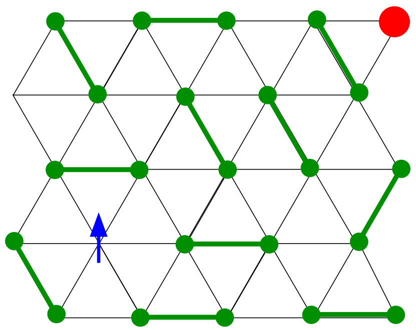
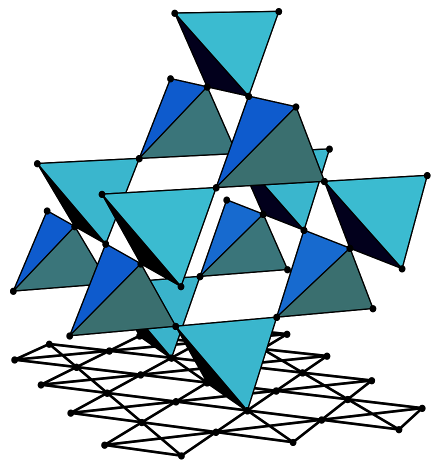
Order and disorder in quantum frustrated magnets



Roderich Moessner

CNRS and ENS Paris



September 2004, Montauk

Overview

- The basic question:
  - interplay of degeneracy and quantum fluctuations
- Ising models of quantum frustration:
  - order by disorder: triangular lattice
  - disorder by disorder: kagome lattice
- High-T$_c$ and the RK quantum dimer model:
  - valence bond solids and RVB liquids in $d = 2$ and $d = 3$
  - excitations: resonons, pi0ns and photons
- Ice in $d = 2$: quantum and sliding ice
- Conclusions and outlook

Collaborators

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Ising models of quantum frustration

- Different choices which bonds to frustrate $\Rightarrow$ different ground states
- On lattice, zero point entropy $\mathcal{S}_0$ is extensive
- Consider only periodic Hamiltonians (no quenched disorder)

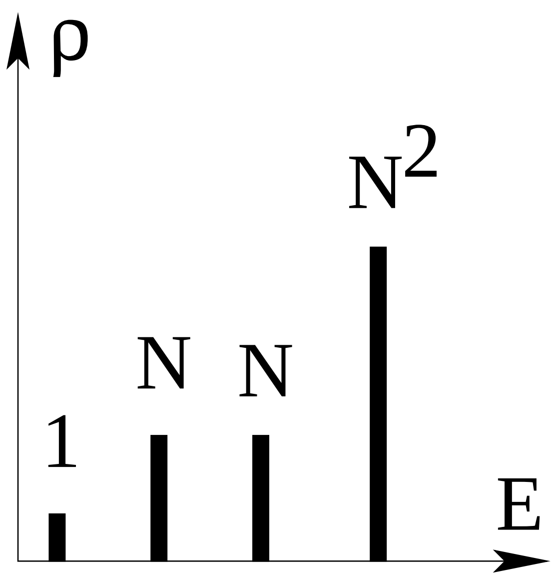
(1) $$H = \sum_{ij} J_{ij} S_i^z S_j^z - \Gamma \sum_i S_i^x$$

$$\langle \uparrow | -\Gamma S^x | \downarrow \rangle = -\Gamma$$

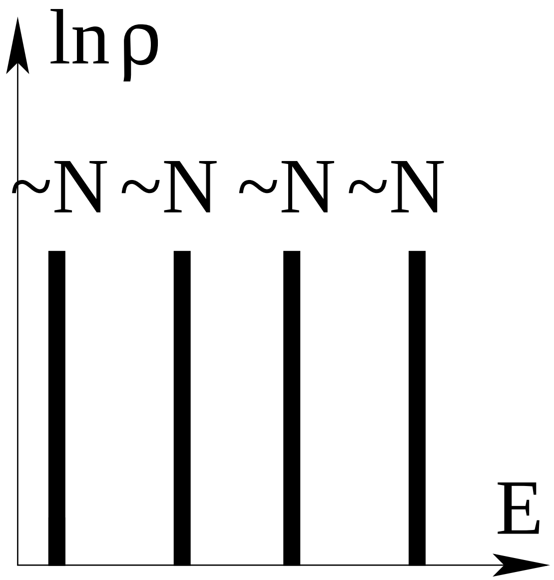
- Transverse field 'flips spins'
  - simplest form of quantum fluctuations
  - matrix elements between degenerate states

An analogy to the quantum Hall effect

d.o.s – unfrustrated magnet



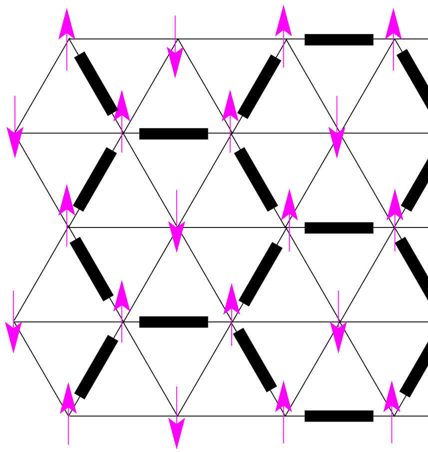
d.o.s – frustrated magnet



- Extensively degnerate ‘Landau levels’
- All perturbations are strong
- New phases?
- New phase transitions?

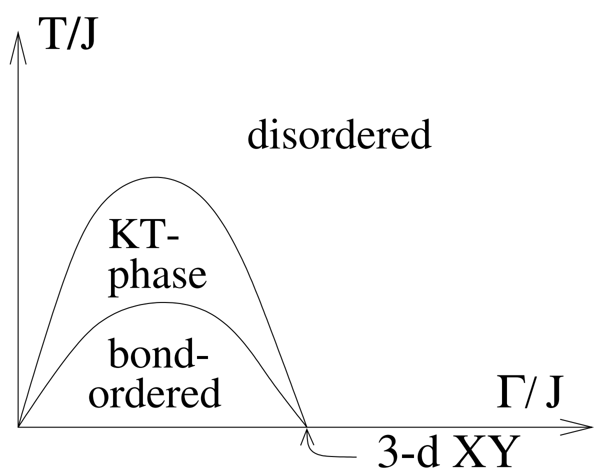
The triangular Ising magnet: order by disorder

- Transverse field ‘likes’ flippable spins: $|S_x = 1\rangle \propto |\uparrow\rangle + |\downarrow\rangle$
- Variational guess: ‘maximally flippable’ configuration forms backbone of ground-state wavefunction



- Close-packing problem of flippable motif $\Rightarrow$ crystalline solution $\Rightarrow$ order by disorder
- Selected state has three-sublattice structure
- Effective action: XY with 6-state clock anisotropy

$$\mathcal{L} = (\partial_\tau \phi)^2 + a_2\phi^2 + a_4\phi^4 + a_6\phi^6$$
$$+b_6\phi^6 \cos 6\theta$$

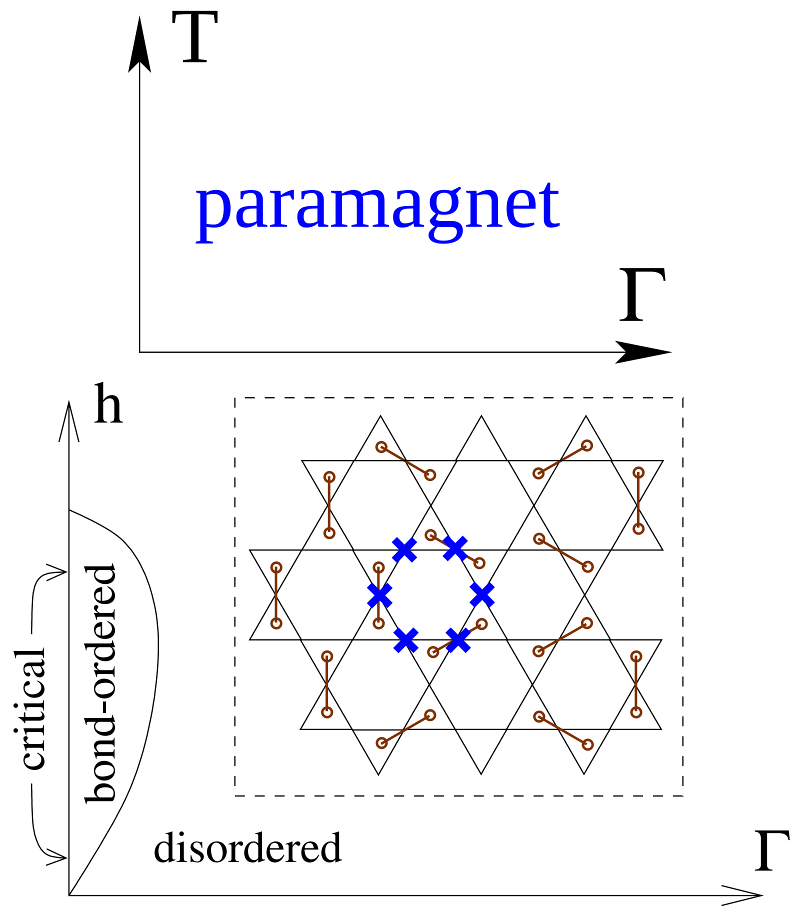


Reformulation as localisation problem

- Define state graph:
  - Nodes are ground states
  - Edges between any pair of ground states connected by single spin flip
- Order by disorder
  - localised ground state
- Disorder by disorder
  - delocalised ground state

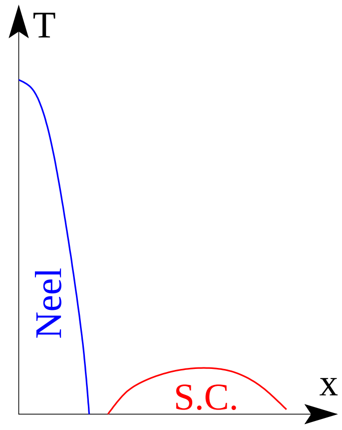
The kagome Ising magnet: disorder by disorder

- Extensively many maximally flippable states
- Dispersionless excitations
- Paramagnetic for all values of T/J, Γ/J
- Longitudinal field suppresses fluctuations $\Rightarrow$ order by disorder

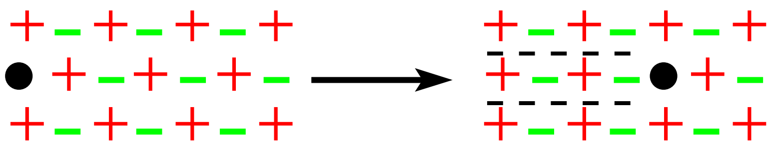


Short-range RVB physics

Basic problem of high-T_c: how do holes hop through an antiferromagnetic Mott insulator?



Hole motion is frustrated:
hopping creates domain walls

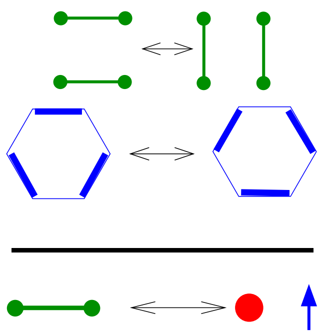


Possible resolution: magnet enters a different phase
resonating valence bond liquid phase
which breaks no symmetries.

Neighbouring electrons form a singlet ("valence") bond
$\longrightarrow$denoted by a dimer.

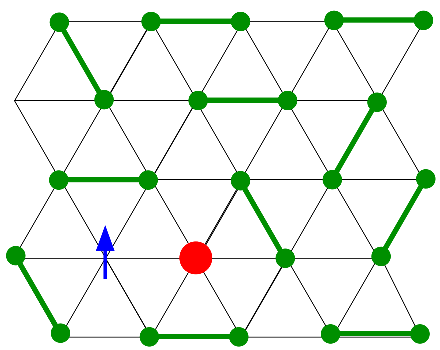
The basic RVB scenario - electron fractionalisation

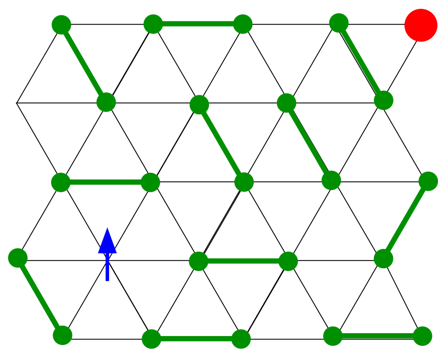
Energetics	RVB	Neel
single pair	valence bond optimal	
higher coordination	energy from resonance	... each neighbour
hole doping	motion unimpeded	motion frustrated



- Basic resonance move is that of benzene

- Removing an electron $\rightarrow$ holon + spinon





spinon and holon are deconfined

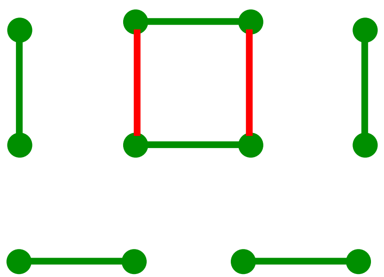
$\downarrow$

(bosonic) holons can condense

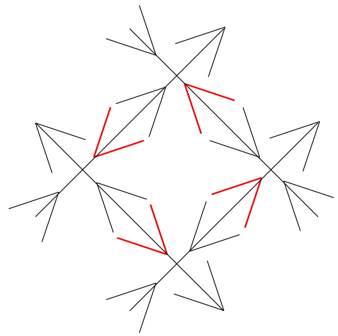
Local constraints and quantum dynamics

- ‘Hard’ constraints are ubiquitous (e.g. single occupancy)
- Effective degrees of freedom encode constraint (sometimes)
- Adding quantum dynamics lifts extensive classical degeneracy (via plaquette resonance; inversion of closed loops; XY or ring exchange, transverse field)

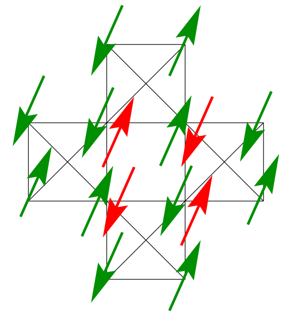
dimer models



vertex models



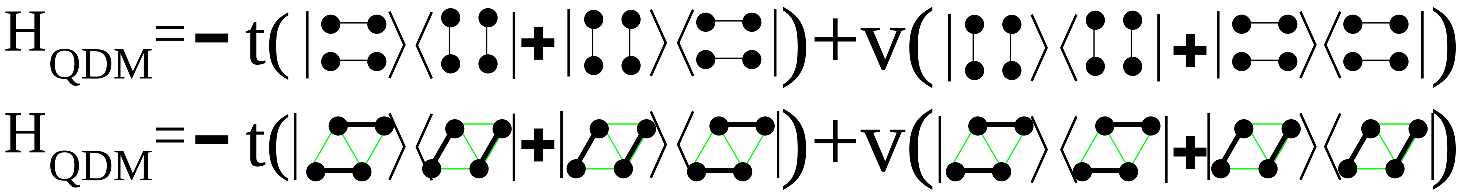
Ising ground states



$\longrightarrow$ degeneracy + quantum dynamics = ???

$\longrightarrow$ non-perturbative + potentially very interesting (see QHE)

The Rokhsar-Kivelson quantum dimer model



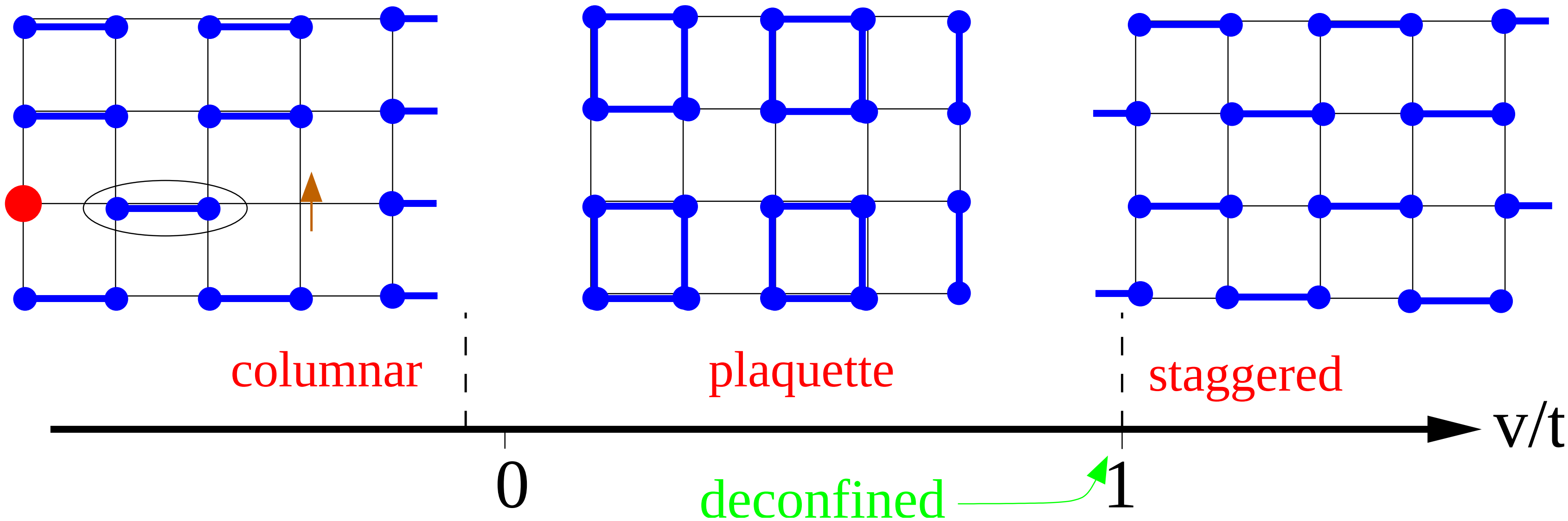
- Resonance (t) and potential (v) term from uncontrolled approximation – one parameter: v/t
- RK point $v/t = 1$ is exactly soluble in $d = 2$ at $T = 0$:

$$|0\rangle = \frac{1}{\sqrt{N_c}} \sum_c |c\rangle \to \langle \hat{P} \rangle = \frac{1}{N_c} \sum_{c,c'} \langle c|\hat{P}|c'\rangle = \frac{1}{N_c} \sum_c p_c$$

$\to$ classical calculation for diagonal operators

- $v/t > 1$ and limits of $v/t \to -\infty$ give solid (staggered and columnar, respectively) phases:

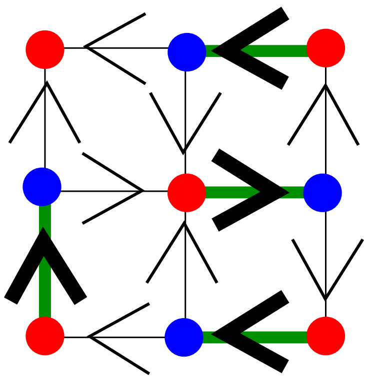
Phase diagram for the square lattice



- all phases confining (break translational symmetry) RK; Read+Sachdev; Leung; ...
- RK point deconfined RM+Sondhi
- RK point highly degenerate RK
- Crucial ingredient: bipartitness allows height (gauge) mapping

Height/gauge mapping of square lattice dimer model

Orientation of dimers (from red to blue sublattice) is possible.



Magnetic analogy: dimer = magnetic flux $\vec{B}$

- Link with dimer $\rightarrow$ flux $\vec{B} = +3$
- Unoccupied link $\rightarrow$ flux $\vec{B} = -1$
- $\nabla \cdot \vec{B} = 0 \rightarrow \vec{B} = \nabla \times \vec{A} = \nabla \times h$

'Vector potential' $\vec{A}$ in $d = 2$ is simple scalar height function h (Youngblood et al.)

Mapping to height takes care of hardcore constraint $\rightarrow$ we can coarse-grain safely to get effective long-wavelength theory.

Height representation in $d = 2$

I Classical (RK point) Blote, Nightingale, Hilhorst, ...
coarse-grain $h \to \tilde{h}$ to get energy functional of entropic origin:

$$Z = \int \mathcal{D}\tilde{h} \exp[\mathcal{S}_{cl}]; \mathcal{S}_{cl} = -\frac{K}{2} \int (\nabla \tilde{h})^2$$

II Quantum: guess effective long-wavelength theory RM et al., Henley

$$\mathcal{S}_q = \int (\partial_\tau \tilde{h})^2 - \rho_2 (\nabla \tilde{h})^2 - \rho_4 (\nabla^2 \tilde{h})^2 + \lambda \cos(2\pi \tilde{h})$$

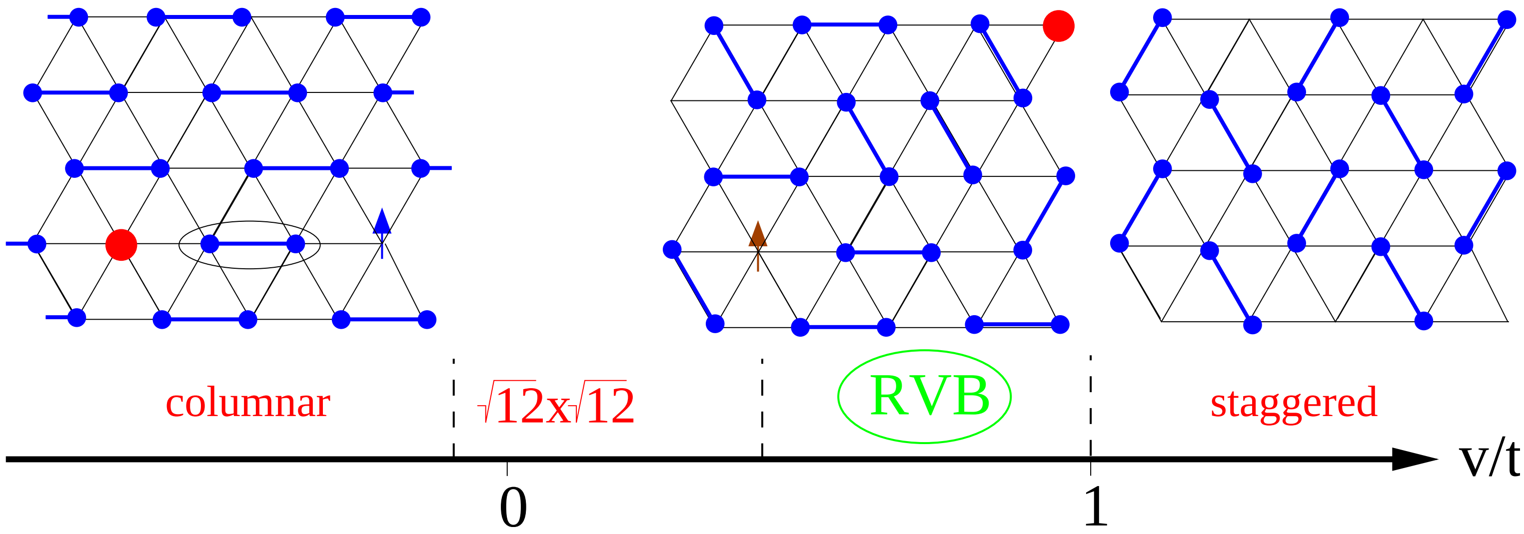
with

- $\rho_2 \propto (v/t - 1) = 0$ at the *critical* RK point $\to$ degeneracy.
- $v/t > 1$ preferring maximal $\nabla \tilde{h} \to$ staggered
- For $v/t < 1$, presence of dangerously irrelevant operator$\to$ flat $\tilde{h} \to$ confining solid (plaquette or columnar).
- RK point is ‘deconfined multicritical’ Fradkin *et al.*

Can we obtain an RVB liquid nonetheless?

- Do all quantum dimer models order?
- In $d = 2 + 1$, height model is never in the rough phase
- Possibilities
  - Non-bipartite lattice $\longrightarrow$ triangular RVB (Z_2) liquid
  - Three dimensions $\longrightarrow$ cubic RVB ($U(1)$) liquid
  - Both $\longrightarrow$ fcc RVB (Z_2) liquid

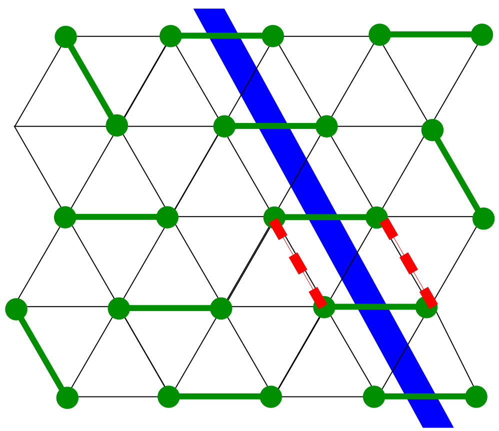
The triangular short-range RVB liquid

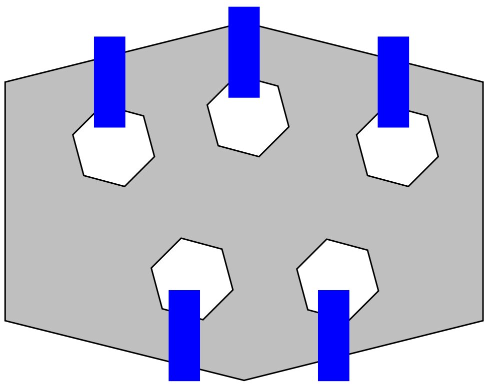


- Point of principle: RVB liquid exists in $d = 2 + 1$
- electron fractionalisation – deconfinement
- gapped excitation spectrum (in single-mode approx.)
- topological order (Wen for QHE)

Topological order in the RVB liquid phase

- Winding parity $(|e\rangle, |o\rangle)$ invariant under action of local Hamiltonian
- Liquids locally indistinguishable $\rightarrow$ sectors degenerate for $L \rightarrow \infty$, and $\langle o|\hat{H}_n|e\rangle \propto \exp(-L)$ for *local* noise $\hat{H}_n$.
- Use as *scalable* q-bit, immune to decoherence? Kitaev *et al.*, Ioffe *et al.* $\rightarrow$ realisation as Josephson junction array?
- Problem: logic gates; non-local operations, ...





Generalisation to $d = 3$: cubic lattice (RK point)

Can again use analogy to electrodynamics by orienting dimers.

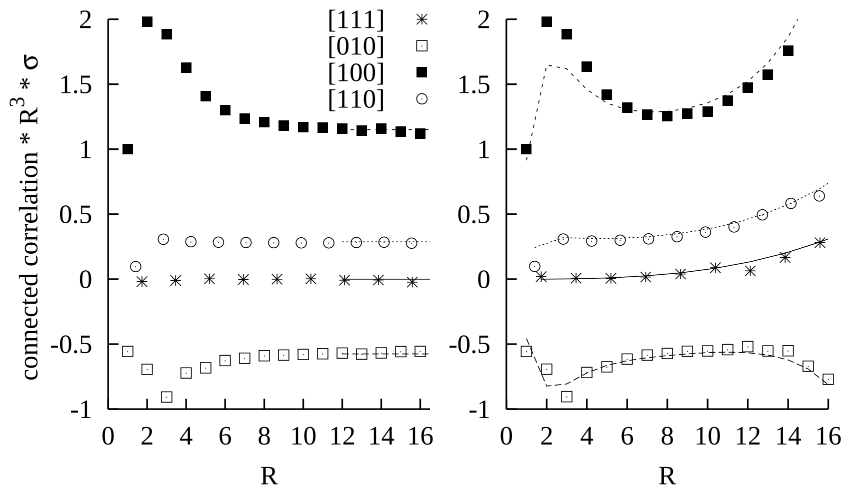
New feature: $\vec{B} = \nabla \times \vec{A}$ is now related to vector potential with local gauge invariance. Youngblood+Axe; Henley; Hermele *et al.*; Huse *et al.*

$$Z = \int \mathcal{D}\vec{A} \exp[\mathcal{S}_{cl}]; \mathcal{S}_{cl} = -\frac{K}{2} \int (\nabla \times \vec{A})^2$$

gives dipolar correlators:

$$c_{xx} \propto (3\cos^2\theta - 1)/r^3$$

which agree well with Monte Carlo (left: $L = 128$; right: $L = 32$):



$U(1)$ ***RVB phase on cubic lattice***

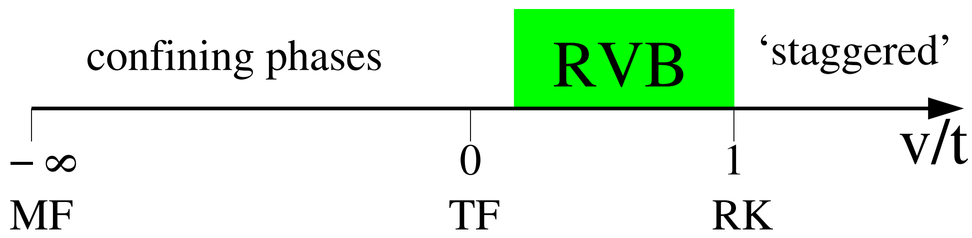
II Quantum: again guess effective long-wavelength theory

$$\mathcal{S}_q = \int \vec{E}^2 - \rho_2 \vec{B}^2 - \rho_4 (\nabla \times \vec{B})^2$$

This is action of compact QED, with monopoles suppressed $(\nabla \cdot \vec{B} = 0) \longrightarrow$

There exists an RVB "Coulomb" liquid phase, with

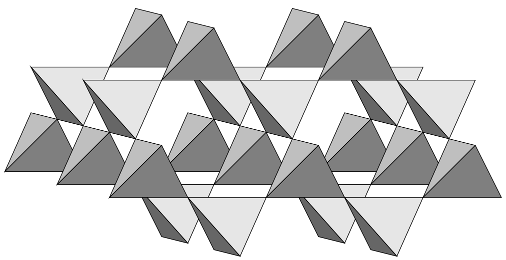
- deconfinement
- gapless photons
- 'quantum order' (Wen)

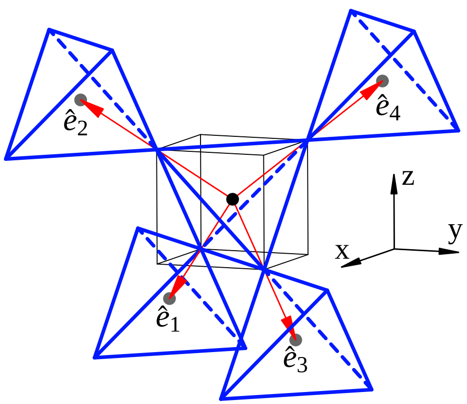


Z_2 RVB phase on face-centred cubic lattice

- The presence/absence of an RVB phase on bipartite lattices is a consequence of the respective presence/absence of deconfining phases in the corresponding $U(1)$ gauge theories in $d = 3 + 1$ and $d = 2 + 1$.
- Similarly, the presence of an RVB phase on the triangular lattice follows from the existence of a deconfined phase in Z_2 gauge theories in $d = 2 + 1$. This carries over to $d = 3 + 1$, where for the non-bipartite face-centred cubic lattice, an Z_2 RVB phase exists (with topological order but without gapless photons).
- Moral: deconfined dimer phases are more easily found in $d = 3 + 1$ than in $d = 2 + 1$ BUT dimer phases are more difficult to stabilise in higher dimensions.

Highly frustrated magnetism in $d = 3$





- Pyrochlore lattice: corner-sharing tetrahedra.
- antiferromagnetic ground states have zero total spin on each tetrahedron
- huge degeneracy
  - Ising: cubic ice=diamond six vertex with residual Pauling entropy $\frac{1}{2} \ln \frac{3}{2}$;
  - H'berg: cooperative paramagnet

No ordering for $T \to 0$

Lattice of tetrahedra is bipartite – we again have conservation law (Henley; R.M. et al.; Hermele et al.)!

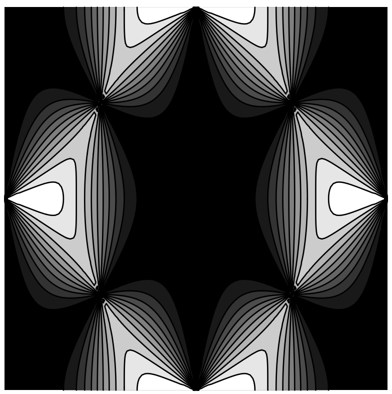
Large-N treatment compared to finite N

Strategy: consider classical $O(N)$ model $N = \infty$. Hope: ‘gross’ features reproduced correctly.

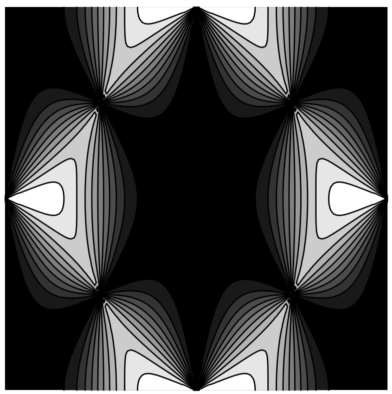
No free parameter.

Structure factor in [hhk] plane for pyrochlore antiferromagnet. (Zinkin; Garanin+Canals)

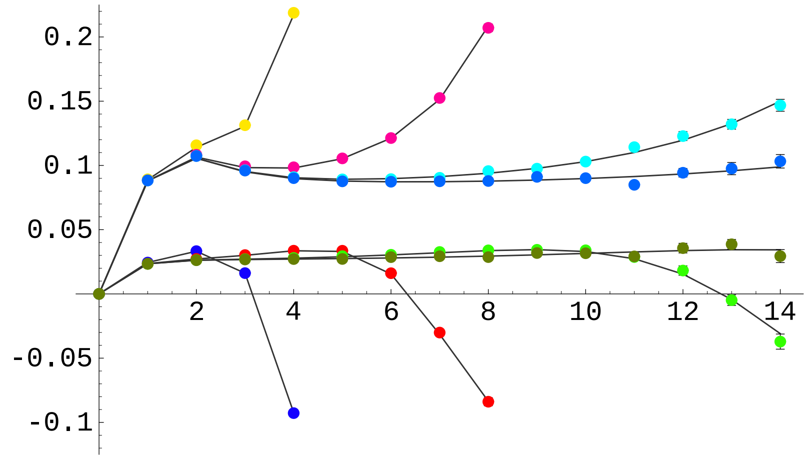
$O(\infty)$



ice I_h $(O(1))$



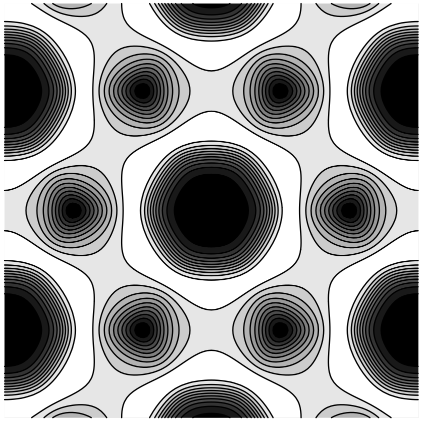
$R^3\times$ Ising real-space correlations (different sizes and directions)



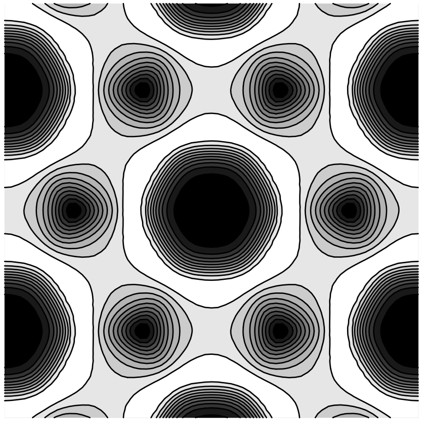
$1/N$ *corrections*

- $1/N$ corrections preserve ‘dipolar’ form of correlations at large distances (conservation law)
- non-perturbative effects: order by disorder and ‘vertex operators’ in $d = 2$ (forbidden in $d = 3$)
- also works for more general set of models, e.g. three-dimer model on triangular lattice (aka kagome ring exchange of Balents *et al.*)

$O(\infty)$



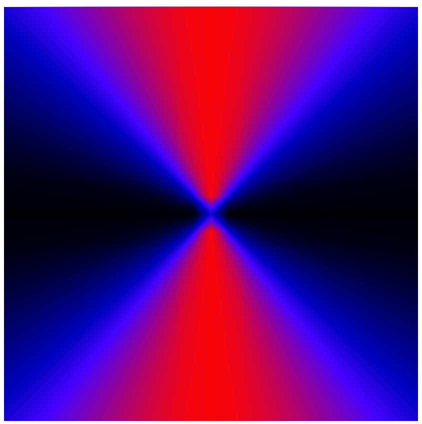
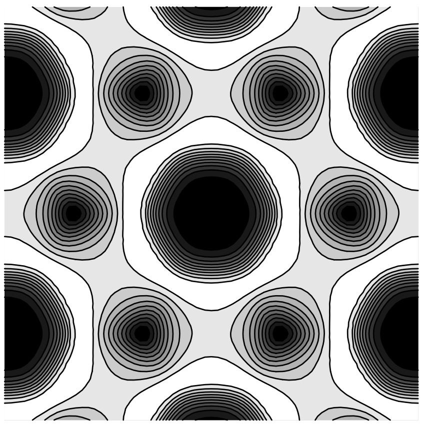
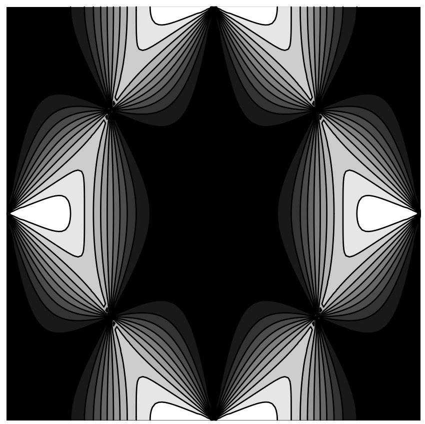
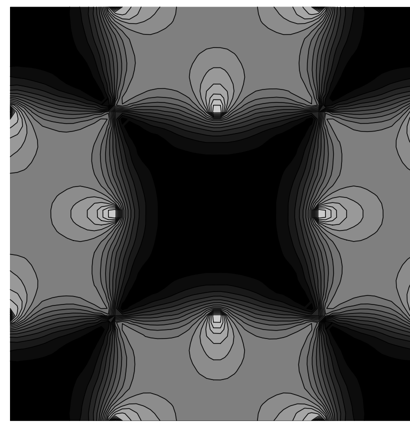
Ising, [$O(1)$]



Treatment is not exact but very accurate

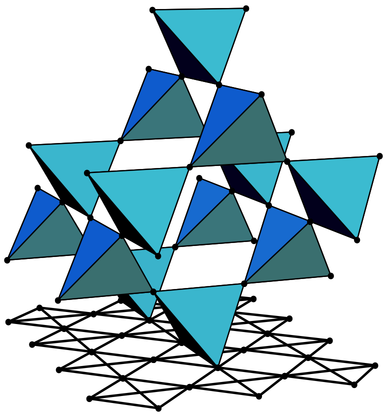
Excitations and the single-mode approximation

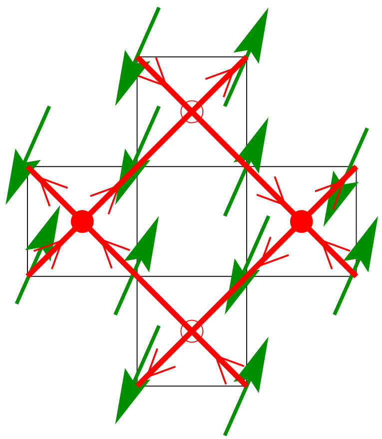
- $\hat{\rho}_{\hat{e}}(k)$: dimer density operator (polarisation $\hat{e}$, wavevector k).
- Ground state: $|0\rangle$, variational excited state $|k\rangle = \hat{\rho}_{\hat{e}}(k)|0\rangle$
- Single-mode approx.: $E_k - E_0 \leq f(k)/s(k)$, where $s(k) = \langle k|k\rangle$ and $f(k) = \langle 0|[\hat{\rho}_{\hat{e}}(k), [H, \hat{\rho}_{\hat{e}}(-k)]]|0\rangle$
- Gapless modes for $f(k) \to 0$ or $s(k) \to \infty$
- For bipartite lattices, near zone-corner Q: $f(Q+k) \propto (k \times \hat{e})^2$

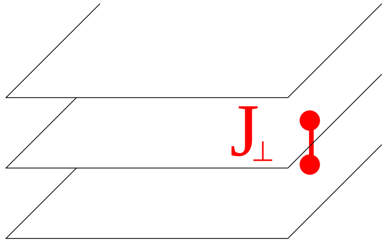
lattice	triangular	pyrochlore	square
excitations	gapped (Z_2)	only photons	resonons+pi0n
			

Sliding ice and the d-DW in $d = 2$

- square ice (six-vertex) = Ising planar pyrochlore ($T = 0$)
- Weakly coupled $d = 2$ planes: $J_\perp / T \ll 1$
- model of d-DW [arrows = conserved currents] (S. Chakrvarty *et al.*)
- Critical correlations of single plane stable for *finite range* of $J_\perp / T \rightarrow$ “Sliding ice”





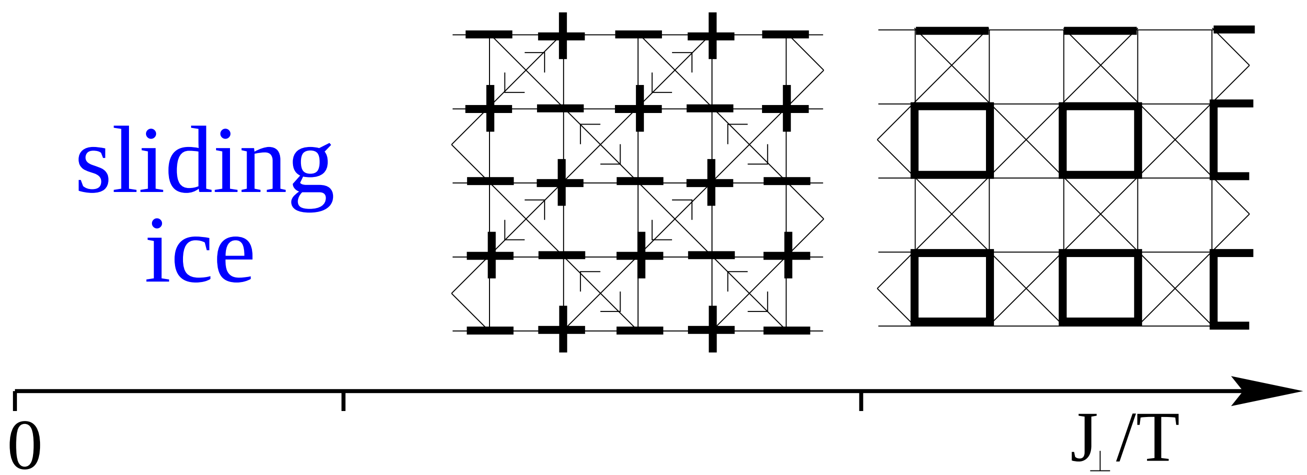


Quantum ice in $d = 2$

- For $J_\perp > J_{crit}$, get antiferroelectric order
- $J_\perp \to \infty$ gives 'quantum ice', also obtained from Ising model plus transverse field ($4^{\rm th}$ order) or J_{xy} ($2^{\rm nd}$ order), with ring-exchange Hamiltonian

$$H_Q = \sum_\Box S^+ S^- S^+ S^- + h.c.$$

- These quantum fluctuations give a 'valence bond solid' (order by disorder): Ph. Sindzingre; RM *et al.*



Summary

- Ising models of quantum frustration
  - cooperative paramagnetism; order by disorder
- RVB liquids:
  - different RVB liquids with fractionalisation, topological order, ...
- range of excitations
  - photons, resonons, pi0ns
- potential realisations:
  - correlated electrons
  - frustrated magnets
  - artificial structures
  - cold atoms