Title: Quantum Spins Simulations - Lecture 3

Date: Apr 07, 2010 11:00 AM

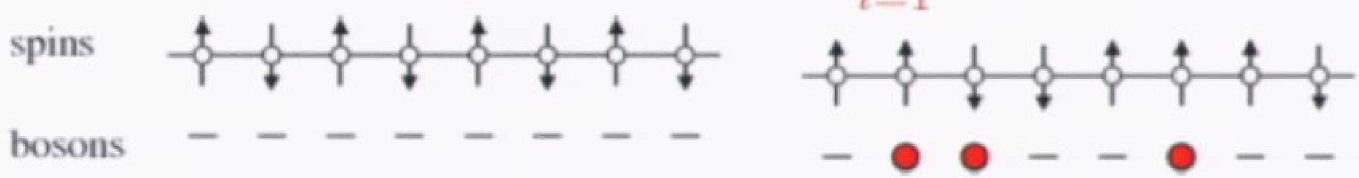
URL: http://pirsa.org/10040045

Abstract:

The ground state has no spin waves

- but it has some density of the original a-bosons
- this density is directly related to the sublattice magnetization

$$\langle m_s \rangle = S - \langle 0|a_i^+ a_i|0\rangle = S - \frac{1}{N}\sum_{i=1}^{N}\langle 0|a_i^+ a_i|0\rangle$$



$(S = 1/2)$

Using the Bogolubov transformation gives

$$\langle m_s \rangle = S - \frac{1}{N}\sum_{\mathbf{k}} \sinh^2(\Theta_{\mathbf{k}}).$$

and one can show with some manipulations that

$$2\sinh^2(\Theta_{\mathbf{k}}) = \frac{1}{\sqrt{1-\gamma_{\mathbf{k}}^2}} - 1$$

Numerical evaluation gives **$\langle m_s \rangle$=0.3034 for S=1/2**

Conclusion: Linear spin-wave theory predicts an ordered ground state

- the quantum fluctuations reduce the order by 40% from the classical value
- this turns out to be very close to the true value (obtained with QMC)

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;

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

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

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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)

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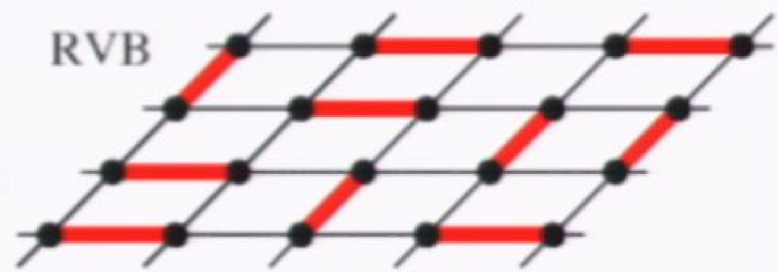
RVB



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)

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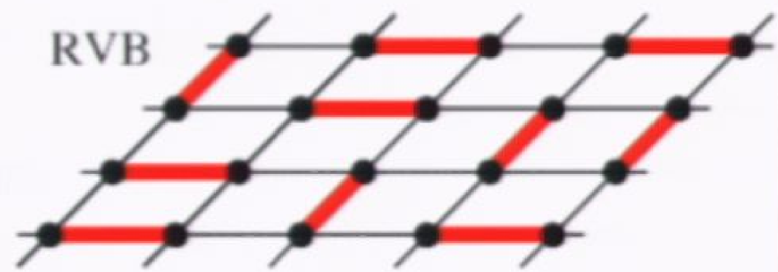

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2D Heisenberg model (e.g., square lattice)

- spin correlation length diverges exponentially fast as T→0

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

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

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

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

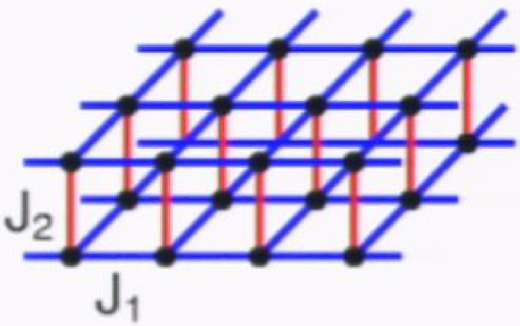
- spin correlations decay exponentially at T=0 (the “Haldane conjecture”)

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

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



$g = J_2/J_1$

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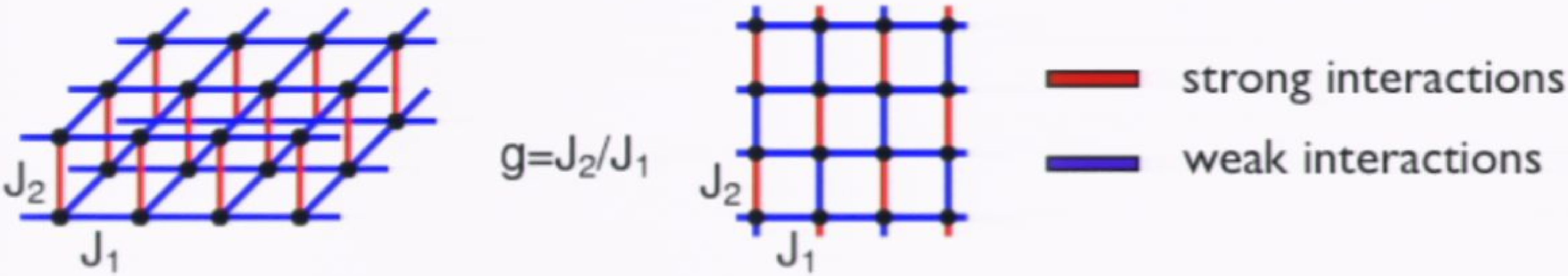
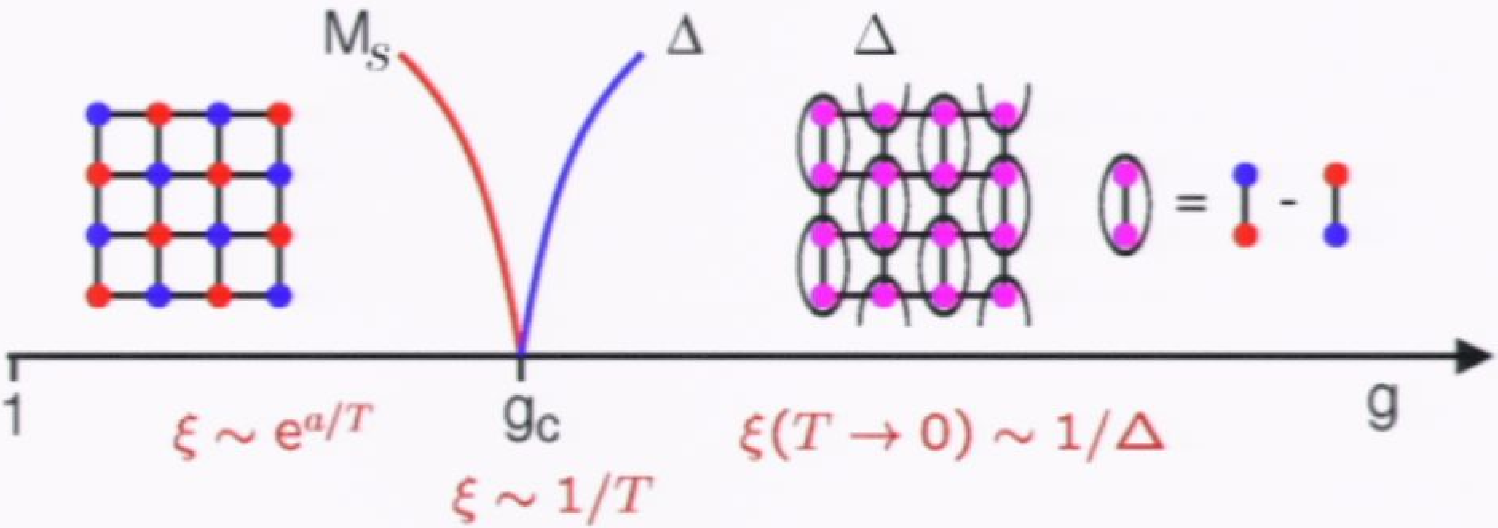


Singlet formation on strong bonds → Neel - disordered transition

Ground state (T=0) phases



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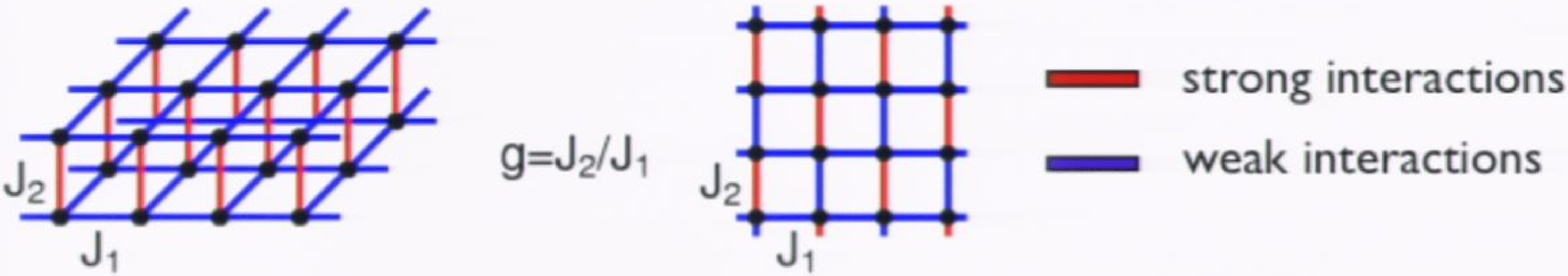

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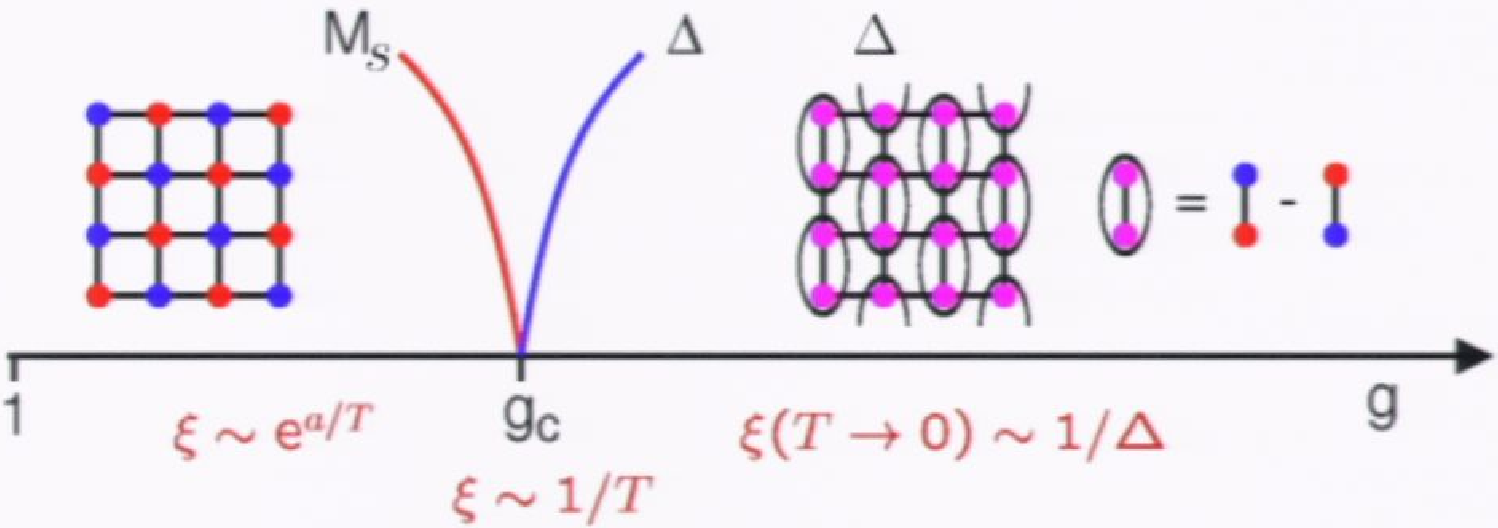
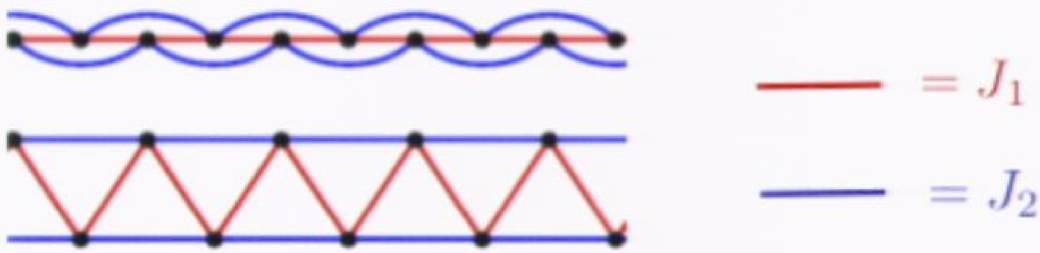


2D quantum spins map onto (2+1)D classical spins (Haldane)

S=1/2 Heisenberg chain with frustrated interactions



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

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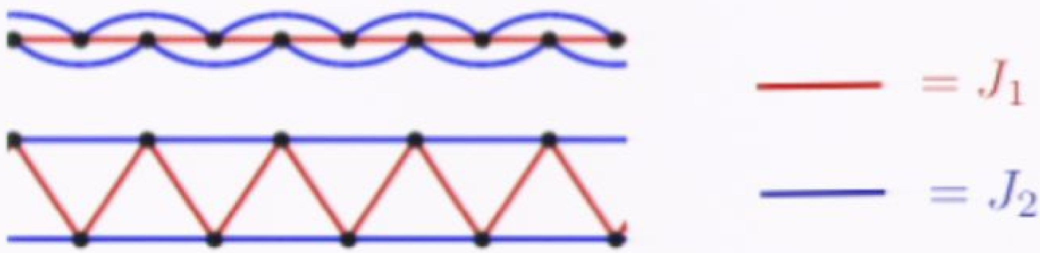

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- **Antiferromagnetic "quasi order" (critical state) for g<0.2411...**
  - exact solution - Bethe Ansatz - for $J_2=0$
  - bosonization (continuum field theory) approach gives further insights
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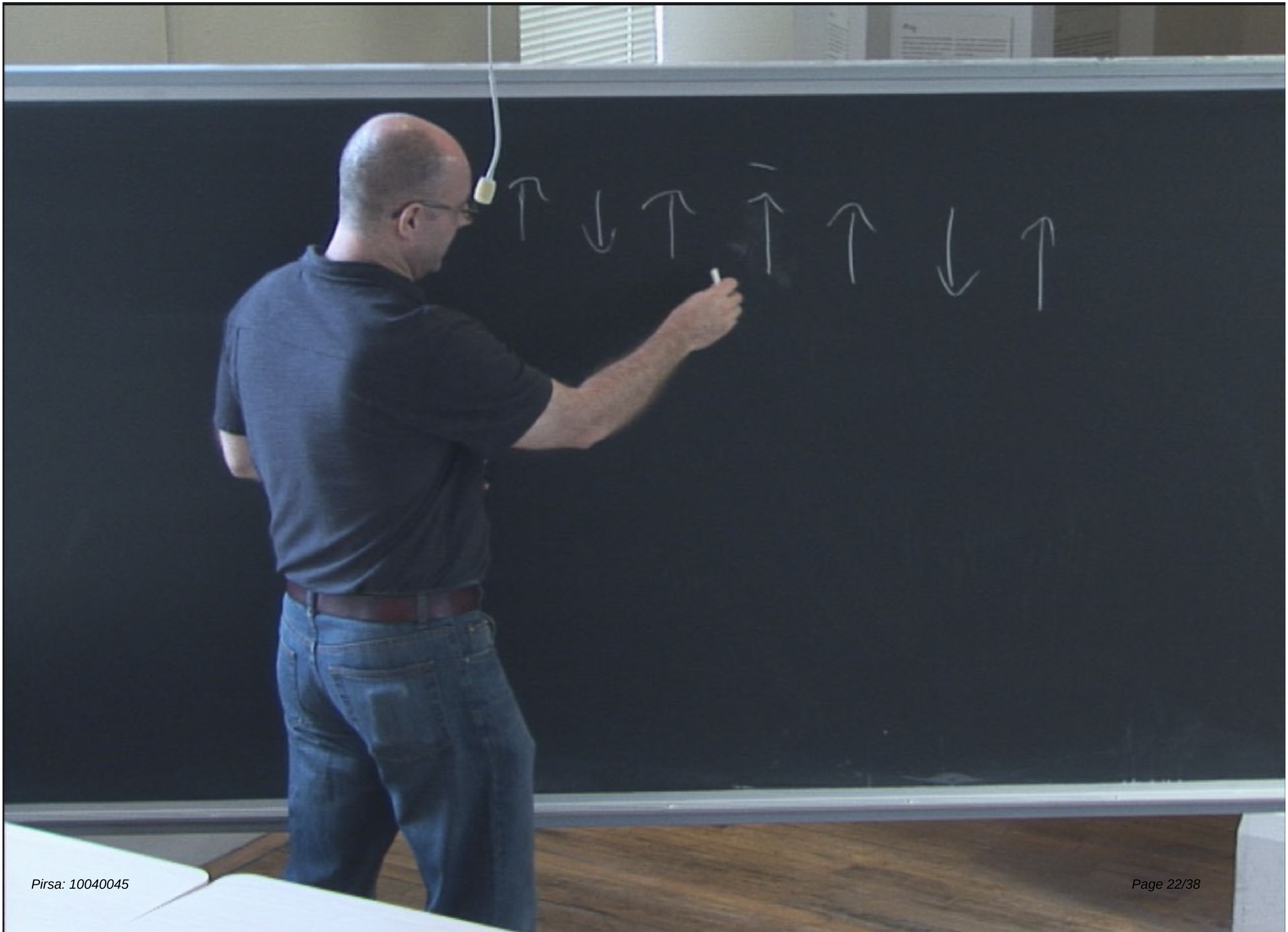

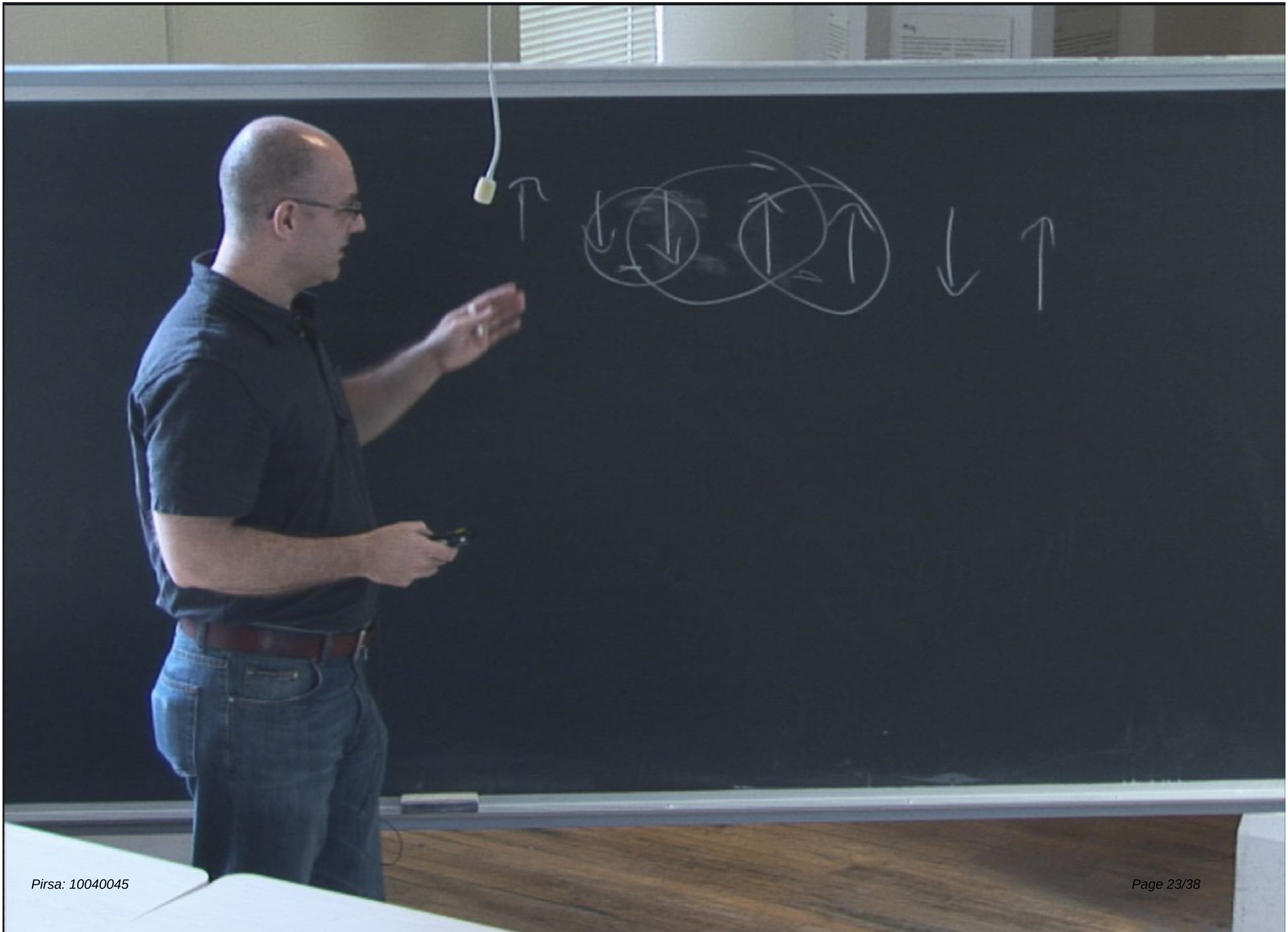

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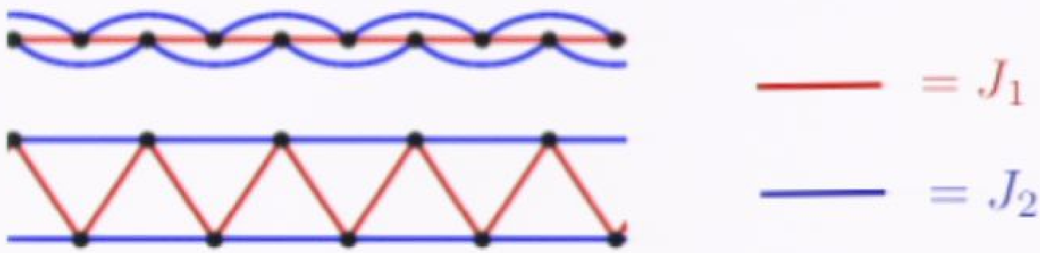

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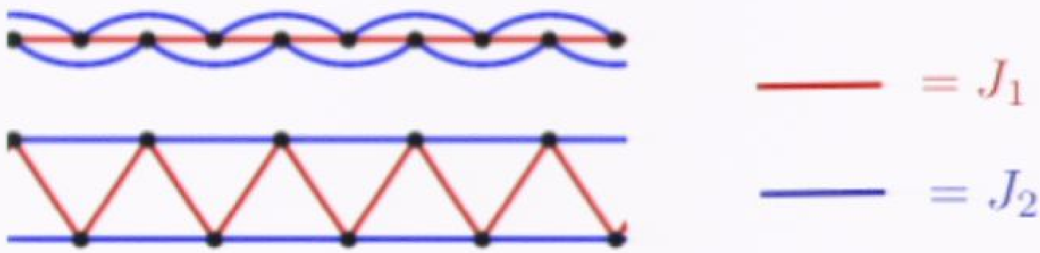

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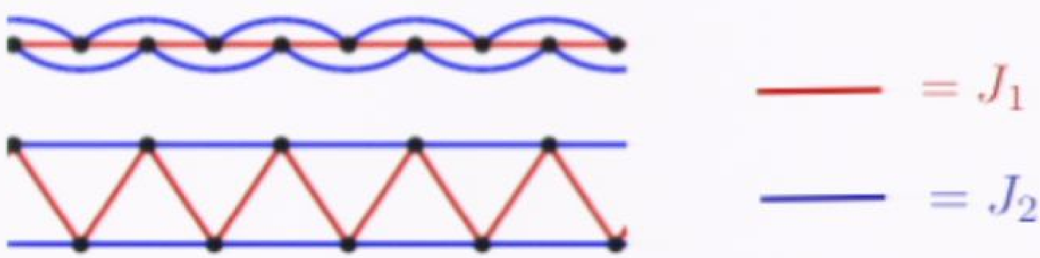

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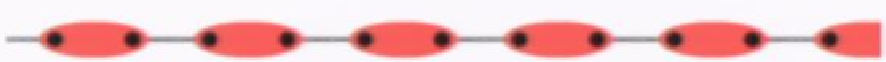
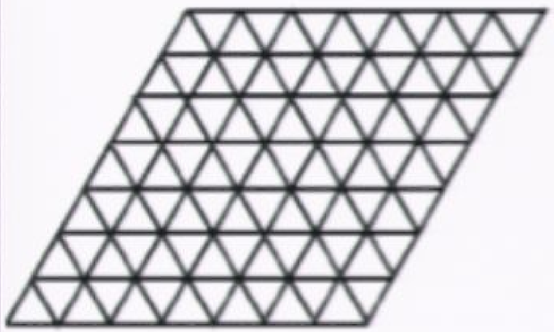


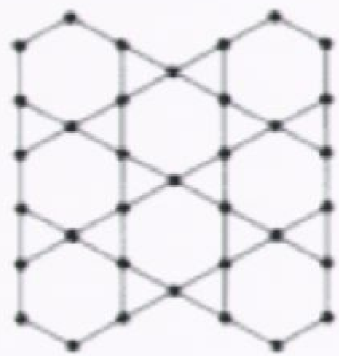
Frustration in higher dimensions

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

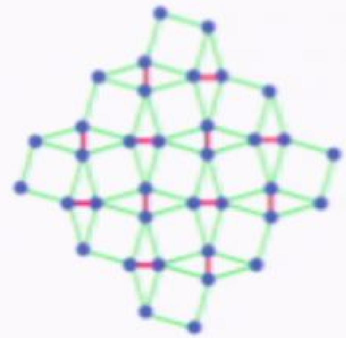
- no classical spin configurations minimiing all bond energies



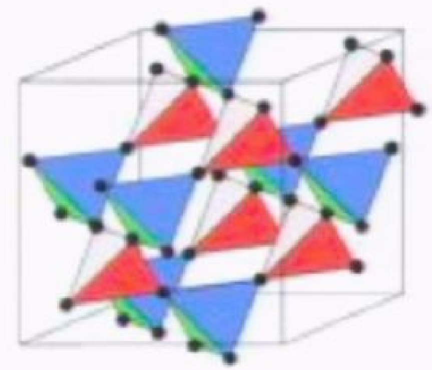
triangular
(hexagonal)



Kagome

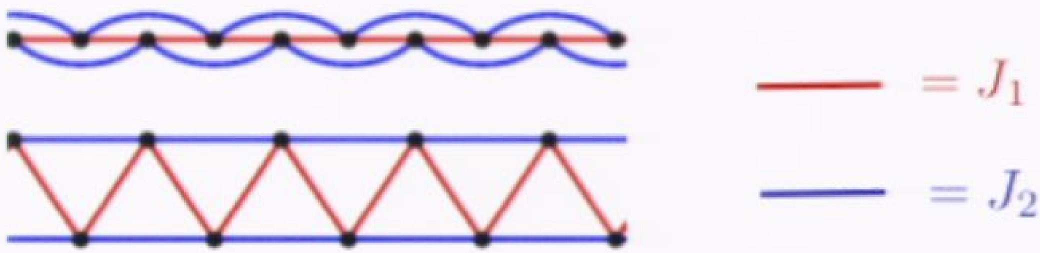


$SrCu_2(BO_3)_2$
(Shastry-Sutherland)



Pyroclore

S=1/2 Heisenberg chain with frustrated interactions



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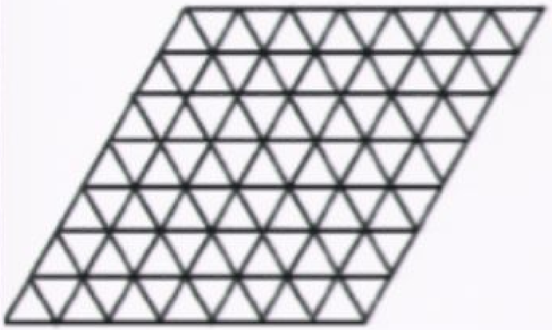

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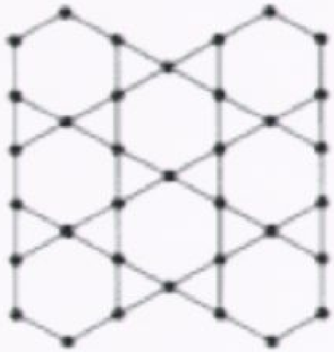

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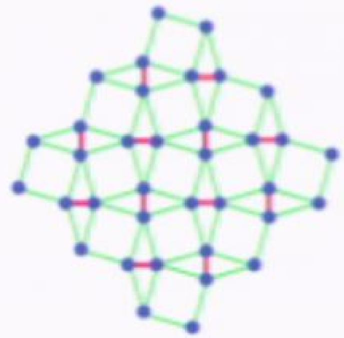

$SrCu_2(BO_3)_2$
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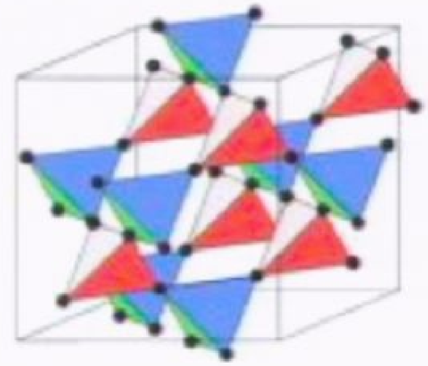
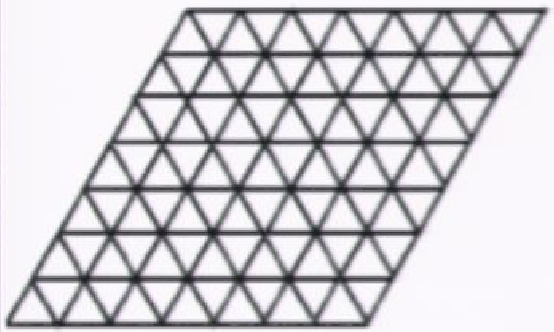


Pyroclore

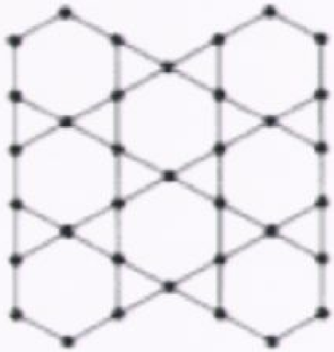
Frustration in higher dimensions

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

- no classical spin configurations minimiing all bond energies



triangular (hexagonal)



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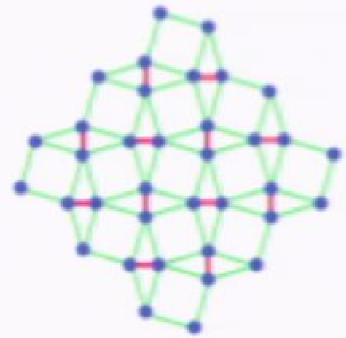

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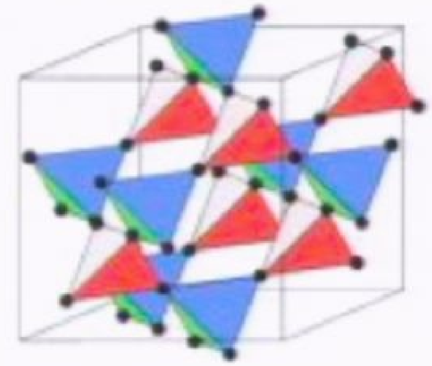
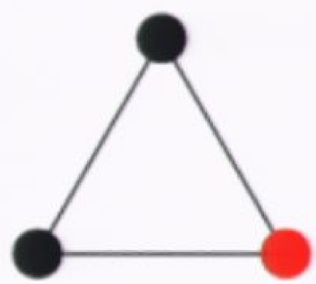
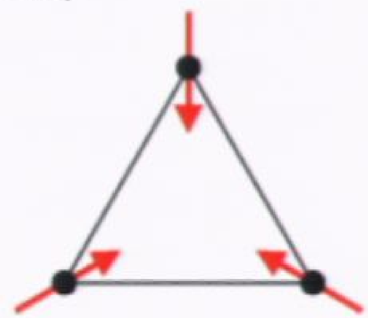


Pyroclore

A single triangular cell:

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





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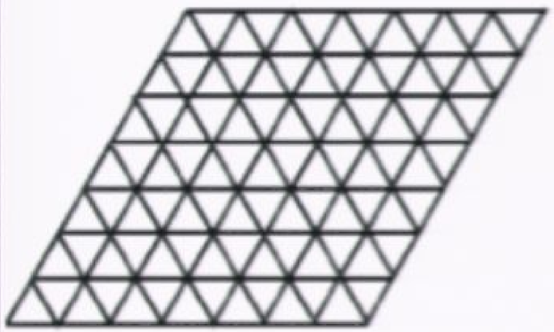

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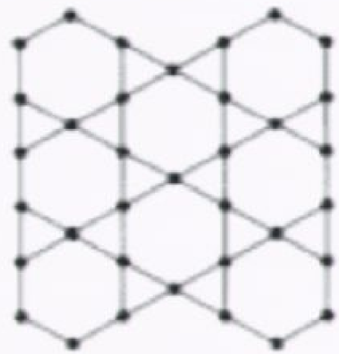

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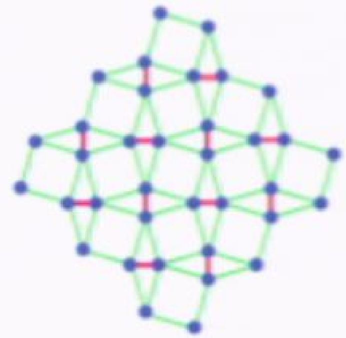

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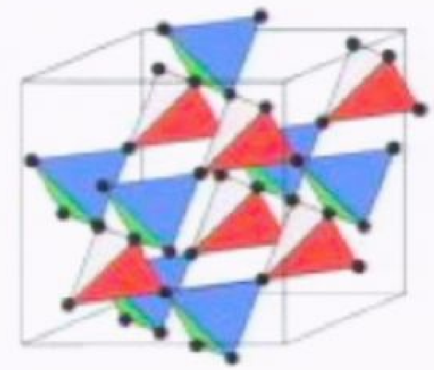

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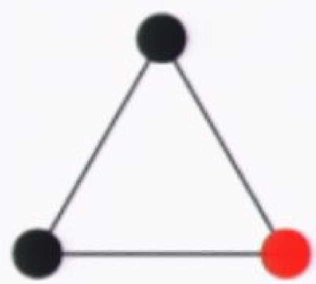

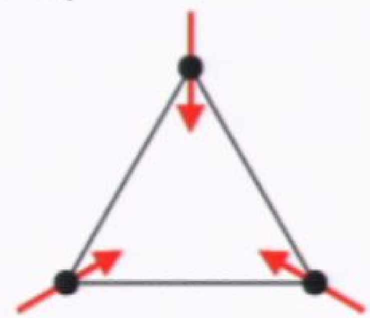

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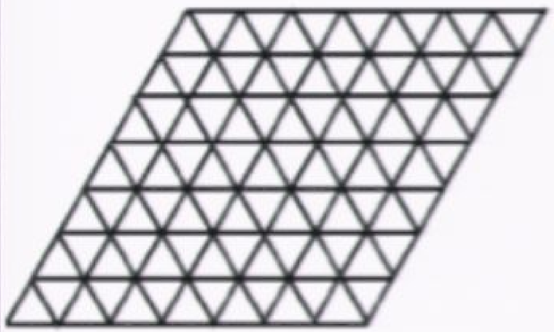

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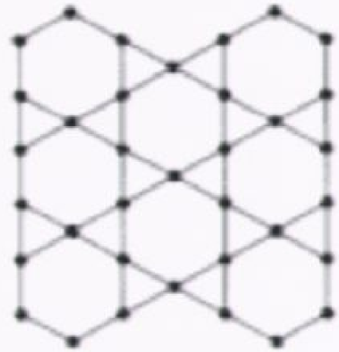

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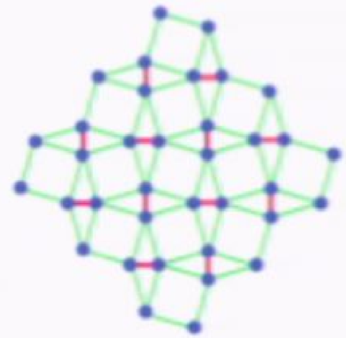

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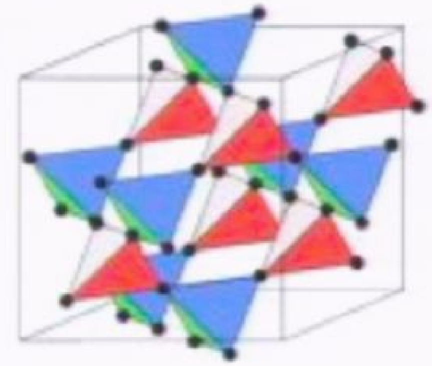

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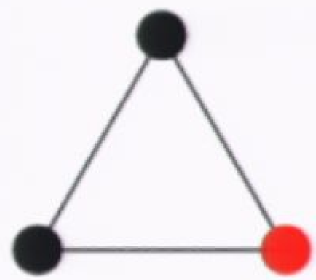

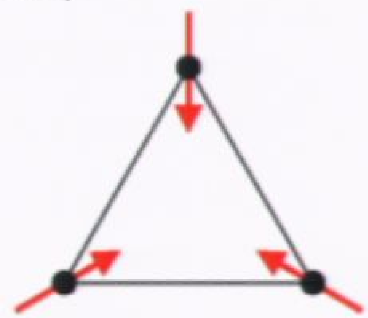

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S=1/2 quantum triangular Heisenberg model

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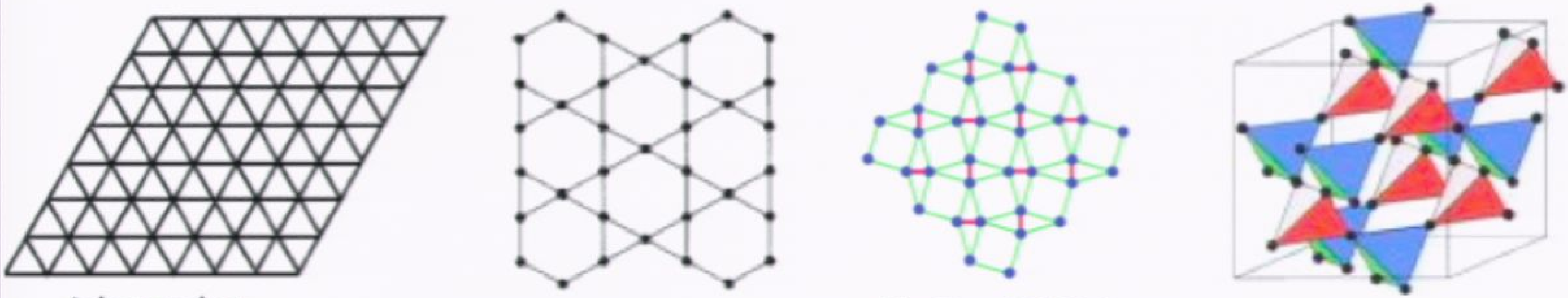

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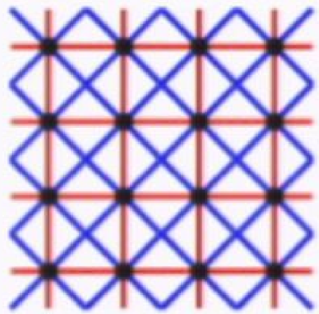
Frustration due to longer-range antiferromagnetic interactions in 2D

Quantum phase transitions as some coupling (ratio) is varied

J1-J2 Heisenberg model is the prototypical example

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



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$$g = J_2/J_1$$

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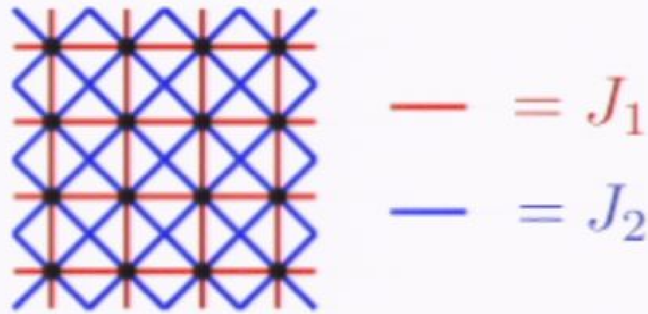

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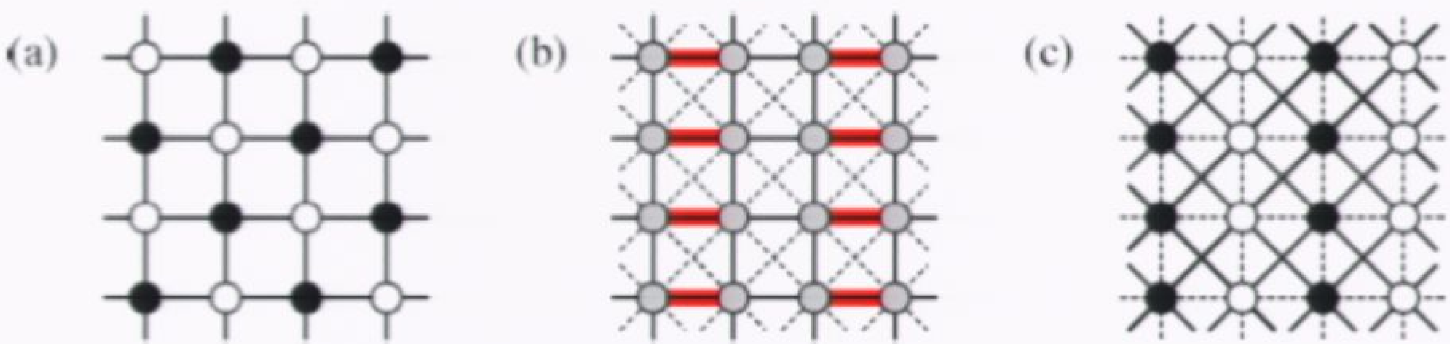
Ground states for small and large g are well understood

- Standard Néel order up to g≈0.45
- collinear magnetic order for g>0.6



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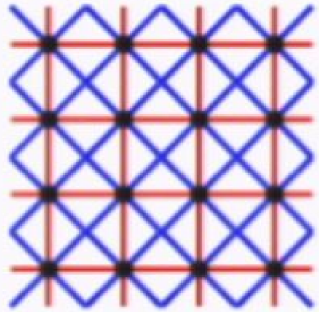

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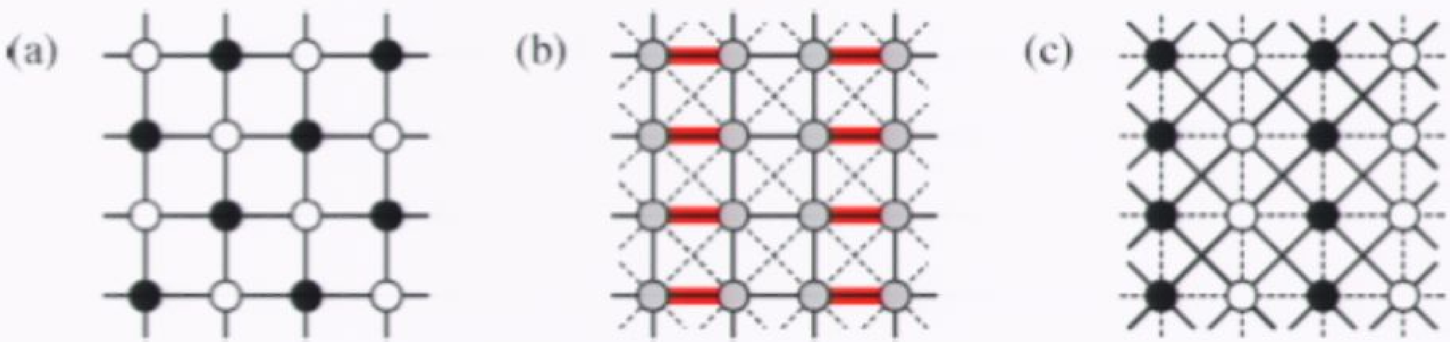

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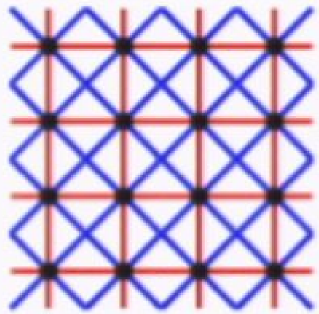

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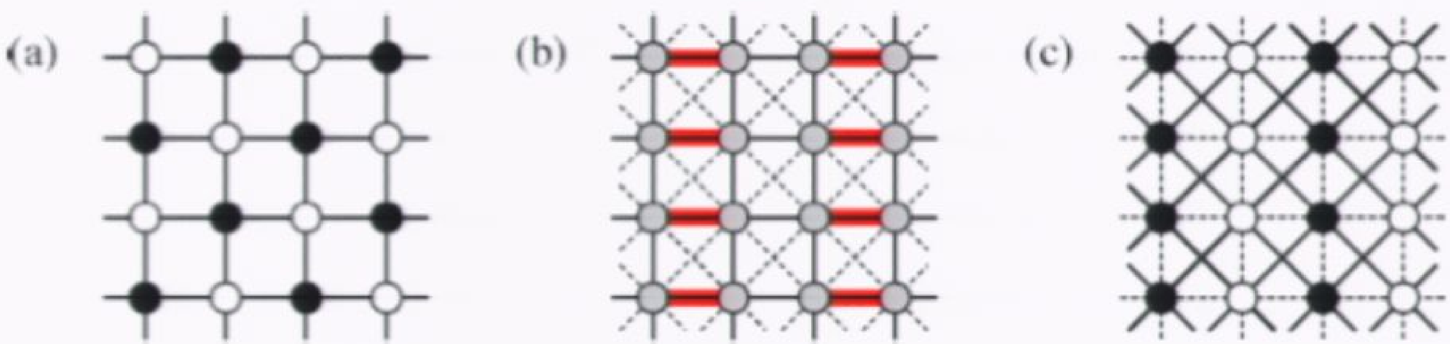

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