Beijing Normal University Mini Course on

Quantum Monte Carlo Simulations of Spin Systems

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Lecture plan

1: Intro to quantum magnetism and QMC simulations

2: Stochastic series expansion QMC (S=1/2 Heisenberg, TFIM)

3: Ground-state projection QMC, valence-bond basis

4: Quantum criticality, finite-size scaling, phenomenological RG

5,6: Deconfined quantum criticality, emergent symmetries

7: Seminar on recent developments

Supporting lectures by Hui Shao

A: Emergent U(1) symmetry in classical and quantum clock models

B: Dynamics from QMC - analytic continuation

Reading material: I will provide a list

Questions: Ask anytime! Write on chat also OK, someone will monitor

Brief introduction to quantum magnetism and quantum phase transitions

arXiv:1101.3281 [pdf, ps, other] cond-mat.str-el hep-lat doi

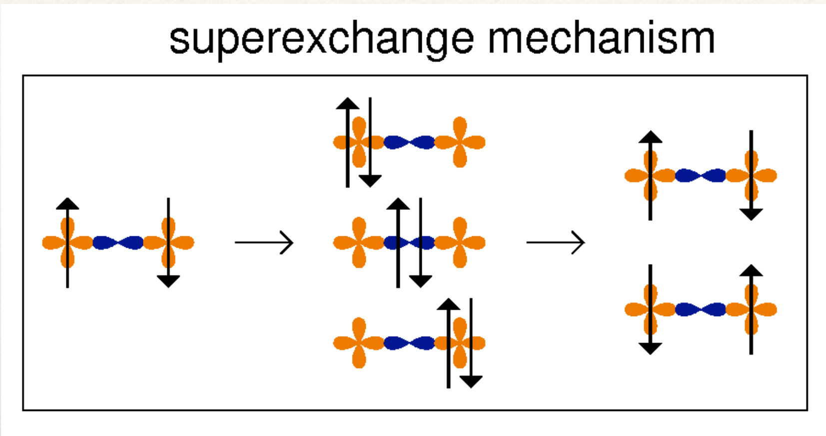
Computational Studies of Quantum Spin Systems

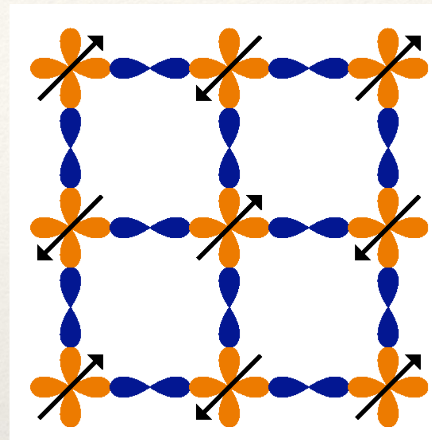
Heisenberg model

$$H = -t \sum_{\sigma} \sum_{\langle i,j \rangle} (c^\dagger_{\sigma i} c_{\sigma j} + c^\dagger_{\sigma j} c_{\sigma i}) + U \sum_i n_{\uparrow i} n_{\downarrow i}$$

- large U/t in Hubbard model
  → few doubly-occupied sites, insulator

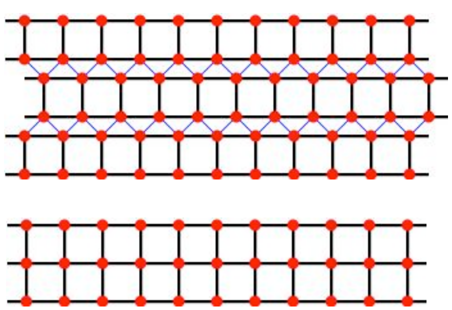
Half-filling → S=1/2 Heisenberg antiferromagnet:



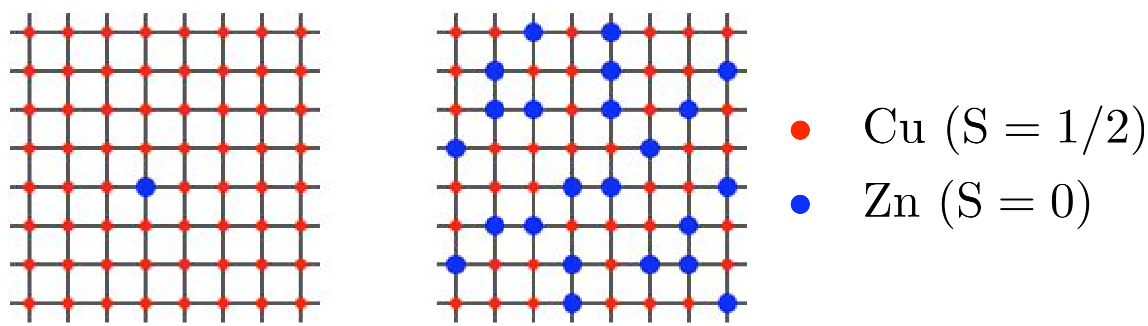


$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

Many variants of Heisenberg model motivated by materials



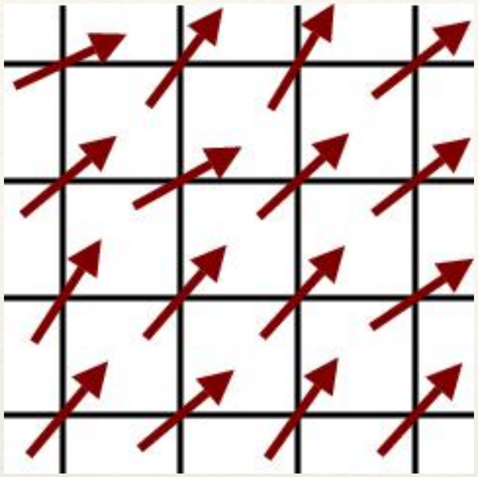
Ladder systems
- even/odd effects



non-magnetic impurities/dilution
- dilution-driven phase transition

Nature of ground state (ordered vs disordered), excitations,…

Quantum versus classical antiferromagnets



Starting point: Heisenberg model

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

- nearest-neighbor interactions (J>0)
- extend by longer-range or multi-spin couplings
- maintain spin-rotation invariance

Consider 2 spins:

- Classical (S=∞) ground state is any anti-parallel configuration
- S=1/2 (extreme quantum) is a singlet (singlet-triplet gap = J)

$$= \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$$

Extended quantum magnets (N→∞) can have aspects of

- classical-like antiferromagnetic order
- non-classical effects can some times be understood using singlets

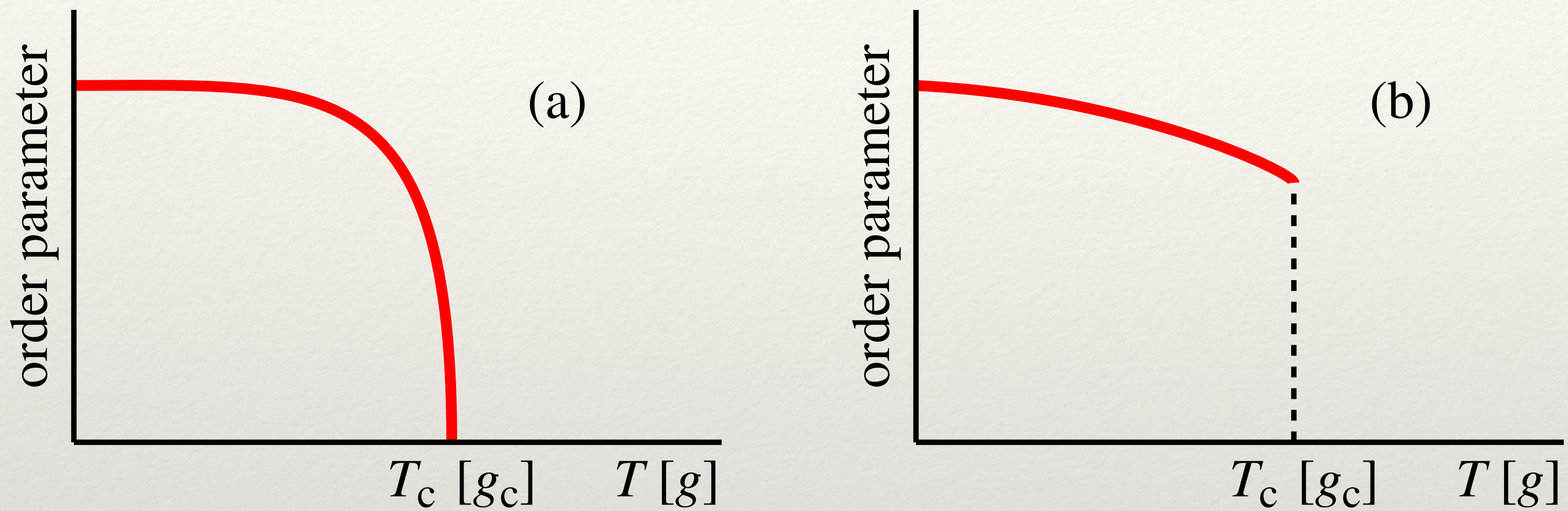
Classical and quantum phase transitions

Classical (thermal) phase transition

- Fluctuations regulated by temperature $T>0$

Quantum (ground state, $T=0$) phase transition

- Fluctuations regulated by parameter g in Hamiltonian



In both cases phase transitions can be

- first-order (discontinuous): finite correlation length ξ as $g \to g_c$ or $g \to g_c$
- continuous: correlation length diverges, $\xi \sim |g-g_c|^{-\nu}$ or $\xi \sim |T-T_c|^{-\nu}$

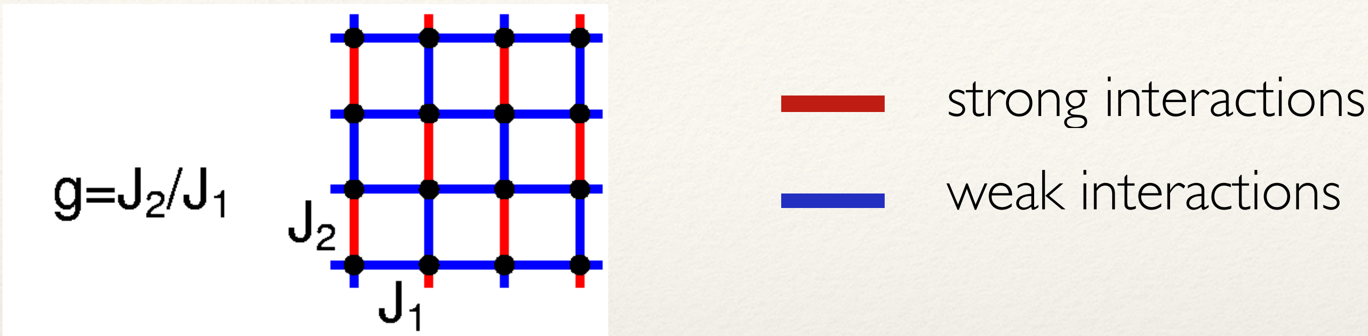
There are many similarities between classical and quantum transitions
- and also important differences

The quantum phases (ground states) can also be highly non-trivial
- even with rather simple lattice models

Example: Néel-paramagnetic quantum phase transition

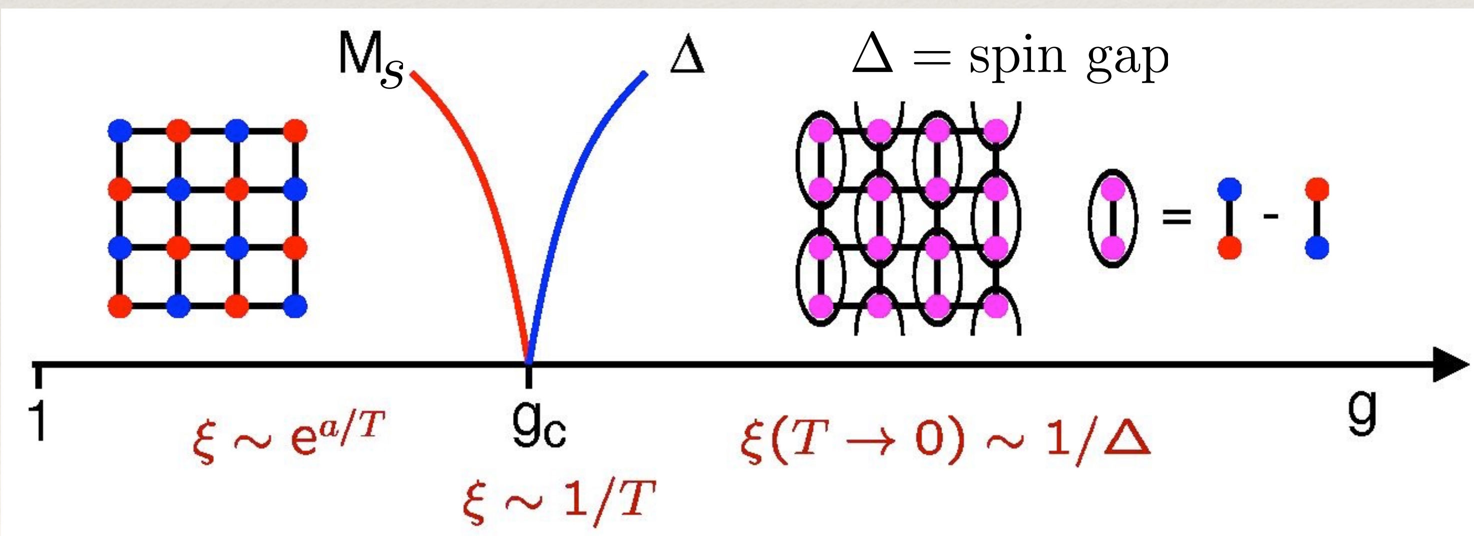
Dimerized S=1/2 Heisenberg models

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



Singlet formation on strong bonds ➙ Néel - quantum-paramagnetic transition

Ground state (T=0) phases



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

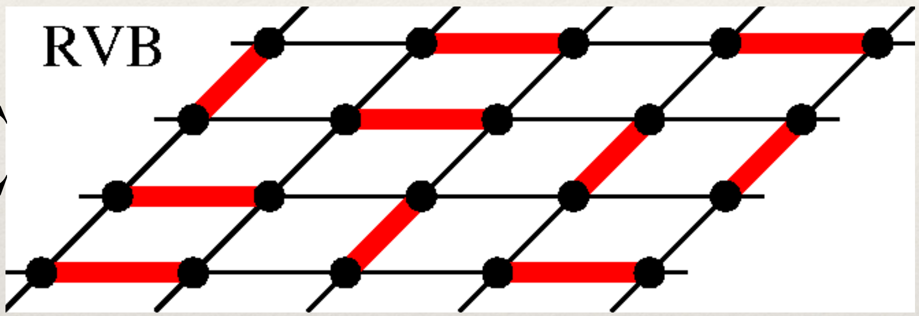
Experimental realization (3D coupled-dimer system): $TlCuCl_3$

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

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

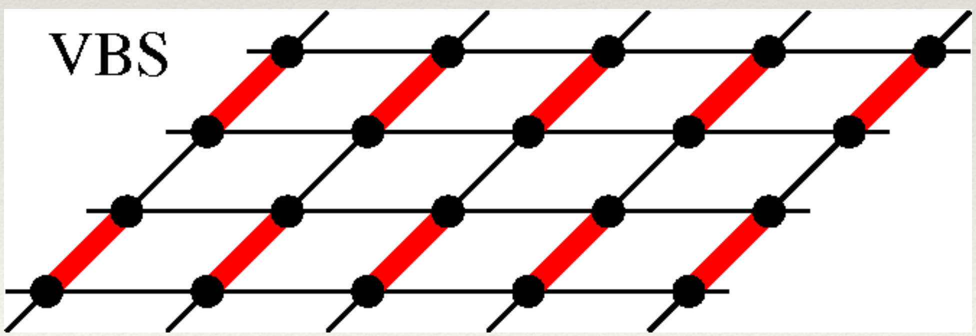
- **highly non-trivial non-magnetic ground states are possible, e.g.,**
  - ➡ resonating valence-bond (RVB) spin liquid
  - ➡ valence-bond solid (VBS)

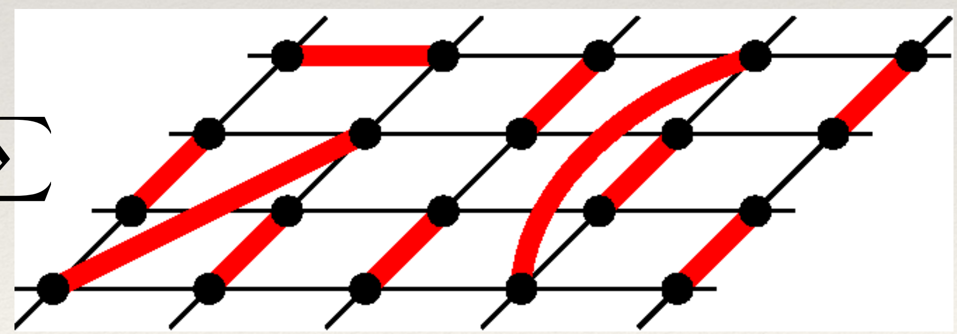
Non-magnetic states often have natural descriptions with **valence bonds**

$\sum$ 

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

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



$\sum$ 

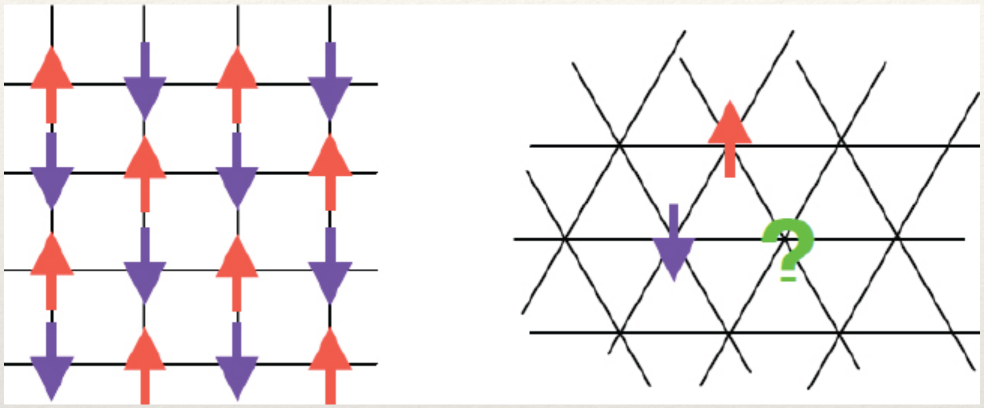
- non-magnetic states dominated by short bonds

Frustrated quantum spins

Competing antiferromagnetic interactions

- structure of ground state can be highly non-trivial
- "spin liquid", other non-trivial quantum paramagnets

Ising spins: $\uparrow, \downarrow$

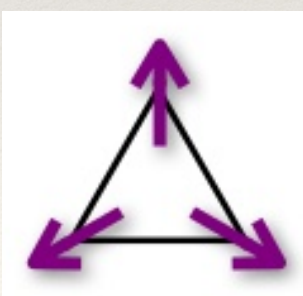


bipartite
un-frustrated

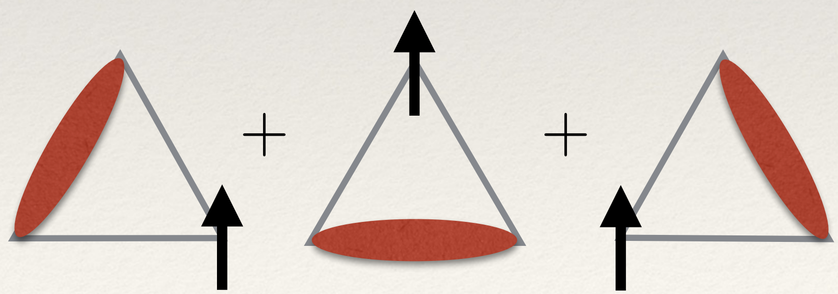
non-bipartite
frustrated

Even classical spin models (Ising, XY, Heisenberg) can be highly non-trivial when the interactions are frustrated

Be careful with classical pictures and intuition:



classical Heisenberg



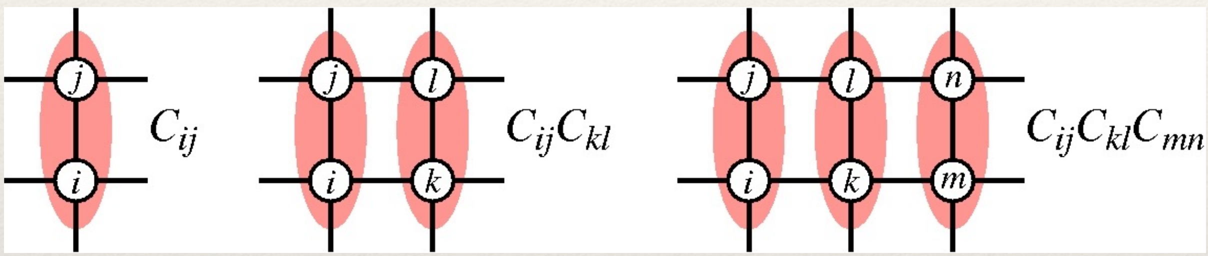
Quantum S=1/2 Heisenberg

Other types of competing interactons: J-Q models

The Heisenberg interaction is equivalent to a singlet-projector

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

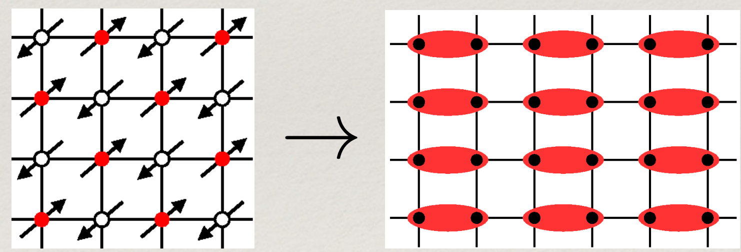
- we can construct models with products of singlet projectors
- no frustration in the conventional sense (QMC can be used)
- correlated singlet projection reduces the antiferromagnetic order



+ all translations and rotations

The J-Q model with two projectors:

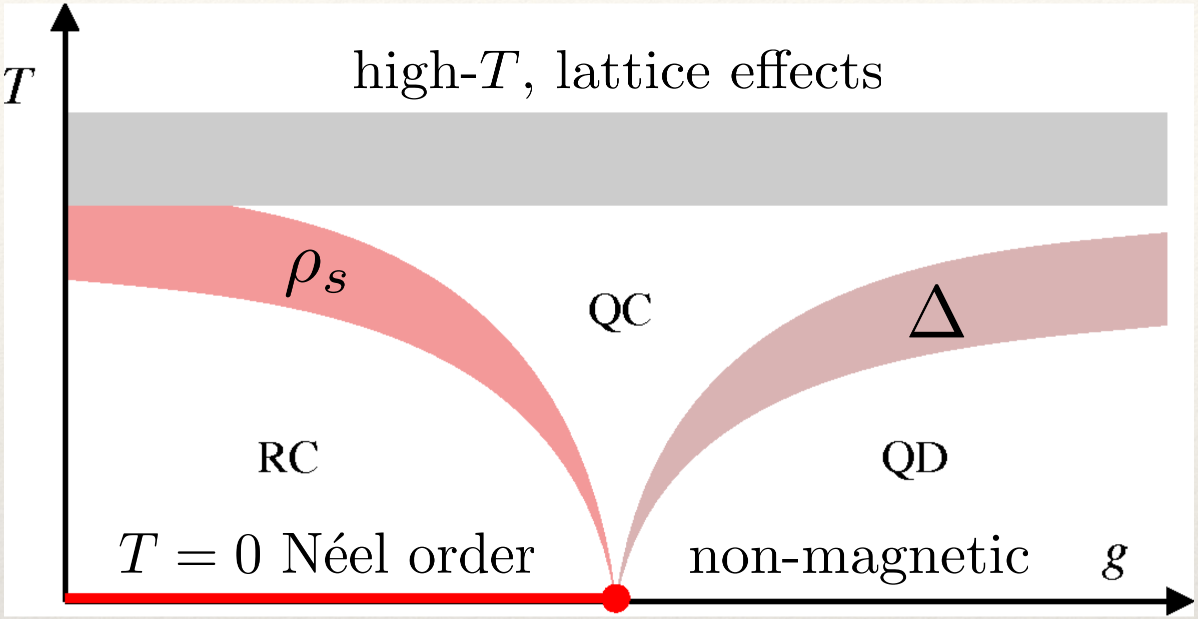
$$H = -J \sum_{\langle ij \rangle} C_{ij} - Q \sum_{\langle ijkl \rangle} C_{ij} C_{kl}$$



- Hosts Néel-VBS quantum phase transition, appears to be continuous
- Not a realistic microscopic model for materials
- "Designer Hamiltonian" for VBS physics and Néel-VBS transition
- Can mimic some aspects of conventional frustrated interactions

What's so special about quantum-criticality?

- large T>0 quantum-critical "fan" where T is the only relevant energy scale
- physical quantities show power laws governed by the T=0 critical point



2D Neel-paramagnet **"cross-over diagram"** [Chakravarty, Halperin, Nelson, PRB 1988]

QC: Universal quantum critical scaling regime

Changing T is changing the imaginary-time size L_τ:

- Finite-size scaling at g_c leads to power laws

$\xi \sim T^{-1}$ (correlation length)

$C \sim T^2$ (specific heat)

$\chi(0) \sim T$ (uniform magnetic susceptibility)

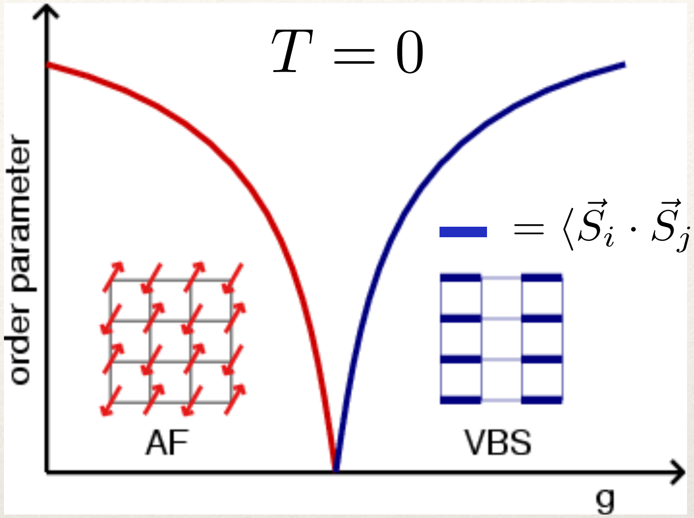
QMC needed to study large lattices; ground states, transitions, T>0,...
- to test predictions, discover new physics,...

Deconfined quantum criticality

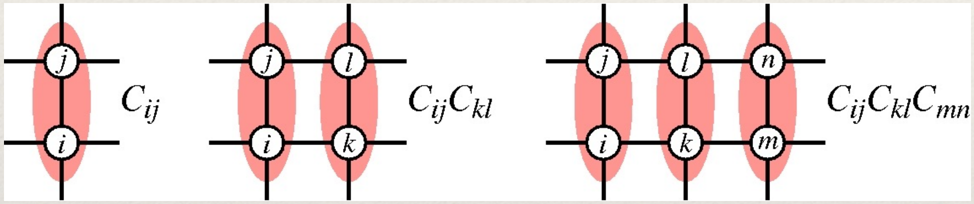
Senthil, Vishwanath, Balents, Sachdev, Fisher (Science 2004)
(+ many previous works; Read & Sachdev, Sachdev & Murthy, Motrunich & Vishwanath….)

Continuous AF - VBS transition at T=0

- would be violation of Landau rule
- first-order would normally be expected
- role of topological defects



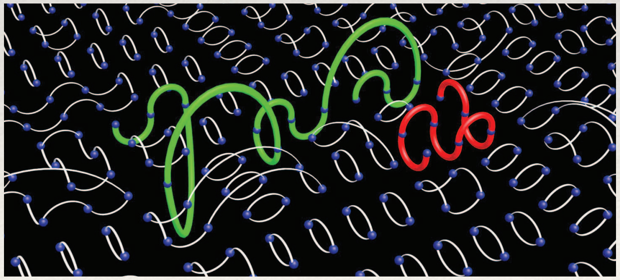
Numerical (QMC) tests using J-Q models



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

The "J-Q" model with two projectors (J-Q_2 model)

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



- **Néel-VBS transition appears to be continuous**
- **Possibly very weakly first-order**
- **Ongoing studies (will be discussed), also J-Q_3 and 'larger' models**

- **Unusual scaling properties, spinons** [Shao, Guo, Sandvik (Science 2016)]

Introduction to quantum Monte Carlo simulations of spin models

arXiv:1101.3281 [pdf, ps, other] cond-mat.str-el hep-lat doi

Computational Studies of Quantum Spin Systems

arXiv:1909.10591 [pdf, other] cond-mat.str-el

Stochastic Series Expansion Methods

Path integrals on the lattice, imaginary time

We want to compute a thermal expectation value

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

where $\beta=1/T$ (and possibly $T\to 0$). 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

Trotter decomposition: error $\propto \Delta_\tau^2$

Trotter decomposition $e^{\Delta(A+B)} = e^{\Delta A}e^{\Delta B} + O(\Delta^2[A,B])$

Example: Heisenberg chain

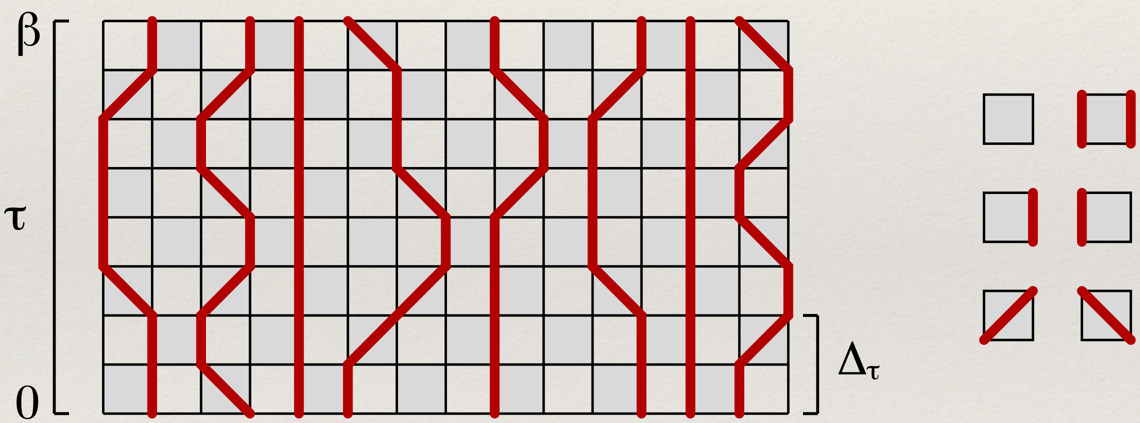
$$H = H_e + H_o, \quad H_e = \sum_{\text{even } i} \mathbf{S}_i \cdot \mathbf{S}_{i+1}, \quad H_o = \sum_{\text{odd } i} \mathbf{S}_i \cdot \mathbf{S}_{i+1}$$

All terms within H_e and H_o commute →

$$e^{-\Delta_\tau(H_e+H_o)} = \prod_{i=1,3,\ldots} e^{-\Delta_\tau \mathbf{S}_i\cdot\mathbf{S}_{i+1}} \prod_{i=2,4,\ldots} e^{-\Delta_\tau \mathbf{S}_i\cdot\mathbf{S}_{i+1}} + O(\Delta_\tau^2)$$

Use in Z, insert complete sets of states between all exponentials

- graphical representation of terms; world lines



Equivalent to 6-vertex model in classical stat mech

Looks like error should be $L\Delta_\tau^2 \sim \beta\Delta_\tau$

- actually $\sim\beta\Delta_\tau^2$ because trace is taken
- procedure is equivalent to using higher-order Trotter dcomposition

$$e^{-\Delta_\tau(H_e+H_o)} = e^{-\Delta_\tau H_e/2} e^{-\Delta_\tau H_o} e^{-\Delta_\tau H_e/2} + O(\Delta_\tau^3)$$

Example of linear approximation and $\Delta_\tau \to 0$: hard-core bosons

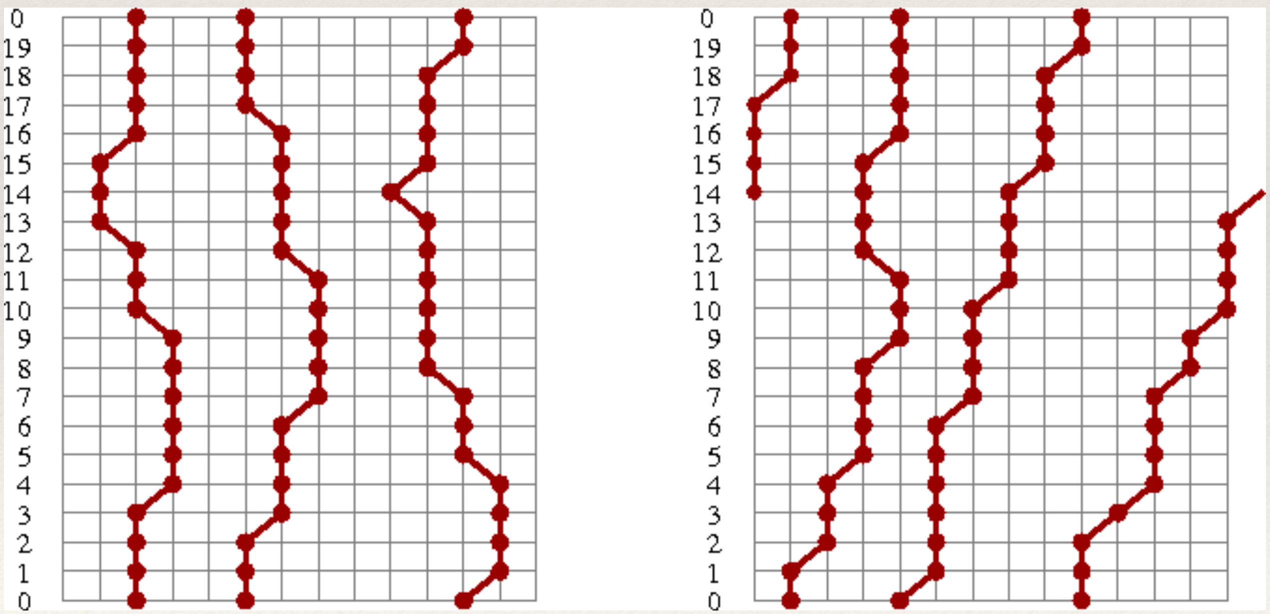
$$H = K = -\sum_{\langle i,j \rangle} K_{ij} = -\sum_{\langle i,j \rangle} (a_j^\dagger a_i + a_i^\dagger a_j) \qquad n_i = a_i^\dagger a_i \in \{0,1\}$$

Equivalent to S=1/2 XY model

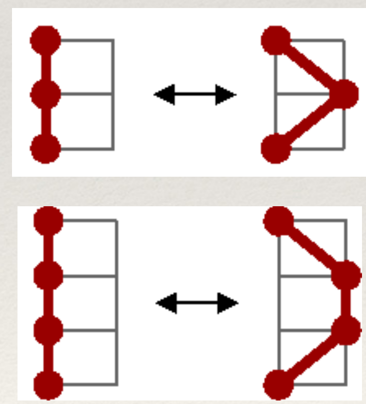
$$H = -2\sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y) = -\sum_{\langle i,j \rangle} (S_i^+ S_j^- + S_i^- S_j^+), \quad S^z = \pm\frac{1}{2} \sim n_i = 0,1$$

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

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

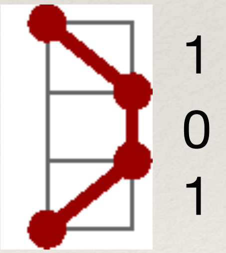
$$W(\{\alpha\}) = \text{weight}$$
$$A(\{\alpha\}) = \text{estimator}$$

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). Multiply and divide by W,

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



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)

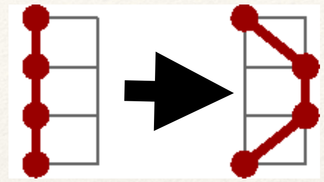
Including interactions

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 →

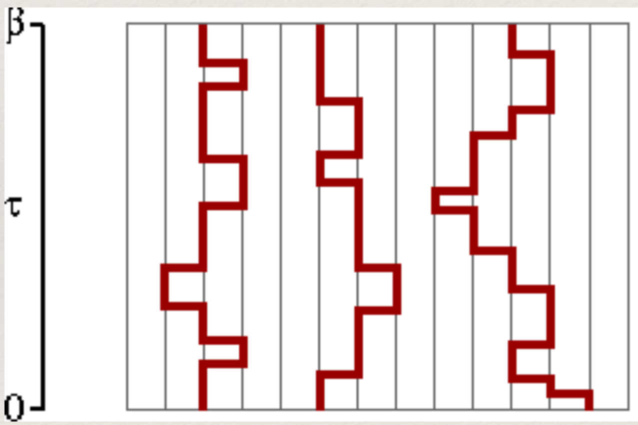
$$W(\{\alpha\}) = \Delta_\tau^{n_K}\exp\left(-\Delta_\tau\sum_{l=0}^{L-1} V_l\right)$$



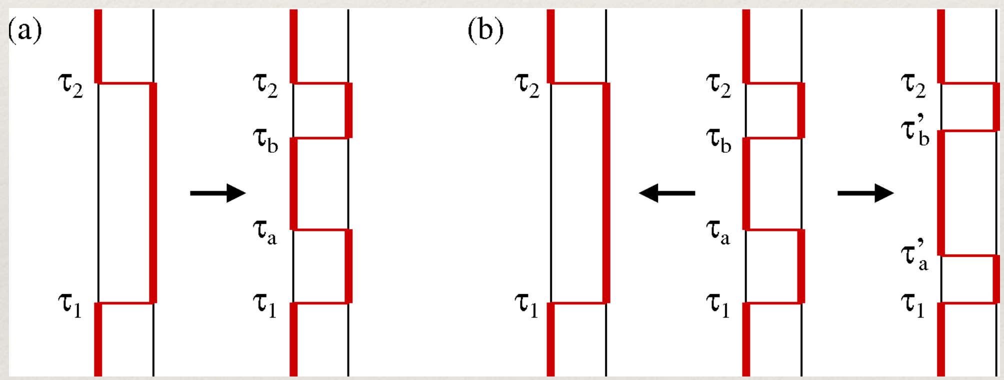
$$P_{\rm acc} = \min\left[\Delta_\tau^2 \exp\left(-\frac{V_{\rm new}}{V_{\rm old}}\right), 1\right]$$

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
- non-zero integrated probabilitis for insertion at all times, choose random time.