Non-magnetic states

Two spins, i and j, in isolation, $H_{ij} = J_{ij}\vec{S}_i \cdot \vec{S}_j = J_{ij}[S_i^z S_j^z + \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)]$

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 (expectations; not eigenstates)

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

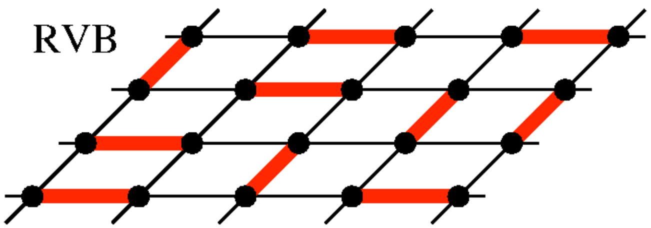
The Néel states are product states; $|\phi_{ij}^{N_a}\rangle = |\uparrow_i\downarrow_j\rangle = |\uparrow_i\rangle \otimes |\downarrow_j\rangle$

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

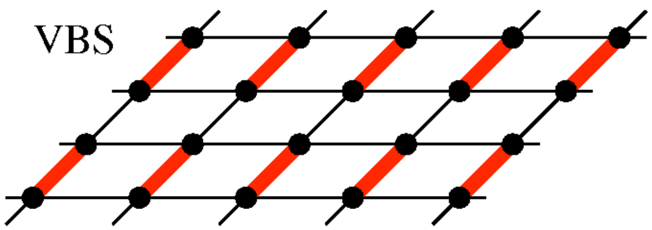
N>2: each spin tends to entangle with its neighbors
(spins it interacts with)

- 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



VBS



Conditions on magnetic order: The Mermin-Wagner theorem

A continuous symmetry cannot be broken for

- a 2D system (classical or quantum-mechanical) at T>0
- a 1D system at T=0,T>0
  - quantum to classical mapping gives 2D T>0 system (path integral)

The Heisenberg model has a continuous symmetry

- spin-rotation invariance [global SU(2) rotation invariance]
- so cannot have Néel order at T>0 in 2D and not at all in 1D

2D Heisenberg model (e.g., square lattice)

- spin correlation length diverges exponentially fast as T→0

$$C(r_{ij}) = \langle \vec{S}_i \cdot \vec{S}_j \rangle \sim (-1)^{x_{ij}+y_{ij}} \mathrm{e}^{-r_{ij}/\xi}, \quad \xi \to \infty \text{ as } T \to 0$$

1D Heisenberg chain (S = 1/2, 3/2, ...)

- spin correlations decay algebraically (almost) at T=0

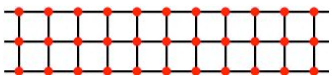
$$C(r) = \langle \vec{S}_i \cdot \vec{S}_{i+r} \rangle \sim (-1)^r \frac{\ln^{1/2}(r/r_0)}{r}, \qquad (T=0)$$

1D Heisenberg chain (S = 1, 2, ...)

- spin correlations decay exponentially at T=0 (the "Haldane conjecture")

$$C(r) = \langle \vec{S}_i \cdot \vec{S}_{i+r} \rangle \sim (-1)^r \mathrm{e}^{-r/\xi_S}, \quad \xi_S \to \infty \text{ as } S \to \infty$$

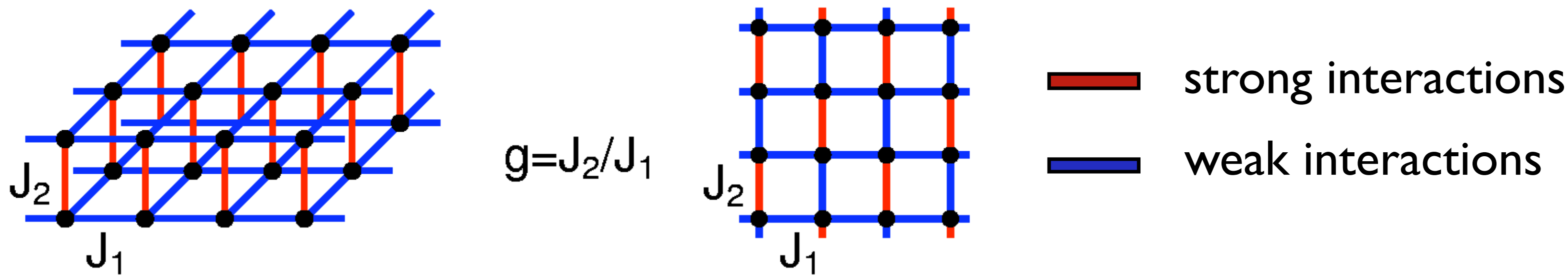
Similar (even-odd n) behavior in n-leg S=1/2 spin ladders



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

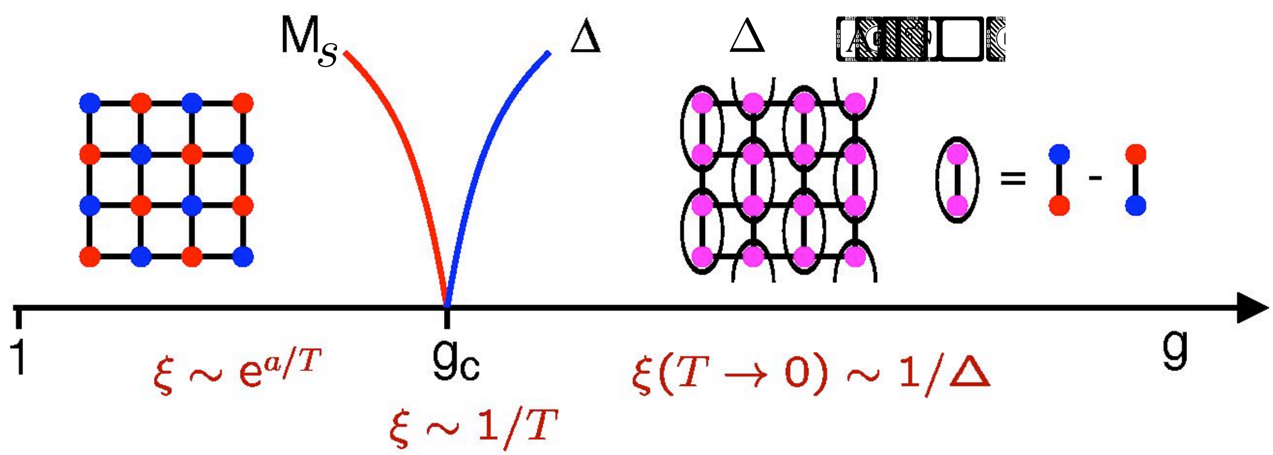
Example: Dimerized S=1/2 Heisenberg models

- 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

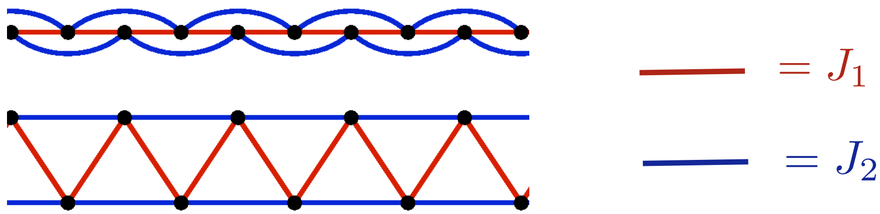


2D quantum spins map onto (2+1)D classical spins (Haldane)

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

⇒ 3D classical Heisenberg (O3) universality class expected

S=1/2 Heisenberg chain with frustrated interactions



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

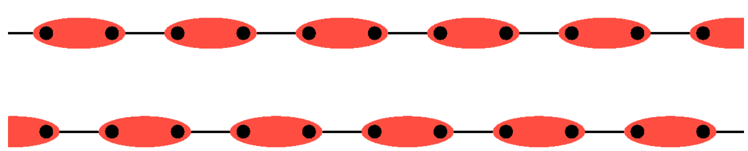
- **Antiferromagnetic "quasi order" (critical state) for g<0.2411...**
  - exact solution - Bethe Ansatz - for $J_2=0$
  - bosonization (continuum field theory) approach gives further insights
  - spin-spin correlations decay as 1/r

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

  - 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

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

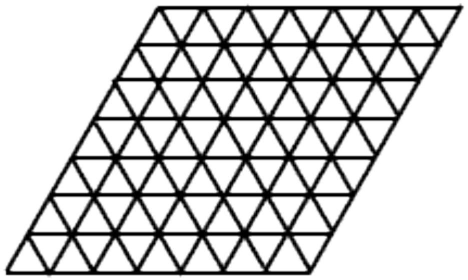
  - singlet-product state is exact for g=0.5 (Majumdar-Gosh point)



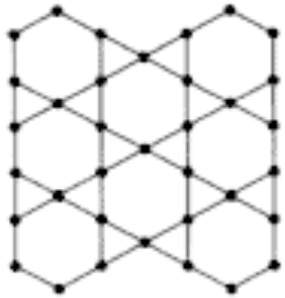
Frustration in higher dimensions

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

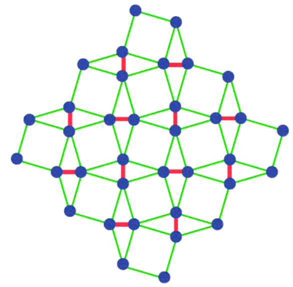
- no classical spin configuration can minimize all bond energies



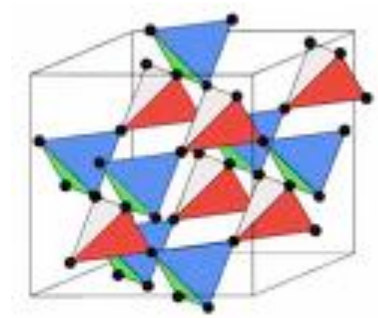
triangular (hexagonal)



Kagome



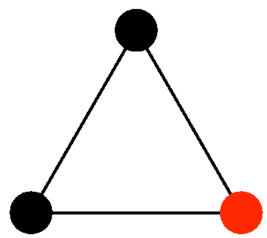
$SrCu_2(BO_3)_2$ (Shastry-Sutherland)

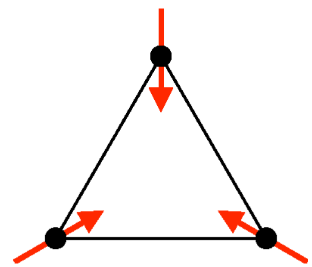


Pyroclore

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

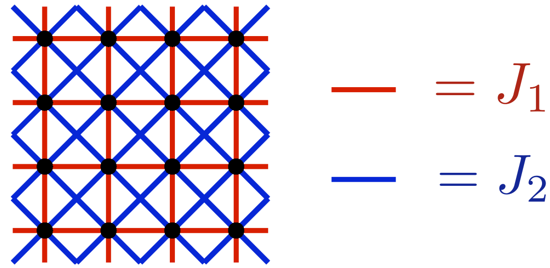
- very challenging, active research field; VBS or spin liquid?

Frustration due to longer-range antiferromagnetic interactions in 2D

Quantum phase transitions as some coupling (ratio) is varied

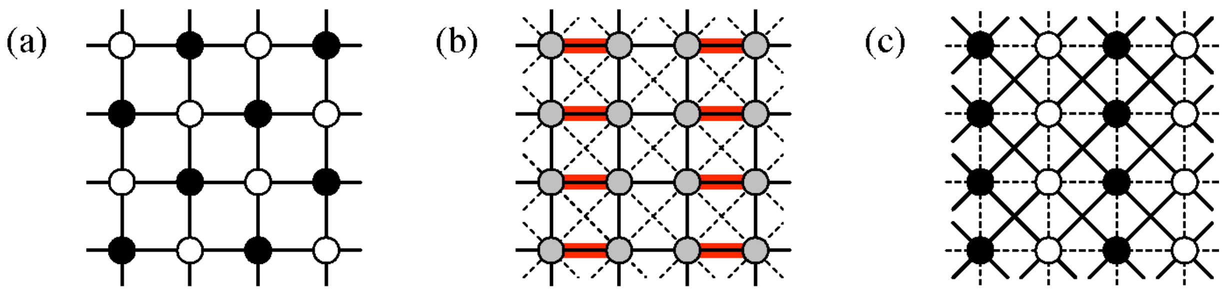
- J_1-J_2 Heisenberg model is the prototypical example

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



$$g = J_2/J_1$$

- 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



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