Frustrated spin systems

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Scope

- Competing interactions and degeneracy
- Classical ground-state correlations
- Order by disorder
- Spin liquids
  - → RVB spin liquids
  - → Algebraic spin liquids
  - → Chiral spin liquids
  - → Spin nematics
- Conclusions

The basic models

- Ising $$H = \sum_{(i,j)} J_{ij} S_i S_j, \quad S_i, S_j = \pm 1 \text{ or } \uparrow, \downarrow$$

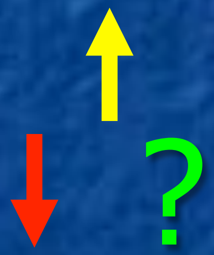
- Heisenberg model $$H = \sum_{(i,j)} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

$$[S_i^\alpha, S_i^\beta] = i\epsilon^{\alpha\beta\gamma} S_i^\gamma, \text{ and } \vec{S}_i^2 = S(S+1)$$

Classical limit $\vec{S}_i$ are unit vectors

Geometrical frustration

Not frustrated



Frustrated

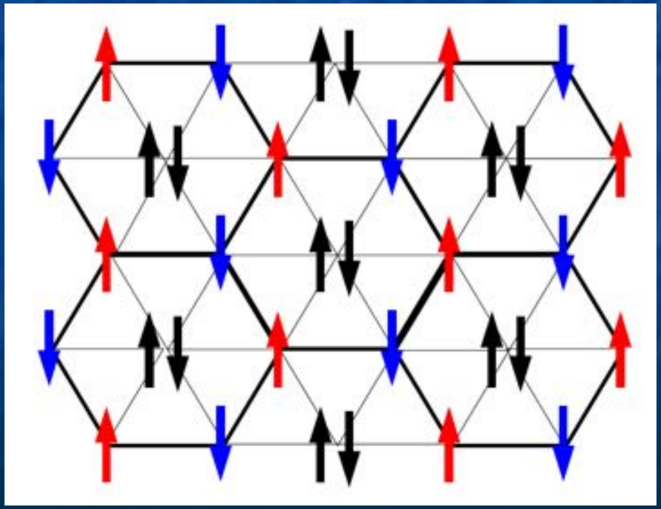
Antiferromagnetic coupling + odd loops

⬇

Competition between exchange paths = frustration

Ising on triangular lattice

- At least one unsatisfied bond per triangle
- Infinite number of ways to achieve only one unsatisfied bond on each triangle



At least $2^{N/3}$ GS

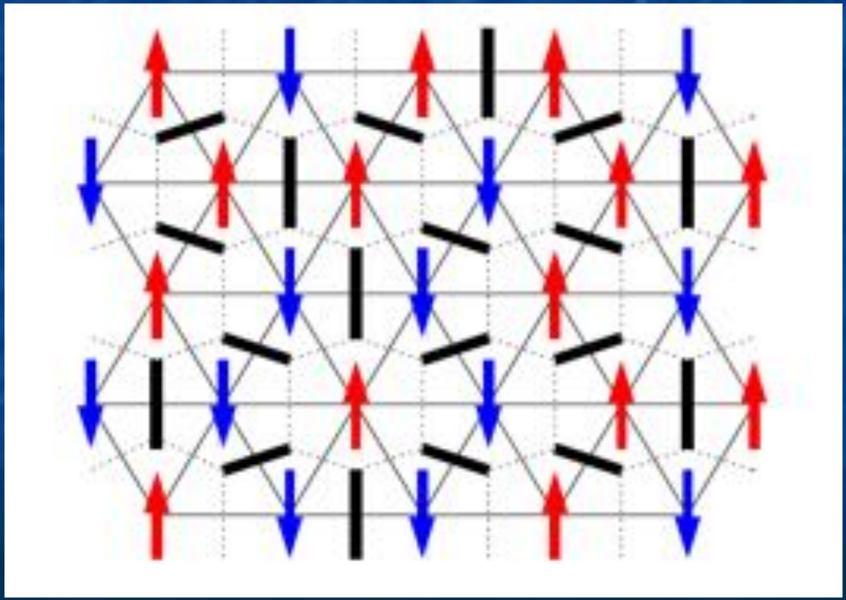
↓

Residual entropy

$S/N > (1/3)\ln 2 = 0.210\ldots$

Entropy of triangular Ising model

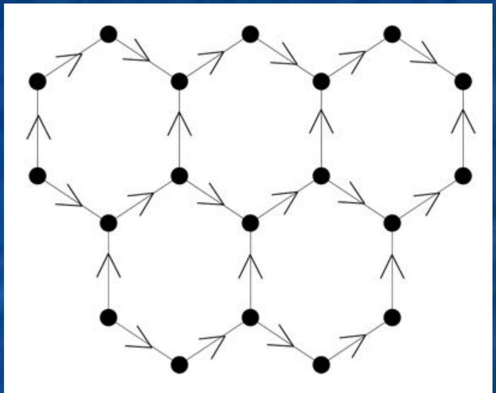
- Wannier (1950): S/N = 0.3230…
- Alternative: dimer problem on dual lattice



GS = 2 times
dimer coverings on
honeycomb lattice

Kasteleyn matrix

Bonds oriented with odd number of clockwise arrows on even plaquettes



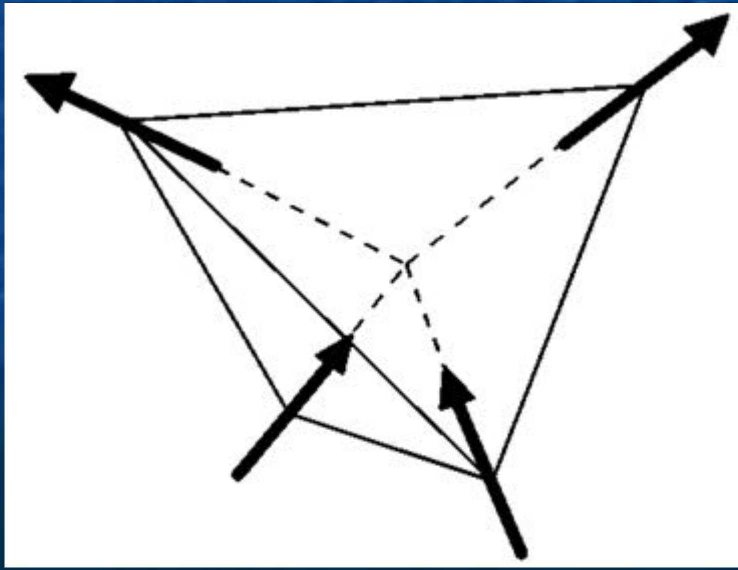
$$a(i,j) = \begin{cases} 1 \text{ if } i,j \text{ ajdacent and } i \rightarrow j \\ -1 \text{ if } i,j \text{ ajdacent and } i \leftarrow j \\ 0 \text{ otherwise.} \end{cases}$$

$$Z = \sqrt{\det a}$$

$$\frac{1}{N_{h_c}} \ln Z = \frac{1}{4} \int_0^1 \mathrm{d}x \int_0^1 \mathrm{d}y \ln |3 + 2\cos(2\pi y) - 2\cos(2\pi(x+y)) - 2\cos(2\pi x)| \simeq 0.1615$$

Spin Ice

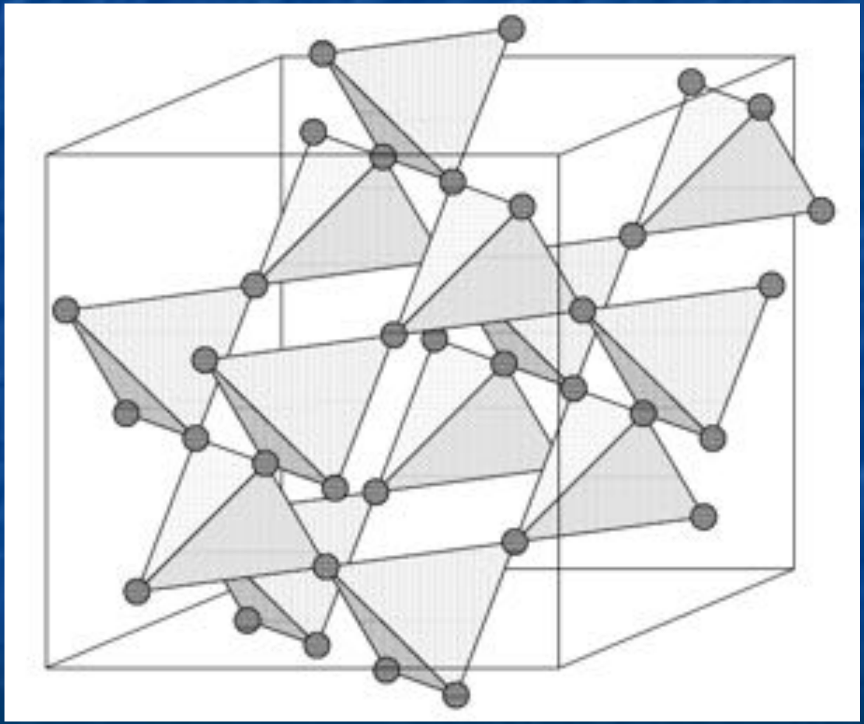
- $Dy_2Ti_2O_6$, $Ho_2Ti_2O_6$
- Pyrochlore lattice
- Ferromagnetic exchange interactions
- Strong anisotropy: spins 'in' or 'out'

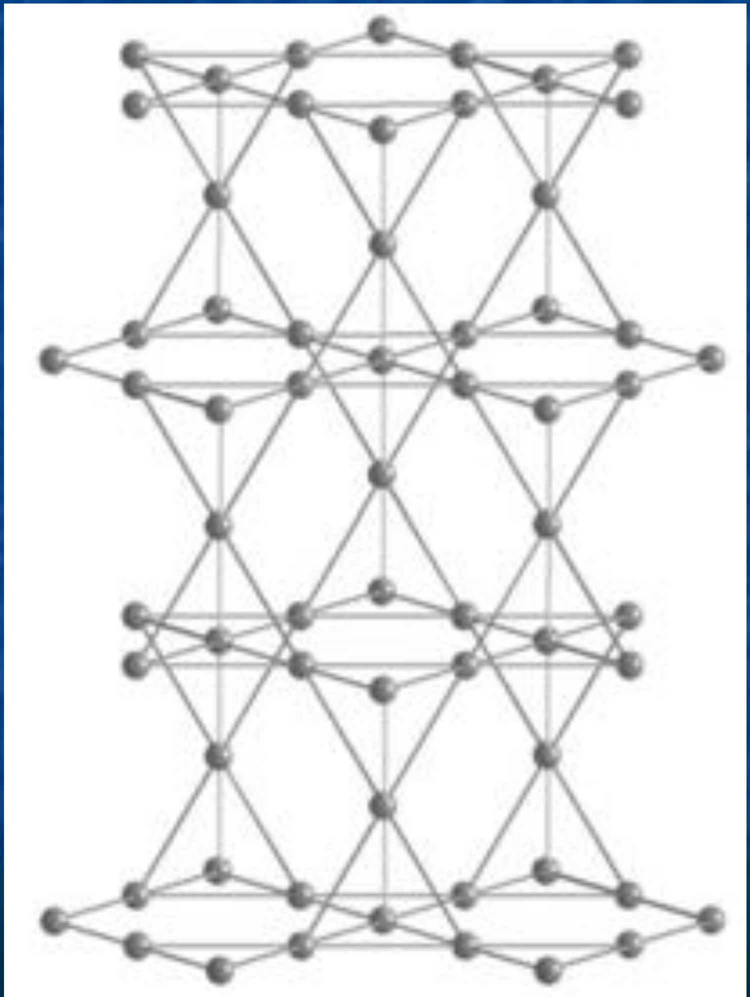


Ground state:
2 spins in, 2 spins out

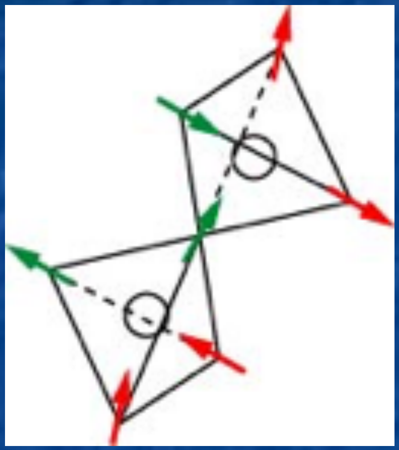
Residual entropy:
the 'ice problem'

Pyrochlore lattice

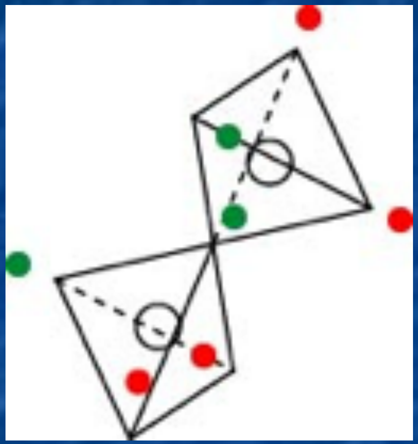




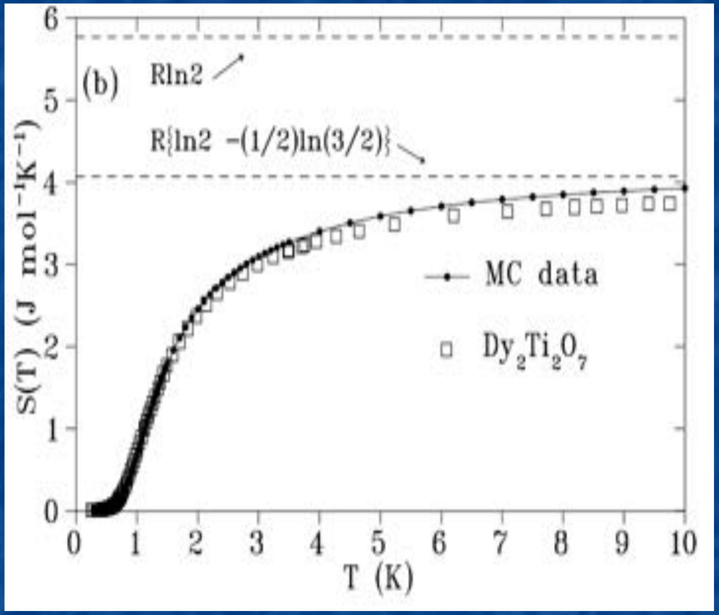
Residual entropy



Spin ice



Ice



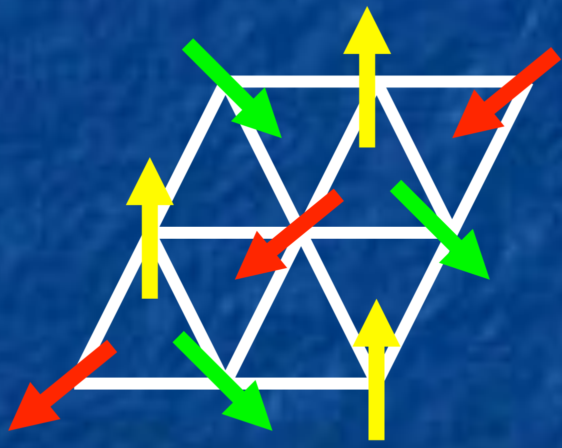
'Exact' : $S/k_B \approx 0.20501$
(Nagle, 1966)

Ramirez et al, 1999

Pauling (1945): $S/k_B \approx (1/2)\ \ln\ (3/2) = 0.202732$

Heisenberg model

- Bravais lattice: helical order
  → pitch vector = minimum of J(q), FT of J_{ij}

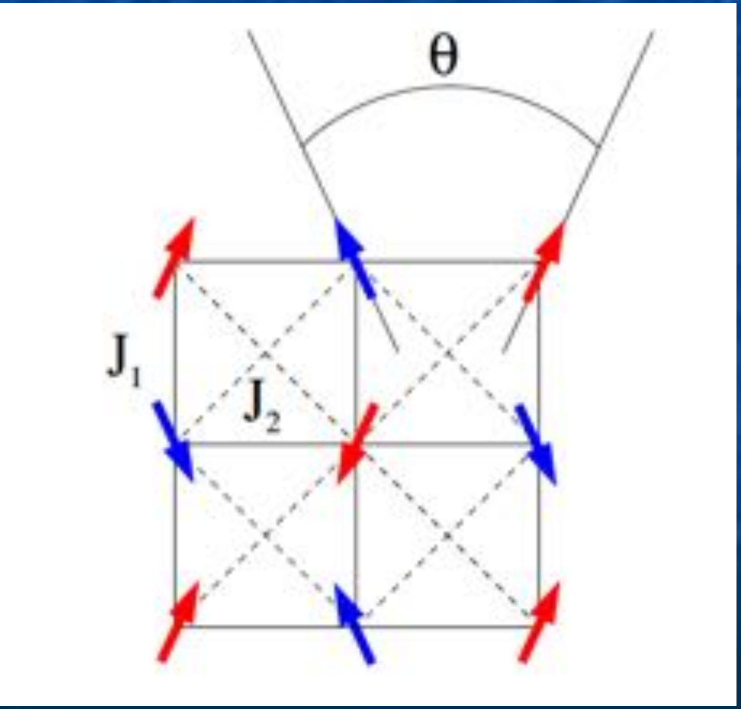


Triangular lattice:
3-sublattice order

Sum of spins = 0 on each triangle

Infinite degeneracy

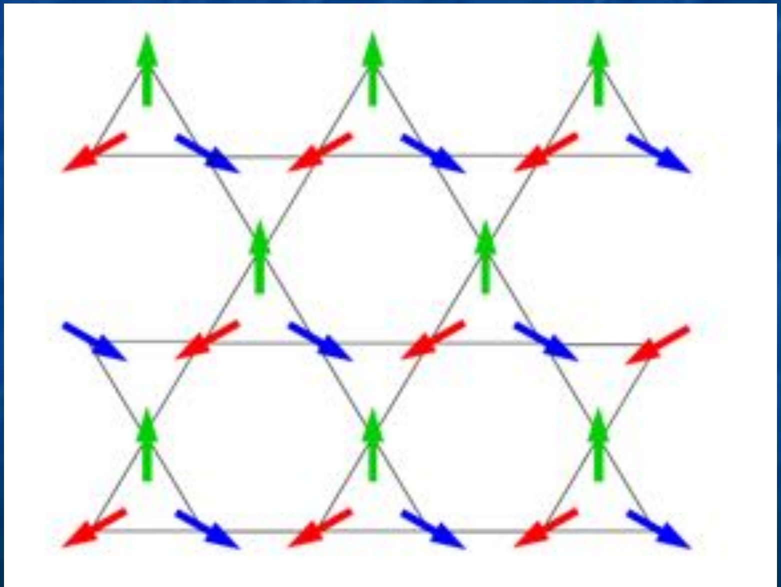
- J_1-J_2 model on square lattice



Classical energy independent of θ

Kagome

- Coplanar ground states: sum of spins = 0 on each triangle → degeneracy of 3-state Potts model
- Non-coplanar ground states



Rotate a chain of blue and red spins around green direction

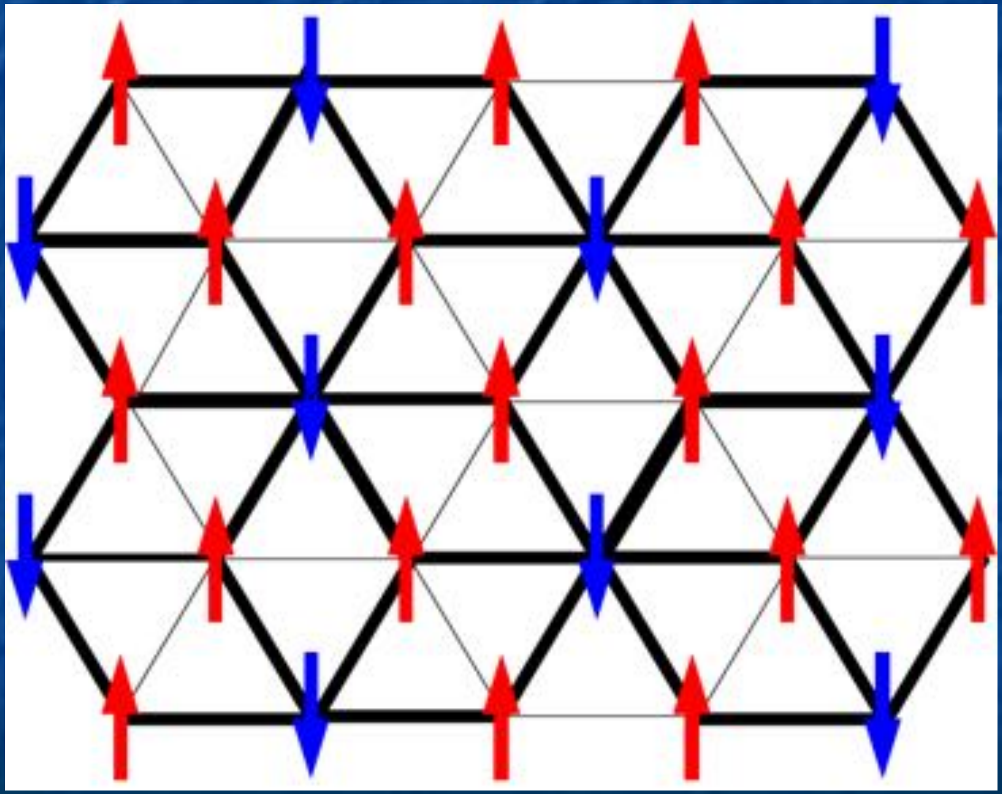
Classical GS correlations (Ising)

- Correlations = average over all GS
- Triangular lattice (Stephenson, 1964)

$$\langle \sigma(\vec{r})\sigma(\vec{0})\rangle \propto 1/r^{1/2}$$

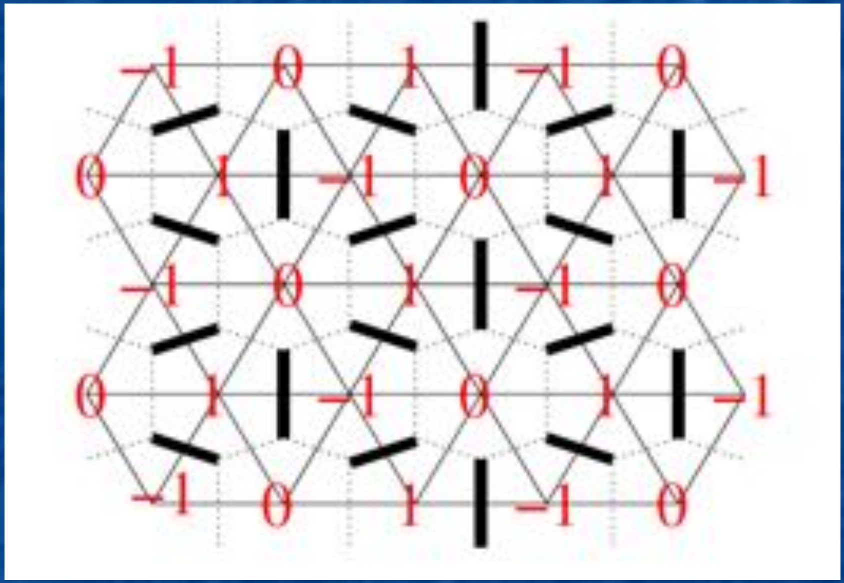
- Simple argument: Kasteleyn matrix on honeycomb gapless (Dirac points at 0)
- Physical interpretation: the maximally flippable configuration dominates the sum

Maximally flippable state



All red spins flippable (2/3)

Mapping on height model



on up triangles, height z(r):
increases by + 2 clockwise if dimer
decreases by 1 otherwise

Coarse graining

$$h(\vec{x}) = [z(\vec{r}_1) + z(\vec{r}_2) + z(\vec{r}_3)]/3$$

Maximally flippable state = flat surface (h=0)

$$F(\{h(\vec{x})\}) = \int \mathrm{d}\vec{x} \frac{K}{2} \left|\vec{\nabla} h(\vec{x})\right|^2$$

$$\langle \sigma(\vec{r})\sigma(\vec{0})\rangle \propto \left(\frac{\pi r}{a}\right)^{-\frac{2\pi}{36K}}$$

Consistent with $1/\,r^{1/2}$ if $K = \pi/9$

Rough phase

Pyrochlore

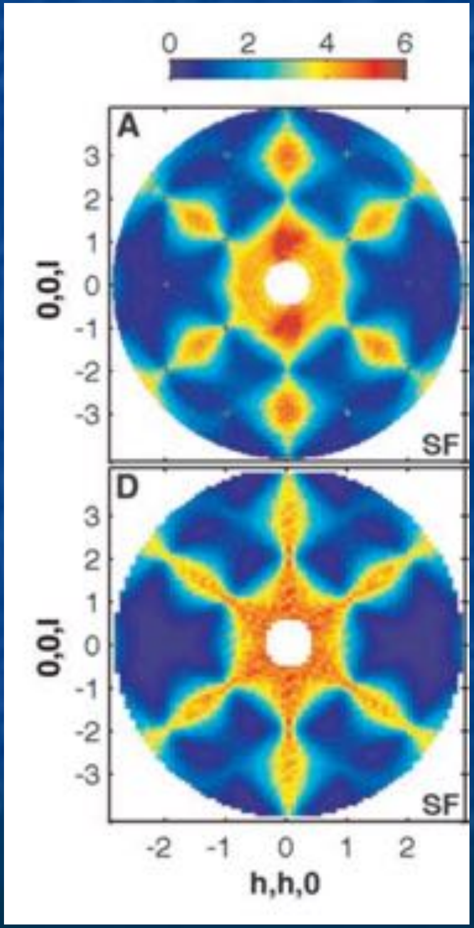
- 2 in - 2 out on each tetrahedron
- Continuum limit: magnetic field $\operatorname{div} \vec{B} = 0$

$$S(\vec{B}(\vec{x})) = \exp\left[-\frac{K}{2}\int \mathrm{d}^3\vec{r}\vec{B}(\vec{r})^2\right]$$

$$\left\langle S_\alpha(\vec{r})S_\beta(\vec{0})\right\rangle = \frac{1}{4\pi K}\frac{3(\hat{e}_\alpha\cdot\vec{r})(\hat{e}_\beta\cdot\vec{r}) - (\hat{e}_\alpha\cdot\hat{e}_\beta)r^2}{r^5}$$

Dipolar correlations

Pinch points in $Ho_2Ti_2O_7$



← Experiment

← Theory

T. Fennel et al, 2009

Quantum fluctuations

Holstein-Primakoff

$$\begin{cases} S_i^{z_i} = S - a_i^\dagger a_i \\ S_i^+ = \sqrt{2S - a_i^\dagger a_i}\ a_i \\ S_i^- = a_i^\dagger \sqrt{2S - a_i^\dagger a_i} \end{cases}$$

1/S expansion + Fourier transform

$$H = E_{\text{classical}} + \sum_{\vec{k}} \left[B_{\vec{k}} a_{\vec{k}}^\dagger a_{\vec{k}} + \frac{1}{2} A_{\vec{k}} \left(a_{\vec{k}}^\dagger a_{-\vec{k}}^\dagger + a_{\vec{k}} a_{-\vec{k}} \right) \right]$$

Zero-point energy

Bogoliubov rotation

$$\alpha_{\vec{k}} = u_{\vec{k}} a_{\vec{k}} + v_{\vec{k}} a^{\dagger}_{-\vec{k}}$$

$$\mathcal{H} = E_0 + \sum_{\vec{k}} \omega_{\vec{k}} \left(\alpha^{\dagger}_{\vec{k}} \alpha_{\vec{k}} + \frac{1}{2} \right)$$

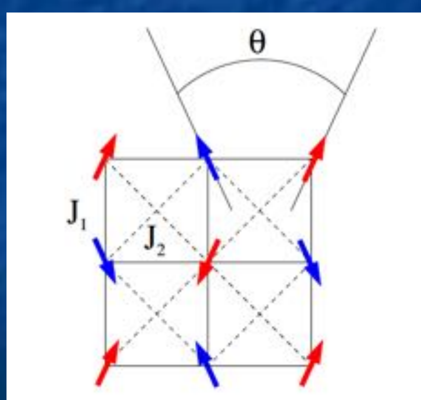
Zero-point energy

$$E(\theta) = E_0 + \frac{1}{2} \sum_{\vec{k}} \omega_{\vec{k}}(\theta)$$

Order by disorder

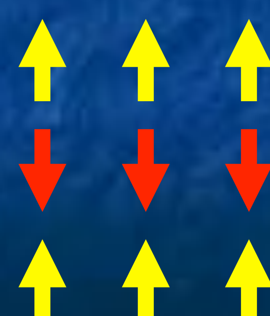
Chris Henley

- Even if the GS is degenerate, the spectrum depends on GS
  → selection by zero-point energy



J_1-J_2

$\theta = 0$

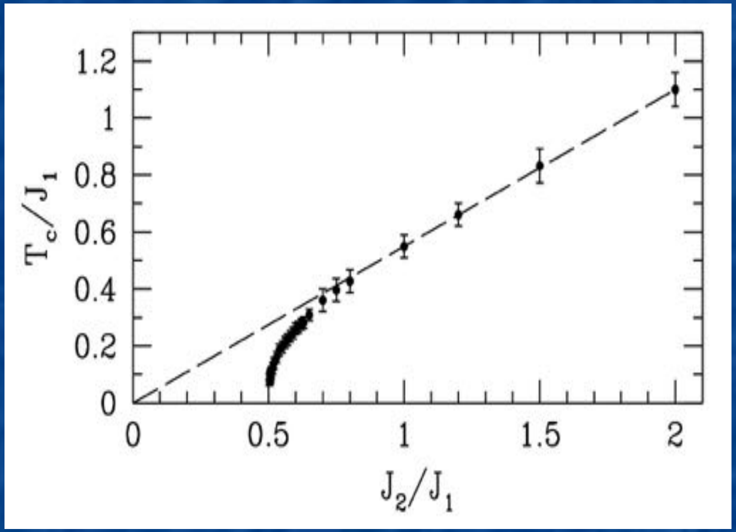


$\theta = \pi$

Ising transition

2 collinear states → Ising degree of freedom

↓



Ising transition for any S

Chandra, Coleman, Larkin, PRL' 89

MC: Ising transition for classical spins

C. Weber, L. Capriotti, G. Misguich, F. Becca, M. Elhajal, FM, PRL' 03

Thermal fluctuations

$$\vec{S}_i = \left(x_i, y_i, \sqrt{1 - x_i^2 - y_i^2} \right)$$

$$F = F_0 - \frac{1}{2} N_h T \ln T + T \sum_{\vec{k}} \ln \omega_{\vec{k}}$$

In general, minimize $\sum_{\vec{k}} \ln \omega_{\vec{k}}$

Exception: zero (harmonic) modes

$$F = F_0 - \frac{1}{2} N_h T \ln T - \frac{1}{4} N_q T \ln T + \dots$$

Selection of the state(s) with maximal number of zero modes

Spin liquids

- Quantum correction to local magnetization

$$\delta_m \equiv S - \langle S_i^z \rangle = \frac{1}{N} \sum_{\vec{k}} \langle a_{\vec{k}}^\dagger a_{\vec{k}} \rangle$$

$$\langle a_{\vec{k}}^\dagger a_{\vec{k}} \rangle = v_{\vec{k}}^2 \propto 1/\omega_{\vec{k}}$$

- Frustration
  → soft spectrum
  → strong (often diverging) correction
  → no magnetic long-range order

Spin gap

J_1-J_2 chain

$$\mathcal{H}_{J_1-J_2} = \sum_i (J_1 \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \vec{S}_i \cdot \vec{S}_{i+2})$$

Majumdar-Ghosh point: $J_2/J_1 = 1/2$

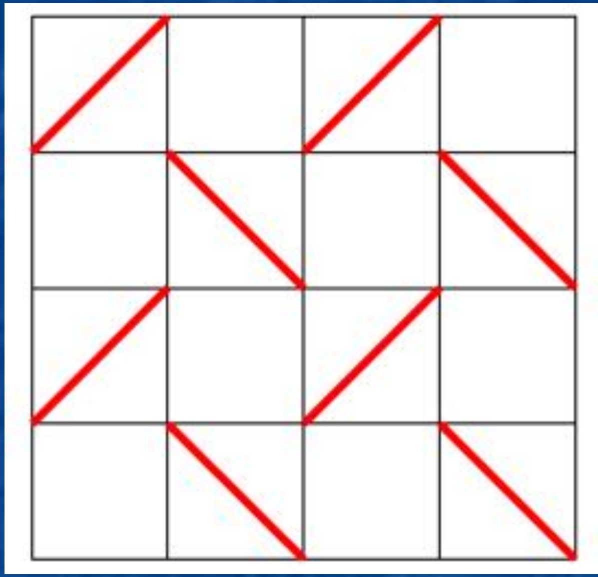
2 exactly dimerized ground states

$$|\psi_{\text{even}}\rangle = \prod_{i \text{ even}} |S(i, i+1)\rangle$$

$$|\psi_{\text{odd}}\rangle = \prod_{i \text{ odd}} |S(i, i+1)\rangle$$

$$|S(i, i+1)\rangle = \text{singlet}$$

Shastry-Sutherland



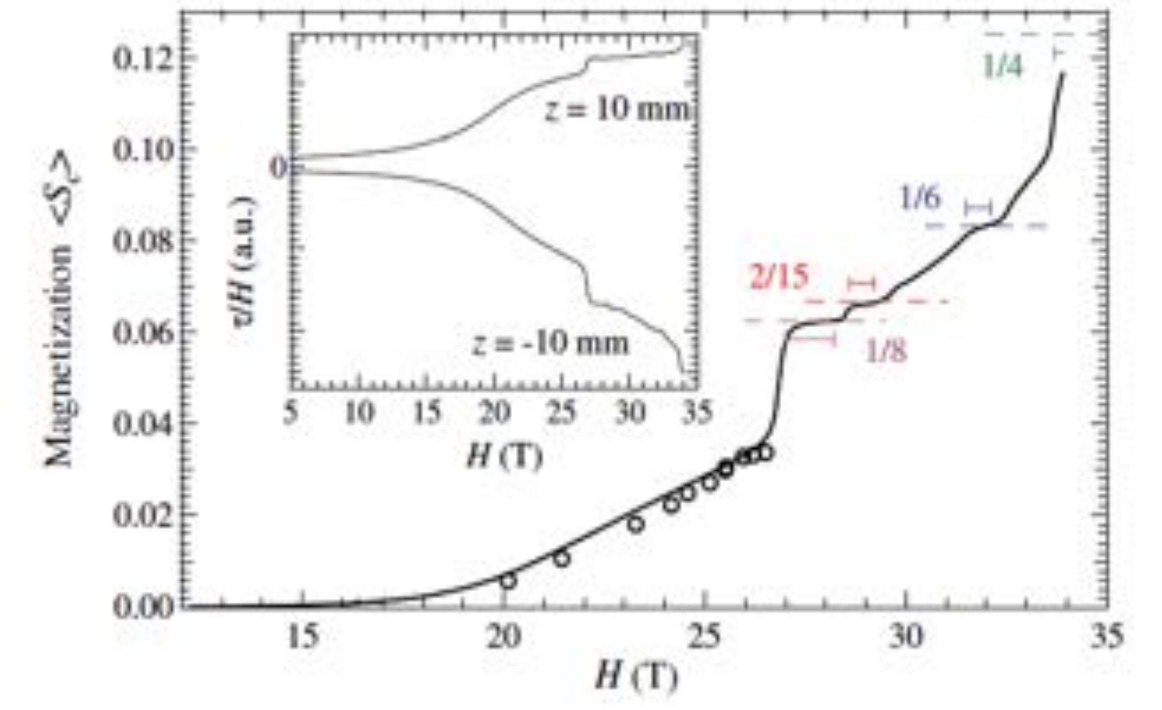
Product of singlets on red bonds:
→ always an eigenstate
→ GS if inter-dimer coupling not too large

- Spin gap
- Magnetization plateaux

PRL 110, 067210 (2013) PHYSICAL REVIEW LETTERS week ending 8 FEBRUARY 2013

Incomplete Devil's Staircase in the Magnetization Curve of $SrCu_2(BO_3)_2$

M. Takigawa,[1,*] M. Horvatić,[2] T. Waki,[3] S. Krämer,[2] C. Berthier,[2] F. Lévy-Bertrand,[2,†] I. Sheikin,[2] H. Kageyama,[4] Y. Ueda,[1] and F. Mila[5]

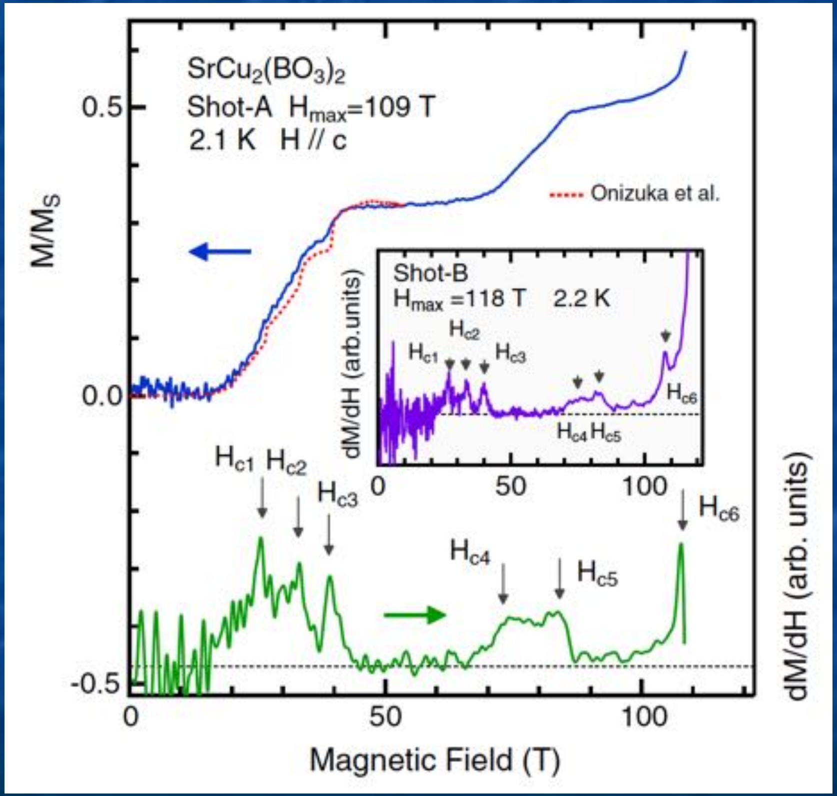


1/8, 2/15, 1/6, 1/4,...

PRL 111, 137204 (2013) PHYSICAL REVIEW LETTERS week ending 27 SEPTEMBER 2013

Magnetization of $SrCu_2(BO_3)_2$ in Ultrahigh Magnetic Fields up to 118 T

Y. H. Matsuda,[1,*] N. Abe,[1] S. Takeyama,[1] H. Kageyama,[2] P. Corboz,[3] A. Honecker,[4,5] S. R. Manmana,[4]
G. R. Foltin,[6] K. P. Schmidt,[6] and F. Mila[7]

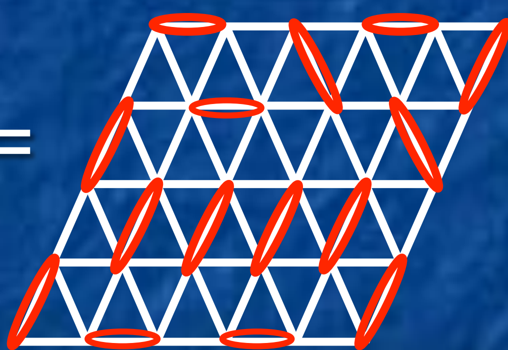
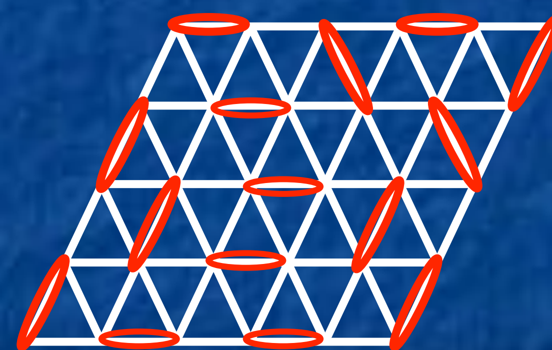


…1/3, 1/2

RVB spin liquids

- Anderson, 1973: restore translational symmetry by a superposition of dimer coverings

→ Resonating Valence Bond spin liquid

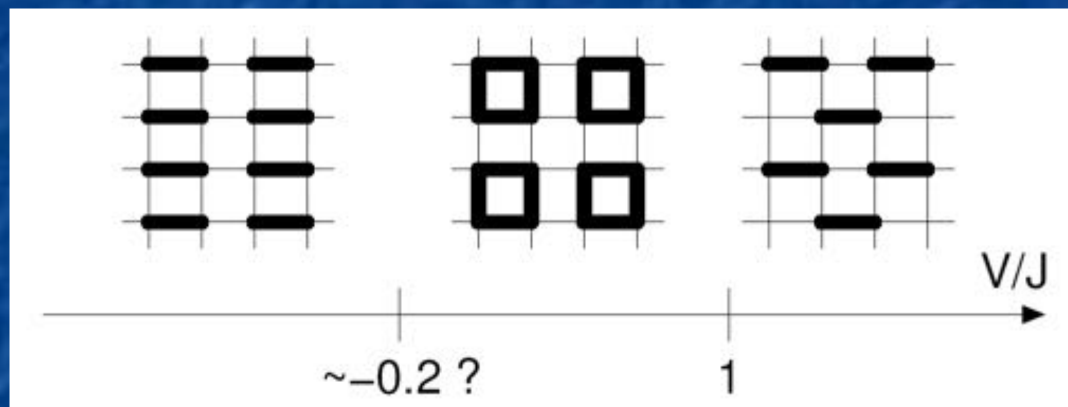
| GS > =  +  + …

Not realized on triangular lattice (3-sublattice LRO)

Quantum dimer model

$$\mathcal{H} = \sum_{\text{Plaquette}} \left[-J \left(|\,\|\,\rangle \langle\,=\,| + \text{H.c.} \right) + V \left(|\,\|\,\rangle \langle\,\|\,| + |\,=\,\rangle \langle\,=\,| \right) \right]$$

Rokhsar-Kivelson 1988



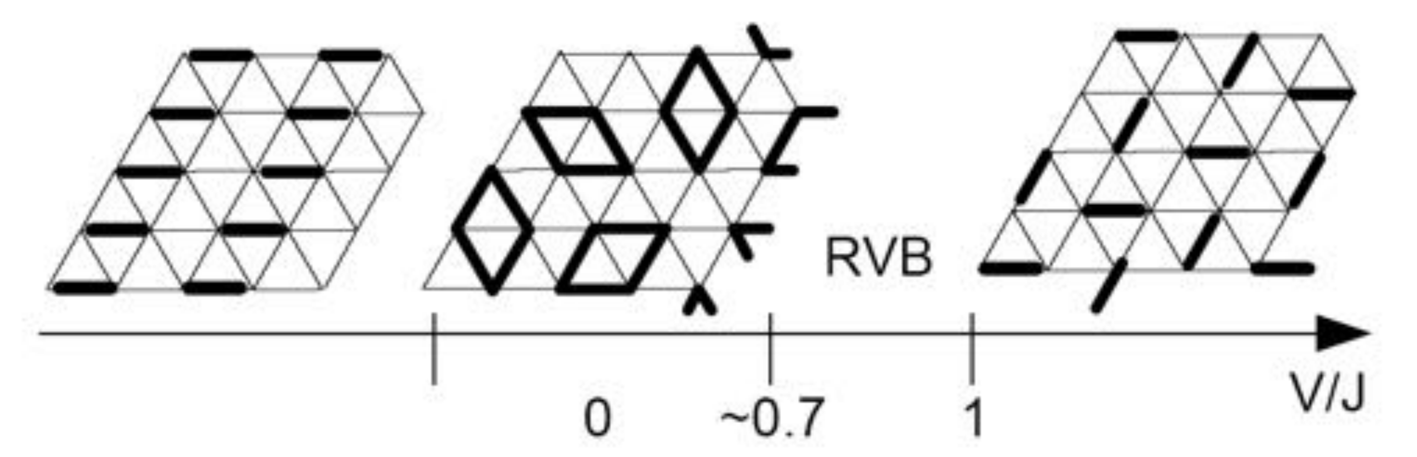
RK point: V/J=1 → GS = sum of all configurations

Correlations: algebraic (Kasteleyn matrix gapless)

→ Isolated point, no RVB phase

QDM on triangular lattice

Moessner and Sondhi, PRL 2001



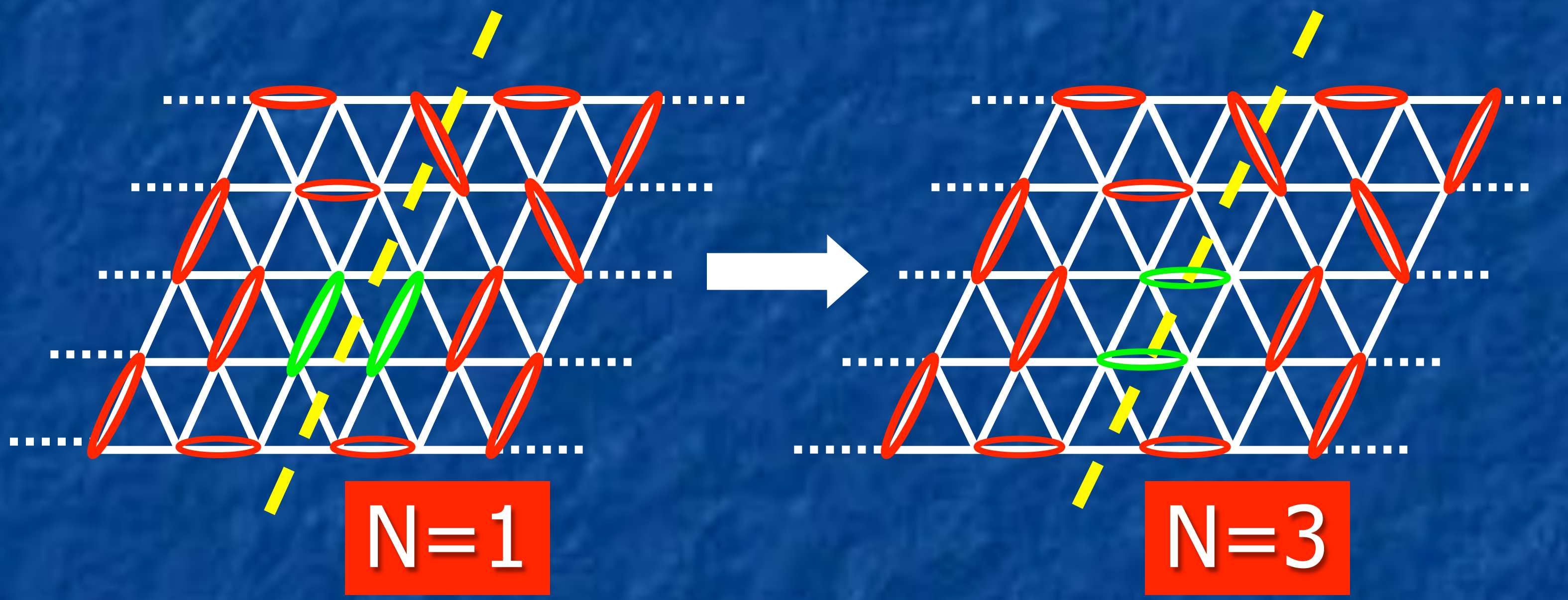
RK point V/J=1 → Kasteleyn matrix gapped

→ exponentially decaying correlations

→ RVB phase

Topological sectors

Number of dimers cutting a given line



Parity conserved → 2 topological sectors (N even or N odd)

Torus: four topological sectors (two cuts)

Numerical proof: Ralko, Ferrero, Becca, Ivanov, FM (2005)

RVB phase in Heisenberg model?

- Spin-1/2 kagome antiferromagnet
  → DMRG simulations
    Han, Huse, White, 2011
  → Effective QDM
    Rousochatzakis, Wan, Tchernyshov, FM, 2014
- Experimental realization?
  → Problematic (residual interactions, DM,…)

Algebraic spin liquids

- Spin-1/2 chain: algebraic correlations (Bethe ansatz, bosonisation)
- Extension in 2D?

$$\begin{cases} S_i^+ = c_{i\uparrow}^\dagger c_{i\downarrow} \\ S_i^- = c_{i\downarrow}^\dagger c_{i\uparrow} \\ S_i^z = \frac{1}{2}\left(n_{i\uparrow} - n_{i\downarrow}\right) \end{cases}$$

Abrikosov fermions

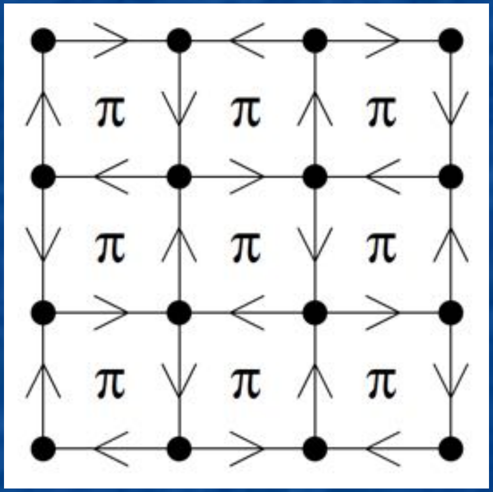
$$H = \frac{1}{2}\sum_{i,j} J_{ij}\left[\frac{1}{2}\left(c_{i\uparrow}^\dagger c_{i\downarrow} c_{j\downarrow}^\dagger c_{j\uparrow} + \mathrm{h.c.}\right) + \frac{1}{4}\left(c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}\right)\left(c_{j\uparrow}^\dagger c_{j\uparrow} - c_{j\downarrow}^\dagger c_{j\downarrow}\right)\right]$$

Mean-field decoupling

$$\chi_{ij} = c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow}$$

$$\chi^0_{ij} = \chi_0 e^{i\theta_{ij}}$$

$$\theta_{ij} = \pi/4$$



Affleck-Marston 1988

$$E = \pm J \chi_0 \sqrt{\cos^2 k_x + \cos^2 k_y}$$

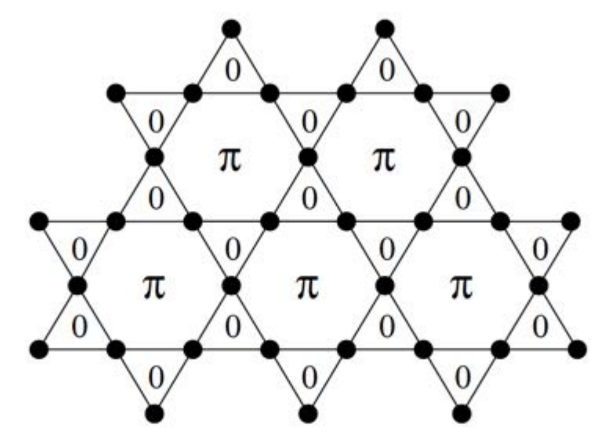
Dirac points

$$k_x, k_y = \pm\pi/2$$

→ Algebraic correlations

Variational approach

- Gutzwiller projection: $P_G = \prod_i (1 - n_{i\uparrow} n_{i|\downarrow})$
- Variational wave-functions: $P_G|\psi_{\text{fermion}}\rangle$



Good variational energy for spin-1/2 kagome

Ran, Hermele, Lee, Wen, 2007

Chiral spin liquids

- The order parameter breaks P and T, but not PT
- Example: $\vec{S}_1.(\vec{S}_2 \times \vec{S}_3)$
- Simple approach: Gutzwiller projected wave functions with fractional fluxes
- Best candidate: a small parameter range in the J_1-J_2-J_3 model on kagome

Gong, Zhu, Sheng 2014

Nematic order

- Order parameter: 2-spin operator
- p-nematic: $\vec{S}_i \times \vec{S}_j$
- n-nematic: rank-2 tensor with 5 components

$$\vec{Q}_{ij} = \begin{pmatrix} S_i^x S_j^x - S_i^y S_j^y \\ \frac{1}{\sqrt{3}}\left(3 S_i^z S_j^z - \vec{S}_i \cdot \vec{S}_j\right) \\ S_i^x S_j^y + S_i^y S_j^x \\ S_i^y S_j^z + S_i^z S_j^y \\ S_i^z S_j^x + S_i^y S_j^z \end{pmatrix}$$

Simple example: S=1

Consider $|S^z = 0\rangle$

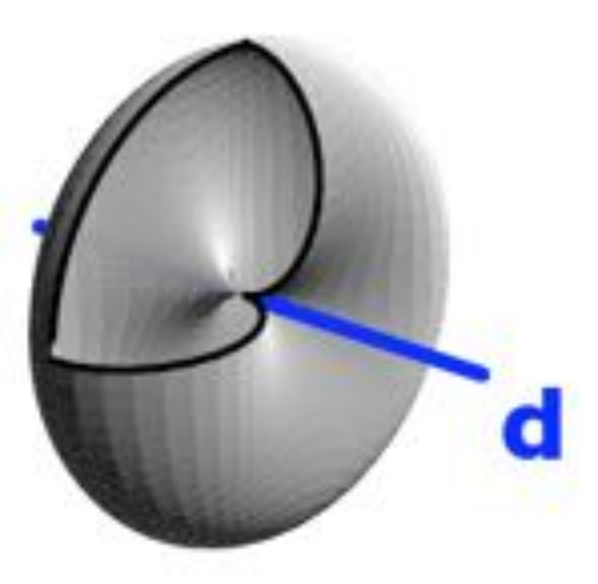
$$\langle S^\alpha \rangle = 0 \qquad \langle (S^z)^2 \rangle = 0 \qquad \langle (S^{x,y})^2 \rangle \neq 0$$

True for any α → Not magnetic

Broken SU(2) symmetry

Quadrupole states and directors

$$|Q(\zeta,\phi)\rangle = i\frac{\sin\zeta}{\sqrt{2}}\left(e^{-i\phi}|1\rangle - e^{i\phi}|\bar{1}\rangle\right) - i\cos\zeta|0\rangle$$



Rotation of | S_z=0>

$$\mathbf{d} = (\sin\zeta\cos\phi, \sin\zeta\sin\phi, \cos\zeta)$$

« director »

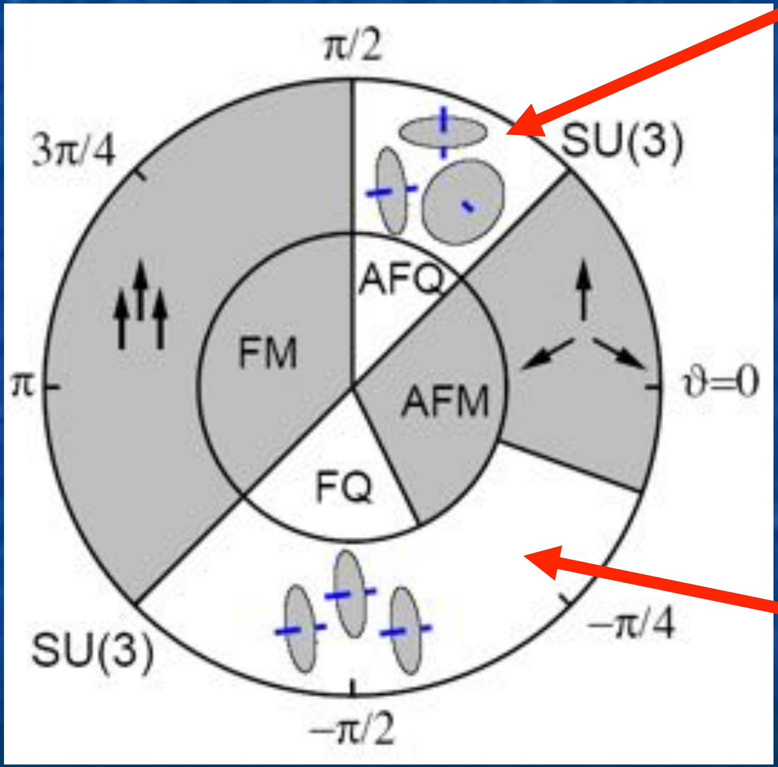
S=1 with biquadratic interaction

$$\mathcal{H} = J \sum_{i,j} \left[\cos\vartheta \mathbf{S}_i \mathbf{S}_j + \sin\vartheta \left(\mathbf{S}_i \mathbf{S}_j\right)^2 \right] - h \sum_i S_i^z$$

$$\hat{\mathbf{Q}}_i = \begin{pmatrix} \hat{Q}_i^{x^2-y^2} \\ \hat{Q}_i^{3z^2-r^2} \\ \hat{Q}_i^{xy} \\ \hat{Q}_i^{yz} \\ \hat{Q}_i^{xz} \end{pmatrix} = \begin{pmatrix} (S_i^x)^2 - (S_i^y)^2 \\ \frac{1}{\sqrt{3}} \left[2(S_i^z)^2 - (S_i^x)^2 - (S_i^y)^2\right] \\ S_i^x S_i^y + S_i^y S_i^x \\ S_i^y S_i^z + S_i^z S_i^y \\ S_i^x S_i^z + S_i^z S_i^x \end{pmatrix}$$

$$\hat{\mathbf{Q}}_i \hat{\mathbf{Q}}_j = 2\left(\hat{\mathbf{S}}_i \hat{\mathbf{S}}_j\right)^2 + \hat{\mathbf{S}}_i \hat{\mathbf{S}}_j - 8/3$$

S=1 on triangular lattice



A. Läuchli, FM, K. Penc, PRL (2006)

Antiferroquadrupolar

Directors mutually perpendicular on 3 sublattices

(see also Tsunetsugu-Arikawa, '06)

Ferroquadrupolar

Parallel directors

Conclusions

- A lot of exotic phases have been predicted
- Only a few of them have been found in realistic models or in actual compounds

  → room for important discoveries

Further reading:

Introduction to Frustrated Magnetism
Eds C. Lacroix, P. Mendels, and F. Mila
(Springer, New York, 2011).