Columnar Order and Ashkin-Teller Criticality in Mixtures of Hard-Squares and Dimers

Kabir Ramola

Martin Fisher School of Physics
Brandeis University

In collaboration with Kedar Damle and Deepak Dhar

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Real gases display a **complex and rich phase diagram**, and modelling the behaviour of a large collection of particles represents a theoretical challenge.

Although low density properties can be understood (gas-like behaviour), 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 such complex physical systems.
Why Study Hard Core Gases?

- Hard-Cores serve as an important first approximation of real gases.

- Temperature plays no role thus purely entropic phase transitions.

- Hard-core interactions are important in understanding fluids, granular materials, glassy systems etc.

- Several studies on single-species models.

- Polydisperse systems are physically relevant models mixtures, granular materials.
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The dimer model is useful in the context of RVB ground states of spin models, high $T_c$ superconductivity, quantum spin liquids etc.

- Exact Solution at full packing (Pfaffian of Signed Adjacency Matrix) (P. W. Kasteleyn, Physica 27, 1209 (1961)).
- Ising Model $\rightarrow$ Dimer model on Fisher Lattice.
- Power law correlations at full packing.
The Dimer Model: Height Mapping

- One-to-One mapping to a scalar height field.

- Global Symmetries \( \{ h \} \rightarrow \{ -h \} \) and \( \{ h \} \rightarrow \{ h + \text{Const.}\} \)

- Long range action:
  \[ S \sim \kappa \int d^2r |\nabla h|^2. \]

Interacting dimer models can have several phases (F. Alet, J. L. Jacobsen, G. Misguich, V. Pasquier, F. Mila, and M. Troyer, Phys. Rev. Lett. 94, 235702 (2005)).

Aligning interactions lead to Columnar order, with KT transitions from fluid to ordered states.


Recent interest in Mathematics: CFT, 2D Limiting shapes.
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The 2D XY Model

\[ \mathcal{H} = \sum_{\langle i,j \rangle} J \cos(\Theta_i - \Theta_j) \]  

1. **2D XY model** arises in several contexts (2D superfluidity, defects in 2D crystals etc).

2. Long range action of the sine-gordon model:  
   \[ S \sim \int d^2 r [g|\nabla \Theta|^2 + \lambda \cos \beta \phi]. \]

3. RG Analysis by **integrating out the contribution from the fast modes**.

4. **Kosterlitz–Thouless** transition from temperature dependent power-law order to disorder.

5. **Vortices proliferate and destroy the power-law ordering** in the system for \( T > T_{KT} \).
The XY Model with Symmetry Breaking

- J. V. Jose, L. P. Kadanoff, S. Kirkpatrick, and D. R. Nelson, Phys. Rev. B 16, 1217 (1977) considered the following action:

\[ S \sim \pi g \int d^2 r |\nabla h|^2 + \sum_{p=4,8,12\ldots} \epsilon_p \int dx dy \cos(2\pi ph) \]  

(2)

- RG analysis suggests that there is a line of fixed points of second order transitions with non-universal exponents.

- Additionally Kadanoff has argued that this line belongs to the Ashkin-Teller Universality class, (L. P. Kadanoff Phys. Rev. Lett. 39, 903 (1977)).

- Has been used extensively in the study of spin models, quantum dimer models.
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The Hard Square Lattice Gas

- Lattice gas of particles where each particle is a $2 \times 2$ square that occupies 4 elementary plaquettes of the square lattice.

Figure: (Left) Low density disordered state (Right) High density columnar ordered state

- Simplest extension to Lee-Yang Lattice Gas.
- Long history of study.
- The system is disordered at low density and columnar ordered at high density.
- Relevant to antiferromagnetic spin systems with plaquette interactions, (M. E. Zhitomirsky and H. Tsunetsugu, Phys. Rev. B 75, 224416 (2007)).
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In the columnar ordered state, **even (odd)** rows or columns are preferentially occupied over the others. There are **four ordered states**.

Characterised by **deconfinement of half-vacancies**, (K. Ramola and D. Dhar, Phys. Rev. E 86, 031135 (2012)).

The leading order correction to the high-activity expansion of order $1/\sqrt{z}$ (where $z = \exp(\mu)$, $\mu = \text{chemical potential}$).

There is as yet **no rigorous proof** of the existence of this type of order in this system.

The disorder-columnar order transition is in the **Ashkin-Teller Universality Class**, (K. Ramola, Ph. D. Thesis, Tata Institute of Fundamental Research (2012)).
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The Ashkin-Teller-Potts Model

- Two Ising degrees of freedom at every site with a \textbf{four spin coupling} term.

- The Hamiltonian of the \textbf{isotropic square lattice Ashkin-Teller model} is given by \cite{AshkinTeller1943}.

\[
H = - \left[ \sum_{\langle i,j \rangle} J_2 \sigma_i \sigma_j + J_2 \tau_i \tau_j + J_4 \sigma_i \sigma_j \tau_i \tau_j \right] \tag{3}
\]

- This model has several phases, separated by \textbf{lines of critical points}.
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.
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The Partition function of this model is given by

$$Z_{dsv} = \sum_{C_{dsv}} z_s^{N_s} z_d^{N_d} z_v^{N_v}.$$ (4)

- $z_r, z_s$ and $z_v$ are the fugacities of the rods, squares and vacancies.
- $N_s, N_d, N_v$ are the number of squares, dimers and vacancies.
- Convention $z_s + z_d^2 + z_v^4 = 1$. $v = z_v / z_s^{1/4}$, and $w = z_d / \sqrt{z_s}$. 

Figure: (Left) Low density disordered state (Right) High density columnar ordered state
At Full Packing: **generalized height mapping** → \( S \sim g \int d^2 r |\nabla h|^2 \).

The introduction of squares causes a \( \mathbb{Z}_4 \) anisotropy \( \sum_{n=4,8,\ldots} \epsilon_n \cos(2n\pi h) \) to this action.

Vacancies introduce **vorticity**.

Dimers, Squares and Vacancies: Expected Phase Diagram

- **Order**
- **Disordered**
- **Hard Squares**
- **Decoupled Ising**
- **Ashkin−Teller Behavior**

- **KT Transition**
- **Power−Law Order**
- **Disordered Fluid**

- **Columnar Order**

- **Columnar Order and Ashkin-Teller Criticality in Mixtures of Hard-Squares and Dimers**

\[ D (\rho_d = 1) \]

\[ S (\rho_s = 1) \]

\[ V (\rho_v = 1) \]
What is the **Order Parameter** in this case?

![Diagram](image)

**Figure:** Values of the columnar order parameter field $\psi(\vec{r})$.

We define the local complex order parameter:

$$
\psi_1 = (-1)^m, \quad \psi_2 = -i(-1)^n, \quad \psi_3 = [(-1)^m - i(-1)^n]/\sqrt{2}.
$$

At full packing $\rightarrow$ reduces to the well-known dimer model height mapping.
In terms of the microscopic Ising variables

\[ \psi(\vec{r}) \equiv \frac{\sigma(\vec{r}) + \tau(\vec{r})}{2} + i \frac{\sigma(\vec{r}) - \tau(\vec{r})}{2}. \]  

(6)

Lattice symmetries imply:

\[ \langle \sigma(\vec{r}_1)\tau(\vec{r}_2) \rangle = 0, \langle \sigma(\vec{r})\sigma(0) \rangle = \langle \tau(\vec{r})\tau(0) \rangle. \]  

(7)

Along the AT phase boundary: 

\[ \langle \psi^*(\vec{r})\psi(0) \rangle \sim 1/r^{1/4}, \]

while 

\[ \langle \text{Re}(\psi^2(\vec{r}))\text{Re}(\psi^2(0)) \rangle \sim 1/r^{\eta_2(\nu)}, \text{ with } \eta_2(\nu) \in [0, 1]. \]

The Ashkin-Teller behaviour implies \( \eta_2 = 1 - 1/(2\nu). \)
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At high packing fractions we encounter Jamming.

We thus need to simulate the model in a different way (columnar order occurs only at very high densities).

We make non-local moves that successfully avoids this problem.

We update an entire $2 \times L$ ladder of the lattice at once.
Update Algorithm

Figure: Steps in the transfer-matrix based algorithm.

- We **empty out an entire** $2 \times L$ **ladder** on the lattice.
- We compute the **restricted partition function** of this ladder subject to the hard-core constraints of objects above and below.
- We then refill the ladder with a **configuration chosen with the correct weight** from the partition function.
There are additional constraints due to the presence of particles immediately above and below this ladder.

**Figure:** The four possible underlying morphologies $\sigma = 1, 2, 3, 4$ of a two-plaquette rung.

**Figure:** The six possible states of a two-plaquette rung.
The Transfer Matrices

- We then construct the **restricted partition function** of the ladder subject to these constraints.

\[
Z_{\text{track}}^{\text{closed}} = \text{Tr}(\mathcal{T}_L \ldots \mathcal{T}_3 \mathcal{T}_2 \mathcal{T}_1).
\]  

(8)

- For Example:

\[
\mathcal{T}_{1,1} = \begin{pmatrix}
0 & 0 & 0 & z_s & 0 & 0 \\
0 & 0 & 0 & z_d^2 & 0 & 0 \\
z_d & z_d & z_d & z_d z_v^2 & z_d z_v & z_d z_v \\
1 & 1 & 1 & z_v^2 & z_v & z_v \\
0 & 0 & 0 & z_d z_v & 0 & z_d \\
0 & 0 & 0 & z_d z_v & z_d & 0
\end{pmatrix}.
\]
**Exact Enumeration Checks**

- **Does the algorithm work?**

- **We enumerate all the possible states** on a $4 \times 4$ lattice with periodic BCs

- **1228** for fully packed, **69941** states for dimers+squares+vacancies
Monte Carlo Simulations

- The correlation lengths in the columnar ordered state are very large.

- **Strong finite-size effects**: Thus we need very large lattice sizes.

- We performed simulations on lattices upto size $L = 1024$ with $10^8$ MCS.
Results: Full-Packing (No Vacancies)
Results: Dimers+Squares (No Vacancies)

\[ \left\langle \frac{|\Psi_L|^4}{|\Psi_L|^2} \right\rangle \]

\[ C(L)w \]

\[ L = 384 \quad \text{red} \]
\[ L = 512 \quad \text{green} \]
\[ L = 768 \quad \text{blue} \]
\[ L = 1024 \quad \text{black} \]

\[ w = 0.198 \quad \eta = 0.250 \]
\[ w = 0.204 \quad \eta = 0.252 \]
\[ w = 0.217 \quad \eta = 0.276 \]
\[ w = 0.230 \quad \eta = 0.295 \]
\[ w = 0.253 \quad \eta = 0.332 \]
\[ w = 0.295 \quad \eta = 0.404 \]
\[ w = 0.333 \quad \eta = 0.460 \]

Figure: \( w_c^0 \approx 0.198(2) \).

\[ \Psi_L \equiv \sum_{\vec{r}} \psi(\vec{r}), \quad C(L) = \left\langle \left| \sum_{\vec{r}} \psi(\vec{r}) \right|^2 \right\rangle / L^2, \]

\[ \Re(L) = \left\langle \left( \sum_{\vec{r}} \text{Re}(\psi^2(\vec{r})) \right)^2 \right\rangle / L^2, \quad I(L) = \left\langle \left[ \sum_{\vec{r}} \text{Im}(\psi^2(\vec{r})) \right]^2 \right\rangle / L^2. \]

(9)
Results: Dimers + Vacancies + Squares

\[ D (\rho_d = 1) \]

\[ V (\rho_v = 1) \]

\[ S (\rho_s = 1) \]

Disordered Fluid

Columnar Order

II
Figure: \( \nu_c = 0.0623(1), \nu_c = 0.1600(1) \). \( \nu = 1.70(5) \). \( \eta_2 = 0.70(5) \).
Results: Squares + Vacancies

- Disordered Fluid
- Columnar Order
- $S(\rho_s = 1)$
- $V(\rho_v = 1)$
- $D(\rho_d = 1)$
Results: Squares + Vacancies

\begin{align}
\mathcal{N}(L) &= \langle \left( \sum_{\vec{r}} T(\vec{r}) \right)^2 \rangle / L^2 \sim L^{2-\eta_2^*}, \eta_2^* \approx 0.46(3). \quad (10)
\end{align}

- Consistent with Ashkin-Teller Criticality.
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Outlook

- Columnar ordering is **ubiquitous in a wide variety of strongly-correlated systems**.

- The emergent U(1) symmetry at full-packing is closely related to the U(1) symmetry of the thermal AT transition to columnar valence-bond solid (VBS) in **frustrated square-lattice antiferromagnets**.

- In the $T \to 0$ along the AT phase boundary (with $\psi(\vec{r})$ the complex VBS order parameter): should $\text{Re}(\psi^2(\vec{r}))$, the **valence-bond nematic order parameter** decay with the same exponent as the **next-nearest-neighbour bond-energy** ($\text{Im}(\psi^2(\vec{r}))$)?

- Additionally, are $\eta_{\text{VBN}}$ and $\nu$ related on the AT phase boundary via the Ashkin-Teller relation?
Conclusions

- We discussed a polydisperse system where critical exponents can be tuned with the relative densities of particles.

- The hard-square lattice gas is one point on this parameter space.

- We verified the Ashkin-Teller nature of the fluid-columnar order transition.

- Has interesting implications for frustrated systems which exhibit columnar ordering.

- Would be interesting to extend to systems with different shapes and types of particles.
Thank You.