Sigma^y_n \Sigma^x_{n+1}$ for **each bond** $(n, n+1)$ of the system, where $\Sigma^a_n = e^{i\pi S^a_n}$. Thus the Hilbert space breaks up into sectors for different values of $\{W_n\}$.
- The dimension of each sector can be expressed as a **trace of products of** 2×2 **transfer matrices** depending on the values of $W_n = \pm 1$. We have

$$\begin{aligned} \mathbb{T}_+ &= \frac{1}{2} \begin{bmatrix} S-1 & S+1 \\ S+1 & S+1 \end{bmatrix} \text{ for } S \text{ odd,} \\ &= \frac{1}{2} \begin{bmatrix} S+2 & S \\ S & S \end{bmatrix} \text{ for } S \text{ even.} \end{aligned}$$

and $\mathbb{T}_- = \mathbb{T}_+ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$.

Spin-1 Chain

- We consider the case with $S = 1$.
- We use the basis $|x\rangle, |y\rangle, |z\rangle$ in which the spin operators have the action $S_\alpha|\alpha\rangle = 0$ with $\alpha \equiv x, y, z$.
- A state with all $W_n = 1$ is the **fully polarized** z **state** ...$zzzz$....
- $\{W_n\}$ is left invariant by the interchange $zz \rightleftharpoons yx$. This can be thought of as a **dimer evaporation/deposition process**.

Spin-1 Chain: Ground state

- We postulate a **ground state variational wavefunction** of the type

$$|\psi\rangle = \sum_{\mathbf{C}} \sqrt{\mathrm{Prob}(\mathbf{C})}\, |\mathbf{C}\rangle \tag{14}$$

$\mathrm{Prob}(\mathbf{C})$ is the probability of a lattice gas configuration $\mathbf{C}$ in a given ensemble.

- Analysis of the eigenvalues for small systems shows that the ground state lies in the **sector with all** $W_n = +1$ with an energy per site $E_g = -0.60356058$

- Using the above wavefunction we obtain an estimate of -0.60333 for the ground state energy, that **agrees with the exact answer to** $< 0.1\%$ **accuracy**.

Spin-1 Chain: Energy Gap

- We then consider the sector with **one W negative** to obtain an estimate of the gap in the excitation spectrum.

- We use a trial wave function of the type

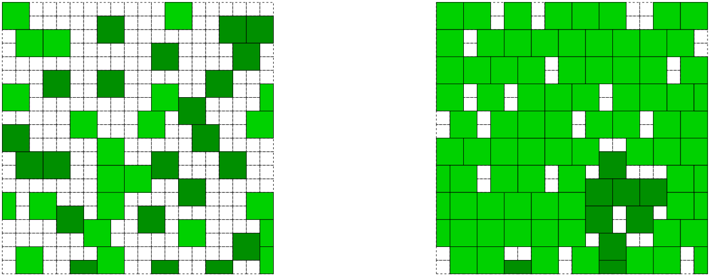
$$|\psi\rangle = \frac{1}{\sqrt{2}}\left[\sum_{U}\sqrt{\mathrm{Prob}(\mathbf{U})}|x\mathbf{U}\rangle - \sum_{V}\sqrt{\mathrm{Prob}(\mathbf{V})}|\mathbf{V}y\rangle\right] \qquad (15)$$

- We assign **position dependent weights** for the lattice gas configurations.

- Using a **ten parameter wavefunction** we obtain an estimate of the energy gap $\Delta \simeq 0.15556$.

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.

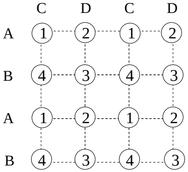
Activity Expansions

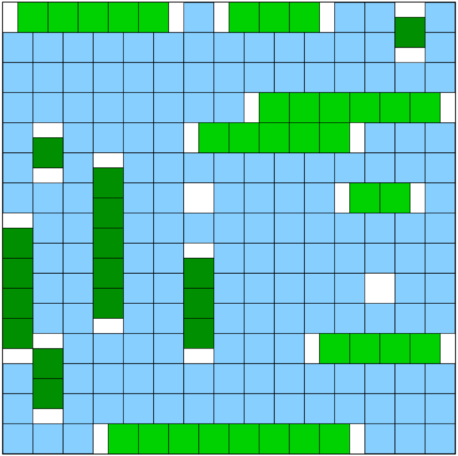
- The **low-activity** series of this model can be computed easily

$$-f(z) = z - \frac{9}{2!}z^2 + \frac{194}{3!}z^3 - \frac{6798}{4!}z^4 + \ldots \qquad (16)$$

- 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

$$O_r = 4[(\rho_1 + \rho_2) - (\rho_3 + \rho_4)], \tag{17}$$

- The **column order parameter** is

$$O_c = 4[(\rho_1 + \rho_4) - (\rho_2 + \rho_3)]. \tag{18}$$

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

$$O_{Z4} = 4\sqrt{2}[(\rho_1 - \rho_3) + i(\rho_2 - \rho_4)]. \tag{19}$$

- 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.

$$\frac{\Omega(z_A, z_B)}{\Omega(z_A, 0)} = 1 + z_B W_1(z_A) + \frac{{z_B}^2}{2!} W_2(z_A) + \ldots \tag{20}$$

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

$$\frac{1}{N} \log \frac{\Omega(z_A, z_B)}{\Omega(z_A, 0)} = z_B \kappa_1(z_A) + \frac{{z_B}^2}{2!} \kappa_2(z_A) + \ldots \tag{21}$$

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

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

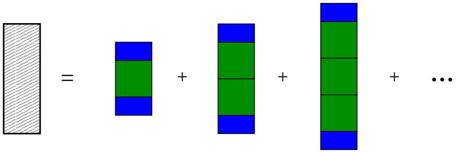
and

$$\frac{\kappa_2(z_A)}{2!} = \frac{1}{16}\left(\frac{1}{{z_A}^3}\right) + \frac{3}{64}\left(\frac{1}{{z_A}^{7/2}}\right) - \frac{21}{64}\left(\frac{1}{{z_A}^4}\right) + \mathcal{O}\left(\frac{1}{{z_A}^{9/2}}\right) \quad (22)$$

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

High-Activity Expansion: Order $1/z$

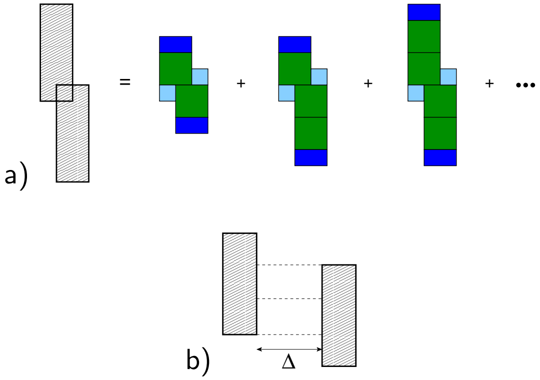
- We **regroup the terms** of the series in powers of $\sqrt{z}$.
- At order $1/z$ the contributing objects are **defects aligned in the vertical direction (rods of arbitrary length)**.



- 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

$$\rho(z) = \frac{1}{4} - \frac{1}{8z^{1/2}} - \frac{1}{4z} - \frac{\left(\frac{9}{2}\log\left(\frac{9}{8}\right) + \frac{11}{64}\right)}{z^{3/2}} + \mathcal{O}\left(\frac{1}{z^2}\right) \qquad (23)$$

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

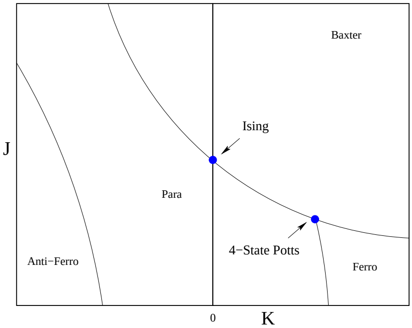
- Two Ising degrees of freedom at every site with a **four spin coupling** term.

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

$$H = -\left[\sum_{\langle i,j\rangle} J_2\sigma_i\sigma_j + J_2\tau_i\tau_j + J_4\sigma_i\sigma_j\tau_i\tau_j\right] \tag{24}$$

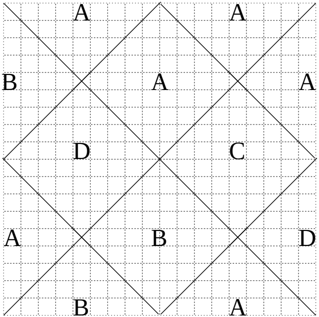
- This model has several phases, separated by **lines of critical points**.

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**.

Mapping to the Ashkin-Teller model



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

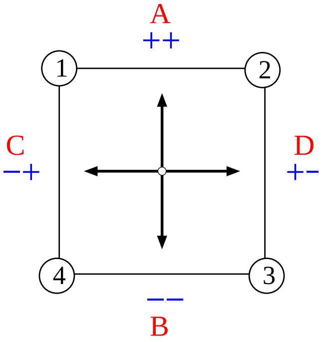
- From symmetry, there are **two types of surface tensions** in this high density phase. $\sigma_{AB} = \sigma_{CD}$ and $\sigma_{AC} = \sigma_{CB} = \sigma_{BD} = \sigma_{DA}$.

- 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

$$\Theta_{AT} = \exp\left(\frac{i\pi}{4}\right)\frac{(\sigma + i\tau)}{\sqrt{2}} \tag{25}$$



We obtain:

$$\begin{aligned} E(\sigma) &\cong (\rho_1 + \rho_3) \\ E(\tau) &\cong (\rho_2 + \rho_4) \end{aligned} \tag{26}$$

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

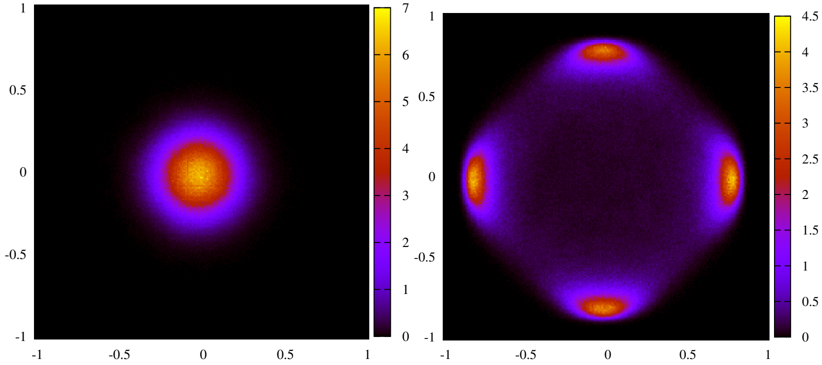


Figure: A histogram of the complex order parameter $O_r + iO_c$ at z = 50 (Left) and z = 100 (Right)

Monte Carlo Simulations: Results

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

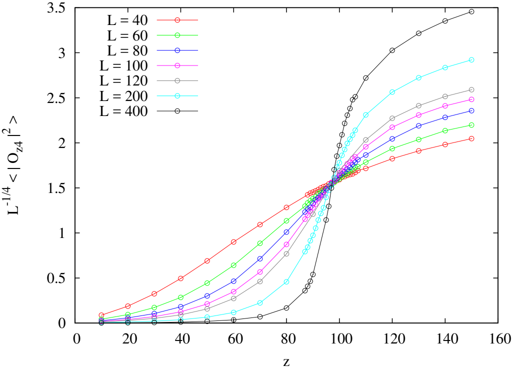
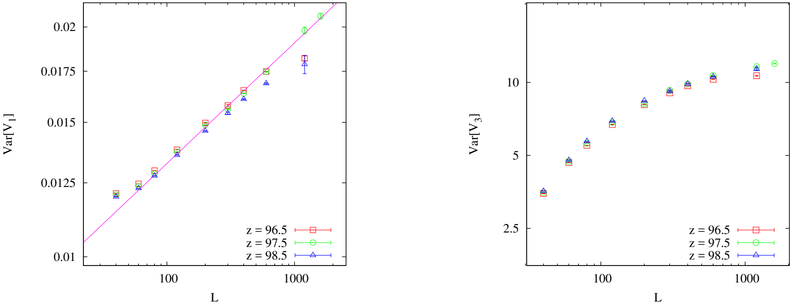


Figure: Plot of $L^{-7/4}\langle|O_{Z4}|^2\rangle$ with respect to z, showing a critical crossing at the value $z_c = 97.5$.

Monte Carlo Simulations: Results

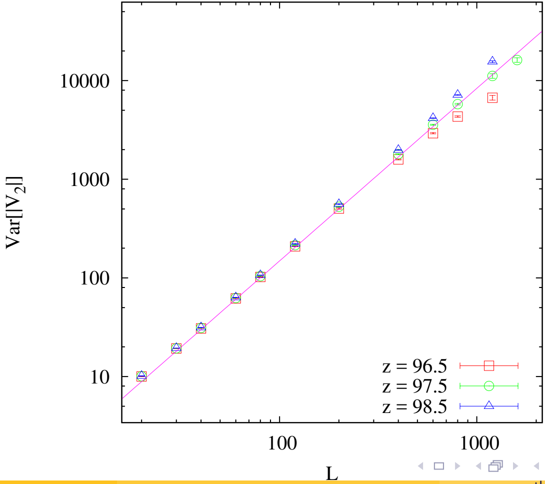
- We monitor the **variance of** $V_i = \rho_1 + \omega_i \rho_2 + {\omega_i}^2 \rho_3 + {\omega_i}^3 \rho_4$, where ω_i with $i = 1$ to 4 are the fourth roots of unity.



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**.

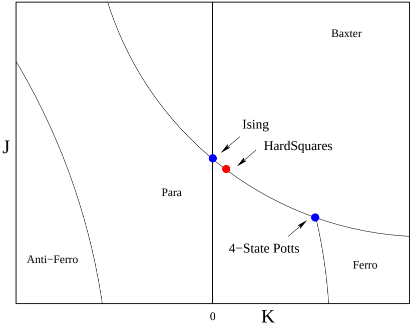
Monte Carlo Simulations: Results

- 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

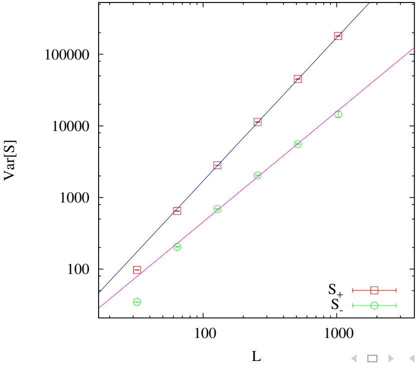
- We place the critical point of this model **slightly to the ferromagnetic side of the Ising point** of the Ashkin-Teller model.



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.



Summary

- We have shown that the classical limit of the spin-S Kitaev model **does not order even at $T = 0$, but has power law correlations**.
- The corresponding spin-S chain (for $\text{S} = 1$) has a **finite energy gap**.
- We developed a **large-z expansion** for the hard square lattice gas.
- We showed that the phase transition in this model is in the **Ashkin-Teller universality class**.

Thank You.

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**.