# Frustrated spin systems

F. Mila Ecole Polytechnique Fédérale de Lausanne Switzerland

### Scope

Competing interactions and degeneracy Classical ground-state correlations Order by disorder Spin liquids  $\rightarrow$  RVB spin liquids  $\rightarrow$  Algebraic spin liquids  $\rightarrow$  Chiral spin liquids  $\rightarrow$  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

#### Antiferromagnetic coupling + odd loops

Frustrated

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

### 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



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

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

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

# Spin Ice

Dy<sub>2</sub>Ti<sub>2</sub>O<sub>6</sub>, Ho<sub>2</sub>Ti<sub>2</sub>O<sub>6</sub>
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**



'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 $J_{ii}$



Triangular lattice: 3-sublattice order

Sum of spins = 0 on each triangle

#### Infinite degeneracy

#### J<sub>1</sub>-J<sub>2</sub> model on square lattice



Classical energy independent of θ



■ 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)

$$F\left(\{h(\vec{x})\}\right) = \int \mathrm{d}\vec{x} \frac{K}{2} \left|\vec{\nabla}h(\vec{x})\right|^2 \quad \left\langle\sigma(\vec{r})\sigma(\vec{0})\right\rangle \propto \left(\frac{\pi r}{a}\right)^{-\frac{2\pi}{36K}}$$

Consistent with  $1/r^{1/2}$  if

$$K = \pi/9$$

Rough phase

### Pyrochlore Ising AF

2 up – 2 down on each tetrahedron
Continuum limit: magnetic field div *B* = 0

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

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

**Dipolar correlations** 

### Pinch points in Ho<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>



#### Experiment



T. Fennel et al, 2009

### Effects of quantum fluctuations

Lifting of degeneracy:  $\rightarrow$  Order by disorder Large (often divergent) fluctuations:  $\rightarrow$  No long-range order What then?  $\rightarrow$  Spin gap and short-range correlations  $\rightarrow$  Algebraic order and fractional excitations  $\rightarrow$  Variations around these themes: RVB liquid, chiral spin liquid, nematic order

### Quantum fluctuations

#### Holstein-Primakoff

$$\left\{ \begin{array}{l} S_i^{z_i} = S - a_i^{\dagger} a_i \\ S_i^+ = \sqrt{2S - a_i^{\dagger} a_i} \; a_i \\ S_i^- = a_i^{\dagger} \sqrt{2S - a_i^{\dagger} a_i} \end{array} \right.$$

#### 1/S expansion + Fourier transform

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

### Zero-point energy

#### **Bogoliubov rotation**

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

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

#### Zero-point energy

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

### Order by disorder



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

**Chris Henley** 





### Local fluctuations

#### 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

### Gapped systems

Exponential decay of correlations

 Correlation length ξ
 The system is effectively of finite size
 'Finite-size' gap
 Start from a product of quantum eigenstates on small clusters, e.g. dimer singlets

$$|\psi\rangle = \prod_{(i,j)} \frac{|\uparrow_i \downarrow_j - \downarrow_i \uparrow_j\rangle}{\sqrt{2}}$$

### Example: spin-1/2 ladders



 $GS \approx product of singlets on rungs$ 

$$|\psi\rangle = \prod_{(i,j)} \frac{|\uparrow_i \downarrow_j - \downarrow_i \uparrow_j\rangle}{\sqrt{2}}$$

Unique ground state for J'=0 $\rightarrow$  non-degenerate perturbation theory in J'/J

### Excitations in spin-1/2 ladders

Triplet on rung *i* 

Singlet on rung j

$$|\psi_i\rangle = T(i)\prod_{j\neq i} S(j)$$

J'=0: all states degenerate with energy J
 → degenerate perturbation theory in J'/J
 → triplet hopping
 → gap Δ = J − O(J')
 Field theory: Δ > 0 even if J'/J large

#### Frustrated spin-1/2 J<sub>1</sub>-J<sub>2</sub> chain

 $J_1 - J_2$  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

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

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

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

### 2D analog: Shastry-Sutherland



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

Spin gapMagnetization plateaux

#### Algebraic spin liquids

 Spin-1/2 chain: gapless, 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

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

#### Mean-field theory on square lattice

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

$$\chi_{ij}^0 = \chi_0 e^{i\theta_{ij}} \qquad \theta_{ij} = \pi/4$$

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



#### Affleck-Marston 1988



#### Dirac points → Algebraic correlations

#### Gutzwiller projection

Mean-field → unphysical wave-function (large deviations from 1 fermion/site)
 Apply Gutzwiller projection

$$P_G = \prod_i (1 - n_{i\uparrow} n_{i|\downarrow})$$

→ physical wave function
 ■ Evaluation of physical properties: Monte Carlo simulations

#### Variational approach

Basic idea: why to start from MF solution?
 Variational wave-functions: apply Gutzwiller projection on the ground state of a family of Hamiltonians

 $\rightarrow$  Variational Monte Carlo (VMC)



 → Good variational energy for spin-1/2 kagome
 → Algebraic spin liquid
 Ran, Hermele, Lee, Wen, 2007

### Excitations in algebraic liquid

No long-range order

 > no gapless spin-waves

 Algebraic correlations

 > gapless spectrum

 Nature of low-lying excitations?

 > fractional excitations

# Example: spinons in 1D S=1



#### **Excitation spectrum**



A spin-1 excitation = 2 spinons → continuum

Early theory Des Cloiseaux – Pearson PRB '62

Stone et al, PRL '03

### 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<sub>1</sub>-J<sub>2</sub>-J<sub>3</sub> model on kagome Gong, Zhu, Sheng 2014

### **RVB** spin liquids

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

 $\rightarrow$  Resonating Valence Bond spin liquid





Not realized on triangular lattice (3-sublattice LRO)

### Quantum dimer model

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

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  $\rightarrow$  DMRG simulations Han, Huse, White, 2011  $\rightarrow$  Effective QDM Rousochatzakis, Wan, Tchernyshov, FM, 2014 More recent results  $\rightarrow$  Algebraic spin liquid (see other talks)

#### Nematic order

#### Order parameter: 2-spin operator

**p**-nematic:  $\vec{S}_i \times \vec{S}_j$ 



#### n-nematic: rank-2 tensor with 5 components

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

#### Simple example: S=1

 $Consider \qquad |S^z = 0\rangle$ 

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

True for any  $\alpha$  Broken SU(2) symmetry

#### Not magnetic

### Quadrupole states and directors

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



Rotation of  $|S_z=0>$ 

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

« director »

### S=1 with biquadratic interaction

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

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

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

### 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

#### Nematic state in spin-1/2 systems

Basic idea: ferromagnetic n.n. coupling

 → effective spin-1 on a bond

 J<sub>1</sub>-J<sub>2</sub> model on chain and square lattice with J<sub>1</sub><0</li>
 J<sub>1</sub>-J<sub>2</sub> chain with J<sub>1</sub><0 just below saturation
 <ul>
 → Antiferroquadrupolar

Zhitormirsky and Tsunetsugu EPL 2010



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#### G

#### Nuclear Magnetic Resonance Signature of the Spin-Nematic Phase in LiCuVO<sub>4</sub> at High Magnetic Fields

A. Orlova,<sup>1,\*</sup> E. L. Green,<sup>2,†</sup> J. M. Law,<sup>2,‡</sup> D. I. Gorbunov,<sup>2</sup> G. Chanda,<sup>2</sup> S. Krämer,<sup>1</sup> M. Horvatić,<sup>1</sup> R. K. Kremer,<sup>3</sup> J. Wosnitza,<sup>2,4</sup> and G. L. J. A. Rikken<sup>1</sup>



#### Conclusions

A lot of exotic quantum 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).