Title: Quantum spin liquid phases in the absence of spin-rotation symmetry

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Abstract: We investigate possible quantum spin liquid phases in the presence of a variety of spin-rotational-symmetry breaking perturbations. Projective symmetry group analysis on slave-particle representations is used to understand possible spin liquid phases on the Kagome lattice. The results of this analysis are used to make connections to the exiting and future experiments on Herbertsmithites. Applications to other systems are also discussed.

Quantum Spin Liquid in the absence of Spin-Rotation Symmetry

Yong Baek Kim
University of Toronto

"Emergence and Entanglement",
Perimeter Institute, May 6, 2013

Canada Research Chairs NSERC CRSNG CIFAR CANADIAN INSTITUTE for ADVANCED RESEARCH

Outline

Warm-up (Honeycomb Iridates):

Heisenberg-Kitaev Model on Honeycomb Lattice

R. Schaffer, S. Bhattacharjee, YBK (2012)

Herbertsmithite (Kagome Lattice):

Spin Liquid Phases with Spin Anisotropies

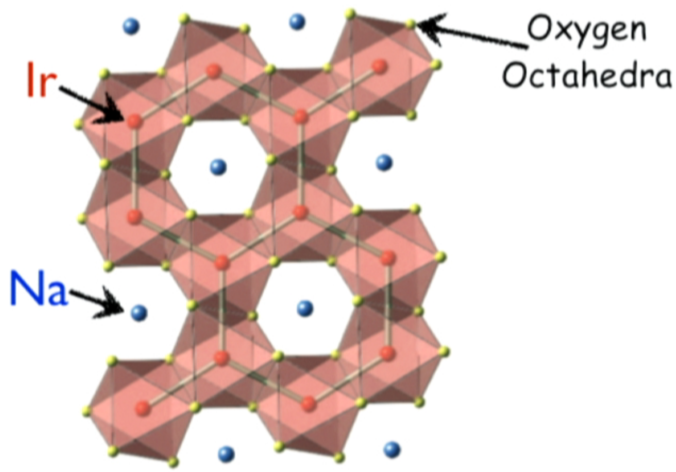
T. Dodds, S. Bhattacharjee, YBK (2013)

Non-Kramers Magnets (Kagome Lattice)

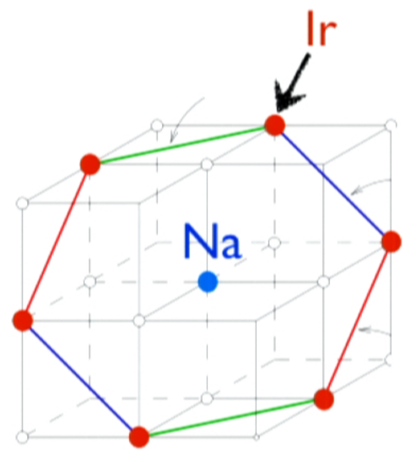
R. Schaffer, S. Bhattacharjee, YBK (2013)

Honeycomb Lattice of Ir^{4+}

Na_2IrO_3 *5d* transition metal oxides



Plane perpendicular
to the [111] direction



Edge-Sharing
Oxygen Octahedra

Strong Coupling Limit the Kitaev Model ?

Including Hund's coupling
direct exchange,
spin-orbit

$$\mathcal{H}_{ij}^{(\gamma)} = -J_1\, S_i^\gamma S_j^\gamma + J_2\, \boldsymbol{S}_i \cdot \boldsymbol{S}_j \qquad \gamma = x, y, z$$

Heisenberg-Kitaev Model

J. Chaloupka, G. Jackeli and G. Khaliullin, PRL 105, 027204 (2010)

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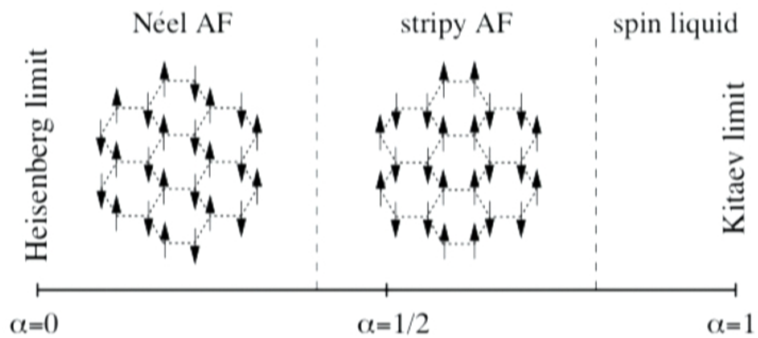
$$H_{\mathrm{HK}} = (1-\alpha)\sum_{\langle i,j \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j - 2\alpha \sum_{\gamma-\mathrm{links}} \sigma_i^\gamma \sigma_j^\gamma$$



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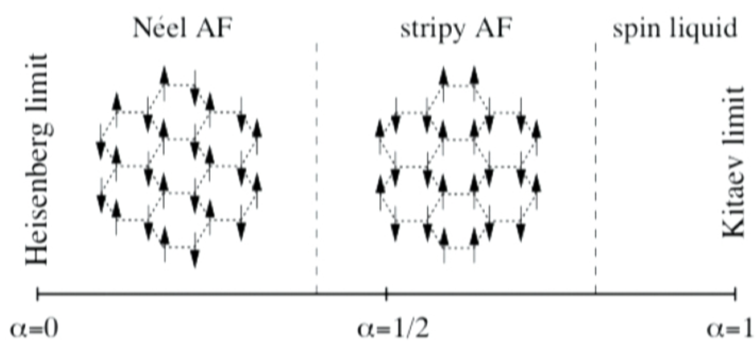
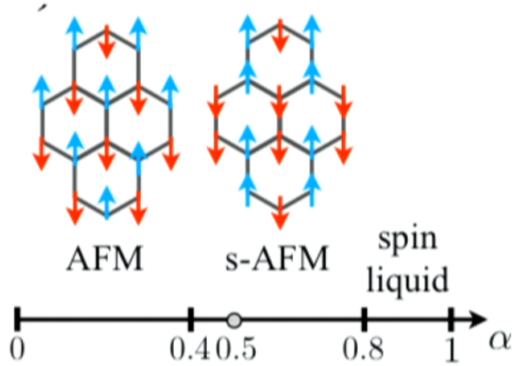
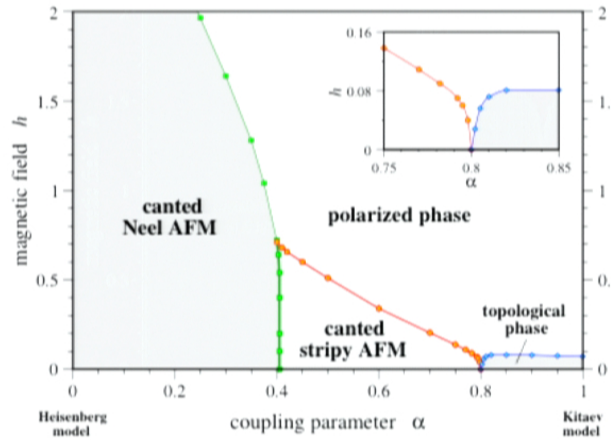


$$H_{\mathrm{HK}} = (1-\alpha)\sum_{\langle i,j\rangle}\vec{\sigma}_i \cdot \vec{\sigma}_j - 2\alpha \sum_{\gamma-\mathrm{links}} \sigma_i^\gamma \sigma_j^\gamma \qquad H_{\mathrm{HK+h}} = H_{\mathrm{HK}} - \sum_i \vec{h}\cdot\vec{\sigma}_i$$





J. Reuther, R. Thomale, S. Trebst, arXiv:1105.2005 (2011)

fRG Study

H.-C. Jiang, Z.-C. Gu, X.-L. Qi, S. Trebst, arXiv:1101.1145 (2011)

DMRG Study

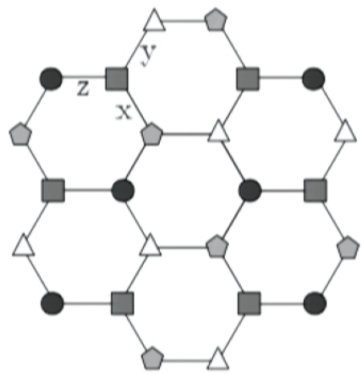
Quantum Phase Transition between Stripy Phase and Spin Liquid

$$H = (1-\alpha)H_{\mathrm{H}} - 2\alpha H_{\mathrm{K}}$$

$$H_{\mathrm{H}} = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \qquad H_{\mathrm{K}} = \sum_{\beta=x,y,z} \sum_{\langle ij \rangle, \beta-links} S_i^\beta S_j^\beta$$

Can the slave-particle (fermion) formulation describe this transition starting from the exactly solvable Kitaev limit of this model (solved in Majorana representation) ?

Rotation of Spin Basis

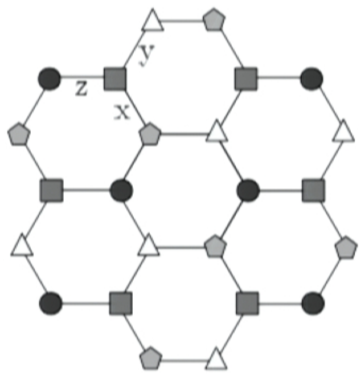


$$H_{\rm H} \rightarrow -H_{\rm H} + 2H_{\rm K}$$

$$H_{\rm K} \rightarrow H_{\rm K}$$

$$H \rightarrow H = -(1-\alpha)H_{\rm H} - 4(\alpha - \frac{1}{2})H_{\rm K}$$

Rotation of Spin Basis



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$$H \to H = -(1-\alpha)H_{\rm H} - 4(\alpha - \frac{1}{2})H_{\rm K}$$

$\alpha = 0.5$ is the SU(2) invariant ferromagnetic Heisenberg model

Hidden SU(2) symmetry;

Stripy phase ==> Ferromagnet (exact ground state at $\alpha = 0.5$)

Transition between a ferromagnetic state to the Z_2 spin liquid

Slave-particle theory in the rotated basis

$$H = -(\frac{1}{2} - \delta)H_{\mathrm{H}} - 4\delta H_{\mathrm{K}} \qquad \delta = \alpha - \frac{1}{2} \qquad \delta \in [0, 0.5]$$

$\delta = 0$ Hidden SU(2) $\qquad \delta = 0.5$ Kitaev limit

Slide-particle theory in the rotated basis

$$H = -(\frac{1}{2} - \delta)H_{\rm H} - 4\delta H_{\rm K} \qquad \delta = \alpha - \frac{1}{2} \qquad \delta \in [0, 0.5]$$

$\delta = 0$ Hidden SU(2) $\qquad \delta = 0.5$ Kitaev limit

$$S_j^\mu = \frac{1}{2} f_{j\alpha}^\dagger [\sigma^\mu]_{\alpha\beta} f_{j\beta} \qquad f_{i\uparrow}^\dagger f_{i\uparrow} + f_{i\downarrow}^\dagger f_{i\downarrow} = 1$$

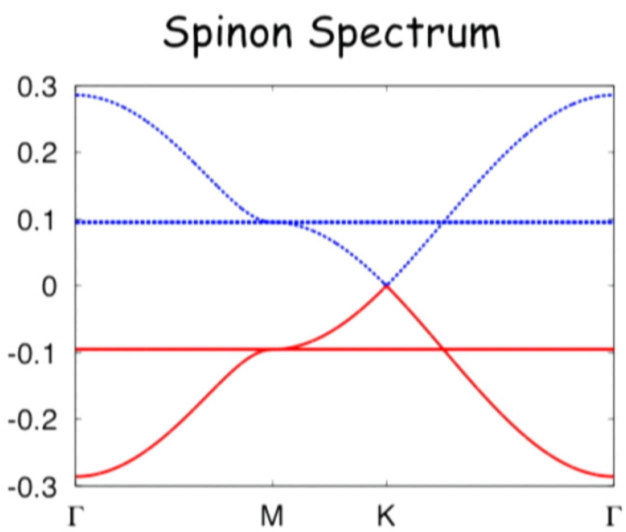
α -th component in the link-p

$$S_i^\alpha S_{i+p}^\alpha = \frac{1}{2} \sum_{\beta=x,y,z} (1 - \delta_{\alpha,\beta}) \left[E_{i,p}^{\beta\dagger} E_{i,p}^\beta + D_{i,p}^{\beta\dagger} D_{i,p}^\beta \right] - \frac{n_i}{4}$$

$$E_{i,p}^\mu = \frac{1}{2} f_{i+p\alpha}^\dagger [\sigma^\mu]_{\alpha\beta} f_{i\beta} \qquad D_{i,p}^\mu = \frac{1}{2} f_{i+p\alpha} [i\sigma^y \sigma^\mu]_{\alpha\beta} f_{i\beta}$$

$$m_j = \frac{1}{2} \langle f_{j\alpha}^\dagger [\sigma^z]_{\alpha\beta} f_{j\beta} \rangle$$ magnetic order

Kitaev Limit



Gapless Z_2 spin liquid

Heisenberg-Kitaev Model

Ferromagnet* (gapped U(1) spin liquid) $\langle m \rangle \neq 0$ $\Leftrightarrow$ Gapless Z_2 spin liquid $E \neq 0$ (charge-2 Higgs)

U(1) spin liquid in 2D with gapped spinons are unstable due to instantons ==> confinement

Ferromagnet $\langle m \rangle \neq 0$ $\Leftrightarrow$ Gapless Z_2 spin liquid

In mean-field theory, this transition is first order (two competing "order parameters")

Open questions ?

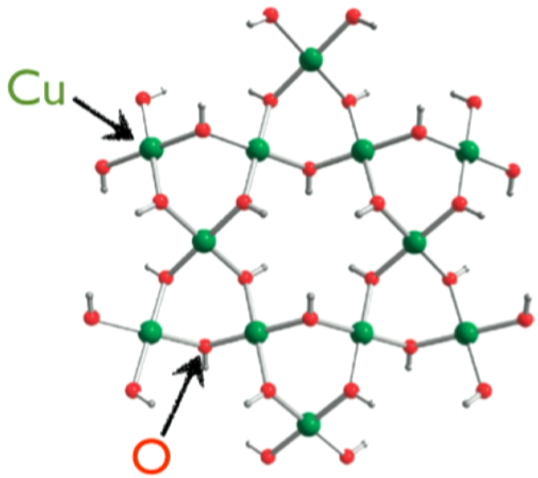
But "E" is not a physical order parameter;
there is no order parameter for the Z_2 spin liquid

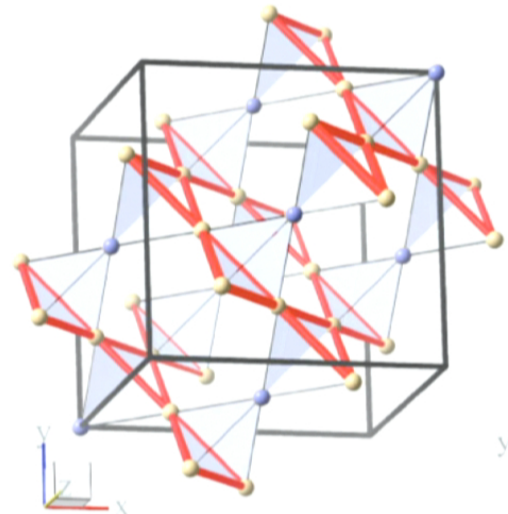
Can we have a continuous transition ?
Collinear magnet and a gapless Z_2 spin liquid

Higgs transition and confinement should occur
at the same time

Herbertsmithite:
Effect of Spin-anisotropies

Herbertsmithite $ZnCu_3(OH)_6Cl_2$





Cu^{2+} S=1/2 Kagome layers

Close to nearest-neighbor AF Heisenberg model

J ~ 200K

Nearest-neighbor AF Heisenberg Model

DMRG: Gapped Spin Liquid	S. Yan et al. (2011) S. Depenbrock et al. (2012)

Nearest-neighbor AF Heisenberg Model

DMRG: Gapped Spin Liquid	S. Yan et al. (2011) S. Depenbrock et al. (2012)
DMRG: Entanglement Entropy with $J_2/J_1 \sim 0.1$: Z_2 spin liquid	H.-C. Jiang et al. (2011)

Which spin liquid state ?

Which Z_2 spin liquid state ?

Herbertsmithite: Model

NN AF Heisenberg interaction

$$\mathcal{H}_{\rm NN-KHAF} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

J ~ 200K

Helton (2007)
Mendels (2007)

Dzyaloshinsky-Moriya

$$\mathcal{H}_{\rm DM} = D \sum_{\langle ij \rangle} \hat{\mathbf{D}}_{ij} \cdot \mathbf{S}_i \times \mathbf{S}_j$$

D ~ J/10

Zorko (2008)
Han (2012) Ofer (2009, 2010)

Ising Easy Axis Interaction

$$\mathcal{H}_{\rm Ising} = \Delta \sum_{\langle ij \rangle} S_i^z S_j^z \qquad \Delta \sim J/10$$

Next-Nearest-Neighbor Interaction

$$\mathcal{H}_{\rm NNN} = J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

may be important for stabilizing Z_2 spin liquid

Slave Particle Construction

$$S_j^\mu = \frac{1}{2} f_{j\alpha}^\dagger [\rho^\mu]_{\alpha\beta} f_{j\beta} \qquad f_{i\uparrow}^\dagger f_{i\uparrow} + f_{i\downarrow}^\dagger f_{i\downarrow} = 1.$$

Spin-rotation Invariant case:

$$\chi_{ij} = \langle f_{i\alpha}^\dagger f_{j\alpha} \rangle^* \qquad \eta_{ij} = \langle f_{i\alpha} \left[i\tau^2 \right]_{\alpha\beta} f_{j\beta} \rangle^*$$

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In absence of spin-rotation invariance

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$$E_{ij}^a = \langle f_{i\alpha}^\dagger \left[\tau^a \right]_{\alpha\beta} f_{j\beta} \rangle^* \qquad D_{ij}^a = \langle f_{i\alpha} \left[i\tau^2 \tau^a \right]_{\alpha\beta} f_{i\beta} \rangle^*$$

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In our case, it is sufficient to keep E^z, D^z
(E^x, E^y, D^x, D^y become repulsive channels in MF theory)

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Quadratic MF Hamiltonian

$$H_Q = \sum_{ij} \Psi_i^\dagger U_{ij} \Psi_j \qquad \Psi_i^\dagger = \left[f_{i\uparrow}^\dagger \;\; f_{i\downarrow} \;\; f_{i\downarrow}^\dagger \;\; -f_{i\uparrow} \right]$$

U_{ij} are functions of $\{\chi_{ij}, \eta_{ij}, \mathbf{E}_{ij}, \mathbf{D}_{ij}\}$

QSL Label	Singlet Ansatz[10]	[Singlet + Triplet] Ansatz
$U(1)[0,0]$	Fermi surface (F.S.)	F.S. is altered but not gapped out
$U(1)[0,\pi]$	Dirac point (D.Pt.)	D. Pt. is gapped out (∗)
$U(1)[\pi,\pi]$ $U(1)[\pi,0]$	Flat bands & D.Pt.	The Flat band acquires dispersion while the D. Pt. remains intact.
$Z_2[0,0]A$	F.S. gapped out to Band touching points	Band touching points remain
$Z_2[0,\pi]\beta$	F. S. becomes fully gapped	Gap is altered
$Z_2[0,0]B$	F.S. shrinks compared to parent $U(1)$	F.S. gapped out to band touching points
$Z_2[0,\pi]\alpha$	D.Pt. changes to band touching points	Band touching points remain
$Z_2[0,0]D$	F.S. shifted compared to parent $U(1)$	F.S. gapped out to band touching points
$Z_2[0,\pi]\gamma$	D.Pt. changes to band touching points	Band touching points remain
$Z_2[\pi,\pi]B$	Negligible change compared to parent $U(1)$	Bands gapped to D.Pt. and band touching points
$Z_2[\pi,0]B$	Flat Bands are gapped to form a F. S.	F.S. gapped to band touching point

Spinon Excitations

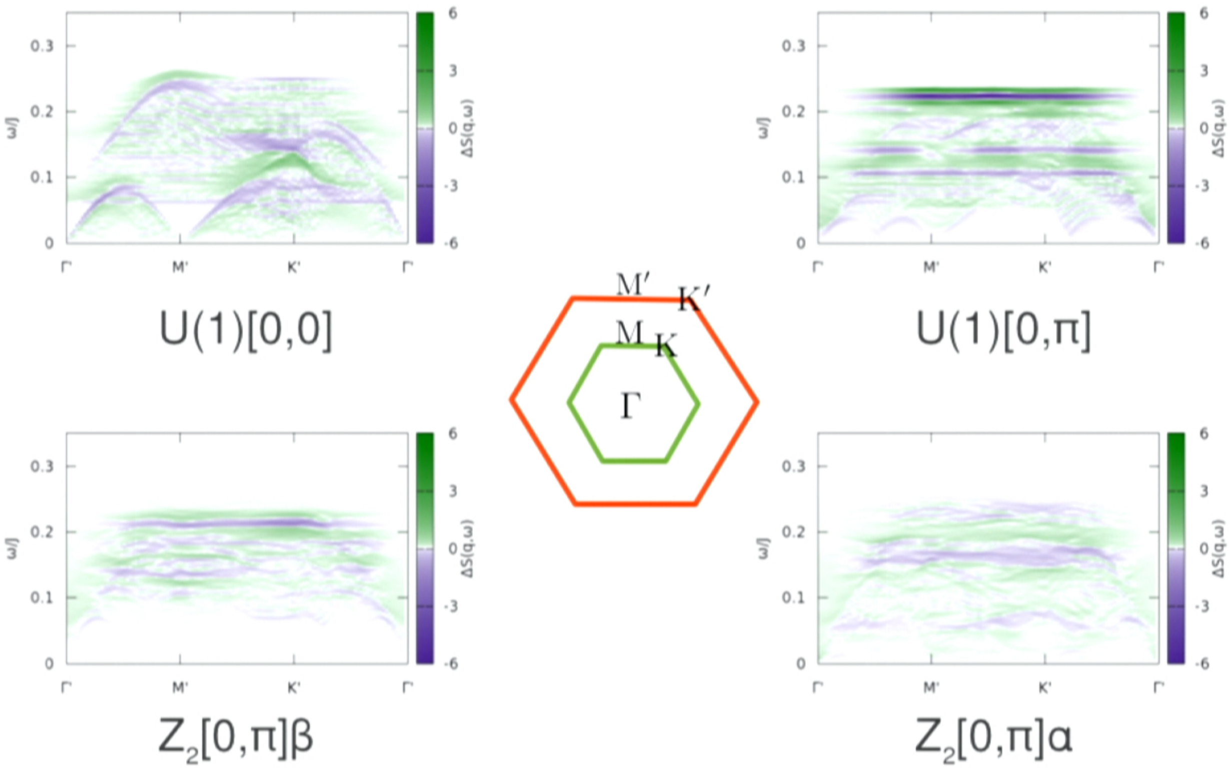
Eight Z2 spin liquid if only the 1st and 2nd neighbor amplitudes are finite

U(1)[a,b]

a: flux through △

b: flux through ⬡

Change from Singlet to Singlet+Triplet



Dynamic Spin Structure Factor

Generally there is a lot of "diffuse" scattering

Consistent with Neutron Scattering ?

When spin-rotation symmetry is broken, there is spectral weight transfer to the zone center (q=0):

generally less dispersive or less momentum dependence

Small intensity at zone center (q=0)

Spin anisotropy is weak

Still difficult to distinguish different spin liquid phases ...

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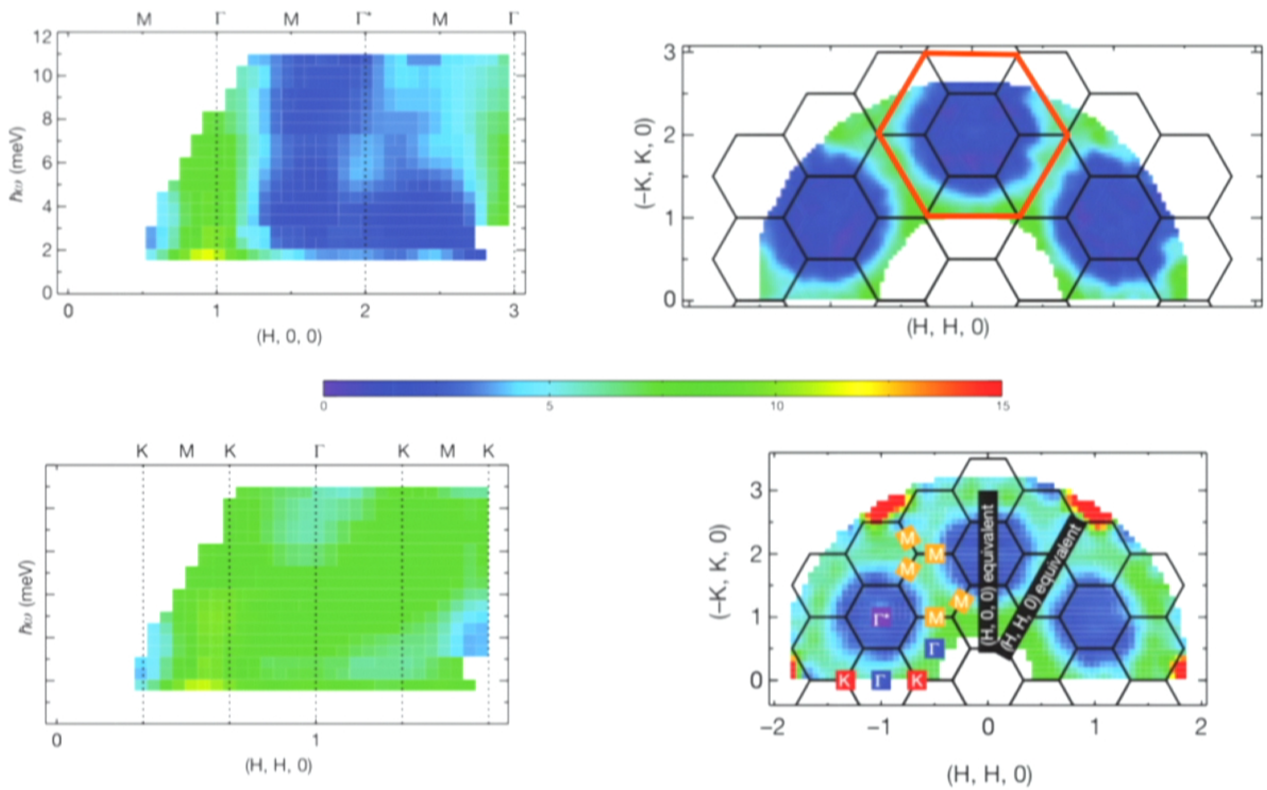
Neutron Scattering



Tian-Heng Han *et. al.*, Nature **492**, 406 (2012)

Electron Spin Resonance (ESR)

ESR may be a useful tool to
distinguish different
quantum spin liquid phases !

Take the advantage of
spin-anisotropy to probe
the underlying spin liquid phases

Spin-Orbital Liquids in Non-Kramers Magnets

Non-Kramers Doublet

Pr^{3+} ($4f^2$) in local D_{3d} crystal field environment

e.g. $Pr_2Sn_2O_7$ or $Pr_2Ti_2O_7$

J=4 (S=1, L=5) multiplet split due to local crystal field by surrounding O^{2-} ions

$$\Gamma_{J=4} = 3E_g \oplus 2A_{1g} \oplus A_{2g}$$

Y. Matchida et al. (2007), S. Onoda and Y. Tanaka (2010)

The ground state is a non-Kramers doublet

$$|\pm\rangle = \alpha|J_z = \pm 4\rangle \pm \beta|J_z = \pm 1\rangle - \gamma|J_z = \mp 2\rangle \quad \alpha \gg \beta, \gamma$$

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Non-Kramers pseudospin degrees of freedom

$\sigma_z \sim J_z$ dipolar

$\sigma_\pm \sim \{J_z, J^\pm\}$ quadrupolar

Non-Kramers Doublet

Time-reversal symmetry $T = \sigma_1 K \quad T^2 = 1$

$$(\sigma_1, \sigma_2, \sigma_3) \longrightarrow (\sigma_1, \sigma_2, -\sigma_3)$$

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Pseudospin model (written in local coordinate axis) is generically non-Heisenberg-like

$$H_{\rm nK} = \sum_{ij} \left[J_{zz}\sigma_i^3\sigma_j^3 - J_{\pm}(\sigma_i^+\sigma_j^- + h.c.) + J_{\pm\pm}(\gamma_{ij}\sigma_i^+\sigma_j^+ + h.c.) \right]$$

Onoda & Tanaka (2010) Savary & Balents (2011)

Consider quantum spin liquid phases (spin-orbital liquid) on frustrated lattices such as Kagome and Pyrochlore lattices

Differences between Kramers and non-Kramers cases ?

Action of time-reversal symmetry is different

Projective Symmetry Group (PSG)

Algebraic PSG is essentially the same for Kramers and non-Kramers doublets on Kagome lattice

But allowed solutions for mean-field Hamiltonians or U_{ij} are DIFFERENT

Solutions to PSG requires $G_T^2 = \eta_T I$

$\eta_T = \pm 1$ if IGG=Z_2

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Non-Kramers case:

Both $\eta_T = +1$ and $\eta_T = -1$ lead to non-trivial solutions

NEW SPIN LIQUIDS