Entanglement in Strongly Correlated Systems
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Introduction to Quantum Monte Carlo

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Why bother?

Estimating scaling dimension by TRG, TNR, etc is very elegant, and when it works it produces very accurate results.

But so far not many universality classes have been examined in this way.

Quantum Monte Carlo is still one of the standard methods for studying large systems to obtain reliable characterization of critical points of a given system.

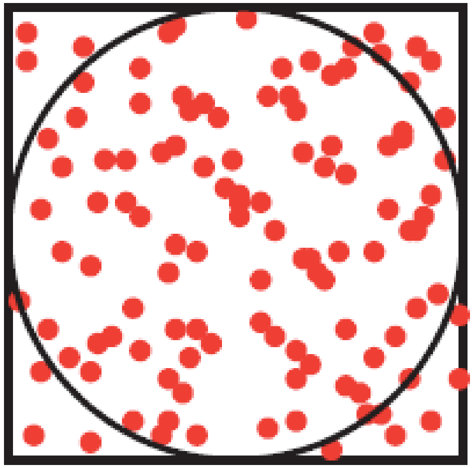
Importance Sampling

Problem: Compute the momentum of inertia of a circle.

$$X = \int_{x^2+y^2 \le 1} dxdy \left(x^2 + y^2\right)$$

<u>Strategy I (random sampling)</u>

1) Generate a point in [-1,1]x[-1,1] uniform randomly.
2) If the point is in the circle, S += x^2+y^2.
3) Repeat 1) and 2), N times.
4) X := 4 x S / N



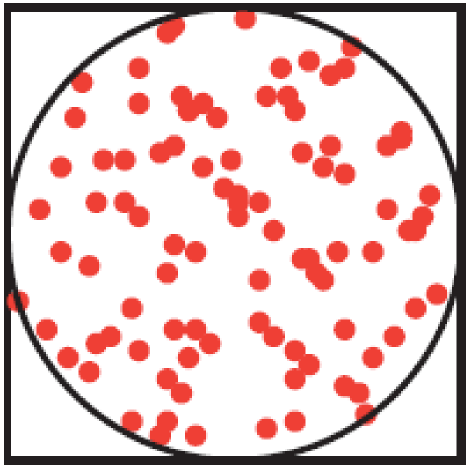
Importance Sampling

Problem: Compute the moment of inertia of a circle.

$$X = \int_{x^2+y^2\le 1} dxdy \left(x^2 + y^2\right)$$

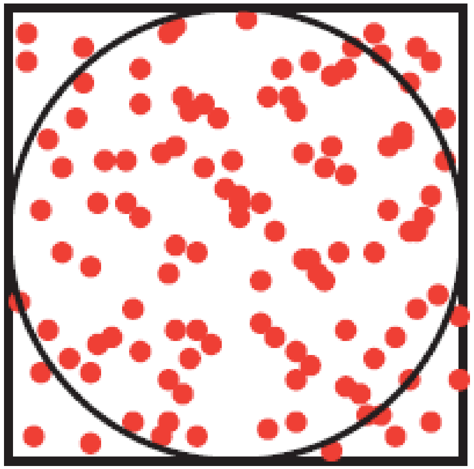
Strategy II (importance sampling)

0) Choose any point (x,y) in **the circle.**
1) Shift the point by a uniform random vector (dx,dy) where dx, dy is a uniform random number in [-D,D]
2) If the point (x+dx,y+dy) is still in the circle x := x+dx, y := y+dy
3) S += x^2+y^2.
4) Repeat 1) through 3), N times.
5) X := π x S / N

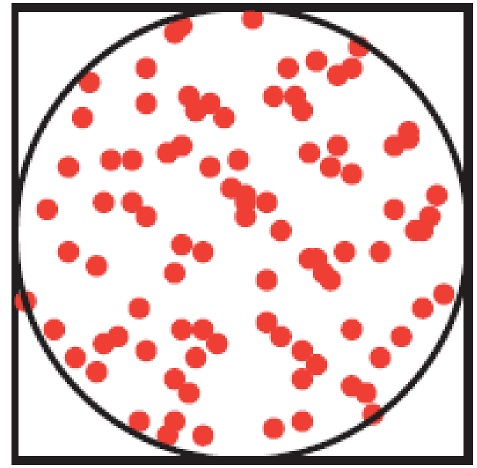


Importance Sampling

Random Sampling



Importance Sampling



$$\frac{V_d}{2^d} \approx \frac{\pi^{d/2}}{2^d \Gamma\left(\frac{d}{2}+1\right)} \approx \left(\frac{\pi e}{2d}\right)^{\frac{d}{2}} \to 0$$

High dimensions kill random sampling.

Markov Chain

$$X_0 \rightarrow X_1 \rightarrow X_2 \rightarrow X_3 \rightarrow \cdots$$

X_t :state at the t-th step

$T(X' \mid X)$:transition probability

$P_t(X_t)$: the probability of having X_t at the t-th step

$$P_{t+1}(X_{t+1}) = \sum_{X_t} T(X_{t+1} \mid X_t) P_t(X_t)$$

or simply,

$$\boldsymbol{P}_{t+1} = T\boldsymbol{P}_t$$

Detailed Balance

Designing a Markov chain

We demand,

$$T_{ij}W_j = T_{ji}W_i$$

e.g. $W_i = e^{-\beta E_i}$

W_i : the target distribution

$$\Rightarrow \quad \boldsymbol{TW} = \boldsymbol{W}$$

Ergodicity

"After a sufficiently long time, any state can appear with non-zero probability."

$$\exists t_0 \, \forall t > t_0 \, \forall (i, j) \left(\left(T^t \right)_{ij} > 0 \right)$$

- T must be irreducible.
- Cyclic solution should be excluded.

Renyi (1960)
Gubernatis, Werner, NK (2016)

Convergence and H-Theorem

"Error" $\varepsilon(\boldsymbol{p}) \equiv \left|\boldsymbol{p} - \boldsymbol{p}^*\right|_1$

$$\left(\boldsymbol{p}^* \equiv \frac{\boldsymbol{W}}{\left|\boldsymbol{W}\right|_1} \text{ : the target distribution} \right)$$

Free energy (or Kulback-Leibler Information)

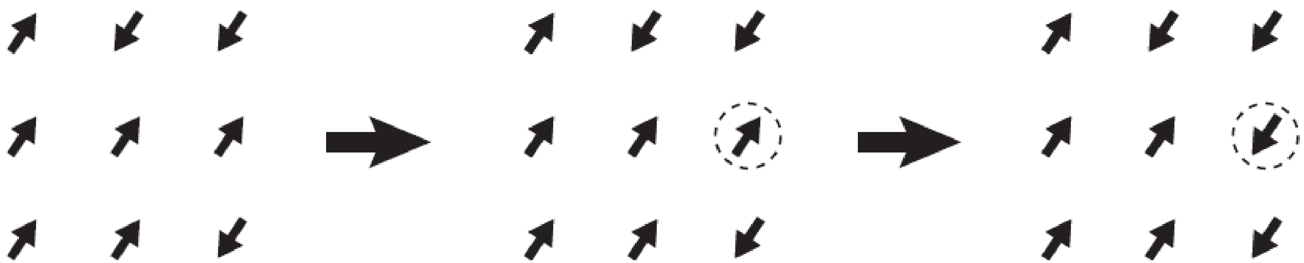
$$F \equiv T I_{\mathrm{KL}} \ , \quad I_{\mathrm{KL}}\left(\boldsymbol{p} \,\|\, \boldsymbol{p}^*\right) \equiv \sum_i p_i \log \frac{p_i}{p_i^*}$$

Both $\varepsilon(\boldsymbol{p}_t)$ and $I_{\mathrm{KL}}\left(\boldsymbol{p}_t \,\|\, \boldsymbol{p}^*\right)$ monotocally decrease,

and converge to 0 in the limit $t \to \infty$.

Local Update for Ising Model

$W_i \propto e^{-K}$ $\qquad$ $W_j \propto e^{K}$



$$T_{ji} = \frac{W_j}{W_i + W_j} = \frac{e^{K}}{e^{-K} + e^{K}}$$

satisfies the detailed balance condition, $T_{ij} W_j = T_{ji} W_i$

Failure of Local Update

The configuration changes only locally at each step.

Similar to a diffusion process, or a random walk.

It takes a very long time to create/annihilate large magnetic clusters.

Autocorrelation time diverges near the critical point.

Fortuin-Kasteleyn Formula

Fortuin and Kasteleyn (1969)

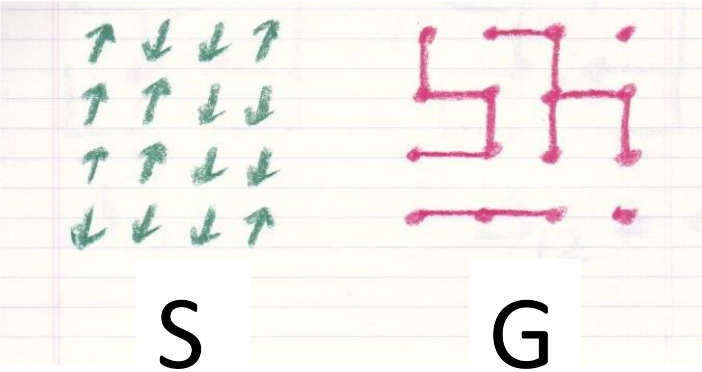
Ising Model

$$e^{KS_1S_2} = e^{-K} + \delta_{S_1,S_2}\left(e^{K} + e^{-K}\right) = \sum_{g=0,1} v_g \Delta_g\left(S_1, S_2\right)$$

g=0 g=1

$$Z = \sum_{S,G} V(G)\Delta(S,G)$$

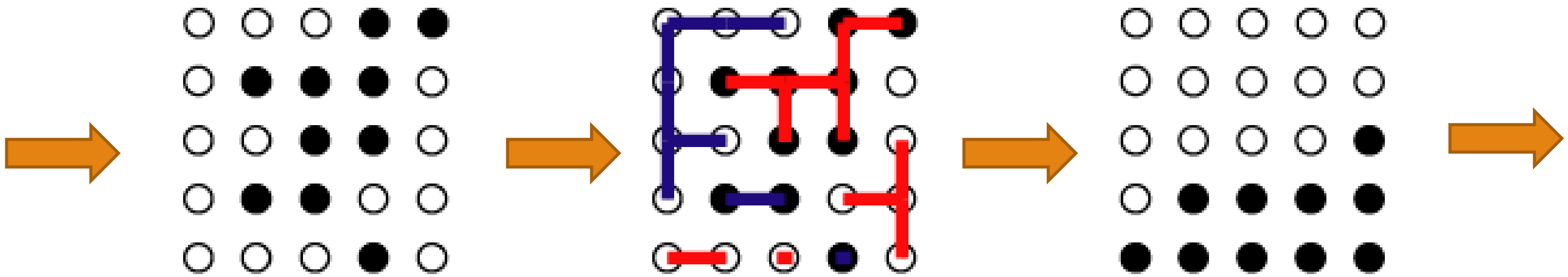
$$S \equiv \{S_i\} \qquad G \equiv \{g_{ij}\}$$



Markov Chain in (S,G) Space

$$Z = \sum_{S,G} W(S,G), \qquad W(S,G) \equiv V(G)\Delta(S,G)$$

$$\cdots \to S_t \to G_t \to S_{t+1} \to G_{t+1} \to \cdots$$



$$T(G|S) = \frac{W(S,G)}{W(S)}, \quad T(S|G) = \frac{W(S,G)}{W(G)}$$

Correlation Functions

$$\langle S_i S_j \rangle = Z^{-1} \sum_{S,G} V(G) \Delta(S,G) S_i S_j$$

$$= Z^{-1} \sum_{G} V(G) 2^{N_c(G)} \chi_{ij}(G) = \langle \chi_{ij}(G) \rangle$$

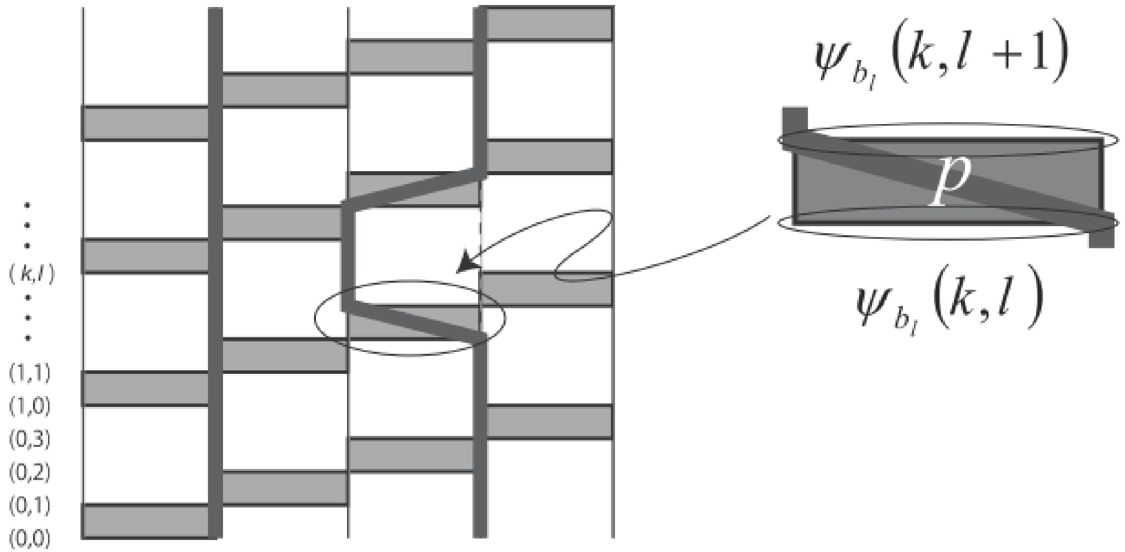
$$\chi_{ij}(G) \equiv \begin{cases} 1 & \text{(if i and j are connected in G)} \\ 0 & \text{(otherwise)} \end{cases}$$

i and *j* are correlated ⟺ *i* and *j* belong to the same cluster

The size of the clusters in G is O(ξ)

Path-Integral

$$Z \approx \sum_{S=\{\psi(k,l)\}} \prod_{k=0}^{M-1} \prod_{l=0}^{N_l-1} \langle \psi(k,l+1) \left| e^{-\Delta\tau H_l} \right| \psi(k,l) \rangle$$



Graph Expansion

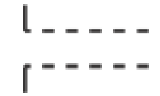
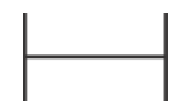
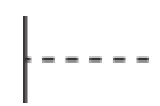
$$-H_{ij} = \sum_{g} a_g \, \hat{\Delta}_{ij}(g)$$

Ex: S=1/2 Antiferromagnetic Heisenberg Model

$$-H_{ij} = -\frac{J}{4} + \frac{J}{2}\begin{pmatrix} 0 & & & \\ & 1 & 1 & \\ & 1 & 1 & \\ & & & 0 \end{pmatrix}$$

$$\left\langle S_i', S_j' \middle| -H_{ij} \middle| S_i, S_j \right\rangle = -\frac{J}{4} + \frac{J}{2}\delta\left(S_i', -S_j'\right)\delta\left(S_i, -S_j\right)$$

$$-H_{ij} = -\frac{J}{4} + \frac{J}{2}\hat{\Delta}_{ij}\left(g_H\right)$$

	Symbol	Graph
	g_{d}	
AF	g_{h}	
	g_{b}	
	g_{ab}	

Loop/Cluster Algorithm

$$Z = \sum_{S=\{S_{i,k}\}} \prod_{(k,b=(ij))} \left\langle S_{i,k+1}\, S_{j,k+1} \middle| 1-(\Delta\tau) H_b \middle| S_{ik}\, S_{jk} \right\rangle$$

$$= \sum_{S} \prod_{(k,b=(ij))} \left\langle S_{i,k+1}\, S_{j,k+1} \middle| 1+(\Delta\tau) \sum_{g} a_g\, \hat{\Delta}_{ij}(g) \middle| S_{ik}\, S_{jk} \right\rangle$$

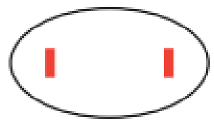
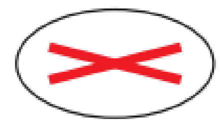
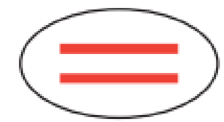
$$= \sum_{S} \sum_{G=\{g_{k,b}\}} \prod_{(k,b=(ij))} (\Delta\tau)^{|G|} a_{g_{k,b}} \left\langle S_{i,k+1}\, S_{j,k+1} \middle| \hat{\Delta}_{ij}(g_{k,b}) \middle| S_{ik}\, S_{jk} \right\rangle$$

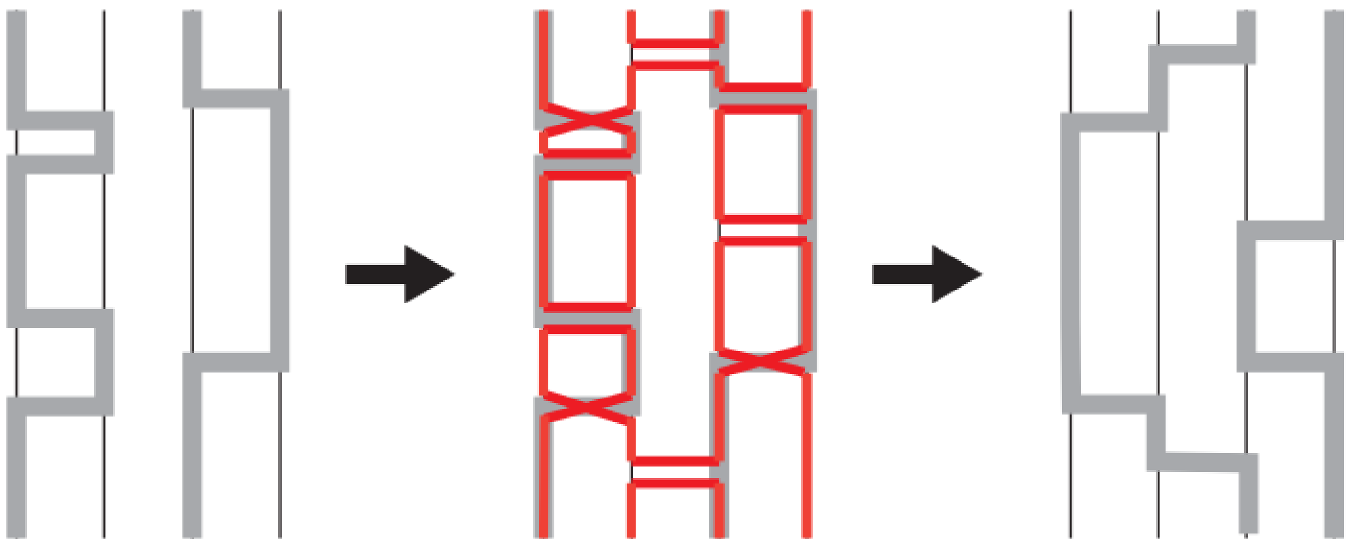
$$= \sum_{S} \sum_{G} W(S,G)$$

The same as the Fortuin-Kasteleyn formula!

Loop/Cluster Algorithm

S=1/2 XY Model

$\langle \psi'_p | 1 - \Delta\tau H_p | \psi_p \rangle =$  $+ (\Delta\tau)\frac{J}{4}($  $+$  $)$



Continuous-Time Limit

$$\lim_{\Delta\tau \to 0}\begin{pmatrix}\text{Placing a stone with probability} \\ \Delta\tau \times a \text{ in a cell of height } \Delta\tau\end{pmatrix}$$

$$= \left(\text{Placing a stone with density } a\right)$$

S=1/2 XY Model (Loop Algorithm)

Super Fluid Density ∝ Stiffness

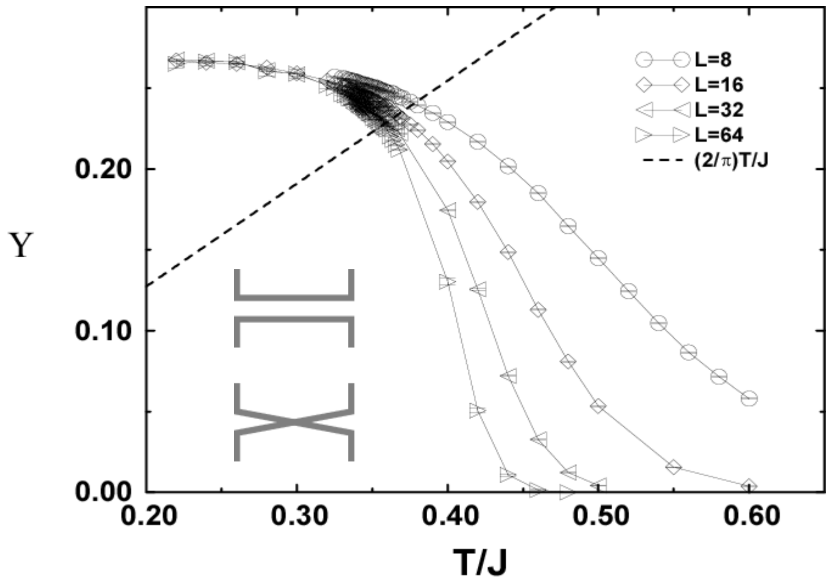
$$\rho_s = \frac{\partial^2 F(\theta)}{\partial \theta^2} = \frac{1}{L_y \beta}\left\langle W_x^2 \right\rangle$$

$$e^{-\beta F(\theta)} \equiv \mathrm{Tr}\, e^{-\beta H(\theta)}$$

$$H(\theta) \equiv -\sum_{(ij)} \left(t_{ij}(\theta) b_j^+ b_i + h.c.\right) + \sum_i (\mathrm{interaction})_i$$

$$t_{ij}(\theta) = t_{ij}\, e^{i\Delta\theta_{ij}} T \quad \left(\Delta\theta_{ij} = \frac{\theta}{L_x} \text{ iff } \vec{ij} \,//\, \vec{e}_x\right)$$

Harada-Kawashima 1998



Tc = 0.34271(5)J

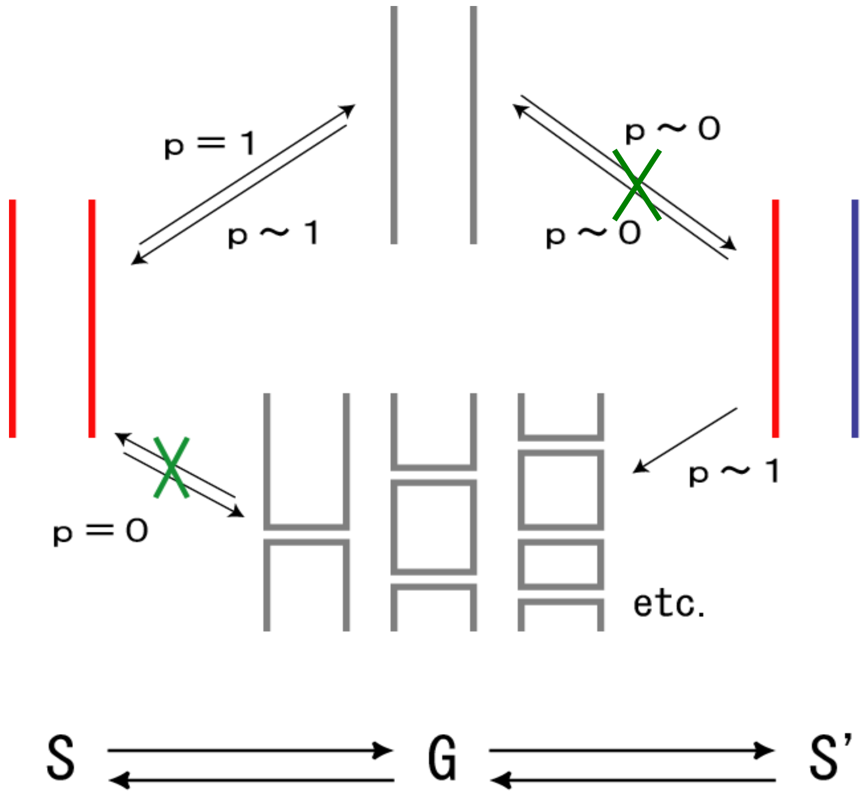
When Loop Update Fails

A two-site problem

$$H = J\, S_i \cdot S_j - H\left(S_i^z + S_j^z\right)$$

Magnetic Field competing against exchange couplings

The cause of the problem ... The effect of magnetic field is NOT taken into account in the graph generation.



High-T Expansion and Worms

Ising Model

$$Z = \sum_{S} \prod_{(ij)} \left(1 + (\tanh K) S_i S_j\right) = \sum_{G \in \Omega_0} (\tanh K)^{|G|}$$

$$W(G) = (\tanh K)^{|G|} \qquad \Omega_0 \equiv \{\text{closed graphs}\}$$

How can we construct a Markov chain for effective sampling?

Extending Graph Space

Ising Model

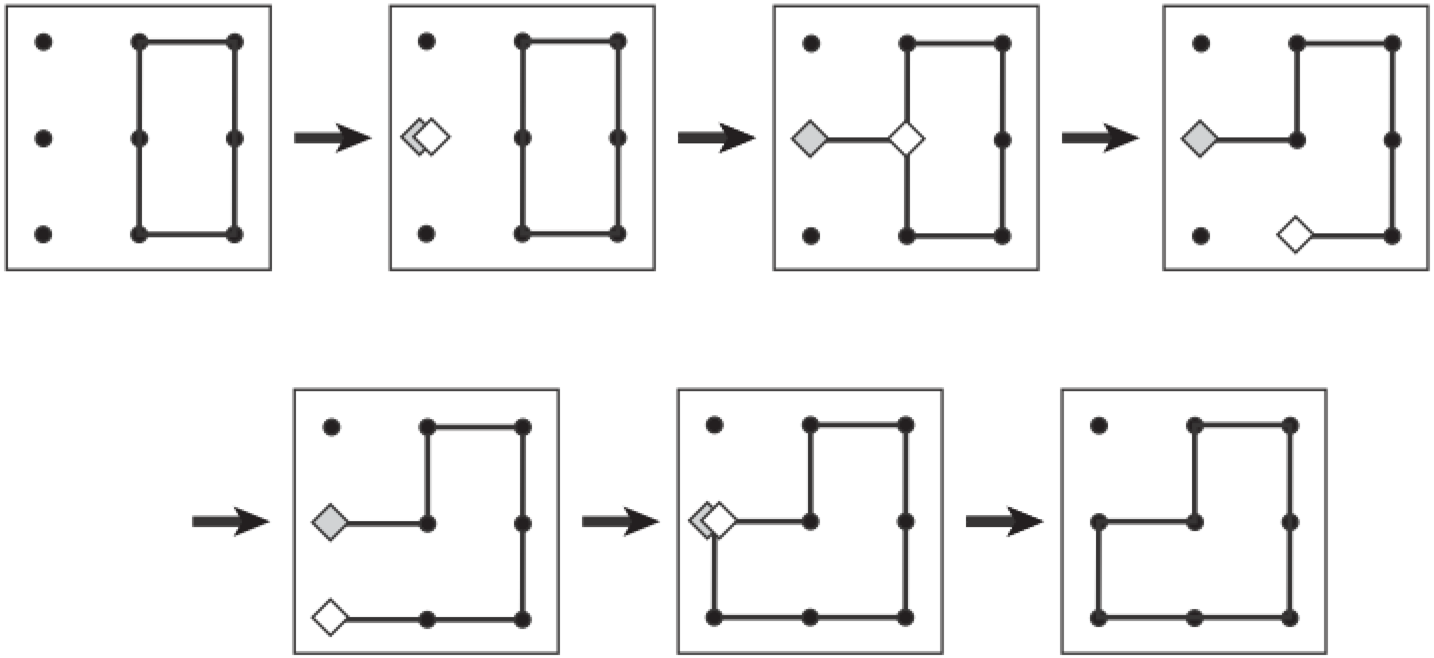
$$\Omega_0 \Rightarrow \Omega_0 \cup \Omega_2$$

$$\Omega_2 \equiv \{\text{graphs with 2 odd vertices}\}$$

$$W(G) = a^{\nu(G)} (\tanh K)^{|G|}$$

$$\nu(G) = \text{"the number of odd vertices in G"}$$

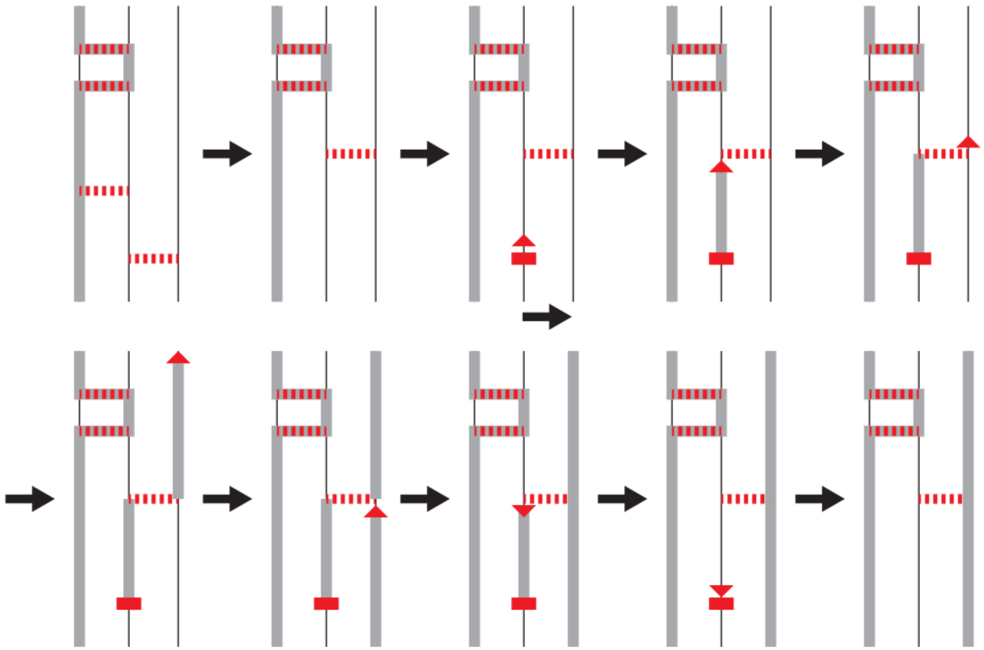
Worm Update for Ising Model



Prokof'ev and Svistunov (2001)

SSE (Worm Update Version)

Worm update for S=1/2 AF Heisenberg model



The effect of magnetic field is taken into account in the "scattering probability" of the worm.

Application of Classical Monte Carlo

--- AKLT state ---

TN representation of AKLT State

Schwinger boson representation

$$\left|S_i^z = m\right\rangle \equiv \frac{1}{\sqrt{m!(z-m)!}}\left(a_i^+\right)^m\left(b_j^+\right)^{z-m}\left|\mathrm{vac}\right\rangle$$

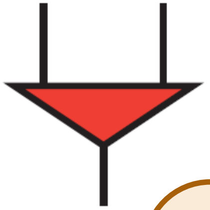
Unitary transformation for bipartite lattice

$$\left(a_i^+ b_j^+ - b_i^+ a_j^+\right)\left|\mathrm{vac}\right\rangle \Rightarrow \left(a_i^+ a_j^+ + b_i^+ b_j^+\right)\left|\mathrm{vac}\right\rangle$$

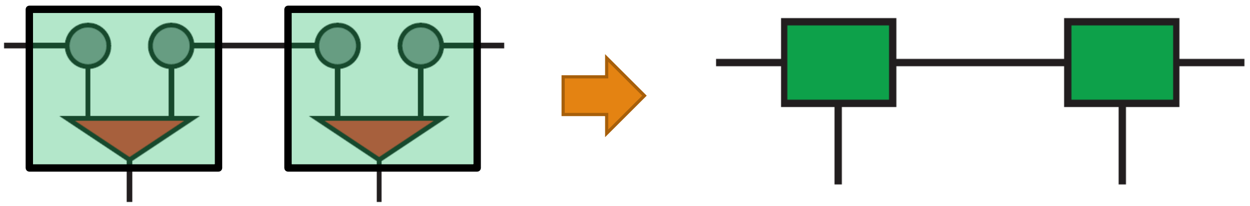
spin singlet

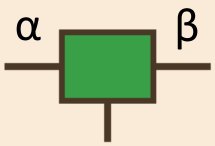
Projection to S=1 states

$$P = |0\rangle\langle 00| + |1\rangle\left(\frac{\langle 01| + \langle 10|}{\sqrt{2}}\right) + |2\rangle\langle 11|$$



projector



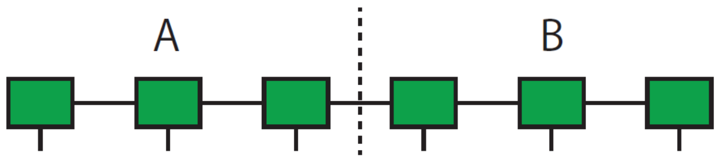


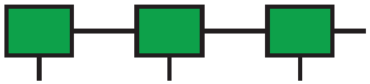
$$T_0^{\alpha\beta} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

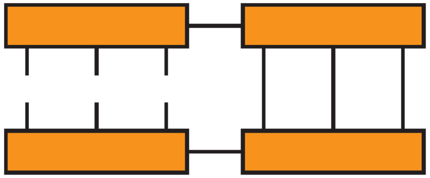
$$T_1^{\alpha\beta} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$T_2^{\alpha\beta} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

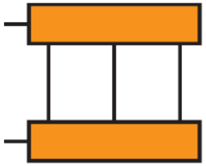
Reduced Density Operator

$|\Psi\rangle =$ 

$\Gamma \equiv$  $=$  $= U\Lambda V^{+}$ (SVD)

$\rho_A = \mathrm{Tr}_B |\Psi\rangle\langle\Psi| =$  $= \Gamma\Gamma^{+}\Gamma\Gamma^{+} = U\Lambda^{4}U^{+}$

"Overlap Matrix"

$\Theta \equiv$  $= V\Lambda^{2}V^{+}$

Studying Θ is sufficient.

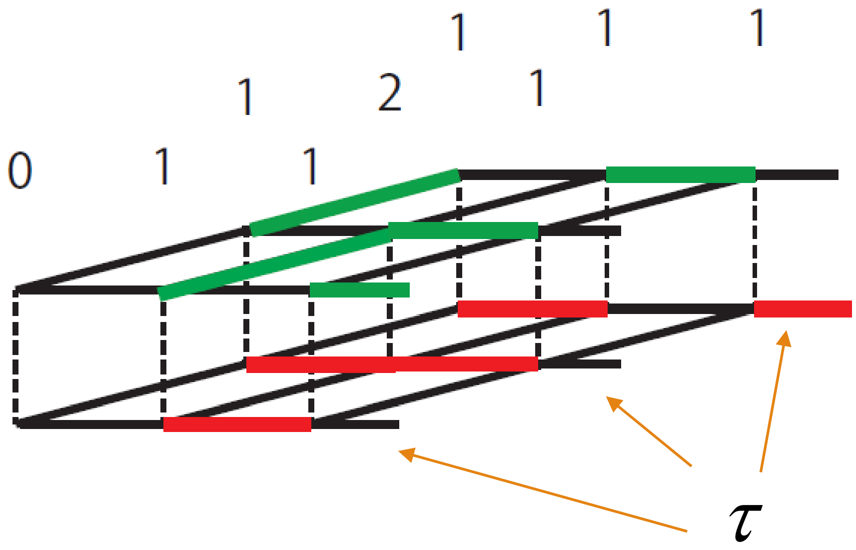
Katsura, NK, Kirillov, Korepin and Tanaka (2010)

2D AKLT State

Katsura, NK, Kirillov, Korepin and Tanaka (2010)
Lou, Tanaka, Katsura, and NK (2011)

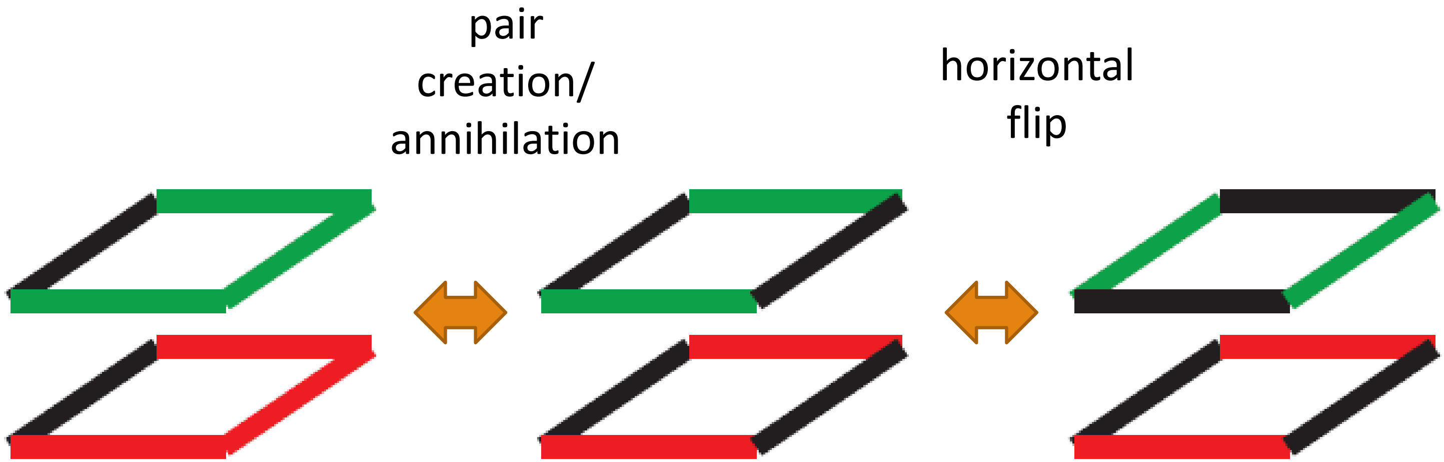
$$\Theta_{\{\tau\}\{\tau'\}} = \sum_{\{\sigma,\sigma'\}} \prod_i \delta_{n_i,n_i'} \binom{z_i}{n_i}^{-1}$$

$$n_i \equiv \sum_{j:\,\text{n.n. of } i} \sigma_{ij} \quad \left(\sigma_{ij} = 0,1\right)$$



Monte Carlo sampling of Overlap Matrix

Local update is sufficient



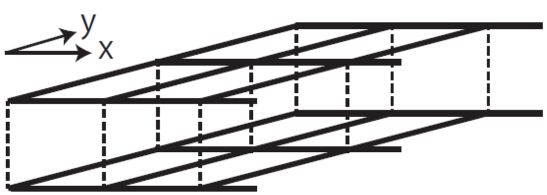
$$\Theta_{\{\tau\}\{\tau'\}} = (\text{const}) \times P(\{\tau\},\{\tau'\})$$

$$P(\{\tau\},\{\tau'\}) = (\text{freq. of having } \{\tau\},\{\tau'\} \text{on the boundary})$$

$$\text{Normalization ... } \quad \mathrm{Tr}\,\Theta = \sum_{\{\tau\}} \Theta_{\{\tau\}\{\tau\}} = 1$$

Katsura, NK, Kirillov, Korepin and Tanaka (2010)

Boundary Hamiltonian

$\Theta \equiv$ 

$$\equiv e^{-\beta H_B} \quad (\ \beta \text{ is arbitrary})$$

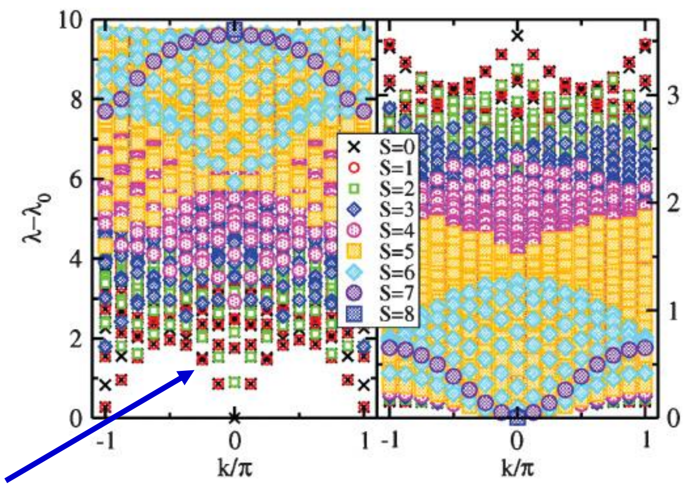
$$U^{+} H_B U = \begin{pmatrix} \lambda_0 & & & \\ & \lambda_1 & & \\ & & \lambda_2 & \\ & & & \ddots \end{pmatrix}$$

$$H_B \left|\psi_0\right\rangle = \varepsilon_0 \left|\psi_0\right\rangle$$

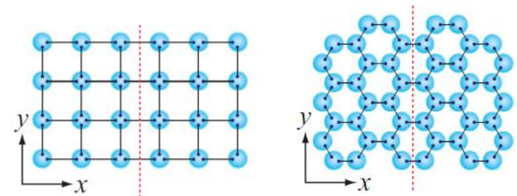
Is H_B meaningful?

Cirac, Poilblanc, Schuch and Verstraete (2011)
Lou, Tanaka, Katsura, and NK (2011)

square honeycomb



des Cloizeaux-Pearson mode?



CFT of Boundary Hamiltonian

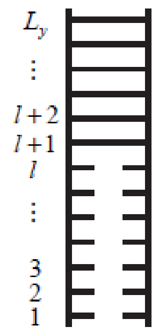
Lou, Tanaka, Katsura, and NK (2011)

$$\Theta = \rho_B \equiv e^{-\beta H_B}$$

The ground state of the boundary Hamiltonian $H_B|\psi_0\rangle = \varepsilon_0|\psi_0\rangle$

Entanglement entropy of T=0 boundary density operator

$$\rho_B^{T=0}(l) \equiv \operatorname*{Tr}_{l+1,l+2,\cdots,L_y} |\psi_0\rangle\langle\psi_0| =$$

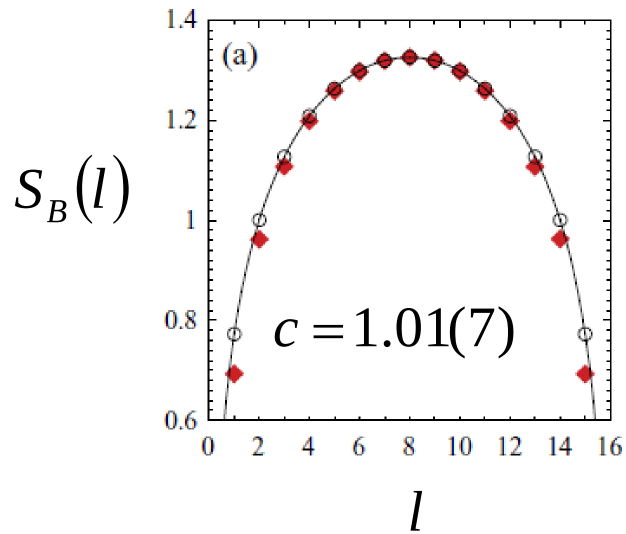


$$S_B(l) = -\mathrm{Tr}\left(\rho_B^{T=0}(l)\log\rho_B^{T=0}(l)\right)$$

cf: Calabrese-Cardy 2004

$$S_B(l) = \frac{c}{3}\ln(f(l)) + \text{const}, \quad f(l) = \frac{L_y}{\pi}\sin\left(\frac{\pi l}{L_y}\right)$$

Ly=16 Lx=5



Application of Loop Update
--- SU(N) Heisenberg Model ---

SU(N) Heisenberg Model

A natural extension of the SU(2) AF Heisenberg model

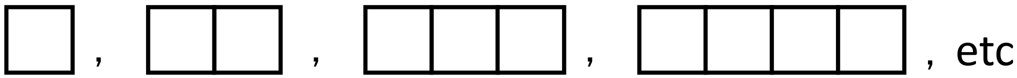
$$H = \frac{J}{N} \sum_{(r,r')} S_\beta^\alpha(r) \bar{S}_\alpha^\beta(r')$$

$S_\beta^\alpha(r) \cdots$ generators of SU(N) rotation represented by some representation R

$\bar{S}_\beta^\alpha(r) \cdots$ the same with the conjugate representation

$$\left[S_\beta^\alpha, S_\delta^\gamma\right] = \delta_\delta^\alpha S_\beta^\gamma - \delta_\beta^\gamma S_\delta^\alpha \qquad \alpha, \beta, \gamma, \delta = 1, 2, \cdots, N$$

Representation:



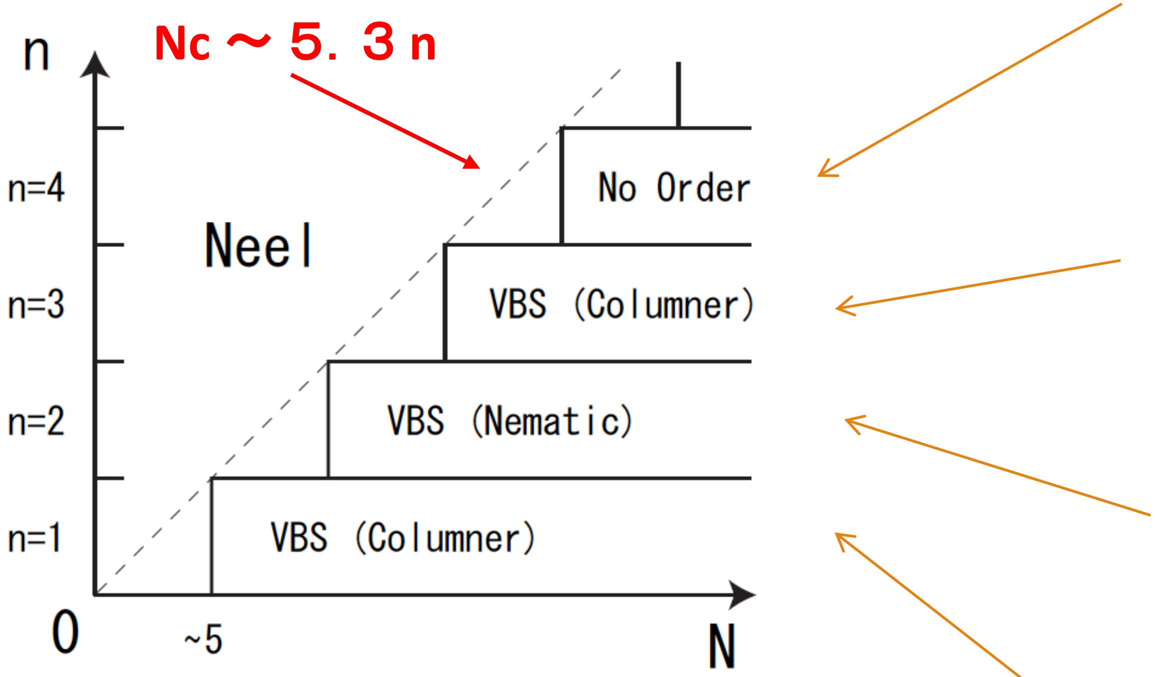
n=1 (fundamental representation.) n=2 n=3 n=4

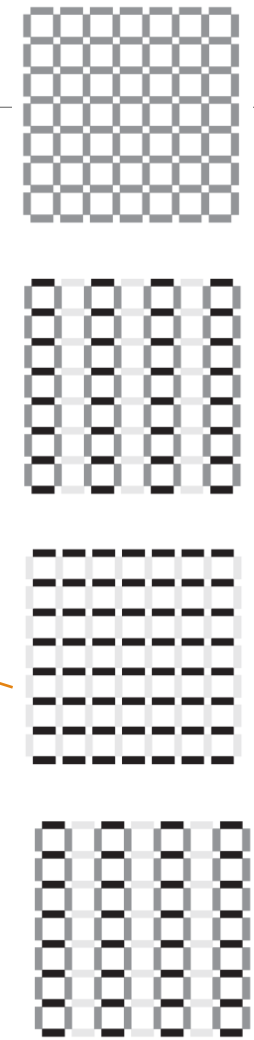
2D Analogue of "Haldane" States

Prediction from 1/N expansion

Arovas & Auerbach (1988)

Read & Sachdev (1989)





For numerical evidences, see

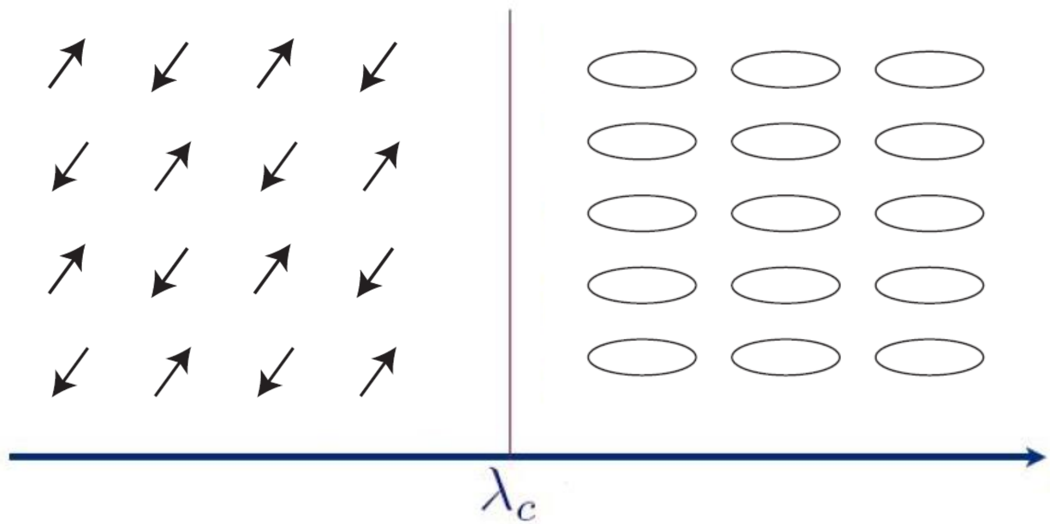
n=1 : Tanabe & NK: PRL 98 057202 (2007)

n=2,3 : Okubo,Harada,Lou & NK : PRB92 134404 (2015)

Magnetic/Non-Magnetic Transition (SU(N) JQ-Model)

SU(2) symmetry broken.
Space symmetry not broken.

SU(2) symmetry not broken.
Space symmetry broken.



λ =Q/J

Text book symmetry breaking paradigm predict the 1st order transition

$$H = J\sum_{(ij)} S_i \cdot S_j - Q \sum_{p=(i,j,k,l)} \left(\frac{1}{4} - S_i \cdot S_j\right)\left(\frac{1}{4} - S_k \cdot S_l\right)$$

SU(3) and SU(4) J-Q Models

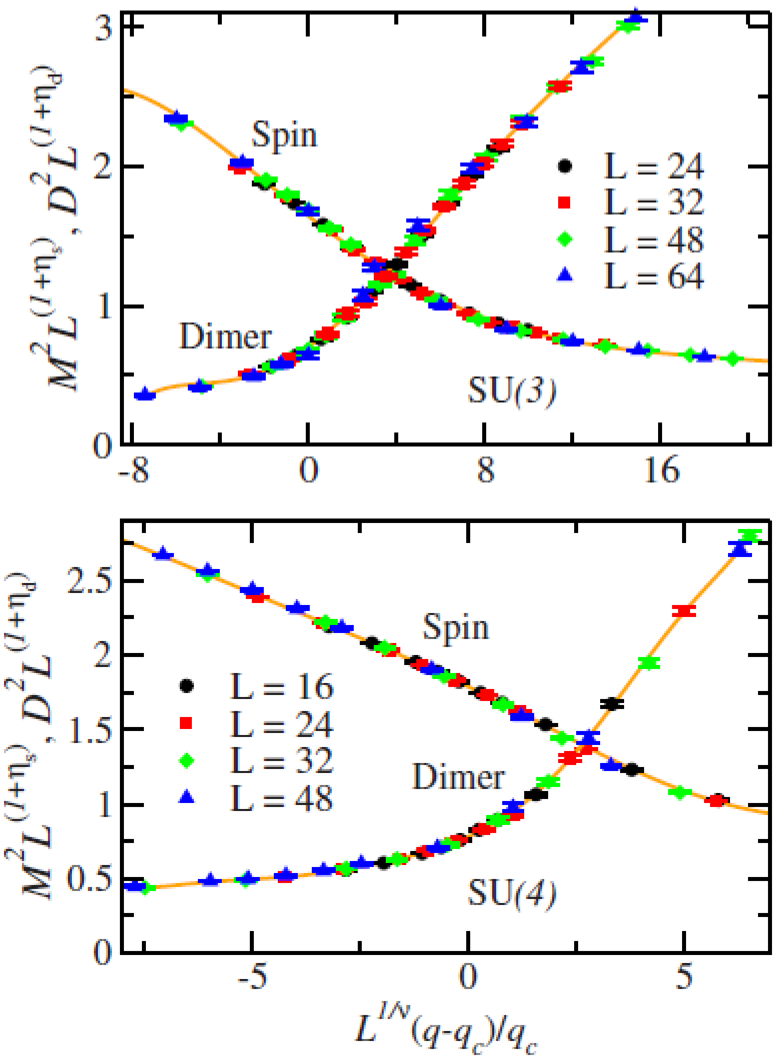
J. Lou, A. Sandvik, N.K (2009)

SU(3) J-Q

$$\eta_s = 0.38(3), \;\; \nu = 0.65(3)$$

SU(4) J-Q

$$\eta_s = 0.42(5), \;\; \nu = 0.70(2)$$



Universality?

Model, symmetry	η_s	η_d	ν	a_4
J-Q_2, SU(2)	0.35(2)	0.20(2)	0.67(1)	
J-Q_3, SU(2)	0.33(2)	0.20(2)	0.69(2)	1.20(5)
J-Q_2, SU(3)	0.38(3)	0.42(3)	0.65(3)	1.6(2)
J-Q_2, SU(4)	0.42(5)	0.64(5)	0.70(2)	1.5(2)

For $N >> 1,\ \eta_\mathrm{s} = 1.$

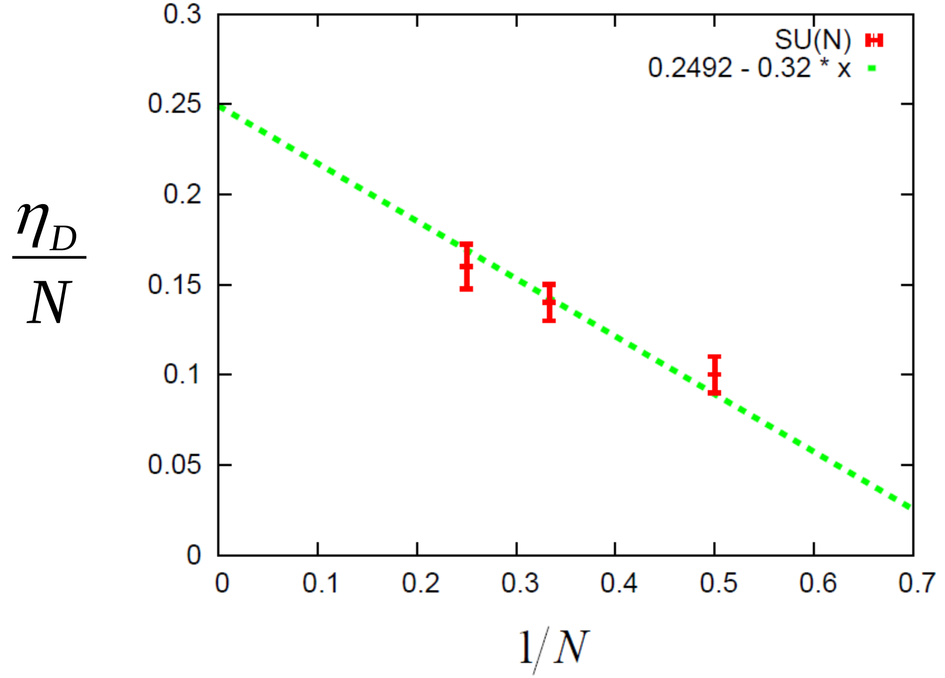
T. Senthil, et al, Science 303, 1490 (2004)
M. Levin and T. Senthil, Phys. Rev. B 70, 220403R (2004).

For $N >> 1,\ \eta_\mathrm{d} \propto N - 1.$

CP^{N-1} Field Theory:
M. A. Metlitski, et al, PRB 78, 214418 (2008)
G. Murthy and S. Sachdev, Nucl. Phys. B 344, 557 (1990).

Monopole Scaling Dimension up to O(N^{-1})

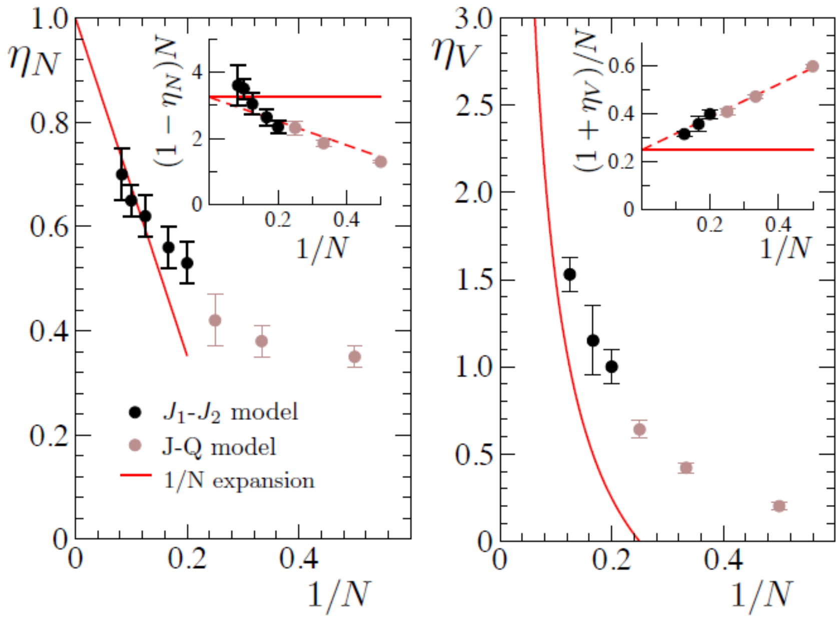
$$\frac{\eta_D}{N} = \frac{2\Delta_1 - 1}{N} = 0.2492 - 0.32\frac{1}{N} + O\left(\frac{1}{N^2}\right)$$

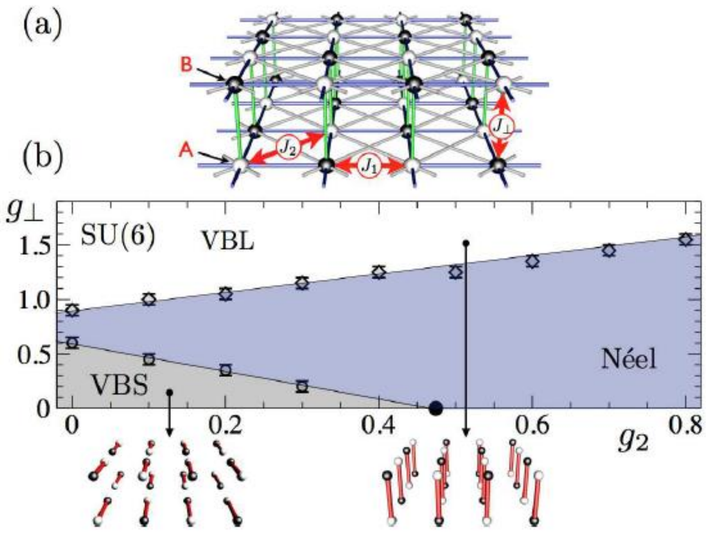


Further Evidences for DCP

Kaul, Sandvik: PRL108_137201 (2012)

Introducing "ferromagnetic" interaction to favor the Neel state for large N.





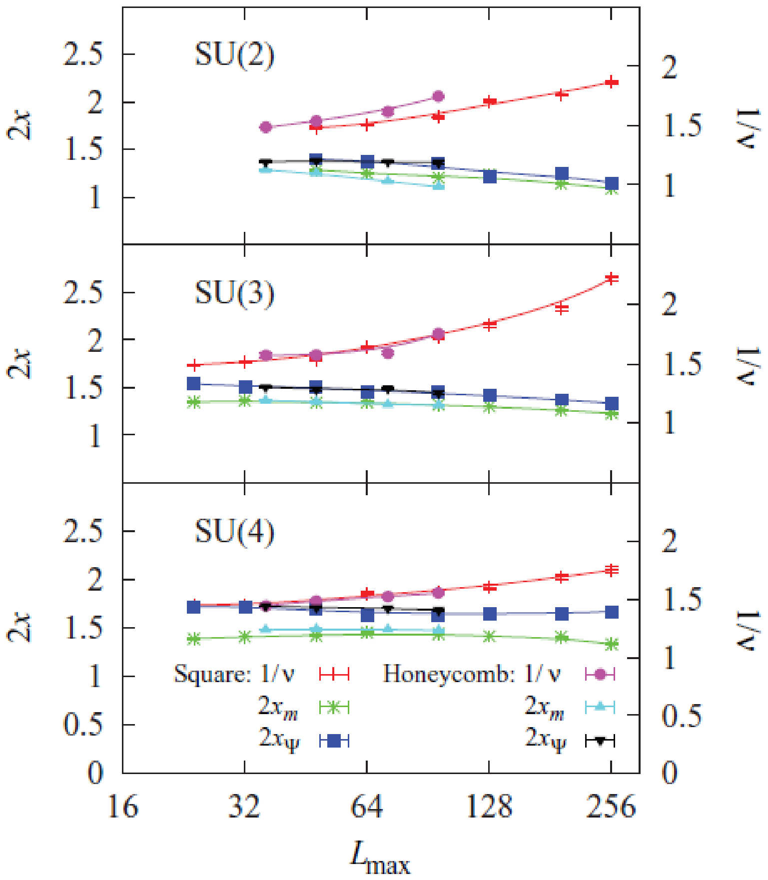
Kaul, Melko and Sandvik: arXiv:1204.5405

Bilayer system show 1st order transition.

An inconvenient truth

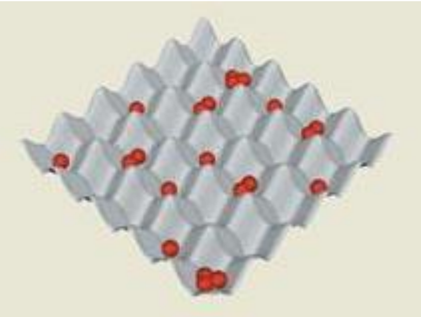
Harada et al (2013)

System-size-restricted finite-size scaling yields strongly size dependent estimates of scaling dimensions

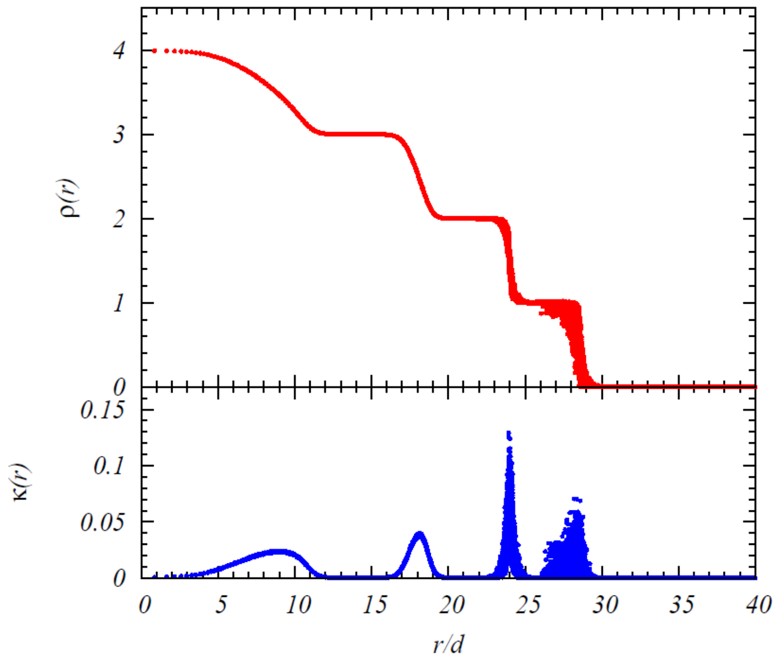


Application of worm update
--- Bose Hubbard Model ---

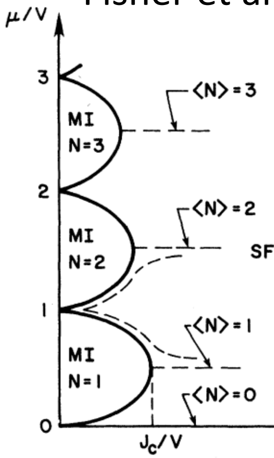
"Big Wedding Cake" in ultracold atoms

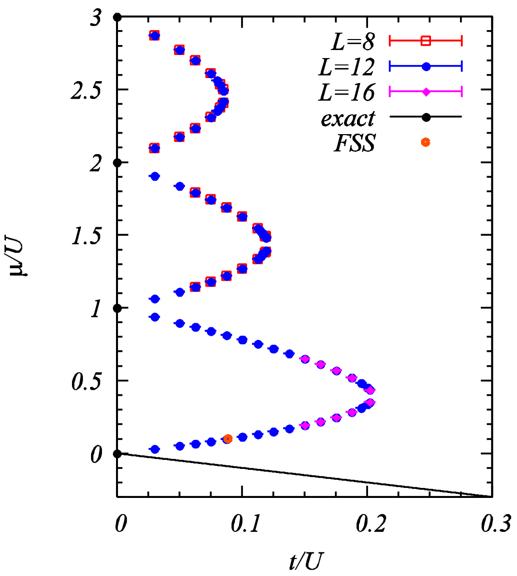


$$t/U = 0.05,\ \mu(r=0)/U = 3.3,$$
$$\Omega = 0.08,\ L^3 = (64^3) \sim 2.6\times 10^5,\ \beta t = 5.0.$$



Fisher et al (1989)





The number of bosons

$$N = 0.6936(1)\times 64^3,$$
$$\sim 1.8\times 10^5.$$

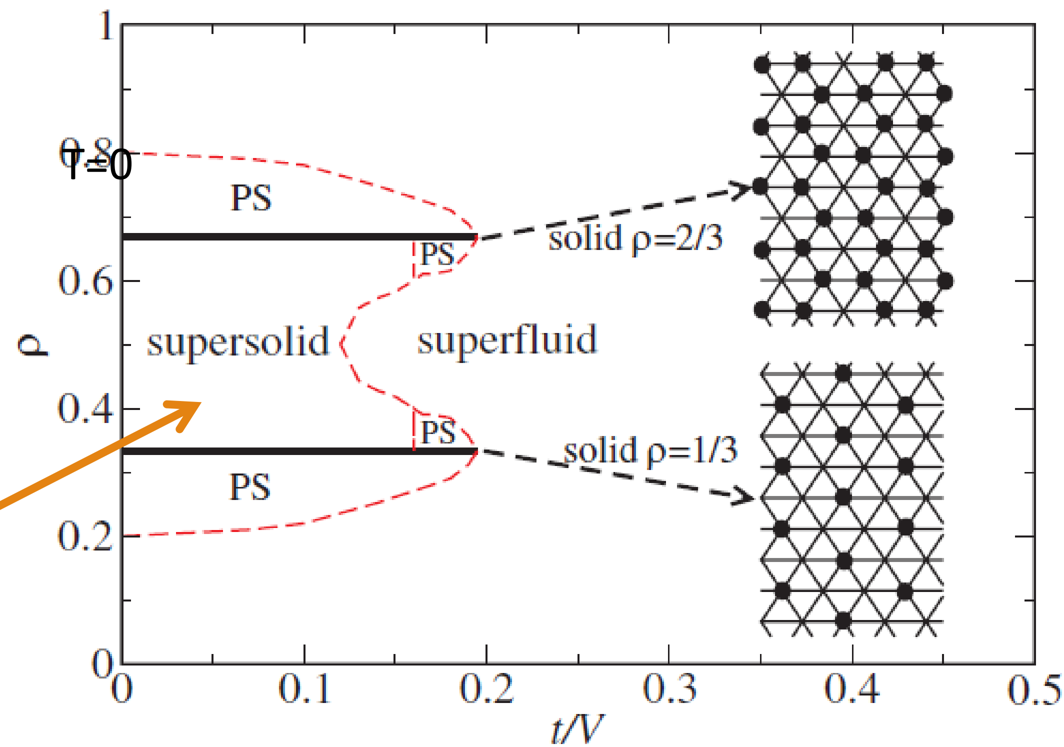
Kato and N.K., PRE79 021104 (2009)

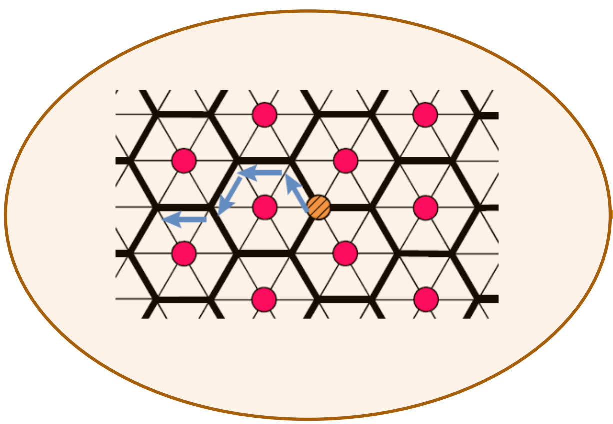
Supersolid on Triangular Lattice

$$H = -t\sum_{\langle i,j\rangle}(a_i^\dagger a_j + a_j^\dagger a_i) + V\sum_{\langle i,j\rangle} n_i n_j - \mu \sum_i n_i$$

Wessel and Troyer:
PRL 95, 127205 (2005)

BHM with hardcores and n.n. interaction



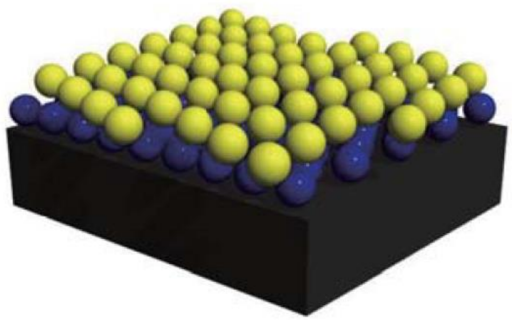


"superflow path"

No vacancy condensation below n=1/3, and no interstitial condensation above n=1/3.

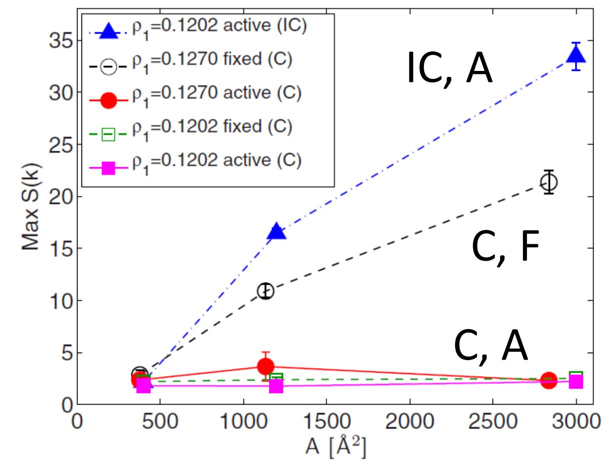
Continuous Space MC

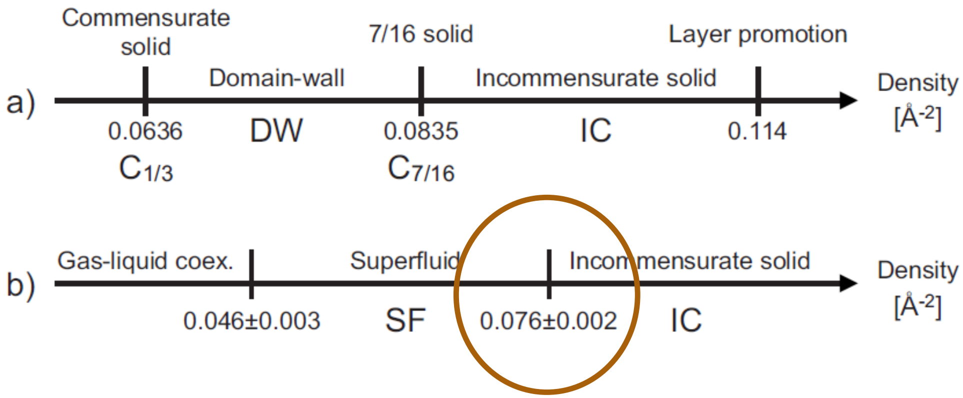
Corboz, Boninsegni, Pollet and Troyer (2008)

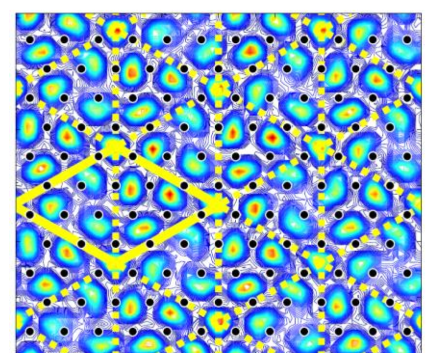


Can Helium-4 on graphite surface be super-solid?

$$T = 0.5K,\ \rho_2 = 0.08\,\text{Å}^{-2}$$





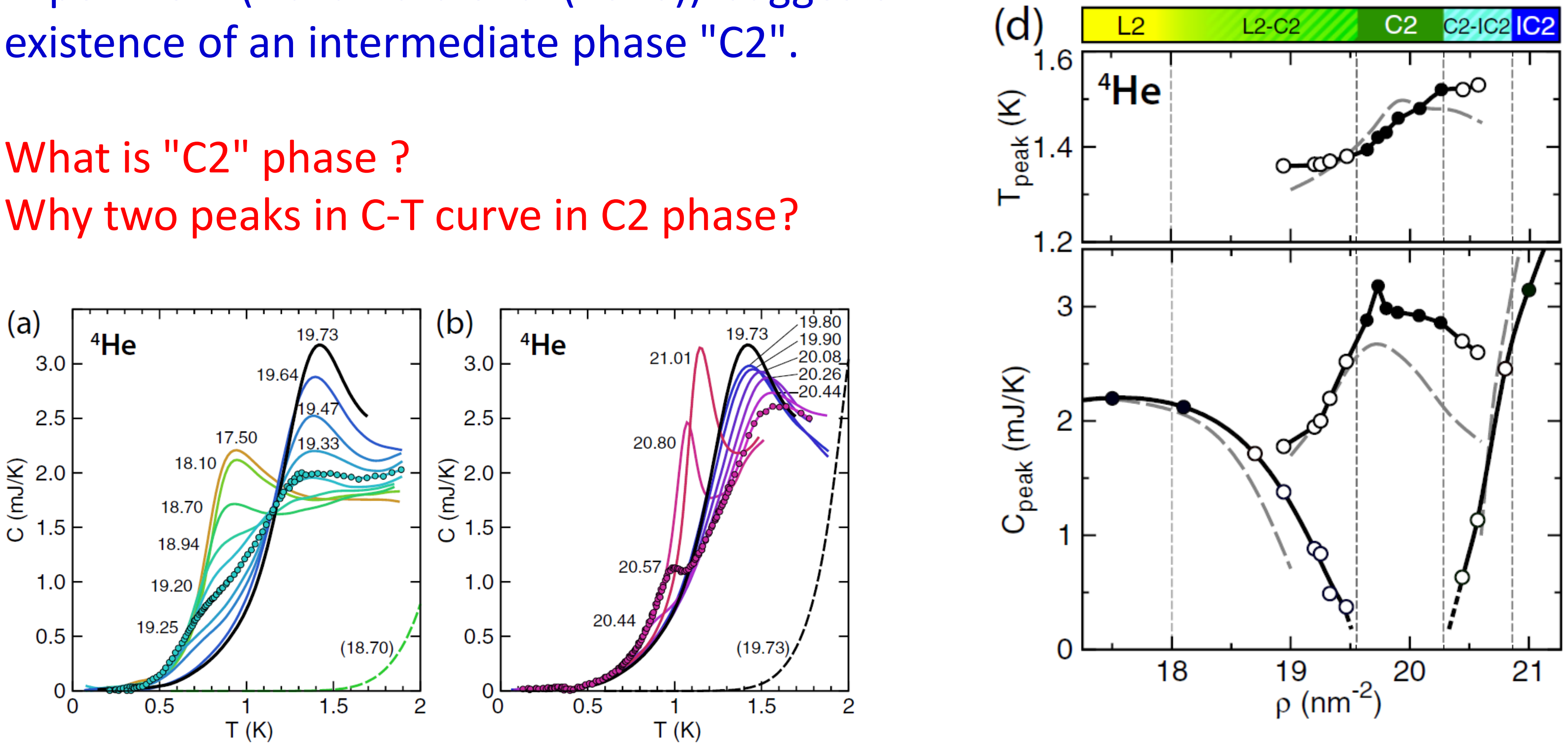


Solid state was observed only when the first layer is fixed.

Remaining Puzzle ...

Experiment (Nakamura et al (2016)) suggests existence of an intermediate phase "C2".

What is "C2" phase ?
Why two peaks in C-T curve in C2 phase?



Summary

When it is not poisoned by negative signs, Monte Carlo method is suitable for many systems, and complementary to the tensor network methods.

END