Title: Mesonic eigenstates for magnetic monopoles in quantum spin ice

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Abstract: <p>The quest for quantum spin liquids is an important enterprise in strongly correlated physics, yet candidate materials are still few and far between. Meanwhile, the classical front has had far more success, epitomized by the exceptional agreement between theory and experiment for a class of materials called spin ices. It is therefore natural to introduce quantum fluctuations into this well-established classical spin liquid model, in the hopes of obtaining a fully quantum spin liquid state.</p>

<p> </p>

<p>The spin-flip excitations in spin ice fractionalize into pairs of effective magnetic monopoles of opposite charge. Quantum fluctuations have a parametrically larger effect on monopole motion than on the spin ice ground states so the leading manifestations of quantum behavior appear when monopoles are present. We study magnetic monopoles in quantum spin ice, whose dynamics is induced by a transverse field term. For this model, we find a family of extensively degenerate excited states, that make up an approximately flat band at the classical energy of the nearest neighbor monopole pair. These so-called mesonic states are exact up to the splitting of the spin ice ground state manifold. In my talk I will discuss their construction and properties that may be relevant in neutron scattering experiments on quantum spin ice candidates.</p>

Mesonic (and hydrogenic!) eigenstates for magnetic monopoles in quantum spin ice

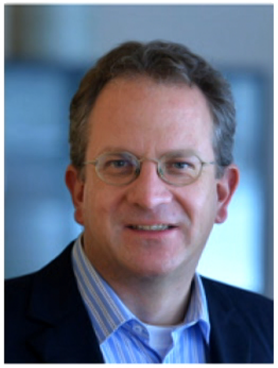
Phys. Rev. B **92**, 100401 (2015)
more on the way

Olga Petrova

École normale supérieure

Département de Physique
École normale supérieure

Collaborators



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MPI PKS
(Dresden, Germany)

Shivaji Sondhi
Princeton University
(Princeton, USA)

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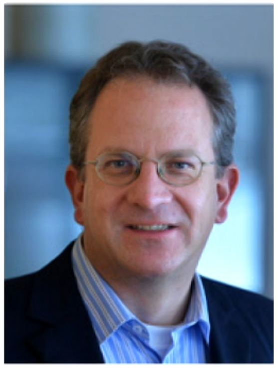

Roderich Moessner
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(Princeton, USA)

Outline

- Why study excitations in quantum spin liquids?
  - because they are interesting!
    fractionalization, Majorana fermions, anyons, etc
  - ground state: no broken symmetries
  - excited states: clear experimental signatures (sometimes)
- Classical spin ice
  - magnetic monopoles
- Quantum spin ice
  - the model
  - the state graph description
  - vacancy problem $\approx$ the Bethe lattice
  - excited mesonic states
- Conclusions

Quantum spin liquids: what are they and why look at their excitations?

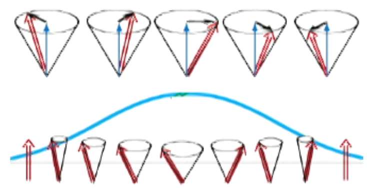
- QSL: a state that cannot be approximated as a product state over any finite blocks [L. Balents]
- No spontaneous symmetry breaking
  - distinct phases with the same symmetry
  - characterized by other properties including excitations
  - local / spatially averaged probes not suitable for the ground state
- Signature of QSL in excitations
  - exotic quasiparticles that can only be found in QSLs
  - fractionalization: spinons, magnetic monopoles, anyons, etc

What does it mean for an excitation to fractionalize?

Regular magnets:

- LRO, broken symmetry, Goldstone mode
- Excitations: magnons

spin wave in a ferromagnet:



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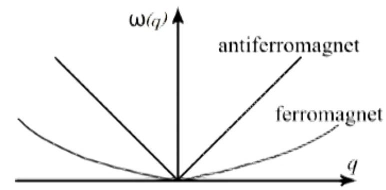

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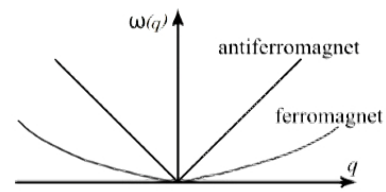
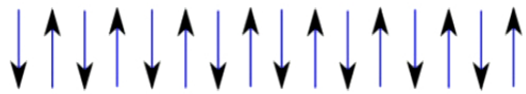


Spin liquids:

- Fractionalized excitations
- Example: Heisenberg AFM chain
- Neutron scattering: continuum

XXZ antiferromagnetic chain:



$$H = J\sum_n (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z)$$

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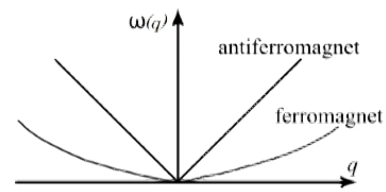

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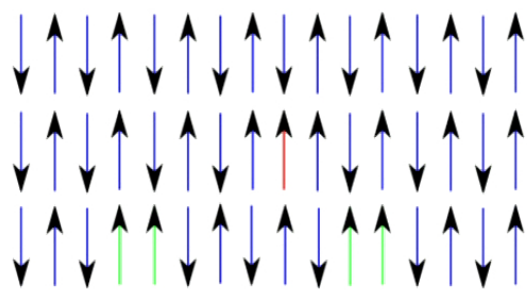
magnon splits into 2 spinons:



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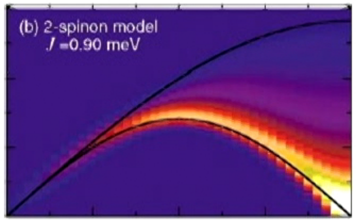

Stone *et al* PRL **91**, 037205 (2003)

Spin liquids:

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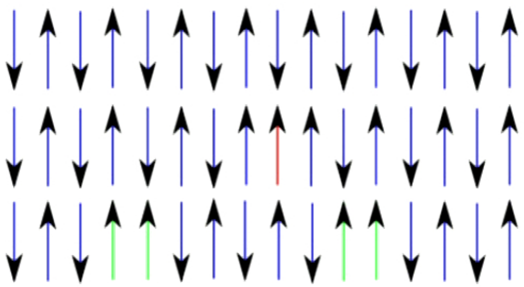

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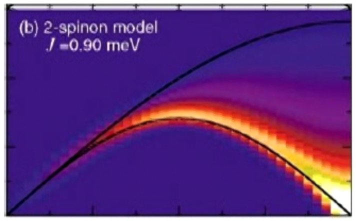

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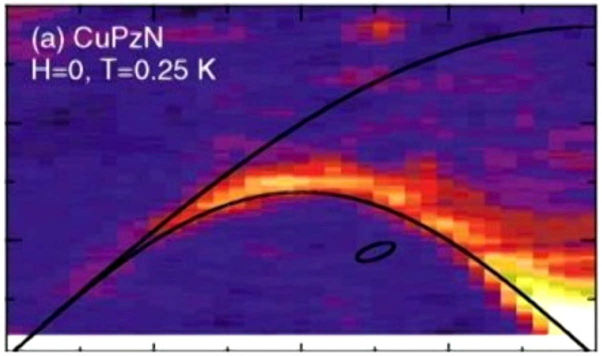
Spin liquids:

- Fractionalized excitations
- Example: Heisenberg AFM chain
- Neutron scattering: continuum

Spin liquids exist!



Outline

1 Why study excitations in QSLs?

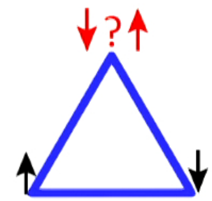
2 Classical spin ice

3 Quantum spin ice
- The vacancy problem
- Excited mesonic states

4 Conclusions

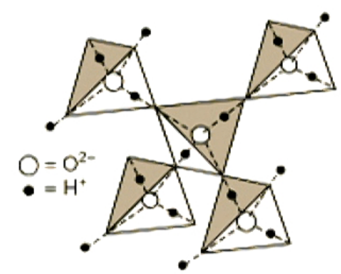
Geometric frustration in water ice

Frustration: all terms in H cannot be minimized
Example: Ising antiferromagnet on a triangle
Leads to classical ground state degeneracy

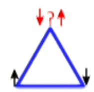


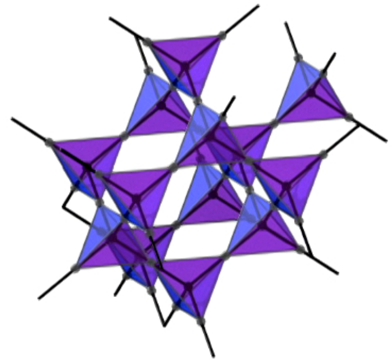
- For every O: 2 H's nearby, 2 H's further away
- 16 possible ways to arrange 4 H's near one O
- Only 6 satisfy the ice condition $\rightarrow$ $\frac{6}{16} = \frac{3}{8}$ of the configurations are allowed
- N water molecules $\rightarrow$ $2N$ hydrogen atoms
- $(\frac{3}{8})^N (2^{2N}) = (\frac{3}{2})^N$ possible configurations
- Residual entropy: $R \ln \frac{3}{2}$

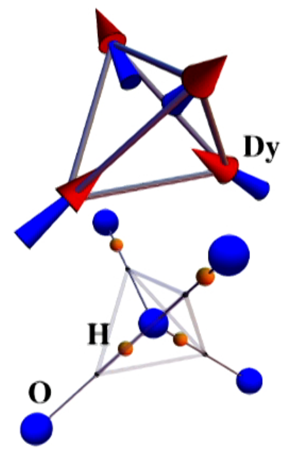
[Pauling 1935]



Classical spin ice: the basics

- $Dy_2Ti_2O_7$, $Ho_2Ti_2O_7$
- Ground state of the magnetic ion: doublet
- Crystal field → easy axis anisotropy
- Effective Ising antiferromagnet
- Pyrochlore lattice → frustration 
- Ice rules: 2-in 2-out
- Excitations: magnetic monopoles





Spin ice: the dumbbell model

$$H_{\rm spin} = \sum_{\langle ij \rangle} J_{zz} S_i^z S_j^z + \text{dipolar interactions}$$

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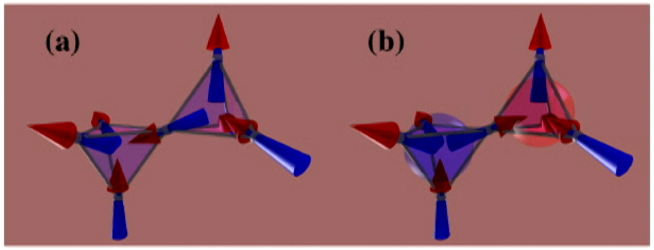
Dumbbell model

Magnetic moment $\rightarrow$ pair of charges

Charges on the diamond lattice: $Q = 0, \pm 2, \pm 4$

$$H \approx \frac{v_0}{2} \sum_{\alpha} Q_\alpha^2 + \frac{\mu_0}{4\pi} \sum_{\alpha<\beta} \frac{Q_\alpha Q_\beta}{r_{\alpha\beta}}$$

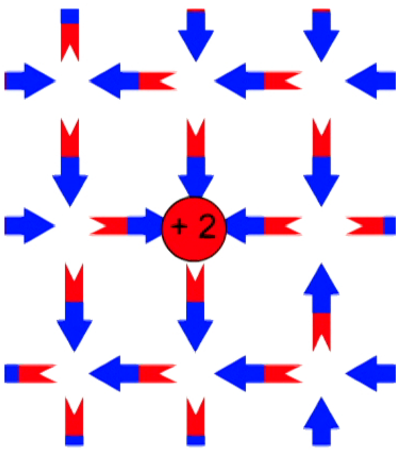
ground state: zero charges

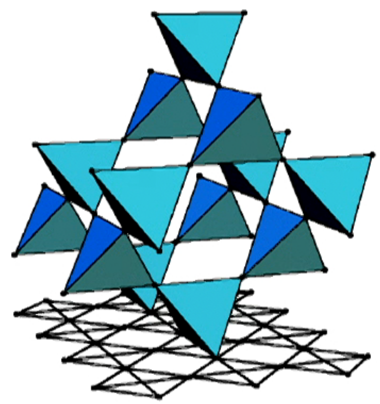


Castelnovo, Moessner, Sondhi

Spin ice: magnetic monopoles

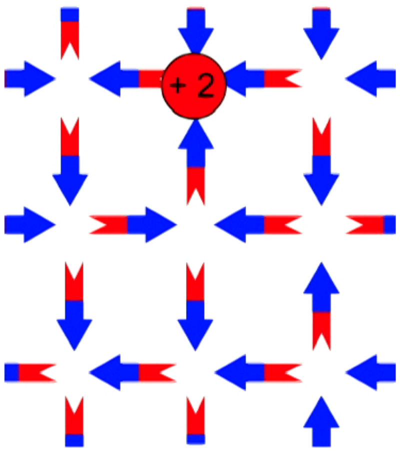
- ±2 charge: 3 in/out (majority), 1 out/in (minority)

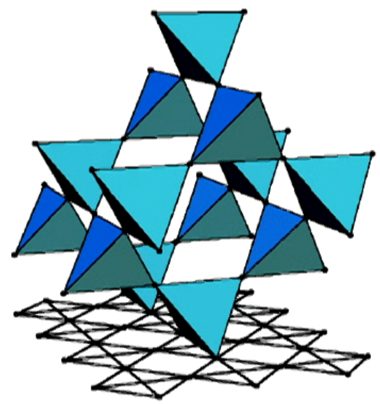




Spin ice: magnetic monopoles

- ± 2 charge: 3 in/out (majority), 1 out/in (minority)
- Flipping a majority spin: shifts a monopole





Spin ice: magnetic monopoles

- ± 2 charge: 3 in/out (majority), 1 out/in (minority)
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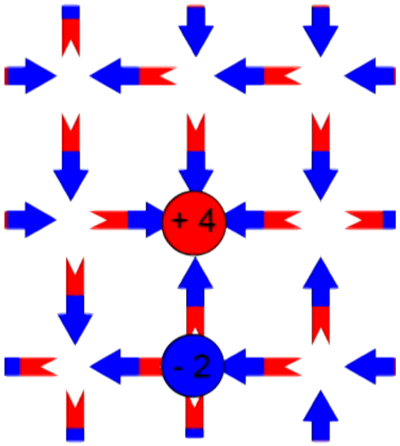
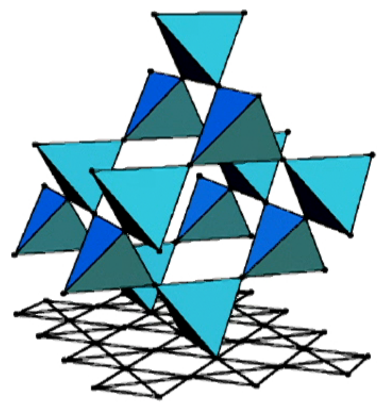
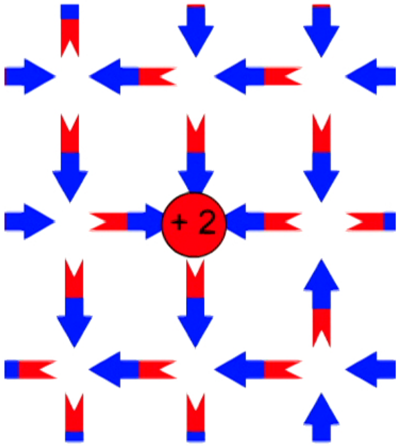
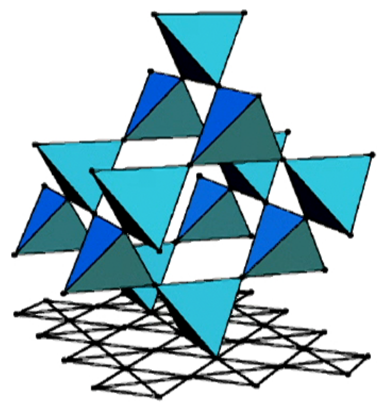




Spin ice: magnetic monopoles

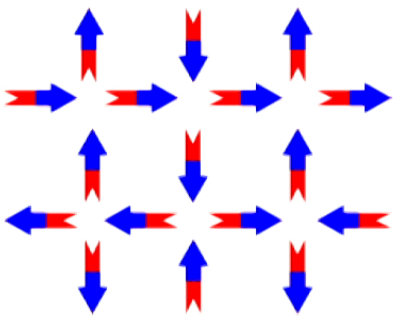
- ± 2 charge: 3 in/out (majority), 1 out/in (minority)
- Flipping a majority spin: shifts a monopole
- Flipping a minority spin: creates ± 4 and ∓ 2 charges
- Three ways for the monopole to go

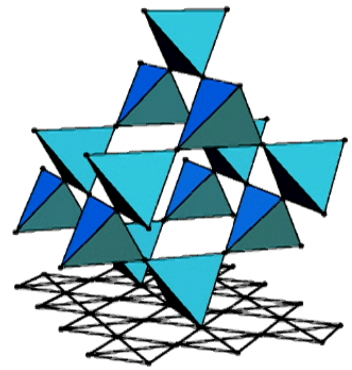




Quantum spin ice: what happens to the ice states?

$$H_{\mathrm{QSI}} = \sum_{\langle ij \rangle} J_{zz} S_i^z S_j^z - \sum_i t S_i^x + \text{dipolar interactions}$$



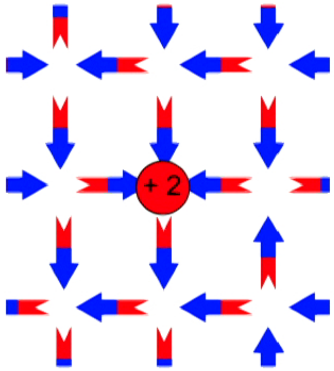


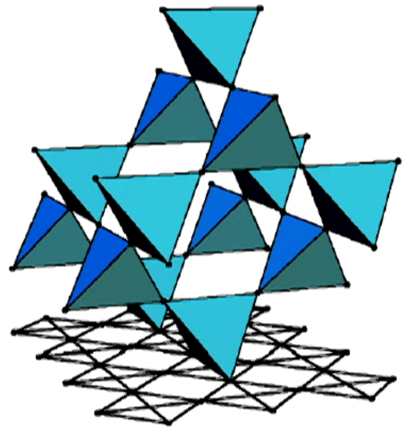
Quantum tunneling between different ice states

- Shortest closed loop on pyrochlore: hexagon
- Ground state degeneracy (only) lifted at $O(t^6)$
- Unique ground state, photon excitations Huse et al., Henley, Hermele et al.
- Is there a better place to look for quantum effects?

What if there is a monopole present?

$$H_{\mathrm{QSI}} = \sum_{\langle ij \rangle} J_{zz} S_i^z S_j^z - \sum_i t S_i^x + \text{dipolar interactions}$$



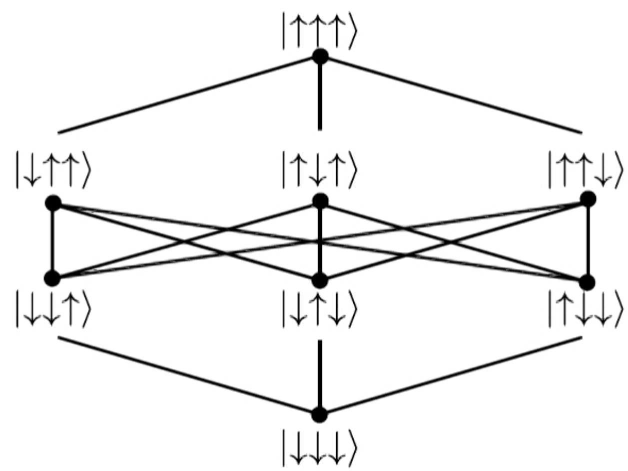


- Monopole hops at $O(t)$
- $\frac{t^6}{(\text{monopole cost})^5} < \mathrm{T} < t$

What is the signature of monopoles in QSI?

State graph

$$H_{\text{3 spins}} = -\sum_{\langle ij \rangle} J_{zz} S_i^z S_j^z - \sum_i t S_i^x$$

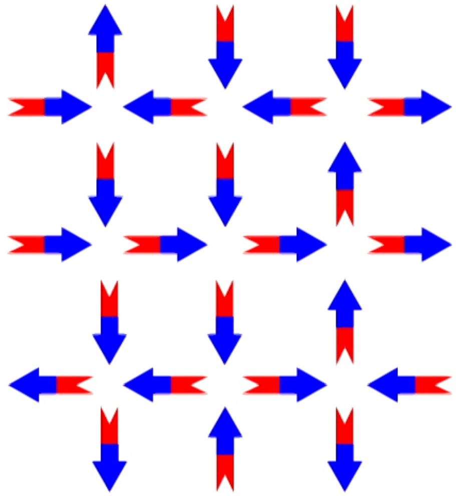


- vertices: spin configurations
- edges: connect vertices connected by H

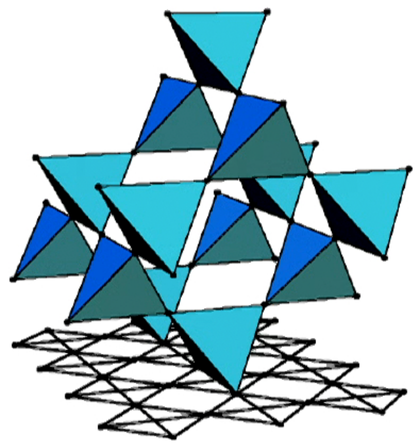
Vacancies in spin ice

[Sen, Moessner 2014]

Ghost spins: pairs of charged tetrahedra



$$H \approx \frac{V_0}{2} \sum_{\alpha} Q_{\alpha}^2 + \dots$$



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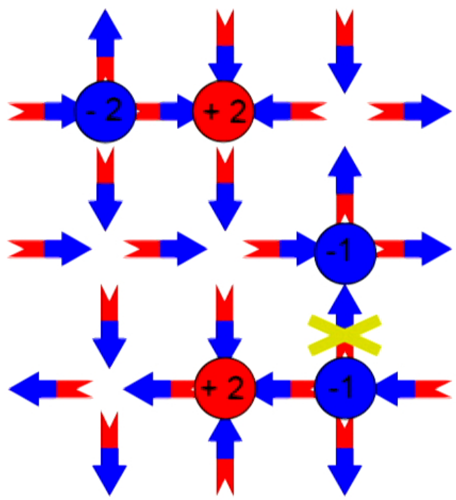
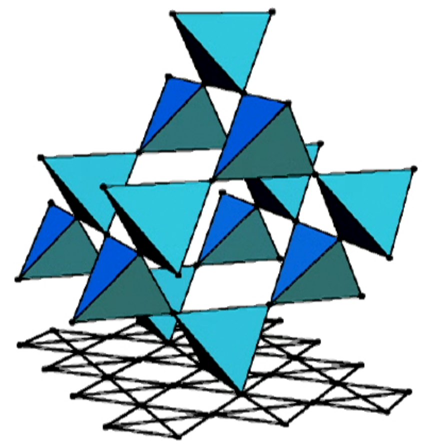




One bulk monopole hopping

What happens on the state graph?

- 4 ways to emit a monopole from the vacancy

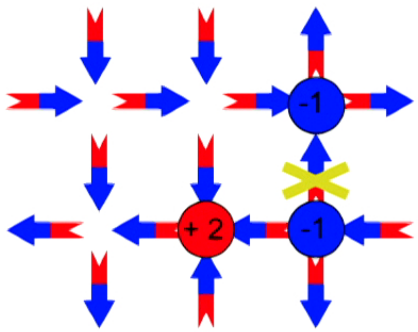
$$H|0\rangle = -t\sum_{m=1}^{4}|m\rangle, \qquad |0\rangle \to \text{no bulk charge}$$

t: transverse field = hopping

- 3 ways for the monopole in the bulk to hop

$$H|n\rangle = \left(I + \frac{C}{d_n}\right)|n\rangle - t\sum_{m=1}^{3}|n_m\rangle, \qquad |n\rangle \neq |0\rangle$$

$I > 0$: cost of ionizing vacancy
$C < 0$: vacancy-monopole Coulomb interaction



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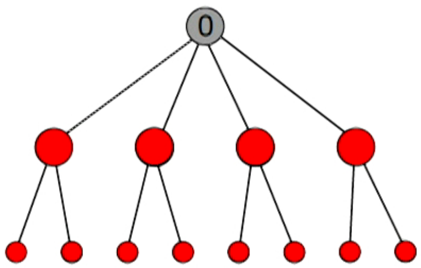
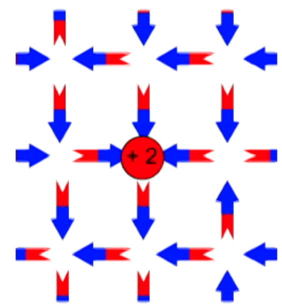
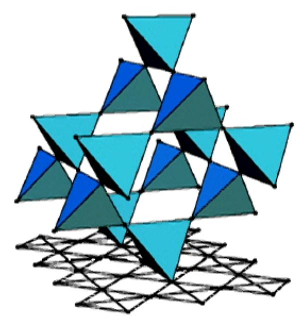


State lattice:
states $\rightarrow$ vertices

Closed cycles on the state graph

- shortest cycle in pyrochlore: hexagon
- t^6 changes state of the system
- t^{12} brings to same state, but self-retracing
- shortest closed cycle: 20 spin flips
  $\approx \frac{t^{20}}{(\text{monopole cost})^{19}}$ effect





Chen, Onsager, Bonner, Nagle 1974

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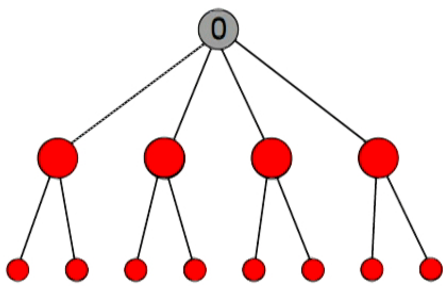
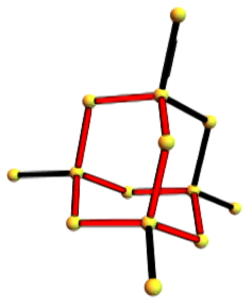
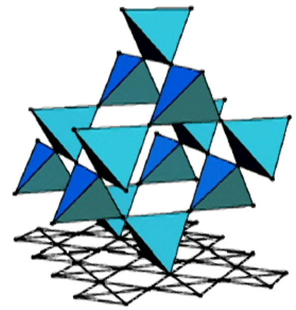
- t^{12} brings to same state, but self-retracing
- shortest closed cycle: 20 spin flips
  $\approx \frac{t^{20}}{(\text{monopole cost})^{19}}$ effect
- Ignore closed cycles $\rightarrow$ Bethe lattice

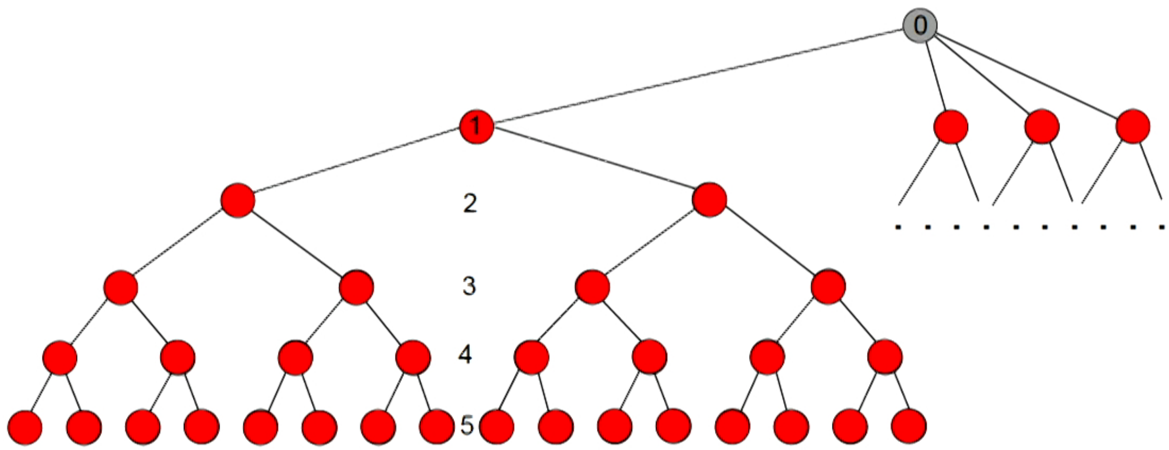






Chen, Onsager, Bonner, Nagle 1974

Coulomb problem on the Bethe lattice



Single particle hopping on the Bethe lattice

- $H|n\rangle = \left(I + \frac{C}{d_n}\right)|n\rangle - t\sum_{m=1}^{3}|n_m\rangle$
- Distance between monopoles $\equiv$ generation of the Bethe lattice
- $H|n\rangle = \left(I + \frac{C}{k}\right)|n\rangle - t\sum_{m=1}^{3}|n_m\rangle$ (site $n \in k^{\text{th}}$ generation)

The Bethe lattice problem ...

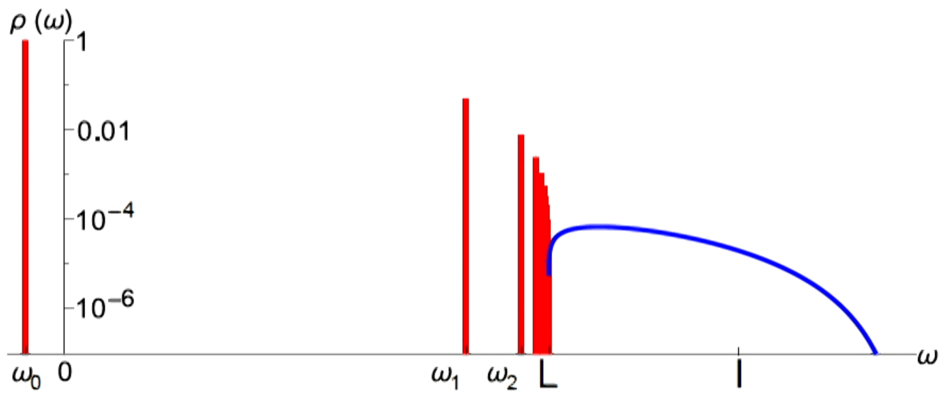
... is exactly solvable!

$$G_k(w) = \frac{2k/w}{\sqrt{1+x^2}+1} \frac{1}{k - \frac{C/w}{\sqrt{1+x^2}}} \frac{F_1^2\left(1 - \frac{C/w}{\sqrt{1+x^2}}, k+1, k+1-\frac{C/w}{\sqrt{1+x^2}}, \frac{1-\sqrt{1+x^2}}{1+\sqrt{1+x^2}}\right)}{F_1^2\left(1 - \frac{C/w}{\sqrt{1+x^2}}, k, k-\frac{C/w}{\sqrt{1+x^2}}, \frac{1-\sqrt{1+x^2}}{1+\sqrt{1+x^2}}\right)}$$

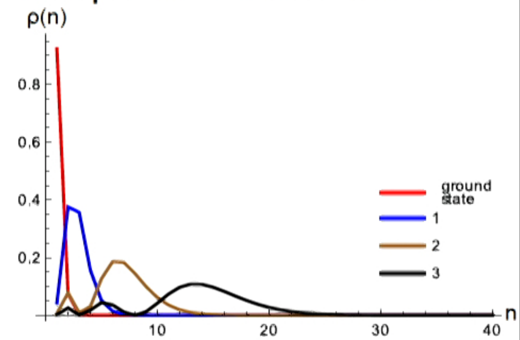
Local density of states at site 0

- Infinitely many bound states
- $w_0 < 0$ due to $t \neq 0$
- Gap to w_1 less than I due to C and $t \neq 0$
- Bound states accumulate below continuum
- Continuum band: $w^2 - I < 8t^2$

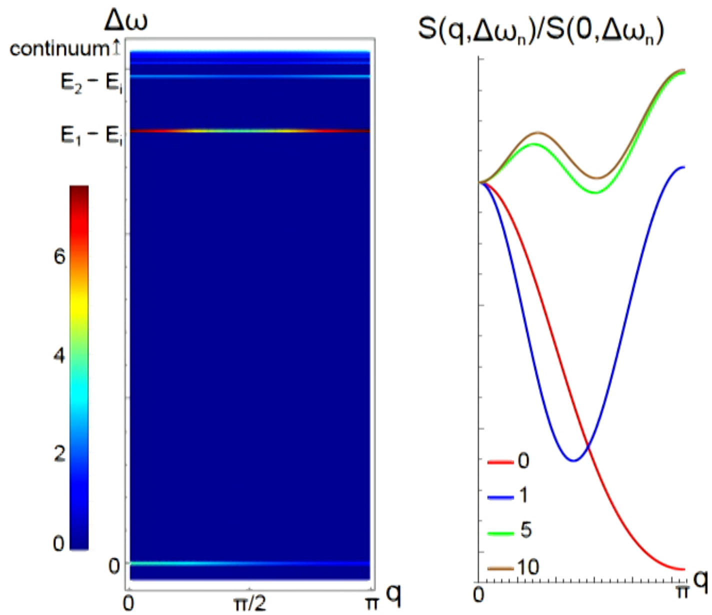
$$C = -I/3$$
$$t = I/10$$
$$L = I - \sqrt{8t^2}$$



Shape of bound states



Dynamic structure factor $S(\vec{q}, \Delta w) = \sum_f \delta(E_f - E_i - \Delta w)|\sum_{\vec{R}} \langle f|S^+_{\vec{R}}|i\rangle e^{i\vec{q}\cdot\vec{R}}|^2$

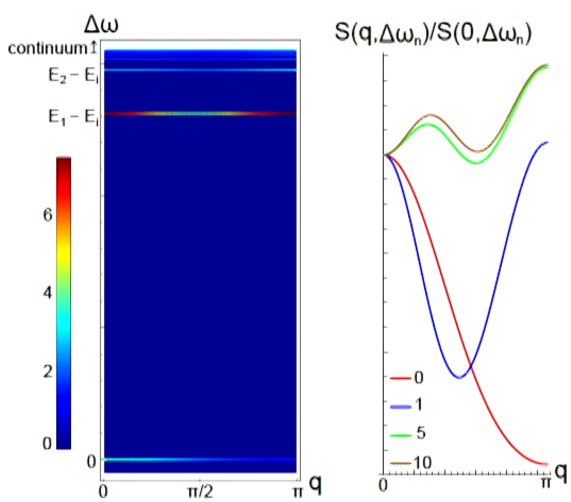


(a) (b)

powder averaged neutron scattering: $S(q, \Delta w)$

Figure (a): color density plot of $S(q, \Delta w)$

Dynamic structure factor $S(\vec{q}, \Delta w)$: summary



(a) (b)

$$S(\vec{q}, \Delta w) = \sum_f \delta(E_f - E_i - \Delta w) \left| \sum_{\vec{R}} \langle f | S^+_{\vec{R}} | i \rangle e^{i\vec{q}\cdot\vec{R}} \right|^2$$

- powder averaged $S(\vec{q}, \Delta w) \to S(q, \Delta w)$
- dilute vacancies limit
- discrete bound states that accumulate below continuum $I - \sqrt{8t^2}$
- If $t = 0$, would only see the $E_1 - E_0$ line
- highly excited states look similar

Constructing excited eigenstates

$$H_{\mathrm{QSI}} = \sum_{\langle ij \rangle} J_{zz} S_i^z S_j^z - \sum_i t S_i^x$$

For a given classical spin ice configuration i:

$$|f_i\rangle = \sum_{\vec{R}} S^x_{\vec{R}} S^z_{\vec{R}} |i\rangle$$

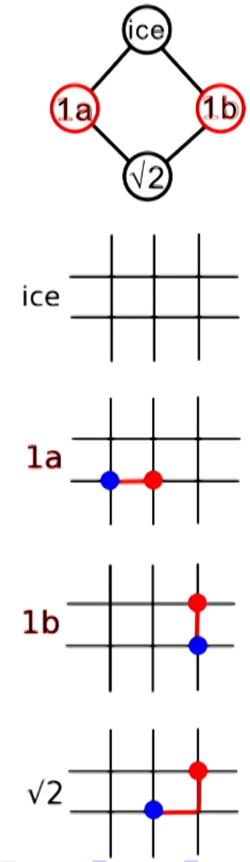
In the zero and two-monopole sector:

$$H_{\mathrm{QSI}}|f_i\rangle = (\text{cost of NN monopole pair})|f_i\rangle$$

Exact excited eigenstate!

Superposition of all nearest-neighbor monopole pairs in i

Remove restriction: eigenstate up to $O(t^6)$



Excited mesonic eigenstates

- Classical degeneracy partially preserved
- These states are quantum: destructive interference
- Delocalized, despite spin backgrounds being disordered!
- Important: bipartite state graph
  Sublattice A: monopoles on the same real space sublattices
  Sublattice B: monopoles on different real space sublattices

  State graph of

  $$H_{=}\sum_{\langle ij\rangle}\left(J_{zz}S_i^z S_j^z - tS_i^+ S_j^-\right)$$

  is not bipartite $\rightarrow$ no mesons
- Vanishing fraction of the dynamic structure factor

Results

- Vacancy problem:
  - exactly solvable model
  - hydrogenic bound states
  - sharp signature in dynamic structure factor
- Mesonic states:
  - (nearly) exact family of excited states
  - extensive degeneracy
  - are they visible in experiments?