Yong Baek Kim
University of Toronto

CIFAR "Spring" School, May 5, 2010

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Emergent Quantum Phases in Frustrated Magnets

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Emergent Quantum Phases

What are good places to look for "Emergent Behavior" of correlated many-body system ?

Competing interactions
No separation of energy scales
Competing phases almost degenerate in energy

Many-Body Frustration

Emergent Quantum Phases

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Quantum fluctuations delicately lift the many-body degeneracy - Possible Emergence of New Phases

Fluctuation leads to Novel Phases

Emergent Quantum Phases

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Competing interactions
No separation of energy scales
Competing phases almost degenerate in energy

Many-Body Frustration

Quantum fluctuations delicately lift the many-body degeneracy - Possible Emergence of New Phases

Fluctuation leads to Novel Phases

Inherently Strong Coupling Problems !

Outline

1. Classical and Quantum Theory of Frustrated Magnets

2. Novel Magnetic Order in Diamond Lattice Spinel

   Quantum Order by Disorder

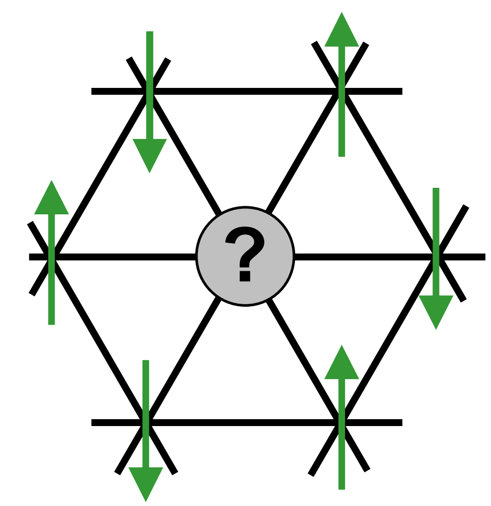
3. Spin Liquid on Hyper-Kagome Lattice $Na_4Ir_3O_8$

   Disorder by Disorder

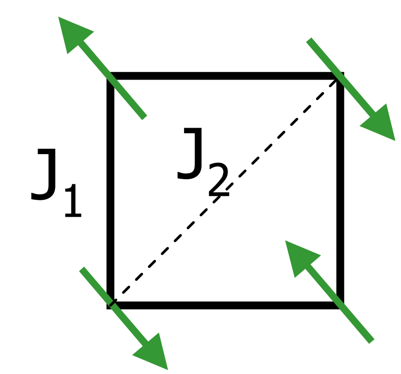
Introduction to Frustrated Magnets

Geometric Frustration:

The arrangement of spins on a lattice precludes (fully) satisfying all interactions at the same time



Large degeneracy of the (classical) ground state manifold $\sim e^{\alpha N}$



Consequence:

No energy scale of its own; any perturbation is strong

Mother of the many conventional and exotic phases

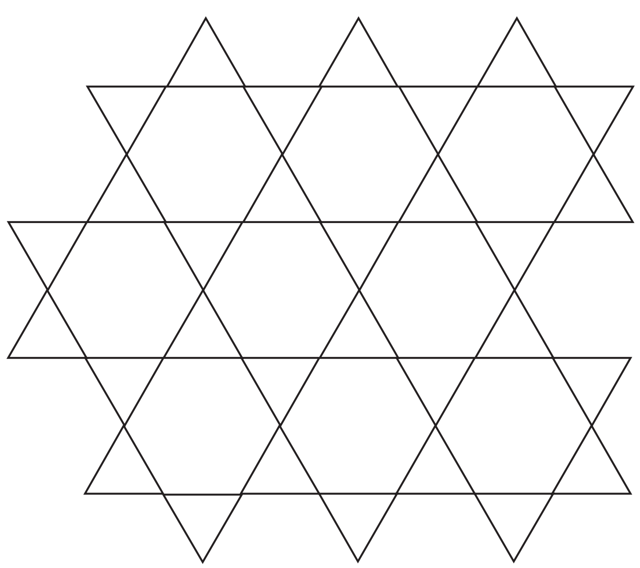
Origin of Classical Ground State Degeneracy

Classical nearest-neighbor antiferromagnetic
Heisenberg model on lattices with corner-sharing simplexes
(simplex = triangle, tetrahedron)

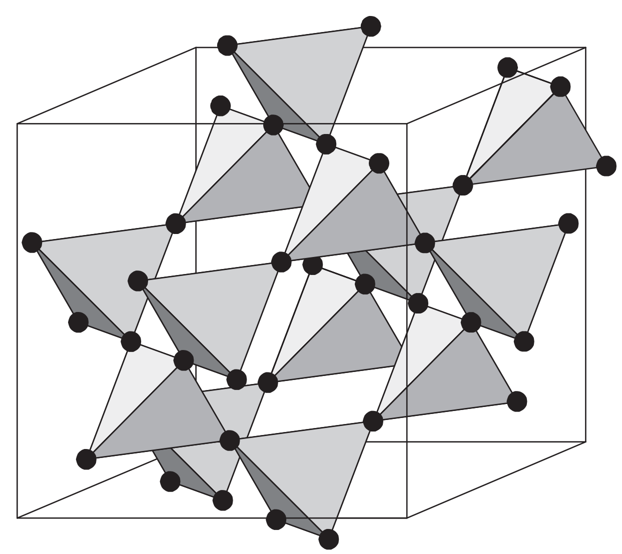
$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = \frac{J}{2} \sum_{\text{simplex}} \left(\sum_{i \,\epsilon\, \text{simplex}} \mathbf{S}_i \right)^2$$

$\mathbf{S}_i$ is a vector with a fixed length

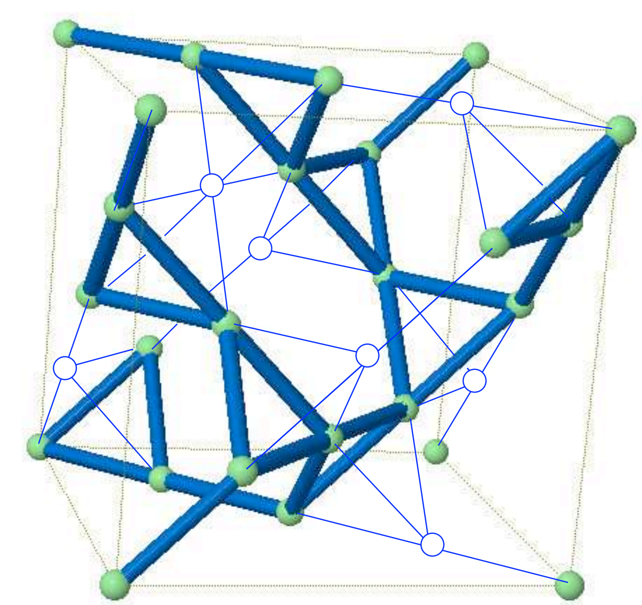
Kagome



Pyrochlore



Hyper-Kagome



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$\mathbf{S}_i$ is a vector with a fixed length

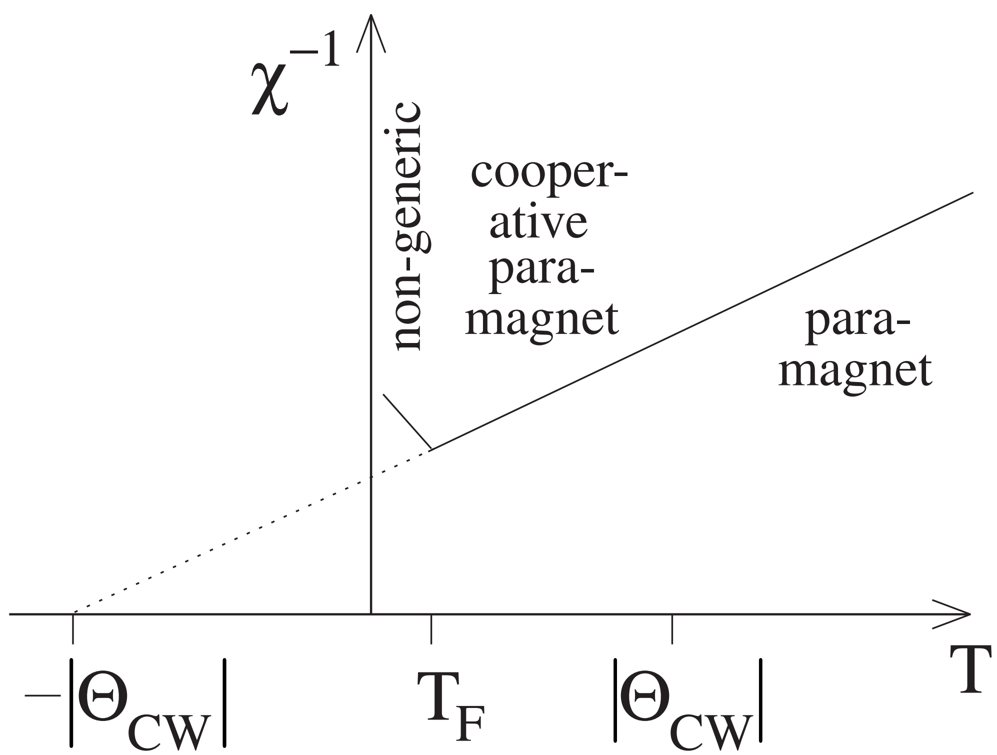
Classical ground state should satisfy $\sum_{i \ \epsilon \ \text{simplex}} \mathbf{S}_i = 0$

These constraints are not independent; counting is subtle

Nonetheless there exists macroscopic degeneracy

Introduction to Frustrated Magnets

Susceptibility 'fingerprint':



Θ_{CW}: Curie-Weiss temperature;
Mean-field Ordering Temperature;
interaction energy scale

$$\chi \sim \frac{1}{T - \Theta_{\mathrm{CW}}} \qquad T \gg |\Theta_{\mathrm{CW}}|$$

$$f = \frac{|\Theta_{\mathrm{CW}}|}{T_F}$$ useful diagnostic of frustration

$f \gg 1$ strong frustration

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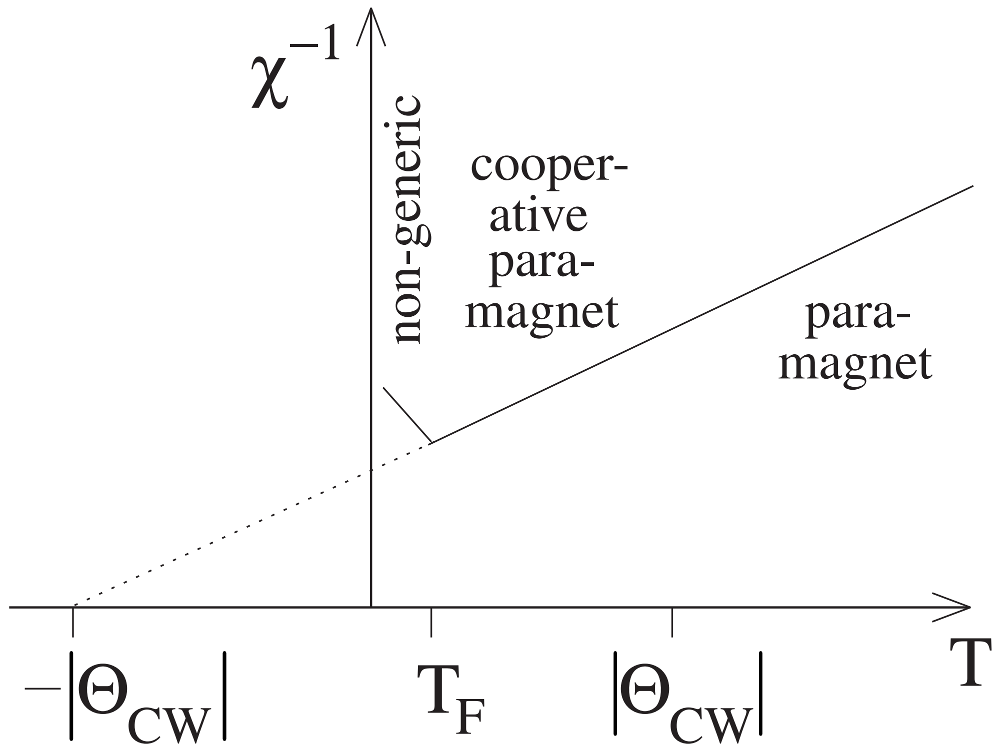

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$T_F < T < |\Theta_{\rm CW}|$

Cooperative paramagnet:
correlations remain weak
more universal

$T < T_F$

Magnetically ordered ?
Spin liquid ? Glassy ?
not universal

Order by Disorder

Order by Disorder via Thermal Fluctuations:

Different entropic weighting to each ground state

Softer the fluctuations around a particular ground state, more likely this ground state will be entropically favored.

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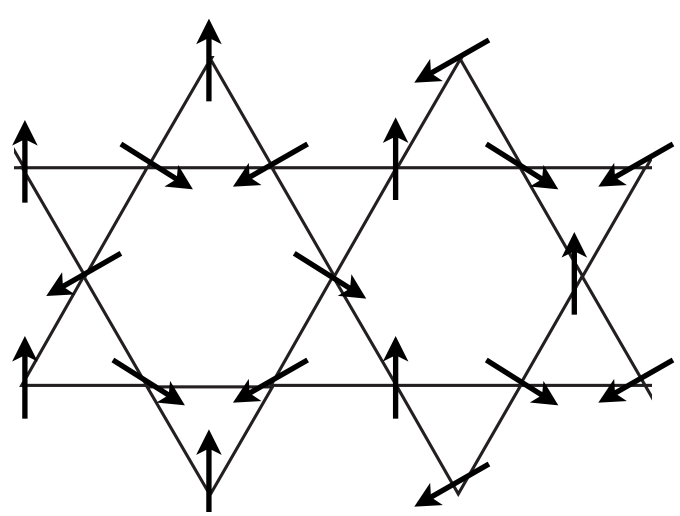
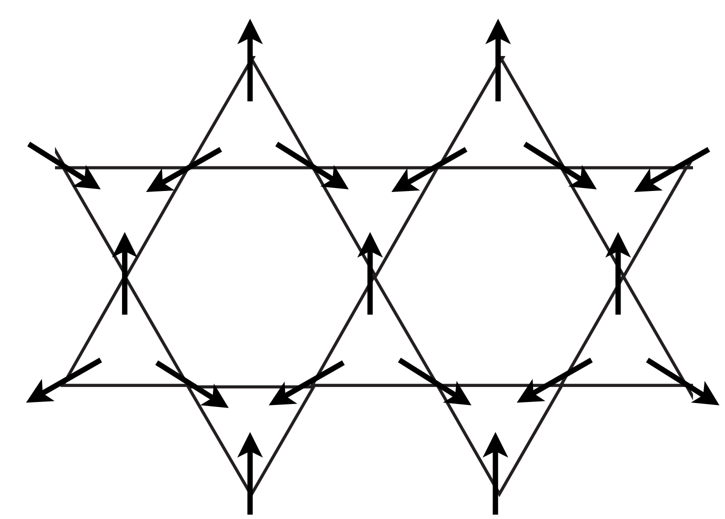
Classical Heisenberg Model on the Kagome lattice

Consider co-planar states $\sum_{i\ \epsilon\ \triangle} \mathbf{S}_i = 0$



$\sqrt{3} \times \sqrt{3}$



$q = 0$

Order by Disorder

Order by Disorder via Thermal Fluctuations:

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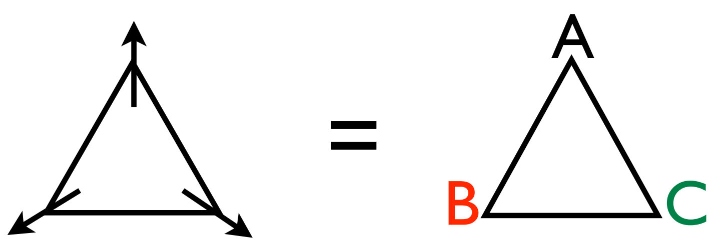
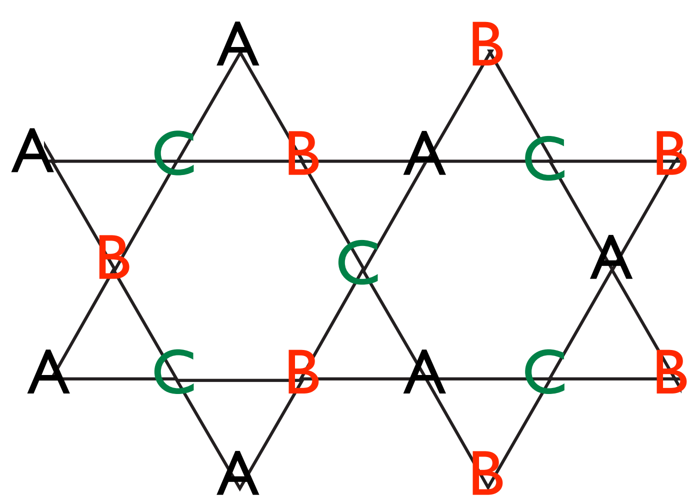
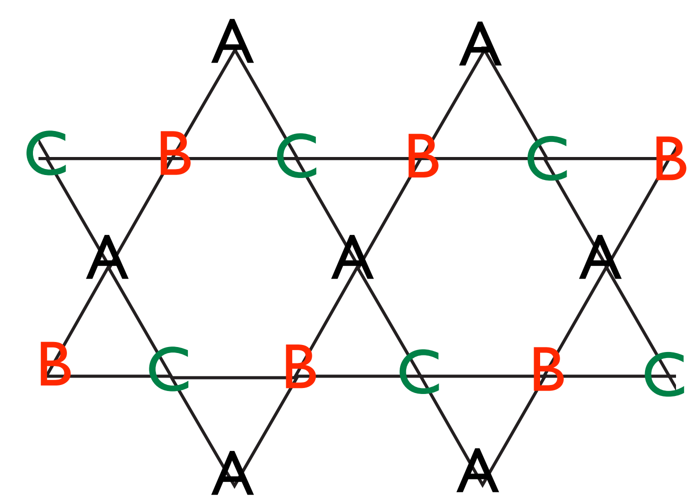


Three-State Potts spins

Degeneracy = $e^{0.379N}$



$\sqrt{3} \times \sqrt{3}$



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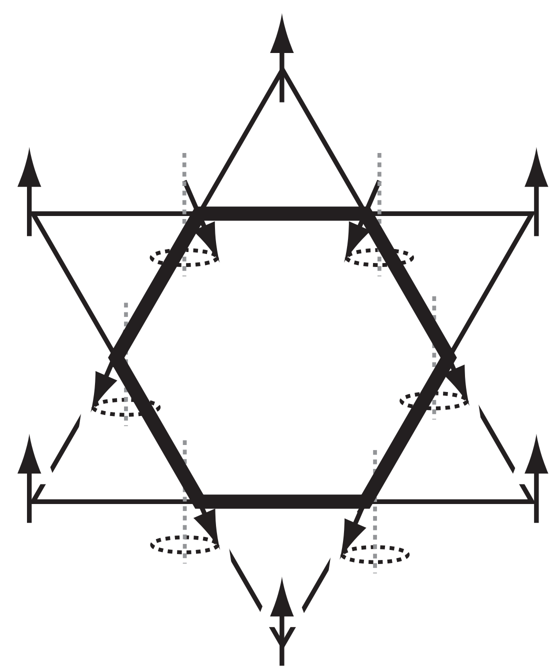

Non-planar states can be generated by continuous distortions of a planar state

Weathervane loop

Planar ground states have more soft modes (introduction of 'defect' removes certain soft modes)

Order by Disorder

Order by Disorder via Thermal Fluctuations:

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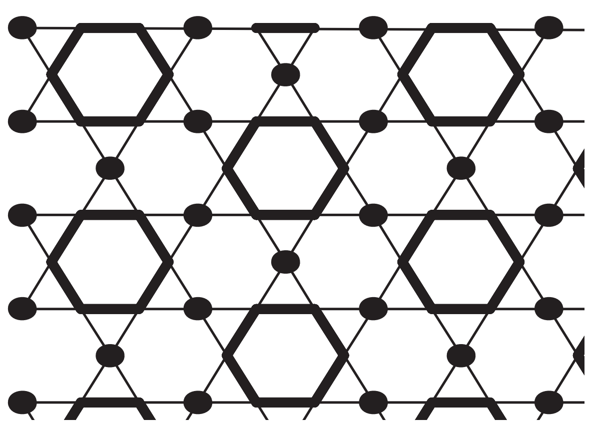
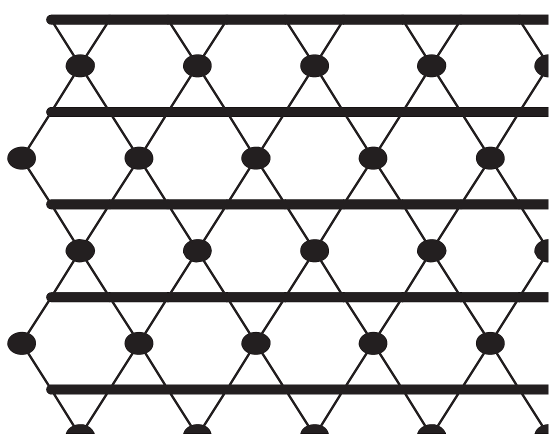


$\sqrt{3} \times \sqrt{3}$



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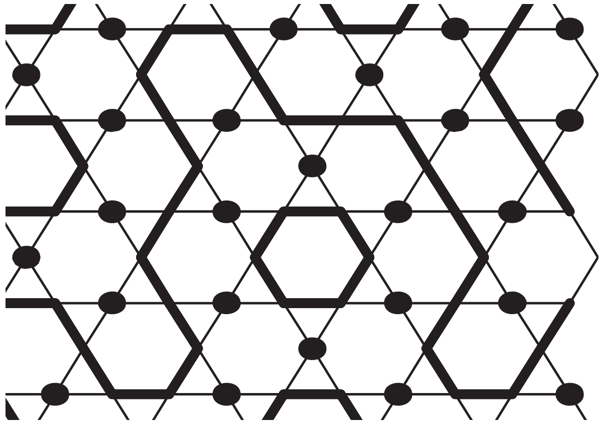


Arbitrary

Softer fluctuations for $\sqrt{3} \times \sqrt{3}$: favored as $T \rightarrow 0$

Order by Disorder

Order by Disorder via Quantum Fluctuations:

Quantum zero point energy and further quantum fluctuations may select an ordered ground state.

Order by Disorder

Order by Disorder via Quantum Fluctuations:

Quantum zero point energy and further quantum fluctuations may select an ordered ground state.

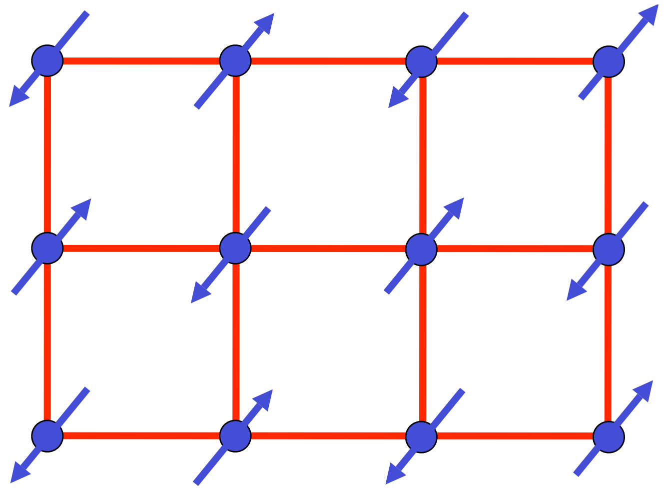
Disorder by Disorder

Sufficiently strong quantum fluctuations (S=1/2 for example), however, may destabilize any ordered phase;
possible quantum spin liquid - Disorder by Disorder

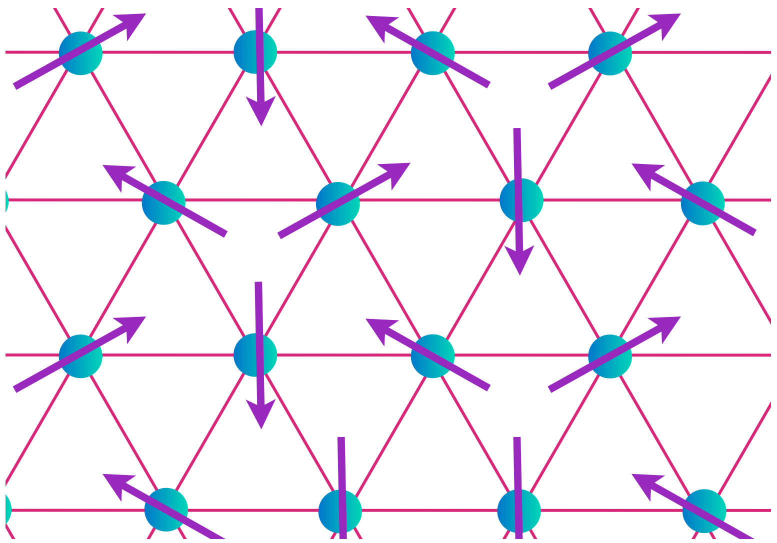
Order by Disorder

Order by Disorder via Thermal/Quantum Fluctuations

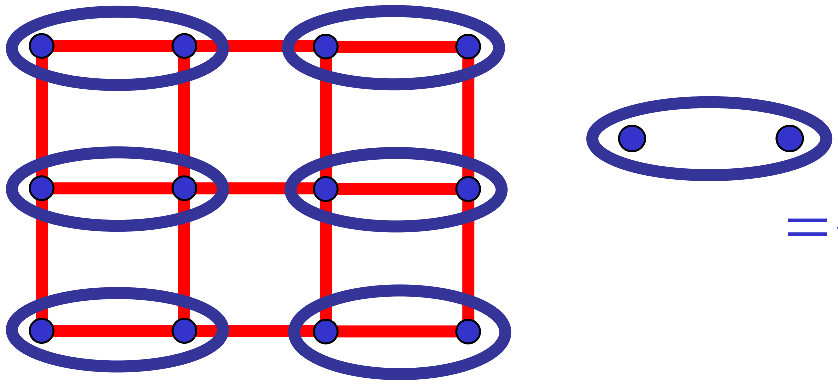
Novel Magnetic Order and/or Valence Bond Solid States



Néel ordered state



Non-collinear ordered antiferromagnet



$$= \frac{1}{\sqrt{2}}\left(\left| \uparrow\downarrow \right\rangle - \left| \downarrow\uparrow \right\rangle \right)$$

Valence Bond Solid

Quantum Fluctuations

Antiferromagnetic Heisenberg Model

$$H = \sum_{\langle i,j \rangle} J \ \vec{S}_i \cdot \vec{S}_j \quad (J \propto t^2/U)$$

Controlling quantum fluctuations - changing S of spin

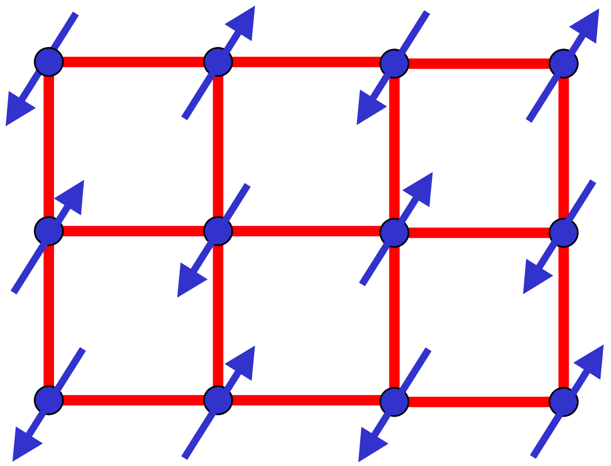
Large-S - Magnetically Ordered

Small-S - Quantum Disordered

Quantum Fluctuations

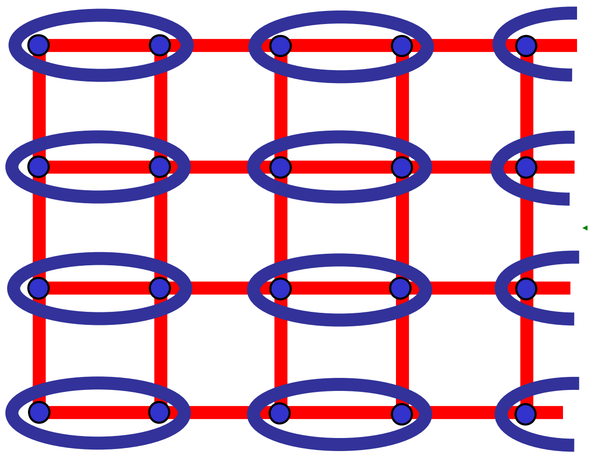
Square lattice

Large-S - Neel Order

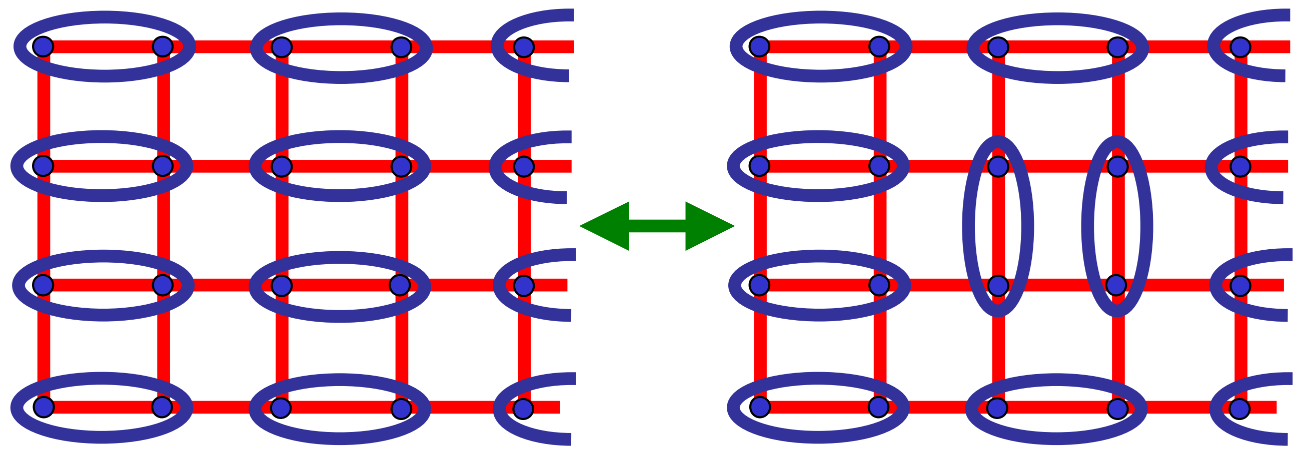


Small-S - Valence Bond Solid (VBS)

Translational symmetry is broken

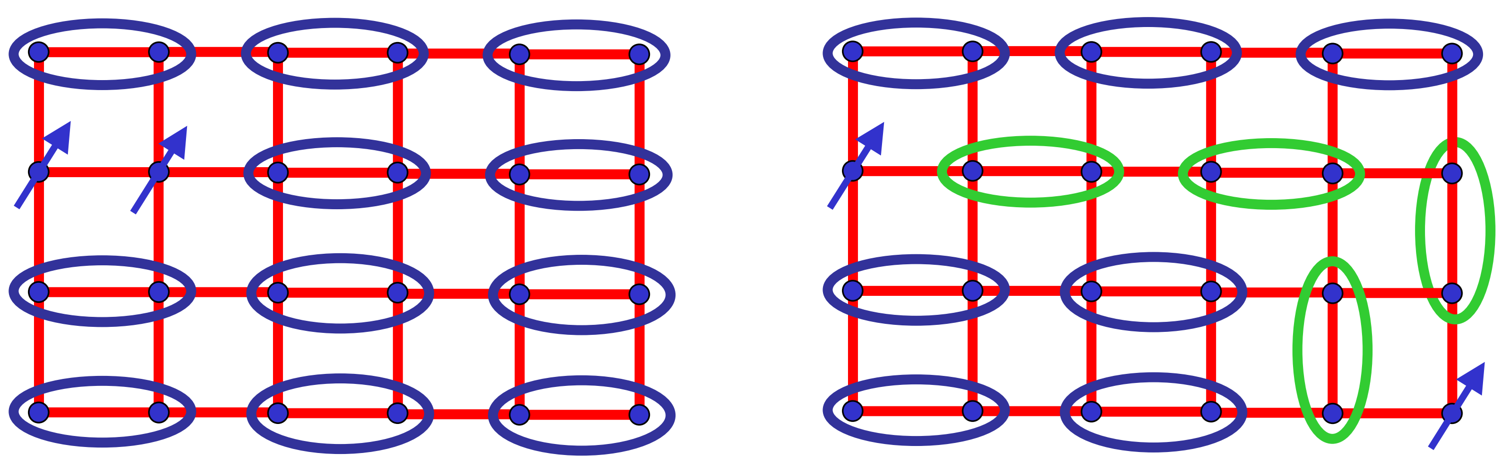


Valence Bond Solid (VBS)



Largest number of singlet pairs can resonate

Breakup and Separation

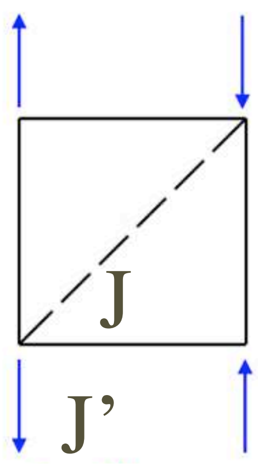


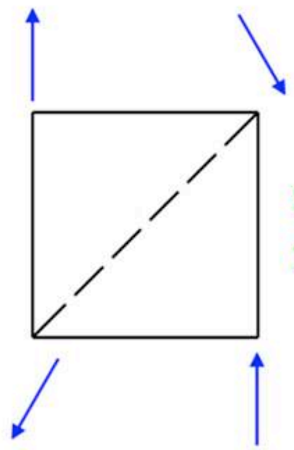
Spinons are ‘confined’ by a linearly confining potential

Frustrated Lattices

Increasing frustration in the large-S or semiclassical limit

Neel order





Spiral order

increasing J'/J

Frustrated Lattices

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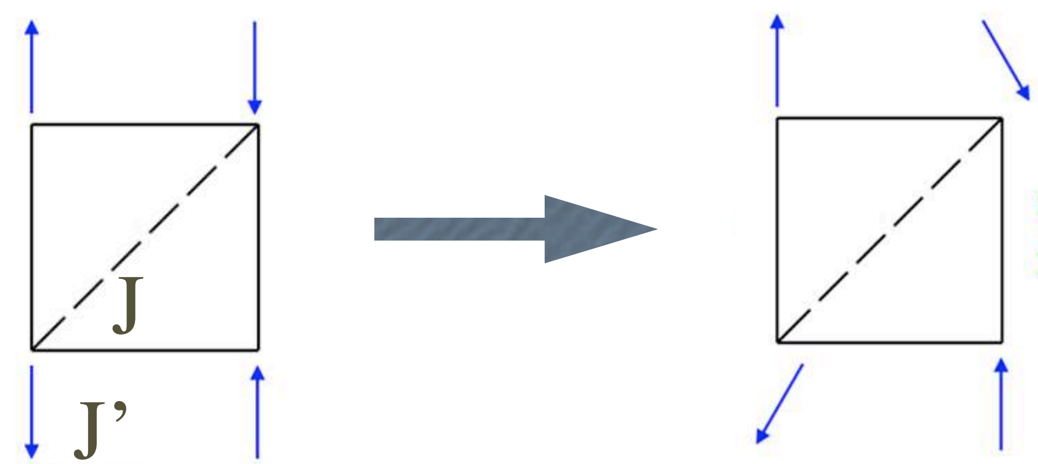


Spiral order

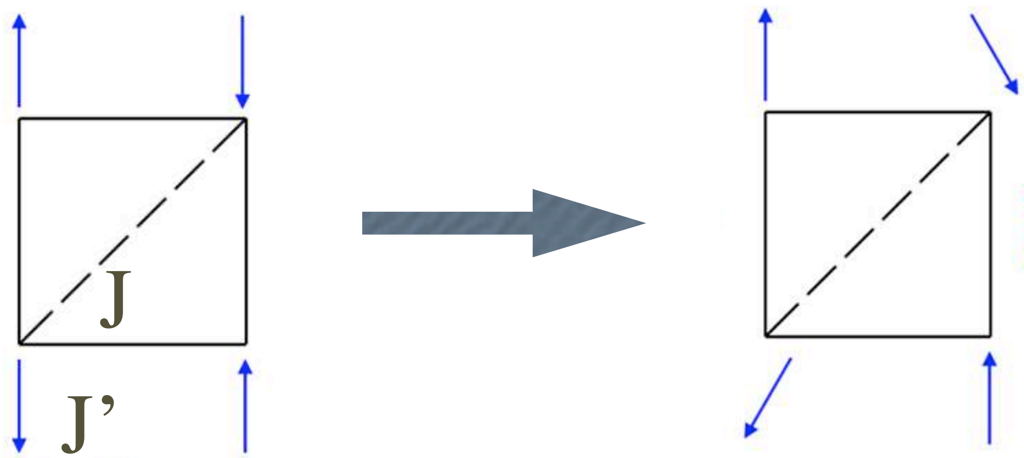
increasing J'/J

Geometric frustration + quantum fluct. in the small-S limit
⇒ Suppression of magnetic long range order

Frustrated Lattices

Increasing frustration in the large-S or semiclassical limit

Neel order



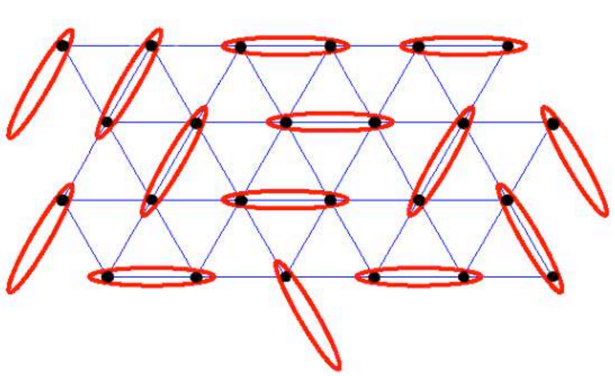
Spiral order

increasing J'/J

Geometric frustration + quantum fluct. in the small-S limit
$\Rightarrow$ Suppression of magnetic long range order

RVB (resonating valence bond) state on frustrated lattices

$|RVB\rangle = \sum_{vb} A_{vb}|vb\rangle$ $\quad\quad$ $|vb\rangle =$



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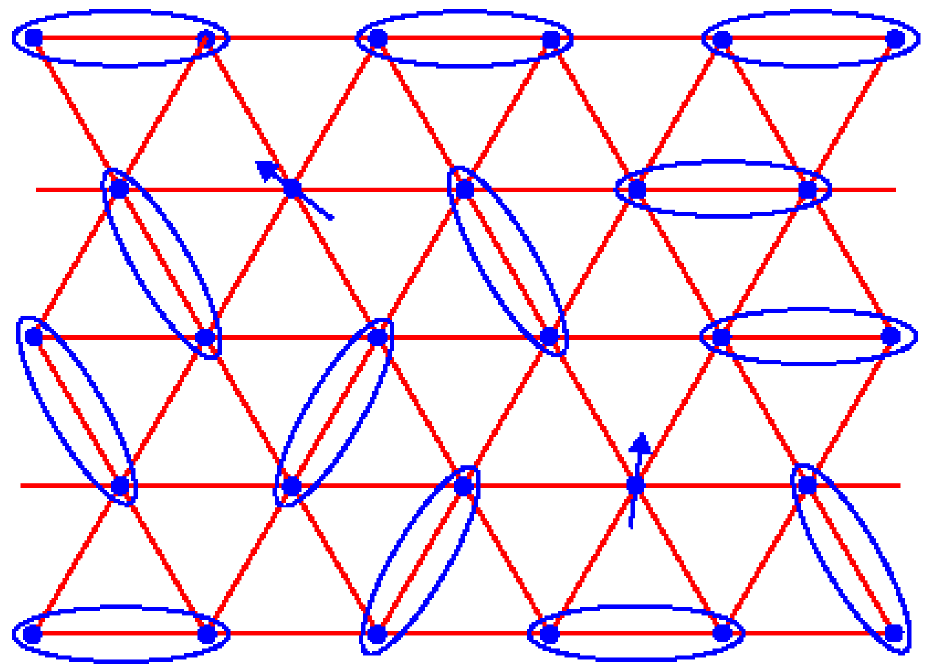
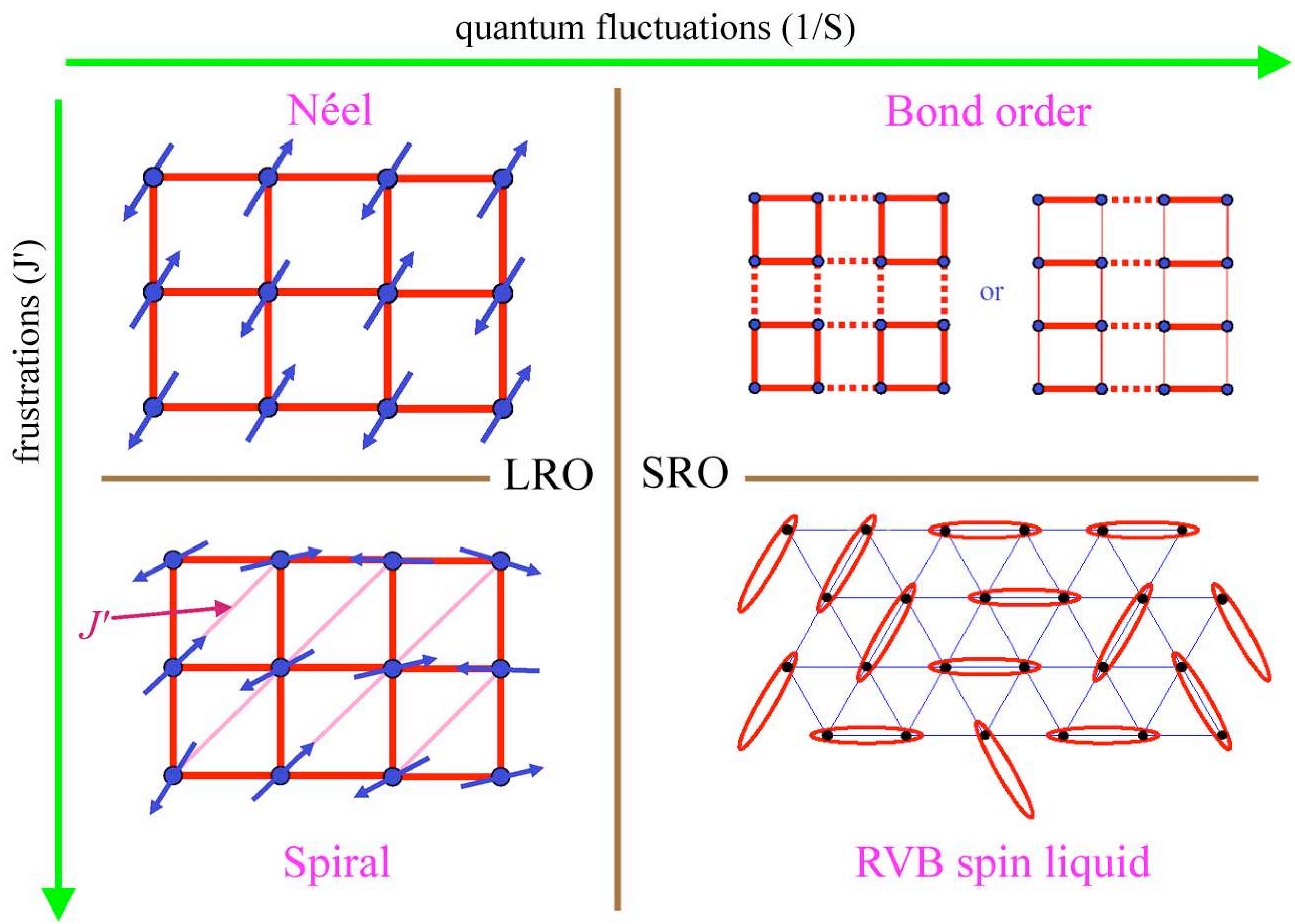


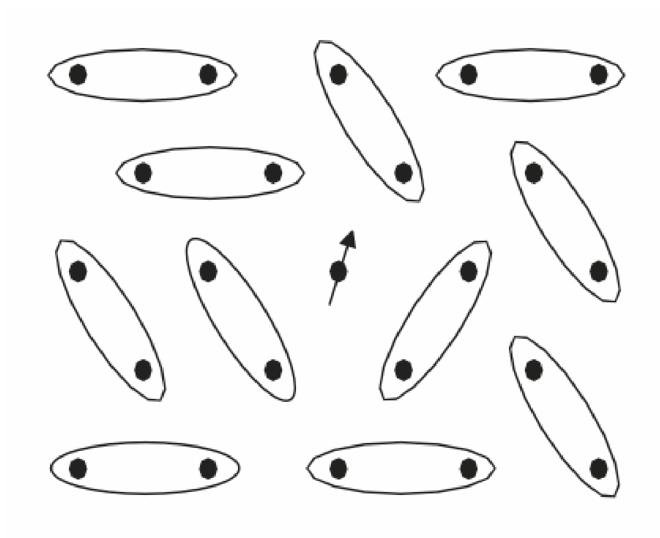
Spinons are 'deconfined'

Spinons: Q=0, S=1/2 excitations

Quantum Phases of Frustrated Mott Insulator

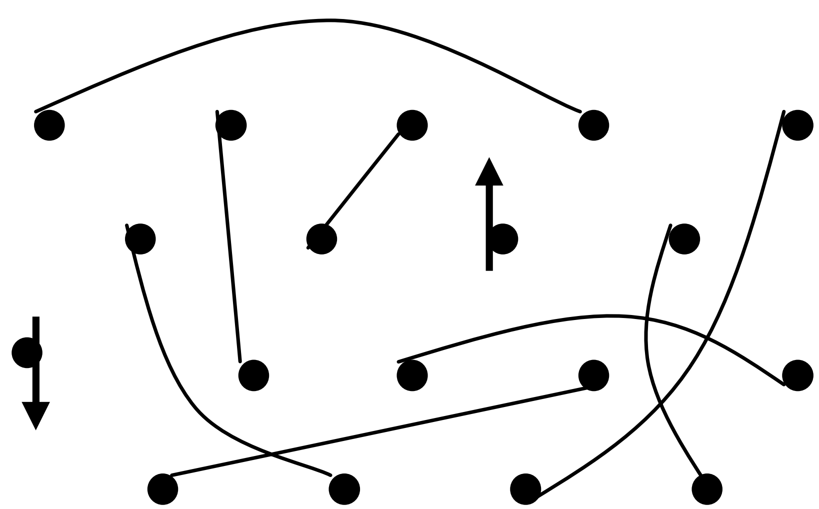


Spin Liquids come in Many Varieties



Short-Range Valence Bond

Excitations with a Gap



Long-Range Valence Bond

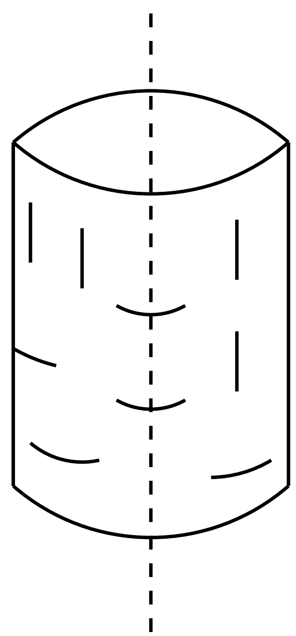
Gapless Excitations

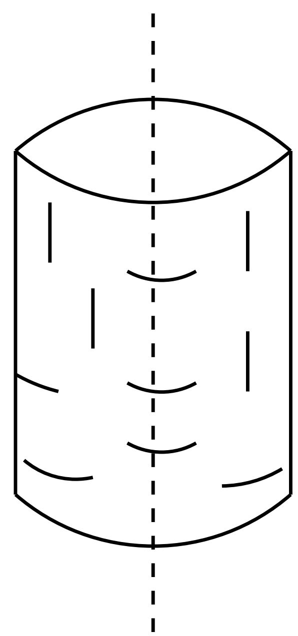
Topological Order ?

$$|RVB\rangle_{\rm even} = \sum_{\rm even} A_{vb}^{\rm even} |vb\rangle_{\rm even} \qquad |RVB\rangle_{\rm odd} = \sum_{\rm odd} A_{vb}^{\rm odd} |vb\rangle_{\rm odd}$$

$|vb\rangle_{\rm even}$ and $|vb\rangle_{\rm odd}$ describe TWO topologically distinct valence bond coverings

intersecting even number of dimers

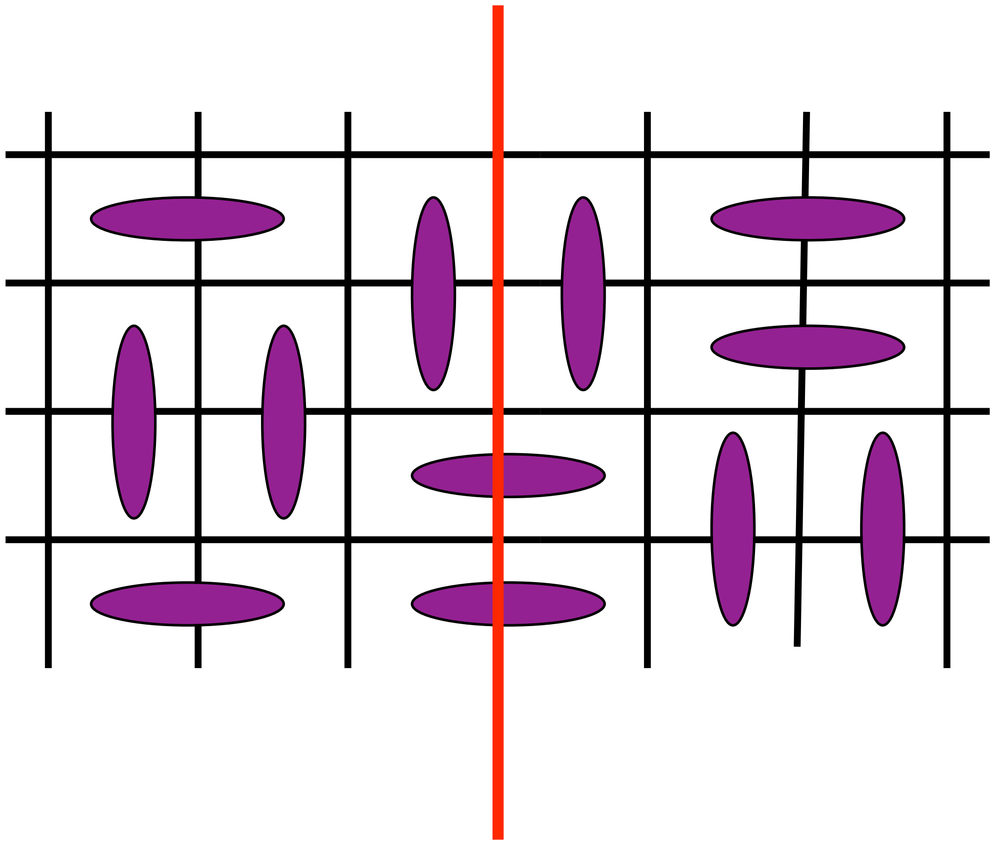




intersecting odd number of dimers

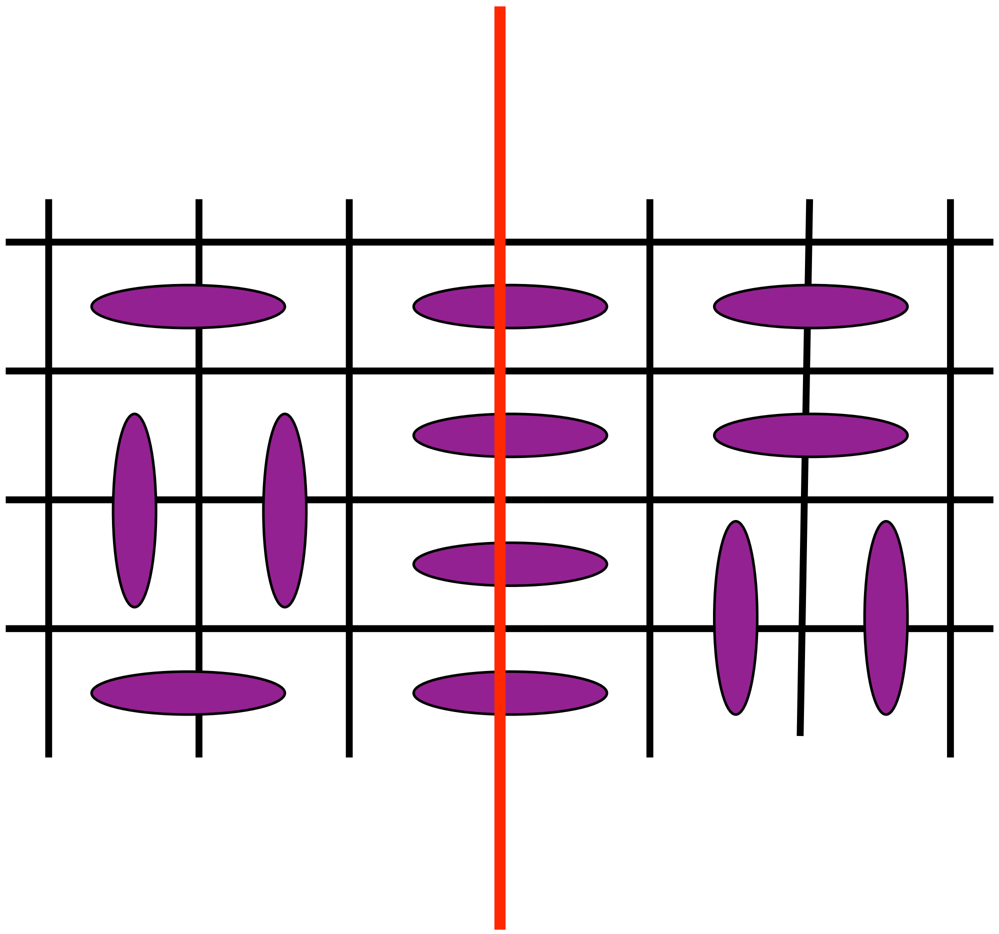
Recall the "cartoon" of the RVB state

Global property unaffected by local dynamics



Red line intersects an even number of bonds

Global property unaffected by local dynamics



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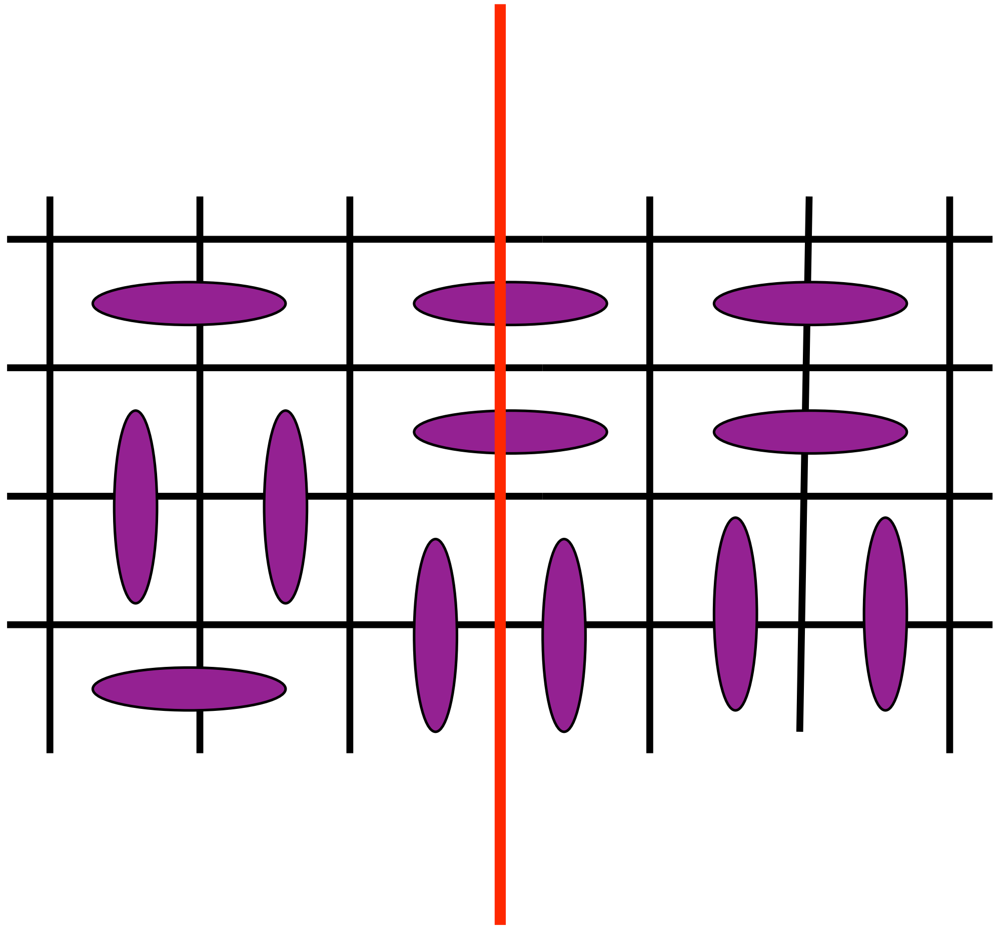

Red line intersects an even number of bonds

Two quantum states: $|even\rangle, \ |odd\rangle$

Topological Order ?

$$|RVB\rangle_{\text{even}} = \sum_{\text{even}} A_{vb}^{\text{even}} |vb\rangle_{\text{even}} \qquad |RVB\rangle_{\text{odd}} = \sum_{\text{odd}} A_{vb}^{\text{odd}} |vb\rangle_{\text{odd}}$$

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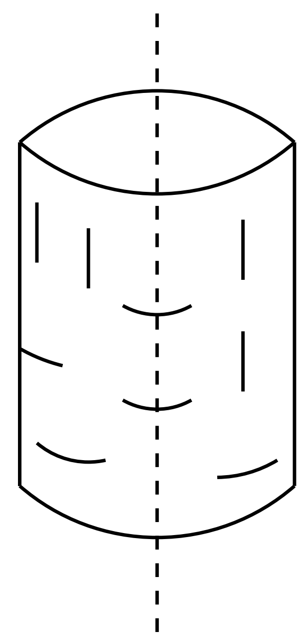
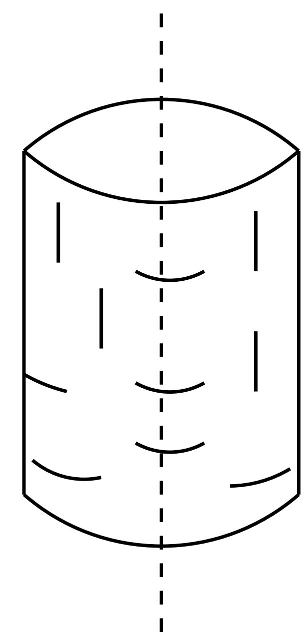
intersecting
even number
of dimers





intersecting
odd number
of dimers

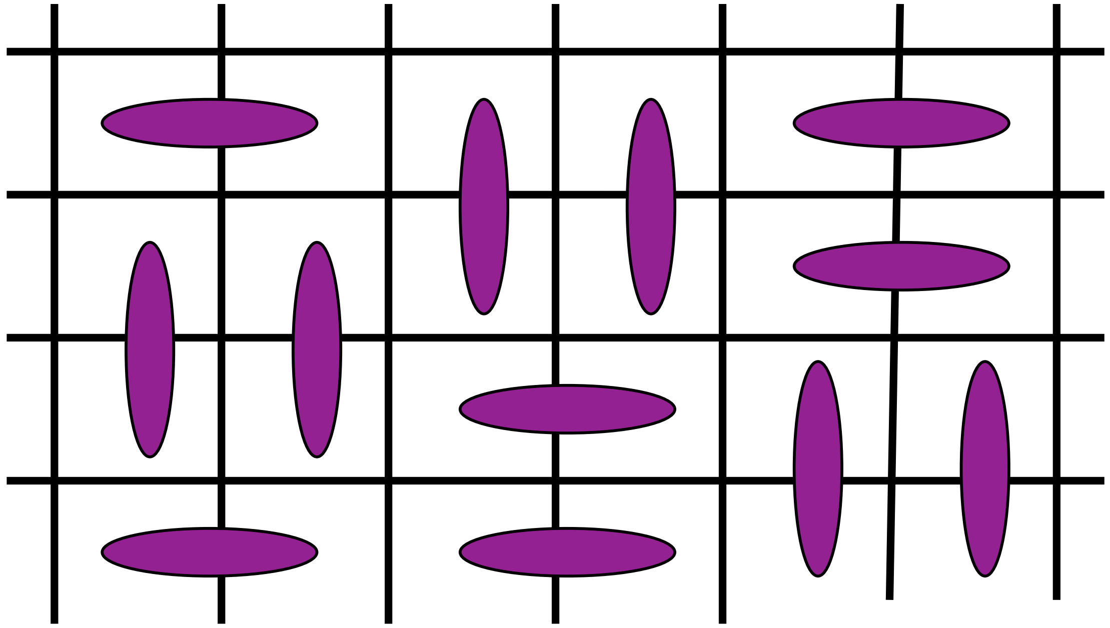
- On the torus, there are FOUR topological sectors

(even,even), (even,odd), (odd,even), (odd,odd)

"A quantum system having particles with "topological" character would be automatically protected against errors caused by local disturbances"

Alexei Kitaev (1995)

Resonating Valence Bond:
Simplest quantum state
with "topological" particles!

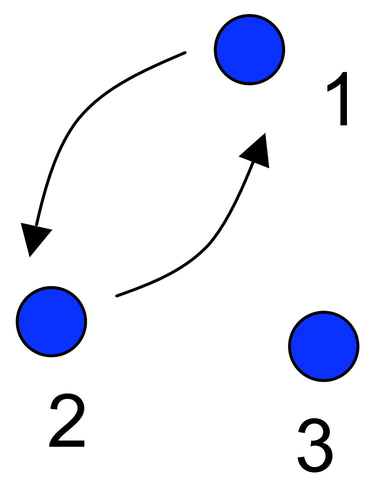


More exotic topological states

Quantum states supporting particles with

"Non Abelian particles"

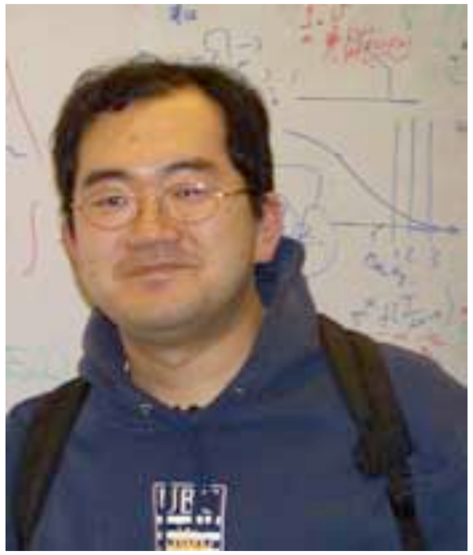
Braid 1 and 2

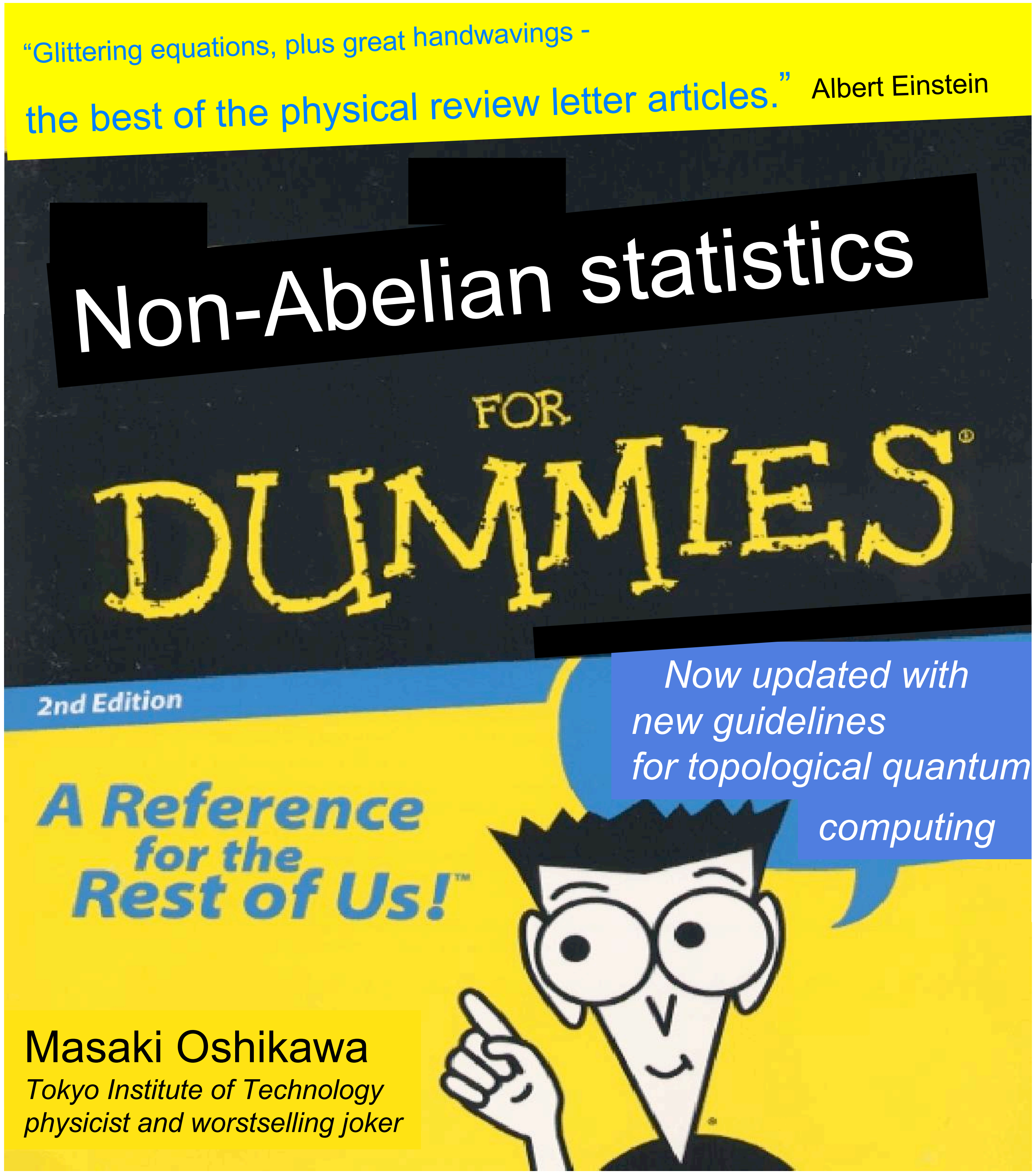


Multiple braids:

$$(1 \leftrightarrow 2, 2 \leftrightarrow 3) \neq (2 \leftrightarrow 3, 1 \leftrightarrow 2)$$

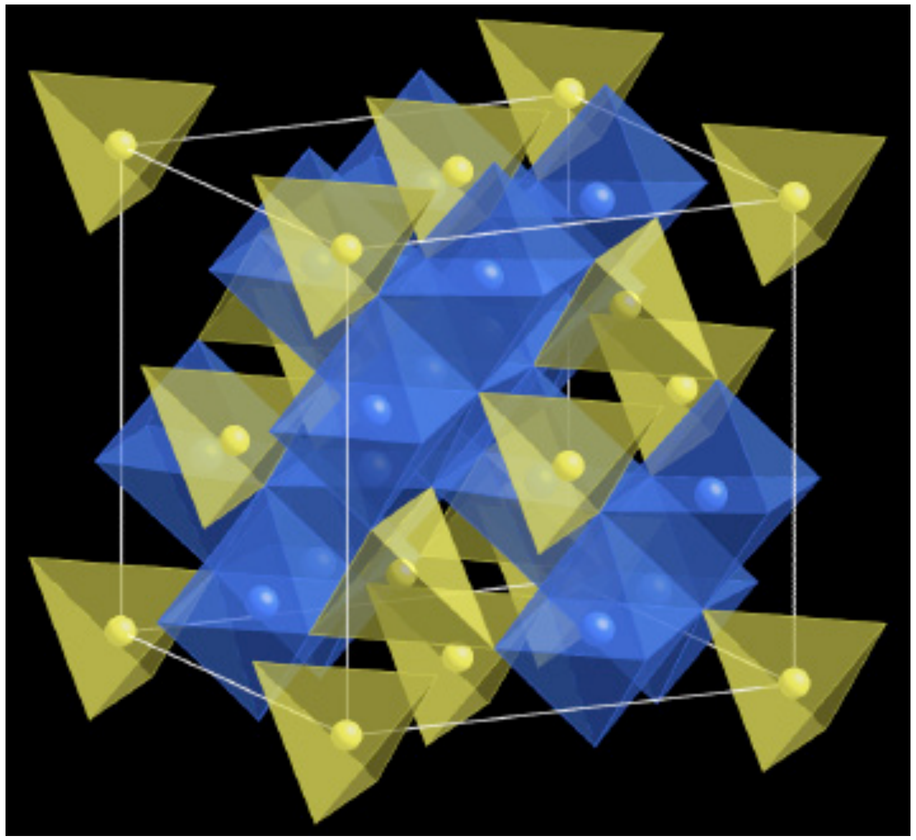
Order of braids matters!




"Glittering equations, plus great handwavings -
the best of the physical review letter articles." Albert Einstein
Non-Abelian statistics
FOR
DUMMIES
2nd Edition
Now updated with
new guidelines
for topological quantum
computing
A Reference
for the
Rest of Us!
Masaki Oshikawa
Tokyo Institute of Technology
physicist and worstselling joker

Quantum Order by Disorder: Frustrated Diamond Lattice Spinel Antiferromagnet

Frustrated Diamond Spinel Antiferromagnets



Spinel Structure

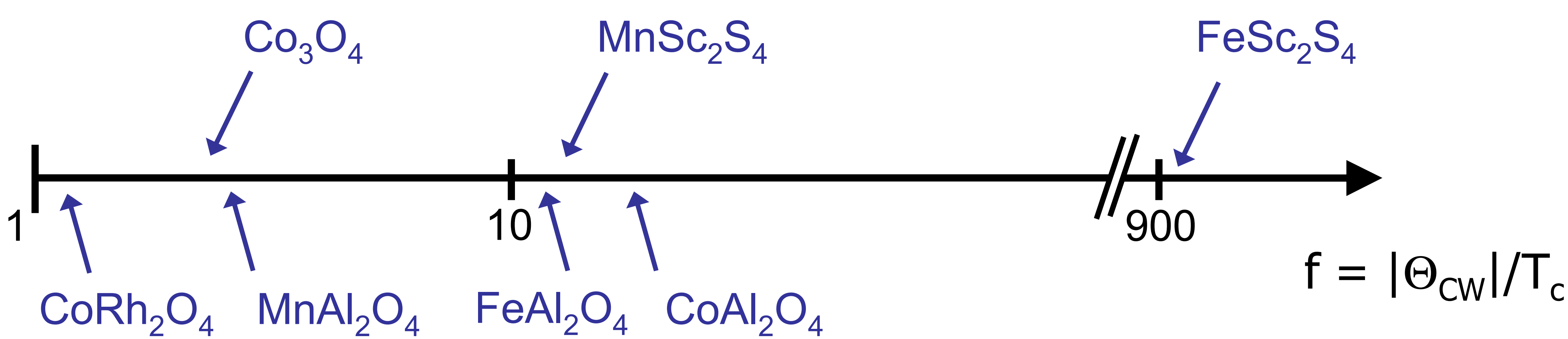
$$\mathrm{AB_2X_4}$$

A-site (Yellow) - diamond lattice

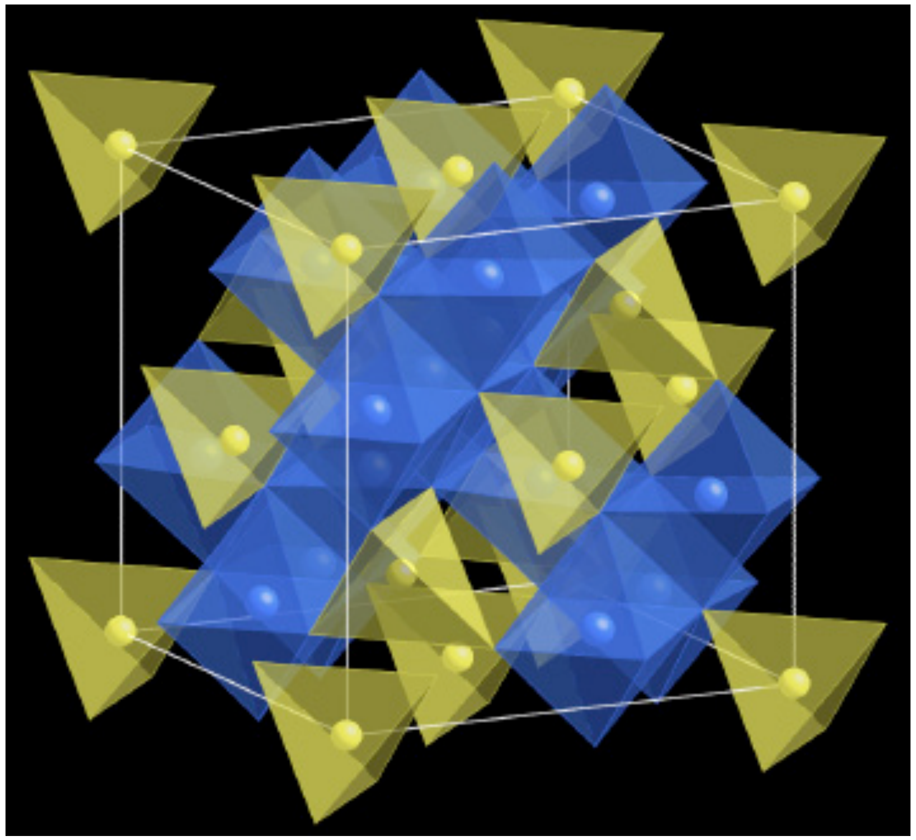
B-site (Blue) - pyrochlore lattice

X-site - vertices

Our interest: Spinel compounds with magnetic A-sites only



Frustrated Diamond Spinel Antiferromagnets



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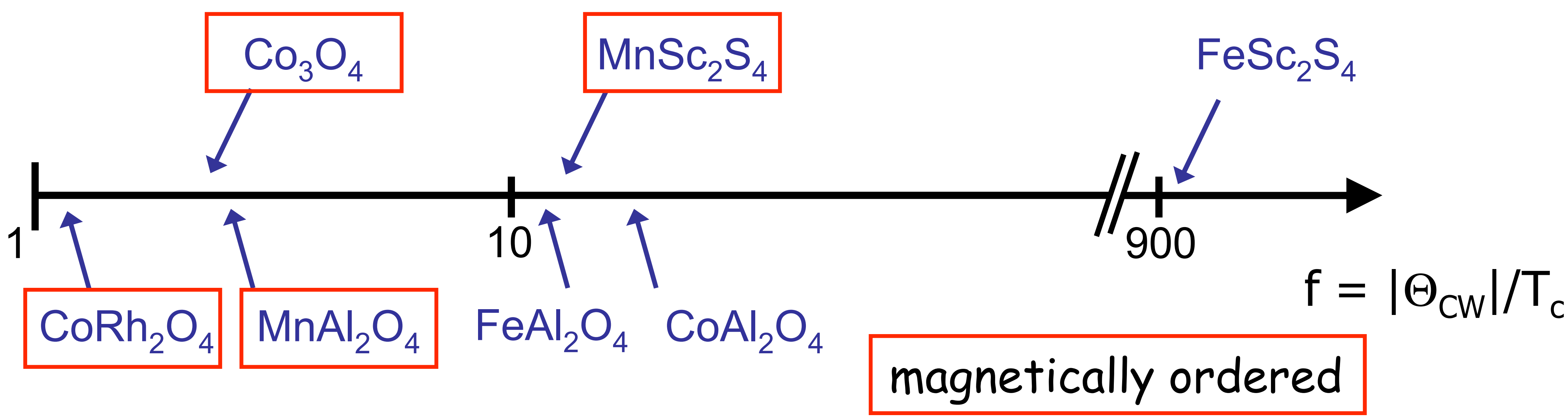
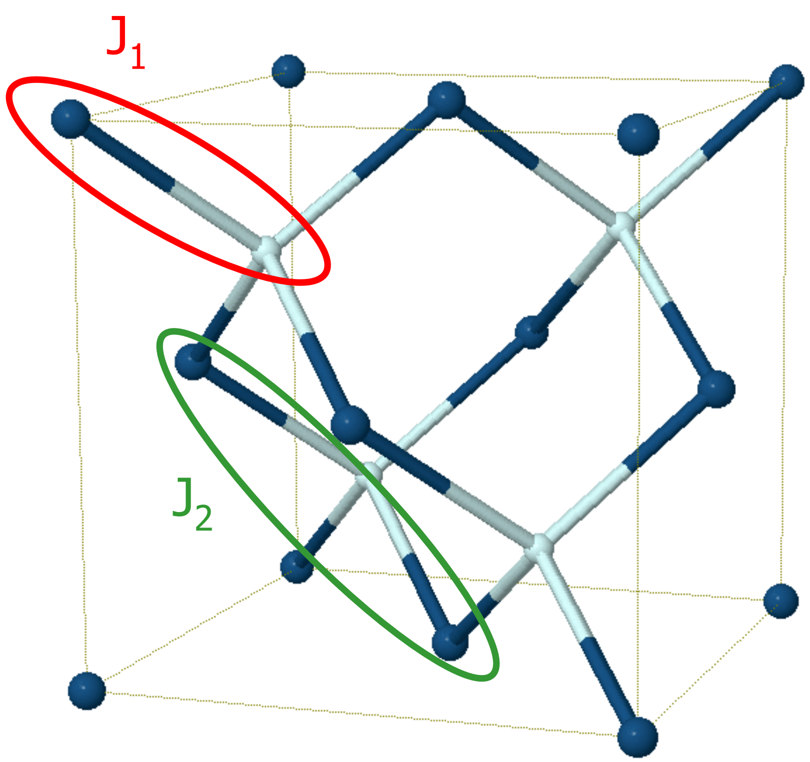


Heisenberg Model on the Diamond Lattice

$$H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



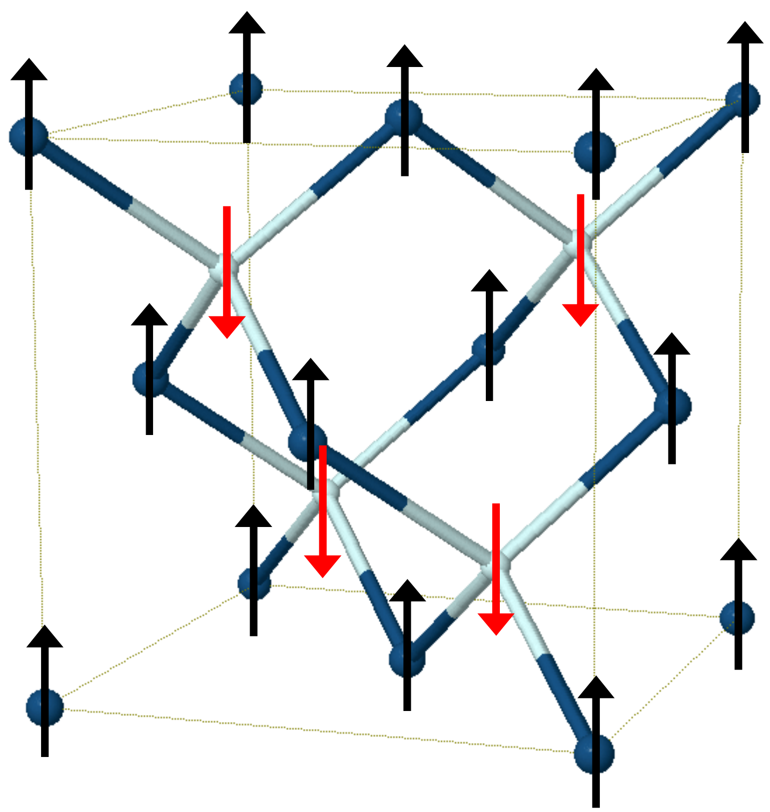
J_1 Not frustrated

favors Neel ordering

J_2 Frustrated !

Heisenberg Model on the Diamond Lattice

$$H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



J_1 Not frustrated

favors Neel ordering

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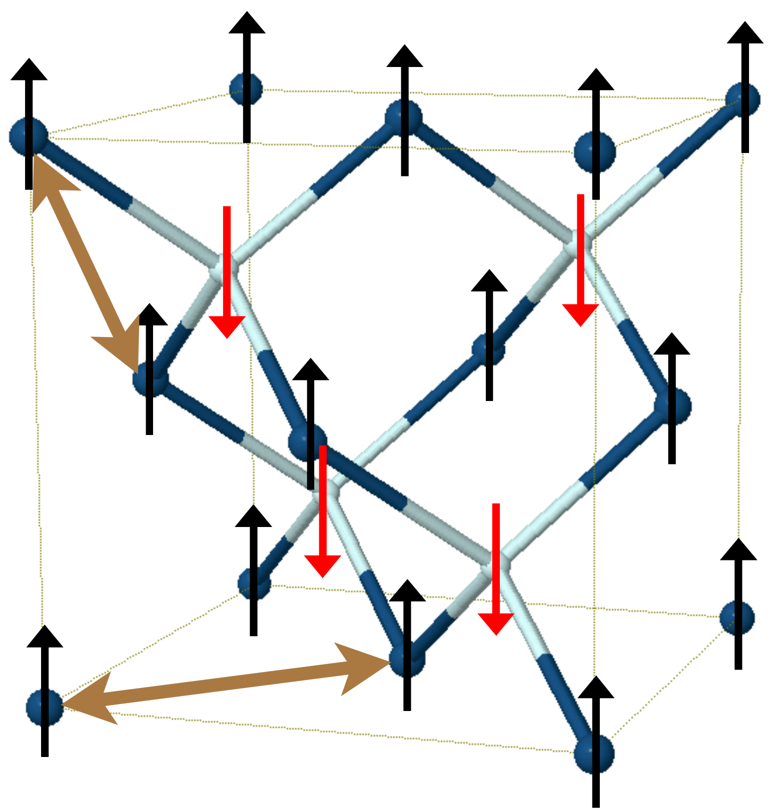


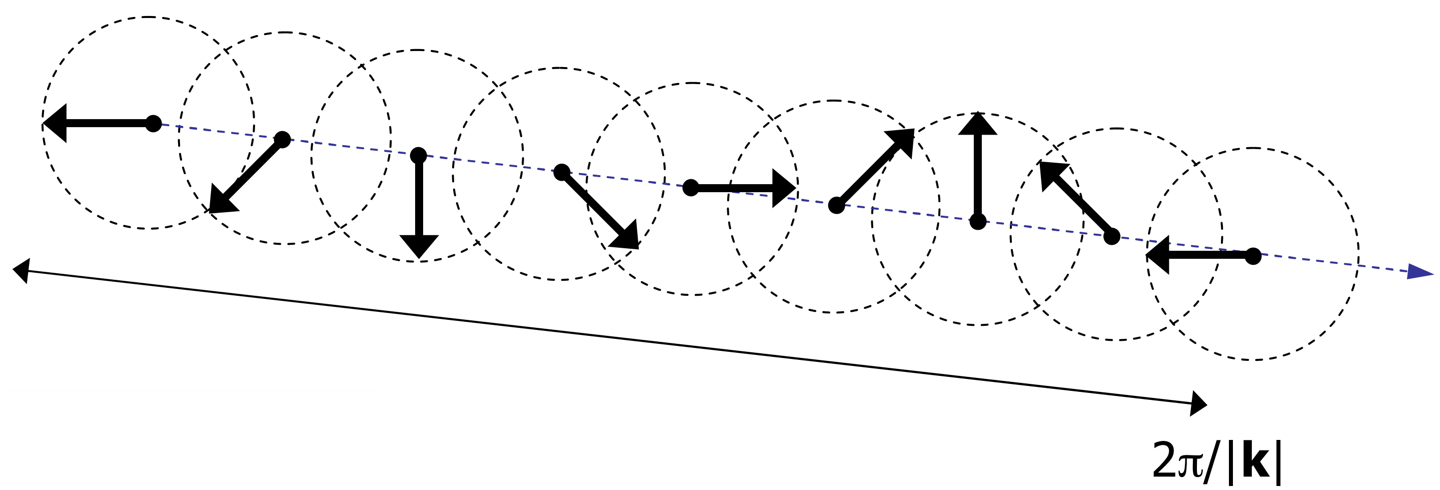
J_1 Not frustrated

favors Neel ordering

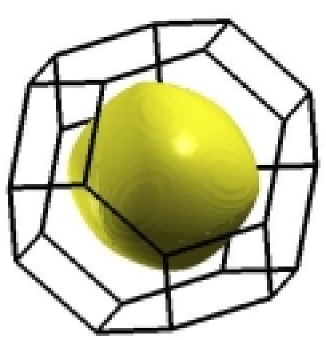
J_2 Frustrated !

Classical Heisenberg Model

Highly degenerate coplanar spiral states for $J_2/J_1 > 1/8$ at T=0



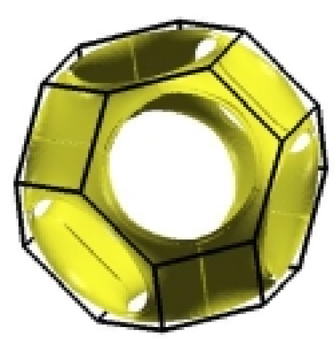
Surface of equal energy in momentum space



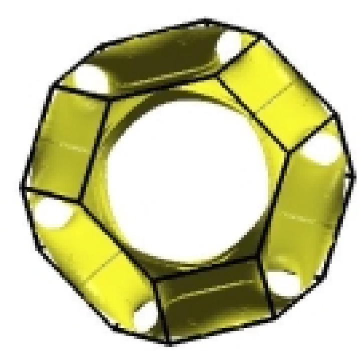
J_2/J_1=0.2

Deformed sphere:

$1/8 < J_2/J_1 < 1/4$



J_2/J_1=0.6



J_2/J_1=0.85

Punctured deformed sphere:

$J_2/J_1 > 1/4$

Quantum Order by Disorder

Expand the ground state energy in $1/\kappa$

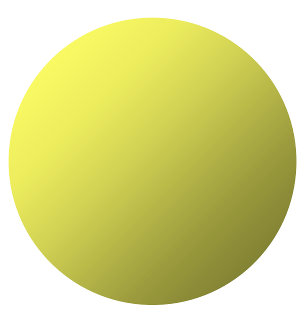
$$E = E_c + \frac{1}{\kappa} E^1 + \ldots$$

$\kappa =$ "$2S$" controls quantum fluctuations

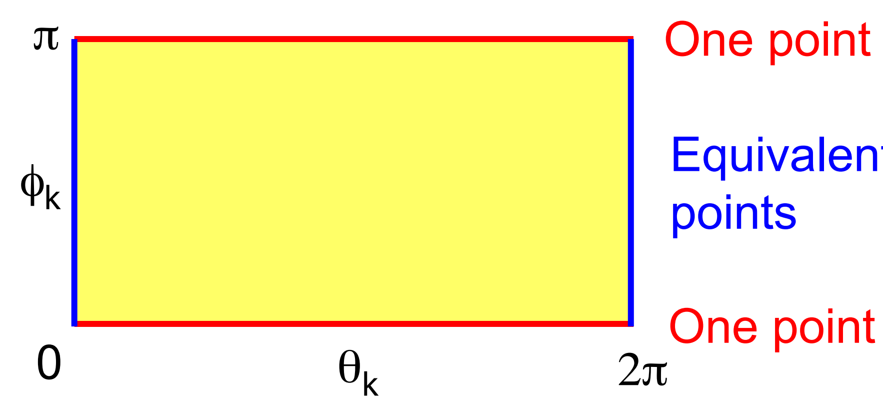
E_c Classical energy

E^1 quantum zero-point fluctuation energy lifts the ground state degeneracy

Represent the resulting energy change/difference

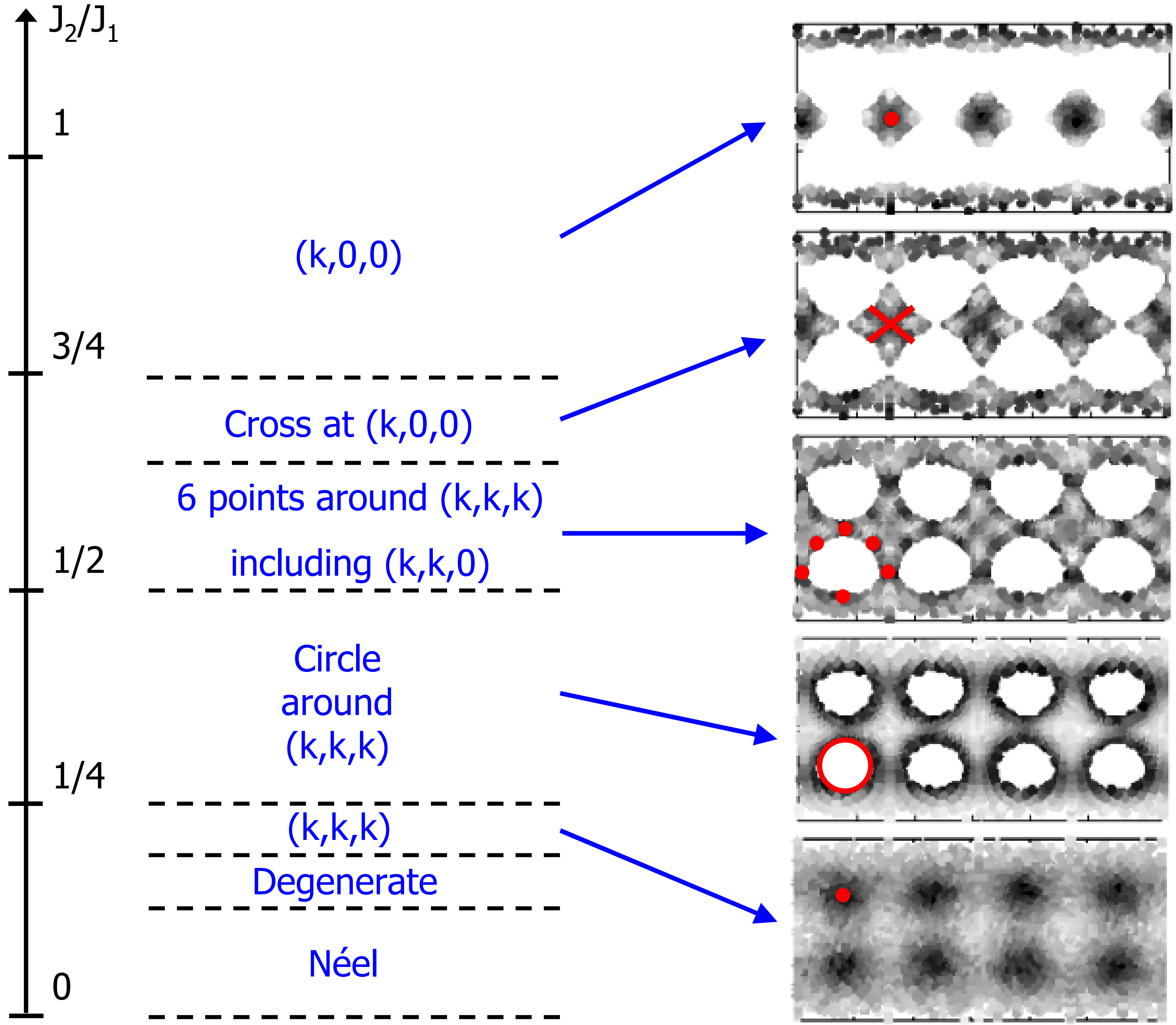


Energy landscape in momentum space: deformed sphere

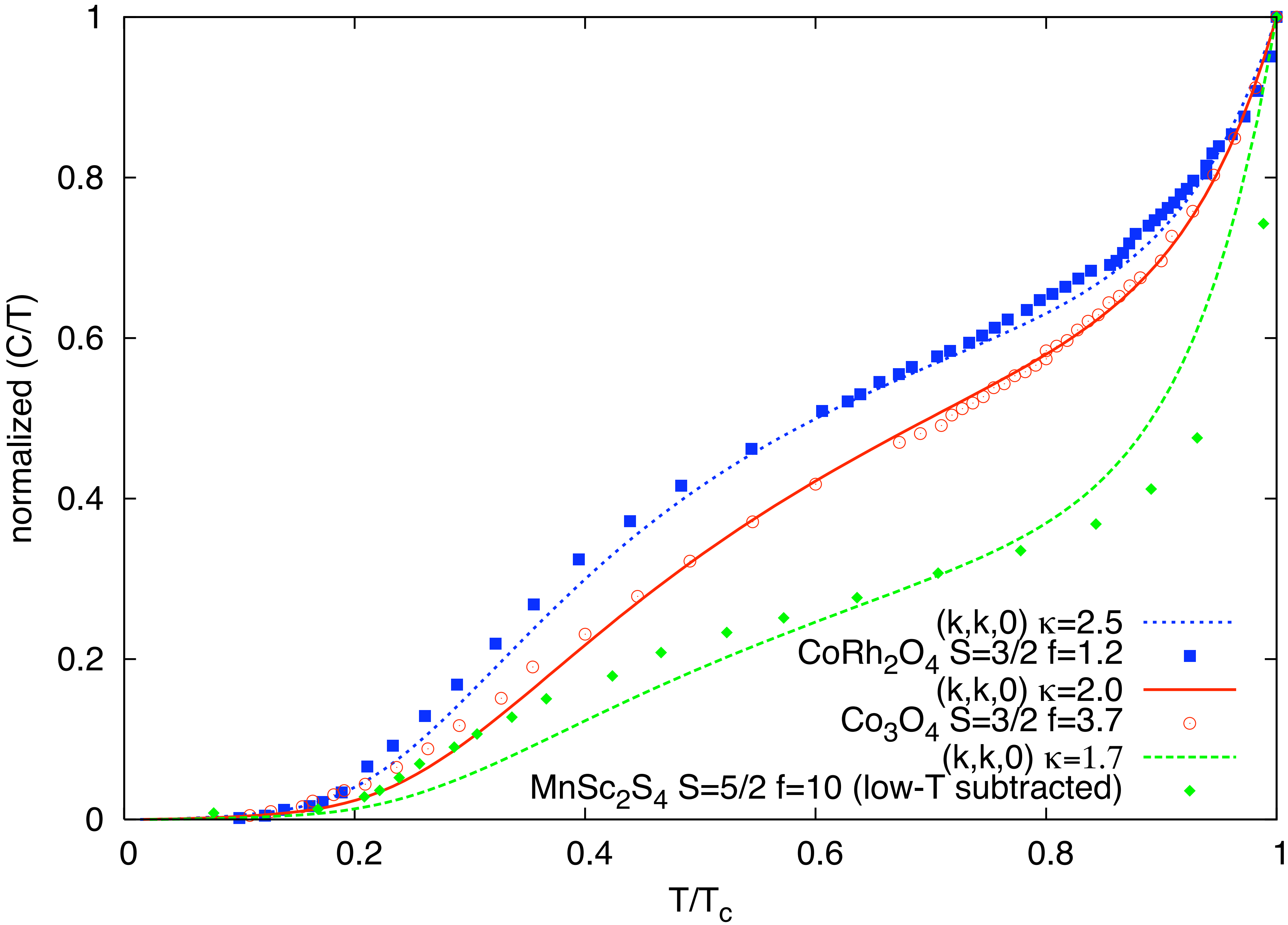


Unfolded "sphere"

Phase Diagram



Finite Temperature Large-N Theory and Specific Heat



(k,k,0) ordering works remarkably well !

Disorder by Disorder:
Spin Liquid on Hyper-Kagome Lattice

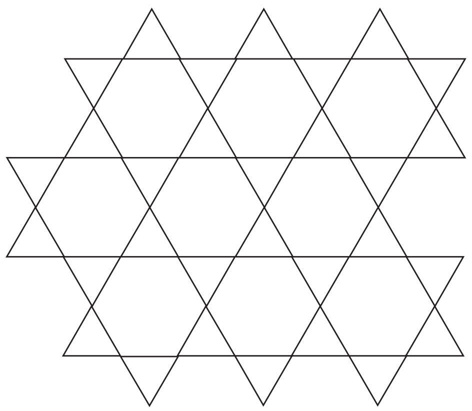
Search for Quantum Spin Liquid (S=1/2)

κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$ Triangular Lattice; near Mott transition

K. Kanoda

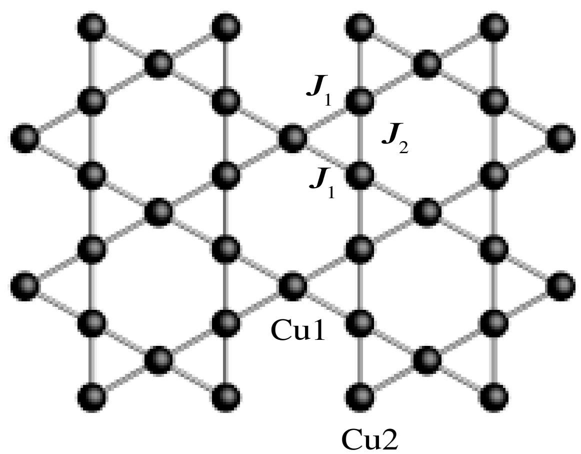
Herbertsmithite "Ideal" Kagome lattice

$ZnCu_3(OH)_6Cl_2$ D. G. Nocera, Y. S. Lee



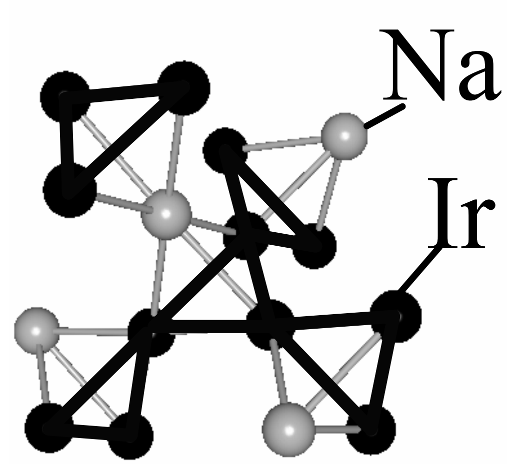
Volborthite Distorted Kagome lattice

$Cu_3V_2O_7(OH)_2 \cdot 2H_2O$ Z. Hiori



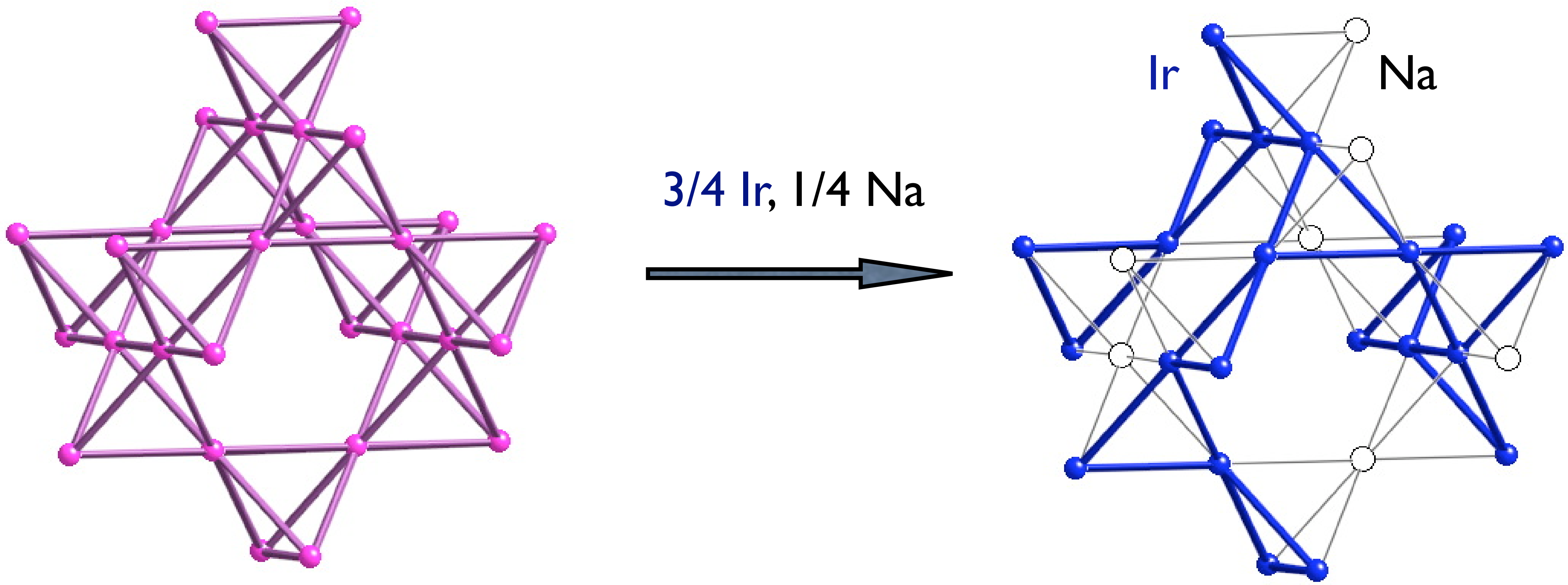
Hyper-Kagome $Na_4Ir_3O_8$

H. Takagi



Three-dimensional S=1/2 Frustrated Magnet

$Na_4Ir_3O_8$ has a Hyper-Kagome sublattice of Ir ions



Pyrochlore

Hyper-Kagome

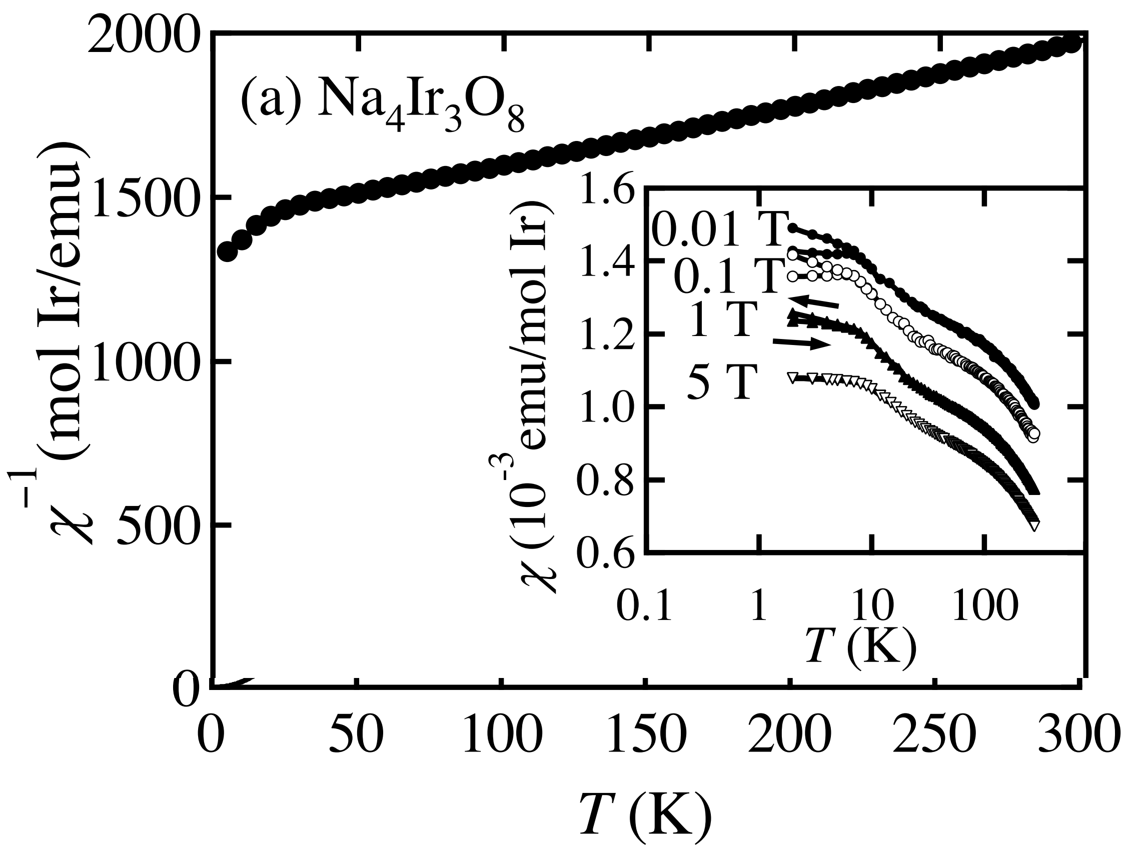
All Ir-Ir bonds are equivalent

Ir^{4+} ($5d^5$) carries "S=1/2" moment ?

Y. Okamoto, M. Nohara, H. Agura-Katrori, and H. Takagi, PRL 99, 137207 (2007)

Inverse Spin Susceptibility; Strong Spin Frustration

Y. Okamoto, M. Nohara, H. Agura-Katrori, and H. Takagi, PRL 99, 137207 (2007)

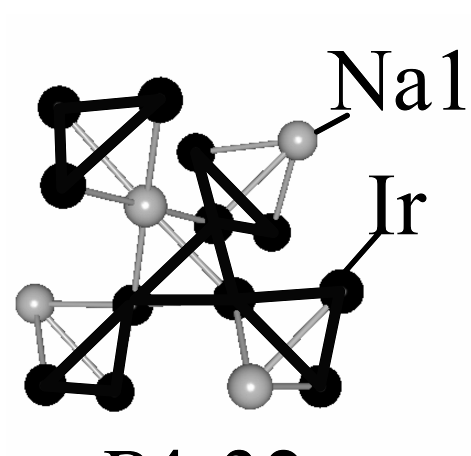


Curie-Weiss fit

$$\Theta_{\rm CW} = -650K$$

No magnetic ordering down to $|\Theta_{\rm CW}|/300$

Large Window of Cooperative Paramagnet

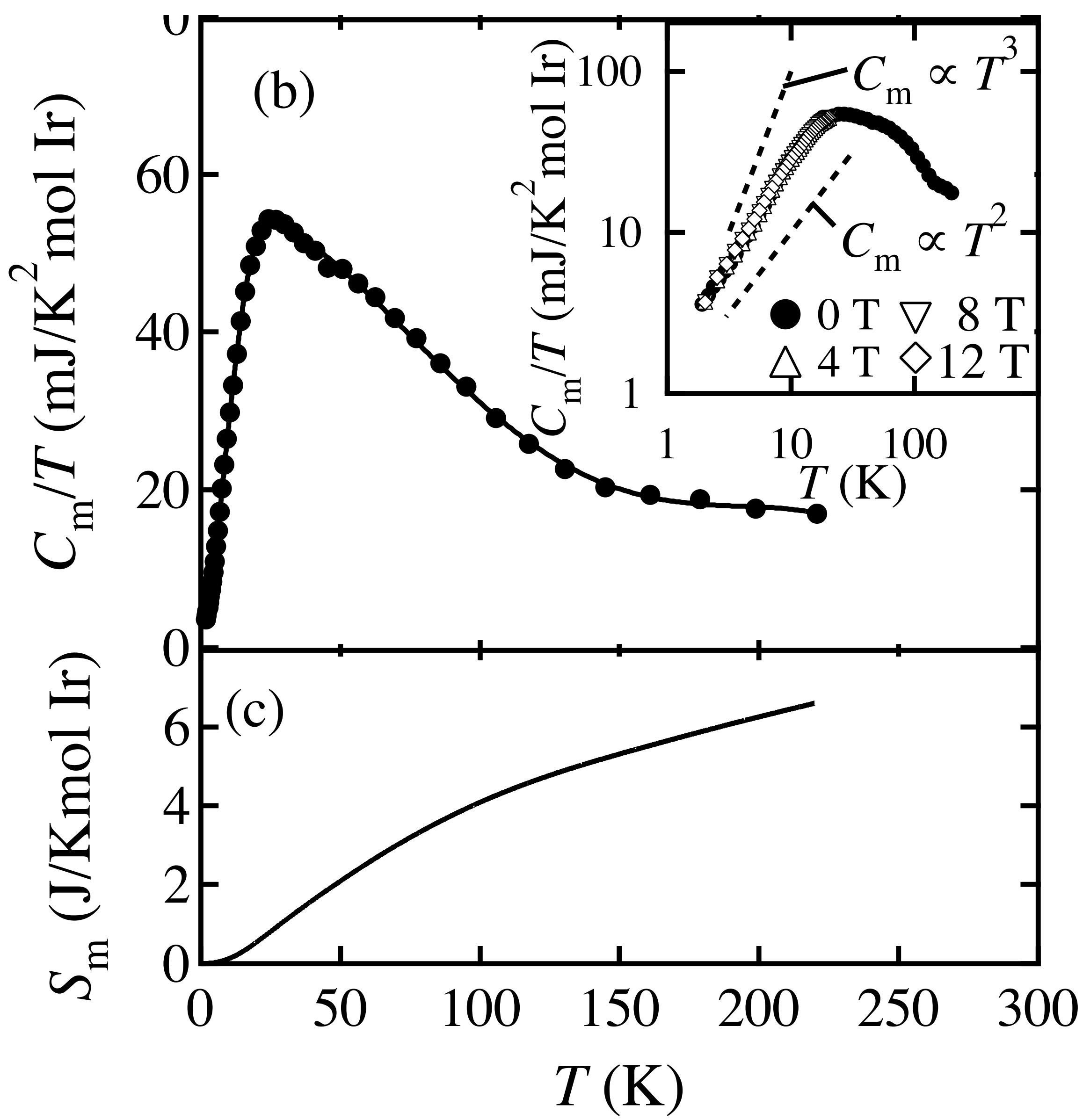


$P4_132$

Strong Frustration - Macroscopic degeneracy of classical ground states

Specific Heat; Low Energy Excitations ?

Y. Okamoto, M. Nohara, H. Agura-Katrori, and H. Takagi, PRL 99, 137207 (2007)



No Magnetic Ordering

Gapless Excitations in an Insulator ?

Field-independent up to 12T

Is the T=0 Ground State a Spin Liquid ?

Theory of Spin Liquid with Fermionic Spinons

Fermionic representation of the spin operator $\alpha, \beta = \{\uparrow, \downarrow\}$

$$\vec{S}_i = \frac{1}{2} f^\dagger_{i\alpha} \vec{\sigma}_{\alpha\beta} f_{i\beta} \quad \text{with the constraint} \quad \sum_\alpha f^\dagger_{i\alpha} f_{i\alpha} = 1$$

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Mean-Field Theory

$\chi_{ij} = \langle f^\dagger_{i\alpha} f_{j\alpha} \rangle$ fermion "kinetic" energy dynamically generated

$\Delta_{ij} = \langle \epsilon_{\alpha\beta} f_{i\alpha} f_{j\beta} \rangle$ possible pairing correlation

The constraint is ONLY imposed on average !

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Projected Wave Function Approach

$\Psi = P_G \Psi_{MF}$

Impose the constraint exactly

Project out unphysical Hilbert space in the mean-field ground states

Theory of Spin Liquid with Fermionic Spinons

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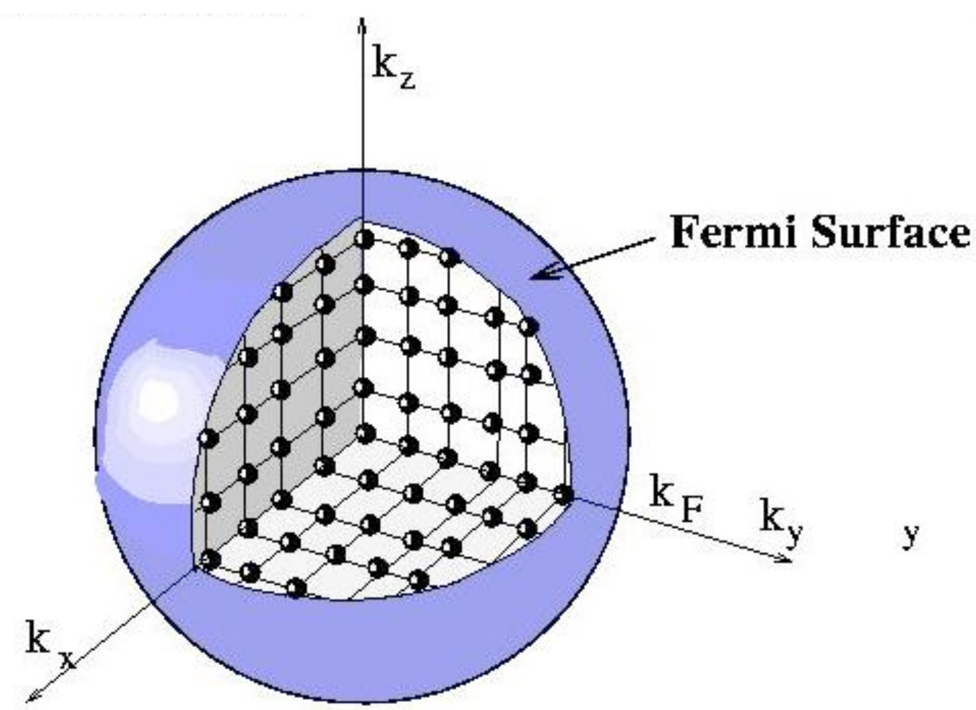
In the spin liquid phases, the fermionic spinons are liberated (deconfined) and become emergent excitations

Theory of Spin Liquid with Gapless Fermionic Spinons

MEAN FEILD THEORY + PROJECTION

The lowest energy state has uniform χ_{ij} and $\Delta_{ij} = 0$

The resulting spin liquid has a "spinon Fermi surface"



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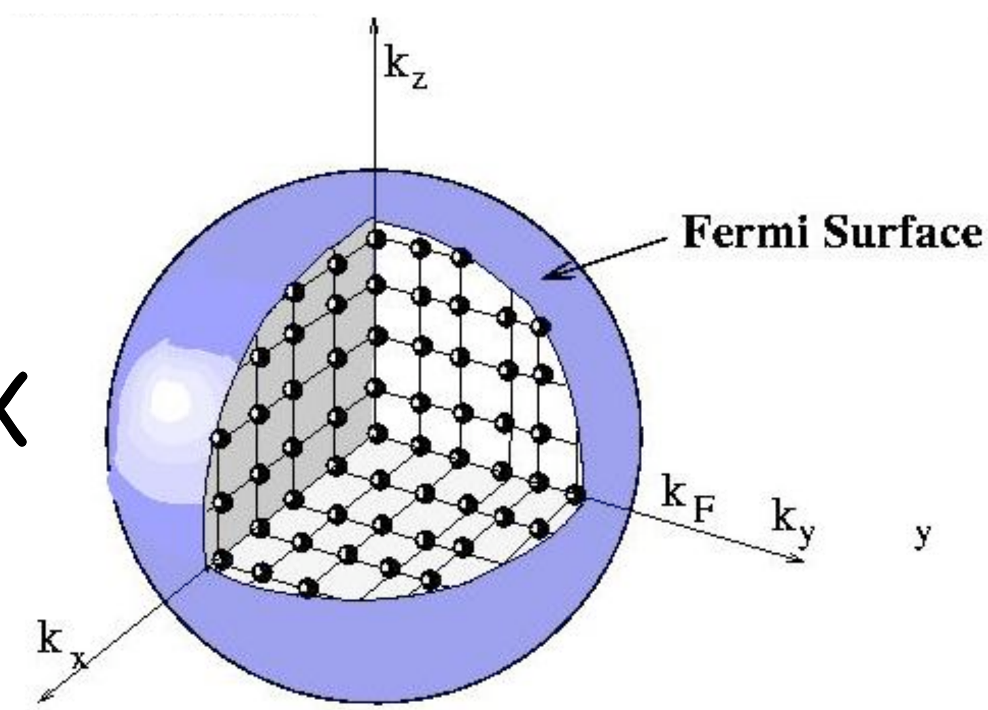
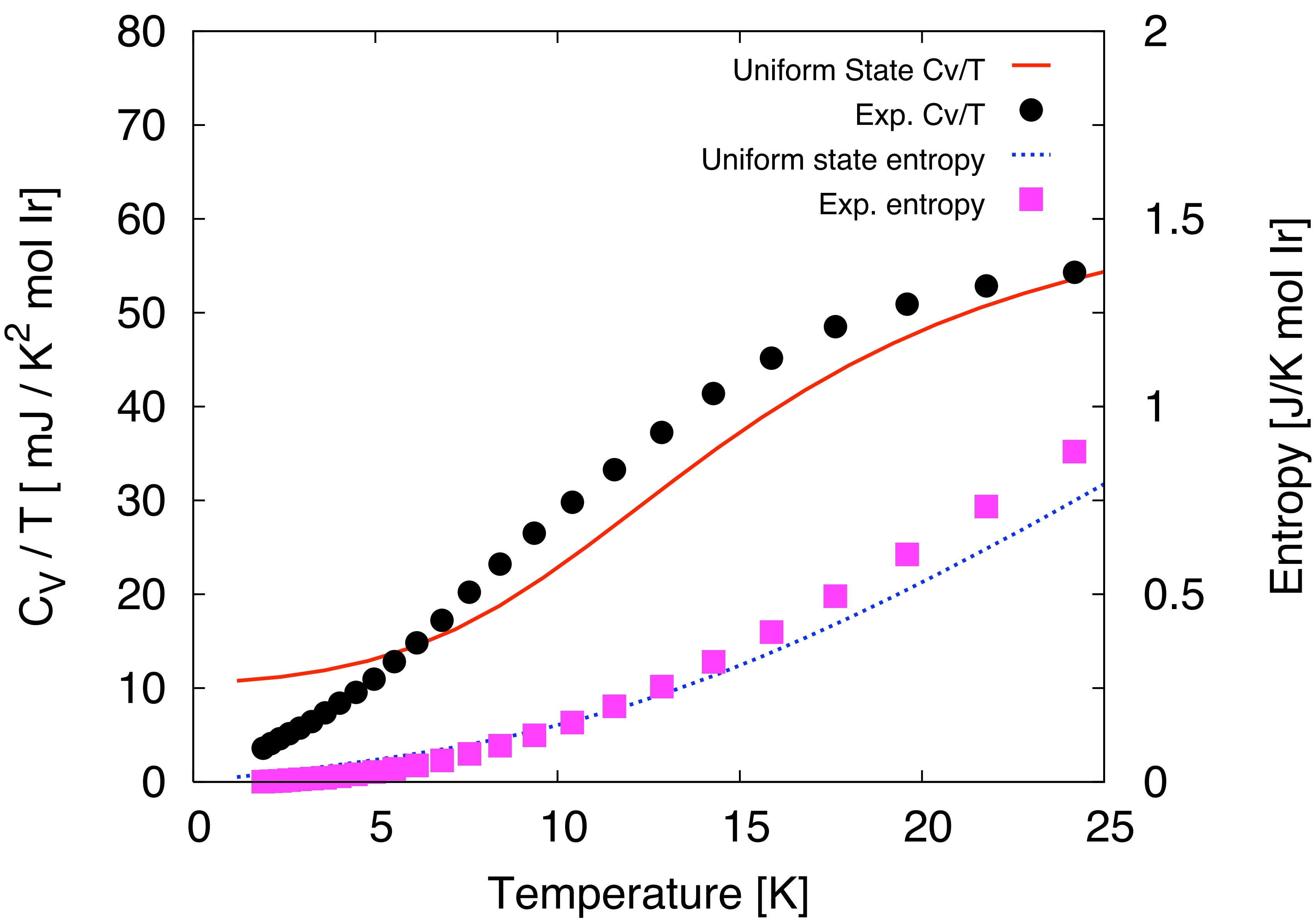
3 X



Theory of Spin Liquid with "Spinon Fermi Surface"



Re-normalized Mean Field Theory with J = 304K

C/T looks linear for 5K < T < 20K

Theory of Spin Liquid with Gapless Fermionic Spinons

The spin liquid with a "spinon Fermi surface" is the ground state of the nearest-neighbor Heisenberg model

At low temperatures, other perturbations may select one of the competing phases as the ground state

If it happens, the resulting phase may be understood as a Fermi surface instability of the "spinon Fermi surface" of the spin liquid

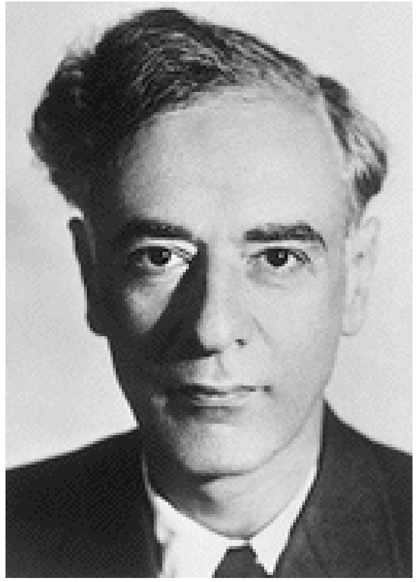
(just like in metals, where magnetic ordering or superconductivity can be understood as an instability of the "electron Fermi surface")

"Spinon Fermi-liquid" Theory of Correlated Insulators ?

Neel Order v.s. Spin Liquid

Louis Neel

Strasbourg meeting
in 1939



Lev Landau

Landau: Quantum Fluctuations will destroy Neel order

e.g. 1D antiferromagnetic Heisenberg model - Spin Liquid with S=1/2 spinons

... leads to his skepticism about the usefulness of quantum mechanics; this was one of the few limitations of this superior mind. (Jacques Friedel, Physics Today)