Numerical approaches to frustrated magnets

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Various Methods

Various powerful methods exist but each with own advantages and limitations

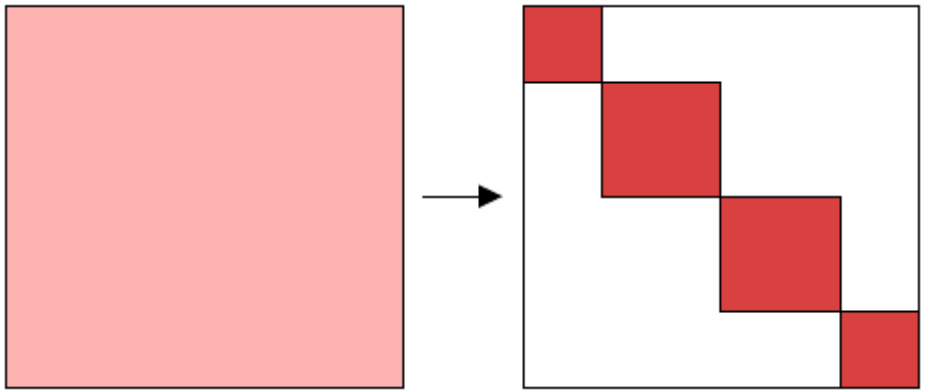
- Monte Carlo methods (Classical Monte Carlo, Quantum Monte Carlo)
- Exact Diagonalization
- Density Matrix Renormalization Group (DMRG) methods
- Series expansion techniques
- Variational wavefunctions
- . . . . . .

Exact Diagonalization

$H|\psi\rangle = E|\psi\rangle$, Many-body (local) Hamiltonian on a (finite) lattice
$\Rightarrow$ (Sparse) Matrix Eigenvalue Problem

- Can use sophisticated black-box program packages for matrix diagonalization, e.g., LAPACK (Linear Algebra PACKage)
- With eigenstates available, any static or dynamic quantity may be computed
- However, exponential increase of the basis size with number of spins N ($M = 2^N$ states for a $S = 1/2$ system)
- Full diagonalization limited to matrices of size $\sim 10^4$ (gives $N \approx 20$ for $S = 1/2$ spins)
- effort to diagonalize $\sim M^3$
- Insights can be gleaned from (small) finite-sized systems in many cases
- Testing the correctness of other methods

Symmetries in ED



- States need to be represented on the computer
- Simple example: $S = 1/2$ sites
  $|\uparrow\uparrow\downarrow\uparrow\downarrow\rangle \rightarrow [11010]$ (let's say S_i^z)
- $H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$ with periodic boundary condition (PBC)
- Symmetries: total spin $\mathbf{S}^2$, total S^z, momentum k
- Symmetry resolved eigenstates very useful $\Rightarrow$ dispersion of excitations, symmetry breaking in thermodynamic limit, locating critical point, $\cdots$

Examples: m_z conservation

- $m_z = \sum_{i=1}^{N} S_i^z$
- Blocks correspond to fixed m_z
- No matrix elemnt of H between states of different m_z
- Number of states in a block of $m_z = N_\uparrow - N_\downarrow$ equals $\frac{N!}{N_\uparrow! N_\downarrow!}$, Largest block for $m_z = 0$
- For $N = 24$, largest block has 1352078 states (compare to $2^{24} = 16777216$)
- Other symmetries can further split the blocks but more complicated (translational symmetry next)

Momentum conserving states

- $T|S^z_1, S^z_2, \cdots, S^z_N\rangle = |S^z_N, S^z_1, \cdots, S^z_{N-1}\rangle$
- We need to construct $|n\rangle$ s.t. $T|n\rangle = e^{ik}|n\rangle$ where $k = \frac{2\pi m}{N}$, $m = 0, 1, \cdots, N-1$
- Choose a representative state $|a\rangle$.

Then $|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr} T^r |a\rangle$

- If $|a\rangle$ and $|b\rangle$ are both representative states, then $T^r|a\rangle \neq |b\rangle$

$[0011] \rightarrow [1001] \rightarrow [1100] \rightarrow [0110]$

$[0101] \rightarrow [1010] \rightarrow [0101] \rightarrow [1010]$

- If $T^R|a\rangle = |a\rangle$ for some $R < N$, then only $kR = 2n\pi$ allowed
- $N_a = N^2/R_a$

Reduction in block size using symmetries

- $k = 0, m_z = 0$ is largest block

Reflection symmetry (parity)
$P|S_1^z, S_2^z, \cdots, S_n^z\rangle = |S_N^z, \cdots, S_2^z, S_1^z\rangle$ $(p = \pm 1)$, Note $[P, T] \neq 0$. However $[P, T] = 0$ if $k = 0, \pi$ since $k = -k$ here

Spin inversion symmetry
$Z|S_1^z, S_2^z, \cdots, S_n^z\rangle = |-S_1^z, -S_2^z, \cdots, -S_N^z\rangle$ $(z = \pm 1)$, can use to further reduce $m_z = 0$ block

N	$(+1,+1)$	$(+1,-1)$	$(-1,+1)$	$(-1,-1)$
8	7	1	0	2
12	35	15	9	21
16	257	183	158	212
20	2518	2234	2136	2364
24	28968	27854	27482	28416
28	361270	356876	355458	359256
32	4707969	4690551	4685150	4700500

Lanczos Algorithm I

$H^{\Lambda}|\Psi_0\rangle = \sum_{n=0}^{M-1} c_n E_n^{\Lambda} |\Psi_n\rangle =$

$c_{\max} E_{\max}^{\Lambda} \left(|\Psi_{\max}\rangle + \sum_{n \neq \max} \frac{c_n}{c_{\max}} \left(\frac{E_n}{E_{\max}} \right)^{\Lambda} |\Psi_n\rangle \right)$, use $(H - c)$

where $c > 0$ to ensure $|E_0 - c| > |E_{M-1} - c|$

Power method can be readily improved by using not only $H^{\Lambda}|\Psi_0\rangle$ but all $H^m|\Psi_0\rangle$ from $m = 0, \cdots, \Lambda$

- For details, Lecture notes by Sandvik, arXiv:1101.3281

Lanczos Algorithm II

- Pick a random state $|\Psi_0\rangle$
- Construct $|\Psi_1\rangle = H|\Psi_0\rangle - \frac{\langle\Psi_0|H|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}|\Psi_0\rangle$
- Then construct $|\Psi_{n+1}\rangle = H|\Psi_n\rangle - a_n|\Psi_n\rangle - b_n^2|\Psi_{n-1}\rangle$, where $a_n = \frac{\langle\Psi_n|H|\Psi_n\rangle}{\langle\Psi_n|\Psi_n\rangle}$, $b_n^2 = \frac{\langle\Psi_n|\Psi_n\rangle}{\langle\Psi_{n-1}|\Psi_{n-1}\rangle}$
- Diagonalize the matrix given by H equals

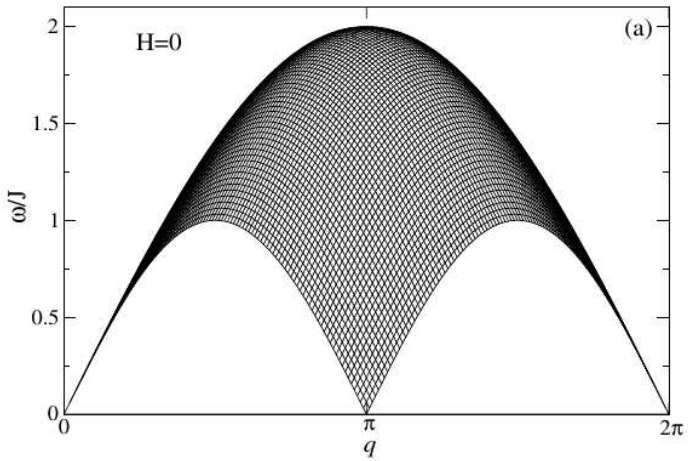
$$\begin{pmatrix} a_0 & b_1 & 0 & 0 & \cdots \\ b_1 & a_1 & b_2 & 0 & \cdots \\ 0 & b_2 & a_2 & b_3 & \cdots \\ 0 & 0 & b_3 & a_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

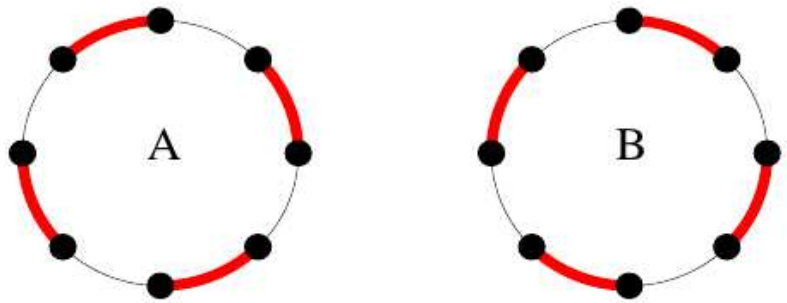
- If ground state energy not converged to desired accuracy, proceed to step 3 by increasing n by 1

Due to finite-precision arithmetic, orthogonality between $|\Psi_n\rangle$ quickly lost. Need to use improved algorithms based on re-orthogonalization of the states

Quantum phase transition in Majumdar-Ghosh model

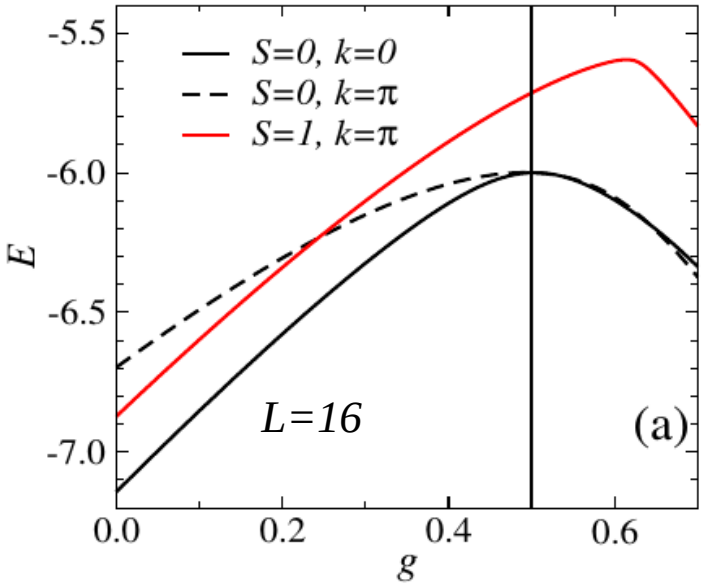
$H = J_1 \sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+2}$, $g_c \approx 0.2411$

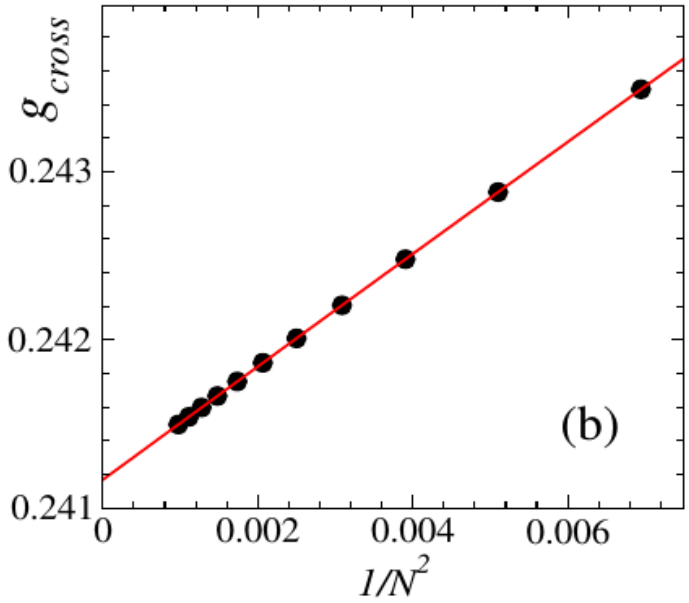




- At $g = 1/2$, degenerate ground states at $k = 0$ and $k = \pi$ respectively (Majumdar and Ghosh (1969))
  $|\psi(0)\rangle = (|\psi_A\rangle + |\psi_B\rangle)/\sqrt{2}$, $|\psi(\pi)\rangle = (|\psi_A\rangle - |\psi_B\rangle)/\sqrt{2}$
- For $g < g_c$, lowest excitation $S = 1$ at $k = \pi$ with gap $\sim 1/N$
- For $g > g_c$, lowest excitation $S = 0$ at $k = \pi$ with gap $\sim \exp(-N)$

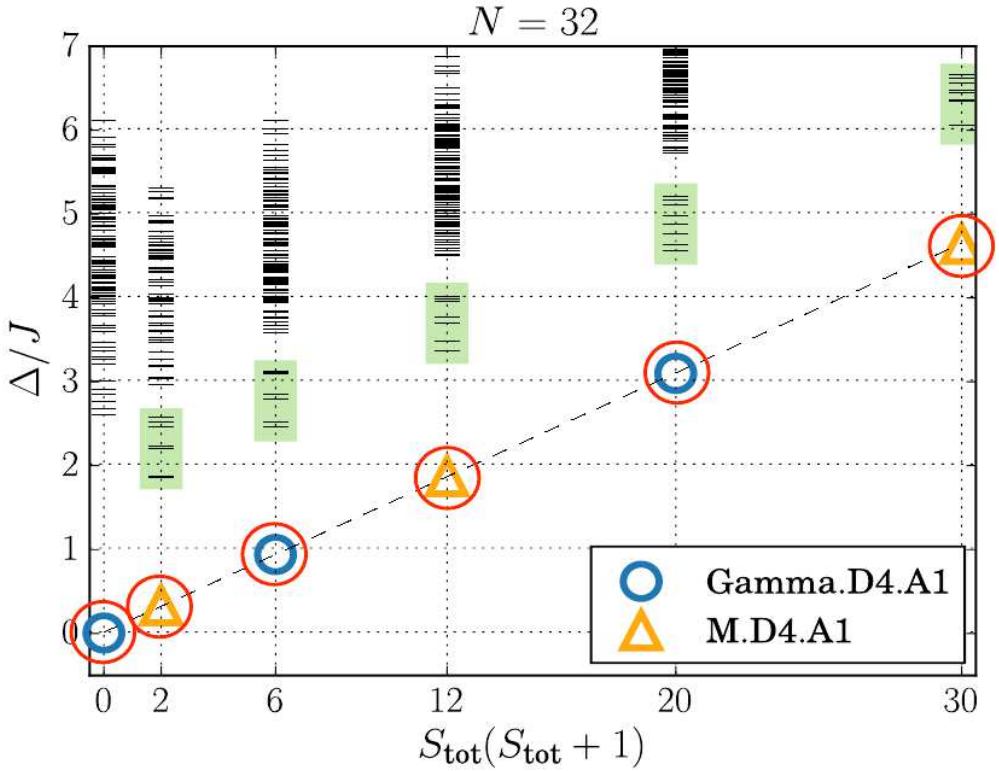
Locating the critical point





- Lecture notes by Sandvik, arXiv:1101.3281
- Fitting to polynomial with leading $1/N^2$ based on $8 \leq N \leq 32$ gives $g_c = 0.2411674(2)$.

Detecting Spontaneous Symmetry Breaking



- Finite size manifestation of continuous symmetry breaking
- Tower of states s.t. gap scales as $1/N$
- Even (odd) S at $\mathbf{k} = (0,0)[(\pi,\pi)]$ $(S \ll \sqrt{N})$
- Gap for the Goldstone modes scale as $1/L$
- **Review by Wietek, Schuler, Läuchli, arXiv:1704.08622**

Monte Carlo methods

- Devise random walk in the space of congifurations ($C_1 \to C_2 \to C_3 \to \cdots$) [Markov process]
- $P(C_n \to C_m)$ depends only on C_n and C_m.

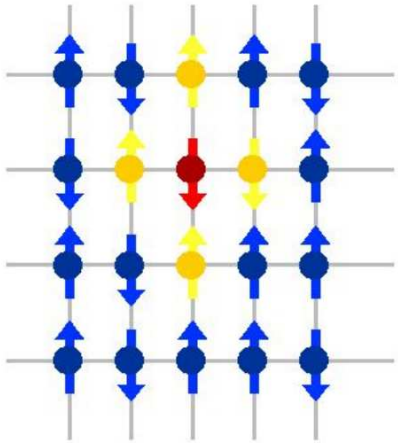
$P(C_n \to C_m) = g(C_n \to C_m)A(C_n \to C_m)$ where $g(C_n \to C_m) =$ Given state C_n, the probability that the algorithm generates a state C_m and $A(C_n \to C_m) =$ acceptance probability of this event

- Condition of ergodicity
- Condition of detailed balance

$p(C_n)P(C_n \to C_m) = p(C_m)P(C_m \to C_n)$ where $p(C_n) = \exp(-\beta E(C_n))/Z$

- $\langle \mathcal{O} \rangle \approx \frac{1}{N_{\mathrm{MCS}}} \sum_n \mathcal{O}(C_n)$–simple arithmetic average over the visited states

Metropolis sampling (1953)

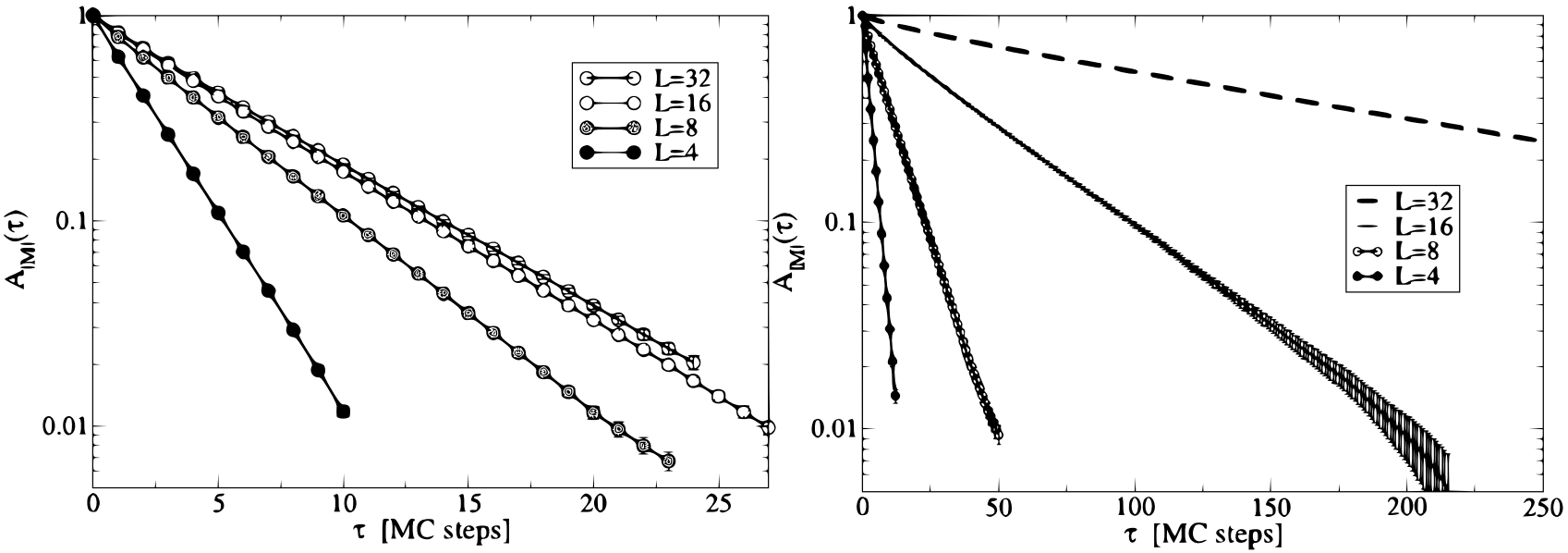


- $g(C_n \to C_m) = 1/N$ and
  $A(C_n \to C_m) = \min[1, \exp(-\beta(E(C_m) - E(C_n)))]$

essential to use good pseudo-random-number generator e.g. Mersenne Twister (period $2^{19937} - 1$) $\Rightarrow$ see Monte Carlo simulations: Hidden errors from "good" random number generators, by Ferrenberg, Landau, Wang (1992)

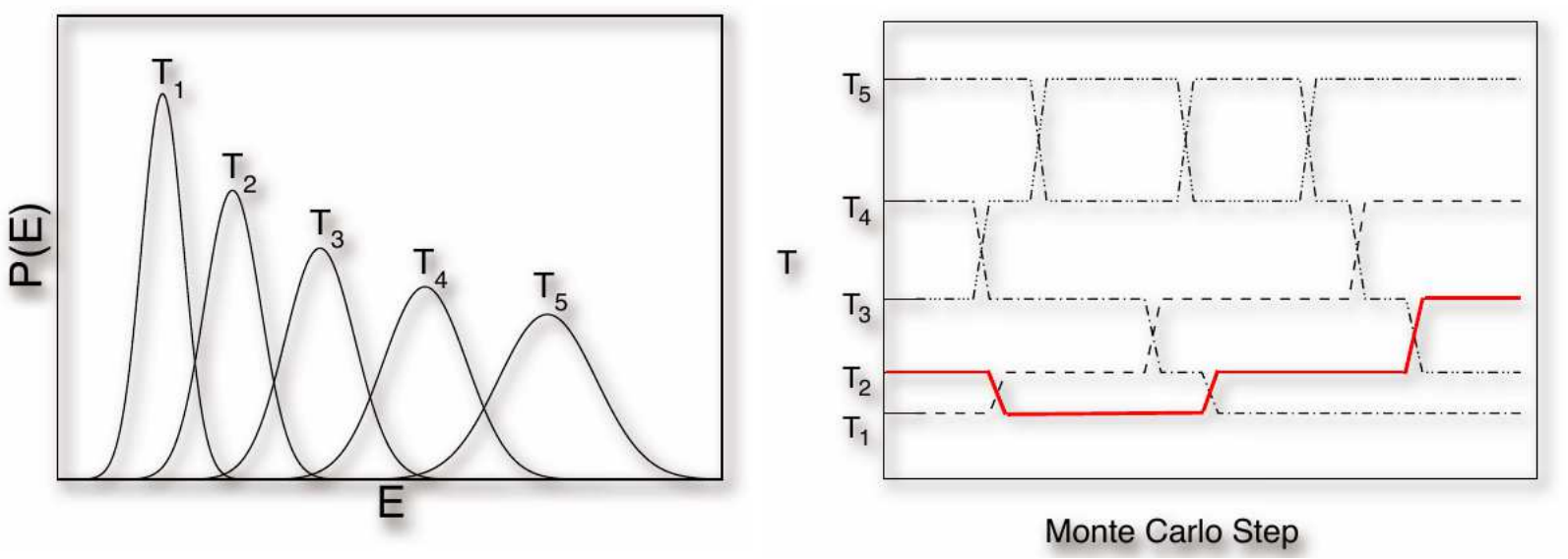
- 1 *Monte Carlo step* equals N attempts to flip randomly selected spins

Autocorrelations



- Need to find statistical error on $\langle \mathcal{O} \rangle \approx \frac{1}{N_{\rm MCS}} \sum_n \mathcal{O}(C_n)$ (binning, bootstrap, jacknife etc, **see Peter Young, arXiv:1210.3781**)
- $A_{\mathcal{O}}(\tau) = \frac{\langle \mathcal{O}_k \mathcal{O}_{k+\tau} \rangle - \langle \mathcal{O}_k \rangle^2}{\langle \mathcal{O}_k^2 \rangle - \langle \mathcal{O}_k \rangle^2} \sim \exp(-\tau/\tau_{\mathcal{O}})$
- Critical slowing down near T_c, $\tau_{\mathcal{O}} \sim L^z$ here $z \approx 2$
- Can be avoided using cluster algorithms (e.g., see Wolff (1989)) [simulate $\sim 1024^2$ spins for the 2D Ising model in the critical regime]

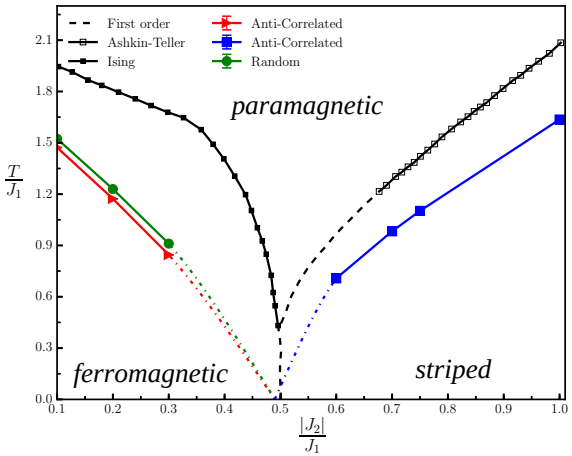
Parallel tempering

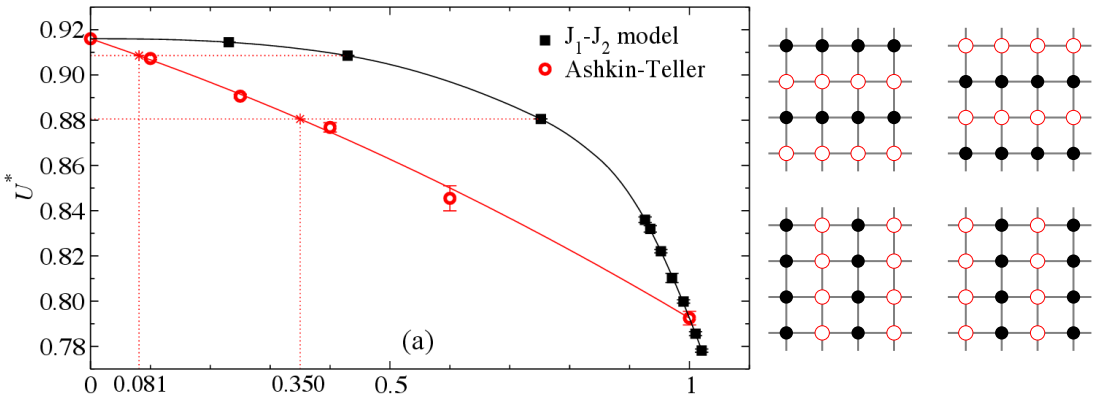


- Configurations at a given T can also be valid configurations (with reasonable probability) also at "slightly" higher or lower T
- Exchange T for M replicas of the system, each with its own temperature .

$$P(\beta_i \rightarrow \beta_j) = min\{1, \exp[(\beta_i - \beta_j)(E_i - E_j)]\}$$

J_1-J_2 Ising model on square lattice





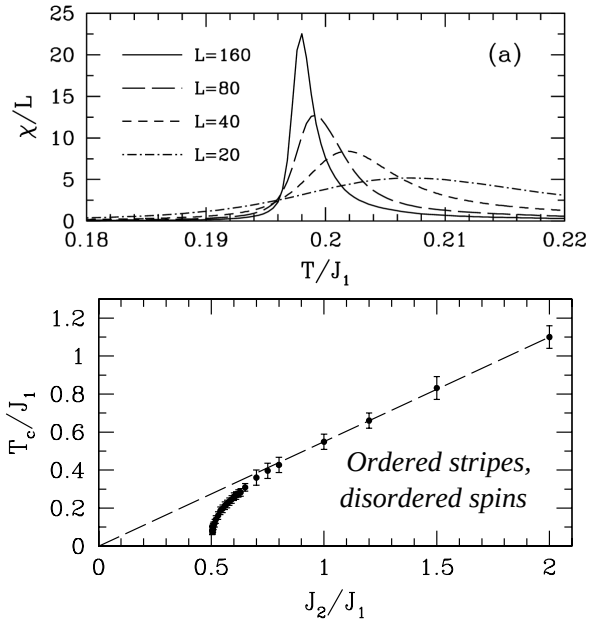
- Striped OP $m_x + im_y$ where $m_{x/y} = \frac{1}{N}\sum_{i=1}^{N} \sigma_i (-1)^{x_i/y_i}$

Binder cumulant $U = 2\left(1 - \frac{1}{2}\frac{\langle m^4 \rangle}{\langle m^2 \rangle^2}\right)$

- AT model $H = -\sum_{\langle ij \rangle}(\sigma_i\sigma_j + \tau_i\tau_j + K\sigma_i\sigma_j\tau_i\tau_j)$
- $\langle \sigma\tau \rangle \neq 0$ AND $\langle \sigma \rangle = \pm\langle \tau \rangle$, OP = $m_\sigma + im_\tau$

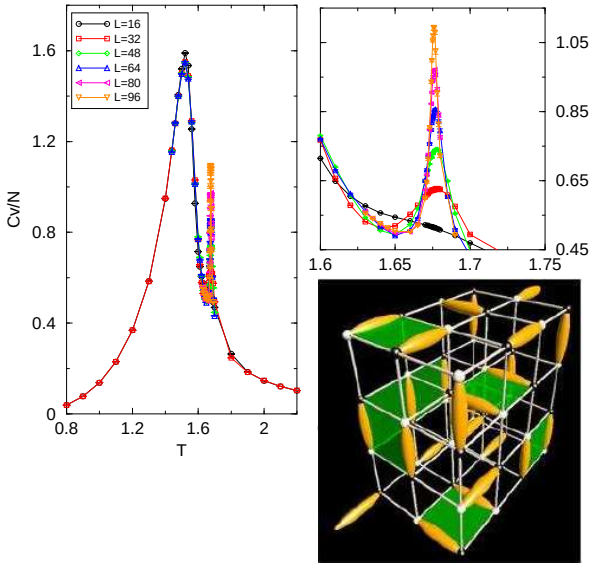
Jin, Sen, Sandvik, PRL (2012), Jin, Sen, Guo, Sandvik, PRB (2013), Kunwar, Sen, Vojta, Narayanan, PRB (2018)

J_1-J_2 Heisenberg model on square lattice



- $H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ik \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_k$
- At finite but low T (and for $J_2/J_1 > 1/2$), two collinear structures are selected due to order by disorder
- Non-trivial discrete degrees of freedom $\sigma_\alpha = \frac{(\mathbf{S}_i - \mathbf{S}_k)(\mathbf{S}_j - \mathbf{S}_l)}{|(\mathbf{S}_i - \mathbf{S}_k)(\mathbf{S}_j - \mathbf{S}_l)|}$ where (i, j, k, l) are the corners with diagonal (i,k) and (j,l)
  P. Chandra et al., PRL (1989), Weber et al., PRL (2003)

Interacting dimers in 3D



- Classical closed packed dimers in 3D, interactions favour parallel dimers on any elementary square plaquette
- Efficient non-local worm updates where $L \sim 100$ (linear dimension)
- Unconventional (Non-Landau) phase transition between dimer crystal and Coulomb phase as a function of T
  Alet et al., PRL (2006), Sreejith, Powell, Nahum, arXiv:1803.11218

Quantum Monte Carlo

- For quantum systems, we have $Z = \mathrm{Tr}\exp(-\beta H)$
- $\langle \mathcal{O} \rangle = \frac{1}{Z}\mathrm{Tr}[\mathcal{O}\exp(-\beta H)]$
- Need to find mapping to an effective "classical" problem in order to perform Monte Carlo simulations
- Will discuss Stochastic Series Expansion (SSE) method for spin systems
- Big issues: The mapping can give "probabilities" which are negative which leads to the notorious sign problem. Often happens for frustrated spin systems
- For details, **Lecture notes by Sandvik, arXiv:1101.3281**

Basic steps

- Choose a basis $|\alpha\rangle$ (e.g. S_i^z)
- Write $H = -\sum_t \sum_a H_{t,a}$ where indices t, a refer to operator "types" and "lattice units"
- $H_{t,a}|\alpha_1\rangle \sim |\alpha_2\rangle$ (no branching)
- $\langle\alpha_2|H_{t,a}|\alpha_1\rangle > 0$ (positivity of weights)

Using these, we get
$Z = \sum_{\{\alpha,n,S_n\}} \frac{\beta^n}{n!} \langle\alpha| \prod_{i=1}^n H_{t_i,a_i}|\alpha\rangle = \sum_{\{\alpha,n,S_n\}} W(\alpha, S_n)$

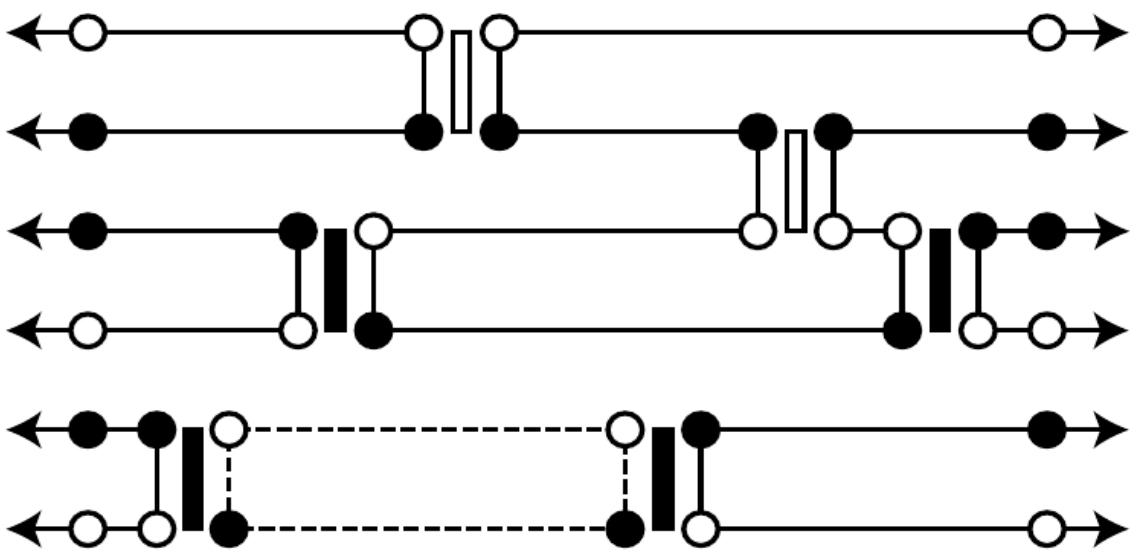
$$\langle A\rangle = \frac{1}{Z} \sum_{\{\alpha,n,S_n\}} \frac{\beta^n}{n!} \langle\alpha|A \prod_{i=1}^n H_{t_i,a_i}|\alpha\rangle = \frac{\sum_{\{\alpha,n,S_n\}} A(\alpha,S_n) W(\alpha,S_n)}{\sum_{\{\alpha,n,S_n\}} W(\alpha,S_n)}$$

- S_n denotes the operator string $S_n = [t_1, a_1], [t_2, a_2], \cdots, [t_n, a_n]$ of length n
- Need to importance sample S_n, the basis state $|\alpha\rangle$, and the expansion power n according to $W(\alpha, S_n)$ AND find $A(\alpha, S_n)$ for operators

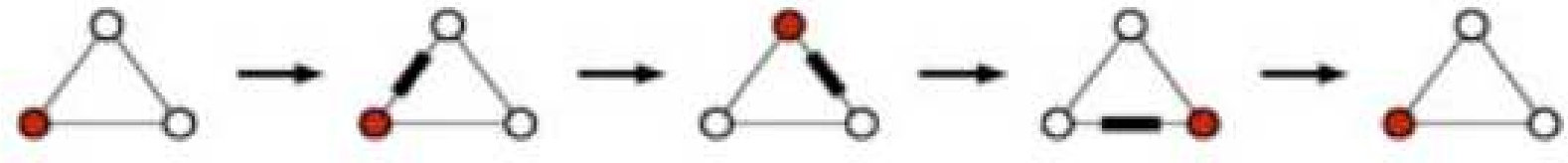
An example

- We also define $H_{0,0} = I$ and work with a fixed operator string of length M where $M > n_{\max}$. Then $Z = \sum_\alpha \sum_{S_M} \frac{\beta^n (M-n)!}{M!} \prod_{i=1}^{M} \langle \alpha_{i-1} | H_{t_i,a_i} | \alpha_i \rangle$
- $H = \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = \sum_{\langle ij \rangle} S_i^z S_j^z + \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)$
- $H_{1,a} = \frac{1}{4} - S_i^z S_j^z$, $H_{2,a} = \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)$

$$\langle \uparrow\downarrow | H_{1,a} | \uparrow\downarrow \rangle = \langle \downarrow\uparrow | H_{1,a} | \downarrow\uparrow \rangle = \frac{1}{2}$$
$$\langle \uparrow\downarrow | H_{2,a} | \downarrow\uparrow \rangle = \langle \downarrow\uparrow | H_{1,a} | \uparrow\downarrow \rangle = \frac{1}{2}$$



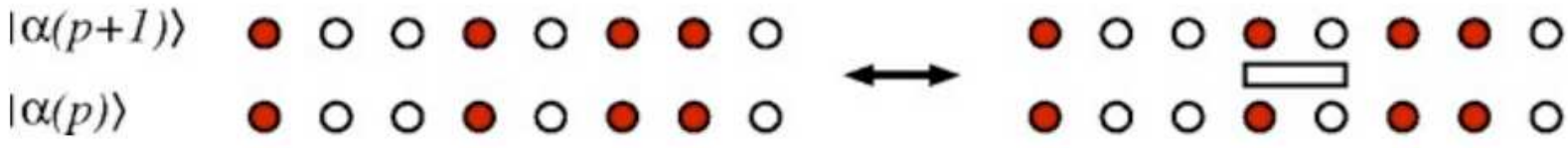
Sign problem



- Take (e.g.) antiferromagnet on kagome lattice
- Cannot do basis transformation to make matrix elements of $H_{2,a}$ positive
- Possible solution–$\langle A \rangle = \frac{\sum_i A_i p_i}{\sum_i p_i}$, sample with $|p_i|$ instead
- $\langle A \rangle = \frac{\sum_i A_i sign(p_i)|p_i| / \sum_i |p_i|}{\sum_i sign(p_i)|p_i| / \sum_i |p_i|} = \frac{\langle A sign \rangle_{|p|}}{\langle sign \rangle_{|p|}}$
- $\langle sign \rangle_{|p|} = \frac{\sum_i p_i}{\sum_i |p_i|} = \frac{Z}{Z_{|p|}} = \exp(-\beta V(f - f_{|p|}))$

$\frac{\Delta sign}{\langle sign \rangle} \approx \frac{\exp(\beta V(f - f_{|p|}))}{\sqrt{N_{MCS}}}$ (NP hard) Troyer and Wiese, PRL (2005)

Diagonal update

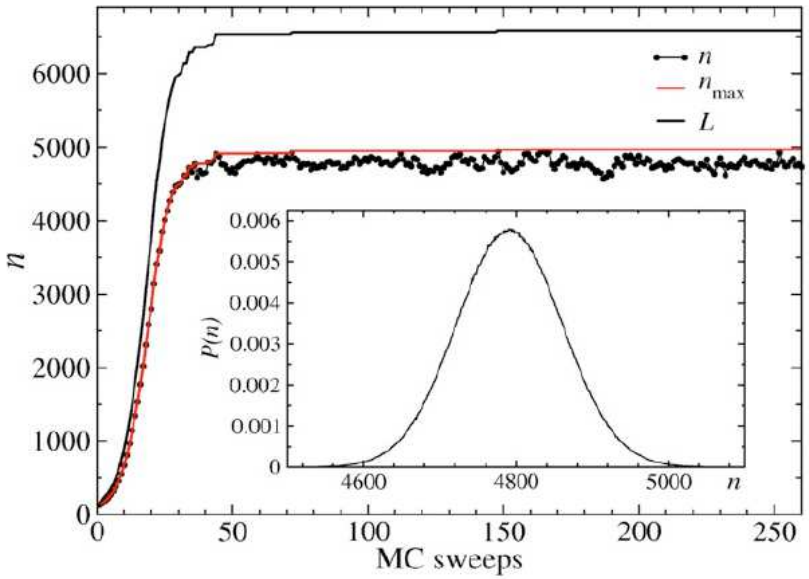


- $W(\alpha, M) = \left(\frac{\beta}{2}\right)^n \frac{(M-n)!}{M!}$
- Diagonal update: $[0,0]_p \leftrightarrow [1,b]_p$
- $P_{select}(0 \to 1) = 1/N_b$ and $P_{select}(1 \to 0) = 1$

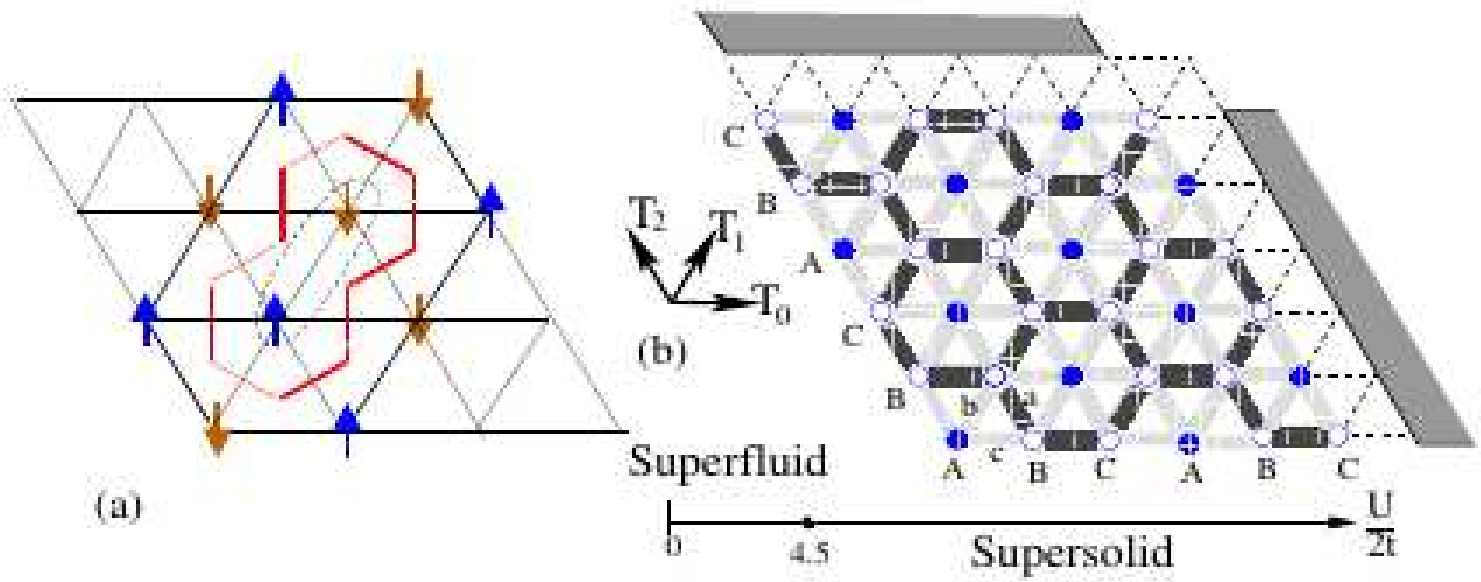
$$P_{accept}([0,0] \to [1,b]) = \min\left[\frac{\beta N_b}{2(M-n)}, 1\right]$$
$$P_{accept}([1,b] \to [0,0]) = \min\left[\frac{2(M-n+1)}{\beta N_b}, 1\right]$$

Some operators

- $|\alpha(p)\rangle \sim \prod_{i=1}^{p} |\alpha(0)\rangle$ where $|\alpha(n) = |\alpha(0)\rangle$
- $\langle A \rangle = \langle \frac{1}{n} \sum_{p=0}^{n-1} A[\alpha(p), S_n(p)] \rangle$
- If A diagonal in the chosen basis, $A(\alpha, S_n) = a(\alpha)$ and $A = \langle \frac{1}{n} \sum_{p=0}^{n-1} a[\alpha(p)] \rangle$
- $\langle H_{t,a} \rangle = \frac{N_{t,a}}{\beta} \rightarrow E = -\frac{\langle n \rangle}{\beta}$
- Specific heat $C = \langle n^2 \rangle - \langle n \rangle^2 - \langle n \rangle$
- For finite L and high β, narrow n distribution with $\langle n \rangle \propto N\beta$, $\sigma_n \propto \sqrt{N\beta}$



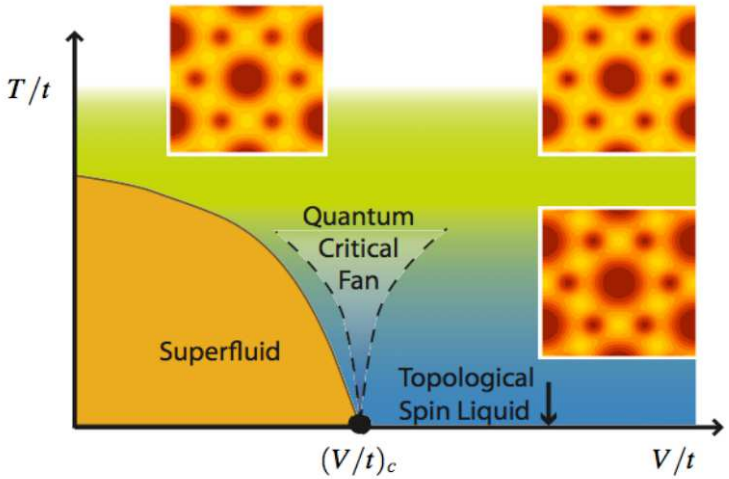
Triangular lattice supersolid at half filling

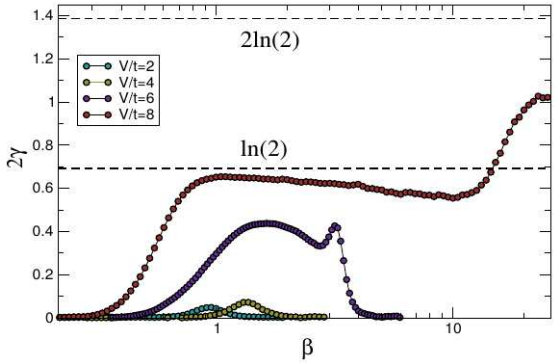


- $H = \sum_{\langle ij \rangle} [U(n_i - 1/2)(n_j - 1/2) - t(b_i^\dagger b_j + b_i b_j^\dagger)] - \mu \sum_i n_i$
- Using SSE method, a supersolid beyond $U/2t \approx 4.5$ was established
- $S = 1/2$ XXZ model with antiferromagnetic $S_i^z S_j^z$ and ferromagnetic transverse couplings on the triangular lattice

Wessel and Troyer, PRL (2005), Heidarian and Damle, PRL (2005), Melko et al., PRL (2005)

Z_2 liquid on the kagome lattice





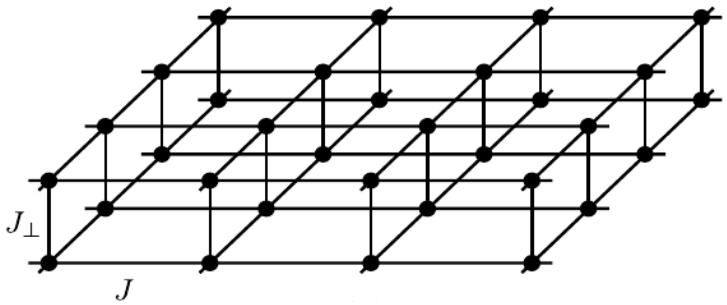
$S = al - \gamma$

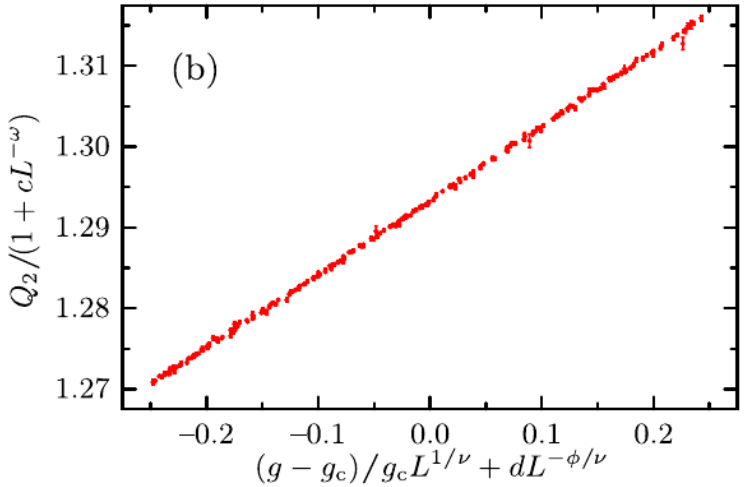
Isakov, Hastings, Melko, Nat. Phys. (2011)

Isakov, Kim, Paramekanti, PRL (2006)

- $H = -J_\perp \sum_{\hexagon}[(S^x_{\hexagon})^2 + (S^y_{\hexagon})^2 - 3] + J_z \sum_{\hexagon}(S^z_{\hexagon})^2$, $J_z, J_\perp > 0$
- $H_b = -t\sum_{(i,j)}(b_i^\dagger b_j + \text{H.c.}) + V\sum_{\hexagon}(n_{\hexagon})^2 - \mu\sum_i n_i$ where $t = J_\perp > 0$, $V = J_z > 0$, $\mu = 12J_z$. Hopping term connects only first, second and third neighbors.
- (Continuous) SF-I transition at $(V/t)_c \approx 19.8$
- Insulating state at half-filling either conventional state with broken lattice symmetry or must have topological order

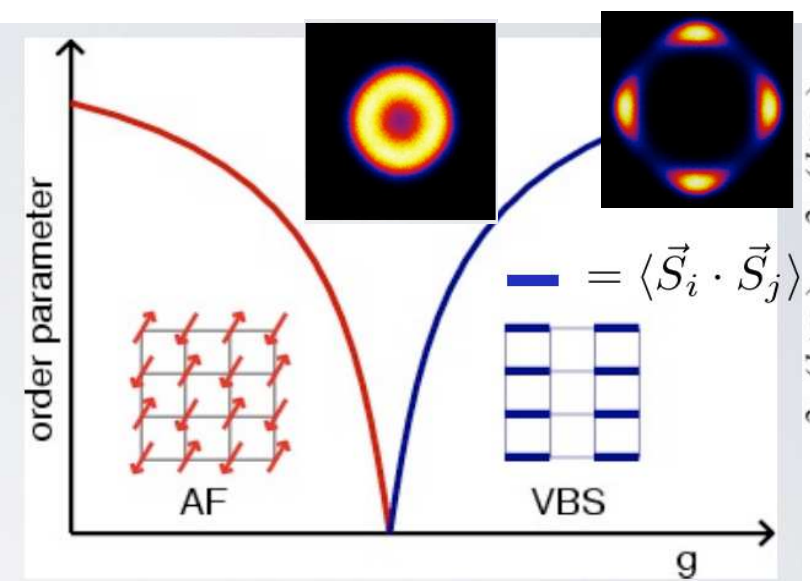
Conventional quantum criticality in $S = 1/2$ Heisenberg bilayers

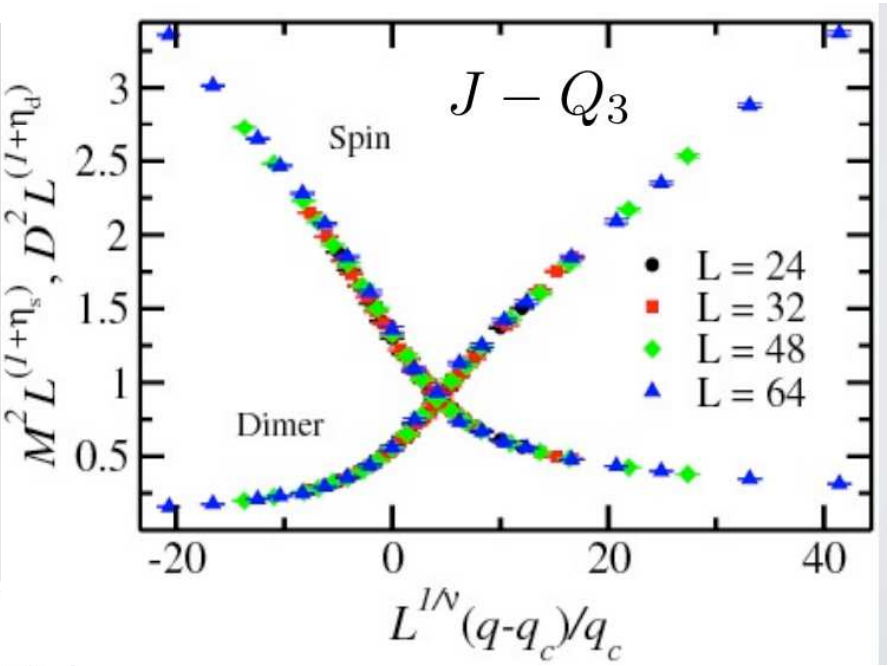




- $H = J\sum_{\langle i,j\rangle}(\mathbf{S}_{1i}\cdot\mathbf{S}_{1j}+\mathbf{S}_{2i}\cdot\mathbf{S}_{2j})+J_\perp\sum_i \mathbf{S}_{1i}\cdot\mathbf{S}_{2i}$
- Néel phase at small g, (trivial) paramagnet at large g
- $g_c = 2.52180(3)$, $\nu = 0.715(2)$ (same universality as the 3D classical Heisenberg model)
  Wang, Beach, Sandvik, PRB (2006)

Unconventional quantum criticality in the $J-Q$ model





- $C_{ij} = \frac{1}{4} - \mathbf{S}_i \cdot \mathbf{S}_j$
  $H = -J \sum_{\langle ij \rangle} C_{ij} - Q \sum_{\langle ijkl \rangle} C_{ij} C_{kl}$ (Sandvik, PRL (2007))
- Néel-VBS transition, $\eta_s = 0.33(2)$, $\eta_d = 0.20(2)$, $\nu = 0.69(2)$ Large η!
- Emergent $U(1)$ symmetry of the dimer fluctuations near critical point