UCDAVIS

Machine Learning of Magnetic, Charge, and Bond Order Phase Transitions

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3. Quantum Models of Itinerant Magnetism
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5. Challenges Posed by Non-Diagonal Order
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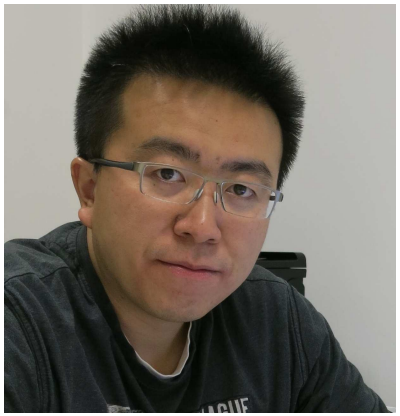

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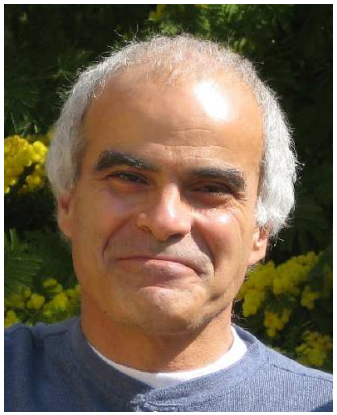

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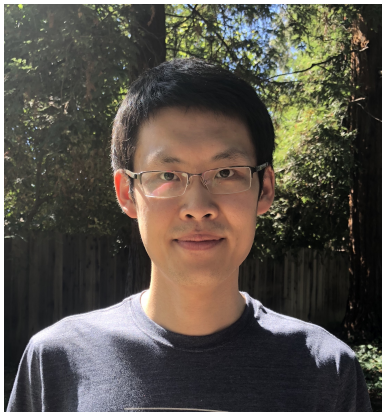

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1. Introduction

Powerful array of existing tools to quantify phase transitions in Monte Carlo:

- Identification of appropriate order parameters.
- Identification of appropriate response functions.
- Finite size scaling.
- Dynamics.

Can require a degree of creativity (even for known order parameter):

- Binder ratio $1 - \langle M^4 \rangle / \langle M^2 \rangle^2$
- Pairing Vertex, $\Gamma = P^{-1} - \bar{P}^{-1}$

Forefront of condensed matter physics today

- Competing types of order

  Cuprates: superconductivity, antiferromagnetism, stripes, nematic, $\cdots$
- More subtle (eg topological) phases.

Develop methods which are useful if the order parameter is not known.

- Recognize novel phases hidden in vast dance of degrees of freedom simulated.

2. Classical Models of Magnetism

Principal Component Analysis

Basic technical data analysis method of many of the results presented here.

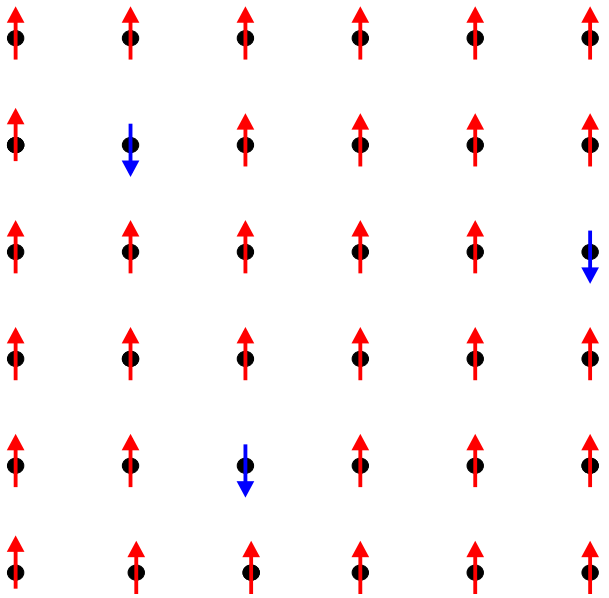
- P simulations at different parameter values (T, U, ρ).
- L configurations (N degrees of freedom S_j) from each simulation.
- Arrange configurations S_j as row j of a matrix X.
- X is rectangular: PL rows and N columns.
- Construct $\mathcal{M} = X^T X$ (square, dimension N).
- Diagonalize $\mathcal{M}$. Eigenvalues λ_i, "relative variance" $\tilde{\lambda}_i = \lambda_i \,/\, \sum_i \lambda_i$
- Inner product of eigenvectors v_i with configurations: $p_{ij} = v_i \cdot S_j$

  "principal components"
- Topology of $\{ (p_{1j}, p_{2j}) \}$ through transition (v_1, v_2: two largest λ_1, λ_2).
- Quantified principal components: $\mathcal{P}_i = \langle \, | \, p_i \, | \, \rangle = \sum_j | \, p_{ij} \, |$

Ising Model $E = -J \sum_{\langle ij \rangle} S_i S_j$ $S_i = \pm 1$

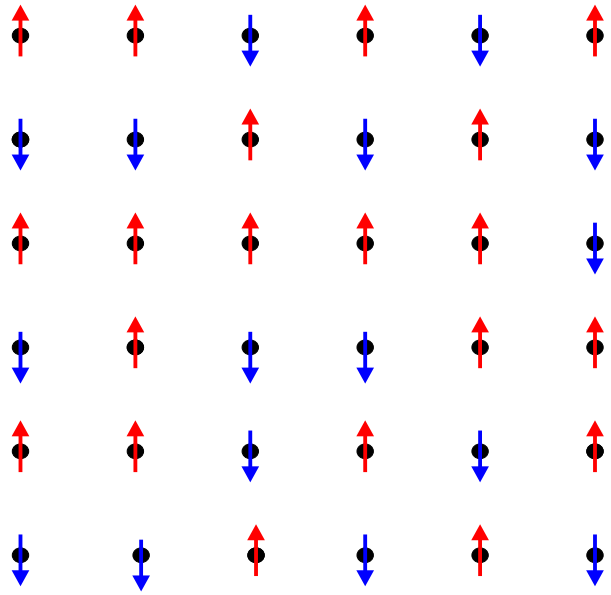
Order parameter $M = \langle \sum_i S_i \rangle$ magnetization

Energy E favors parallel spin configurations:



$M \neq 0$

Entropy S favors random spin configurations:



$M = 0$

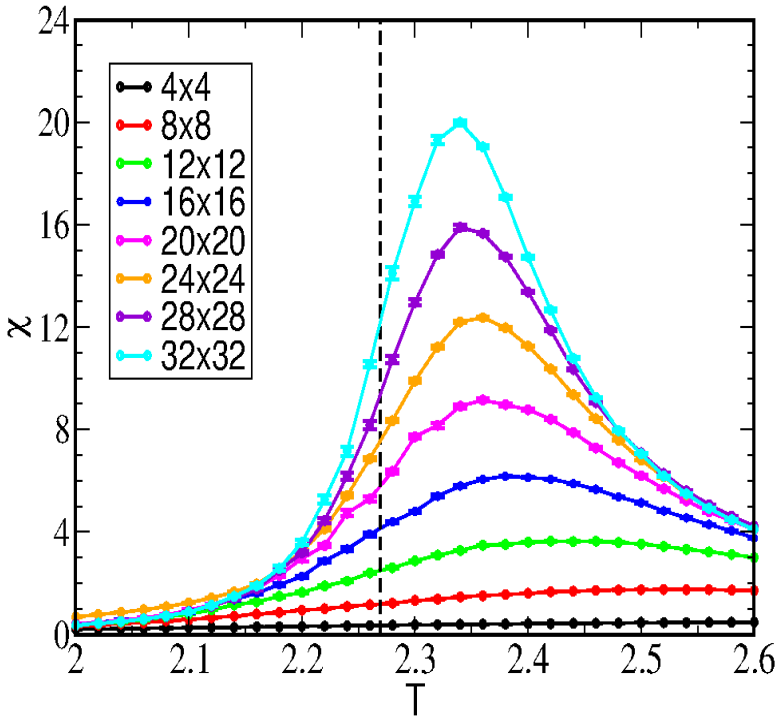
Minimize Free Energy $F = E - TS$

Temperature T controls whether E or S wins.

Ising Model $\quad E = -J \sum_{\langle ij \rangle} S_i S_j \quad S_i = \pm 1$

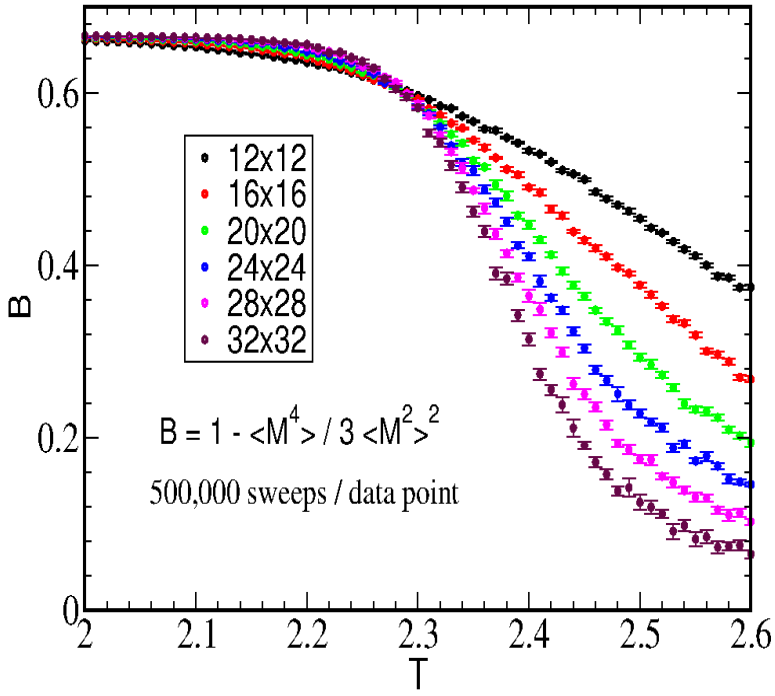
Magnetic susceptibility

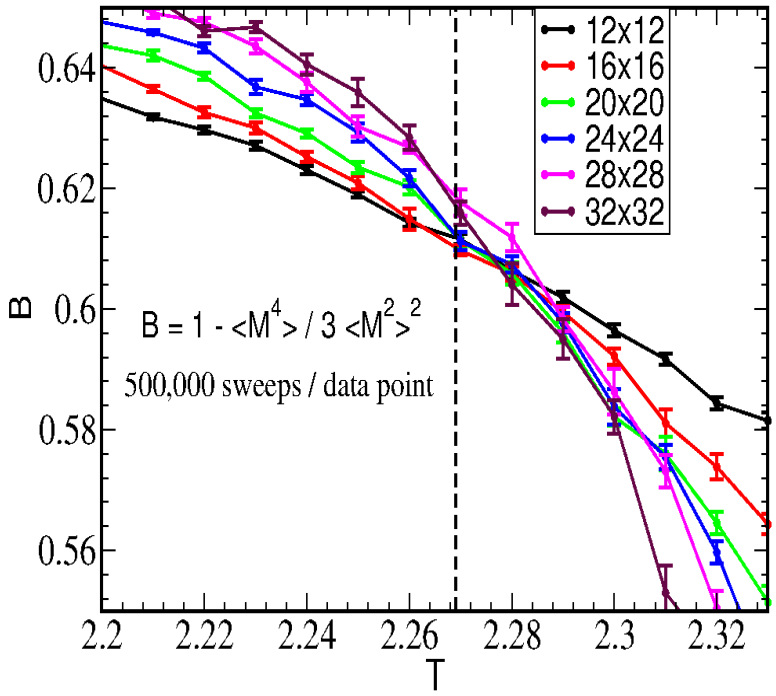
$\chi = \frac{1}{T}(\langle M^2 \rangle - \langle M \rangle^2)$



Ising Model $\quad E = -J \sum_{\langle ij \rangle} S_i S_j \quad S_i = \pm 1$

Binder Ratio provides very accurate T_c

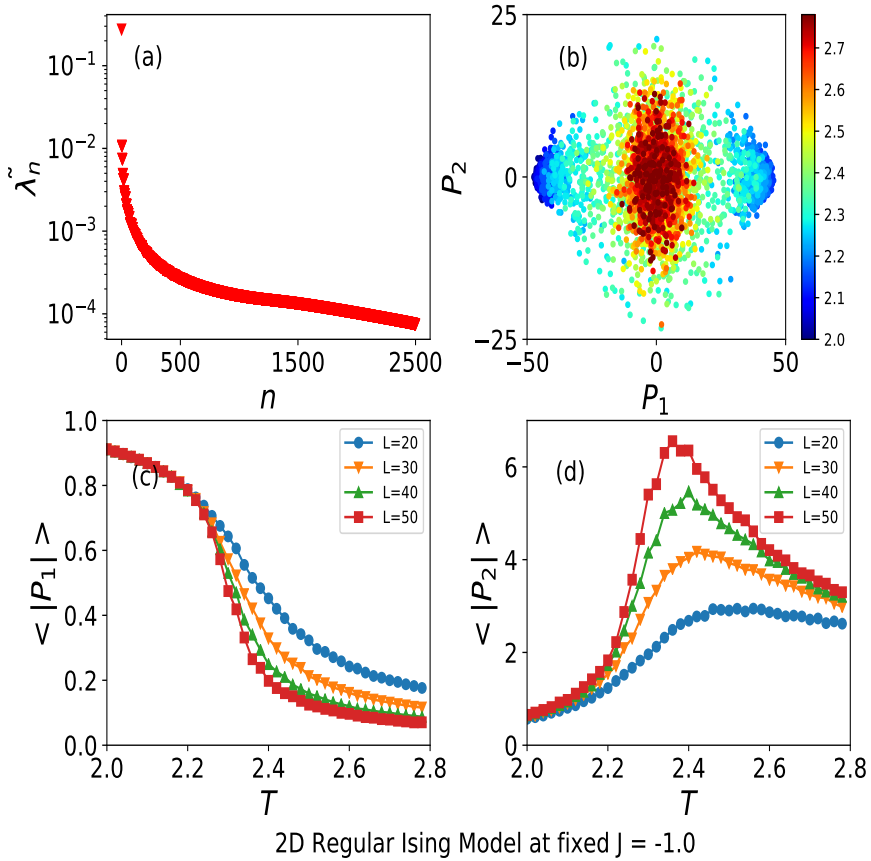




Single spin flip Metropolis $\rightarrow$ cluster algorithms (Wolfe, etc)

Ising Model $E = -J \sum_{\langle ij \rangle} S_i S_j \qquad S_i = \pm 1$

[See also L. Wang, PRB94, 195105 (2016);
J. Liu, Y. Qi, Z.Y. Meng and L. Fu, PRB95, 041101 (2017)]

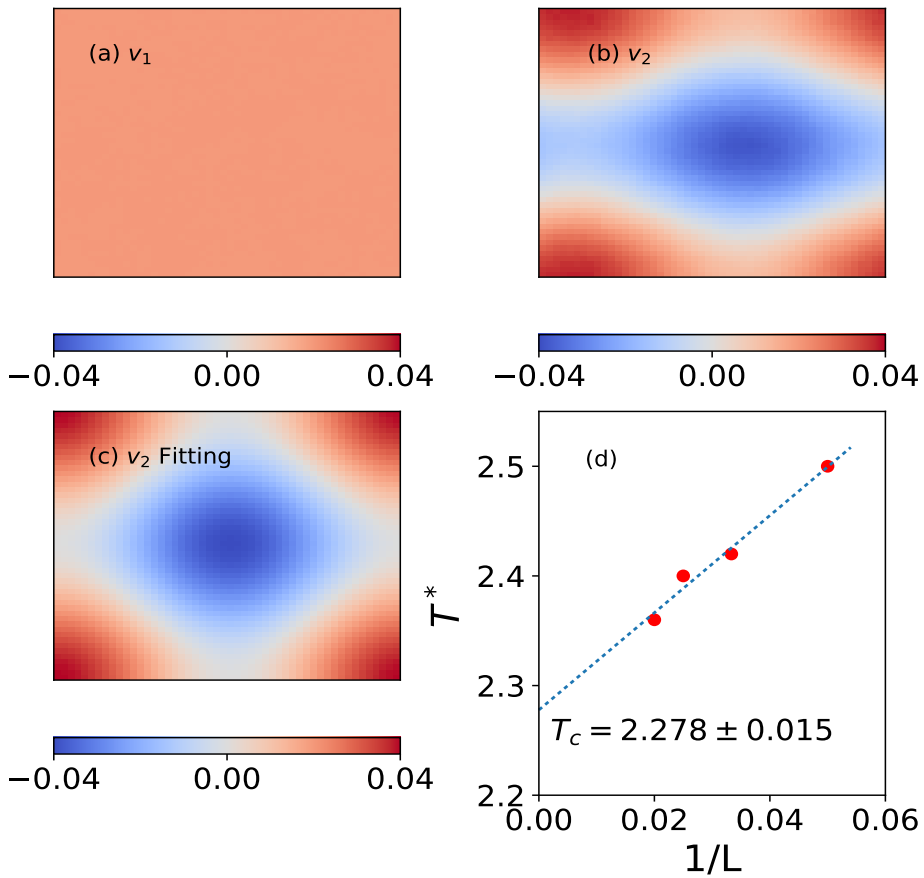


(a) Relative variances $\tilde{\lambda}_i$ drop rapidly with i

(b) $\{ (p_{1j}, p_{2j}) \}$ changes topology at $T_c \sim 2.269$. bifurcates $\rightarrow$ 2 clusters.

(c) $\mathcal{P}_1$ mimics $\langle \, | \, M \, | \, \rangle$.

(d) $\mathcal{P}_2$ mimics χ.



2D Regular Ising Model at fixed J = -1.0

(a) Leading eigenvector v_1 uniform (ferromagnetic).

(b) Subleading eigenvector v_2 domain walls.

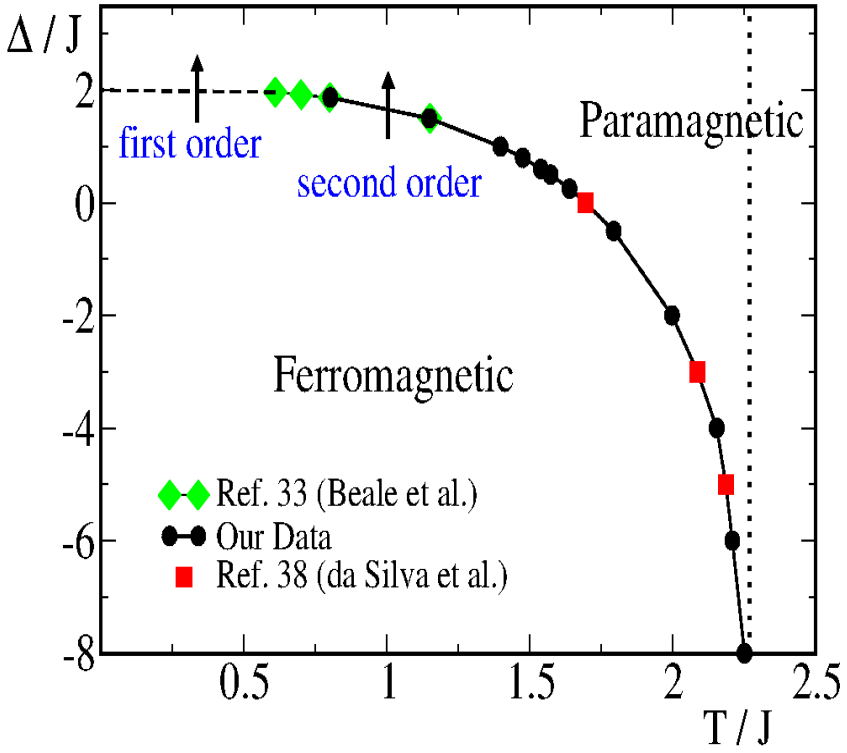
(c) Compare to $v_2' = \big(\cos(r_1 k_1), \cos(r_2 k_1), \cdots\big) + \big(\cos(r_1 k_2), \cos(r_2 k_2), \cdots\big)$
$k_1 = (2\pi/L, 0),\ k_1 = (0, 2\pi/L)$

(d) Extrapolate peaks T^* of $\mathcal{P}_2(T)$ with $1/L$.

Blume-Capel Model $E = -J \sum_{\langle ij \rangle} S_i S_j + \Delta \sum_i S_i^2 \quad S_i = 0, \pm 1$

Δ is "Impurity potential"

$\Delta < 0$ favors $S_i = \pm 1$ $\qquad$ $\Delta > 0$ favors $S_i = 0$

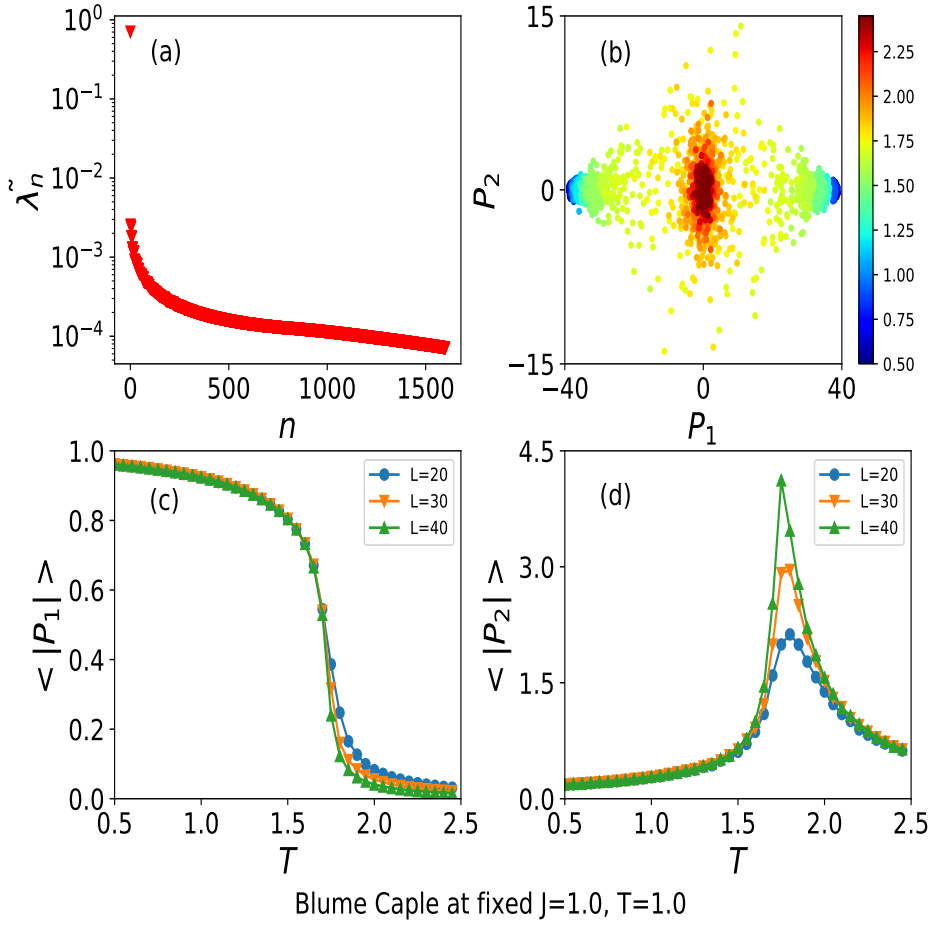


Ising Model in limit $\Delta \to -\infty$

Tricritical point:

$(T/J, \Delta/J) \sim (0.61, 1.97)$

Blume-Capel Model in second order regime, $T = 1.0$.



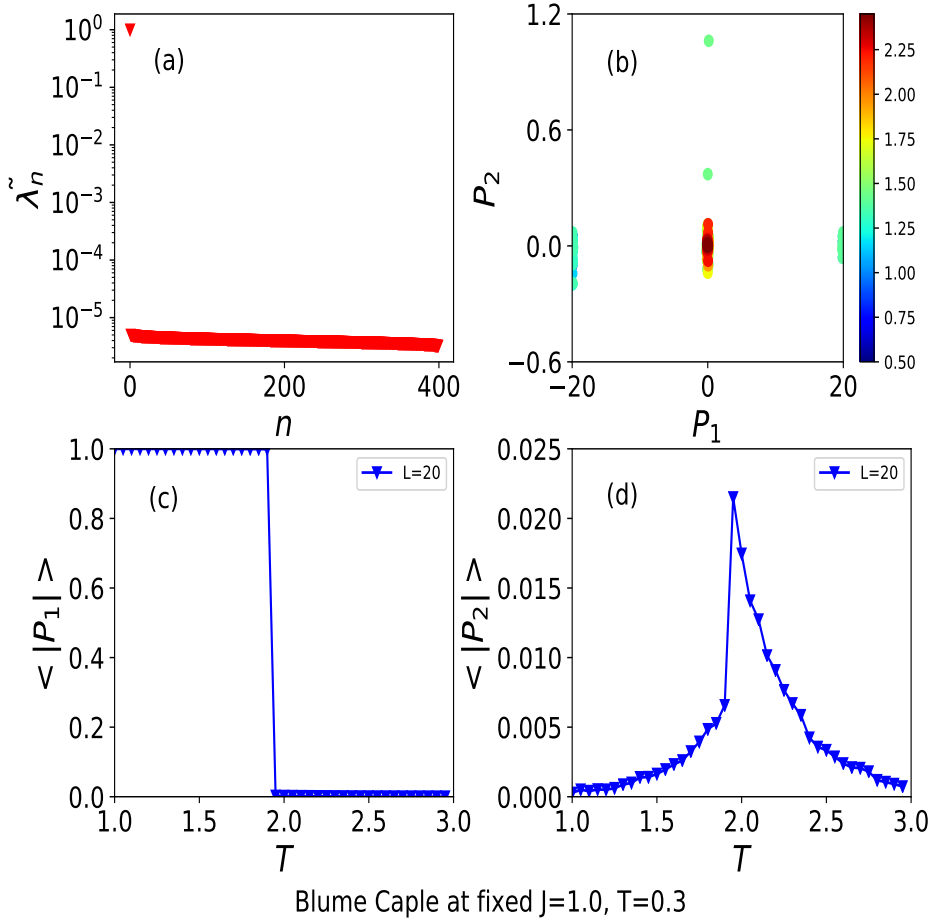
(a) Relative variances $\tilde{\lambda}_i$ drop rapidly with i

(b) $\{ (p_{1j}, p_{2j}) \}$ changes topology at $\Delta_c \sim 1.7$. 2 cluster bifurcation.

(c) $\mathcal{P}_1$ mimics $\langle | M | \rangle$.

(d) $\mathcal{P}_2$ mimics χ.

Blume-Capel Model in first order regime, $T = 0.3$.



(a) Relative variances $\tilde{\lambda}_i$ drop rapidly with i

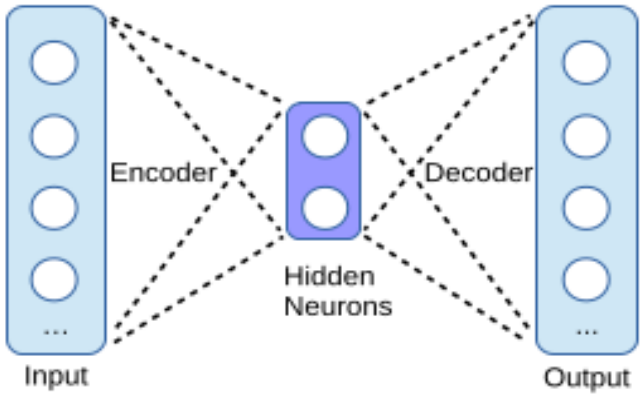
(b) $\{ (p_{1j}, p_{2j}) \}$ changes topology at $\Delta_c \sim 2.0$.

(c) $\mathcal{P}_1$ mimics $\langle | M | \rangle$.

(d) $\mathcal{P}_2$ mimics χ.

First order character is evident!

Autoencoder



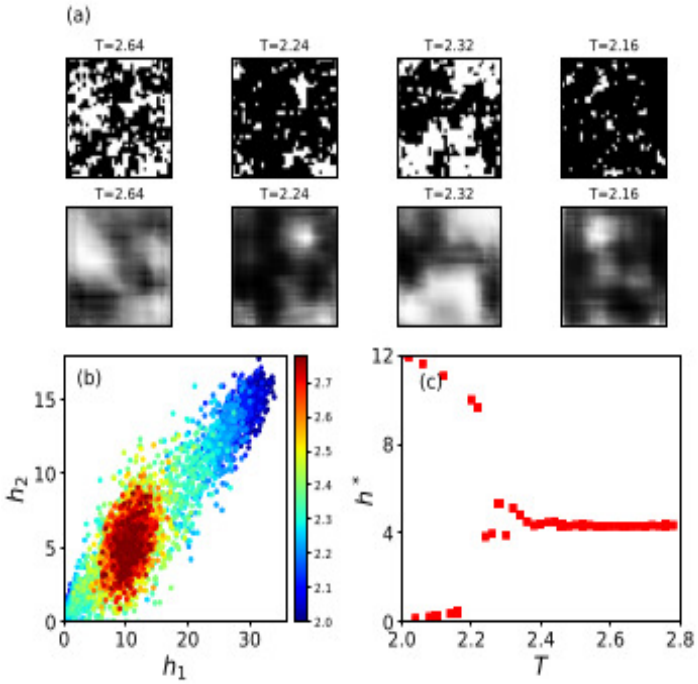
Artificial Neural Network (unsupervised learning)

Like PCA: dimensional reduction

Unlike PCA: nonlinear

Compressed representation:

Reproduce original spin configuration despite reduced hidden layer information storage



(a) Spin configuration (top) $N = 40 \times 40$
Reconstruction (below) 200 hidden neurons

(b) Two hidden neurons activations (h_1, h_2)
Similar to PCA.

(c) Single hidden neuron
average over 10000 samples at each T.

3. Quantum Models of Magnetism and Charge Order

Methodology is determinant Quantum Monte Carlo (DQMC).

Electron-electron interactions decoupled via introduction of discrete 'Hubbard-Stratonovich' field $S_{i\tau}$.

$S_{i\tau}$ has spatial $i = 1, 2, \cdots N$; imaginary time $\tau = 1, 2, \cdots L$ indices.

$L = \beta/\Delta\tau$: number of divisions of inverse temperature.

Sign Problem except in special cases like half-filling (one fermion per site)

*** Can machine learning help with sign problem?! ***

Different Options for PCA:

- Provide $S_{i\tau}$ for all i at single τ, or all τ at single i.
- Provide $S_{i\tau}$ for all i, τ.
- Provide a 'derived quantity': e.g. Greens function.

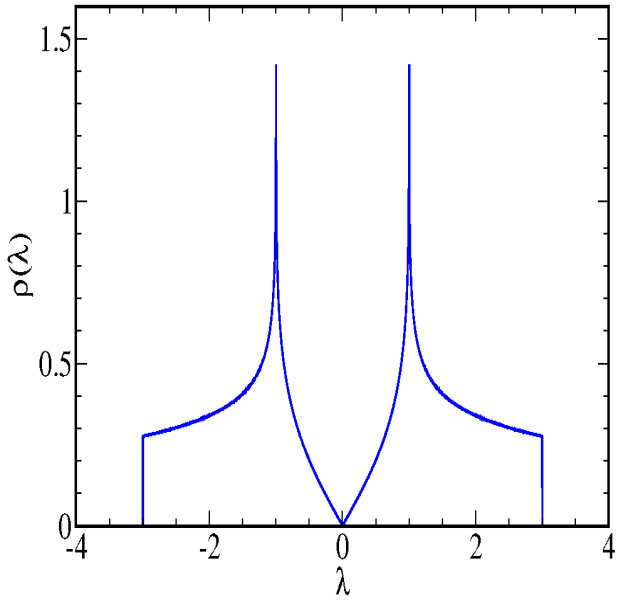
Prior work (very partial list!):
Xiao Yan Xu, Yang Qi, Junwei Liu, Liang Fu, Zi Yang Meng, Phys. Rev. B96 041119R (2017).
K. Ch'ng, J. Carrasquilla, R.G. Melko, and E. Khatami, Phys. Rev. X7 031038 (2017).
P. Broecker, J. Carrasquilla, R.G. Melko, and S. Trebst, Nature Sci. Rep. 7, 8823 (2017).
S. Li, P.M. Dee, E. Khatami, and S. Johnston, Phys. Rev. B100, 020302 (2019).

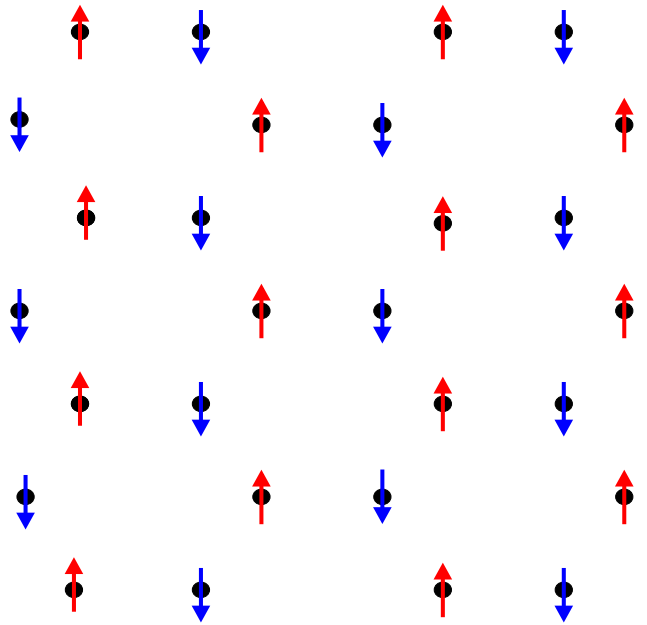
Hubbard Model on honeycomb lattice (graphene).

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Semimetallic density of states at half-filling (one electron per site).

Antiferromagnetic order (at $T = 0$) only if $U > U_c \sim 3.8$.

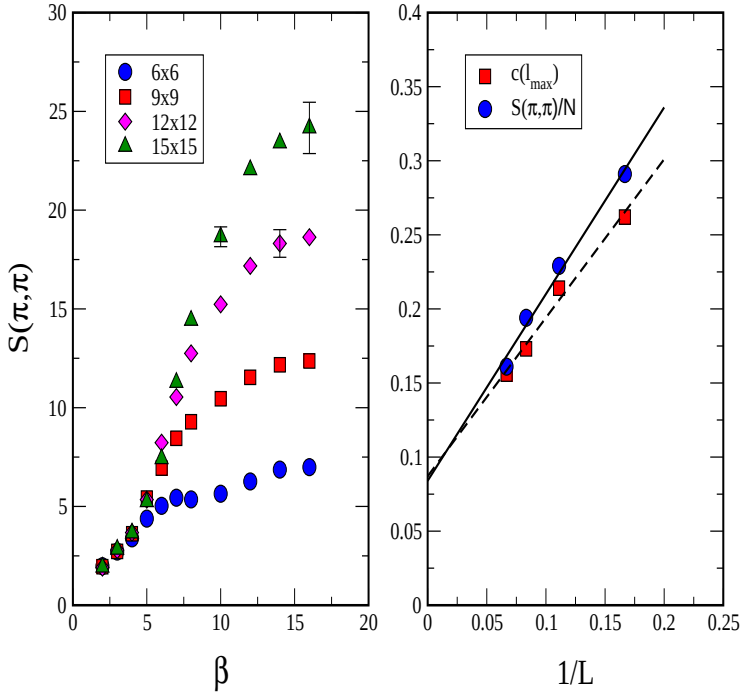




Hubbard Model on honeycomb lattice.

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Honeycomb lattice, half-filling: AF order if $U > U_c \sim 3.8$.



Antiferromagnetic structure factor

$S(\pi, \pi) = \sum_{i,j} (-1)^{i-j} \; c(i-j)$

$c(i-j) = \langle \, m_i m_j \, \rangle$

$m_i = n_{i\uparrow} - n_{i\downarrow}$

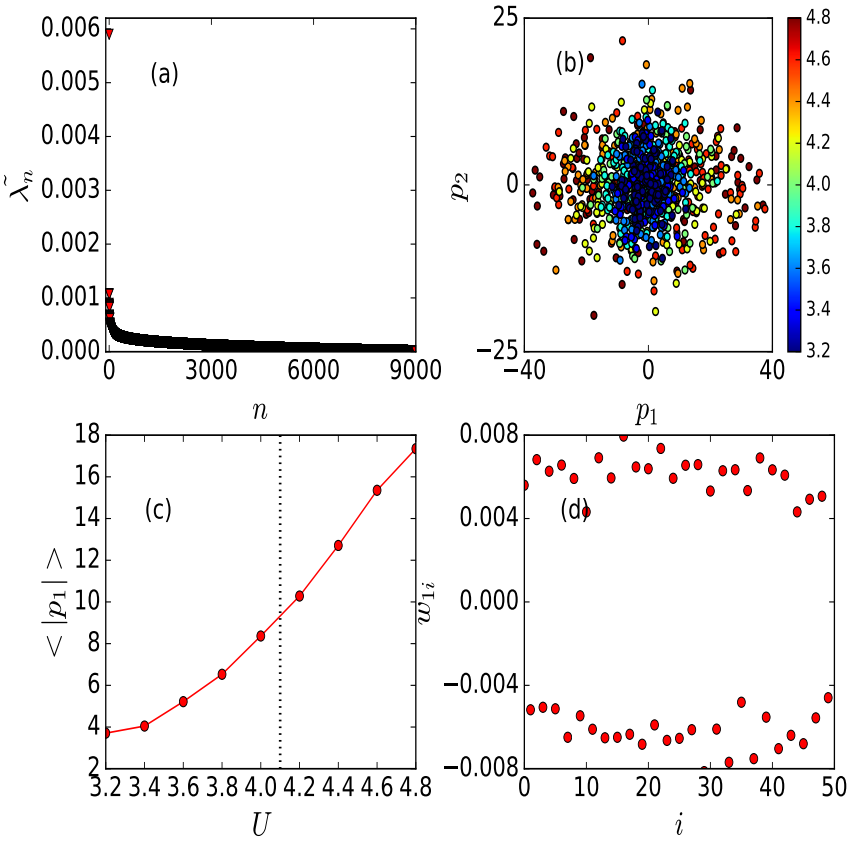
If $c(i-j)$ is long ranged, $S(\pi, \pi) \sim N$

At left: $U = 6.0 > U_c$:

Hubbard Model on honeycomb lattice.

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Honeycomb lattice, half-filling: AF order if $U > U_c \sim 3.8$.



(a) Dominant variance $\tilde{\lambda}_i$

(b) Central $(\mathcal{P}_1, \mathcal{P}_2)$ peak expands as U increases.

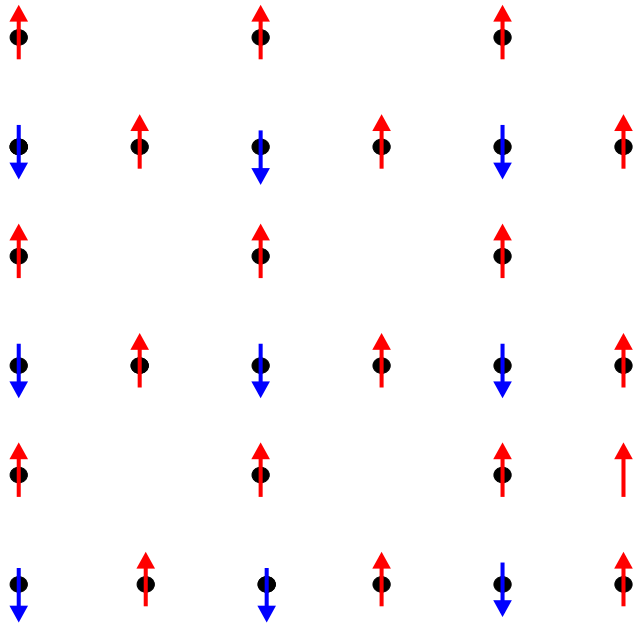
(c) Principal component

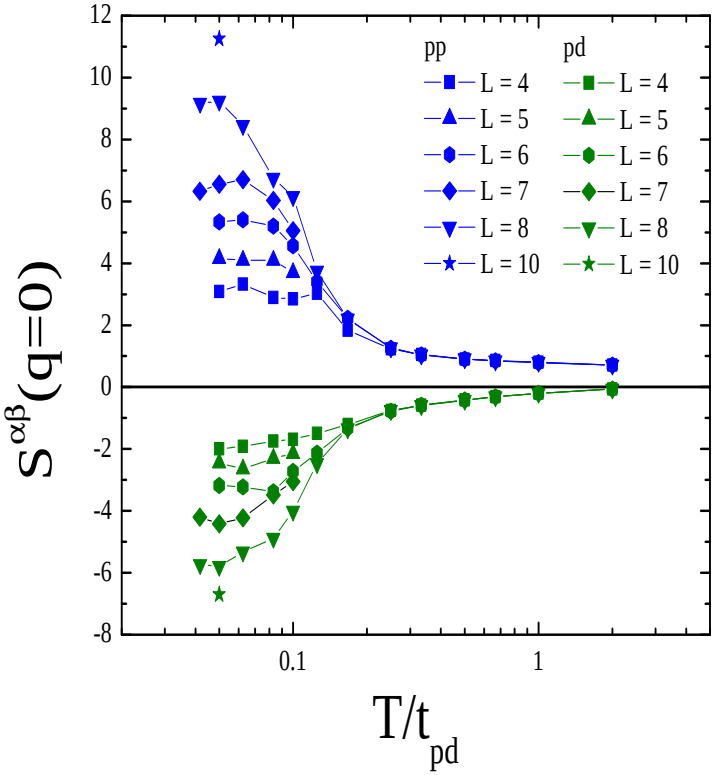
(d) AF pattern.

Hubbard Model on Lieb Lattice

Three bands: two dispersing, bracket flat band.

Ferrimagnetic order at half-filling of whole lattice.





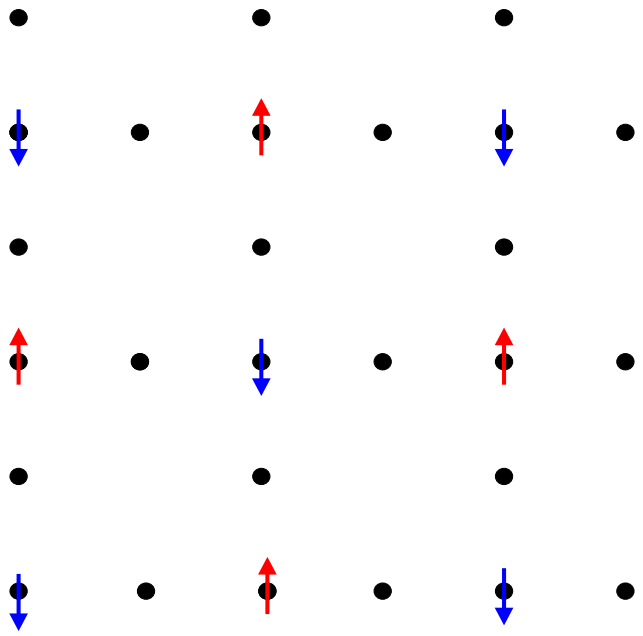
Hubbard Model on Lieb Lattice

Positive site energy to depopulate 'bridging sites'

(oxygen atoms in CuO_2 planes of cuprate superconductors).

Remaining population of square lattice

(copper atoms in CuO_2 planes of cuprate superconductors).

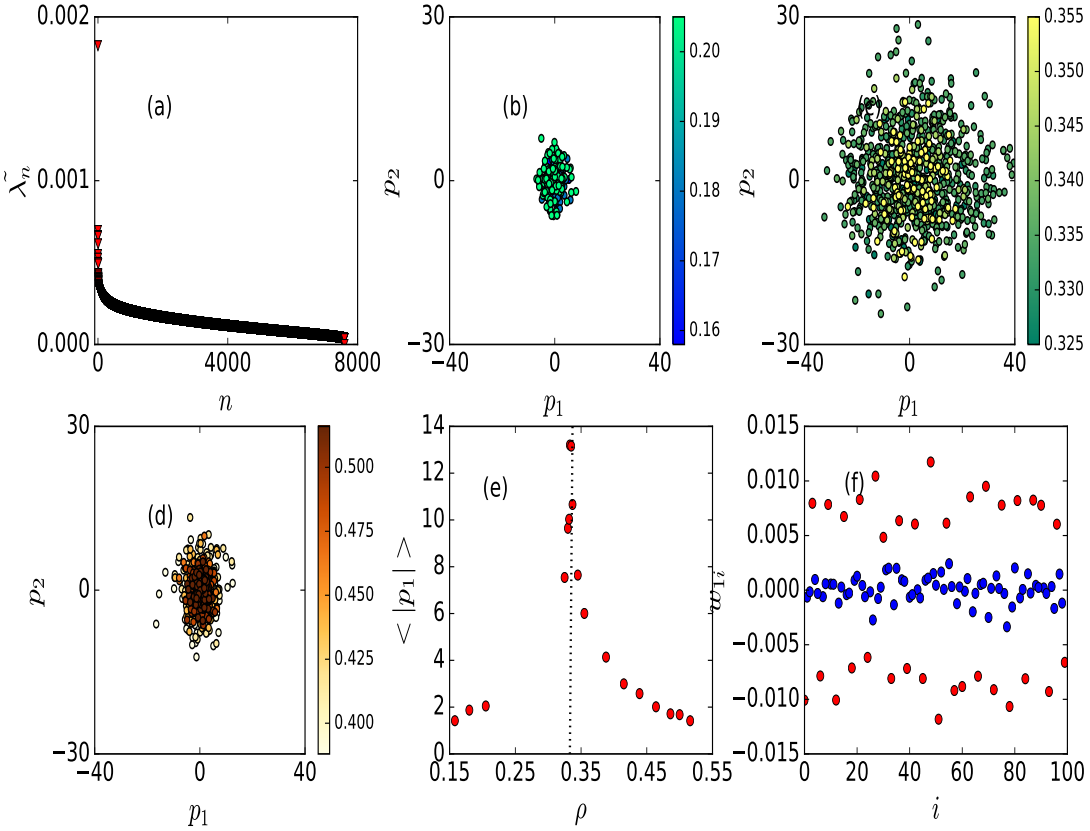


!! Sign Problem !!

Hubbard Model on Lieb Lattice

Three bands: two dispersing, bracket flat band.

Half-filling of lowest band only ($\rho = 1/3$) AF order.



(a) Dominant variance $\tilde{\lambda}_i$

(b,d) Central $(\mathcal{P}_1, \mathcal{P}_2)$ peak

(c) expanded $\rho \sim 1/3$.

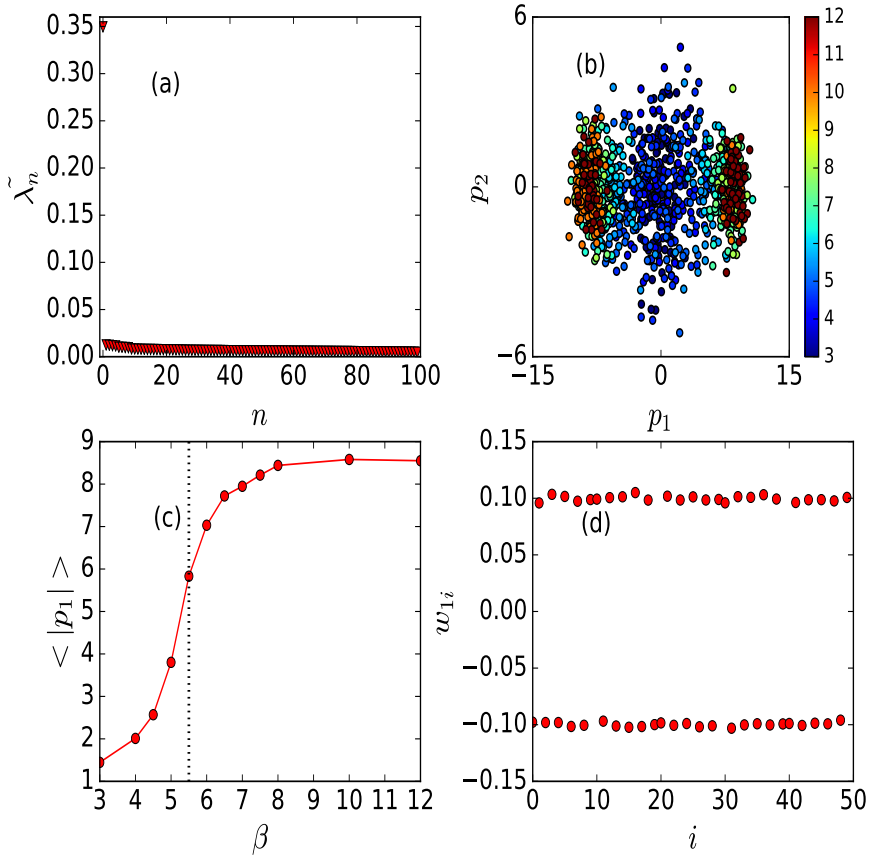
(e) $\mathcal{P}_1$ peak at $\rho = 1/3$.

(f) AF pattern ("copper" sites).

PCA for doped system (weak sign problem).

Holstein model: e^- coupled to phonons: $S_{i\tau} \to x_{i\tau}$.

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma} \right) + \frac{1}{2} \sum_i \left(p_i^2 + \omega^2 x_i^2 \right) + g \sum_i x_i \left(a_i^\dagger + a_i \right)$$



Half-filling: Simultaneous CDW and SC order at $T = 0$.

Doped: SC transition of KT type (these results). $\beta_c \sim 8$.

(a) Dominant variance $\tilde{\lambda}_i$

(b) $(\mathcal{P}_1, \mathcal{P}_2)$ divides at low T.

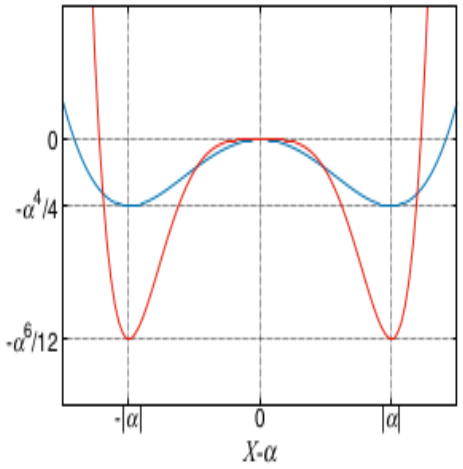
(c) $\mathcal{P}_1$ order onset $\beta \sim 6$.

(d) Remnant CDW order.

P.M. Dee, J. Coulter, K.G Kleiner, and S. Johnston, Comm. Phys. 3, 1 (2020).

S. Li and S. Johnston, Nature Quantum Mat. 5, 1 (2020).

4. Self Learning Monte Carlo, Role of Symmetry

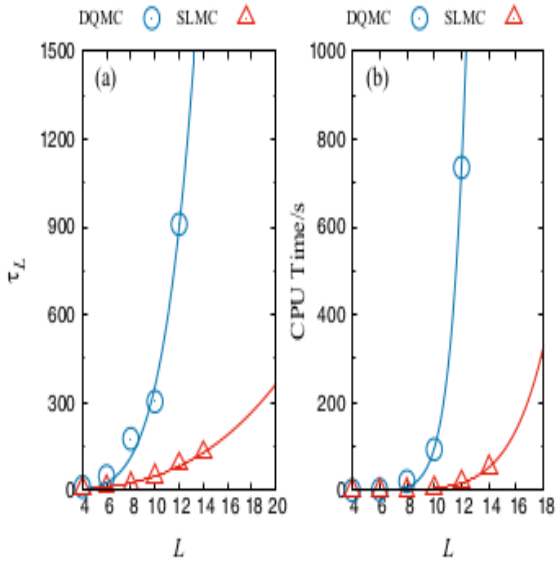


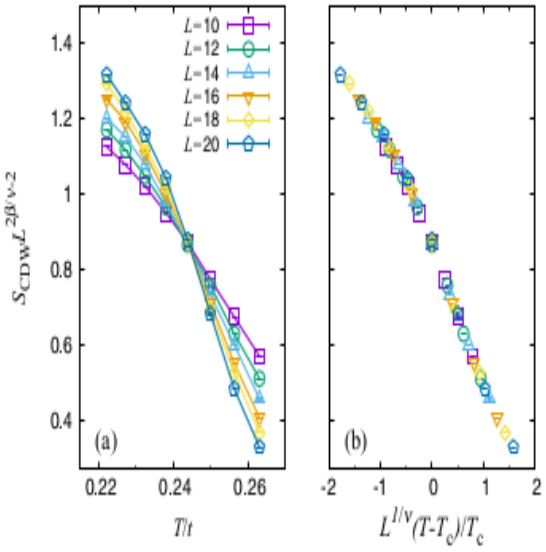
Train local effective model S_{eff}

Reduce $o(N^3)$ fermion determinant evaluation

S_{eff} captures 'polaron' minima $X - \frac{g^2}{\omega^2} = \pm\frac{g^2}{\omega^2}$

couples phonons in space and imaginary time





Autocorrelation time reduced

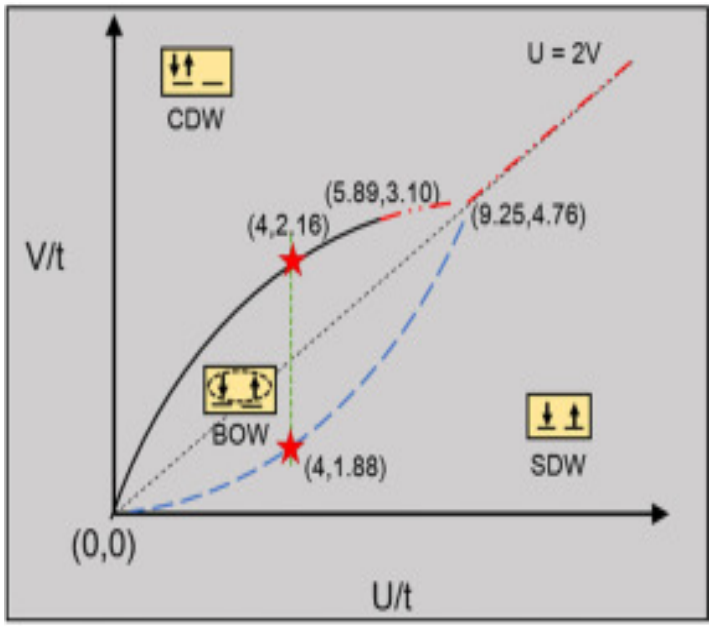
FSS captures T_c

5. Challenges Posed by Non-Diagonal Order

"Visualizing strange metallic correlations in the two-dimensional Fermi-Hubbard model with artificial intelligence," E. Khatami, E. Guardado-Sanchez, B.M. Spar, J.F. Carrasquilla, W.S. Bakr, R. Scalettar, Phys. Rev. A102, 033326 (2020).

An older example: Extended Hubbard Model

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right) + \mathbf{U} \sum_{i} n_{i\uparrow} n_{i\downarrow} + \mathbf{V} \sum_{\langle ij \rangle} n_i n_j$$



$U > 2V$: Spin density wave (AF)

up/down spin alternates

$U < 2V$: Charge density wave

empty, double occupation alternates

$U \sim 2V$: "Bond Ordered Wave"

High/low kinetic energy alternates

Order **not** in density operators.

$\Rightarrow$ Khatami talk

6. Conclusions

Machine learning method can accurately discern phase transitions.

Magnetism: Classical Ising and Blume-Capel

- Dominant principle component $\leftrightarrow$ order parameter;
- Recognizes symmetry breaking; first vs second order transitions.
- Sub-dominant principle components: small q behavior (domain walls).

Magnetic and Charge Order: Quantum Hubbard and Holstein Models

- Similar to classical: principal component bifurcation $\rightarrow$ transition
- Effective even in doped case (sign problem!)

  Configurational snapshots: ML does not require $\frac{\langle \mathcal{S}\mathcal{O} \rangle}{\langle \mathcal{S} \rangle}$!!

  $\Rightarrow$ **Johnston talk**

** Use ML for doing more effective simulations, not just data analysis **

What about more "subtle" situations?

- Bond Ordered Wave phase of extended Hubbard model.
- Strange Metal phase of square lattice Hubbard model (and cuprates)

  $\Rightarrow$ **Khatami talk**