Introduction au magnétisme

F. Mila
Institute of Theoretical Physics
Ecole Polytechnique Fédérale de Lausanne

Plan du cours

1) Modèles de base
   - Ising
   - Heisenberg
2) Modèle de Heisenberg et ordre magnétique
   - Structures hélicoïdales
   - Ondes de spin
3) Dimensionnalité réduite et fluctuations quantiques
   - Gap de spin
   - Ordre algébrique

Plan du cours (suite)

4) Modèle d'Ising et frustration géométrique
- Entropie résiduelle
- Corrélations algébriques et dipolaires

5) Liquides de spin quantiques
- Frustration, modes mous et fluctuations quantiques
- Liquide RVB et modèles de dimères quantiques
- Liquide de spin algébrique

Plan du cours

1) Modèles de base
   - Ising
   - Heisenberg
2) Modèle de Heisenberg et ordre magnétique
   - Structures hélicoïdales
   - Ondes de spin
3) Dimensionnalité réduite et fluctuations quantiques
   - Gap de spin
   - Ordre algébrique

Basic Models

Heisenberg
$$\mathcal{H} = \sum_{i,j} J_{ij}\vec{S}_i \cdot \vec{S}_j - g\mu_B H \sum_i S_i^z$$

Classical $\vec{S}_i \in R^3$ Quantum $[S_i^x, S_i^y] = iS_i^z$ $\vec{S}_i^2 = S(S+1)$

XXZ
$$\mathcal{H} = \sum_{i,j}[J_{ij}^{xy}(S_i^x S_j^x + S_i^y S_j^y) + J_{ij}^z S_i^z S_j^z] - g\mu_B \vec{H} \cdot \sum_i \vec{S}_i$$

Transverse field Ising model
$$\mathcal{H} = \sum_{i,j} J_{ij} S_i^z S_j^z - H \sum_i S_i^x$$

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

Plan du cours

1) Modèles de base
   - Ising
   - Heisenberg
2) Modèle de Heisenberg et ordre magnétique
   - Structures hélicoïdales
   - Ondes de spin
3) Dimensionnalité réduite et fluctuations quantiques
   - Gap de spin
   - Ordre algébrique

Magnetic long-range order

$$H = \sum_{\vec{r}_i, \vec{r}_j} J_{\vec{r}_j - \vec{r}_i} \vec{S}_i . \vec{S}_j, \quad \vec{r}_i \in \text{Bravais lattice}$$

$$J_{\vec{k}} = \sum_{\vec{r}} J_{\vec{r}} \; e^{i\vec{k}.\vec{r}} \text{ minimum at } \vec{k} = \vec{Q}$$

Classical GS: helix with pitch vector Q

$$\langle \vec{S}_i . \vec{S}_j \rangle \propto m_{\vec{Q}}^2 \cos[\vec{Q}.(\vec{r}_i - \vec{r}_j)]$$
$$\text{as} \quad |\vec{r}_i - \vec{r}_j| \to \infty$$

Quantum spins: Large S

Fluctuations around classical GS = bosons

Holstein-Primakoff

$$\begin{aligned} S_i^z &= S - a_i^+ a_i \\ S_i^+ &= (2S - a_i^+ a_i)^{1/2}\ a_i \\ S_i^- &= a_i^+ (2S - a_i^+ a_i)^{1/2} \end{aligned}$$

$$[a_i, a_i^+] = 1$$

$$\Downarrow$$

$$[S_i^x, S_i^y] = i S_i^z$$

$$S_i^+ = S_i^x + i S_i^y \qquad S_i^- = S_i^x - i S_i^y$$

I - Local rotation

$$\vec{S}_i = \begin{pmatrix} 0 \\ \sin(\vec{Q}\cdot\vec{R}_i) \\ \cos(\vec{Q}\cdot\vec{R}_i) \end{pmatrix}$$

$$\theta_i = \vec{Q}\cdot\vec{R}_i$$

$$S^u = S^x,\; S^v = \cos\theta_i S^y - \sin\theta_i S^z \text{ et } S^w = \sin\theta_i S^y + \cos\theta_i S^z$$

$$\begin{aligned} H &= \frac{1}{2}\sum_i \sum_{\vec{R}_n} J_{\vec{R}_n} \vec{S}_i \cdot \vec{S}_{i+\vec{R}_n} \\ &= \frac{1}{2}\sum_i \sum_{\vec{R}_n} J_{\vec{R}_n} \left[S_i^u S_{i+n}^u + \cos(\theta_i - \theta_{i+n}) \left(S_i^v S_{i+n}^v + S_i^w S_{i+n}^w \right) \right. \\ &\left. + \sin(\theta_i - \theta_{i+n}) \left(S_i^w S_{i+n}^v - S_i^v S_{i+n}^w \right) \right] \end{aligned}$$

II – Terms of order S^2 and S

$$\begin{aligned} S_i^w &= S - a_i^+ a_i \\ S_i^+ &\equiv S_i^u + i S_i^v \simeq \sqrt{2S} a_i \\ S_i^- &\equiv S_i^u - i S_i^v \simeq \sqrt{2S} a_i^+ \end{aligned}$$

$$\begin{aligned} H &= \frac{1}{2} \sum_i \sum_{\vec{R}_n} J_{\vec{R}_n} [\frac{S}{2}(a_i a_{i+n} + a_i^+ a_{i+n}^+)(1 - \cos(\theta_i - \theta_{i+n})) \\ &+ \frac{S}{2}(a_i^+ a_{i+n} + a_{i+n}^+ a_i)(1 + \cos(\theta_i - \theta_{i+n})) \\ &+ [S^2 - S(a_i^+ a_i + a_{i+n}^+ a_{i+n})] \cos(\theta_i - \theta_{i+n}) \end{aligned}$$

III – Fourier transformation

$$J_{\vec{R}_n} = \frac{1}{N}\sum_{\vec{k}} J_{\vec{k}} e^{i\vec{k}\cdot\vec{R}_n} \quad , \quad a_i = \frac{1}{\sqrt{N}}\sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}_i} a_{\vec{k}} \quad , \quad a_i^+ = \frac{1}{\sqrt{N}}\sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}_i} a_{\vec{k}}^+$$

$$\begin{aligned} H &= \frac{NS^2}{2} J_{\vec{Q}} + \frac{S}{2}\sum_{\vec{k}} \left[J_{\vec{k}} + \frac{1}{2}\left(J_{\vec{k}+\vec{Q}} + J_{\vec{k}-\vec{Q}} \right) - 2J_{\vec{Q}} \right] a_{\vec{k}}^+ a_{\vec{k}} \\ &+ \frac{S}{4}\sum_{\vec{k}} \left[J_{\vec{k}} - \frac{1}{2}\left(J_{\vec{k}+\vec{Q}} + J_{\vec{k}-\vec{Q}} \right) \right] \left(a_{\vec{k}} a_{-\vec{k}} + a_{\vec{k}}^+ a_{-\vec{k}}^+ \right) \end{aligned}$$

IV – Bogoliubov transformation

$$\alpha_k = u_k a_k + v_k a^+_{-k}$$ with u_k and v_k such that

$$H = \sum_k \omega_k \alpha_k^+ \alpha_k + \text{constant}$$

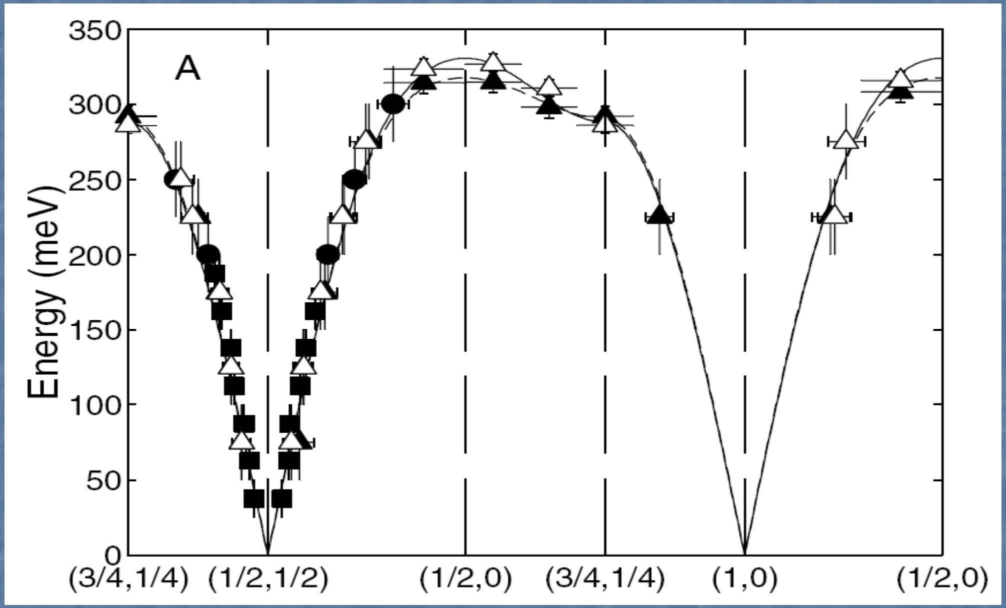
$$\omega_{\vec{k}} = S\sqrt{\left(J_{\vec{k}} - J_{\vec{Q}}\right)\left(\frac{1}{2}\left(J_{\vec{k}+\vec{Q}} + J_{\vec{k}-\vec{Q}}\right) - J_{\vec{Q}}\right)}$$

Goldstone modes

$$\omega_{\vec{k}} = 0 \quad \text{si} \quad \left\{ \begin{array}{c} \vec{k} = 0 \\ \vec{k} = \pm\vec{Q} \end{array} \right.$$

Physical consequences

Inelastic Neutron Scattering → Spin-wave dispersion



La_2CuO_4

(Coldea et al, PRL 2001)

Specific heat: C_v / T^D

Domain of validity

$$\langle S_i^z \rangle = S - \frac{1}{N}\sum_k \langle a_k^+ a_k \rangle > 0$$

Fluctuations around

$$| \, S_i^z = S \rangle$$

Thermal Fluctuations (T>0)

$$< a_{\vec{k}}^+ a_{\vec{k}} > \propto 1/k^2 \text{ for small } k$$

$$\Rightarrow \int < a_{\vec{k}}^+ a_{\vec{k}} > \; \mathrm{d}\vec{k}$$ diverges in 1D and 2D

No LRO at T>0 in 1D and 2D (Mermin-Wagner theorem)

Plan du cours

1) Modèles de base
   - Ising
   - Heisenberg
2) Modèle de Heisenberg et ordre magnétique
   - Structures hélicoïdales
   - Ondes de spin
3) Dimensionnalité réduite et fluctuations quantiques
   - Gap de spin
   - Ordre algébrique

Quantum Fluctuations (T=0)

$$< a_{\vec{k}}^{+} a_{\vec{k}} >= \frac{JSz - \omega_{\vec{k}}}{2\omega_{\vec{k}}} \propto 1/k \text{ for small } k$$

→ $\int < a_{\vec{k}}^{+} a_{\vec{k}} > \, \mathrm{d}\vec{k}$ diverges in 1D

→ No magnetic long-range order in 1D antiferromagnets

Ground-state and excitations in 1D?

Spin gap

$$\int < a_k^{+} a_k > \ \mathrm{d}k$$

infrared singularity

If excitations are spin waves,
there must be a spin gap to produce
an infrared (low-energy) cut-off

First example: spin 1 chain (Haldane, 1983)

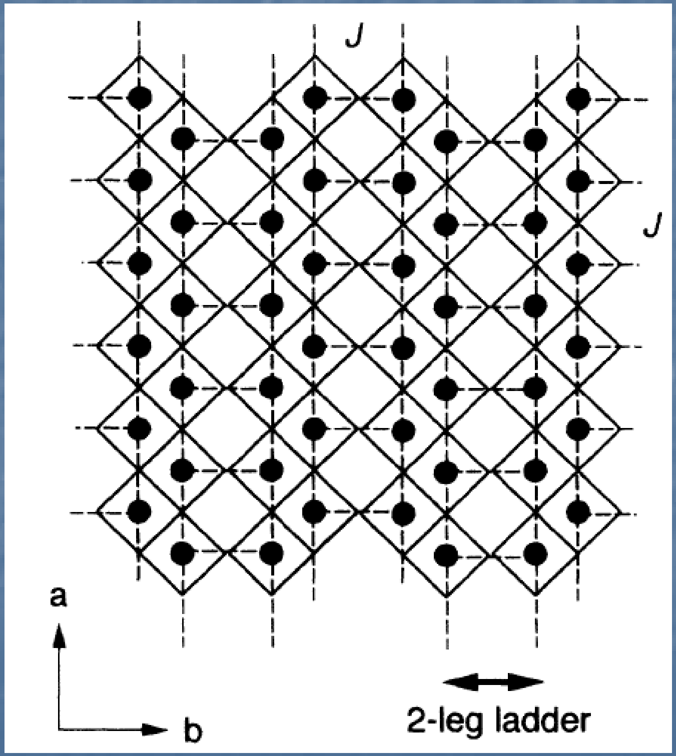
(see below)

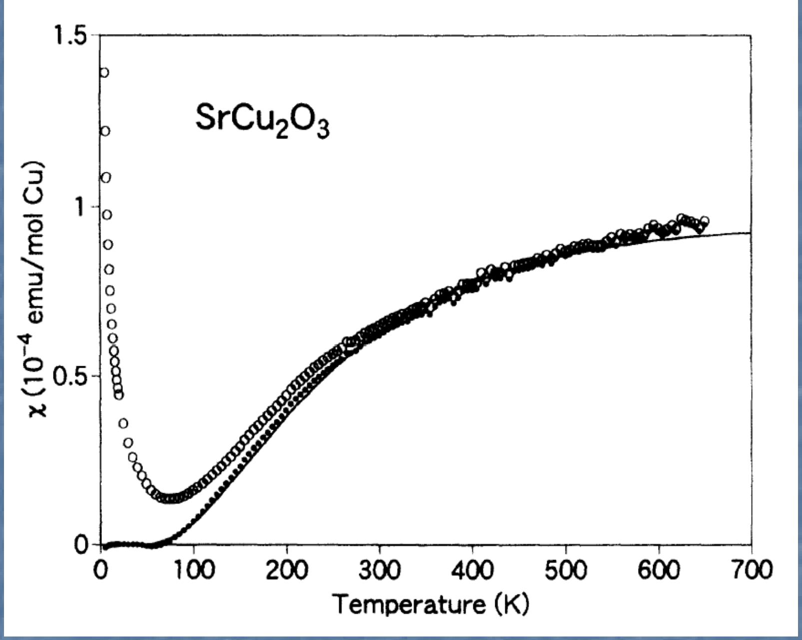
Recent example: spin 1/2 ladders

Spin ladders

(Azuma, PRL ’94)

$SrCu_2O_3$

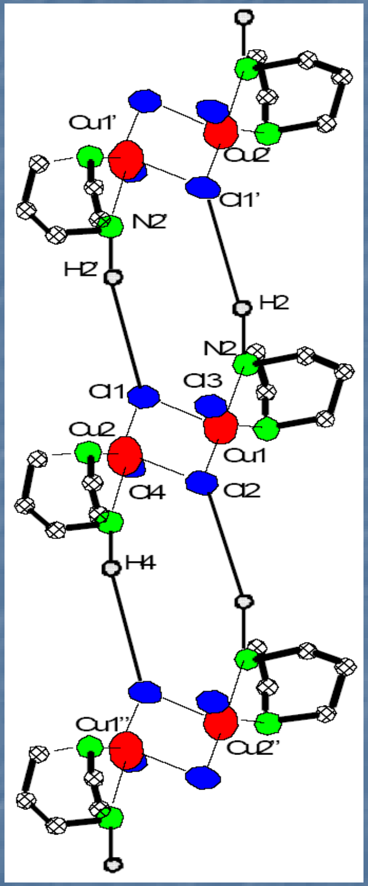




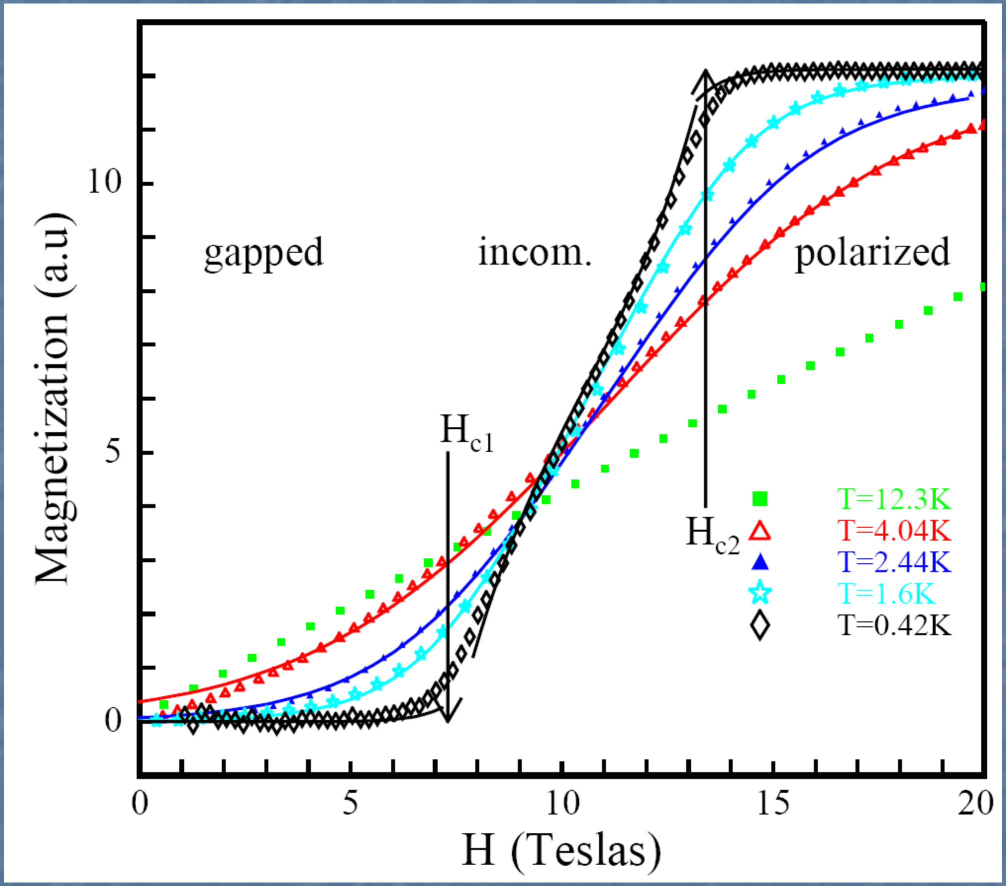
$$\chi(T) = \alpha T^{-1/2} \exp(-\Delta/T)$$

Δ: spin gap

Magnetization of spin ladders



CuHpCl

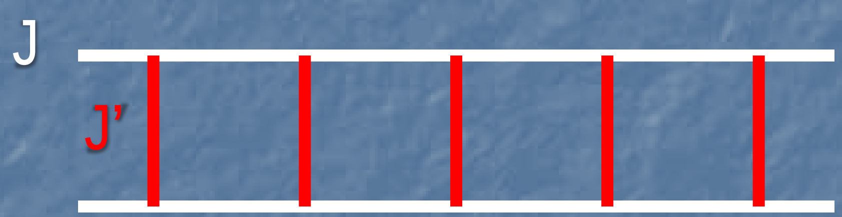


Chaboussant et al, EPJB '98

Origin of spin gap in ladders

Review: Dagotto and Rice , Science '96

Strong coupling



$J=0 \rightarrow \Delta=J'$

$J \ll J' \rightarrow \Delta=J'+O(J)$

Weak coupling

$J' \ll J$ → weakly coupled chains (→ Giamarchi)

Spinons

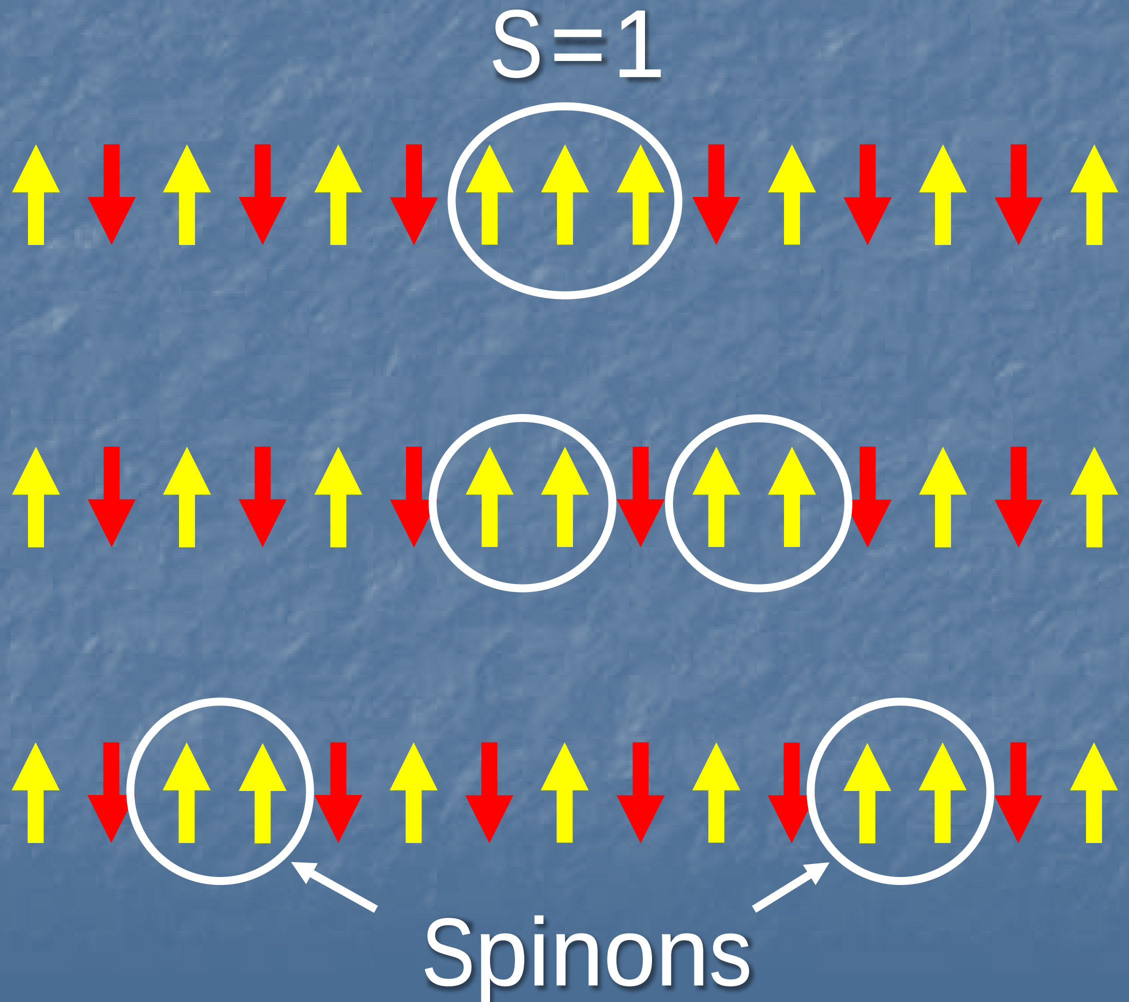
If the spectrum is gapless,
low-lying excitations
cannot be spin-waves

Can the spectrum be gapless in 1D?

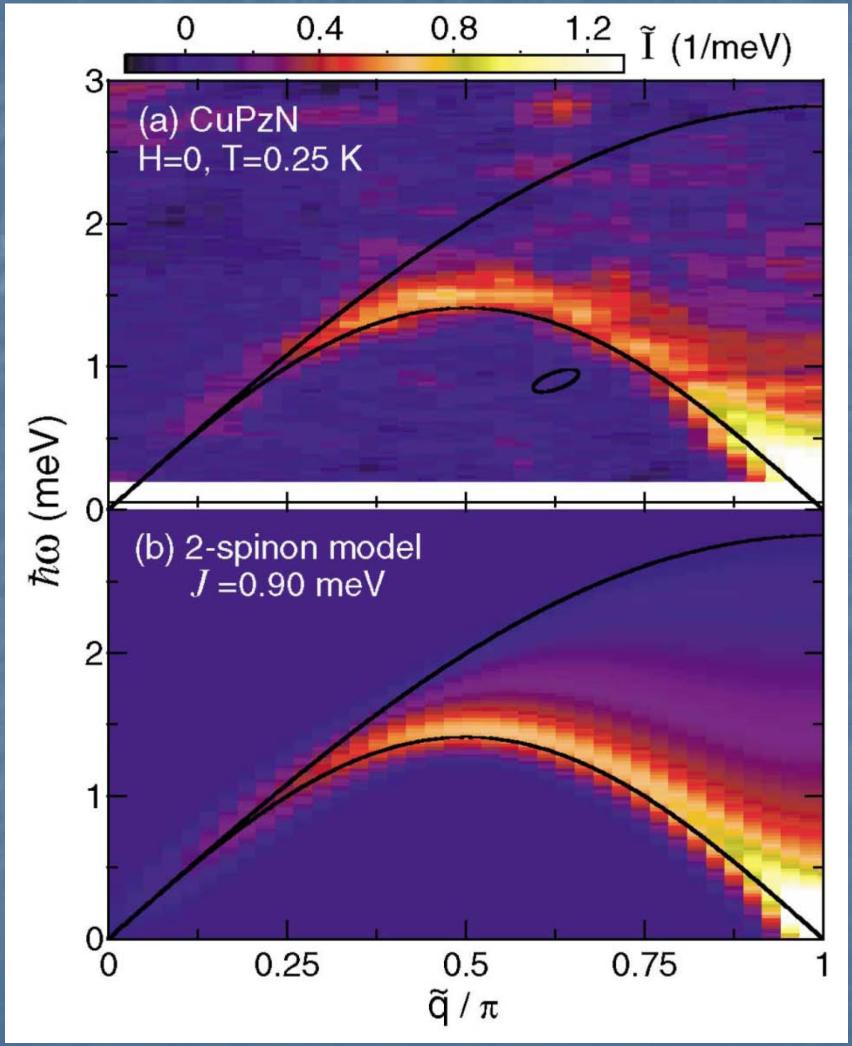
YES!

Example: S=1/2 chain (Bethe, 1931)

Nature of excitations? Spinons!



Excitation spectrum



Stone et al, PRL '03

A spin 1 excitation

= 2 spinons

→ continuum

Early theory

Des Cloiseaux – Pearson

PRB '62

Algebraic correlations

- Jordan-Wigner transformation
  → 1D interacting fermions
- Spin-spin correlation
  → Bosonisation

see Giamarchi's lecture

Unified framework

When to expect spin-waves,
and when to expect spinons?

Haldane, 1983

Integer spins: gapped spin-waves

Half-integer spins: spinons

Field theory approach

Haldane, PRL '88

Path integral formulation

$$\langle \vec{\Omega}_0 \mid \hat{U}(t_1, t_2) \mid \vec{\Omega}_0 \rangle = \int_{\vec{\Omega}(t_1)=\vec{\Omega}(t_2)=\vec{\Omega}_0} D[\vec{\Omega}(t)] e^{iS\omega} e^{-i\int dt H_s(t)/\hbar}$$

Spin coherent state

Evolution operator

Berry phase

$\omega[\vec{\Omega}(t)]$ Solid angle of path (mod 4π)

Field theory approach

In 1D antiferromagnets

$$S\sum_n(-1)^n\omega(x_n) \rightarrow 2\pi S Q_{xt}$$

→ 1 (S integer)

→ ± 1 (S ½-integer)

$$Q_{xy}=(1/4\pi)\int d^2r(\vec{\Omega}.\partial_x\vec{\Omega}\times\partial_y\vec{\Omega})$$

Pontryagin index (integer)

Destructive interferences for ½-integer spins

Plan du cours (suite)

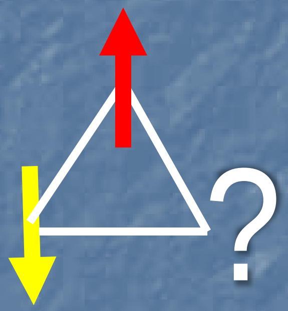
4) Modèle d'Ising et frustration géométrique

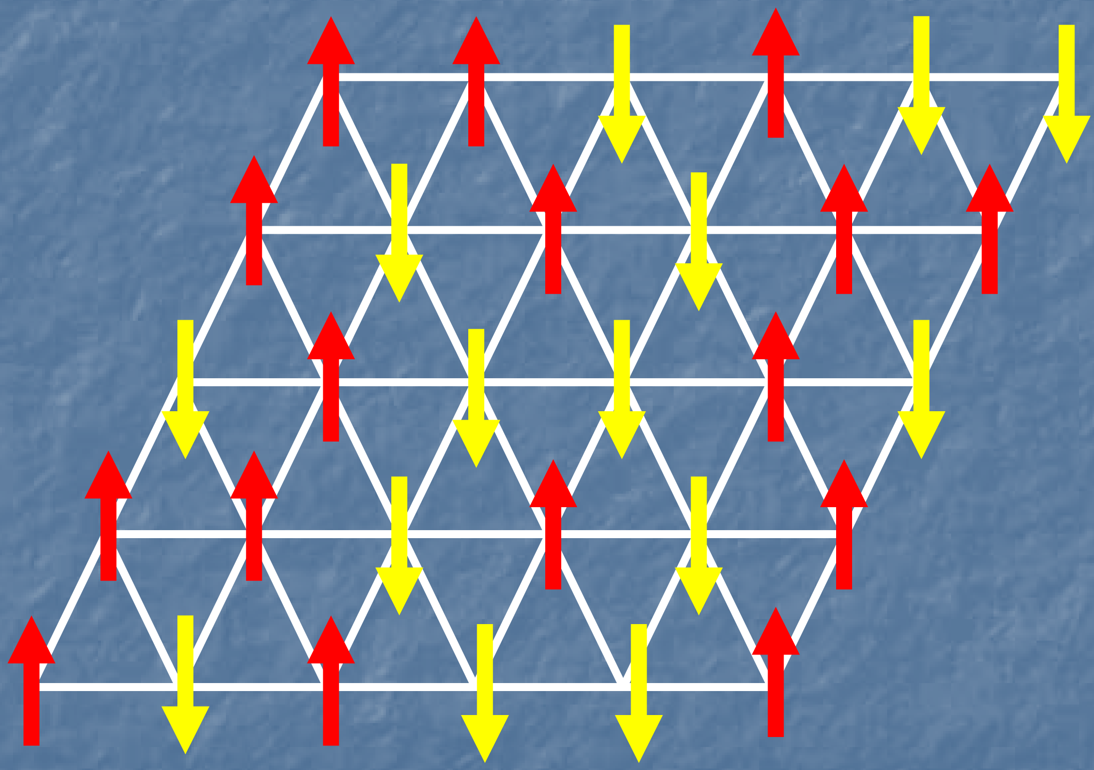
- Entropie résiduelle
- Corrélations algébriques et dipolaires

5) Liquides de spin quantiques

- Frustration, modes mous et fluctuations quantiques
- Liquide RVB et modèles de dimères quantiques
- Liquide de spin algébrique

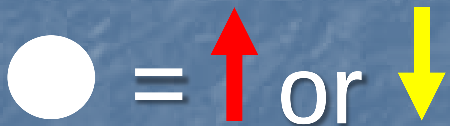
AF Ising model on triangular lattice



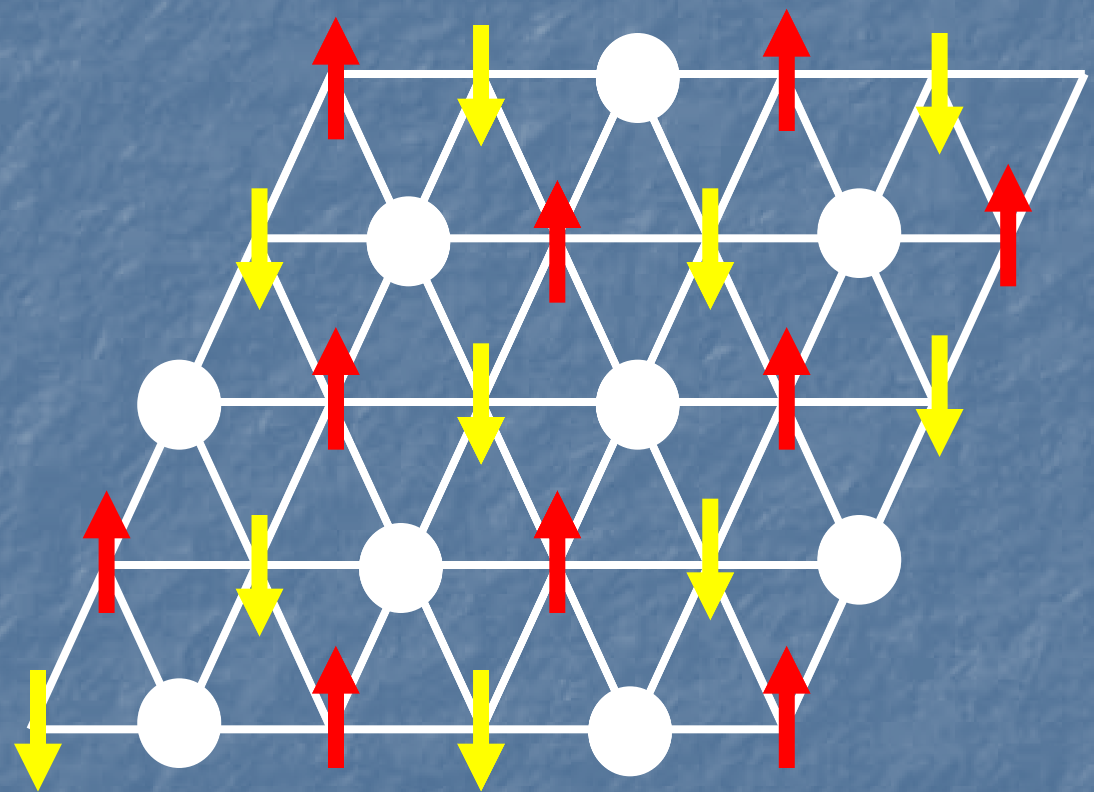


Many different ways of minimizing the energy

Residual entropy



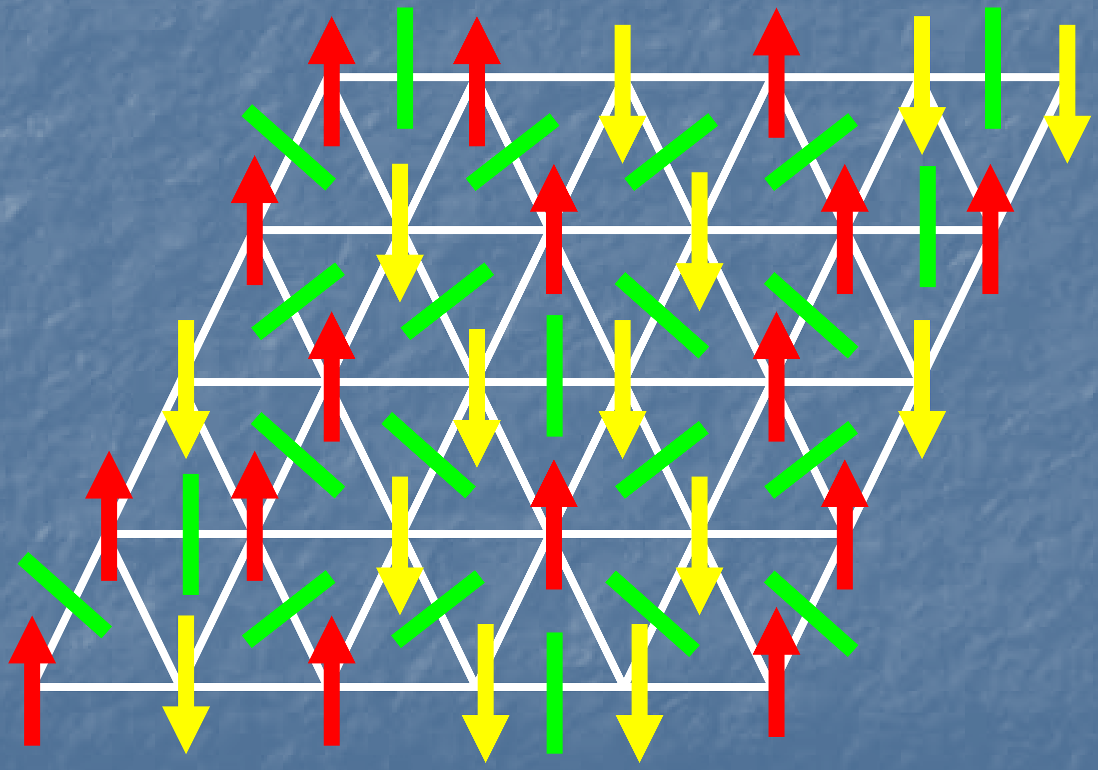
$\Omega = 2^{N/3}$



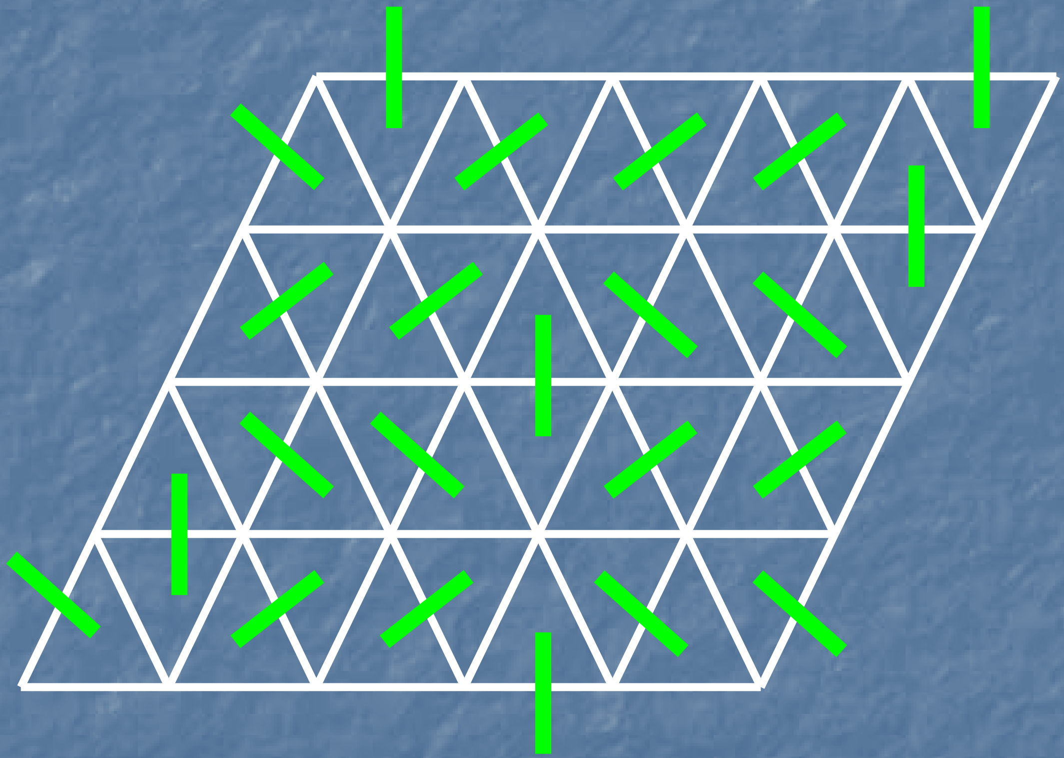
$S > 1/3 \ln 2 = 0.23105...$

Exact entropy?

Mapping onto dimer model - I



Mapping onto dimer model - II



Dimer covering of honeycomb lattice

Counting the dimer coverings

$$Z = \frac{1}{(N/2)!2^{N/2}} \sum_P b(p_1, p_2) b(p_3, p_4) ... b(p_{N-1}, p_N)$$

$$P = \{p_1, ..., p_n\} = \text{permutations of } 1, ..., \text{N}$$

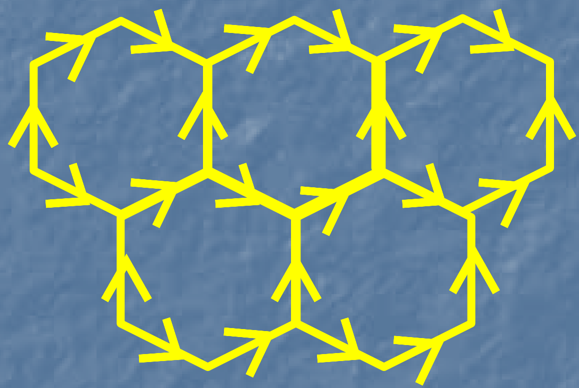
$$b(i, j) = 1 \text{ if } i, j \text{ adjacent}, \ 0 \text{ otherwise}$$

How to calculate it?

Transform it into a determinant!

Kasteleyn's method

Odd number of clockwise arrows in each even loop



$$a(i,j) = 1 \text{ if } i,j \text{ adjacent and } i \rightarrow j$$
$$a(i,j) = -1 \text{ if } i,j \text{ adjacent and } i \leftarrow j$$
$$a(i,j) = 0 \text{ if } i,j \text{ not adjacent}$$

$$Z = \left| \frac{1}{(N/2)!2^{N/2}} \sum_P \epsilon(P) a(p_1,p_2) a(p_3,p_4) \ldots a(p_{N-1},p_N) \right|$$

Z=Pfaffian of a

Calculation of Pfaffian

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

a: periodic, 2 sites per unit cell

det(a)= product on k of eigenvalues of (2x2) Kasteleyn matrix

$$\frac{1}{N_{hc}} \ln Z = \frac{1}{4} \int_0^1 dx \int_0^1 dy \ln |3 + 2\cos 2\pi y - 2\cos 2\pi(x+y) - 2\cos 2\pi x| = 0.161533\ldots$$

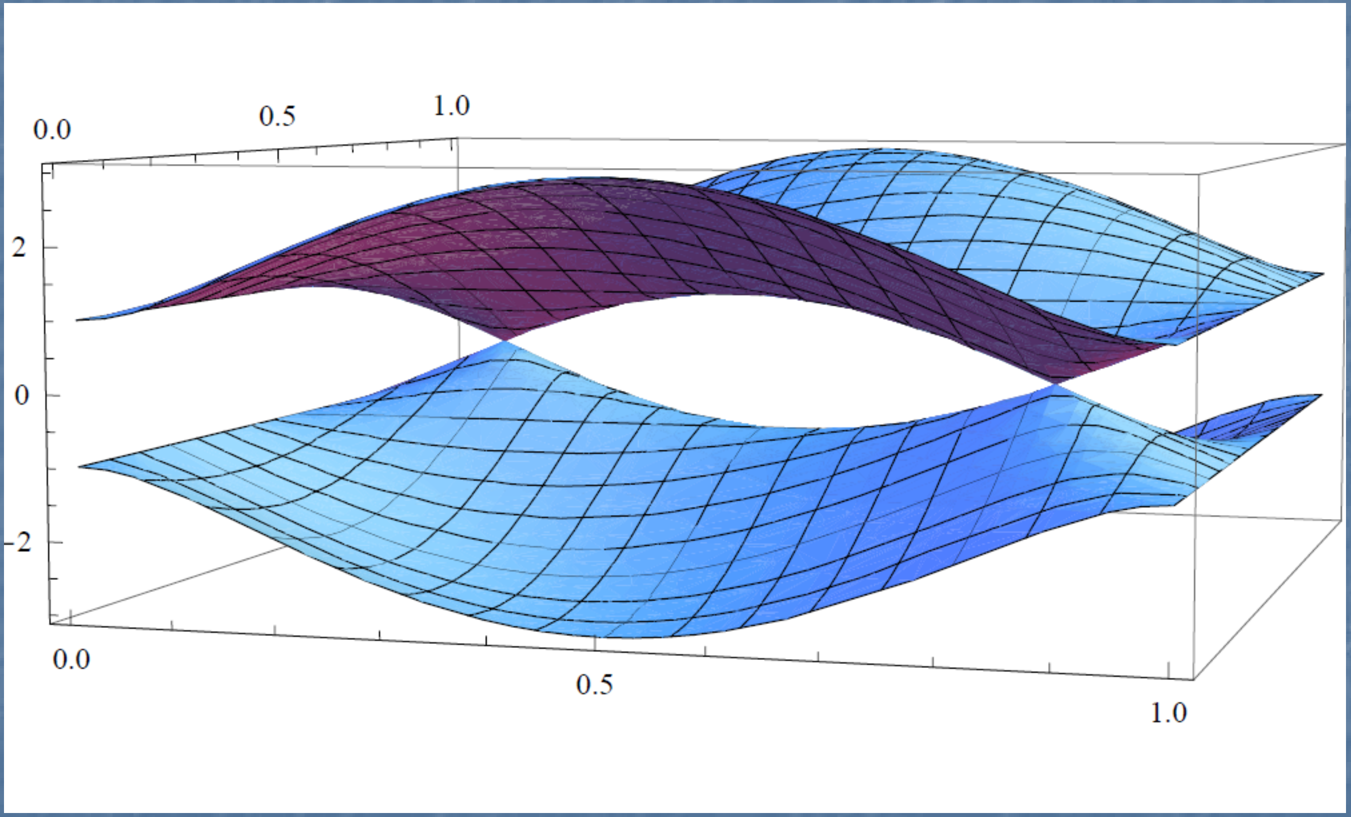
Entropy Ising model

$$S = 0.3230659\ldots$$

Spin-spin correlations

- Many ground states → average over ground states
- Pfaffian representation → inverse of Kasteleyn matrix
- Kasteleyn matrix gapped: exponential decay
- Kasteleyn matrix not gapped: algebraic decay

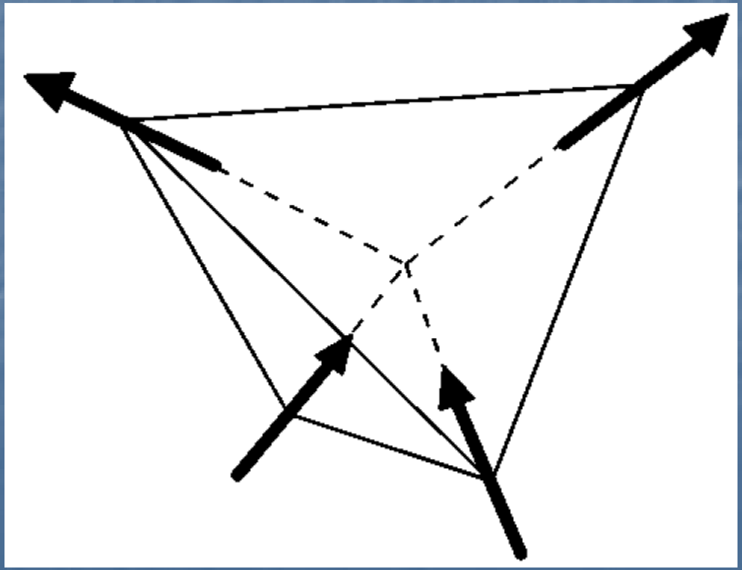
Kasteleyn matrix for honeycomb



→ algebraic correlations

Spin Ice

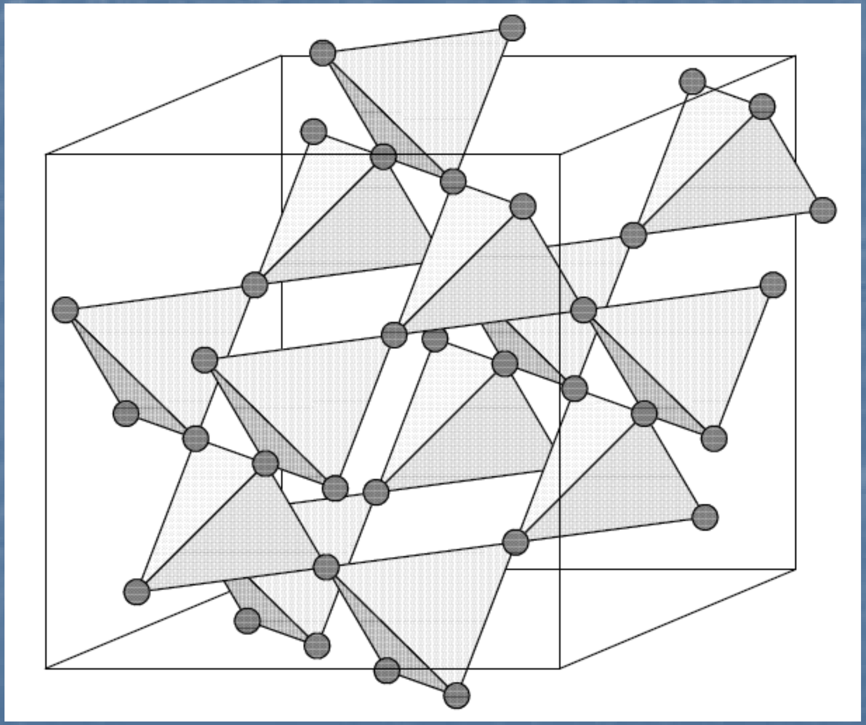
- $Dy_2Ti_2O_6$, $Ho_2Ti_2O_6$
- Pyrochlore lattice
- Ferromagnetic exchange interactions
- Strong anisotropy: spins ‘in’ or ‘out’

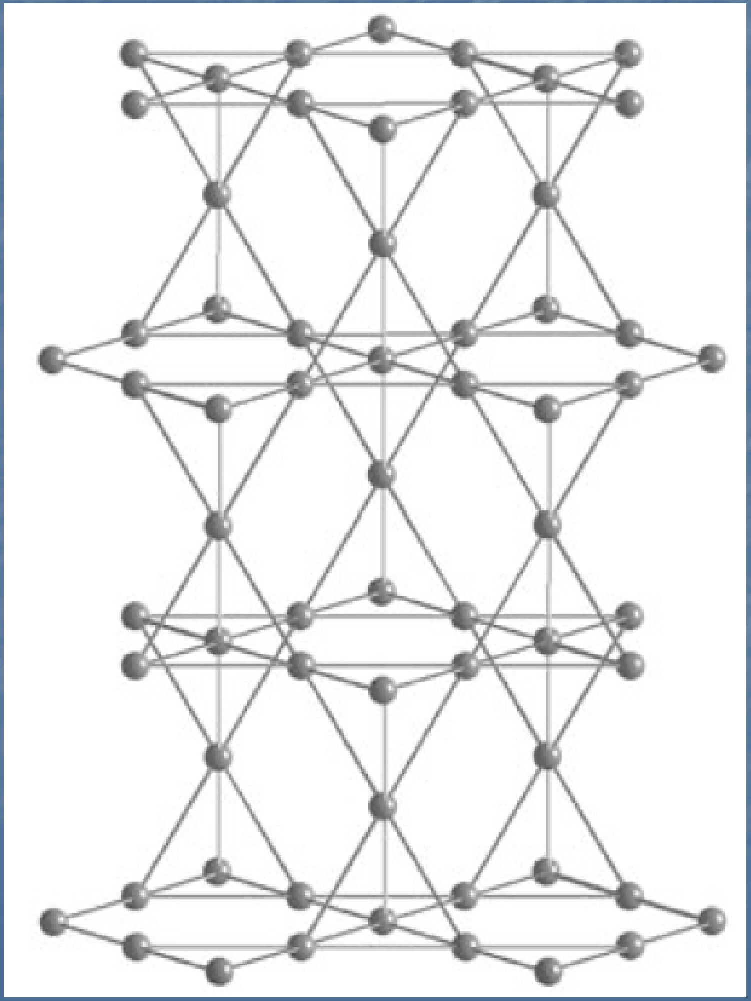


Ground state:
2 spins in, 2 spins out

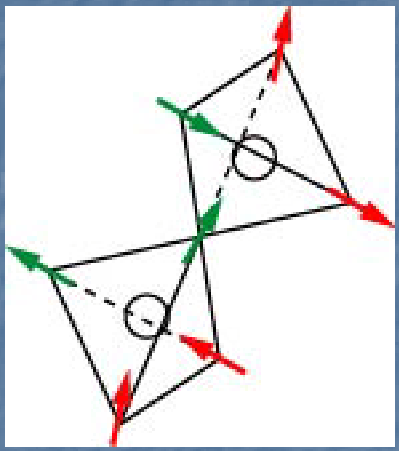
Residual entropy:
the ‘ice problem’

Pyrochlore lattice

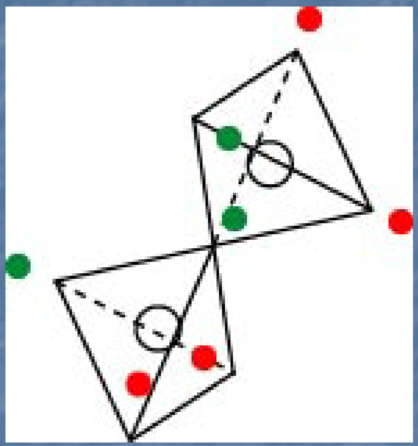




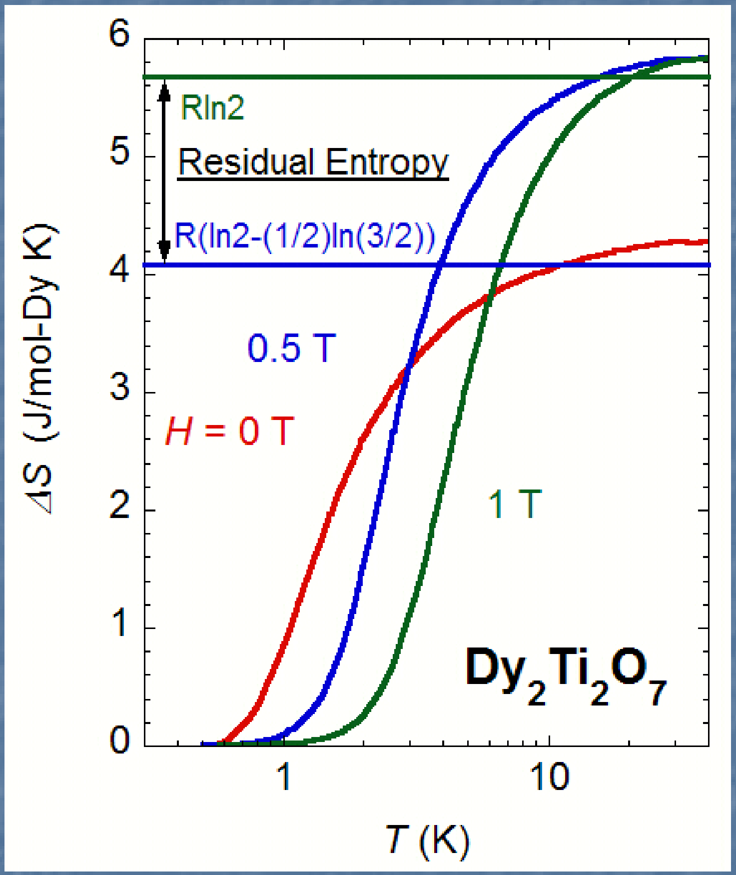
Residual entropy



Spin ice



Ice

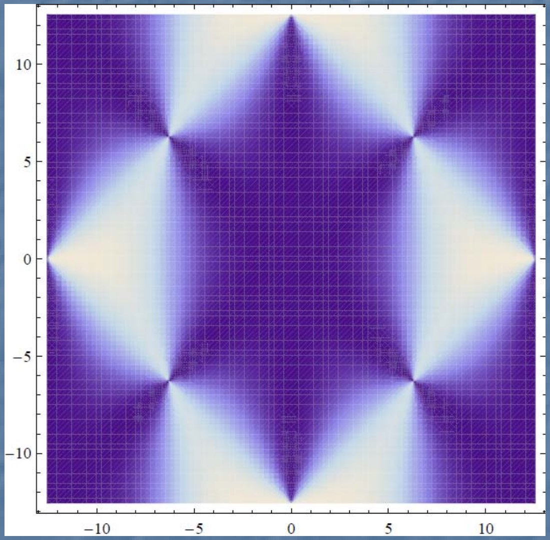


'Exact': $S/k_B \approx 0.20501$
(Nagle, 1966)

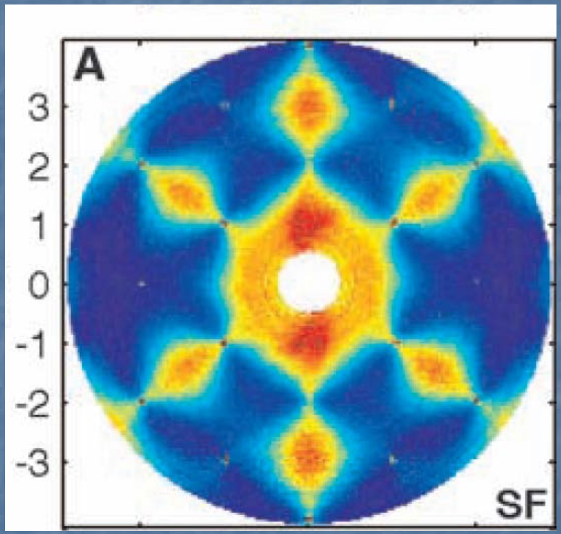
Pauling (1945): $S/k_B \approx (1/2) \ln (3/2) = 0.202732$

Dipolar correlations

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



Theory:
Canals-Garanin, 1999



Experiments:
Fennell, 2009

Why dipolar correlations?

- Height model:

  → algebraic correlations of height variable
- Triangular lattice: spin= exponential of height variable

  → simple algebraic decay
- 2D pyrochlore: spin= gradient of height variable

  → dipolar correlations

Plan du cours (suite)

4) Modèle d'Ising et frustration géométrique
- Entropie résiduelle
- Corrélations algébriques et dipolaires

5) Liquides de spin quantiques
- Frustration, modes mous et fluctuations quantiques
- Liquide RVB et modèles de dimères quantiques
- Liquide de spin algébrique

Strong Quantum effects in 2D

Basic idea

$$\int < a^{+}_{\vec{k}} a_{\vec{k}} > \ \mathrm{d}\vec{k}$$

diverges in 2D as soon as

$$\omega_{\vec{k}} \propto k^2$$

or

$\omega_{\vec{k}}$ has a line of zeroes

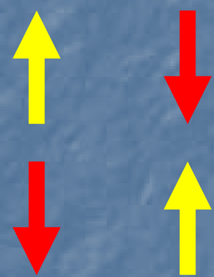
since

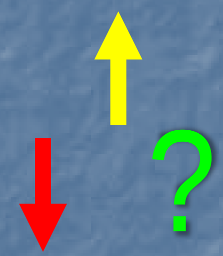
$$< a^{+}_{\vec{k}} a_{\vec{k}} > = \frac{JSz - \omega_{\vec{k}}}{2\omega_{\vec{k}}}$$

Defining frustration I

Frustration = competition between exchange processes

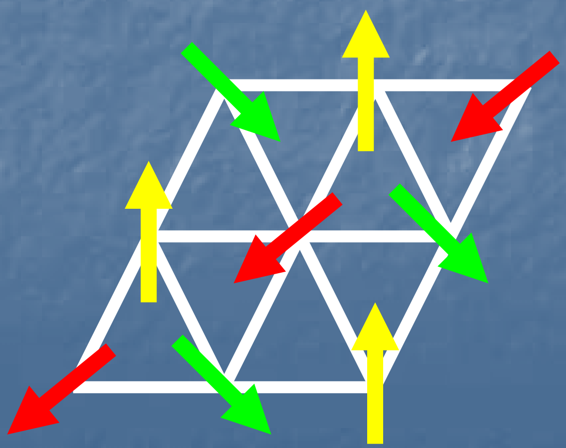
Not frustrated





Frustrated

Not enough!



RVB theory of triangular lattice (Anderson)

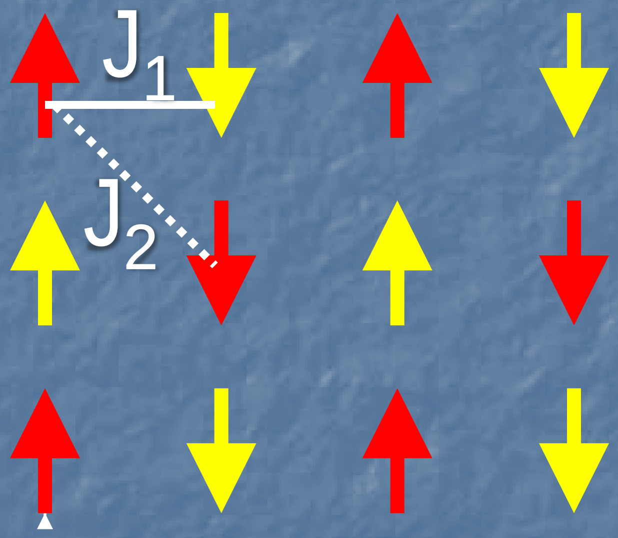
↓

3-sublattice long-range order (Bernu et al, 1990)

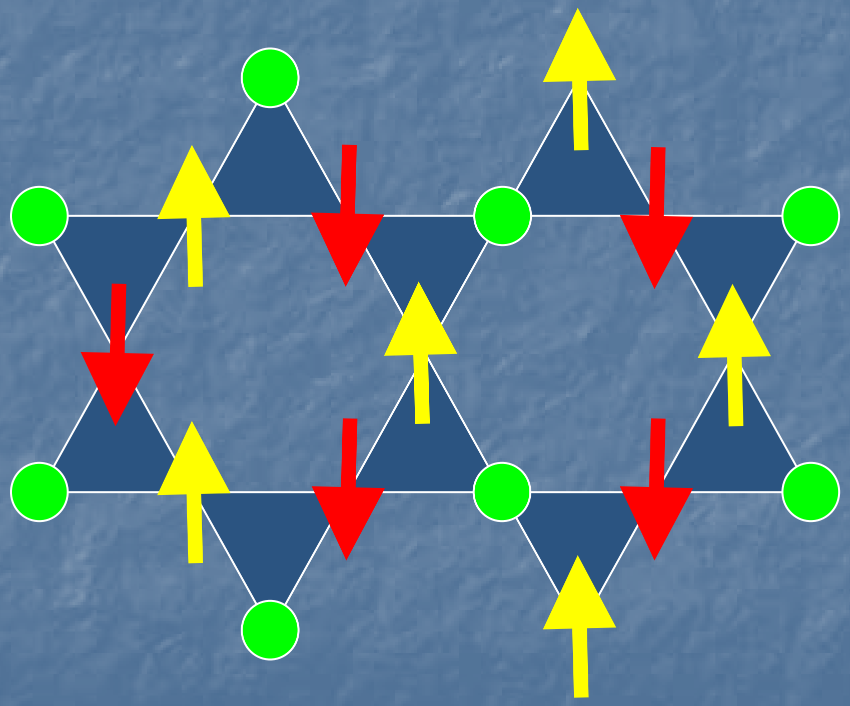
Defining frustration II

Frustration = infinite degeneracy of classical ground state

J_1-J_2 model ($J_2>J_1/2$)



Kagome lattice



Effect of quantum fluctuations?

J_1-J_2 model on square lattice

Infinite number of helical GS for $J_2/J_1=1/2$

$$\omega_{\vec{k}} \propto k^2$$ ⇒ No long-range order

More generally

Frustrated magnets with infinite number of ground states and soft modes

Quantum spin liquids

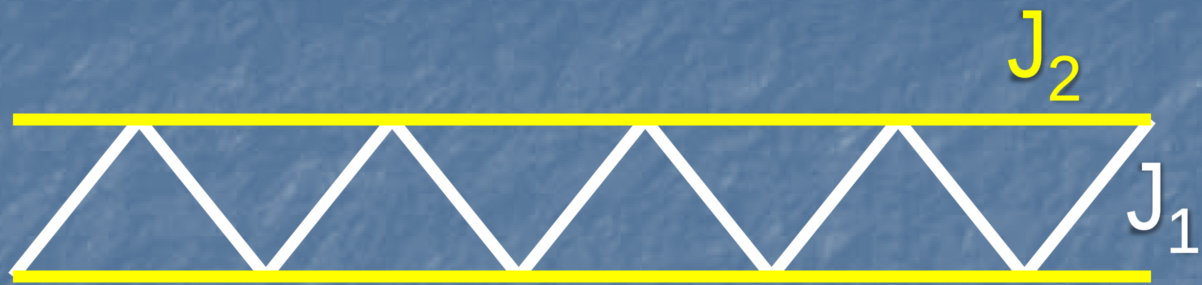
First definition (Shastry-Sutherland, 1981)

Absence of magnetic long-range order
even at T=0

Problem

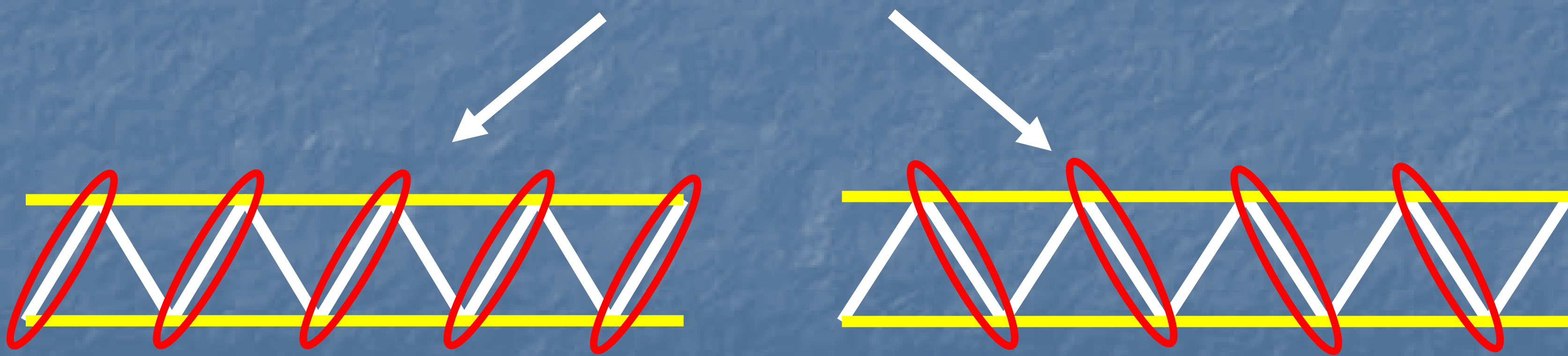
Some systems have a symmetry breaking in the ground state, hence some kind of order, but no magnetic long-range order

Spontaneous symmetry breaking



$J_1 = 2J_2 \rightarrow$ 2 singlet ground states

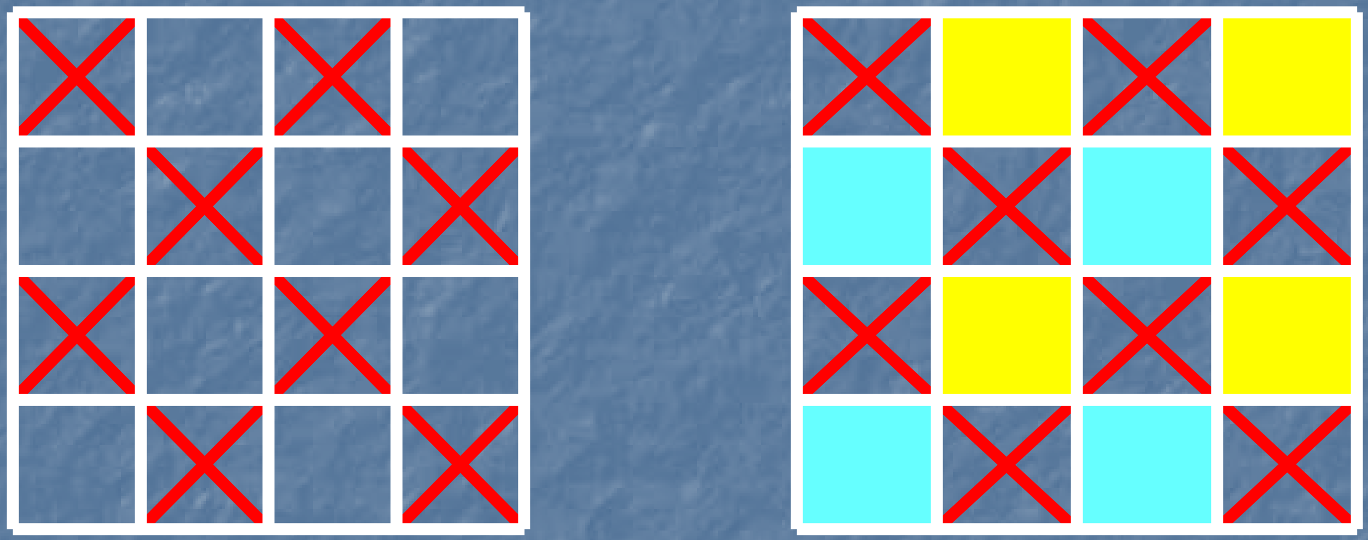
(Majumdar-Ghosh, 1970)



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

Checkerboard lattice

Fouet et al, 2003; Canals, 2003



2 plaquette coverings → 2 groundstates which break the translational symmetry

Spin liquids

New definition

Absence of any kind of order

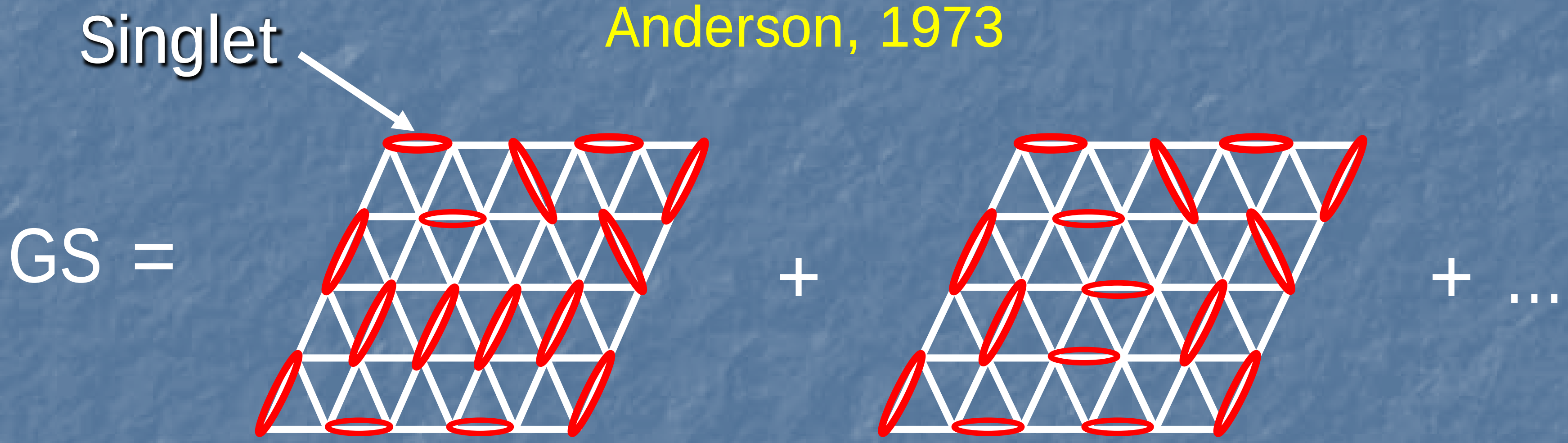
Can quantum magnets
behave as spin liquids?

→ Spin-1/2 kagome?
→ Quantum Dimer models

RVB spin liquids

Question: with one spin ½ per unit cell, can we preserve SU(2) without breaking translation?

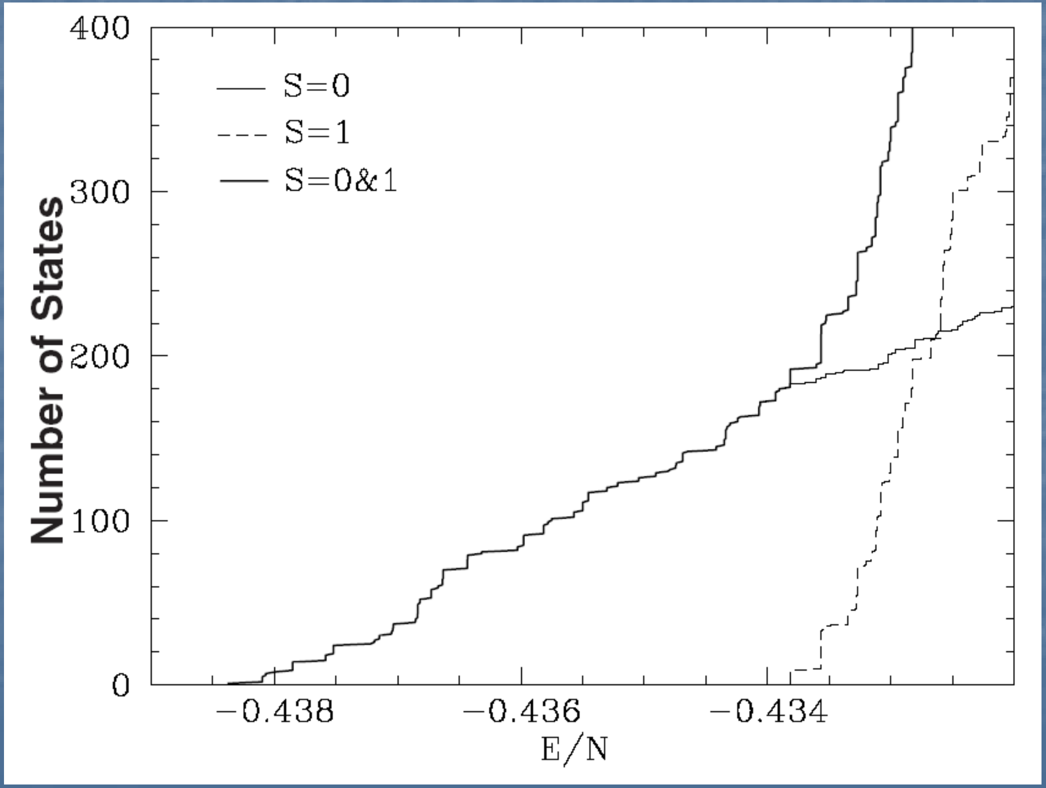
Anderson, 1973



Restore translational invariance with resonances between valence-bond configurations

Spin ½ kagome

Proliferation of low-lying singlets

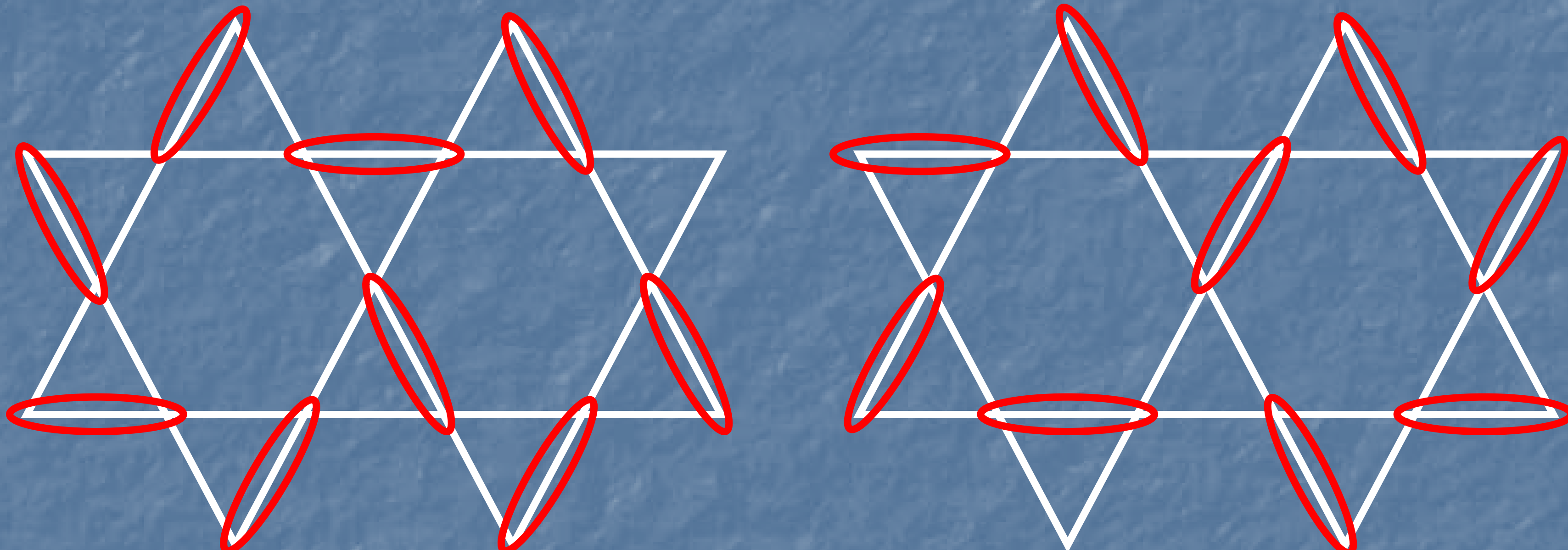


Exact diagonalizations of clusters with up to 36 sites

Lecheminant et al, PRB ‘97

RVB interpretation

Resonance between Valence Bond configurations



→ Proposed for triangular lattice by Anderson and Fazekas ('73)

→ Widely accepted as a good variational basis for kagome after Mambrini and Mila, '00

Quantum Dimer Models

Square lattice (Rokhsar-Kivelson, '88)

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

Assume dimer configurations are orthogonal

V=J: Rokhsar-Kivelson point

GS= superposition of all dimer coverings

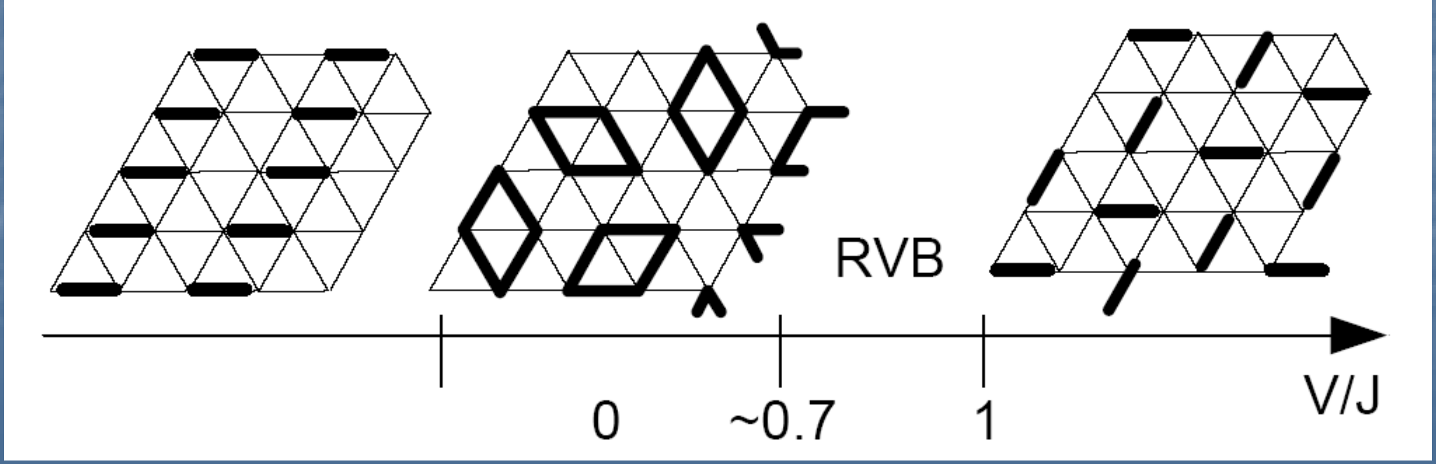
RVB phase? No!

Kasteleyn matrix gapless → algebraic correlations

QDM on triangular lattice

Moessner and Sondhi, '01;
A. Ralko, F. Becca, M. Ferrero, D. Ivanov, FM, '05

Kasteleyn matrix gapped
→ Exponential correlations
→ RVB phase



Algebraic spin liquids

- Hypothetical ground state of Heisenberg antiferromagnets with no long-range order but algebraic correlations, hence a gapless spectrum
- Can be described using the fermionic representation of spin operators
- Has been proposed (as basically everything else) for the spin-1/2 kagome

Fermionic representation

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

Constraint

$$n_{i\uparrow} + n_{i\downarrow} = 1$$

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

Mean-field theory

$$\chi^0_{ij} = \langle \chi_{ij} \rangle = \langle c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow} \rangle$$
$$\eta^0_{ij} = \langle \eta_{ij} \rangle = \langle c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} - c^\dagger_{i\downarrow} c^\dagger_{j\uparrow} \rangle$$

+ constraint on average

Dimerized solution

$$\begin{aligned} \chi^0_{ij} &= 1 \text{ on some bonds} \\ \eta^0_{ij} &= 0 \text{ everywhere} \end{aligned}$$

Fluctuations beyond mean-field

→ Quantum Dimer Models

Flux phase

$$\chi^0_{ij} = \chi_0 e^{i\theta_{ij}}, \quad \theta_{ij} = \frac{\pi}{4}(-1)^{i_x+i_y}$$
$$\eta^0_{ij} = 0 \text{ everywhere}$$

Square lattice

Affleck-Marston, 1988

$$E^{\pm}(\vec{k}) = \pm 4\chi_0 \sqrt{\cos^2 k_x + \cos^2 k_y}$$

Dirac spectrum with 4 gapless points

→ Algebraic correlations

Stability of mean-field solutions

- Compare mean-field energies
  → not very reliable (constraint treated on average+mean-field decoupling)
- Treat constraint with Gutzwiller projection

$$|\psi\rangle \to \prod_i (1 - n_{i\uparrow} n_{i\downarrow}) |\psi\rangle$$

- Treat χ^0_{ij} as variational parameters

Further reading

Interacting electrons and quantum magnetism

Assa Auerbach

A modern discussion of non-frustrated magnets

Introduction to Frustrated Magnetism

C. Lacroix, P. Mendels, F. Mila Eds., Springer, 2010

A recent review of all aspects of frustrated magnets (theory, experiment, synthesis)