Summer School on Computational Statistical Physics
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Quantum spin systems - models and computational methods

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Lecture outline

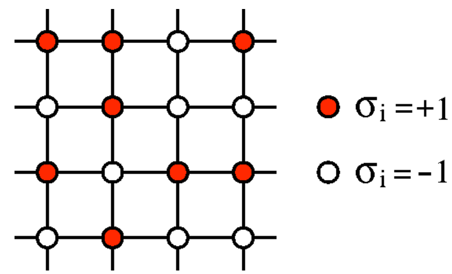
- Introduction to quantum spin systems
- Exact diagonalization methods
  - use of symmetries for block diagonalization
  - full diagonalization and the Lanczos method
- Quantum Monte Carlo
  - introduction to path integrals
  - the stochastic series expansion (SSE) method
- Studies of quantum phase transitions

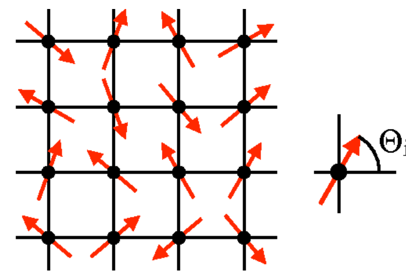
Classical spin models

Lattice models with "spin" degrees of freedom at the vertices

Classified by type of spin:

- **Ising model:** discrete spins, normally two-state σ_i = -1, +1
- **XY model:** planar vector spins (normally of length S=1)
- **Heisenberg model**: 3-dimensional vector spins (S=1)





Statistical mechanics

- spin configurations C
- energy E(C)
- some quantity Q(C)
- temperature T (k_B=1)

$$\langle Q \rangle = \frac{1}{Z} \sum_C Q(C) \mathrm{e}^{-E(C)/T}$$

$$Z = \sum_C \mathrm{e}^{-E(C)/T}$$

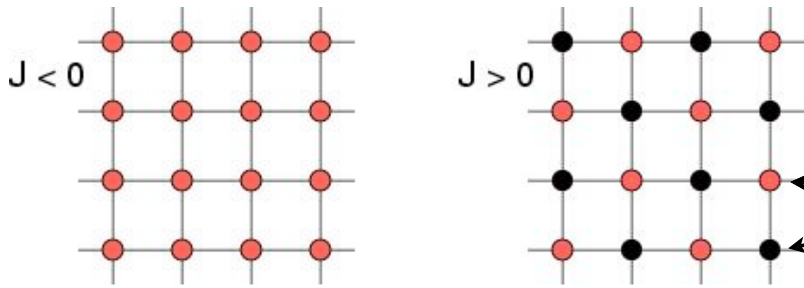
$$E = \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j \qquad \textbf{(Ising)}$$

$$E = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j = \sum_{\langle ij \rangle} J_{ij} \cos(\Theta_i - \Theta_j) \qquad \textbf{(XY)}$$

$$E = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j \qquad \textbf{(Heisenberg)}$$

Phase transition: The 2D Ising model

Ground state (T=0) depends on J, E(0)/N=-2J



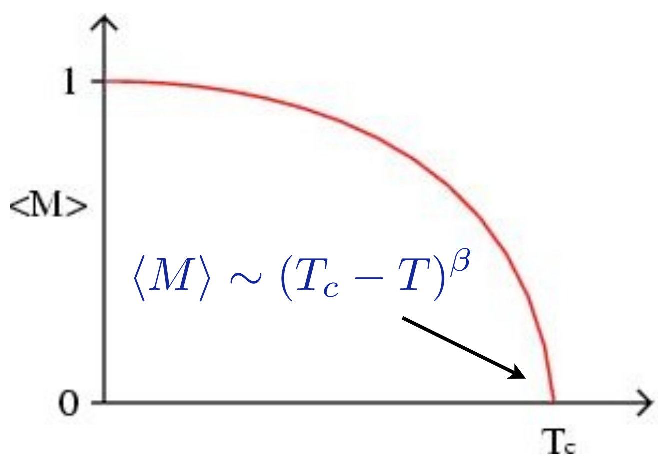
$$E = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \quad \sigma_i = \pm 1$$

- +J and -J systems are trivially related by sublattice transformation

  $\sigma_i \to -\sigma_i \quad \text{for i on sublattice A}$

- Ising ferromagnet and antiferromagnet have identical properties

T > 0, thermal expectation values, **phase transition**



$$\langle A \rangle = \frac{1}{Z} \sum_n A_n \mathrm{e}^{-E_n/T}, \quad Z = \sum_n \mathrm{e}^{-E_n/T}$$

$$M = \frac{1}{N} \sum_i \sigma_i \quad \left(M = \frac{1}{N} \sum_i \sigma_i (-1)^{x_i + y_i} \ \text{ for AF} \right)$$

$$T_\mathrm{c}/J \approx 2.27$$

Quantum spins

Spin magnitude S; basis states $|S^z_1,S^z_2,\ldots,S^z_N\rangle$, S^z_i = -S, ..., S-1, S

Commutation relations:

$$[S_i^x,S_i^y]=i\hbar S_i^z \quad (\text{we set } \hbar=1)$$

$$[S_i^x,S_j^y]=[S_i^x,S_j^z]=\ldots=[S_i^z,S_j^z]=0 \quad (i\neq j)$$

Ladder (raising and lowering) operators:

$$S_i^+=S_i^x+iS_i^y, \qquad S_i^-=S_i^x-iS_i^y$$

$$S_i^+|S_i^z\rangle = \sqrt{S(S+1)-S_i^z(S_i^z+1)}|S_i^z+1\rangle,$$

$$S_i^-|S_i^z\rangle = \sqrt{S(S+1)-S_i^z(S_i^z-1)}|S_i^z-1\rangle,$$

Spin (individual) squared operator: $S_i^2|S_i^z\rangle = S(S+1)|S_i^z\rangle$

S=1/2 spins; very simple rules

$$|S_i^z=+\tfrac{1}{2}\rangle=|\uparrow_i\rangle, \qquad |S_i^z=-\tfrac{1}{2}\rangle=|\downarrow_i\rangle$$

$$S_i^z|\uparrow_i\rangle=+\tfrac{1}{2}|\uparrow_i\rangle \qquad S_i^-|\uparrow_i\rangle=|\downarrow_i\rangle \qquad S_i^+|\uparrow_i\rangle=0$$

$$S_i^z|\downarrow_i\rangle=-\tfrac{1}{2}|\downarrow_i\rangle \qquad S_i^+|\downarrow_i\rangle=|\uparrow_i\rangle \qquad S_i^-|\downarrow_i\rangle=0$$

Quantum spin models

Ising, XY, Heisenberg hamiltonians

- the spins always have three (x,y,z) components
- interactions may contain 1 (Ising), 2 (XY), or 3 (Heisenberg) components

$$H = \sum_{\langle ij \rangle} J_{ij} S_i^z S_j^z = \tfrac{1}{4} \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j \qquad \textbf{(Ising)}$$

$$H = \sum_{\langle ij \rangle} J_{ij} [S_i^x S_j^x + S_i^y S_j^y] = \tfrac{1}{2} \sum_{\langle ij \rangle} J_{ij} [S_i^+ S_j^- + S_i^- S_j^+] \qquad \textbf{(XY)}$$

$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j = \sum_{\langle ij \rangle} J_{ij} [S_i^z S_j^z + \tfrac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)] \qquad \textbf{(Heisenberg)}$$

Quantum statistical mechanics

$$\langle Q \rangle = \frac{1}{Z} \mathrm{Tr} \left\{ Q \mathrm{e}^{-H/T} \right\} \qquad Z = \mathrm{Tr} \left\{ \mathrm{e}^{-H/T} \right\} = \sum_{n=0}^{M-1} \mathrm{e}^{-E_n/T}$$

Large size M of the Hilbert space; $M=2^N$ for S=1/2

- difficult problem to find the eigenstates and energies
- we are also interested in the ground state (T→0)
  - for classical systems the ground state is often trivial

Why study quantum spin systems?

Solid-state physics

- localized electronic spins in Mott insulators (e.g., high-Tc cuprates)
- large variety of lattices, interactions, physical properties
- search for “exotic” quantum states in such systems (e.g., spin liquid)

Ultracold atoms (in optical lattices)

- spin hamiltonians can (?) be engineered
- some boson systems are very similar to spins (e.g., “hard-core” bosons)

Quantum information theory / quantum computing

- possible physical realizations of quantum computers using interacting spins
- many concepts developed using spins (e.g., entanglement)

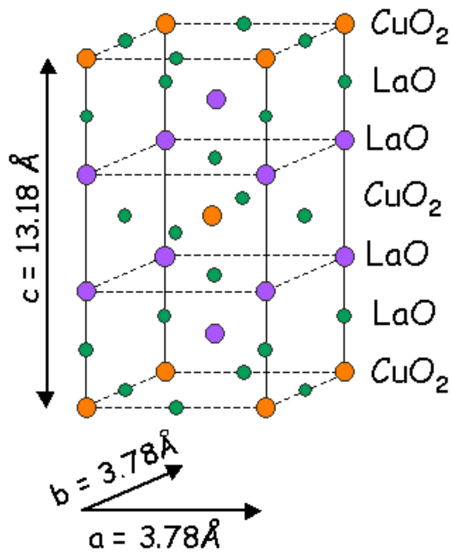
Generic quantum many-body physics

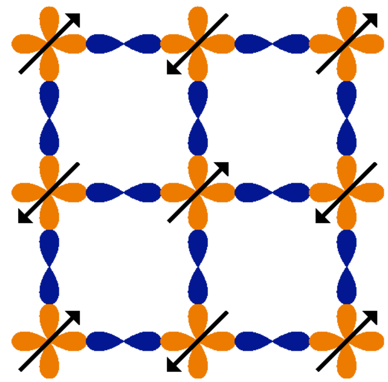
- testing grounds for collective quantum behavior, quantum phase transitions
- identify “Ising models” of quantum many-body physics

Particle physics / field theory / quantum gravity

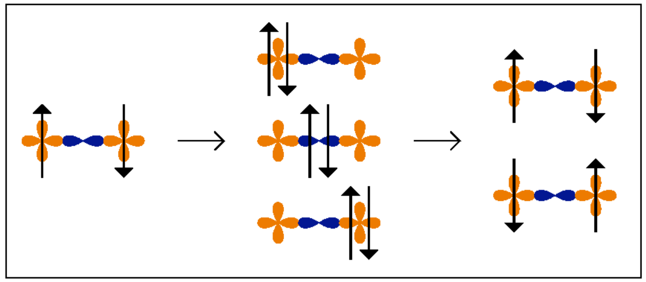
- some quantum-spin phenomena have parallels in high-energy physics
  - e.g., spinon (quark) confinement-deconfinement transition
- spin foams (?)

Prototypical Mott insulator; high-Tc cuprates (antiferromagnets)





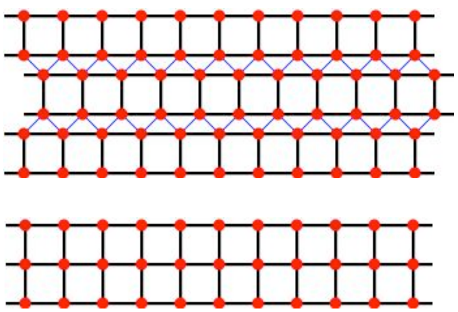
superexchange mechanism



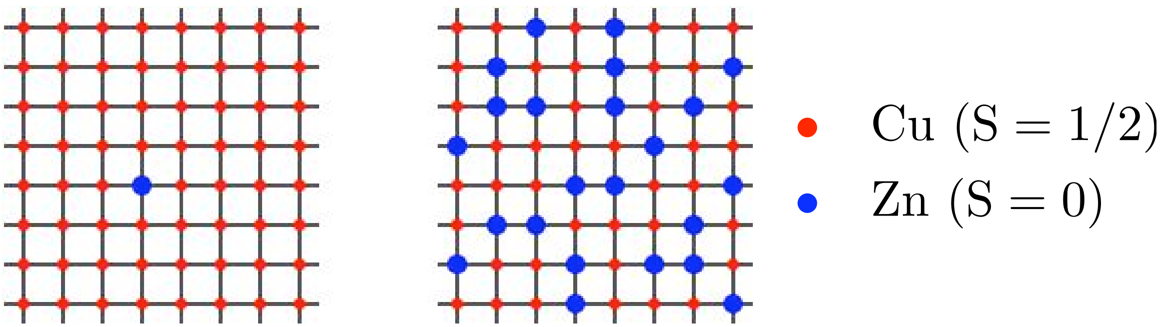
CuO_2 planes, localized spins on Cu sites
- Lowest-order spin model: S=1/2 Heisenberg
- Super-exchange coupling, J≈1500K

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

Many other quasi-1D and quasi-2D cuprates
• chains, ladders, impurities and dilution, frustrated interactions, ...



Ladder systems
- even/odd effects



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

The antiferromagnetic (Néel) state and quantum fluctuations

The ground state of the 2D Heisenberg model

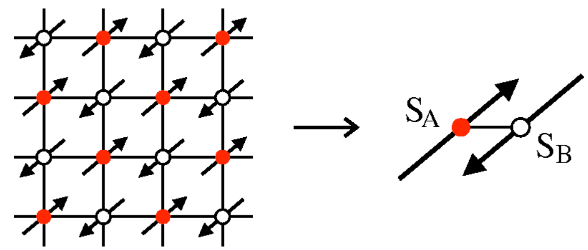
$$H = J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j = J\sum_{\langle ij\rangle}[S_i^z S_j^z + \tfrac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)]$$

Does the "staggered" (Néel) order survive quantum fluctuations?

- order parameter: staggered (sublattice) magnetization

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

$$\vec{m}_s = \frac{1}{N}\left(\vec{S}_A - \vec{S}_B\right)$$



- For S→∞ (classical limit) $\langle m_s\rangle \to S$
- what happens for small S (especially S=1/2)?

- $\langle m_s\rangle \approx 0.31$ (≈60% of classical value 1/2)
- demonstrated using quantum Monte Carlo (Reger and Young, 1989)
- in good agreement with experiments on cuprates
  - neutron scattering, NMR,...
- 1D Heisenberg chain: no magnetic order (Mermin-Wagner theorem)

Non-magnetic states in 2D

Consider two spins, i and j, in isolation:

$$H_{ij} = J_{ij}\vec{S}_i \cdot \vec{S}_j = J_{ij}[S_i^z S_j^z + \tfrac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)]$$

For $J_{ij}>0$ the ground state is the **singlet**;

$$|\phi_{ij}^s\rangle = \frac{|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle}{\sqrt{2}}, \qquad E_{ij} = -3J_{ij}/4$$

The Néel states have higher energy (expectation values; not eigenstates)

$$|\phi_{ij}^{N_a}\rangle = |\uparrow_i\downarrow_j\rangle, \qquad |\phi_{ij}^{N_b}\rangle = |\downarrow_i\uparrow_j\rangle, \qquad \langle H_{ij}\rangle = -J_{ij}/4$$

The Néel states are product states:

$$|\phi_{ij}^{N_a}\rangle = |\uparrow_i\downarrow_j\rangle = |\uparrow_i\rangle \otimes |\downarrow_j\rangle$$

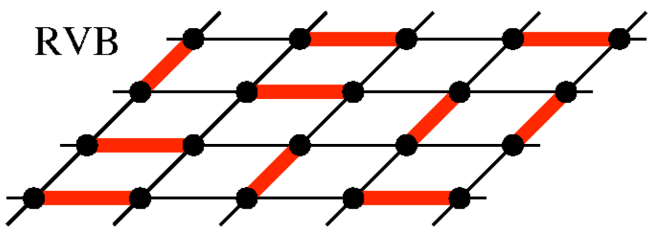
The **singlet is a maximally entangled** state
(furthest from product state)

N>2: each spin tends to entangle with its neighbors

- entanglement is energetically favorable
- but cannot singlet-pair with more than 1 spin
- leads to fluctuating singlets (valence bonds)
  - ➡ less entanglement, $\langle H_{ij} \rangle > -3J_{ij}/4$
  - ➡ closer to a product state (e.g., Néel)

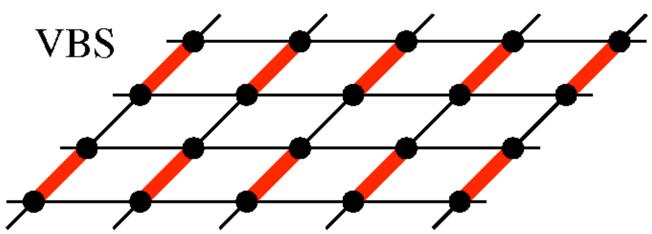
- **non-magnetic states possible** (N=∞)
  - ➡ resonating valence-bond (RVB) spin liquid
  - ➡ valence-bond solid (VBS)

RVB



Translationally invariant state
- no broken symmetries

VBS



Broken translational symmetry
- "strong" and "weak" correlations of neighbors

$$\langle \vec{S}(\mathbf{r}) \cdot \vec{S}(\mathbf{r} + \hat{\mathbf{x}}) \rangle$$

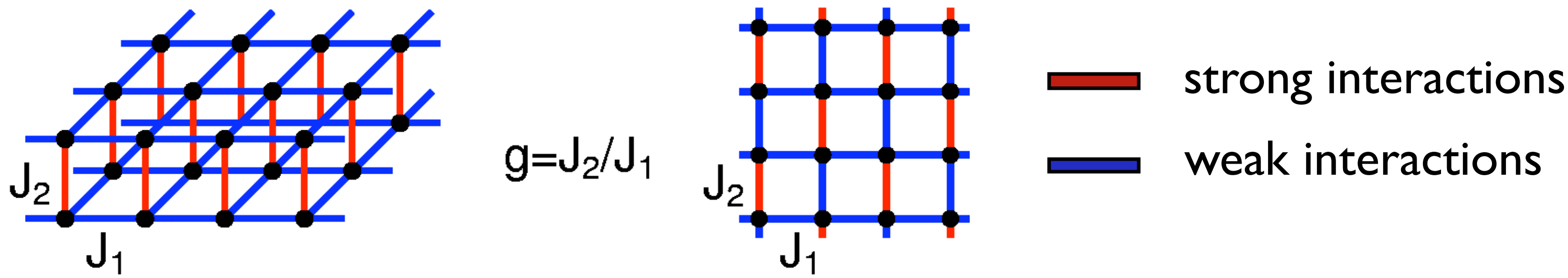
$$\langle \vec{S}(\mathbf{r}) \cdot \vec{S}(\mathbf{r} + \hat{\mathbf{y}}) \rangle$$

$$= (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$$

Quantum phase transitions (T=0; change in ground-state)

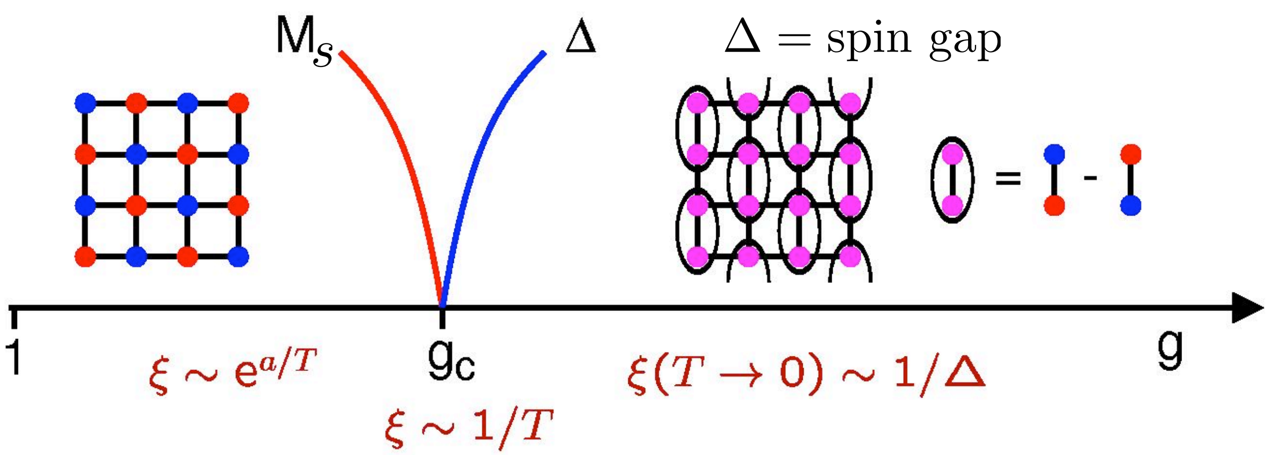
Example: Dimerized S=1/2 Heisenberg models

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



Singlet formation on strong bonds → Neel - disordered transition

Ground state (T=0) phases

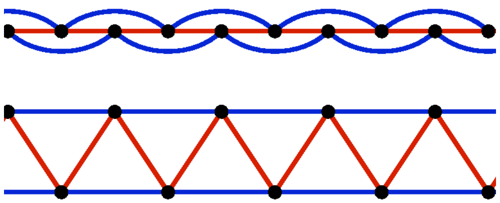


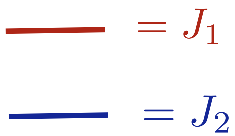
2D quantum spins map onto (2+1)D classical spins (Haldane)

- Continuum field theory: nonlinear σ-model (Chakravarty, Halperin, Nelson)

⇒ 3D classical Heisenberg (O3) universality class expected

S=1/2 Heisenberg chain with frustrated interactions





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

Different types of ground states, depending on the ratio **$g=J_2/J_1$** (both >0)

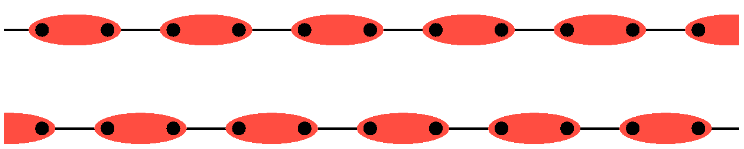
- **Antiferromagnetic "quasi order" (critical state) for g<0.2411...**
  - exact solution - Bethe Ansatz - for $J_2=0$
  - bosonization (continuum field theory) approach gives further insights
  - spin-spin correlations decay as 1/r

$$C(r) = \langle \vec{S}_i \cdot \vec{S}_{i+r} \rangle \sim (-1)^r \frac{\ln^{1/2}(r/r_0)}{r}$$

  - gapless spin excitations ("spinons", not spin waves!)
- **VBS order for g>0.2411... the ground state is doubly-degenerate state**
  - gap to spin excitations; exponentially decaying spin correlations

$$C(r) = \langle \vec{S}_i \cdot \vec{S}_{i+r} \rangle \sim (-1)^r \mathrm{e}^{-r/\xi}$$

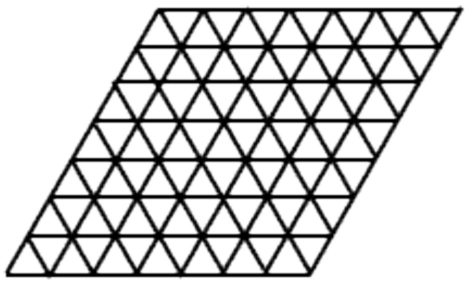
  - singlet-product state is exact for g=0.5 (Majumdar-Gosh point)



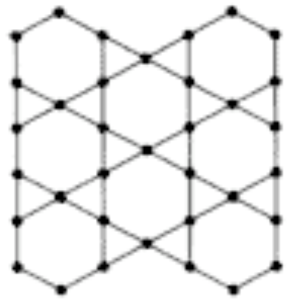
Frustration in higher dimensions

There are many (quasi-)2D and 3D materials with **geometric spin frustration**

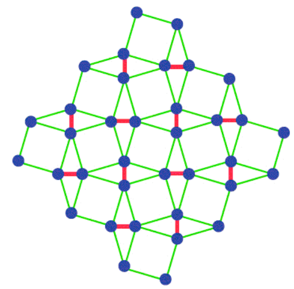
- no classical spin configuration can minimize all bond energies



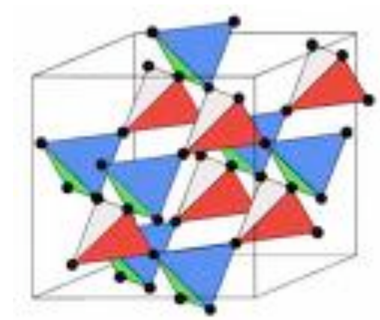
triangular (hexagonal)



Kagome



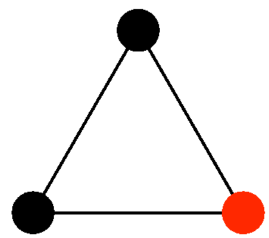
$SrCu_2(BO_3)_2$ (Shastry-Sutherland)

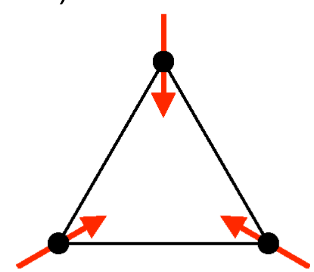


Pyroclore

A single triangular cell:

- 6-fold degenerate Ising model
- “120° Néel” order for vectors





Infinite triangular lattice

- highly degenerate Ising model (no order)
- “120° Néel” (3-sublattice) order for vectors

S=1/2 quantum triangular Heisenberg model

- the classical 3-sublattice order most likely survives
  [White and Chernyshev, PRL 2007]

S=1/2 Kagome system

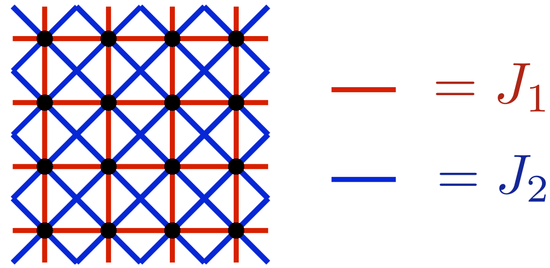
- very challenging, active research field; VBS or spin liquid?

Frustration due to longer-range antiferromagnetic interactions in 2D

Quantum phase transitions as some coupling (ratio) is varied

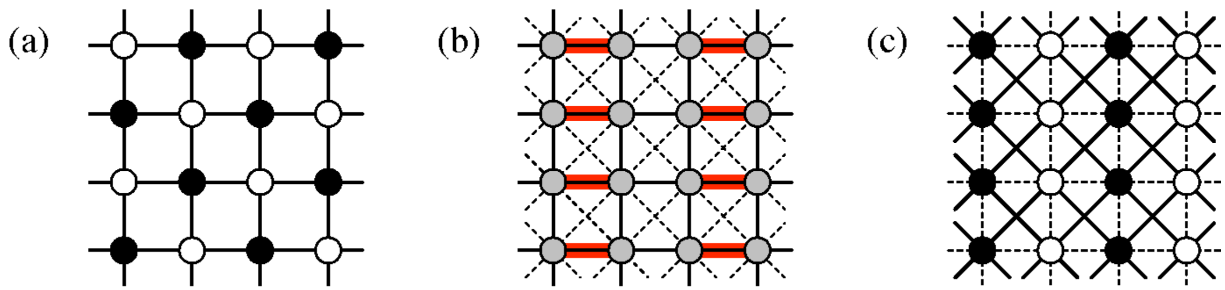
- J_1-J_2 Heisenberg model is the prototypical example

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



$$g = J_2/J_1$$

- 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



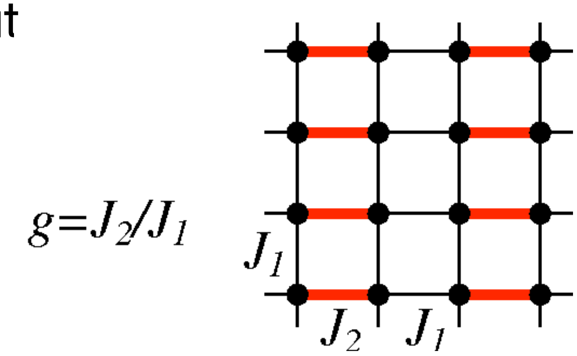
$0 \leq g < 0.45$ $\quad$ $0.45 \leq g < 0.6$ $\quad$ $g > 0.6$

- A non-magnetic state exists between the magnetic phases
  - Most likely a VBS (what kind? Columnar or “plaquette?)
  - Some calculations (interpretations) suggest spin liquid
- 2D frustrated models are challenging
  - no generally applicable unbiased methods (numerical or analytical)

Finite-lattice calculations

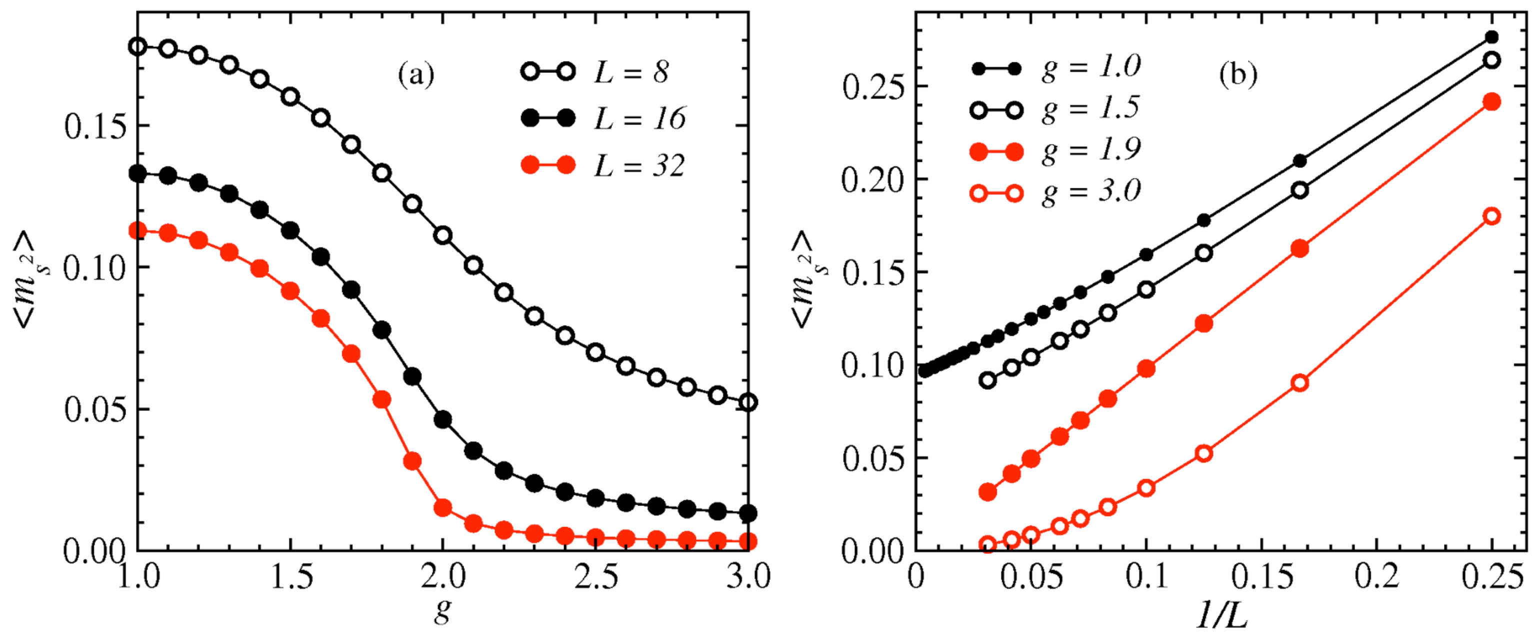
Numerically exact calculations (no approximations) for finite lattices

- extrapolate to infinite size, to learn about
  - the ground state and excitations
  - nature of quantum phase transitions
  - associated T>0 physics



Example: Dimerized Heisenberg model

- QMC results for L×L lattices



It is often known how various quantities should depend on L

- in a Néel state, spin-wave theory → $\langle m_s^2(L)\rangle = \langle m_s^2(\infty)\rangle + a/L + \dots$
- use finite-size scaling theory to study the quantum-critical point