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

Tuesday 17$^{\text{th}}$ February, 2015

Outline

Lattice Gases

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

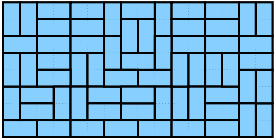
- Although low density properties can be understood (gas-like behaviour), real gases display **significant deviations from ideal behaviour at high densities**.

- **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.

The Dimer Model



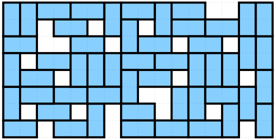
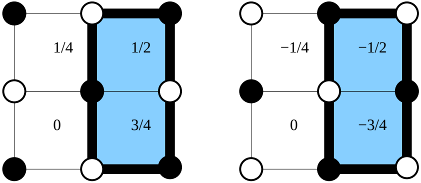
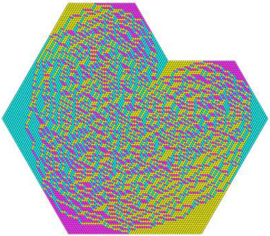


Figure: **(Left)** Fully-Packed state **(Right)** State with Dimers+Vacancies

- 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 → Dimer model on **Fisher Lattice**.
- **Power law correlations** at full packing.
- No order away from full packing: rigorous proof, (O. J. Heilmann and E. H. Lieb, Comm. Math. Phys.**25**, 190-232 (1972)).

The Dimer Model: Height Mapping





- One-to-One mapping to a **scalar height field**.
- Global Symmetries $\{h\} \to \{-h\}$ and $\{h\} \to \{h + \mathrm{Const.}\}$
- Long range action: $\mathcal{S} \sim \kappa \int d^2 r |\nabla h|^2$.

R. Kenyon, Les Houches Lecture notes (2006).

Interacting Dimer Models

- **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.
- Exact **range expansion** of RVB wavefunction $\rightarrow$ interacting dimer models (K. Damle, D. Dhar, and K. Ramola, Phys. Rev. Lett. 108, 247216 (2012)).
- Recent interest in Mathematics: CFT, 2D Limiting shapes.

The 2D XY Model

$$\mathcal{H} = \sum_{\langle i,j \rangle} J \cos(\Theta_i - \Theta_j) \tag{1}$$

- **2D XY model** arises in several contexts (**2D superfluidity, defects in 2D crystals etc**).
- Long range action of the sine-gordon model: $\mathcal{S} \sim \int d^2 r [g |\nabla \Theta|^2 + \lambda \cos \beta \phi]$.
- RG Analysis by **integrating out the contribution from the fast modes.**
- **Kosterlitz–Thouless** transition from temperature dependent power-law order to disorder.
- **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:

$$\mathcal{S} \sim \pi g \int d^2 r |\nabla h|^2 + \sum_{p=4,8,12\dots} \epsilon_p \int dxdy \cos(2\pi p h) \tag{2}$$

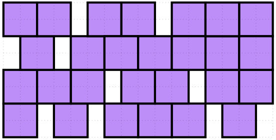
- RG analysis suggests that there is a **line of fixed points of second order transitions** with **non-universal exponents**.

- 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**.

The Hard Square Lattice Gas

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



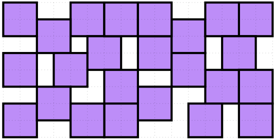


Figure: **(Left)** Low density disordered state **(Right)** High density columnar ordered state

- 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)).

Columnar Order

- 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 $z = \exp(\mu)$, $\mu =$ 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)).

The Ashkin-Teller-Potts Model

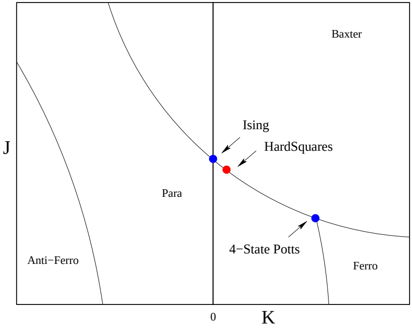
- Two Ising degrees of freedom at every site with a **four spin coupling** term.

- The Hamiltonian of the **isotropic square lattice Ashkin-Teller model** is given by (J. Ashkin and E. Teller, Phys. Rev. 64, 178 (1943)).

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

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

The Ashkin-Teller-Potts Model (Cont.)



- 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**.

Dimers, Squares and Vacancies: A Polydisperse Hard-Core system

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

- The Partition function of this model is given by

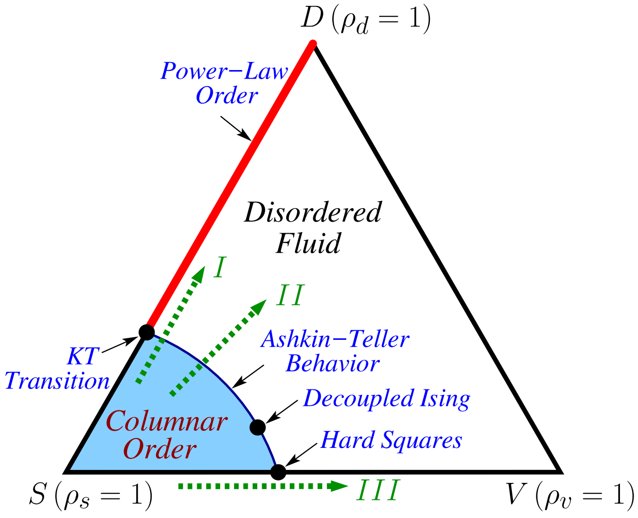
$$Z_{dsv} = \sum_{\mathcal{C}_{dsv}} z_s^{N_s} z_d^{N_d} z_v^{N_v} \ . \tag{4}$$

- 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 $w = z_d / \sqrt{z_s}$.

Dimers, Squares and Vacancies: Theoretical Predictions

- At Full Packing: **generalized height mapping** $\rightarrow \mathcal{S} \sim g \int d^2 r |\nabla h|^2$.
- The introduction of squares causes a $\mathcal{Z}_4$ anisotropy $\sum_{n=4,8...} \epsilon_n \cos(2n\pi h)$ to this action.
- Vacancies introduce **vorticity**.
- We can use the powerful theory developed by **J. V. Jose, L. P. Kadanoff, S. Kirkpatrick, and D. R. Nelson, Phys. Rev. B 16, 1217 (1977)**: vorticity and anisotropy "balance" along a **line of fixed points**, with **continuously varying critical exponents**.

Dimers, Squares and Vacancies: Expected Phase Diagram



Dimers, Squares and Vacancies: Scaling Predictions

- What is the **Order Parameter** in this case?

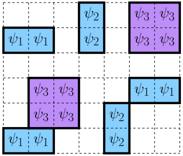


Figure: Values of the columnar order parameter field $\psi(\vec{r})$.

- We define the local complex order parameter:

$$\psi_1 = (-1)^m,\ \psi_2 = -i(-1)^n,\ \psi_3 = [(-1)^m - i(-1)^n]/\sqrt{2}\,. \qquad (5)$$

- At full packing $\rightarrow$ reduces to the well-known dimer model height mapping.

Dimers, Squares and Vacancies: Scaling Predictions (Cont.)

- In terms of the microscopic Ising variables

$$\psi(\vec{r}) \equiv \frac{\sigma(\vec{r}) + \tau(\vec{r})}{2} + i\frac{\sigma(\vec{r}) - \tau(\vec{r})}{2}. \quad (6)$$

- Lattice symmetries imply:

$$\langle \sigma(\vec{r}_1)\tau(\vec{r}_2)\rangle = 0 \ , \ \langle \sigma(\vec{r})\sigma(0)\rangle = \langle \tau(\vec{r})\tau(0)\rangle. \quad (7)$$

- Along the AT phase boundary: $\langle \psi^*(\vec{r})\psi(0)\rangle \sim 1/r^{1/4}$,

- while $\langle \mathrm{Re}(\psi^2(\vec{r}))\mathrm{Re}(\psi^2(0))\rangle \sim 1/r^{\eta_2(v)}$, with $\eta_2(v) \in [0, 1]$.

- The Ashkin-Teller behaviour implies $\eta_2 = 1 - 1/(2\nu)$.

Update Algorithm

- 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

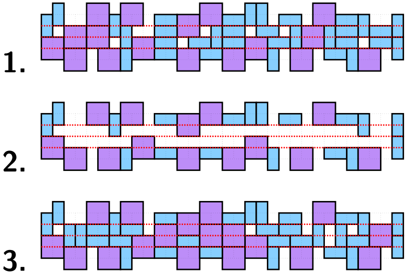


Figure: Steps in the transfer-matrix based algorithm.

- 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.

Transfer-Matrix Based Update: States and Morphology

- There are additional constraints due to the **presence of particles immediately above and below this ladder**.

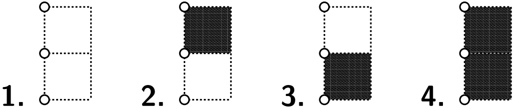


Figure: The four possible underlying morphologies $\sigma = 1, 2, 3, 4$ of a two-plaquette rung.

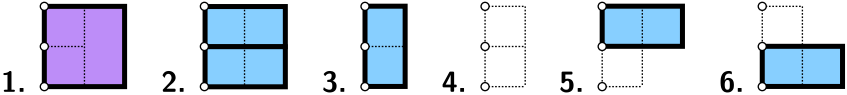


Figure: The six possible states of a two-plaquette rung.

The Transfer Matrices

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

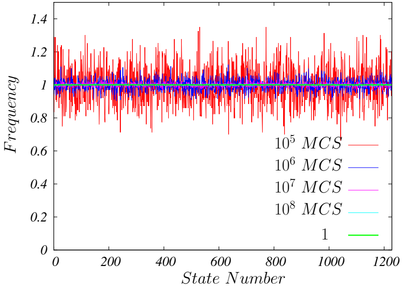
$$Z_{\text{track}}^{closed} = \text{Tr}(\mathcal{T}_L.......\mathcal{T}_3\mathcal{T}_2\mathcal{T}_1). \tag{8}$$

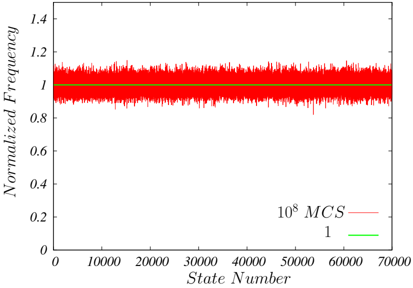
- For Example:

$$\mathcal{T}_{1,1} = \begin{pmatrix} 0 & 0 & 0 & z_s & 0 & 0 \\ 0 & 0 & 0 & z_d^2 & 0 & 0 \\ z_d & z_d & z_d & z_d z_v^2 & z_d z_v & z_d z_v \\ 1 & 1 & 1 & z_v^2 & z_v & z_v \\ 0 & 0 & 0 & z_d z_v & 0 & z_d \\ 0 & 0 & 0 & z_d z_v & z_d & 0 \end{pmatrix}.$$

Exact Enumeration Checks

- Does the algorithm **work**?
- We **enumerate all the possible states** on a 4×4 lattice with periodic BCs
- **1228** for fully packed, **69941** states for dimers+squares+vacancies

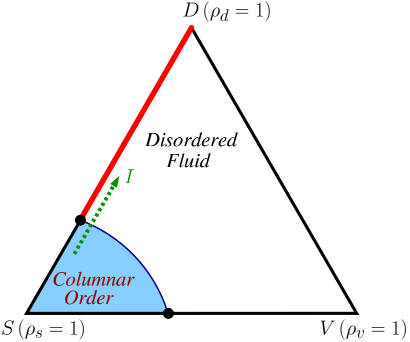




Monte Carlo Simulations

- 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)

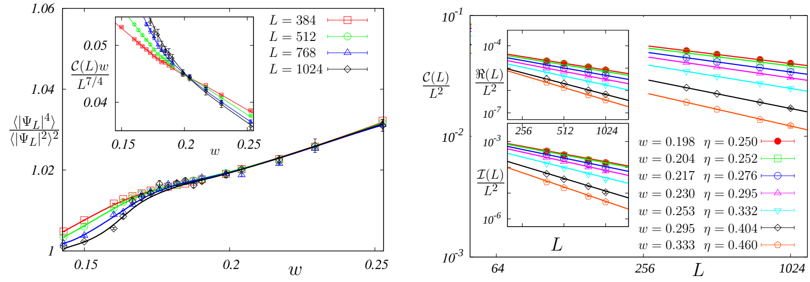
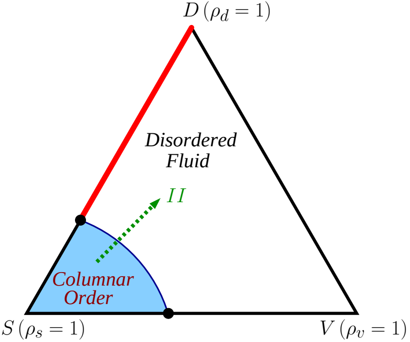


Figure: $w_c^0 \approx 0.198(2)$.

$$\Psi_L \equiv \sum_{\vec{r}} \psi(\vec{r}), \qquad \mathcal{C}(L) = \langle|\sum_{\vec{r}} \psi(\vec{r})|^2\rangle / L^2,$$

$$\Re(L) = \langle(\sum_{\vec{r}} \mathrm{Re}(\psi^2(\vec{r})))^2\rangle / L^2, \qquad \mathcal{I}(L) = \langle[\sum_{\vec{r}} \mathrm{Im}(\psi^2(\vec{r}))]^2\rangle / L^2. \tag{9}$$

Results: Dimers+Vacancies+Squares



Results: Dimers+Vacancies+Squares

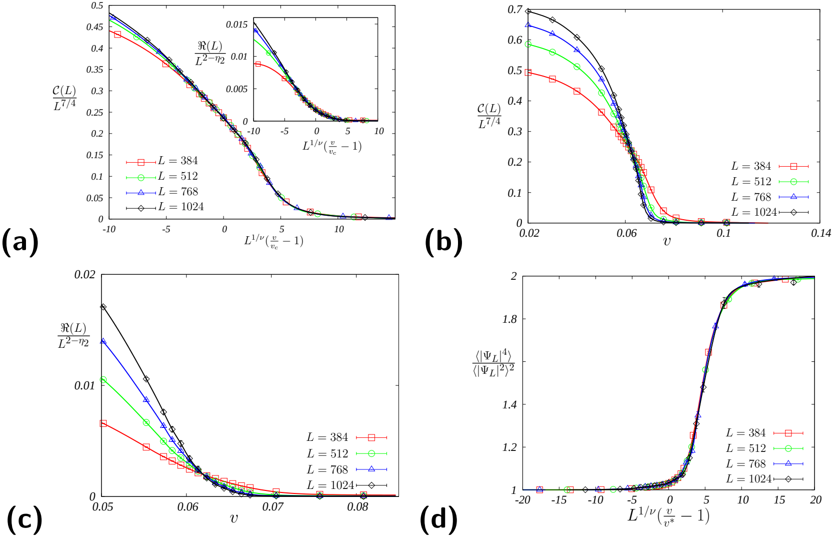
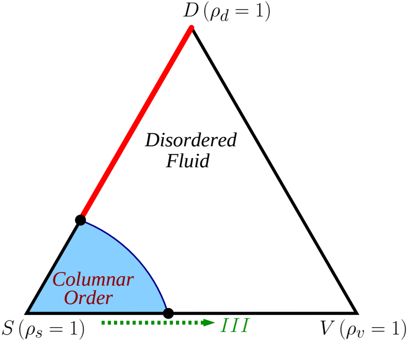


Figure: $v_c = 0.0623(1)$, $w_c = 0.1600(1))$. $\nu = 1.70(5)$. $\eta_2 = 0.70(5)$.

Results: Squares+Vacancies



Results: Squares+Vacancies

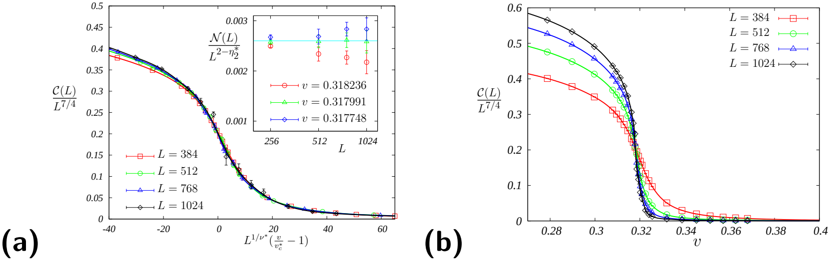


Figure: $v_c^* = 0.31799(30)$, $\nu^* = 0.92(3)$.

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

- Consistent with Ashkin-Teller Criticality.

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 $\mathrm{Re}(\psi^2(\vec{r}))$, the **valence-bond nematic order parameter** decay with the same exponent as the **next-nearest-neighbour bond-energy** $(\mathrm{Im}(\psi^2(\vec{r})))$?
- Additionally, are η_{VBN} and ν **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.