Kagome Lattice Quantum Antiferromagnets

A Quest for Unconventional Quantum Phases

Predrag Nikolić and T. Senthil

Massachusetts Institute of Technology

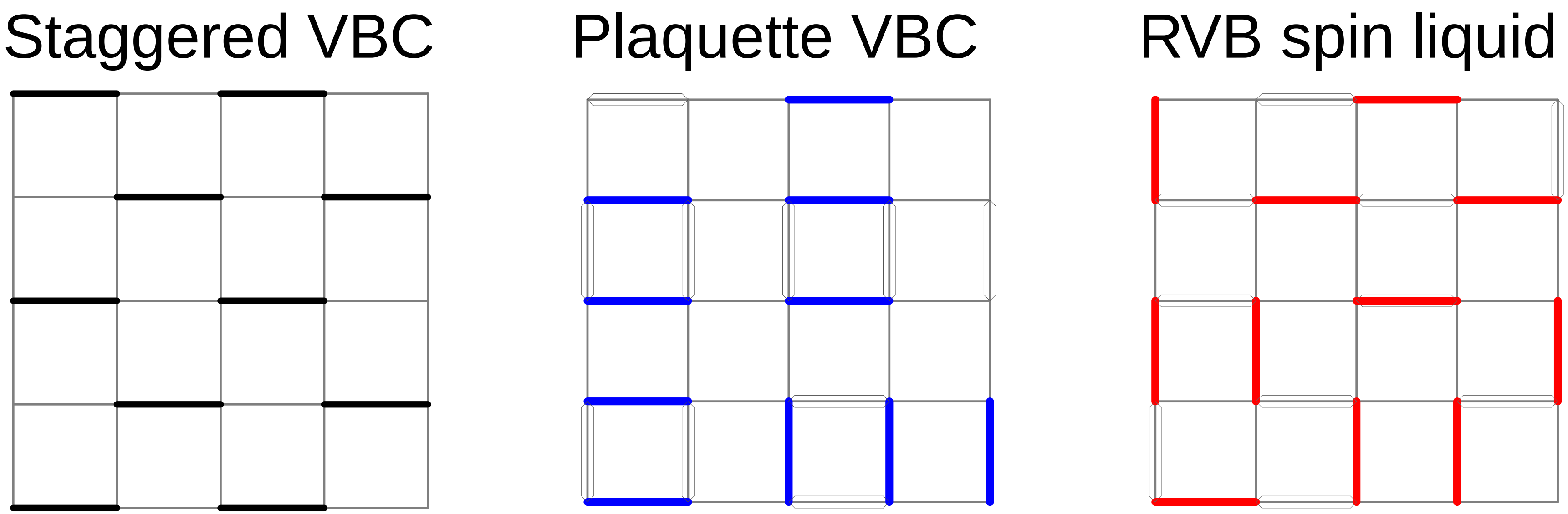
Quantum Phases

System	Conventional	Unconventional
Metals	Fermi liquid	non-Fermi liquid cuprates heavy fermion materials
Magnets	ferromagnet antiferromagnet plain paramagnet	paramagnets: spin-Peierls (VBC) spin liquid (RVB)

Unconventional Quantum Magnets

- Two spins form a valence bond (singlet):

$$|VB\rangle = \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$$



RVB Spin Liquid

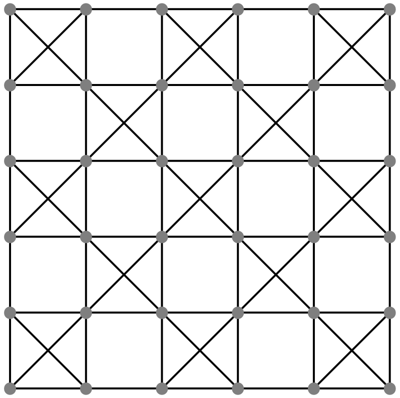
- No broken symmetries (at $T = 0$)
- Fractionalized quasiparticles
  $S = \frac{1}{2}$ spinons
- Topological phase in 2 and more dimensions
  $\mathbb{Z}_2$ vortices (visons)

Motivation/Realizations:

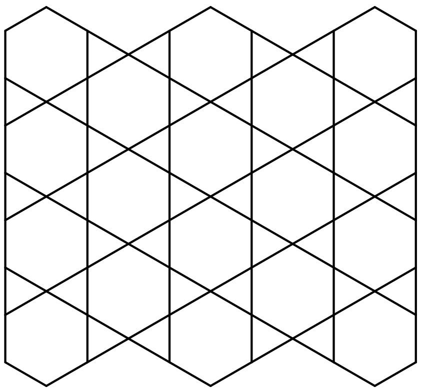
- Heisenberg antiferromagnetic chains (1D)
- Pseudo-gap region of the cuprates?
- Cs_2CuCl_4?
- $\kappa - (BEDT - TTF)_2 - Cu_2(CN)_3$?

Geometric Frustration

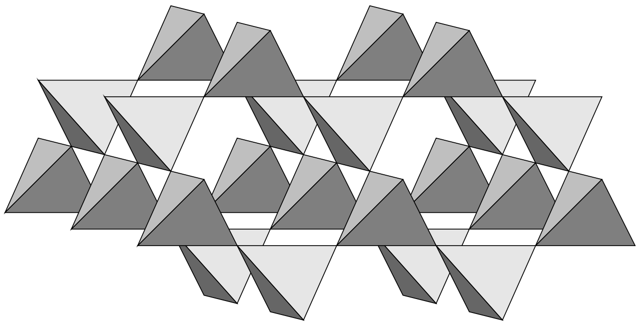
Checkerboard



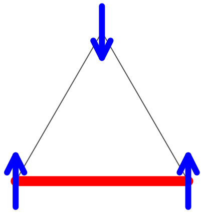
Kagome



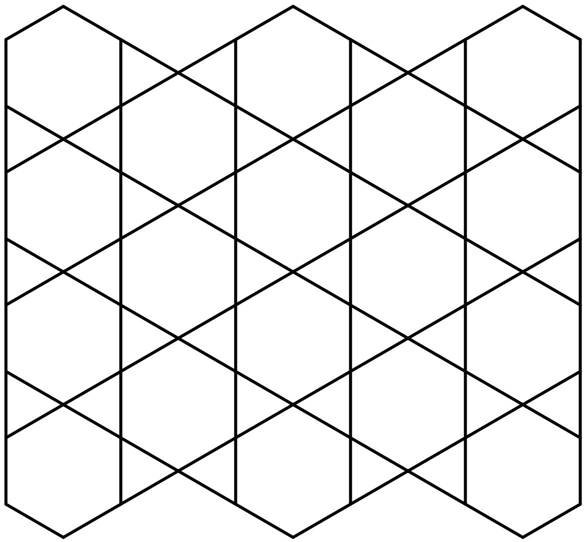
Pyrochlore



- Huge degeneracy of *classical* ground states
- Fluctuations lift the *classical* degeneracy
  incompletely: order-by-disorder
  completely: spin liquid
- New physics emerges at low energy scales



Kagome Lattice
Heisenberg Antiferromagnet



Kagome Experiments

Spin $S = 3/2$ kagome material $SrCr_8Ga_4O_{19}$ (SCGO)

- No magnetic long-range order down to $T = 100mK$
- Spin-glass behavior?
- Missing entropy
- Heat-capacity *not* thermally activated: $C(T) \propto T^2$
  $\Longrightarrow$ gapless excitations
- Heat-capacity virtually independent of magnetic field
  $\Longrightarrow$ singlet excitations

Also, QS-ferrite…

Kagome Numerics (Lhuillier, et.al)

Exact diagonalization of the $S = 1/2$ Heisenberg model (samples with up to 36 sites)

- Disordered ground-state
- Short-range correlations:
  spin-spin, dimer-dimer, chiral-chiral
- Small spin-gap: $\sim J/20$ in thermodynamic limit
- Singlet excitations form a *gapless* band
- Macroscopic number of singlet excitations below the spin-gap: 1.15^N (*not* Goldstone modes)
- Comparison with numerics for $S = 1$:
  large spin-gap, no gapless singlets
  $\Longrightarrow$ topological effects may be important

Questions

- Nature of the ground state:
  spin liquid or order-by-disorder?
- Confined or deconfined spinons?

- Nature of the mysterious gapless singlet excitations?
  1. Why so large number of states below the spin-gap?
  2. Why gapless?

- Great hope for a spin liquid?
- Gauge bosons as low energy excitations?

Kagome Theory

- $SU(N), N \to \infty$ (Marston, Zheng)
- $Sp(N), N \to \infty$ (Sachdev)
- Trimerized Kagome lattice (Mambrini, Mila)
- Quantum dimer model at RK point (Misguich) (exactly solvable)
- Quantum dimer model from overlap expansion (Elser)
- Chiral spin liquid (Yang, Warman, Girvin)
- Hidden long-range order and Goldstone modes
- Some other approaches. . .

New Theoretical Approach

- Describes the singlet states below the spin-gap
- Low energy effective theory

Approaches to paramagnetic phases:

1. Large-N expansion: (Sachdev, Read)
   A gauge theory describes fluctuations
   about the mean-field state
   $\Longrightarrow$ pure $\mathbb{Z}_2$ gauge theory
2. Quantum dimer models:
   (Jalabert, Sachdev; Moessner, Sondhi)
   $\Longrightarrow$ fully frustrated Ising model on the dual lattice
3. Heisenberg model as a theory of
   fermionic *spinons* coupled to a $\mathbb{Z}_2$ gauge field

$\mathbb{Z}_2$ Gauge Theory

Ingredients:

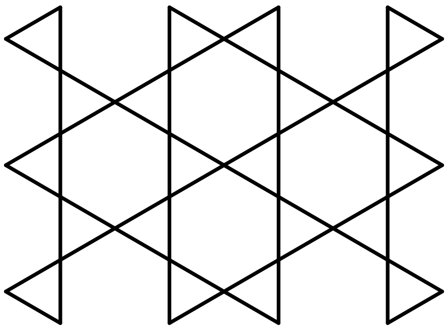
- Kagome spins: $\boldsymbol{S}_i = \frac{1}{2} f^\dagger_{i,\alpha} \boldsymbol{\sigma}_{\alpha\beta} f_{i,\beta}$
- Fermionic *spinons* on the Kagome sites: $f_{i,\alpha}$
- $\mathbb{Z}_2$ gauge field on the Kagome bonds: σ_{ij}

$$H = -h_0 \sum_{\langle ij \rangle} \sigma^x_{ij} - \sum_{\langle ij \rangle} \sigma^z_{ij} \Big[t_{ij} \sum_{\alpha=\uparrow\downarrow} (f^\dagger_{\alpha i} f_{\alpha j} + h.c.) + \Delta_{ij} (f^\dagger_{\uparrow i} f^\dagger_{\downarrow j} - f^\dagger_{\downarrow i} f^\dagger_{\uparrow j} + h.c.) \Big]$$

$$G_i = \prod_{i' \in i} \sigma^x_{ii'} (-1)^{\sum_{\alpha=\uparrow\downarrow} f^\dagger_{\alpha i} f_{\alpha i}} = -1$$

Effective Theory

- Interactions between the spinons are mediated by the $\mathbb{Z}_2$ gauge field $\Longrightarrow$ Heisenberg model
- *Numerics:* the spinons are gapped!
  Integrate out spinons
  $\Longrightarrow$ pure *odd* $\mathbb{Z}_2$ gauge theory

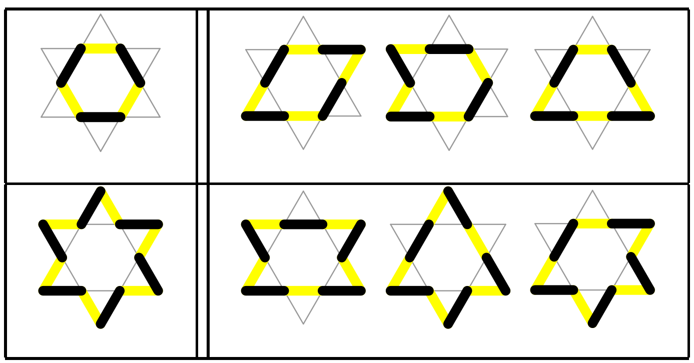


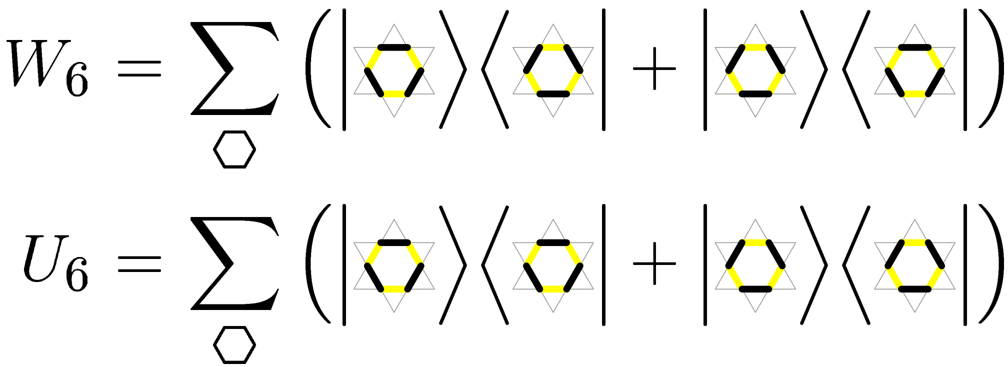
$$H = -h \sum_{\langle ij \rangle} \sigma^x_{ij} - K_3 \sum_{\triangle} \prod_{\triangle} \sigma^z_{ij} - K_6 \sum_{\hexagon} \prod_{\hexagon} \sigma^z_{ij} - K_{3+3} \sum_{\bowtie} \prod_{\bowtie} \sigma^z_{ij} - \cdots$$

Odd theory: $G_i = \prod_{i' \in i} \sigma^x_{ii'} = -1$

Effective Dimer Model: $h \gg K_n$

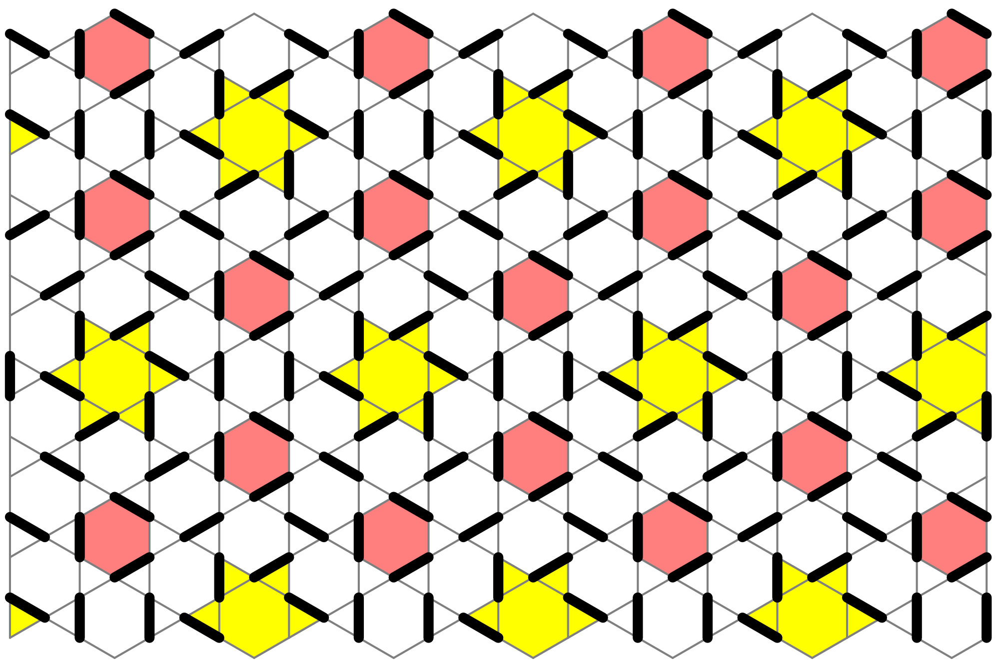
$$
\begin{aligned}
H = & -Nh - K_6 W_6 - \frac{K_6 K_{3+3}}{2h} W_8^{(ar.)} - \\
& - \left(\frac{2}{3}\frac{K_3^2}{h} + \frac{3}{8}\frac{K_{3+3}^2}{h} \right) U_6 - \left(\frac{1}{4}\frac{K_6^2}{h} + \frac{7}{9}\frac{K_3^2}{h} + \frac{1}{2}\frac{K_{3+3}^2}{h} \right) U_8 - \\
& - \left(\frac{1}{8}\frac{K_6^2}{h} + \frac{8}{9}\frac{K_3^2}{h} + \frac{5}{8}\frac{K_{3+3}^2}{h} \right) U_{10} - \left(\frac{1}{12}\frac{K_6^2}{h} + \frac{K_3^2}{h} + \frac{3}{4}\frac{K_{3+3}^2}{h} \right) U_{12} + \\
& + \mathcal{O}\left(\frac{K^3}{h^2} \right)
\end{aligned}
$$





Ground State: $h \gg \; K_n$

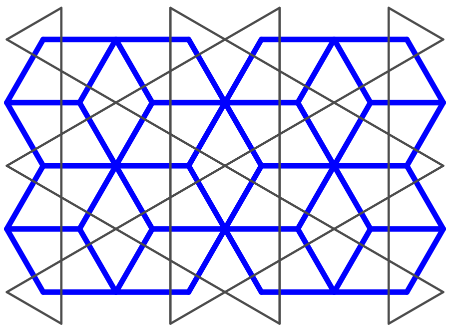
- 1^{st} order: maximum number of “perfect” hexagons
- 2^{nd} order: honeycomb pattern
  macroscopic degeneracy due to the “stars”
- 4^{nd} order: macroscopic degeneracy lifted



- Valence-bond order
- Unit-cell: 36 sites!
- Extremely “small” singlet gap $\sim \frac{K_6 K_{3+3}^3}{h^3}$

Effective Ising Model: $K_n \gg h$

- Dual representation:
  fully frustrated quantum Ising model on the *dice* lattice



$$H = -h \sum_{\langle lm \rangle} \epsilon_{lm} v_l^z v_m^z - K_3 \sum_{l_3} v_{l_3}^x - K_6 \sum_{l_6} v_{l_6}^x - K_{3+3} \sum_{(l_3 m_3)} v_{l_3}^x v_{m_3}^x - \cdots$$

Ground State:

- Ground state is disordered $\Longrightarrow$ spin liquid
- Visons v_l^x are gapped
- Gap is “large” $\sim K_n$

Comparison With Numerics

Reliable Aspects of Numerics

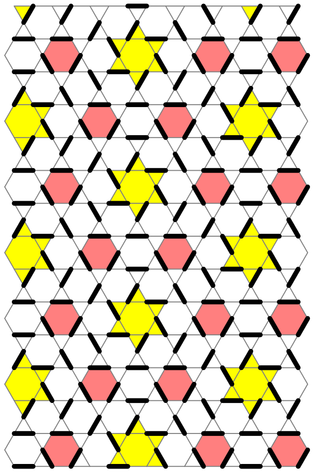
Feature found in numerics	VB	SL
Large number of singlets below the spin-gap	✓	✗
Extremely small singlet energy scale	✓	✗

Aspects of Numerics Sensitive to Finite Size

Feature found in numerics	VB	SL
No long range order	✗	✓
Deconfined spinons	✗	✓
Character of spectrum (gaps, degeneracy. . .)	✗	✗

Proposal for Kagome Heisenberg AF

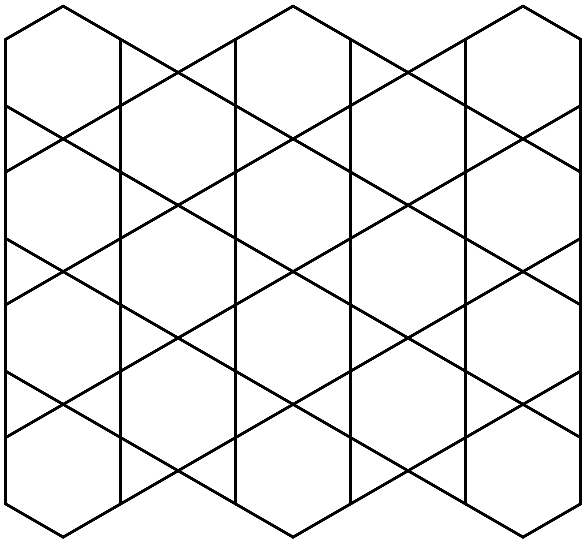
- Exotic valence-bond ordered phase:
  Unit-cell as large as maximum sample size in numerics!
- Lowest lying excitations:
  gapped, heavy singlets
- Singlet gap is extremely small
- Excitations with magnetic moment:
  gapped $S = 1$ magnons
  (confined spinon pairs)



The valence-bond order is also analytically favored. . .

Similar results for the checkerboard lattice:
agreement with numerics

Kagome Lattice
Ising Antiferromagnet



Ising model: Motivation

Physical Motivation:

- More frustrated than the Heisenberg model
- Interesting physics expected:
  valence-bond order, spin liquid?
- Easy-axis anisotropy
  $\Longrightarrow$ a route to the isotropic Heisenberg model

Theoretical Motivation:

- Amenable to reliable Monte Carlo numerics
- Analytical methods available:
  U(1) gauge theory, duality, field theory

Questions

- Nothing conserved: transverse field dynamics

$$H = J \sum_{\langle ij \rangle} S_i^z S_j^z - \Gamma \sum_i S_i^x \quad , \quad \Gamma \ll J$$

- Total spin conserved: XXZ dynamics

$$H = J_z \sum_{\langle ij \rangle} S_i^z S_j^z + J_\perp \sum_{\langle ij \rangle} \left(S_i^x S_j^x + S_i^y S_j^y \right) \quad , \quad J_\perp \ll J_z$$

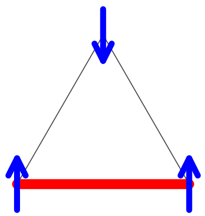
- Including higher order dynamical processes. . .
- What phases are possible?
- Is there a topological spin liquid phase?

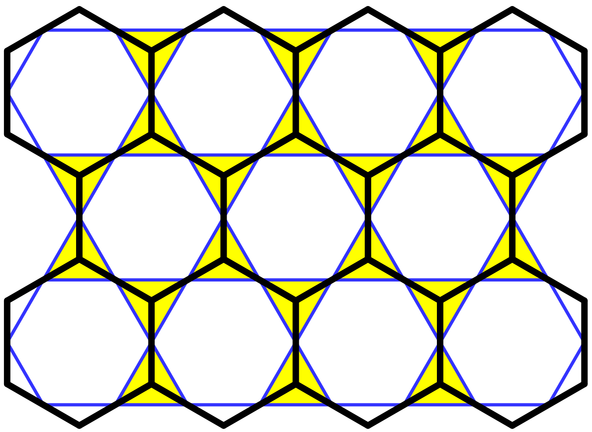
A U(1) Lattice Gauge Theory

$$H_z = J \sum_{\langle ij \rangle} S_i^z S_j^z = \frac{J}{2} \sum_{\triangle} \Big(\sum_{i \in \triangle} S_i^z \Big)^2 + \text{const.}$$

- Minimum frustration $\Longrightarrow$ local constraint

$$(\forall p) \quad s_p^z = \sum_{q \in p} S_{\langle pq \rangle}^z \in \left\{ \pm \frac{1}{2} \right\}$$





Kagome sites i

$\Updownarrow$

honeycomb bonds $\langle pq \rangle$

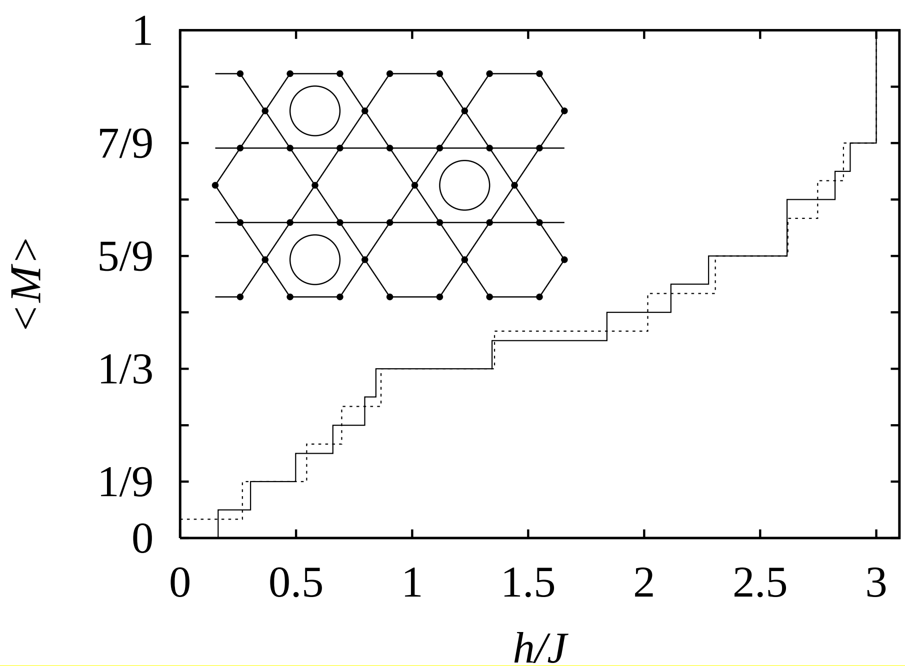
Analysis

- Compact U(1) gauge theory on the honeycomb lattice
- Honeycomb lattice is bipartite:
  - Kagome spin $\Longrightarrow$ electric field vector
  - plaquette spin $\Longrightarrow$ charged boson
- Fixed background charge: breaks lattice symmetries
- Charge=1 bosonic matter field
  $\Longrightarrow$ a non-topological disordered phase exists (in 2D)

Analysis uses a duality transformation, sine-Gordon theory, and field theory methods. . .

Phases: Transverse Field Ising Model

- Disordered non-topological phase
  agrees with Monte-Carlo (Moessner, Sondhi)
- Valence-bond ordered phase
  broken translational symmetry (3-fold degeneracy)
  broken global $\mathbb{Z}_2$ symmetry



Ordered phase corresponds to the $\frac{1}{3}$ of the saturated magnetization. (plateau in magnetization curve)

Dynamics of Frustrated Bonds

- Applicable to other lattices
- Convenient for more *microscopic* insight
- Cannot handle longitudinal field

Analysis:

1. Frustrated bond $\longrightarrow$ dimer on the (bipartite) dice lattice
2. Compact U(1) gauge theory on the dice lattice
3. Dual lattice height theory on the Kagome lattice
   (two coupled height fields)
4. Large degeneracy of saddle-points lifted by fluctuations
5. Study which states are entropically preferred
   (search for *order-by-disorder*)

Microscopic Insight

Transverse Field Dynamics:

- Disordered non-topological ground state
- Probability amplitude concentrated around maximally flippable states
- Quasi-localized excited states
- Wave-function is well approximated by a Gutzwiller projection

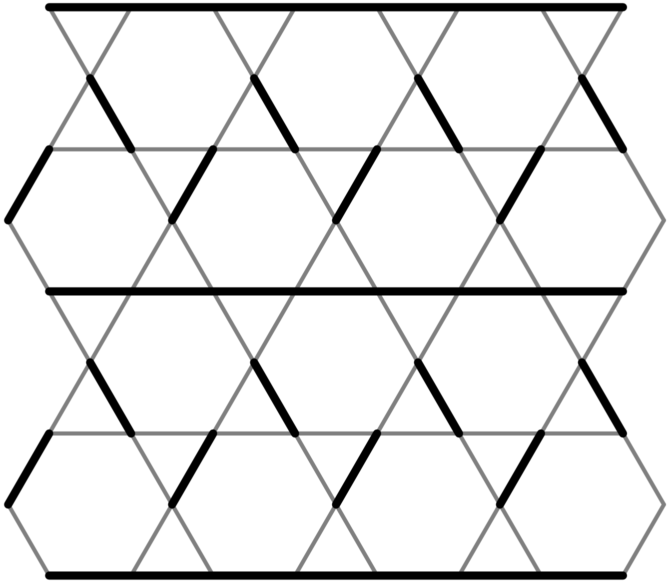
XXZ Dynamics:

- Valence-bond ordered ground state

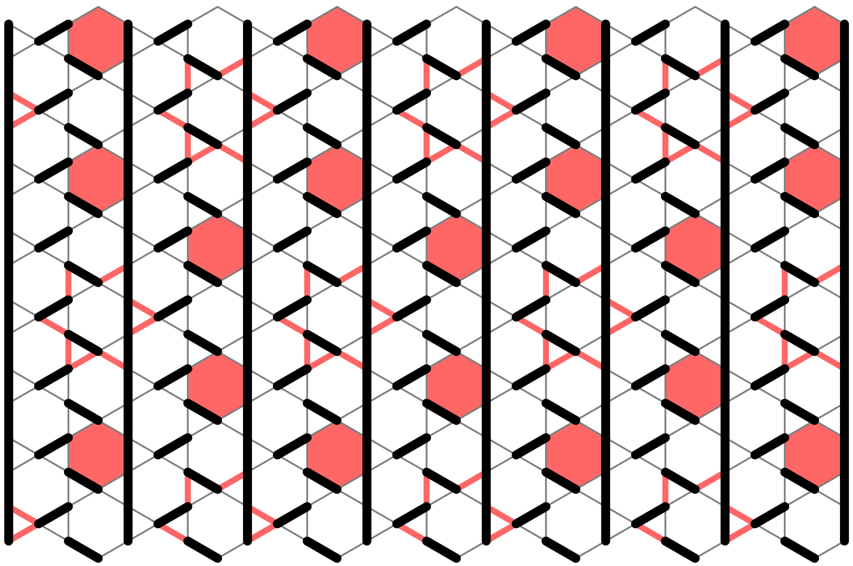
XXZ Dynamics

- Anisotropic Heisenberg model
- Strong easy-axis anisotropy

Frustrated Bonds



Partial Melting?



Conclusions

- Unconventional and fundamental physics emerges at low energies in frustrated magnets

Kagome Lattice Antiferromagnets:

- Isotropic Heisenberg: valence-bond ordered
  - large unit cell
  - extremely small energy scale for singlet states
- Easy-axis Heisenberg: possibly valence-bond ordered
- Ising in external field:
  - disordered, but not topological phase
  - valence-bond ordered magnetized phase