Numerical and Analytical Methods for Strongly Correlated Systems
Benasque, Spain, August 24 - September 13, 2014

Anders W Sandvik, Boston University

Quantum Monte Carlo Techniques
(with a focus on quantum spins)

Lecture 1
Stochastic series expansion and ground state projection

Lecture 2
Non-magnetic and critical states in 2D spin systems

Review article on quantum spin systems and numerical methods**: ArXiv:1101.3281**

Role of numerics/simulations

in studies of many-body ground states and criticality

Obtain **definite results** for "prototypical" model hamiltonians ("Ising models of quantum many-body physics")
- some realized in solid-state materials
- some realizable in cold atoms
- some corresponding to key quantum field theories
- unbiased tests of various analytical calculations
- tools for exploration/discoveries

"Unbiased" methods

(no approximations except finite size)

- exact diagonalization (small systems - be careful!)
- DMRG, 1D systems, recent progress in 2D
- tensor networks, progress in 2D, 3D may be possible (still convergence issues, can become unbiased in principle)
- QMC, for sign-problem free models, any D, large systems

Stochastic Series Expansion and Ground State Projection

Outline

- Path integrals in quantum statistical mechanics
- The series-expansion representation
- Stochastic Series Expansion (SSE) algorithm for the Heisenberg model
- The valence-bond basis for S=1/2 systems
- Ground-state projector algorithm with valence bonds

Reference: AIP Conf. Proc. 1297, 135 (2010); arXiv:1101.3281

Detailed lecture notes on quantum spin models and methods

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Path integrals in quantum statistical mechanics

We want to compute a thermal expectation value

$$\langle A \rangle = \frac{1}{Z} \mathrm{Tr}\{ A \mathrm{e}^{-\beta H} \}$$

where β=1/T (and possibly T→0). How to deal with the exponential operator?

"Time slicing" of the partition function

$$Z = \mathrm{Tr}\{\mathrm{e}^{-\beta H}\} = \mathrm{Tr}\left\{ \prod_{l=1}^{L} \mathrm{e}^{-\Delta_\tau H} \right\} \qquad \Delta_\tau = \beta / L$$

Choose a basis and insert complete sets of states;

$$Z = \sum_{\alpha_0} \sum_{\alpha_1} \cdots \sum_{\alpha_L - 1} \langle \alpha_0 | \mathrm{e}^{-\Delta_\tau H} | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | \mathrm{e}^{-\Delta_\tau H} | \alpha_1 \rangle \langle \alpha_1 | \mathrm{e}^{-\Delta_\tau H} | \alpha_0 \rangle$$

Use approximation for imaginary time evolution operator. Simplest way

$$Z \approx \sum_{\{\alpha\}} \langle \alpha_0 | 1 - \Delta_\tau H | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | 1 - \Delta_\tau H | \alpha_1 \rangle \langle \alpha_1 | 1 - \Delta_\tau H | \alpha_0 \rangle$$

Leads to error $\propto \Delta_\tau$. Limit $\Delta_\tau \to 0$ can be taken

Example: hard-core bosons

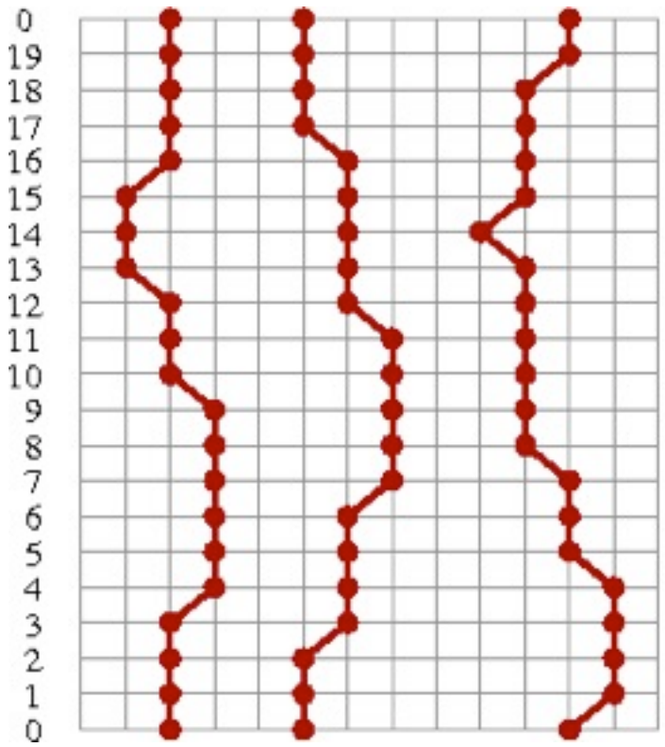
$$H = K = -\sum_{\langle i,j \rangle} K_{ij} = -\sum_{\langle i,j \rangle} (a_j^\dagger a_i + a_i^\dagger a_j) \qquad n_i = a_i^\dagger a_i \in \{0, 1\}$$

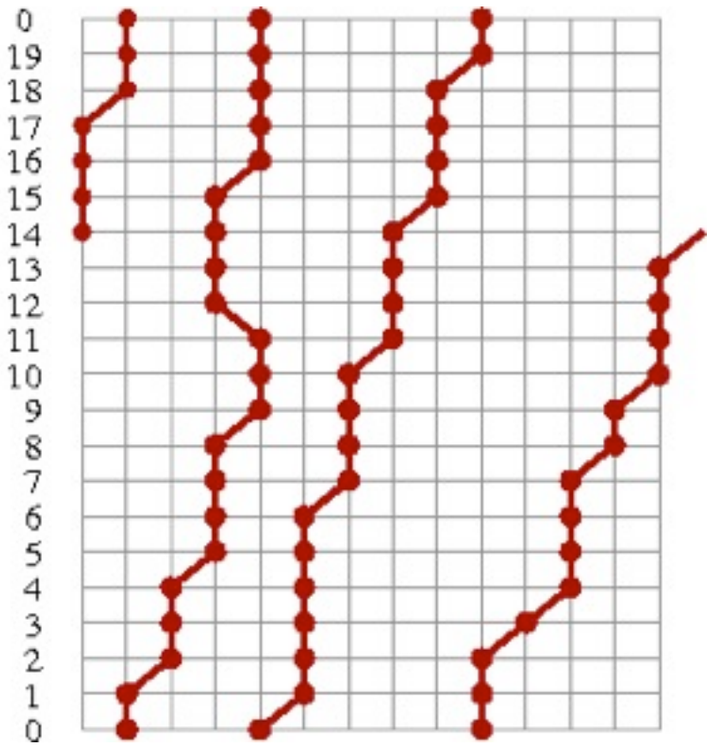
Equivalent to S=1/2 XY model

$$H = -2\sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y) = -\sum_{\langle i,j \rangle} (S_i^+ S_j^- + S_i^- S_j^+), \quad S^z = \pm\frac{1}{2} \sim n_i = 0, 1$$

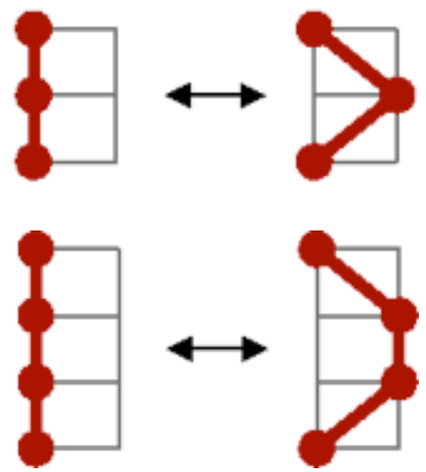
"World line" representation of

$$Z \approx \sum_{\{\alpha\}} \langle \alpha_0 | 1 - \Delta_\tau H | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | 1 - \Delta_\tau H | \alpha_1 \rangle \langle \alpha_1 | 1 - \Delta_\tau H | \alpha_0 \rangle$$





world line moves for Monte Carlo sampling



$$Z = \sum_{\{\alpha\}} W(\{\alpha\}), \quad W(\{\alpha\}) = \Delta_\tau^{n_K}$$

n_K = number of "jumps"

Expectation values

$$\langle A\rangle = \frac{1}{Z}\sum_{\{\alpha\}}\langle\alpha_0|\mathrm{e}^{-\Delta_\tau}|\alpha_{L-1}\rangle\cdots\langle\alpha_2|\mathrm{e}^{-\Delta_\tau H}|\alpha_1\rangle\langle\alpha_1|\mathrm{e}^{-\Delta_\tau H}A|\alpha_0\rangle$$

We want to write this in a form suitable for MC importance sampling

$$\langle A\rangle = \frac{\sum_{\{\alpha\}} A(\{\alpha\})W(\{\alpha\})}{\sum_{\{\alpha\}} W(\{\alpha\})} \quad\longrightarrow\quad \langle A\rangle = \langle A(\{\alpha\})\rangle_W$$

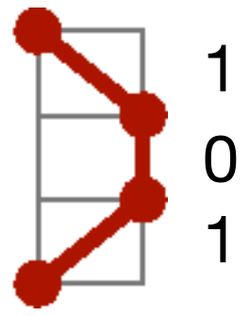
$$W(\{\alpha\}) = \text{weight}$$
$$A(\{\alpha\}) = \text{estimator}$$

For any quantity diagonal in the occupation numbers (spin z):

$$A(\{\alpha\}) = A(\alpha_n) \quad \text{or} \quad A(\{\alpha\}) = \frac{1}{L}\sum_{l=0}^{L-1} A(\alpha_l)$$

Kinetic energy (here full energy). Use

$$K\mathrm{e}^{-\Delta_\tau K} \approx K \qquad K_{ij}(\{\alpha\}) = \frac{\langle\alpha_1|K_{ij}|\alpha_0\rangle}{\langle\alpha_1|1-\Delta_\tau K|\alpha_0\rangle} \in \{0, \frac{1}{\Delta_\tau}\}$$



Average over all slices → count number of kinetic jumps

$$\langle K_{ij}\rangle = \frac{\langle n_{ij}\rangle}{\beta}, \quad \langle K\rangle = -\frac{\langle n_K\rangle}{\beta} \qquad \langle K\rangle \propto N \rightarrow \langle n_K\rangle \propto \beta N$$

There should be of the order βN "jumps" (regardless of approximation used)

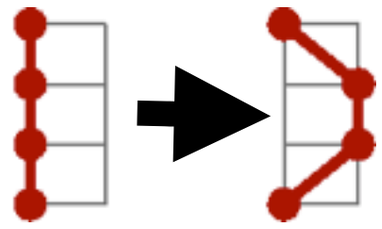
Including interactions

For any diagonal interaction V (Trotter, or split-operator, approximation)

$$\mathrm{e}^{-\Delta_\tau H} = \mathrm{e}^{-\Delta_\tau K}\mathrm{e}^{-\Delta_\tau V} + \mathcal{O}(\Delta_\tau^2) \rightarrow \langle\alpha_{l+1}|\mathrm{e}^{-\Delta_\tau H}|\alpha_l\rangle \approx \mathrm{e}^{-\Delta_\tau V_l}\langle\alpha_{l+1}|\mathrm{e}^{-\Delta_\tau K}|\alpha_l\rangle$$

Product over all times slices →

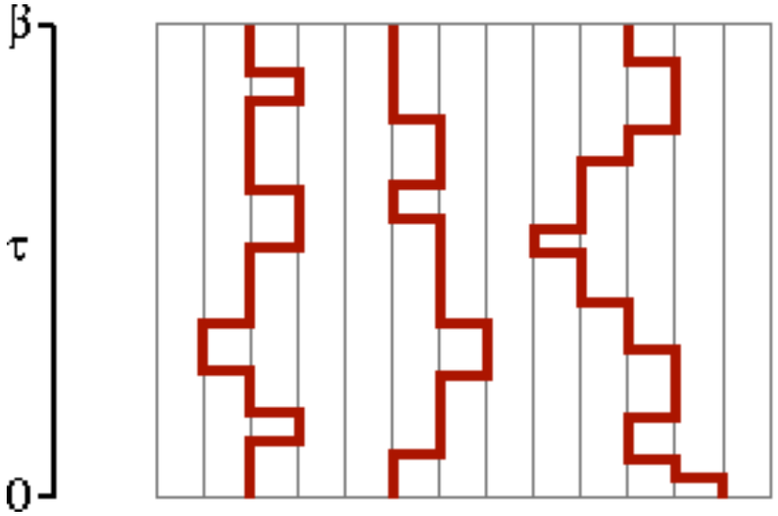
$$W(\{\alpha\}) = \Delta_\tau^{n_K}\exp\left(-\Delta_\tau\sum_{l=0}^{L-1}V_l\right)$$



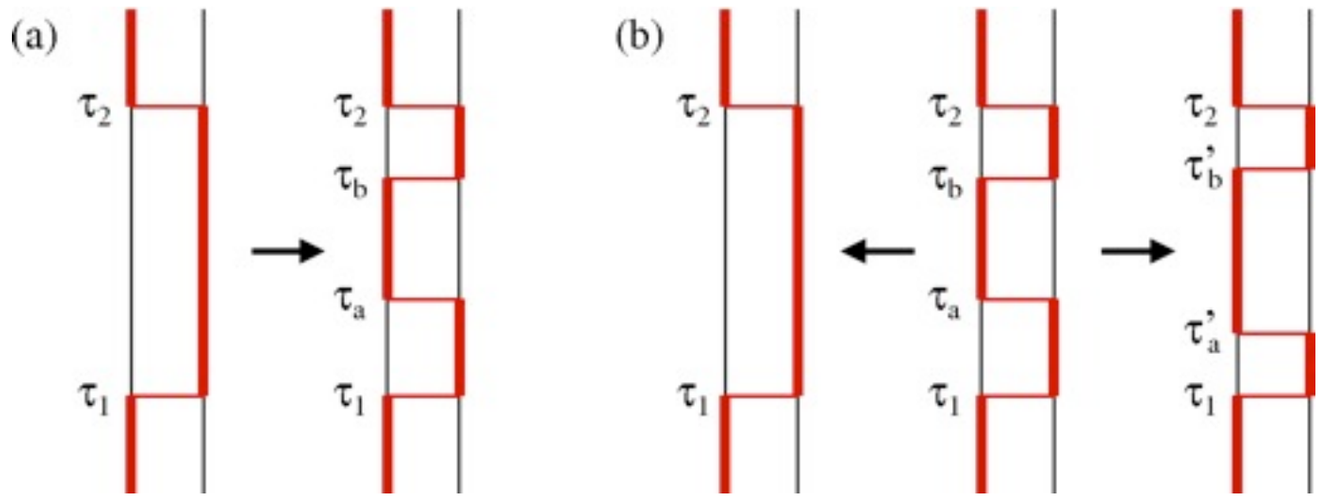
$$P_{\mathrm{acc}} = \min\left[\Delta_\tau^2\exp\left(-\frac{V_{\mathrm{new}}}{V_{\mathrm{old}}}\right),1\right]$$

The continuous time limit

Limit $\Delta_\tau \rightarrow 0$: number of kinetic jumps remains finite, store events only



Special methods (**loop and worm updates**) developed for efficient sampling of the paths in the continuum



local updates (problem when $\Delta_\tau \rightarrow 0$?)

- consider probability of inserting/removing events within a time window

⇐ Evertz, Lana, Marcu (1993), Prokofev et al (1996)
Beard & Wiese (1996)

Series expansion representation

Start from the Taylor expansion $\mathrm{e}^{-\beta H} = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} H^n$ (approximation-free method from the outset)

$$Z = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\{\alpha\}_n} \langle\alpha_0|H|\alpha_{n-1}\rangle \cdots \langle\alpha_2|H|\alpha_1\rangle\langle\alpha_1|H|\alpha_0\rangle$$

Similar to the path integral; $1 - \Delta\tau H \to H$ and weight factor outside

For hard-core bosons the (allowed) path weight is $W(\{\alpha\}_n) = \beta^n/n!$

For any model, the energy is

this is the operator we "measure"

$$E = \frac{1}{Z} \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\{\alpha\}_{n+1}} \langle\alpha_0|H|\alpha_n\rangle \cdots \langle\alpha_2|H|\alpha_1\rangle\langle\alpha_1|H|\alpha_0\rangle$$

one more "slice" to sum over here

$$= -\frac{1}{Z} \sum_{n=1}^{\infty} \frac{(-\beta)^n}{n!} \frac{n}{\beta} \sum_{\{\alpha\}_n} \langle\alpha_0|H|\alpha_{n-1}\rangle \cdots \langle\alpha_2|H|\alpha_1\rangle\langle\alpha_1|H|\alpha_0\rangle = \frac{-\langle n\rangle}{\beta}$$

relabel terms to "get rid of" extra slice

$C = \langle n^2\rangle - \langle n\rangle^2 - \langle n\rangle$

From this follows: narrow n-distribution with $\langle n\rangle \propto N\beta, \quad \sigma_n \propto \sqrt{N\beta}$

Fixed-length scheme

- n fluctuating → varying size of the configurations
- the expansion can be truncated at some n_{max}=M (exponentially small error)
- cutt-off at n=M, fill in operator string with unit operators H_0=I

n=10 | H_4 | H_7 | H_1 | H_6 | H_2 | H_1 | H_8 | H_3 | H_3 | H_5 | ⟹

M=14 | H_4 | I | H_7 | I | H_1 | H_6 | I | H_2 | H_1 | H_8 | H_3 | H_3 | I | H_5 |

- conisider all possible locations in the sequence
- overcounting of actual (original) strings, correct by combinatorial factor:

$$\binom{M}{n}^{-1} = \frac{n!(M-n)!}{M!}$$

Here n is the number of H_i, i>0 instances in the sequence of M operators

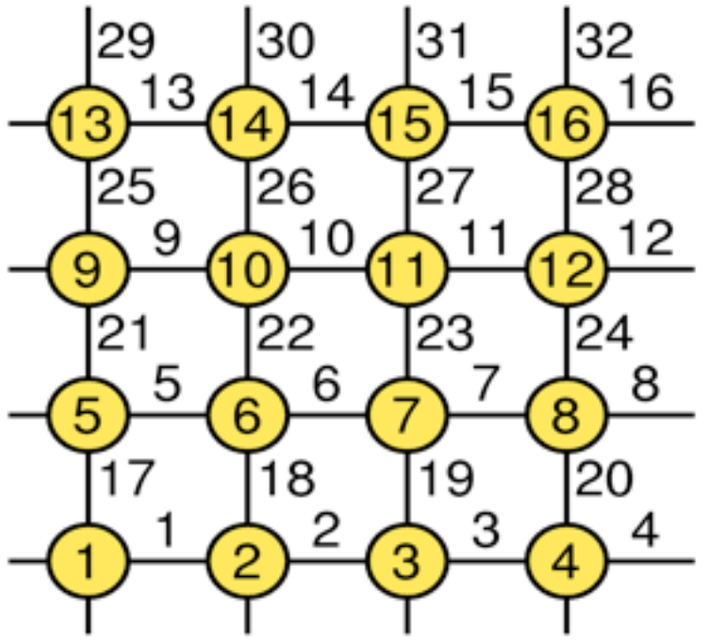
$$Z = \sum_{\{\alpha\}_M} \sum_{\{H_i\}} \frac{(-\beta)^n (M-n)!}{M!} \langle \alpha_0 | H_{i(M)} | \alpha_{M-1} \rangle \cdots \langle \alpha_1 | H_{i(1)} | \alpha_0 \rangle$$

Stochastic Series expansion (SSE): S=1/2 Heisenberg model

Write H as a bond sum for arbitrary lattice

$$H = J \sum_{b=1}^{N_b} \mathbf{S}_{i(b)} \cdot \mathbf{S}_{j(b)},$$

2D square lattice
bond and site labels



Diagonal (1) and off-diagonal (2) bond operators

$$H_{1,b} = \frac{1}{4} - S^z_{i(b)} S^z_{j(b)},$$

$$H_{2,b} = \frac{1}{2}(S^+_{i(b)} S^-_{j(b)} + S^-_{i(b)} S^+_{j(b)}).$$

$$H = -J \sum_{b=1}^{N_b} (H_{1,b} - H_{2,b}) + \frac{J N_b}{4}$$

Four non-zero matrix elements

$$\langle \uparrow_{i(b)} \downarrow_{j(b)} | H_{1,b} | \uparrow_{i(b)} \downarrow_{j(b)} \rangle = \frac{1}{2} \qquad \langle \downarrow_{i(b)} \uparrow_{j(b)} | H_{2,b} | \uparrow_{i(b)} \downarrow_{j(b)} \rangle = \frac{1}{2}$$

$$\langle \downarrow_{i(b)} \uparrow_{j(b)} | H_{1,b} | \downarrow_{i(b)} \uparrow_{j(b)} \rangle = \frac{1}{2} \qquad \langle \uparrow_{i(b)} \downarrow_{j(b)} | H_{2,b} | \downarrow_{i(b)} \uparrow_{j(b)} \rangle = \frac{1}{2}$$

Partition function

$$Z = \sum_{\alpha} \sum_{n=0}^{\infty} (-1)^{n_2} \frac{\beta^n}{n!} \sum_{S_n} \left\langle \alpha \left| \prod_{p=0}^{n-1} H_{a(p),b(p)} \right| \alpha \right\rangle$$

n_2 = number of a(i)=2
(off-diagonal operators)
in the sequence

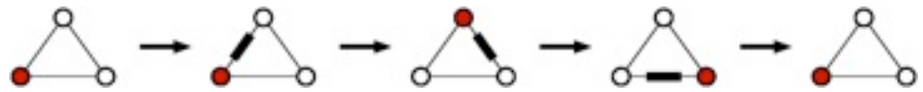
Index sequence: $S_n = [a(0), b(0)], [a(1), b(1)], \ldots, [a(n-1), b(n-1)]$

For fixed-length scheme (string length = L now)

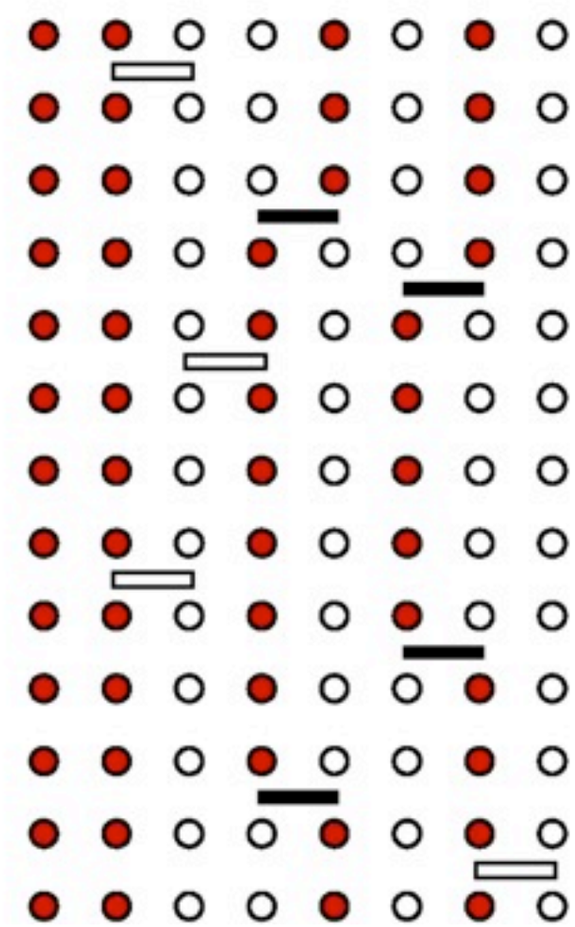
$$Z = \sum_{\alpha} \sum_{S_L} (-1)^{n_2} \frac{\beta^n (L-n)!}{L!} \left\langle \alpha \left| \prod_{p=0}^{L-1} H_{a(p),b(p)} \right| \alpha \right\rangle \qquad W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$$

Propagated states: $|\alpha(p)\rangle \propto \prod_{i=0}^{p-1} H_{a(i),b(i)} |\alpha\rangle$

W>0 (n_2 even) for bipartite lattice
Frustration leads to **sign problem**



i =	1	2	3	4	5	6	7	8
$\sigma(i)$ =	-1	+1	-1	-1	+1	-1	+1	+1



p	$a(p)$	$b(p)$	$s(p)$
11	1	2	4
10	0	0	0
9	2	4	9
8	2	6	13
7	1	3	6
6	0	0	0
5	0	0	0
4	1	2	4
3	2	6	13
2	0	0	0
1	2	4	9
0	1	7	14

In a program:

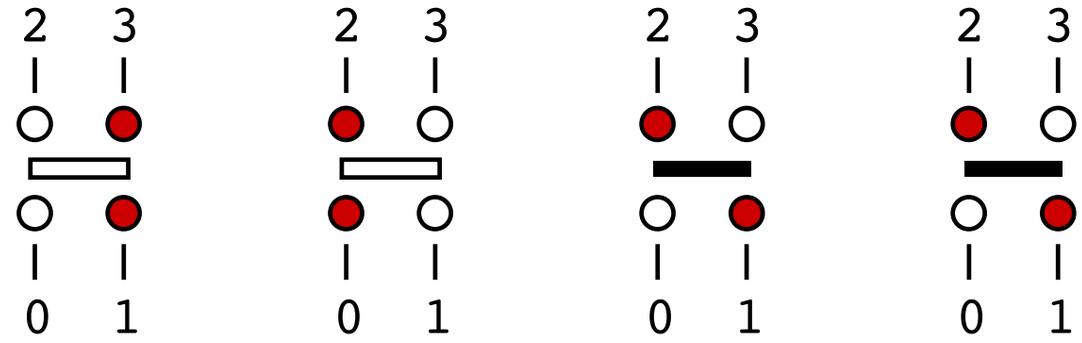
s(p) = operator-index string
- **s(p) = 2*b(p) + a(p)-1**
- diagonal; s(p) = even
- off-diagonal; s(p) = off

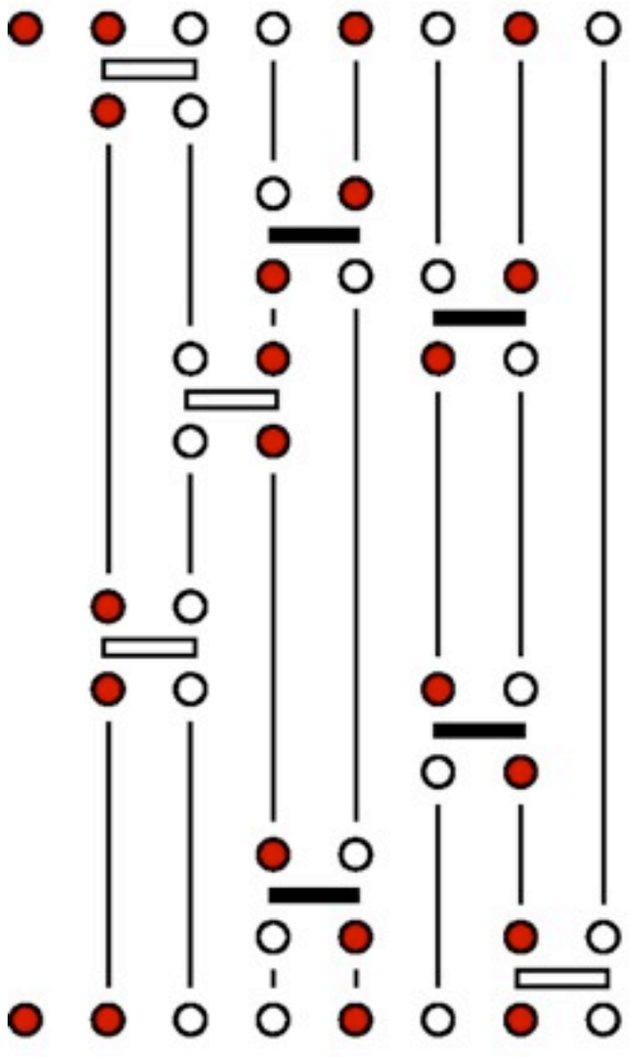
σ(i) = spin state, i=1,...,N
- only one has to be stored

SSE effectively provides a discrete representation of the time continuum
- computational advantage; only integer operations in sampling

Linked vertex storage

The “legs” of a vertex represents the spin states before (below) and after (above) an operator has acted





p	v X(v)		v X(v)		v X(v)		v X(v)	
11	44	18	45	30	46	16	47	17
10	40	-	41	-	42	-	43	-
9	36	31	37	7	38	4	39	5
8	32	14	33	15	34	12	35	0
7	28	19	29	6	30	45	31	36
6	24	-	25	-	26	-	27	-
5	20	-	21	-	22	-	23	-
4	16	46	17	47	18	44	19	28
3	12	34	13	2	14	32	15	33
2	8	-	9	-	10	-	11	-
1	4	38	5	39	6	29	7	37
0	0	35	1	3	2	13	3	1
	l=0		l=1		l=2		l=3	

X( ) = vertex list

- operator at p→X(v)
  v=4p+l, l=0,1,2,3
- links to next and previous leg

Spin states between operations are redundant; represented by links

- network of linked vertices will be used for loop updates of vertices/operators

Monte Carlo sampling scheme

Change the configuration; $(\alpha, S_L) \to (\alpha', S'_L)$

$$W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$$

$$P_{\text{accept}} = \min\left[\frac{W(\alpha', S_L)}{W(\alpha, S_L)} \frac{P_{\text{select}}(\alpha', S'_L \to \alpha, S_L)}{P_{\text{select}}(\alpha, S_L \to \alpha', S'_L)}, 1\right]$$

Diagonal update: $[0,0]_p \leftrightarrow [1,b]_p$

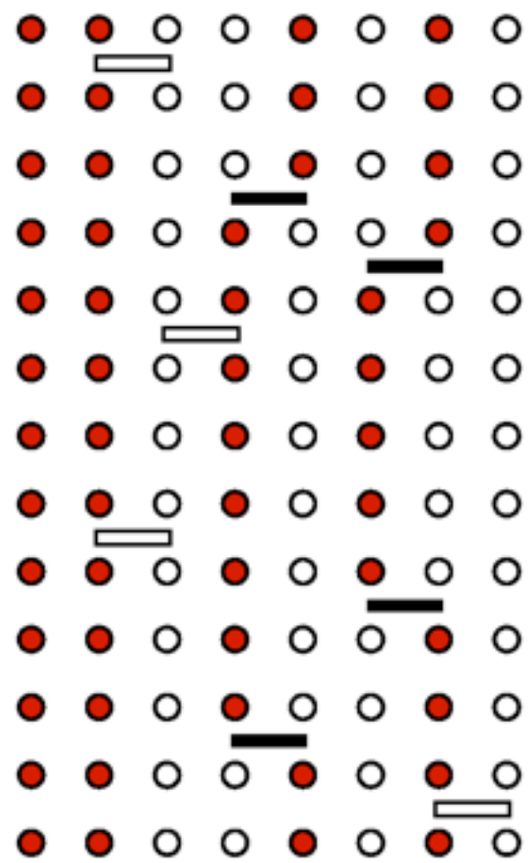
Attempt at p=0,...,L-1. Need to know |α(p)>

- generate by flipping spins when off-diagonal operator

$$P_{\text{select}}(a = 0 \to a = 1) = 1/N_b, \quad (b \in \{1, \ldots, N_b\})$$

$$P_{\text{select}}(a = 1 \to a = 0) = 1$$

$$\frac{W(a=1)}{W(a=0)} = \frac{\beta/2}{L-n} \qquad \frac{W(a=0)}{W(a=1)} = \frac{L-n+1}{\beta/2}$$



n is the current power

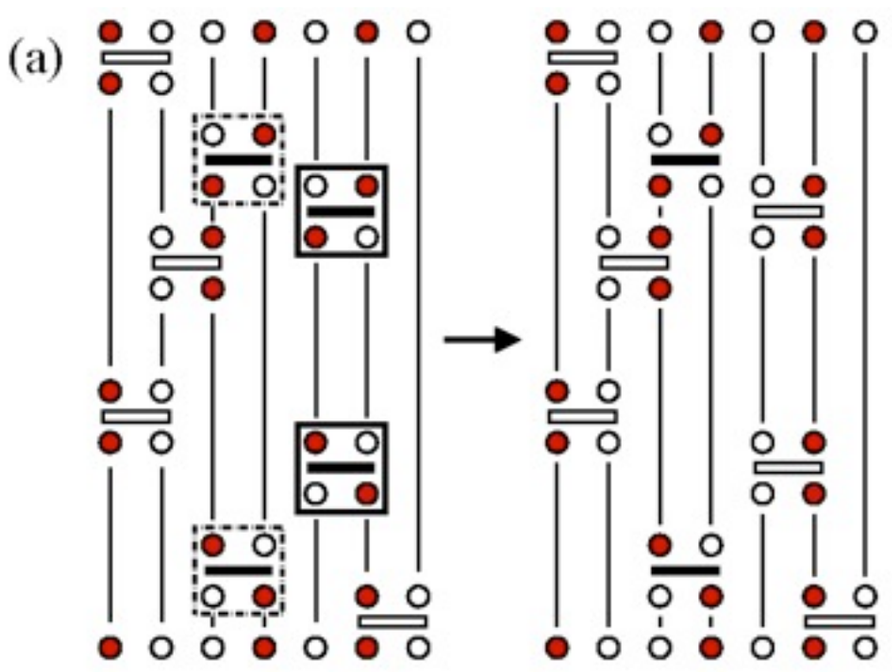
- n → n+1 (a=0 → a=1)
- n → n-1 (a=1 → a=0)

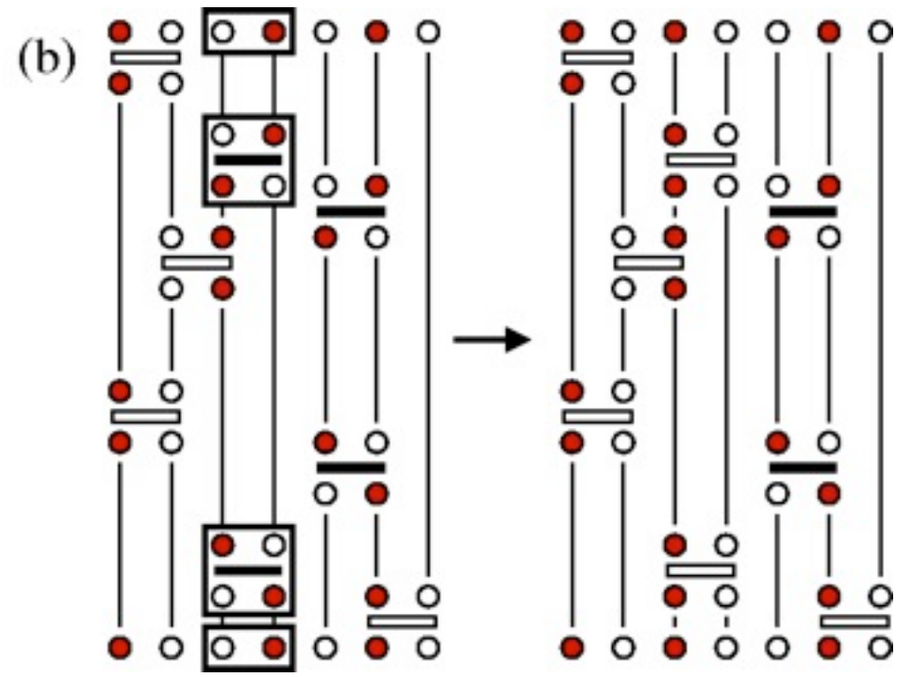
Acceptance probabilities

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

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

Off-diagonal updates

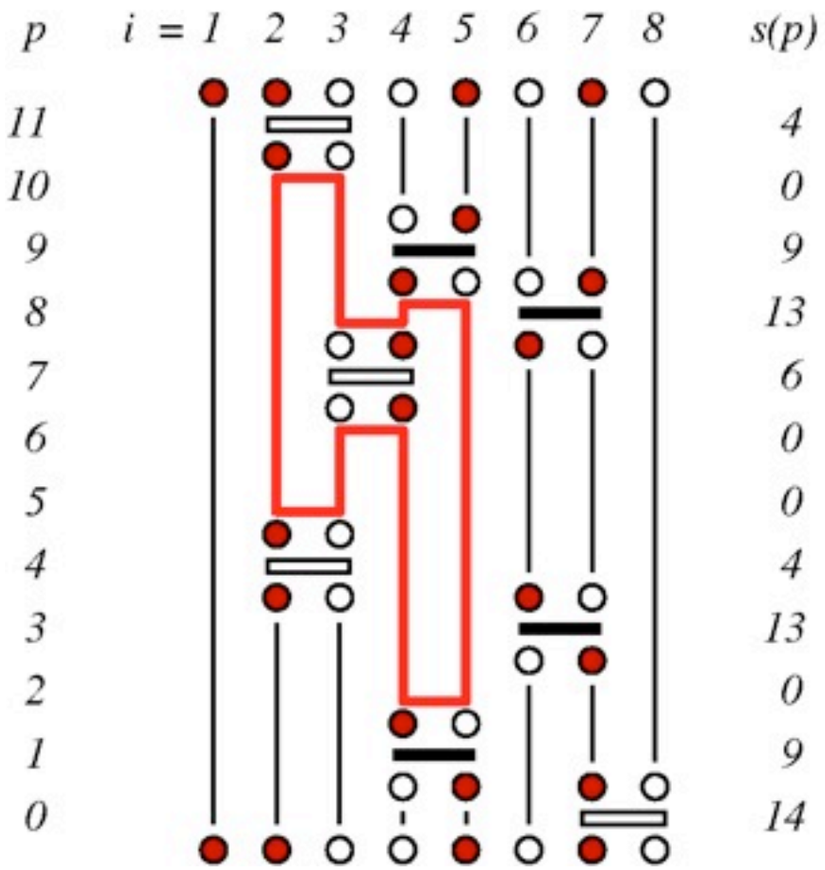


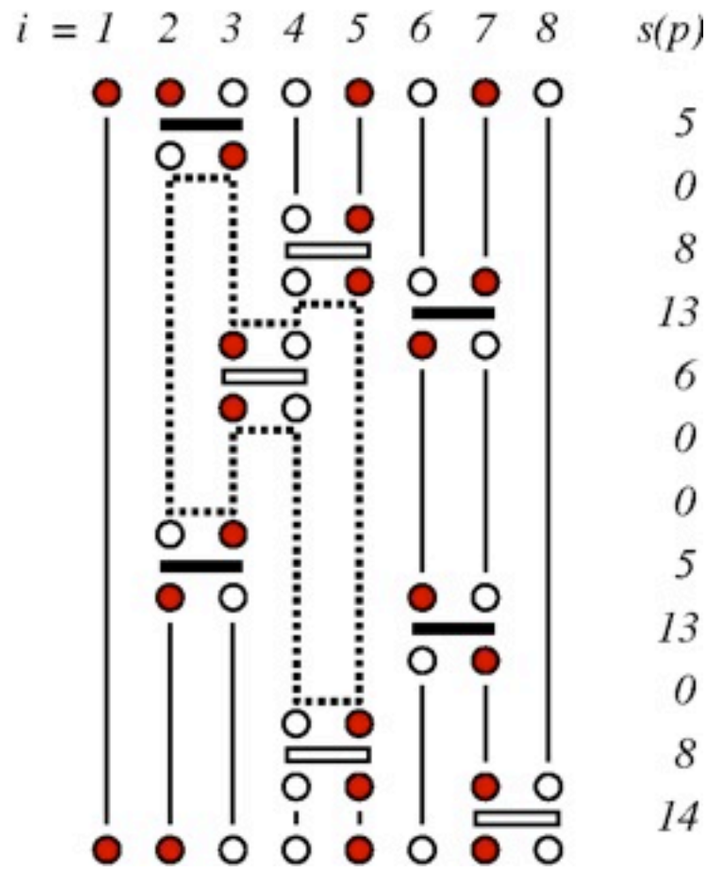


Local update

Change the type of two operators

- constraints
- inefficient
- cannot change winding numbers





Operator-loop update

- Many spins and operators can be changed simultaneously
- can change winding numbers

Determination of the cut-off L

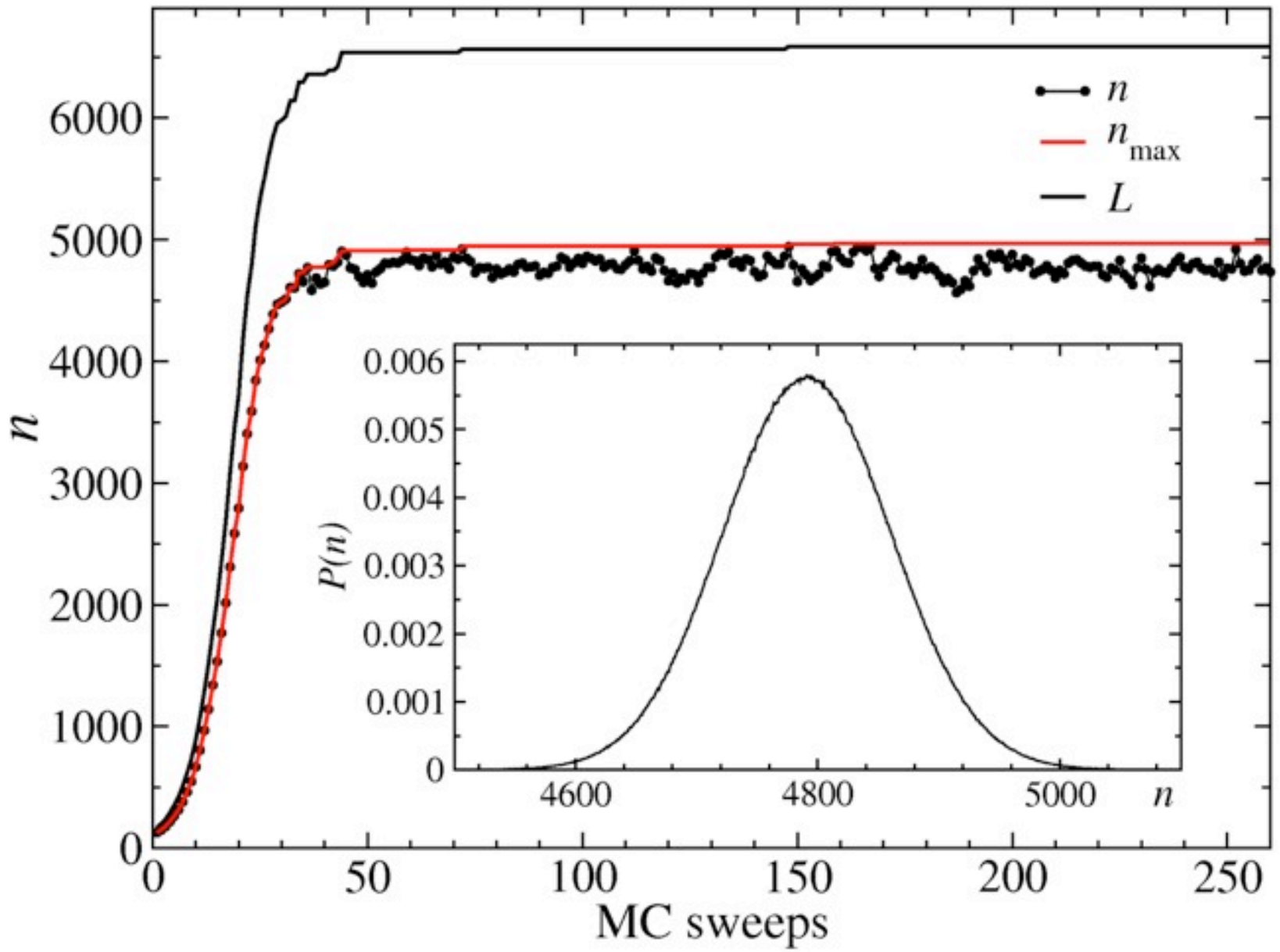
- adjust during equilibration
- start with arbitrary (small) n

Keep track of number of operators n

- increase L if n is close to current L
- e.g., ***L=n+n/3***

Example

- 16×16 system, β=16 ⇒
- evolution of L
- n distribution after equilibration
- truncation is no approximation

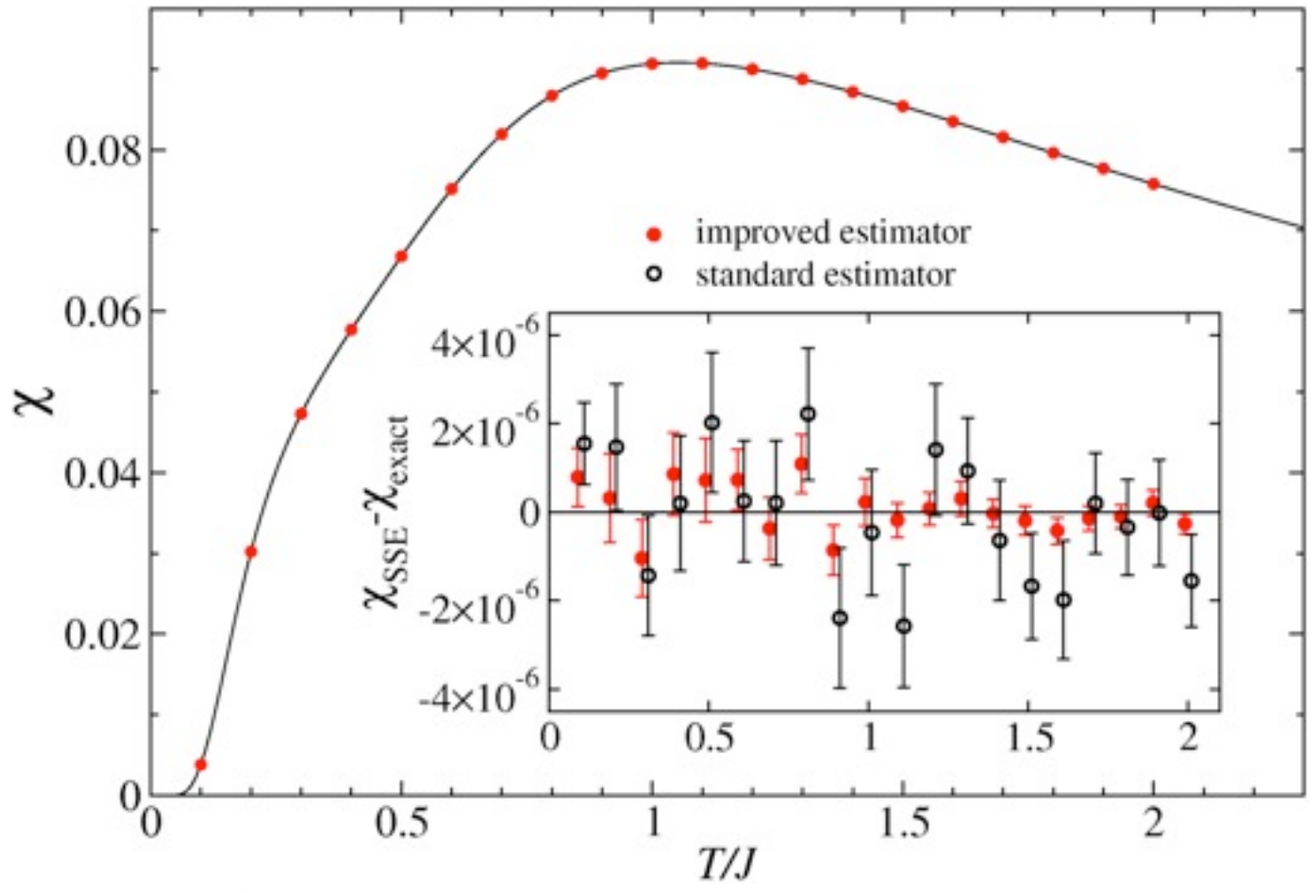


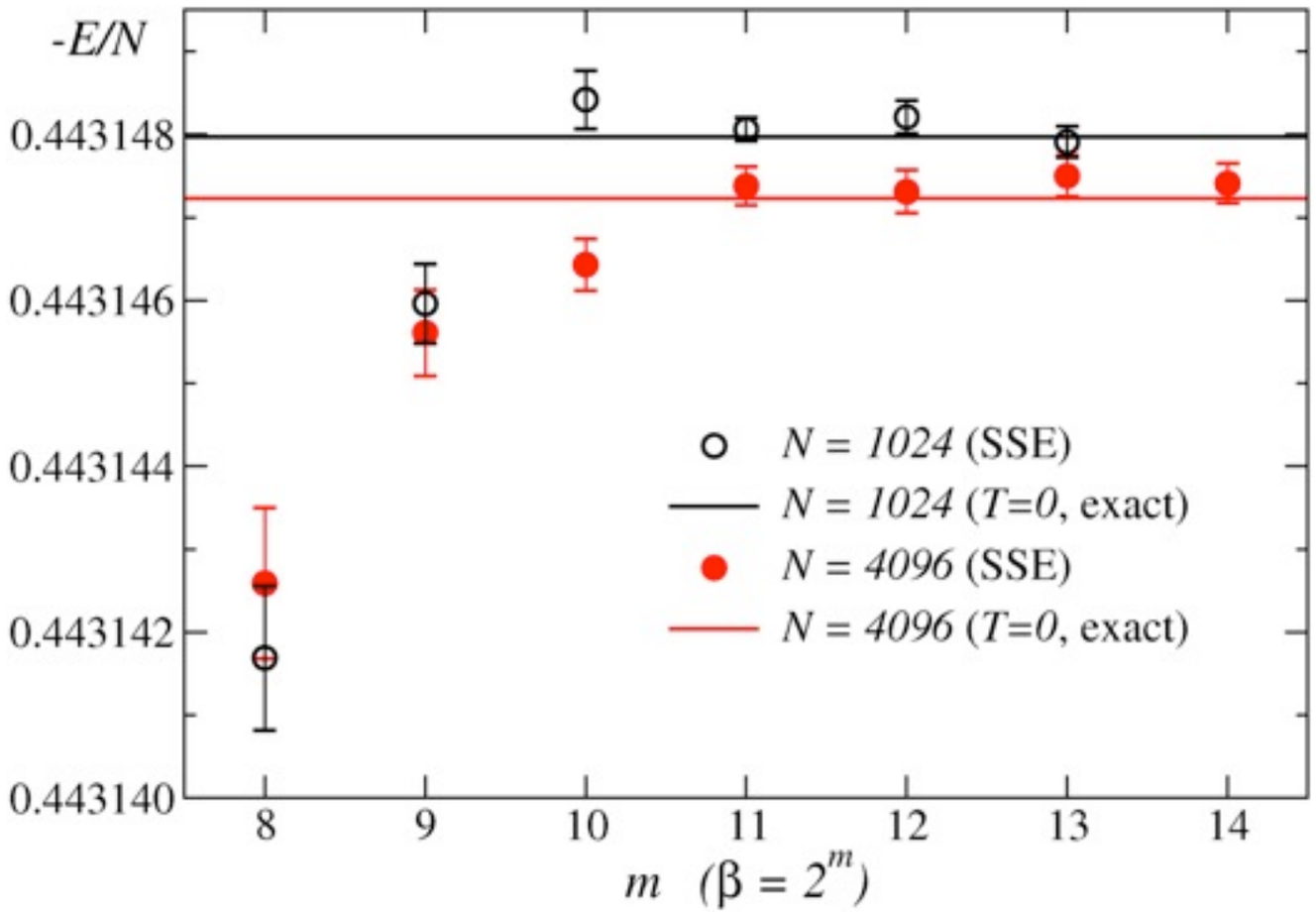
Does it work?
Compare with exact results

- 4×4 exact diagonalization
- Bethe Ansatz; long chains

Susceptibility of the 4×4 lattice ⇒

- SSE results from 10^{10} sweeps
- improved estimator gives smaller error bars at high T (where the number of loops is larger)





⇐ Energy for long 1D chains

- SSE results for 10^6 sweeps
- Bethe Ansatz ground state E/N
- SSE can achieve the ground state limit (T→0)

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Valence bonds and Ground State Projection

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Outline

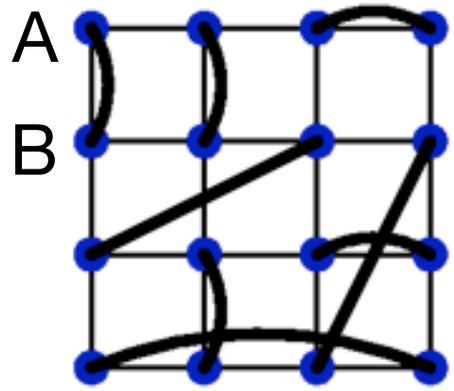
- The valence-bond basis for S=1/2 systems
- Ground-state projector algorithm with valence bonds

The valence bond basis for S=1/2 spins

Valence-bonds between sublattice A, B sites $(i,j) = (|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle)/\sqrt{2}$

Basis states; singlet products

$$|V_r\rangle = \prod_{b=1}^{N/2}(i_{rb}, j_{rb}), \quad r = 1, \ldots (N/2)!$$



The valence bond basis is overcomplete and non-orthogonal

- expansion of arbitrary singlet state is not unique

$$|\Psi\rangle = \sum_r f_r |V_r\rangle$$ (all f_r positive for non-frustrated system)

All valence bond states overlap with each other

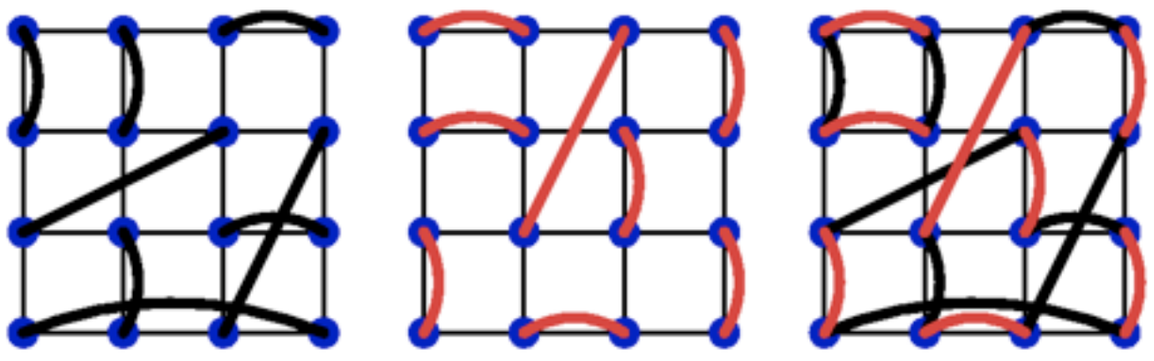
$$\langle V_l|V_r\rangle = 2^{N_\circ - N/2} \qquad N_\circ = \text{ number of loops in overlap graph}$$

Spin correlations from loop structure

$$\frac{\langle V_l|\vec{S}_i\cdot\vec{S}_j|V_r\rangle}{\langle V_l|V_r\rangle} = \begin{cases} \frac{3}{4}(-1)^{x_i - x_j + y_i - y_j} & \textit{(i,j in same loop)} \\ 0 & \textit{(i,j in different loops)} \end{cases}$$

More complicated matrix elements (e.g., dimer correlations) are also related to the loop structure

K.S.D. Beach and A.W.S.,
Nucl. Phys. B 750, 142 (2006)



Projector Monte Carlo in the valence-bond basis

Liang, 1991; AWS, Phys. Rev. Lett 95, 207203 (2005)

(-H)^n projects out the ground state from an arbitrary state

$$(-H)^n|\Psi\rangle = (-H)^n \sum_i c_i|i\rangle \rightarrow c_0(-E_0)^n|0\rangle$$

S=1/2 Heisenberg model

$$H = \sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j = -\sum_{\langle i,j\rangle} H_{ij}, \qquad H_{ij} = (\tfrac{1}{4} - \vec{S}_i \cdot \vec{S}_j)$$

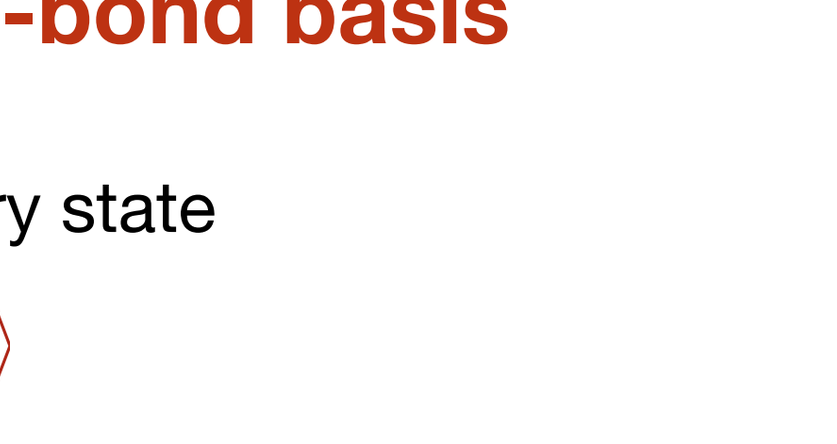
Project with string of bond operators

$$\sum_{\{H_{ij}\}} \prod_{p=1}^{n} H_{i(p)j(p)}|\Psi\rangle \rightarrow r|0\rangle$$ (r = irrelevant)

Action of bond operators

$$H_{ab}|...(a,b)...(c,d)...\rangle = |...(a,b)...(c,d)...\rangle$$

$$H_{bc}|...(a,b)...(c,d)...\rangle = \frac{1}{2}|...(c,b)...(a,d)...\rangle$$



$$(i,j) = (|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle)/\sqrt{2}$$

Simple reconfiguration of bonds (or no change; diagonal)

- no minus signs for A→B bond 'direction' convetion
- sign problem does appear for frustrated systems

Expectation values: $\langle A\rangle = \langle 0|A|0\rangle$

Strings of singlet projectors

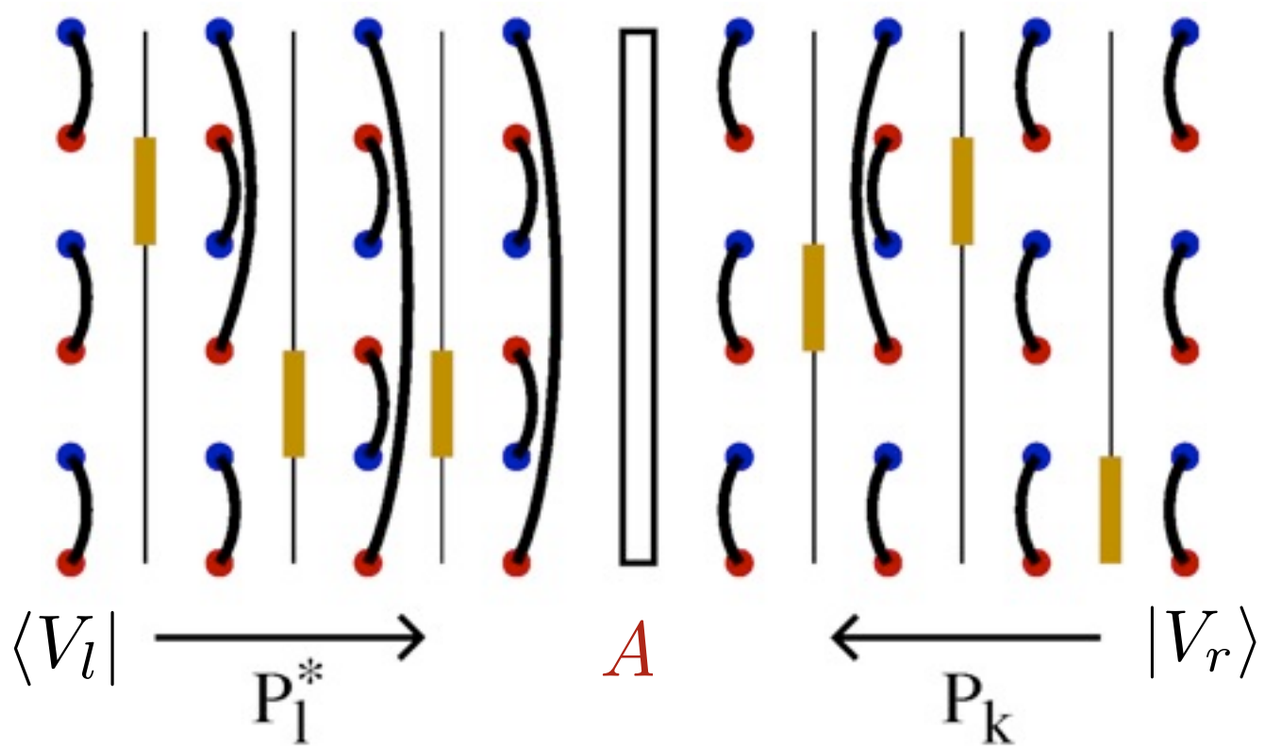
$$P_k = \prod_{p=1}^{n} H_{i_k(p)j_k(p)}, \quad k = 1, \ldots, N_b^n \quad (N_b = \text{number of interaction bonds})$$

We have to project bra and ket states

$$\sum_k P_k|V_r\rangle = \sum_k W_{kr}|V_r(k)\rangle \rightarrow (-E_0)^n c_0|0\rangle$$

$$\sum_g \langle V_l|P_g^* = \sum_g \langle V_l(g)|W_{gl} \rightarrow \langle 0|c_0(-E_0)^n$$

6-spin chain example:



$$\langle A\rangle = \frac{\sum_{g,k}\langle V_l|P_g^* A P_k|V_r\rangle}{\sum_{g,k}\langle V_l|P_g^* P_k|V_r\rangle} = \frac{\sum_{g,k} W_{gl}W_{kr}\langle V_l(g)|A|V_r(k)\rangle}{\sum_{g,k} W_{gl}W_{kr}\langle V_l(g)|V_r(k)\rangle}$$

- Monte Carlo sampling of operator strings
- Estimators based on transition graphs

More efficient ground state QMC algorithm → larger lattices

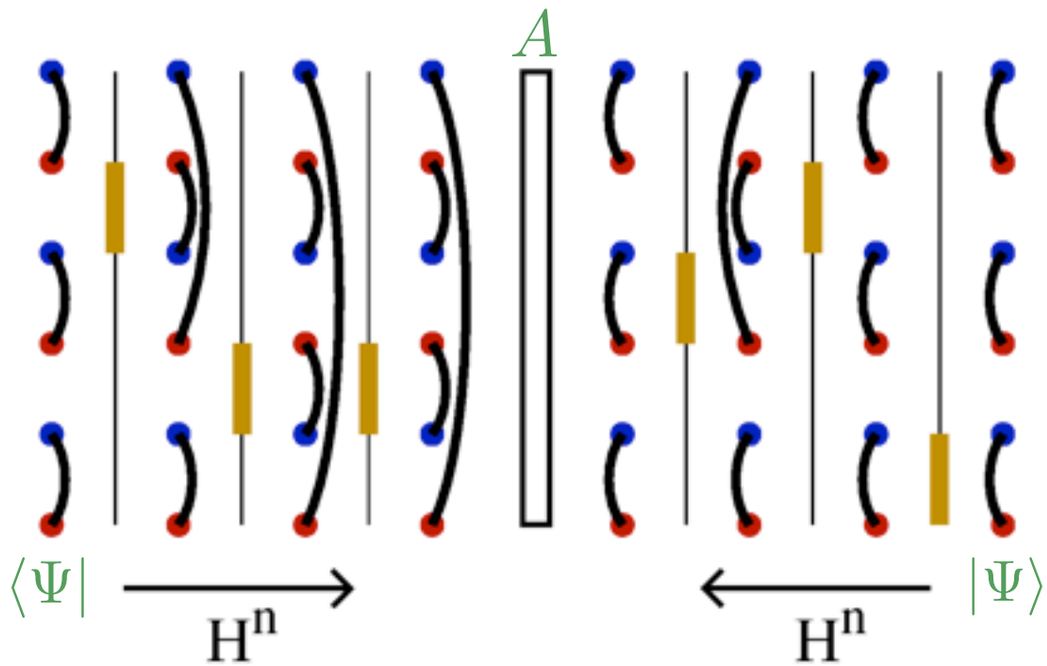
Loop updates in the valence-bond basis

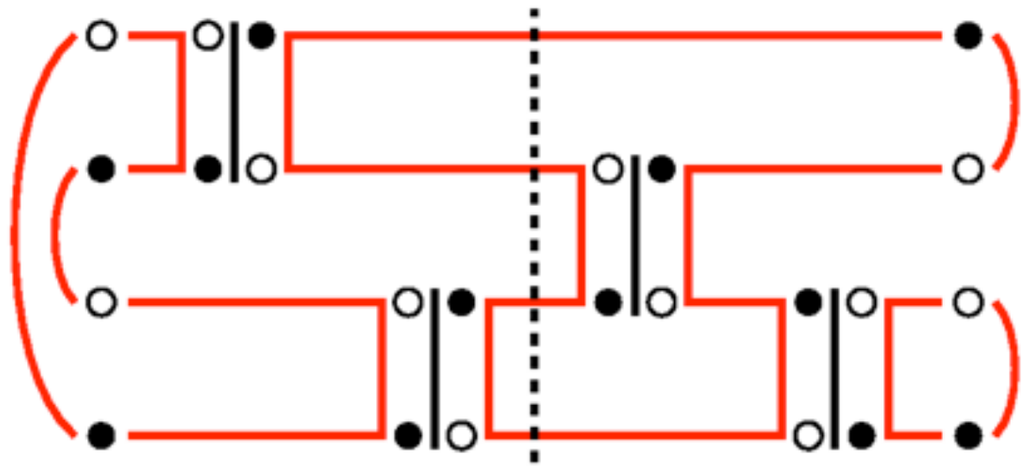
AWS and H. G. Evertz, PRB 2010

Put the spins back in a way compatible with the valence bonds

$$(a_i, b_i) = (\uparrow_i \downarrow_j - \downarrow_i \uparrow_j)/\sqrt{2}$$

and sample in a combined space of spins and bonds





Loop updates similar to those in finite-T methods
(world-line and stochastic series expansion methods)

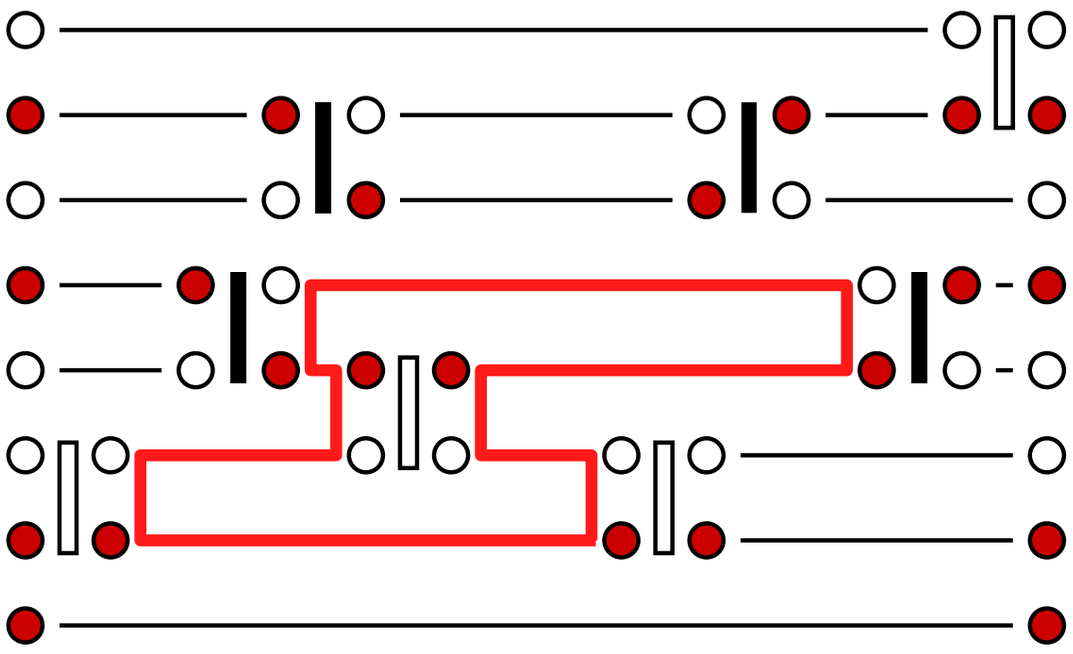
- good valence-bond trial wave functions can be used
- larger systems accessible
- sample spins, but measure using the valence bonds

T>0 and T=0 algorithms side-by-side

Finite-temperature QMC

(world lines, SSE,...)

$$\mathrm{tr}\{\mathrm{e}^{-\beta H}\} = \sum_n \frac{\beta^n}{n!} \langle\alpha|(-H)^n|\alpha\rangle$$

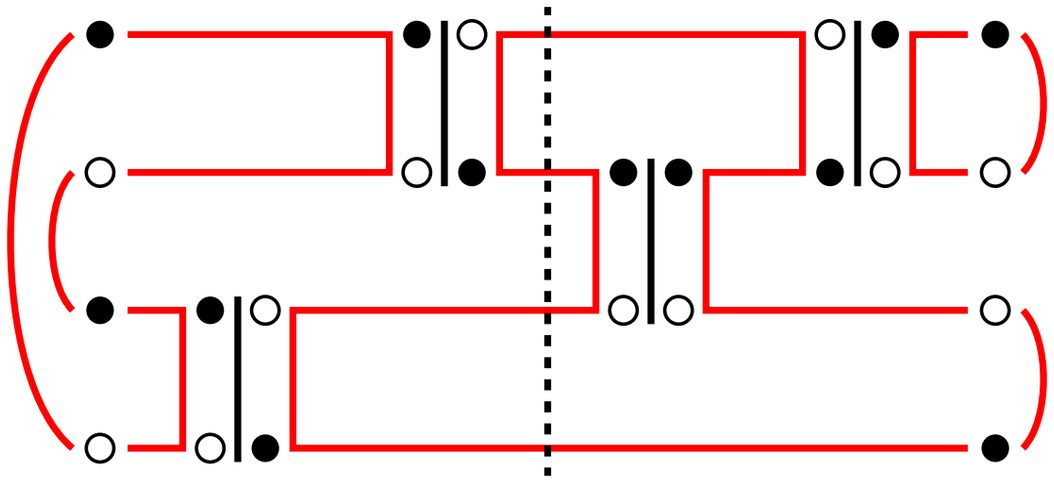


periodic time boundary conditions

- Computer implementations similar

Ground state projection

$$\sum_{\alpha\beta} f_\beta f_\alpha \langle\beta|(-H)^m|\alpha\rangle$$

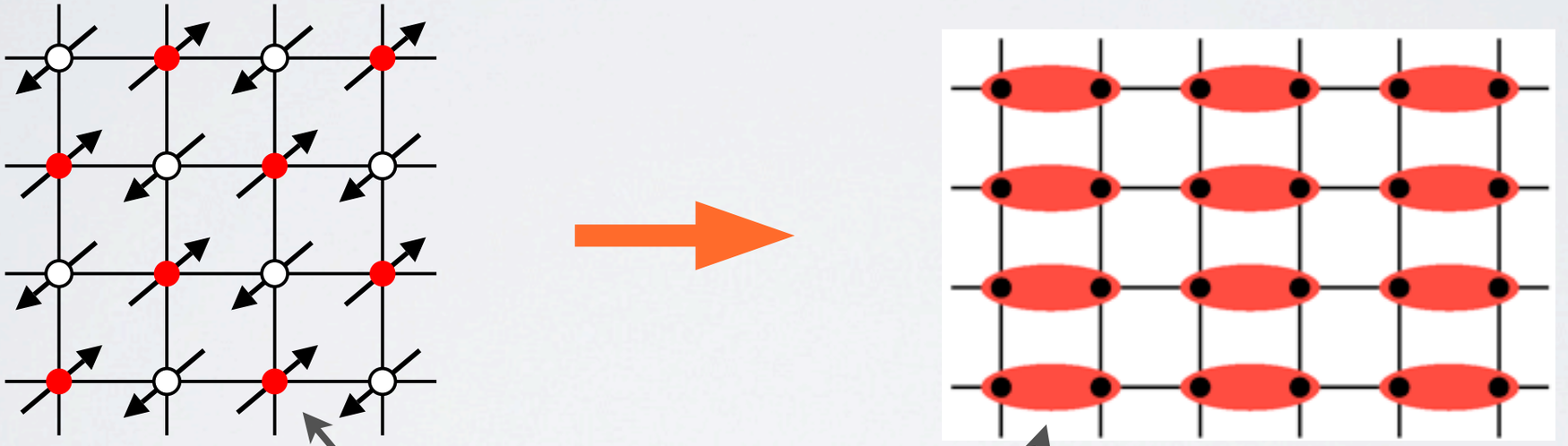


open boundaries capped by valence bonds (2-spin singlets) [AWS, HG Evertz, 2010]

Trial state can conserve relevant ground state quantum numbers (S=0, k=0,...)

Numerical and Analytical Methods for Strongly Correlated Systems
Benasque, Spain, August 24 - September 13, 2014

Nonmagnetic and Critical Ground States of 2D Quantum Spin Systems



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Outline

Conventional quantum phase transition in 2D antiferromagnets

- Néel to non-degenerate quantum paramagnet

Unconventional transition (deconfined quantum criticality?)

- Néel to valence-bond-solid (4-fold degenerate ground state)
- Sign-free QMC realization: “J-Q” models

Studies of criticality in J-Q models

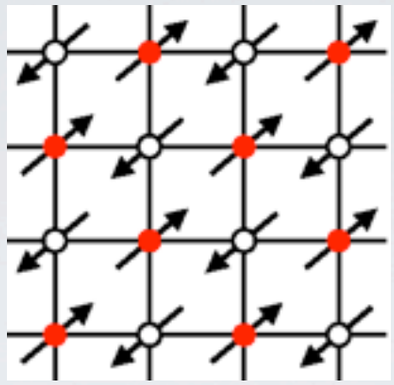
- Finite-size scaling

Universality: Correspondence in frustrated spin models?

- comparisons with recent results for J1-J2 Heisenberg model

Starting point: S=1/2 antiferromagnetic Heisenberg model

$$H = J \sum_{\langle i,j \rangle} S_i \cdot S_j$$



Sublattice magnetization

$$\vec{m}_s = \frac{1}{N} \sum_{i=1}^{N} \phi_i \vec{S}_i, \qquad \phi_i = (-1)^{x_i + y_i} \quad \text{(2D square lattice)}$$

Long-range order: **$\langle m_s^2 \rangle > 0$ for $N \to \infty$**

Quantum Monte Carlo

- finite-size calculations
- no approximations
- extrapolation to infinite size

Reger & Young 1988

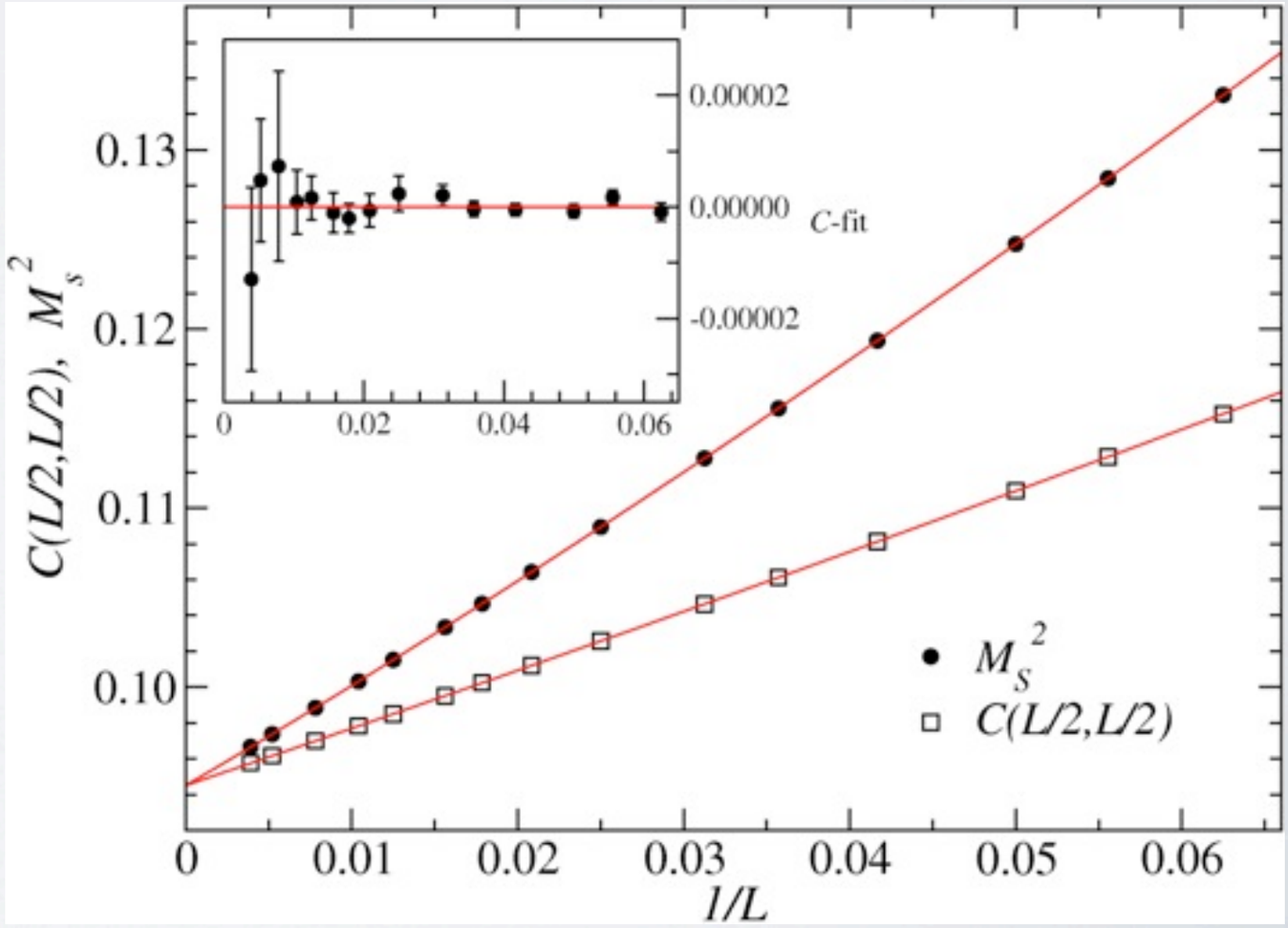
$$m_s = 0.30(2)$$

$$\approx 60\ \%\ \text{of classical value}$$

AWS & HG Evertz 2010

$$m_s = 0.30743(1)$$

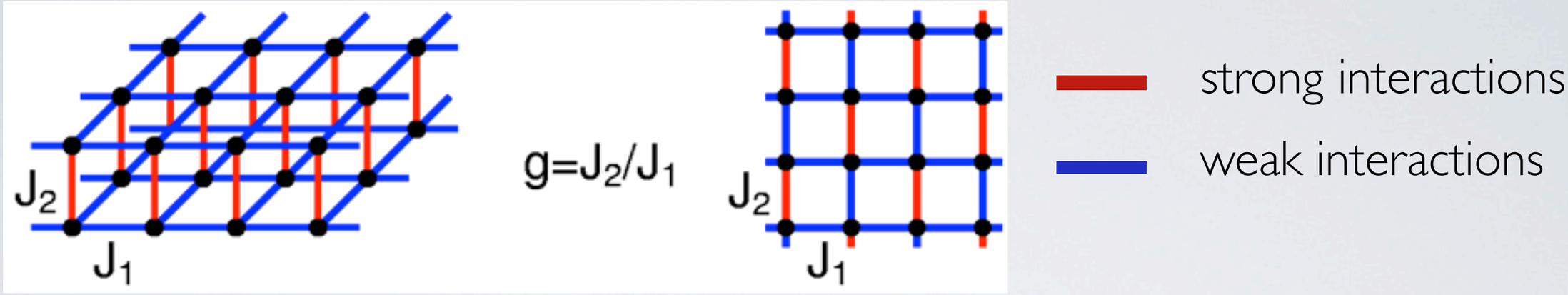
L×L lattices up to 256×256, T=0



T=0 Néel-paramagnetic quantum phase transition

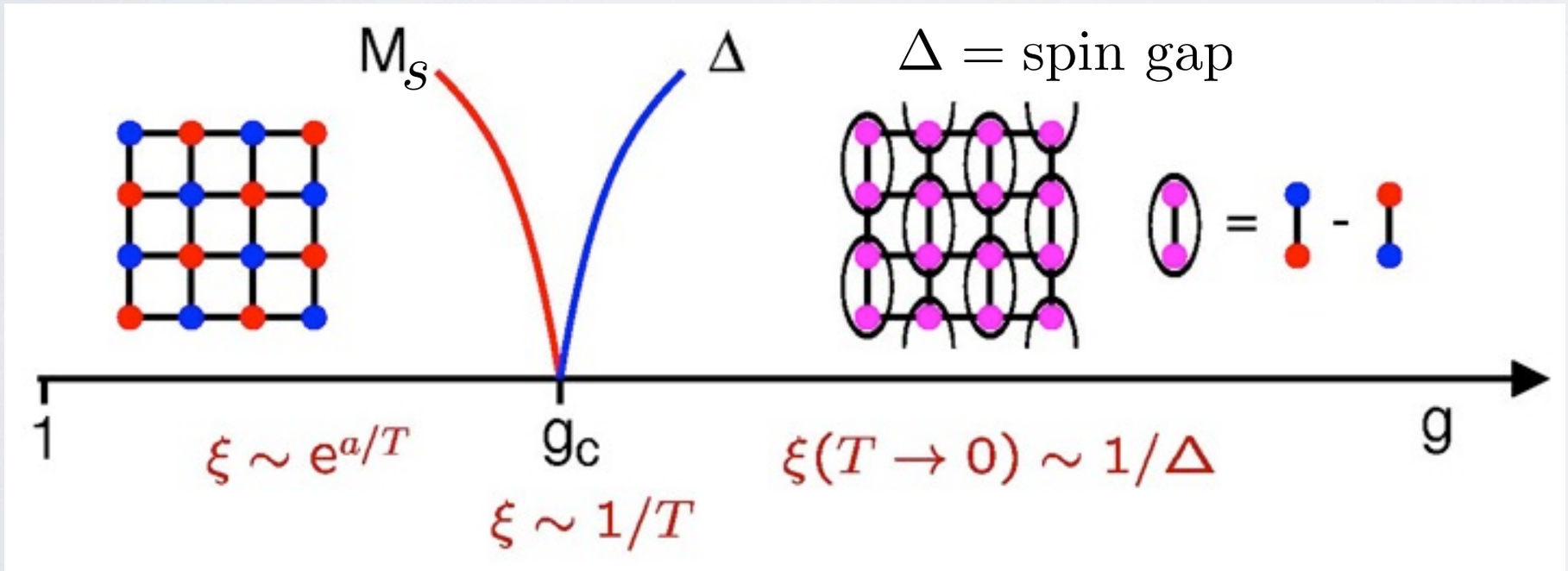
Example: Dimerized S=1/2 Heisenberg models

- every spin belongs to a dimer (strongly-coupled pair)
- many possibilities, e.g., bilayer, dimerized single layer



Singlet formation on strong bonds ➙ Néel - disordered transition

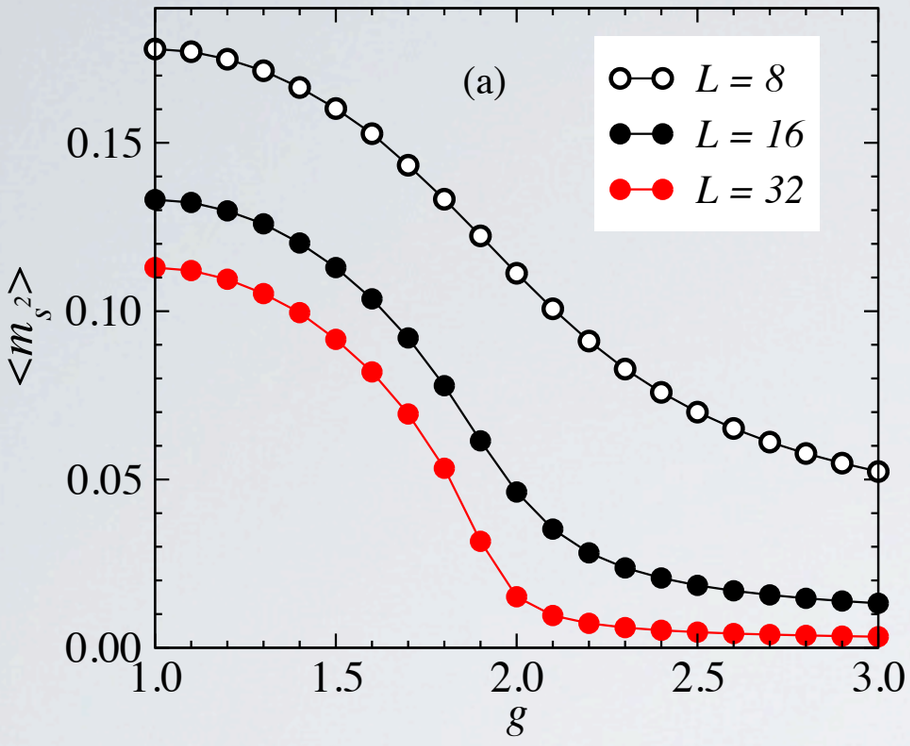
Ground state (T=0) phases

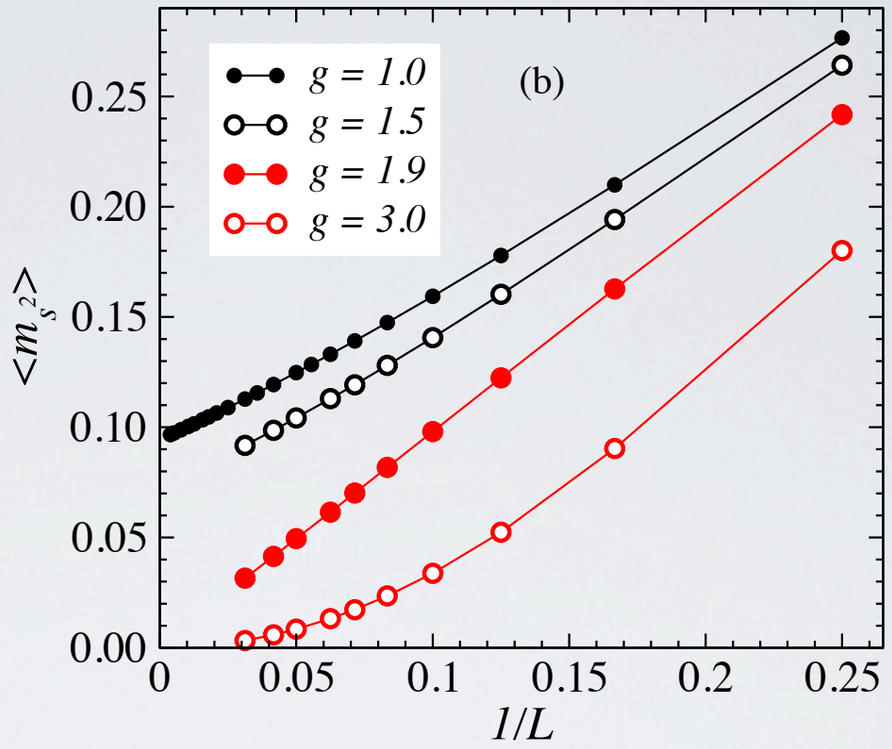


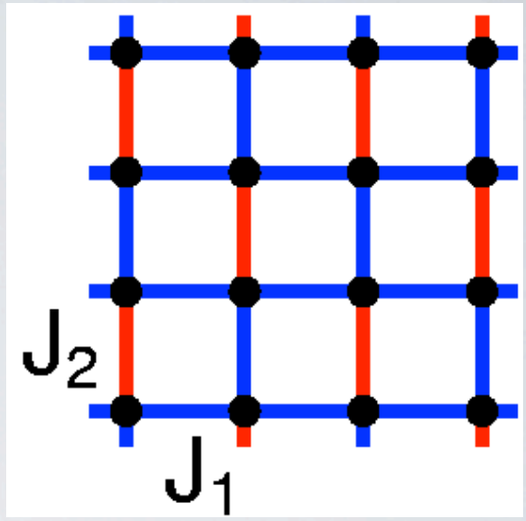
⇒ 3D classical Heisenberg (O3) universality class; QMC confirmed

Experimental realization (3D coupled-dimer system): $TlCuCl_3$

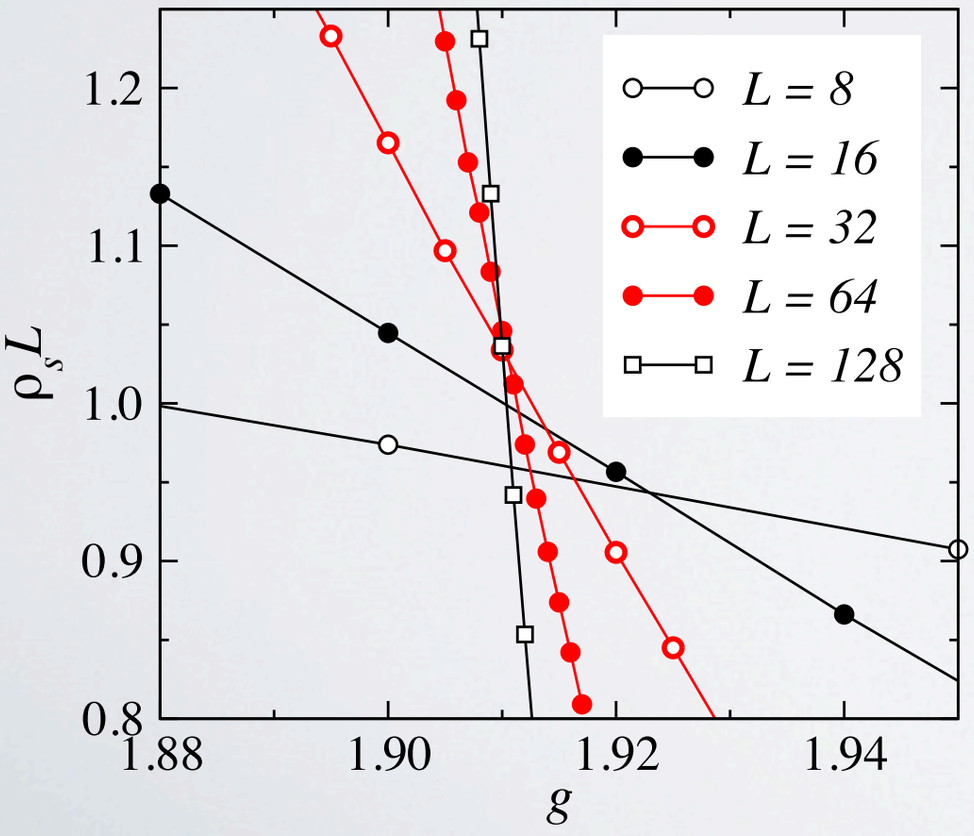
Example of finite-size scaling scaling studies; dimerized Heisenberg







$$g = J_2/J_1$$



According to theory, spin stiffness at the critical point should scale according to (T=0)

$$\rho_s \sim \frac{1}{L} \rightarrow L\rho_s \text{ constant}$$

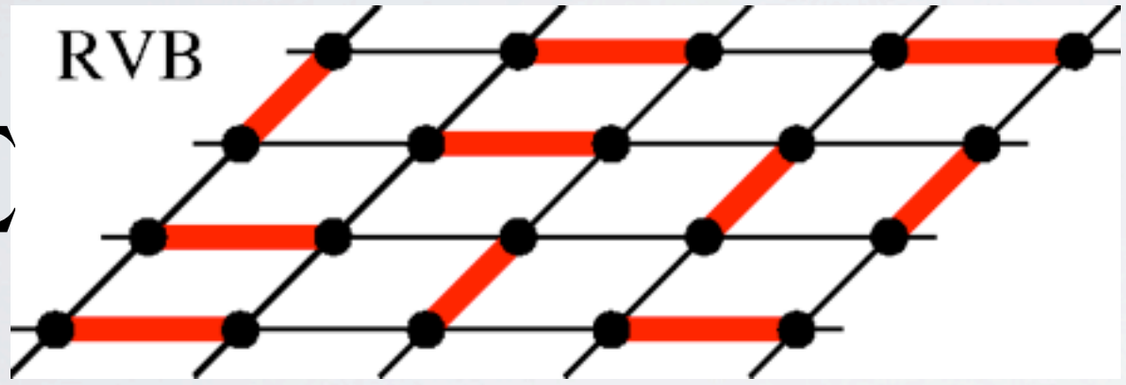
Allows accurate determination of the critical point (curve crossings)

More complex non-magnetic states; systems with 1 spin per unit cell

$$\mathbf{H} = \mathbf{J}\sum_{\langle \mathbf{i},\mathbf{j}\rangle} \mathbf{S_i}\cdot\mathbf{S_j} \quad + \quad \mathbf{g}\times\cdots$$

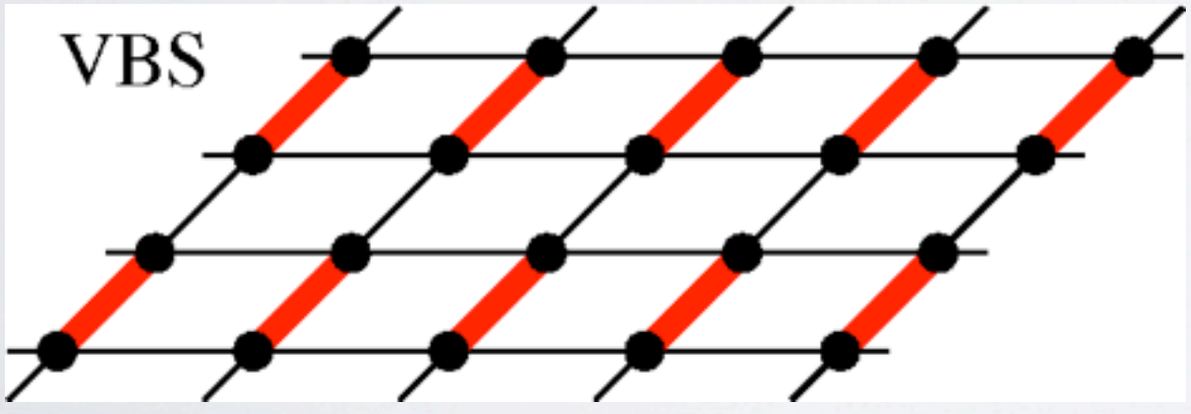
- **non-trivial non-magnetic ground states are possible, e.g.,**
  - ➡ resonating valence-bond (RVB) spin liquid
  - ➡ valence-bond solid (VBS)

Non-magnetic states often have natural descriptions with **valence bonds**

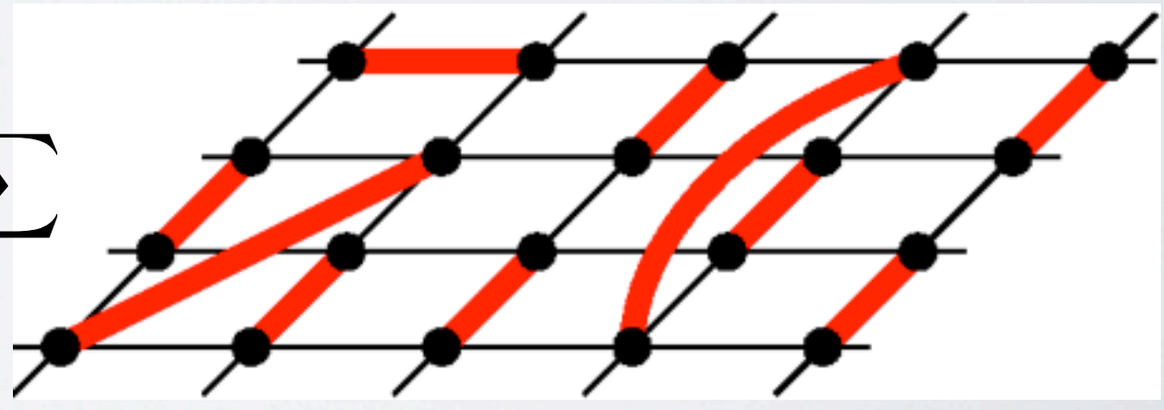
$\sum$ 

$$= (\uparrow_i\downarrow_j - \downarrow_i\uparrow_j)/\sqrt{2}$$

The basis including bonds of all lengths is **overcomplete** in the singlet sector



Spontaneous symmetry breaking
(different from dimerized Hamiltonian)

$\sum$ 

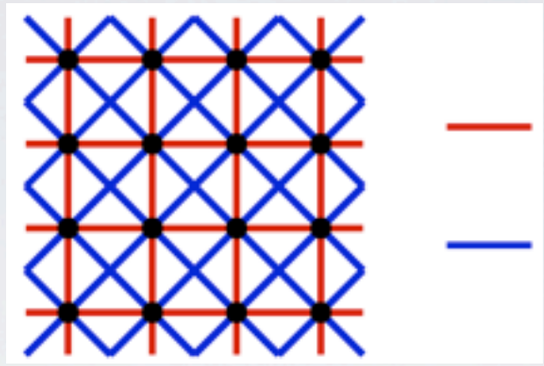
- non-magnetic states dominated by short bonds

Non-magnetic states from frustrated spin interactions

Quantum phase transitions as some coupling (ratio) is varied

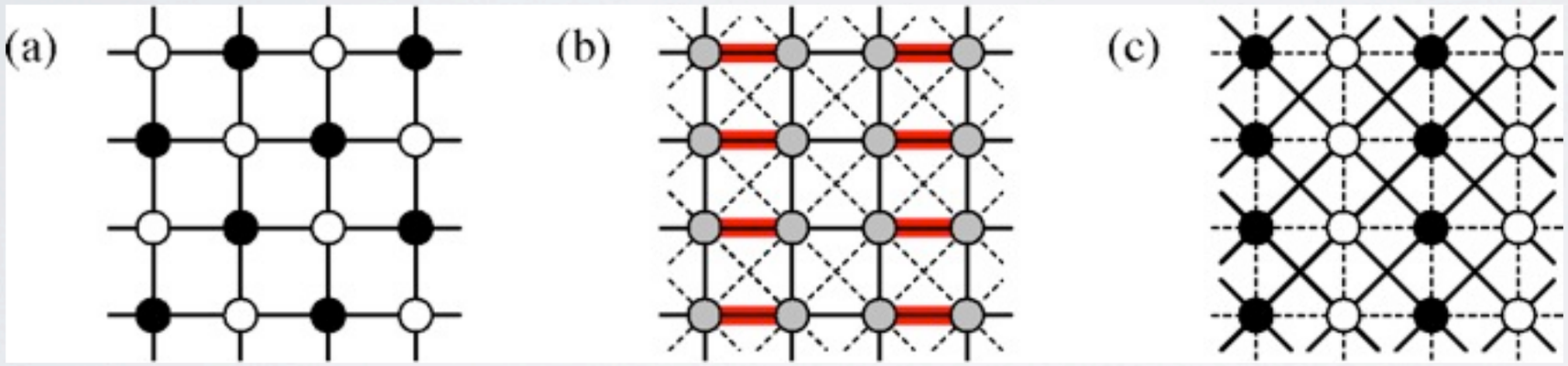
- J_1-J_2 Heisenberg model is the prototypical example

$$H = \sum_{\langle i,j \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$



$$g = J_2/J_1$$

- Ground states for small and large g are well understood
  - Standard **Néel order up to g≈0.45; collinear magnetic order for g>0.6**



$0 \leq g < 0.45$ $\quad$ $0.45 \leq g < 0.6$ $\quad$ $g > 0.6$

- A non-magnetic state exists between the magnetic phases
  - Most likely a VBS (what kind? Columnar or plaquette?)
  - Some recent calculations suggest spin liquid (but I doubt it...).
- 2D frustrated models are challenging: QMC sign problems

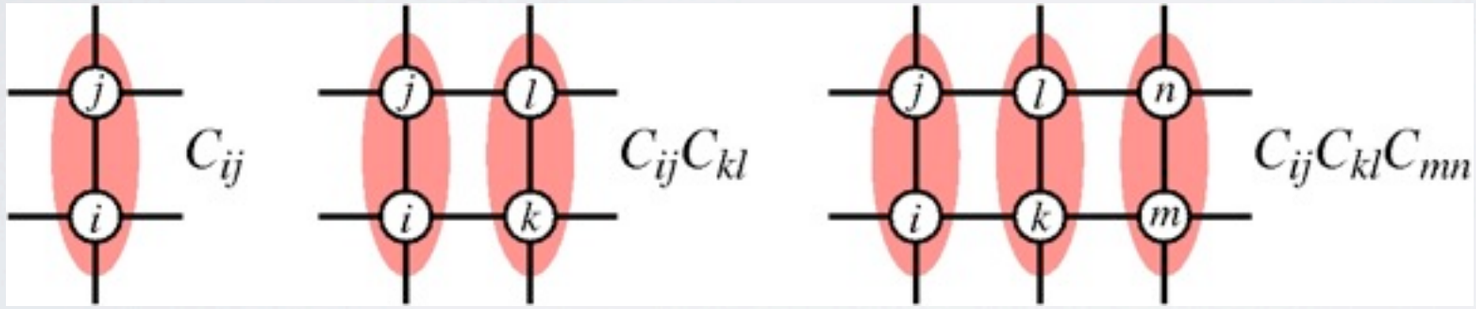
VBS states from multi-spin interactions (AWS, PRL 2007)

The Heisenberg interaction is equivalent to a singlet-projector

$$C_{ij} = \frac{1}{4} - \vec{S}_i \cdot \vec{S}_j$$

$$C_{ij}|\phi^s_{ij}\rangle = |\phi^s_{ij}\rangle, \qquad C_{ij}|\phi^{tm}_{ij}\rangle = 0 \quad (m = -1, 0, 1)$$

- we can construct models with products of singlet projectors
- no frustration in the conventional sense (QMC can be used)
- correlated singlet projection reduces the antiferromagnetic order



+ all translations and rotations

The "J-Q" model with two projectors is

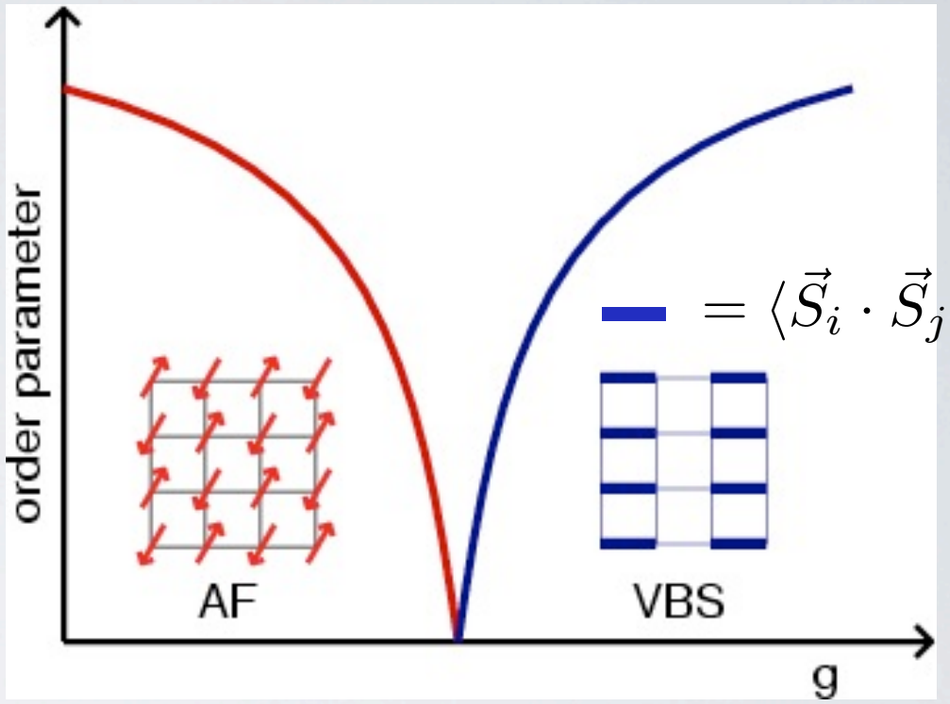
$$H = -J \sum_{\langle ij \rangle} C_{ij} - Q \sum_{\langle ijkl \rangle} C_{ij}C_{kl}$$

- Has Néel-VBS transition, appears to be continuous
- Not a realistic microscopic model for materials
- Intended to study VBS and Néel-VBS transition (universal physics)

VBS states and "deconfined" quantum criticality

Read, Sachdev (1989),....,Senthil, Vishwanath, Balents, Sachdev, Fisher (2004)

$$\mathbf{H} = \mathbf{J}\sum_{\langle \mathbf{i},\mathbf{j}\rangle} \mathbf{S_i}\cdot\mathbf{S_j} \quad + \quad \mathbf{g}\times\cdots$$



Neel-VBS transition in 2D

- generically continuous
- violating the "Landau rule" stating 1st-order transition

Description of critical point with spinor field (2-component complex vector)

$\mathbf{\Phi} = z_\alpha^* \boldsymbol{\sigma}_{\alpha\beta} z_\beta$ gauge redundancy: $z \longrightarrow e^{i\gamma(r,\tau)} z$

$$\mathcal{S}_z = \int \mathrm{d}^2 r \mathrm{d}\tau \left[|(\partial_\mu - iA_\mu) z_\alpha|^2 + s|z_\alpha|^2 + u(|z_\alpha|^2)^2 + \frac{1}{2e_0^2}(\epsilon_{\mu\nu\lambda}\partial_\nu A_\lambda)^2 \right]$$

A is a U(1) symmetric gauge field

- CP^1 action (non-compact)

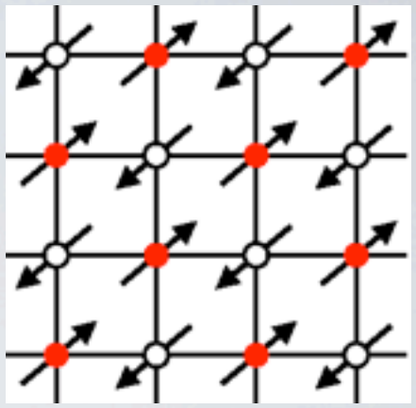
- proposed as critical theory separating Neel and VBS states

- SU(N) generalization: large-N calculations for CP^{N-1} theory [can be carried out with similar QMC as SU(2) models]

T=0 Néel-VBS transition in the J-Q model

Ground-state projector QMC calculations

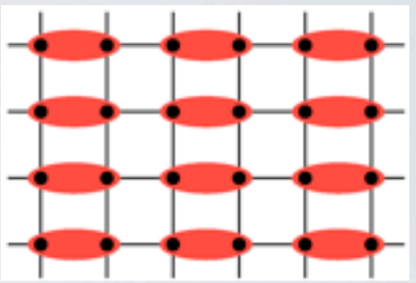
(Sandvik, 2007; Lou, Sandvik, Kawashima, 2009)



Néel order parameter (staggered magnetization)

$$\vec{M} = \frac{1}{N}\sum_i (-1)^{x_i+y_i}\vec{S}_i$$

VBS vector order parameter (D_x,D_y) (x and y lattice orientations)



$$D_x = \frac{1}{N}\sum_{i=1}^{N}(-1)^{x_i}\mathbf{S}_i\cdot\mathbf{S}_{i+\hat{x}}, \quad D_y = \frac{1}{N}\sum_{i=1}^{N}(-1)^{y_i}\mathbf{S}_i\cdot\mathbf{S}_{i+\hat{y}}$$

No symmetry-breaking in simulations; study the squares

$$M^2 = \langle \vec{M}\cdot\vec{M}\rangle, \qquad D^2 = \langle D_x^2 + D_y^2\rangle$$

Finite-size scaling: a critical squared order parameter (A) scales as

$$A(L,q) = L^{-(1+\eta)} f[(q-q_c)L^{1/\nu}]$$

Data "collapse" for different system sizes L of $AL^{1+\eta}$ graphed vs $(q-q_c)L^{1/\nu}$

coupling ratio

$$q = \frac{Q}{J+Q}$$

J-Q_2 model; q_c=0.961(1)

$$\eta_s = 0.35(2)$$

$$\eta_d = 0.20(2)$$

$$\nu = 0.67(1)$$

J-Q_3 model; q_c=0.600(3)

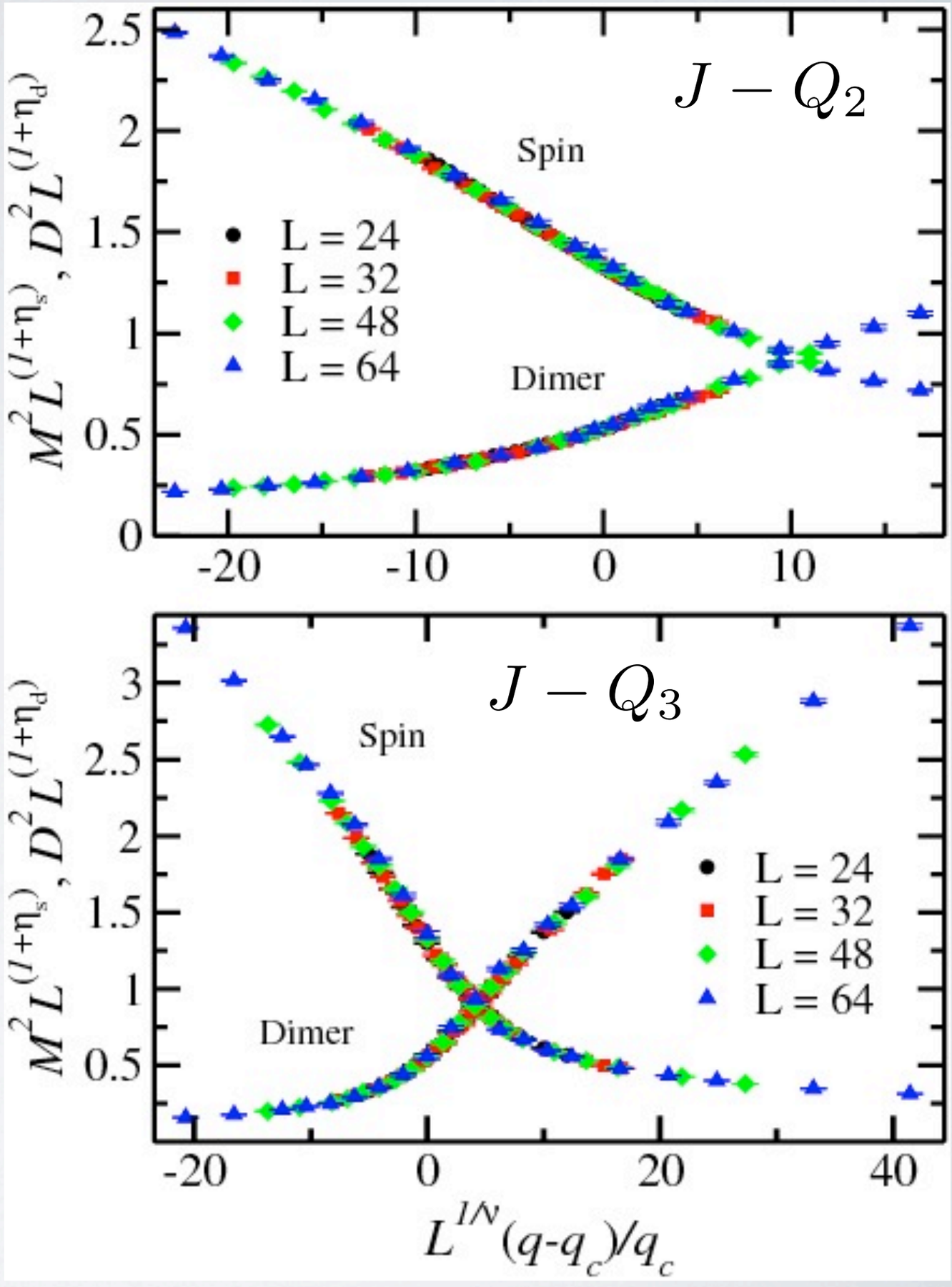
$$\eta_s = 0.33(2)$$

$$\eta_d = 0.20(2)$$

$$\nu = 0.69(2)$$

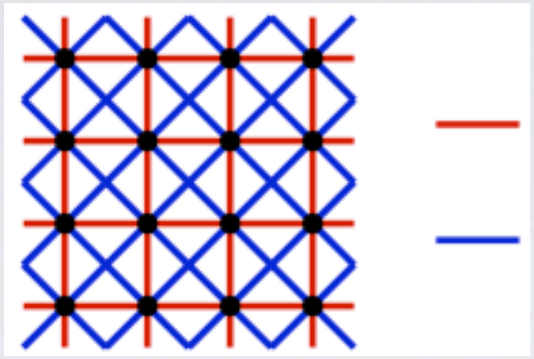
Exponents universal
(within error bars)
Comparable results for honeycomb J-Q model
Alet & Damle, PRB 2013
Block, Melko, Kaul, PRL 2013

Exponents drift for large L
Kawashima et al, PRB 2013
- weak first-order transition?
- or large scaling corrections?



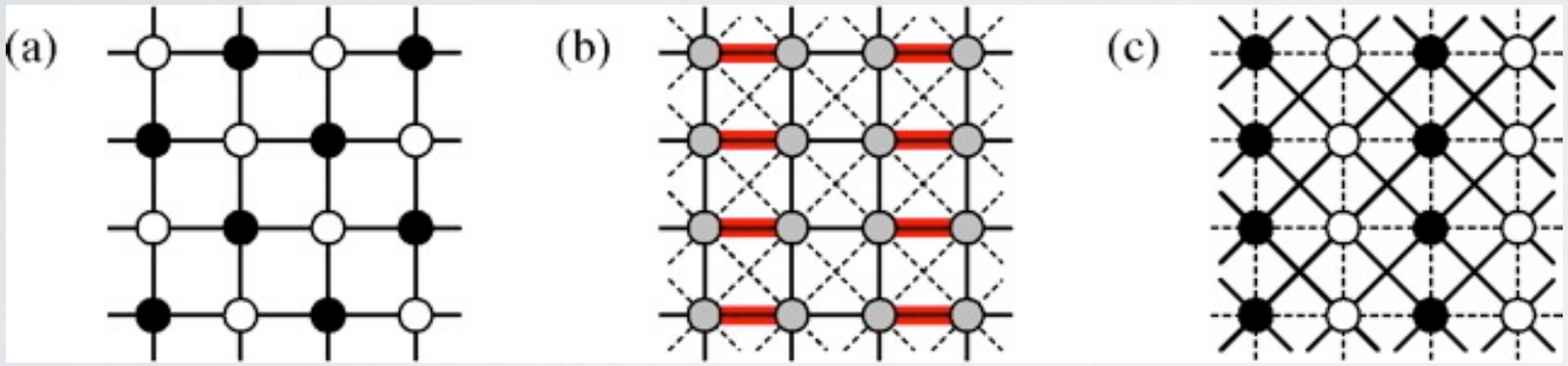
Universality of J-Q physics: Frustrated spin models

$$H = \sum_{\langle i,j \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$



$$g = J_2/J_1$$

Until recently, most calculations indicated VBS around $J_2/J_1=1/2$

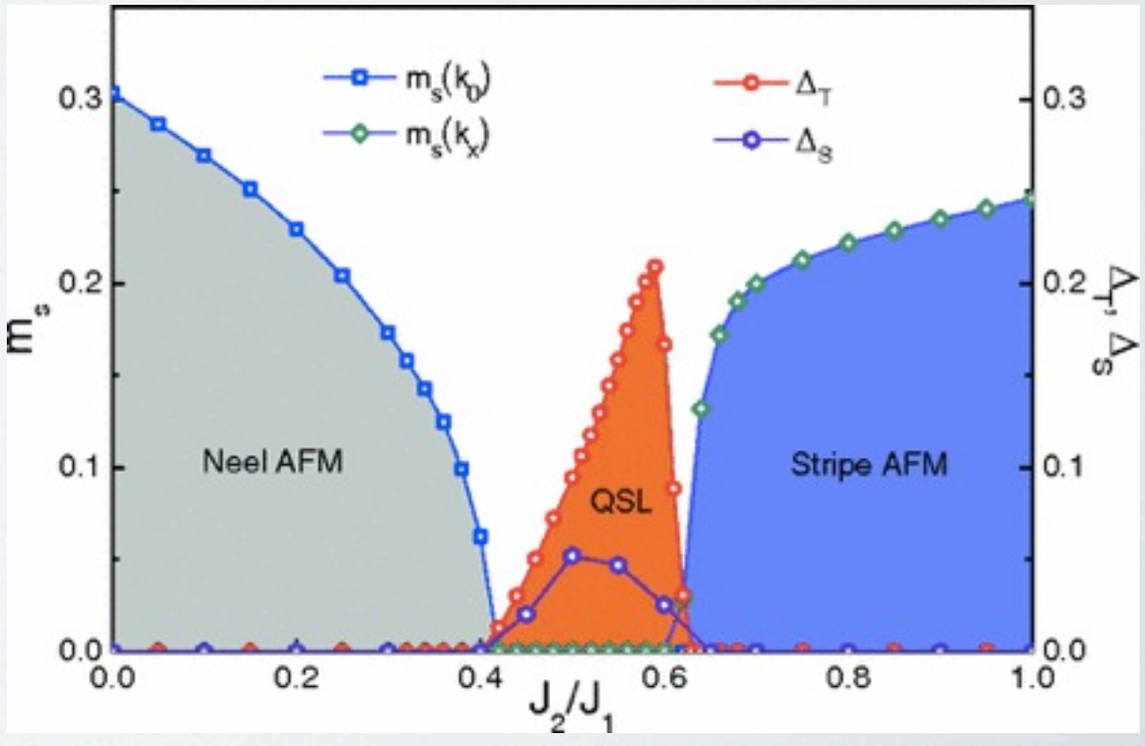


$0 \le g < 0.45$ $\quad$ $0.45 \le g < 0.6$ $\quad$ $g > 0.6$

Recent DMRG calculations claim a spin liquid

1) Jiang, Yao, Balents (PRB 2012)

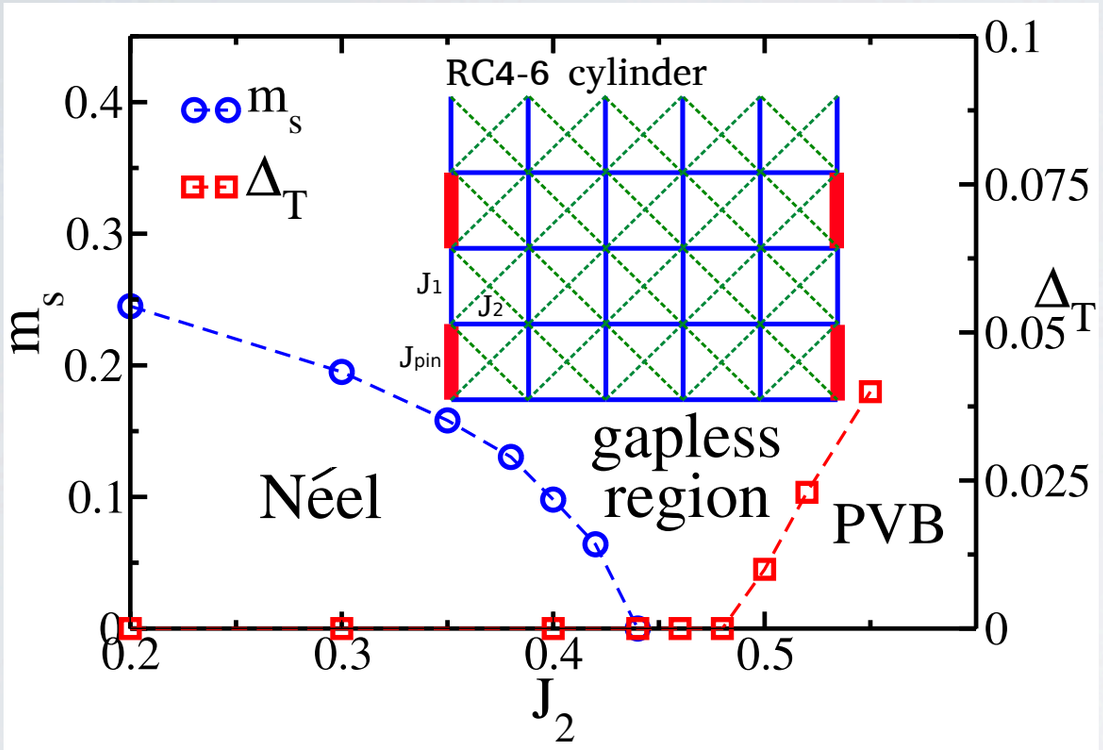
2) Gong, Zhu, Sheng, Motrunich, Fisher (arXiv 2014)



Plaquette ordered phase and quantum spin liquid in the spin-$\frac{1}{2}$ J_1-J_2 square Heisenberg model

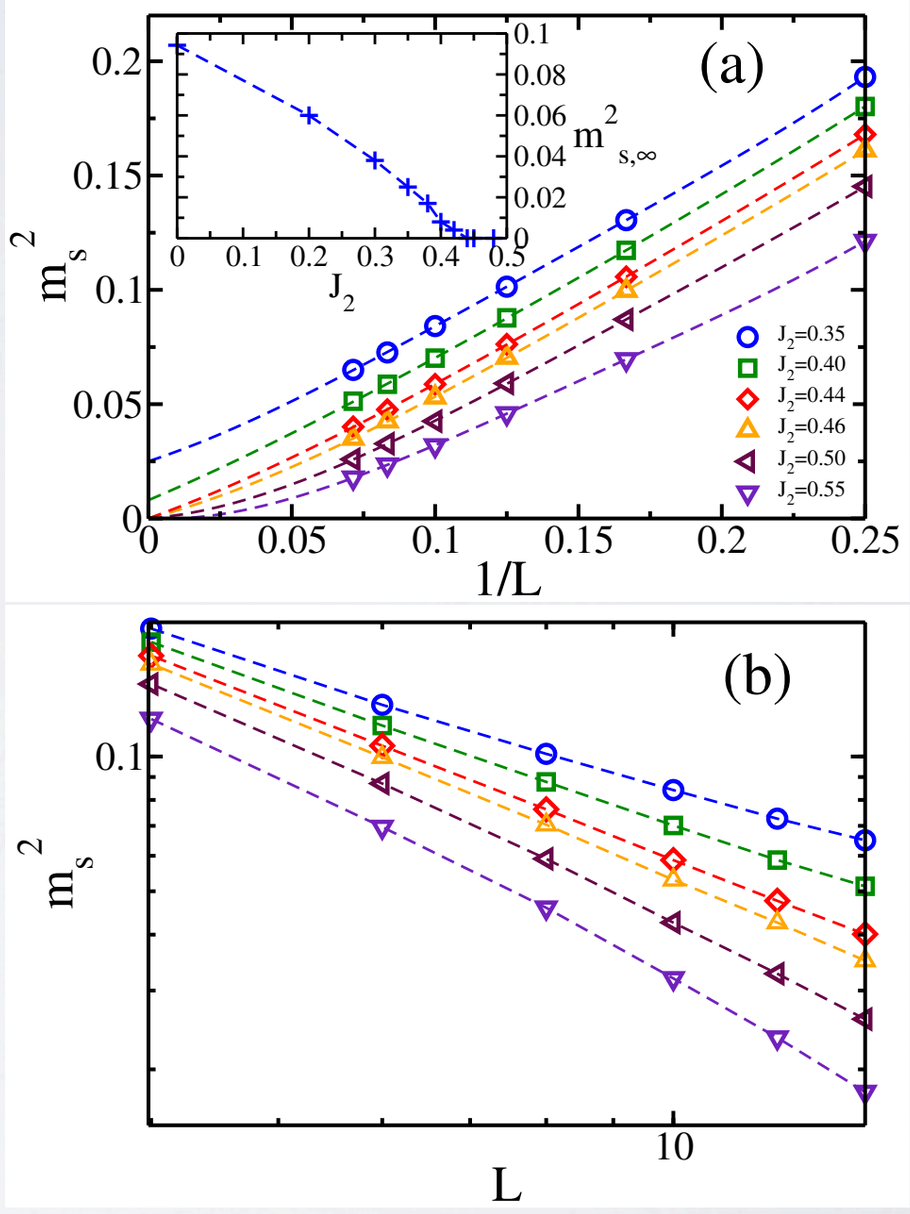
Shou-Shu Gong[1], Wei Zhu[1], D. N. Sheng[1], Olexei I. Motrunich[2], Matthew P. A. Fisher[3]

arXiv:1311.5962v1



Order-parameter extrapolations indicate disordered phase, **but extrapolations are no reliable close to a critical point**

- most likely dqc point as in J-Q



DMRG results should be compared in detail with J-Q QMC

... New version of the paper [PRL 113, 027201 (2014)]

Plaquette ordered phase and **quantum phase diagram** in the S=1/2 J_2-J_1 square Heisenberg model

"The critical exponents obtained from the finite-size spin and dimer correlations could be compatible with the deconfined criticality"

Conclusion from studies of J-Q and frustrated square lattice

- the J-Q model can mimic the behavior of (some) frustrated systems!
- many more insights into deconfined criticality and VBS states obtained by large-scale QMC studies of J-Q models

K. Harada et al, PRB 88, 220408 (2013)
M. Block, R. Melko, R. Kaul, PRL 111, 137202 (2013)
S. Pujari, K. Damle, F. Alet PRL 111, 087203 (2013)
Y. Tang, AWS, PRL 110, 217213 (2013)
S. Jin, AWS, PRB 87, 108040 (2013)
AWS, PRB 84, 134407 (2012)
A. Banerjee, K. Damle, F. Alet, PRB 83, 235111 (2011)
.....