The Abdus Salam International Centre for Theoretical Physics

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Miniworkshop on Strong Correlations in Materials and Atom Traps

4 - 15 August 2008

Fluctuations and degenracy breaking in some frustrated magnet.

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Searching for Quantum Spin Liquids

and finding surprises

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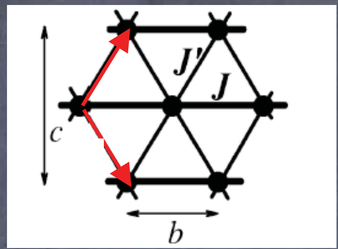
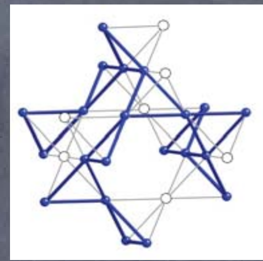
The David and Lucile Packard Foundation

Collaborators





- Oleg Starykh, U. Utah

- Masanori Kohno, NIMS, Japan

- Gang Chen, UCSB

- Michael Lawler, Toronto

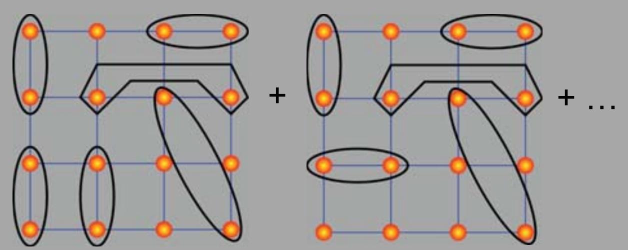
- Yong-Baek Kim, Toronto

- Arun Paramekanti, Toronto

Quantum Spin Liquids

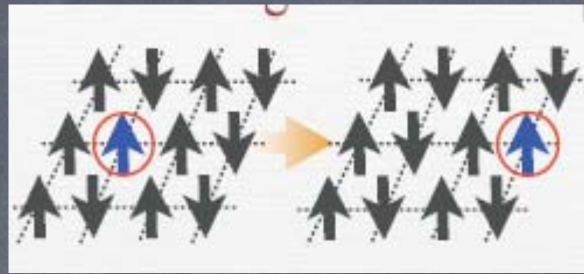
- QSL: a state of a magnet in which quantum fluctuations prevent order even at T=0.
- Many theoretical suggestions since Anderson (73)
  - "Resonating Valence Bond" QSL states

$\Psi =$

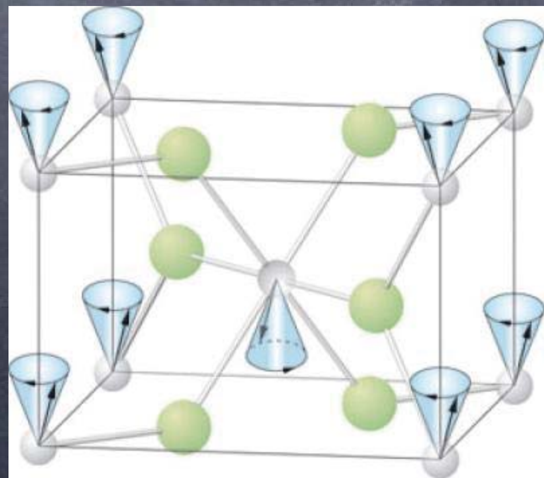


Magnons

- Basic excitation: spin flip
  - Carries "S^z"$=\pm 1$



- Periodic Bloch states: spin waves
  - Quasi-classical picture: small precession



MnF_2

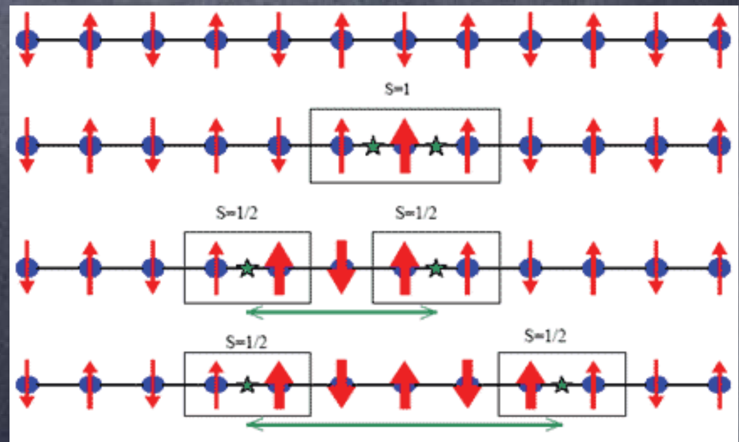
$\vec{k}$

$\epsilon = \hbar\omega(\vec{k})$

Image: B. Keimer

One dimension

- Heisenberg model is a *spin liquid*
  - No magnetic order $\langle \vec{S}(x) \cdot \vec{S}(x') \rangle \sim \frac{(-1)^{x-x'}}{|x-x'|} + \cdots$
  - Power law correlations of spins and dimers
- Excitations are s=1/2 *spinons*
  - General for 1d chains

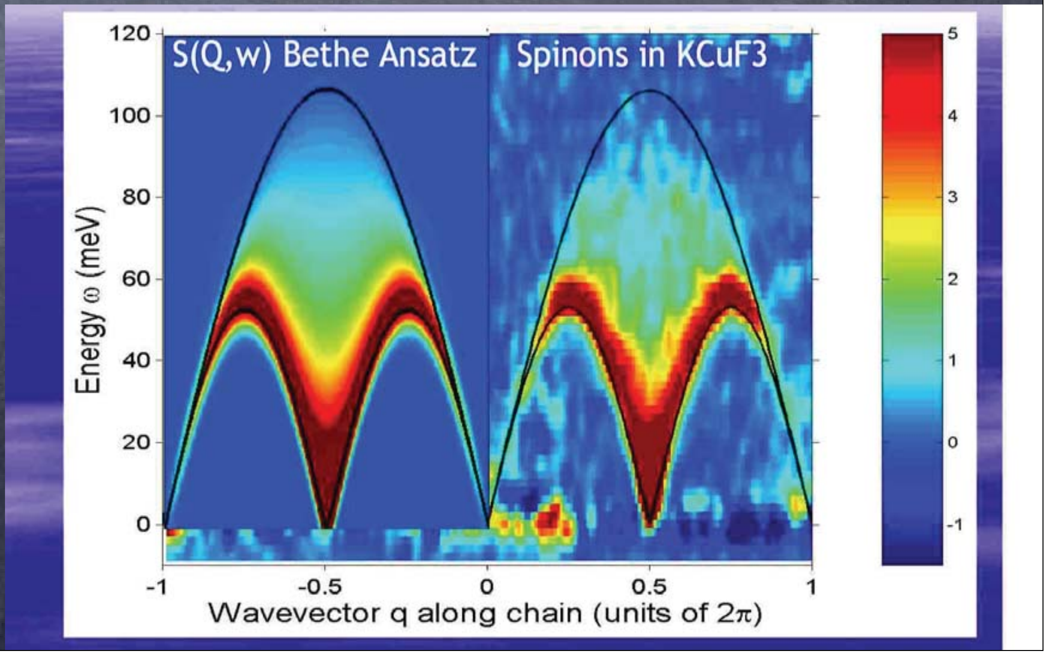


Spinons by neutrons

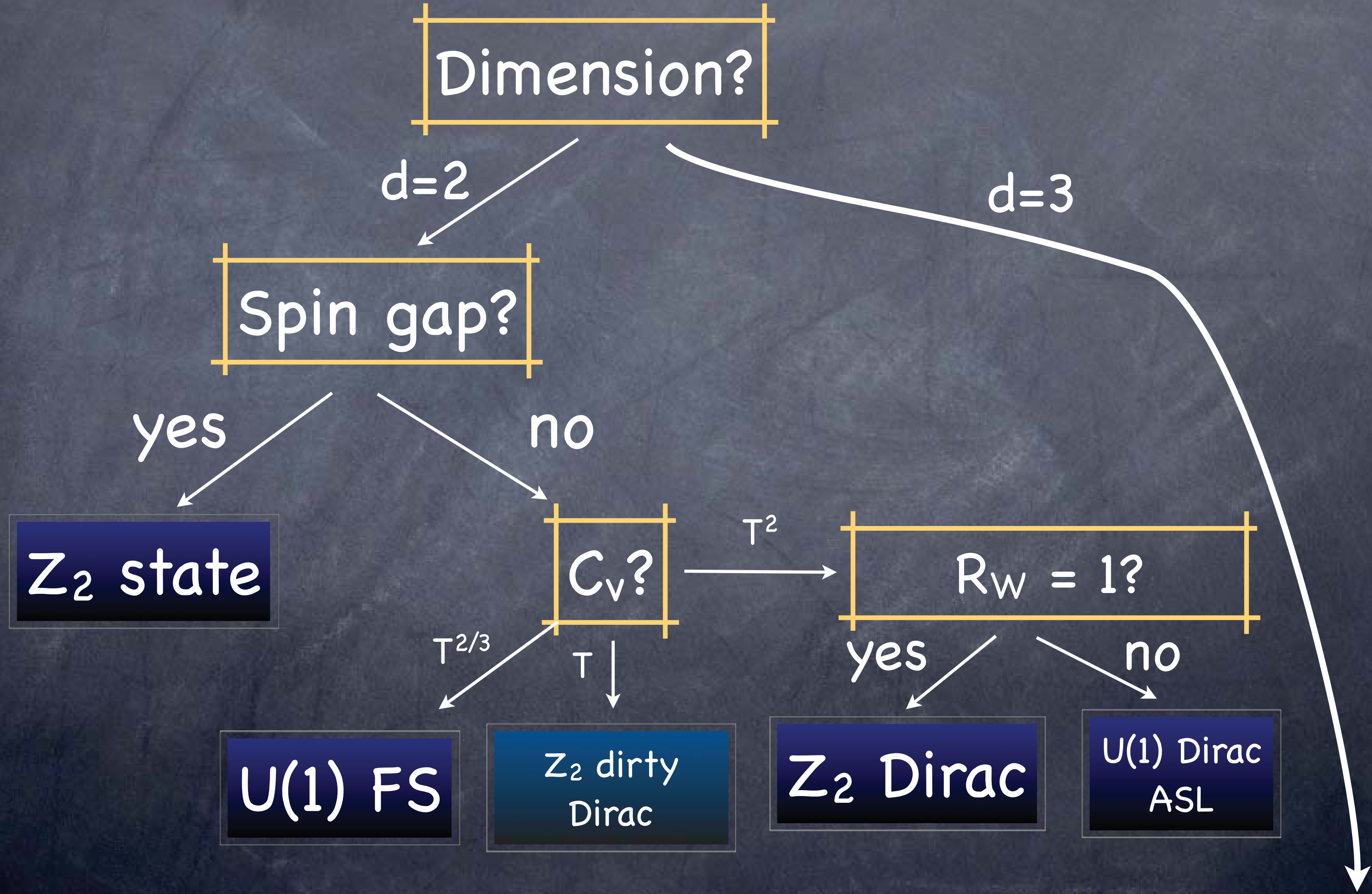
- Bethe ansatz: $$\epsilon_s(k) = \frac{\pi J}{2}|\sin k|$$
  - Spinon energy $$k = k_1 + k_2$$
  - Spin-1 states $$\epsilon = \epsilon_s(k_1) + \epsilon_s(k_2)$$

2-particle continuum

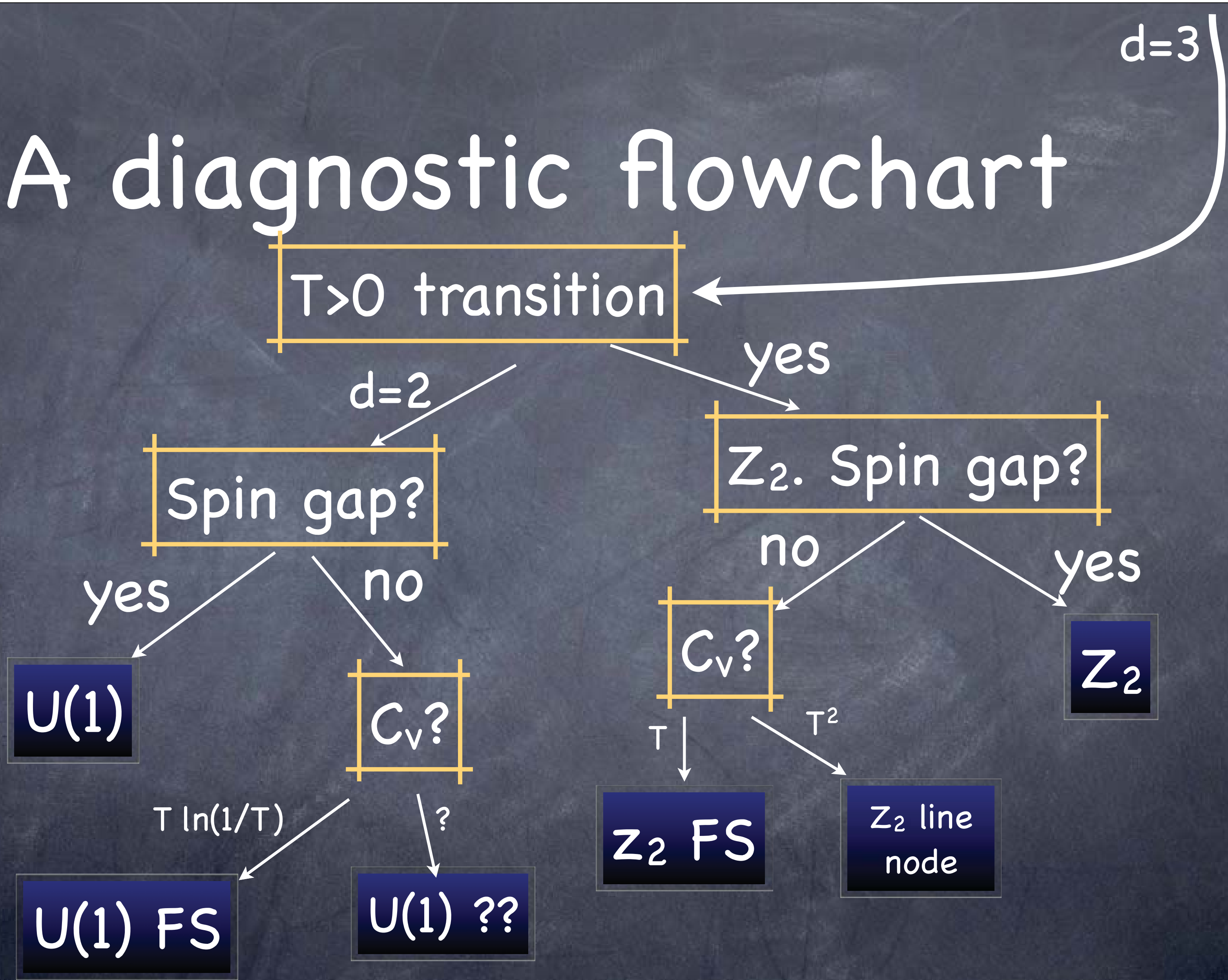
- Theory vs experiment for $KCuF_3$ with anisotropy ≈30
  - B. Lake, HMI



Many spin liquids in theory!



A diagnostic flowchart



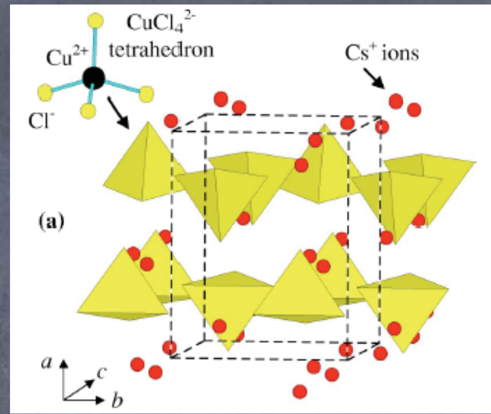
disordered possibilities neglected

QSL candidates

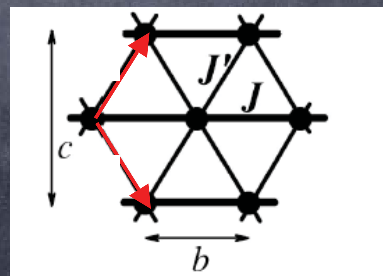
- $CsCu_2Cl_4$ - spin-1/2 anisotropic triangular lattice
- ? $NiGa_2S_4$ - spin-1 triangular lattice
- κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$, $EtMe_3Sb[Pd(dmit)_2]_2$ - triangular lattice organics
- ? $FeSc_2S_4$ - orbitally degenerate spinel
- $Na_4Ir_3O_8$ - hyperkagome
- $ZnCu_3(OH)_6Cl_2$ - kagome

Cs_2CuCl_4

- Spatially anisotropic triangular lattice
  - Cu^{2+} spin-1/2 spins



$$\boxed{H = \frac{1}{2}\sum_{ij}\left[J_{ij}\vec{S}_i\cdot\vec{S}_j - \vec{D}_{ij}\cdot\vec{S}_i\times\vec{S}_j\right]}$$



$$\vec{D} = D\hat{a}$$

- couplings:

J=0.37meV

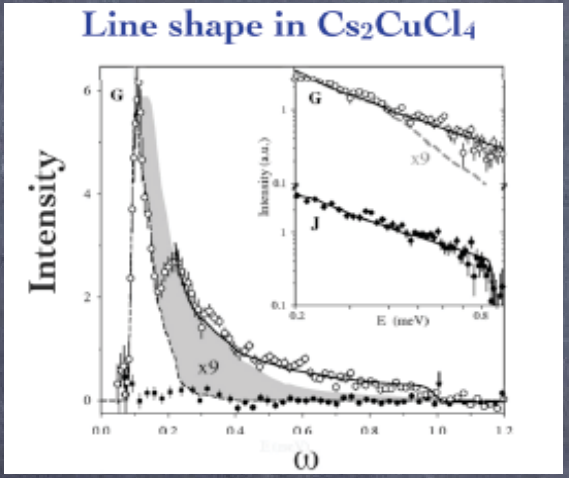
J'=0.3J

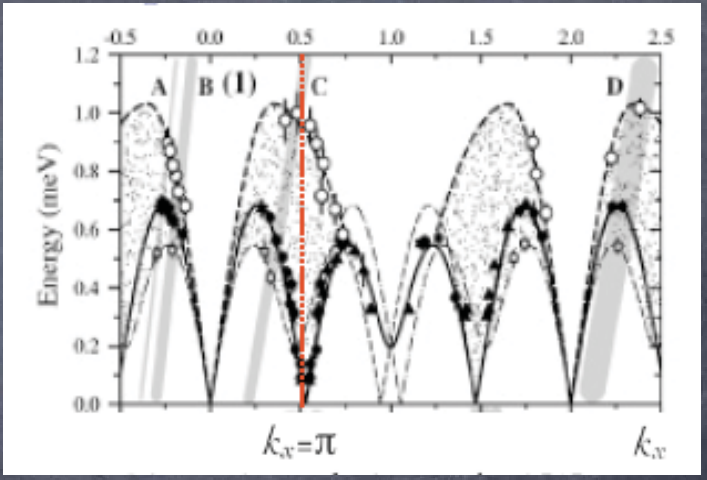
D=0.05J

R. Coldea et al

Neutron scattering

- Coldea et al, 2001/03: a 2d spin liquid?



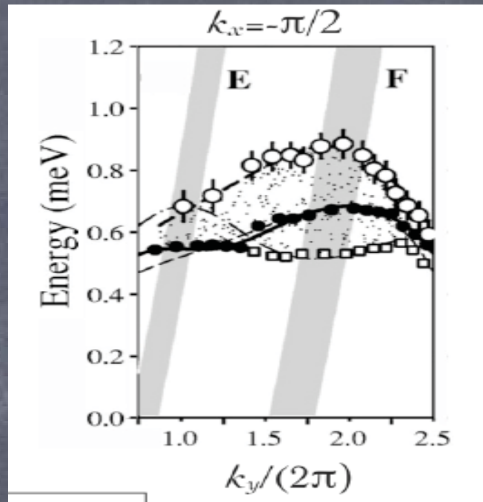


Very broad spectrum similar to 1d (in some directions of k space). Roughly fits power law.

Fit of "peak" dispersion to spin wave theory requires adjustment of J,J′ by 40% – in opposite directions!

2d theories

- Arguments for 2d:
  - $J'/J = 0.3$ *not very small*
  - Transverse dispersion
- Exotic theories:



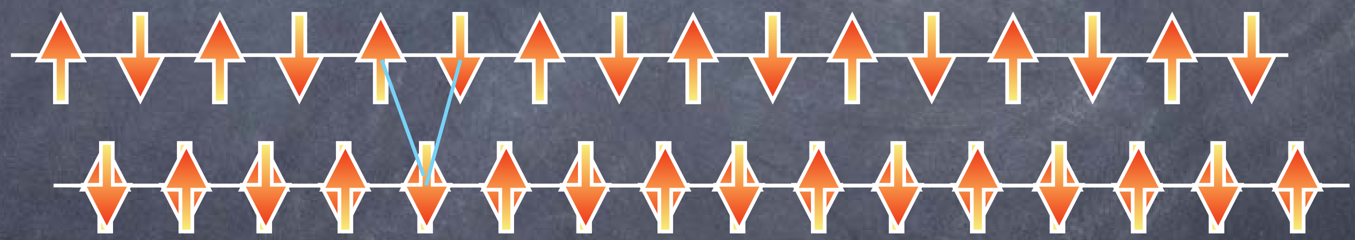
- J.Alicea, O.I.Motrunich & M.P.Fisher: Phys. Rev. Lett. **95**, 247203 (2005).
- S.V.Isakov, T.Senthil & Y.B.Kim: Phys. Rev. B **72**, 174417 (2005).
- Y.Zhou & X.-G.Wen: cond-mat/0210662.
- F.Wang & A.Vishwanath: Phys. Rev. B **74**, 174423 (2006).
- C.-H.Chung, K.Voelker & Y. B. Kim: Phys. Rev. B **68**, 094412 (2003).

- Spin waves

- M.Y.Veillette, A.J.A.James & F.H.L.Essler: Phys. Rev. B **72**, 134429 (2005).
- D.Dalidovich, R.Sknepnek, A.J.Berlinsky, J.Zhang & C.Kallin: Phys. Rev. B **73**, 184403 (2006).
- R.Coldea, D.A.Tennant & Z.Tylczynski: Phys. Rev. B **68**, 134424 (2003).

Dimensional reduction?

- Frustration of interchain coupling makes it less "relevant"
  - First order energy correction vanishes

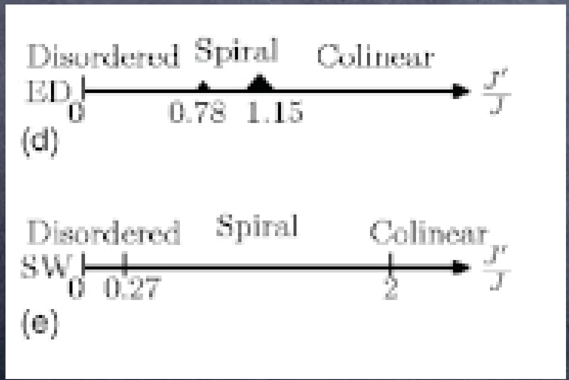


  - Leading effects on correlations are in fact $O[(J')^4/J^3]$!

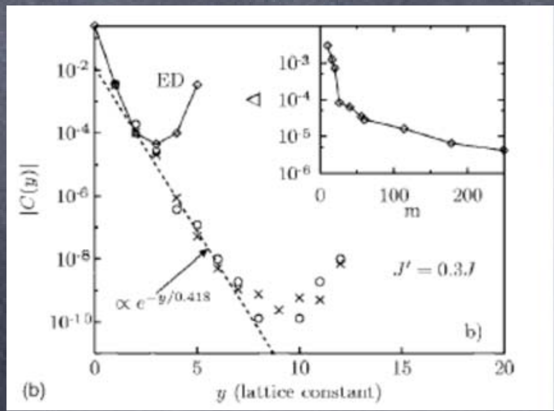
Dimensional reduction?

- Frustration of interchain coupling makes it less "relevant"
  - First order energy correction vanishes.
  - Numerics: J'/J < 0.7 is "weak"

Weng et al, 2006



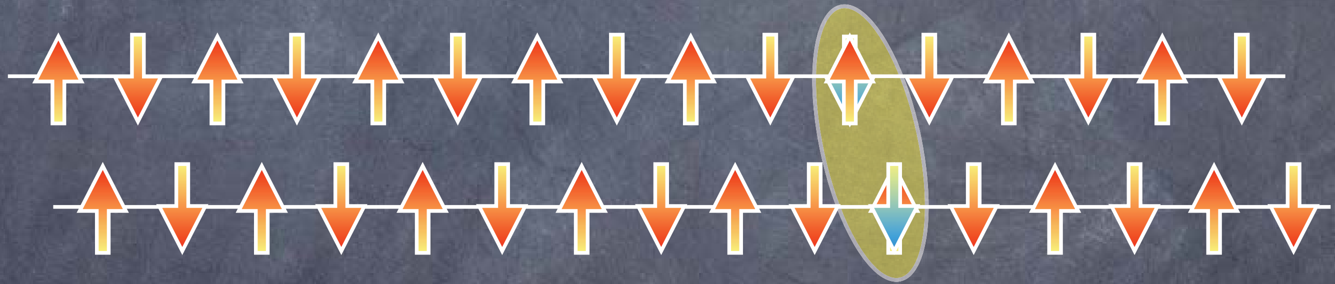
Very different from spin wave theory



Very weak inter-chain correlations

Excitations

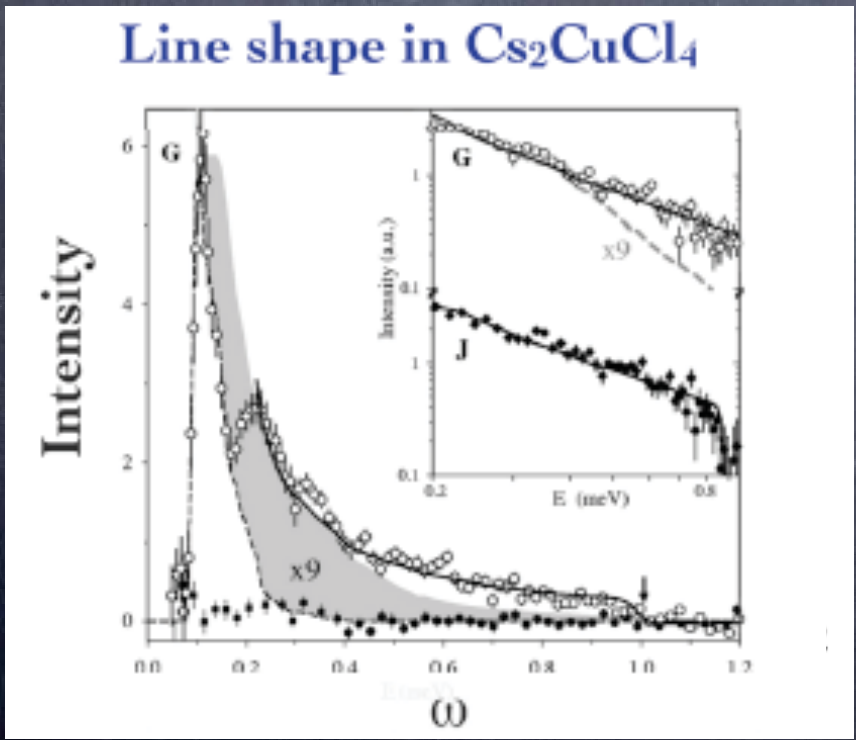
- Build 2d excitations from 1d spinons
  - Exchange: $$\frac{J'}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)$$

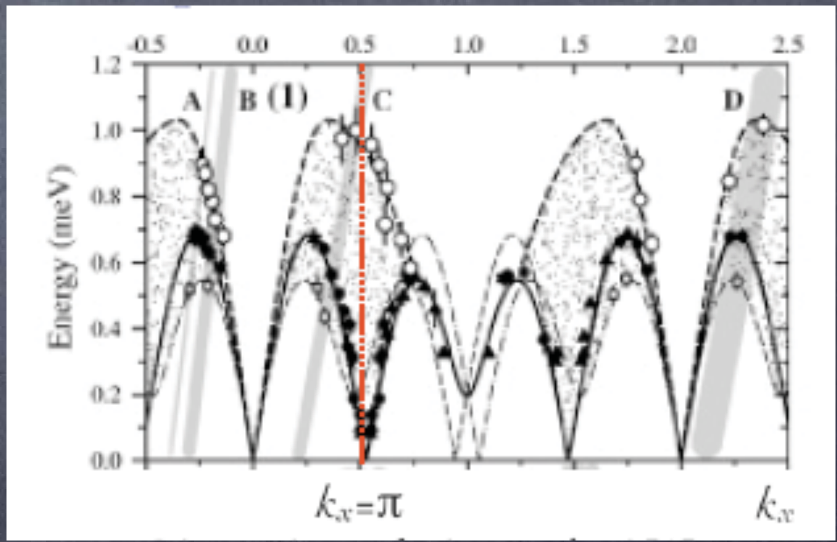


- Expect spinon binding to lower inter-chain kinetic energy
  - Use 2-spinon Schroedinger equation

Broad lineshape: “free spinons”

- “Power law” fits well to free spinon result
  - Fit determines normalization

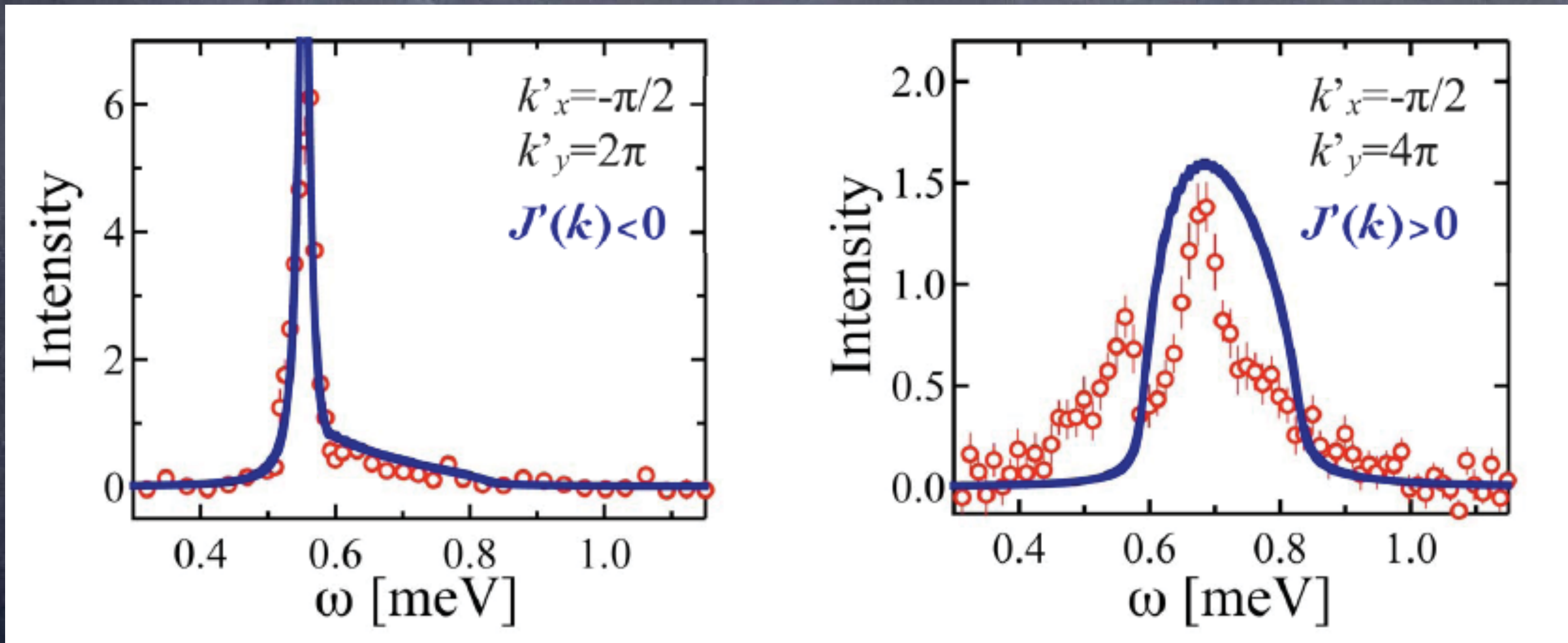




J’(k)=0 here

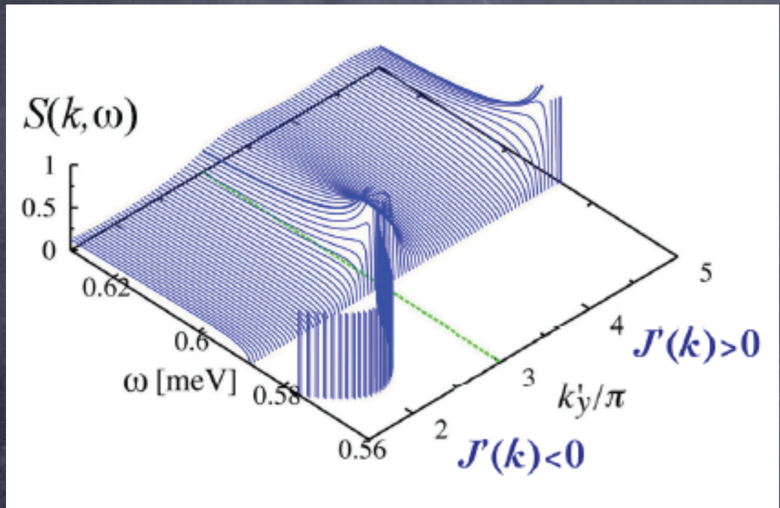
Bound state

- Compare spectra at J'(k)<0 and J'(k)>0:

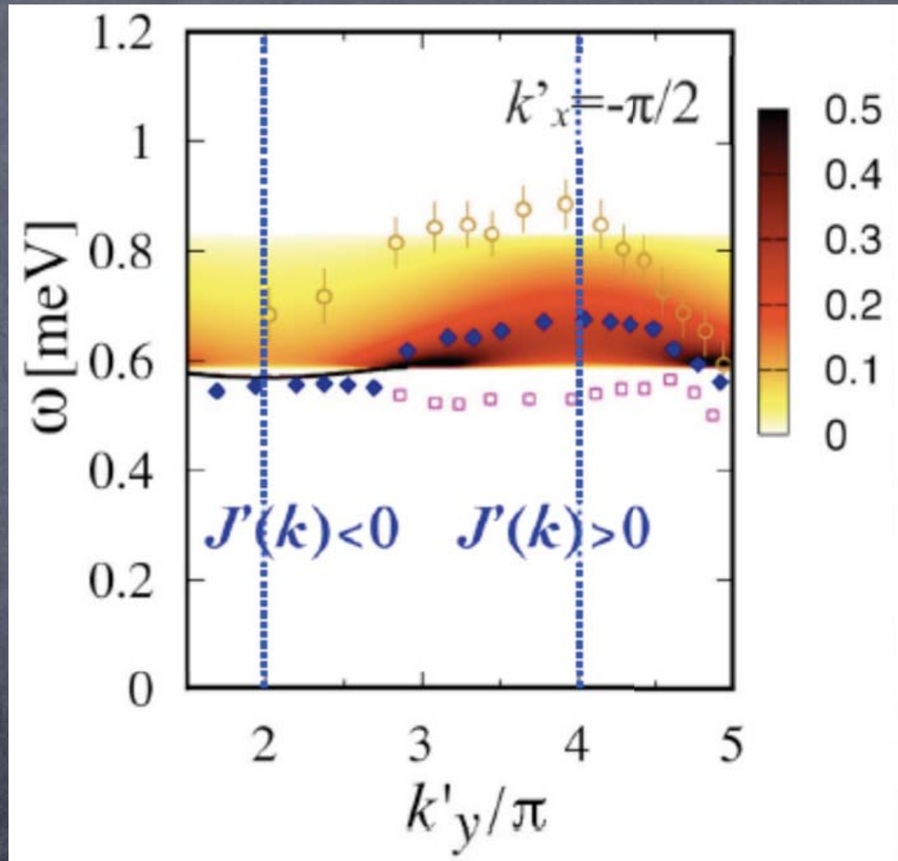


- Curves: 2-spinon RPA w/ experimental resolution
- Curves: 4-spinon theory w/ experimental resolution

Transverse dispersion

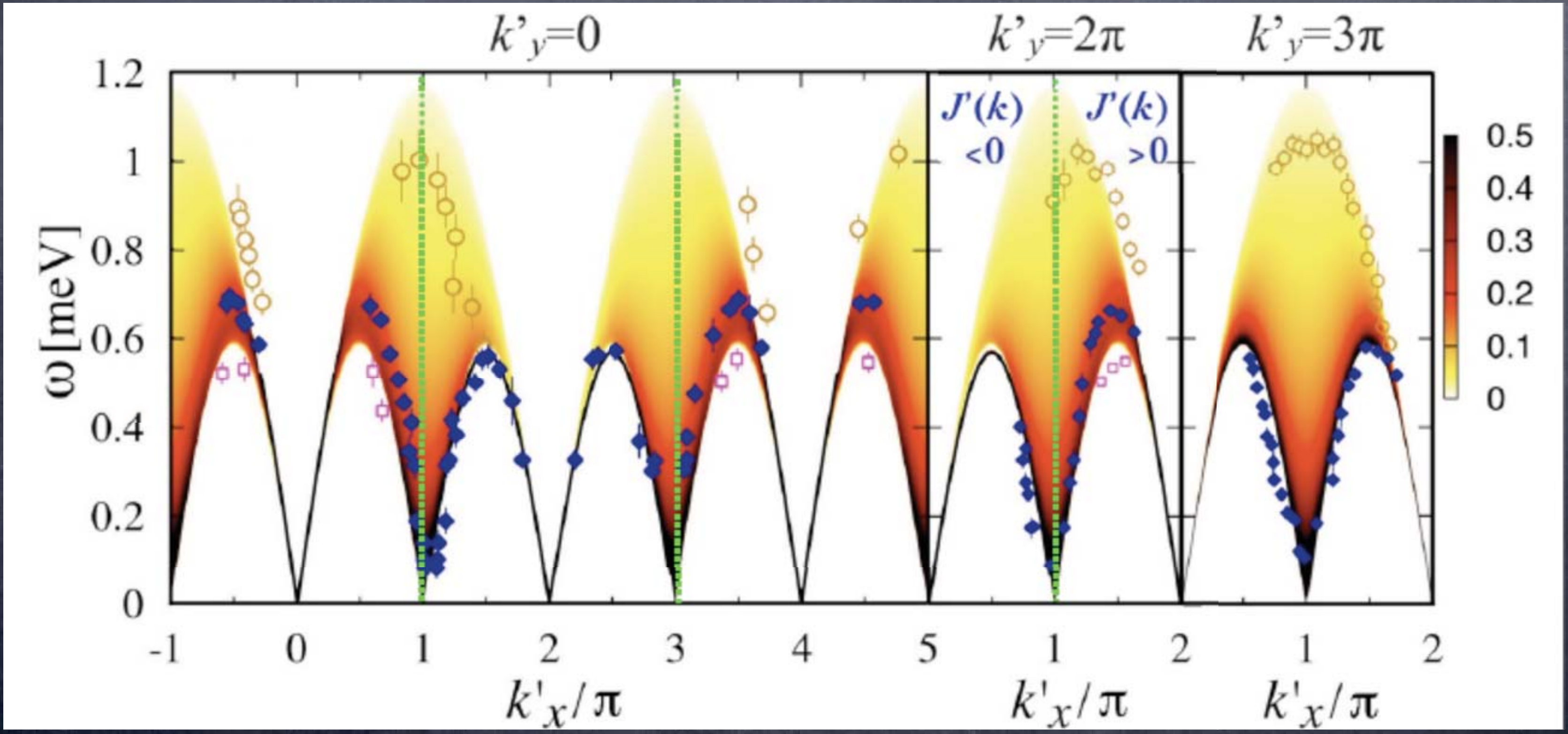


Bound state and resonance



Solid symbols: experiment
Note peak (blue diamonds) coincides with bottom edge only for J'(k)<0

Spectral asymmetry



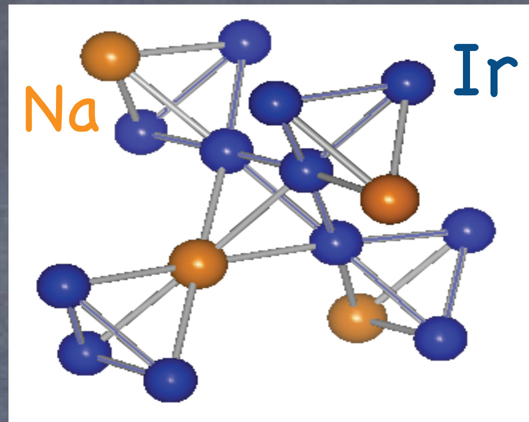
- Vertical lines: J'(k)=0.

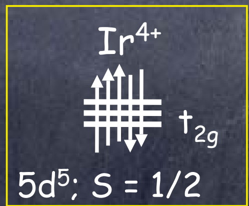
Conclusions on Cs_2CuCl_4

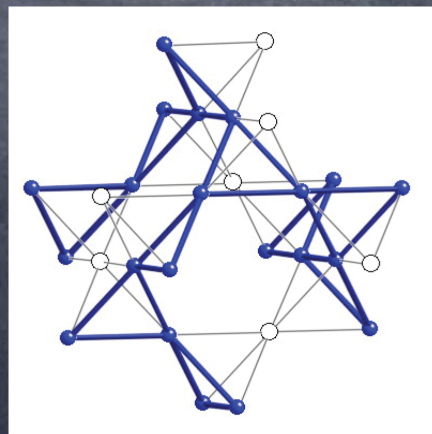
- Simple theory works well for frustrated quasi-1d antiferromagnets
  - Frustration leads to a strong enhancement of one-dimensionality
- The mystery of Cs_2CuCl_4 should be considered solved
  - Many (nearly all) other details of diverse experiments on this material may be understood in the same framework

$Na_4Ir_3O_8$

- An "hyperkagome" lattice of Ir^{4+} spins
- Expect S=1/2 spin state - orbital state unclear?



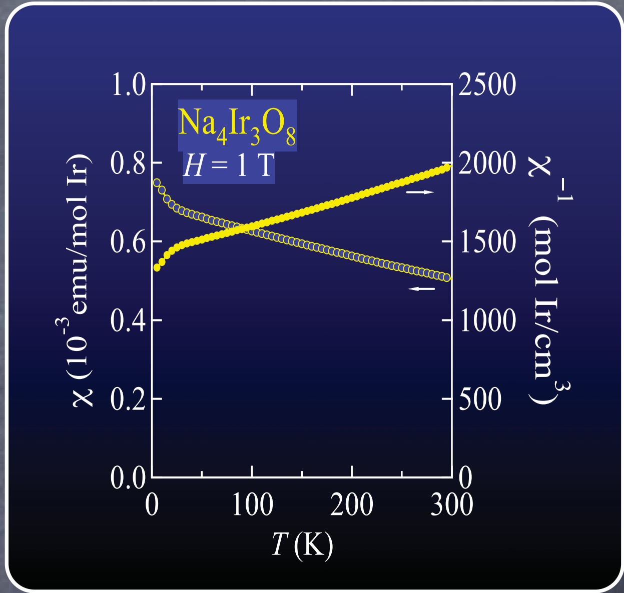


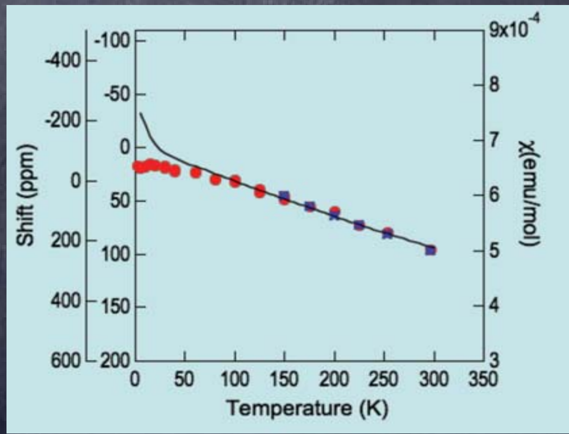


Takagi group

$Na_4Ir_3O_8$

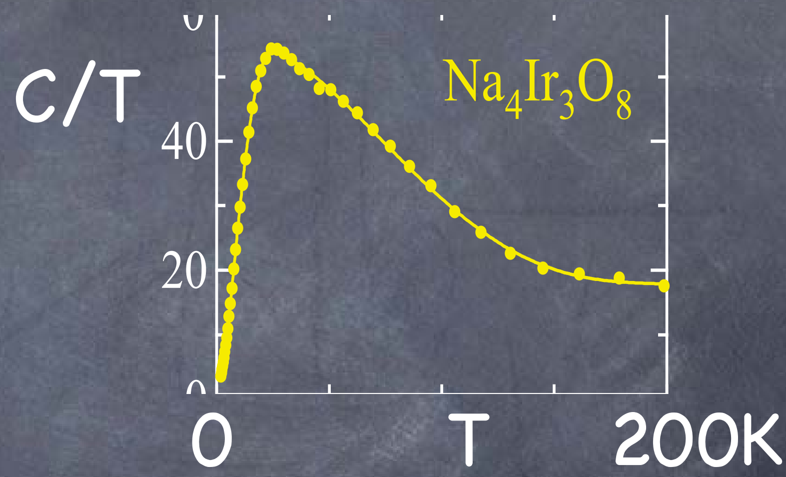
- Susceptibility
  - Curie-Weiss temperature $\Theta_{CW} \approx$ -650K
  - Large χ at low T
  - μ_{eff} = 1.96 μ_B/Ir ≈ 1.73 μ_B/Ir (s=1/2)
- Consistent with Knight shift
  - low-T upturn not seen in K: extrinsic

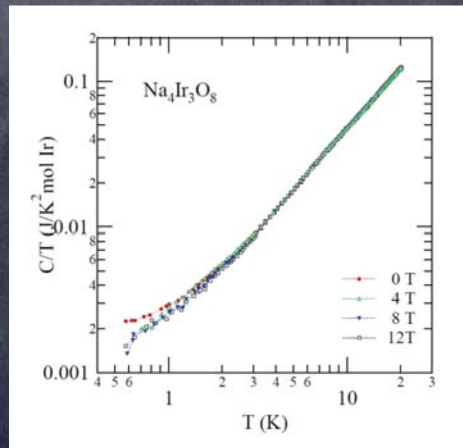




$Na_4Ir_3O_8$

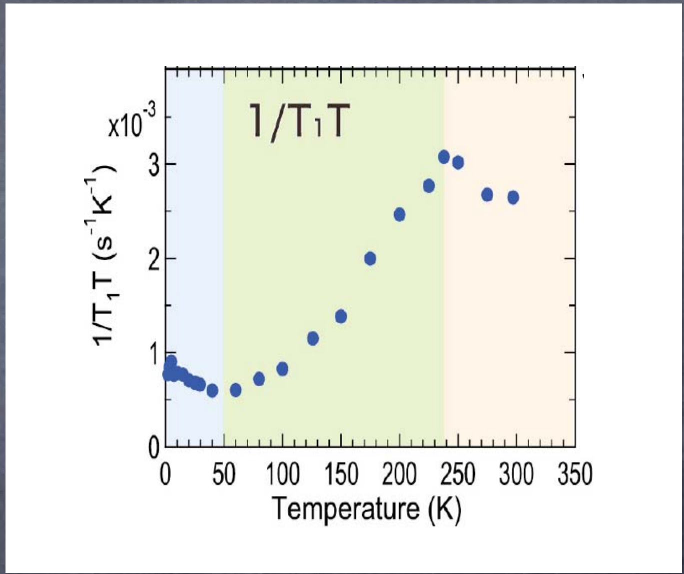
- Specific Heat
  - broad peak around 30K
  - power-law (between T and T^2) at low T indicates gapless excitations





$Na_4Ir_3O_8$

- NMR $1/T_1$ rate is power law for 50<T<200, suggestive of low energy excitations

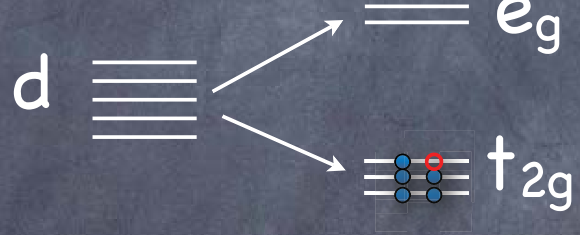


Theory

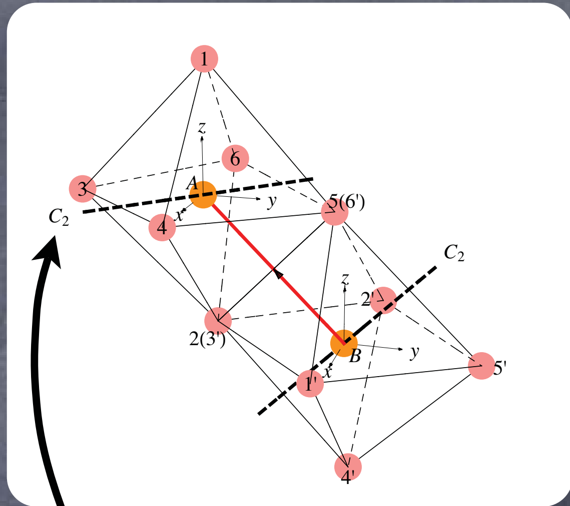
- Write down Heisenberg model
  - start doing all standard things...
    - Classical Heisenberg model J. M. Hopkinson, S. V. Isakov, H.-Y. Kee, Y. B. Kim, PRL 99, 037201 (2007).
    - Quantum bosonic SP(N) MFT M. J. Lawler, H.-Y. Kee, Y. B. Kim, and A. Vishwanath, PRL 100, 227201 (2008)
  - but wait...

Quantum Chemistry

- Cubic approximation:



- Orbital degeneracy?
  - non-cubic splittings
  - spin-orbit coupling



C_2 axis is the only point group operation of the Ir site

Ir-O distances are:
2.043Å < 2.048Å < 2.096Å

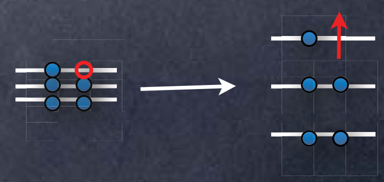
Quantum Chemistry (2)

- Effective Hamiltonian

$$H_{\text{eff}} = \sum_m \delta\epsilon_m |m\rangle\langle m| + \lambda \vec{\ell} \cdot \vec{S}$$

- Two limits:
  - "weak" spin orbit: $\lambda \ll |\delta\epsilon_m|$

t_{2g}



Quantum Chemistry (2)

- Effective Hamiltonian

$$H_{\text{eff}} = \sum_m \delta\epsilon_m |m\rangle\langle m| + \lambda \vec{\ell} \cdot \vec{S}$$

- Two limits:
  - "weak" spin orbit: $\lambda \ll |\delta\epsilon_m|$
  - "strong" spin orbit $\lambda \gg |\delta\epsilon_m|$

t_{2g}  $\longrightarrow$?

Strong spin orbit

- Orbital angular momentum

$$\vec{\ell} = \hat{P}_{t_{2g}} \vec{L} \hat{P}_{t_{2g}} = -\vec{\mathsf{L}}\ !$$

$$|\vec{\mathsf{L}}|^2 = L(L+1)$$

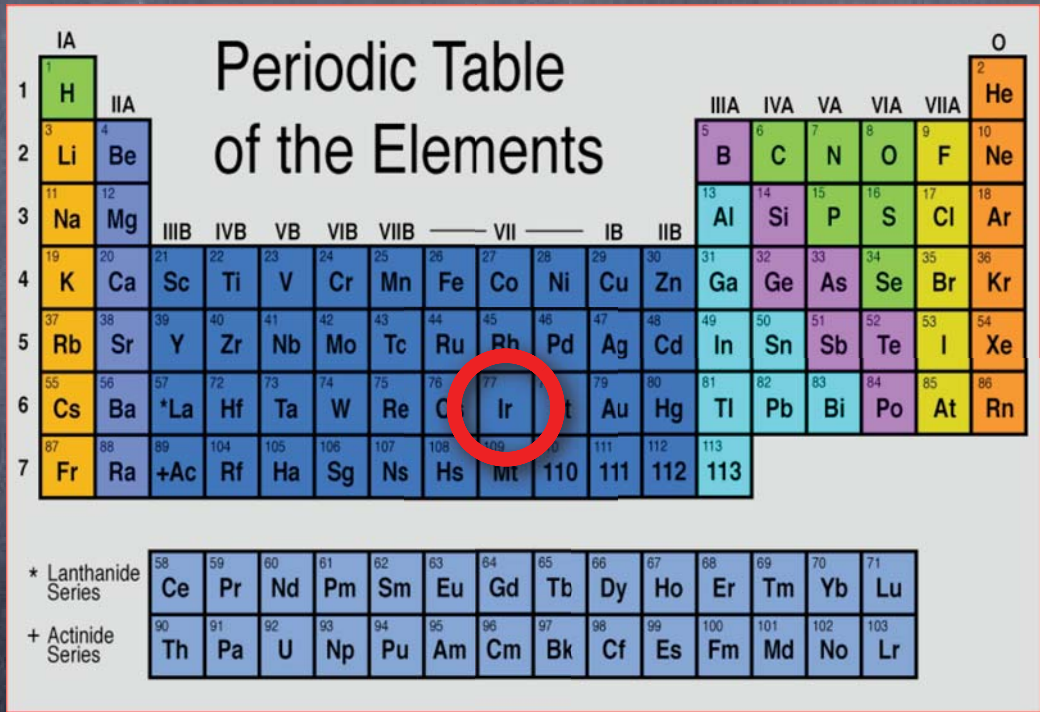
L=1

- Spin-orbit coupling

$$\lambda \vec{\ell} \cdot \vec{S} = -\lambda \vec{\mathsf{L}} \cdot \vec{S} \qquad \vec{\mathsf{J}} = \vec{\mathsf{L}} + \vec{S}$$

- Ground state has J=1/2: no orbital degeneracy
  - but g=-2!

Spin orbit coupling

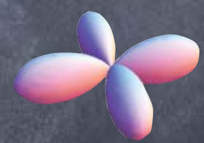


- Estimate (?) $\lambda \approx 0.5$ eV
- Probably much larger than $\Delta\varepsilon_m$

Exchange Anisotropy

- J eigenstates: "spin" has strong orbital component

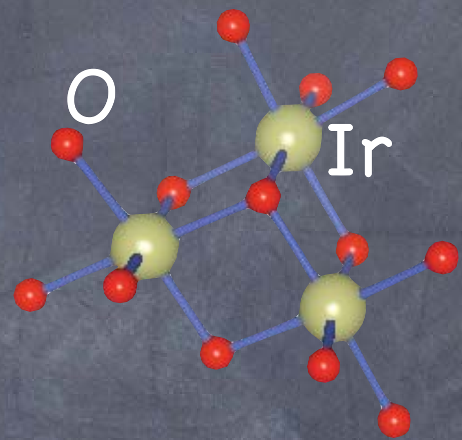
  e.g. $$\left|\Uparrow\right\rangle = \sqrt{\tfrac{2}{3}}\left|L^z=1\right\rangle\left|\downarrow\right\rangle - \sqrt{\tfrac{1}{3}}\left|L^z=0\right\rangle\left|\uparrow\right\rangle$$

  - generally expect O(1) exchange anisotropy
- Heisenberg model may be totally wrong!
  - If so, what is going on?

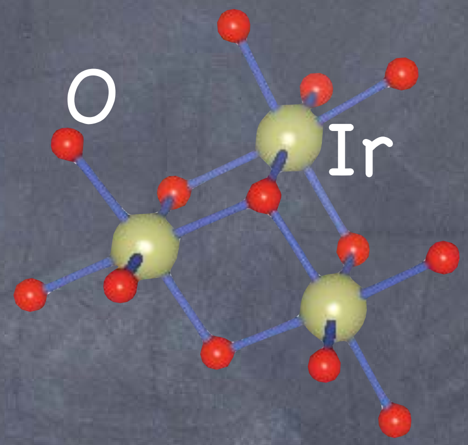
Ir-O-Ir Superexchange

- Resulting exchange Hamiltonian is indeed highly anisotropic
- Actually unfrustrated:
  - unique ground state up to global spin rotations!
- Obviously inconsistent with experiments!



Ir-Ir Direct Exchange

- Miraculously
  - Exchange is pure antiferromagnetic Heisenberg!
- Deviations from strong SO limit give Dzyaloshinskii-Moriya terms $D \sim |\Delta\varepsilon_n|/\lambda$
- Frustration preserved!



J + D

Quantum Spin Liquid?

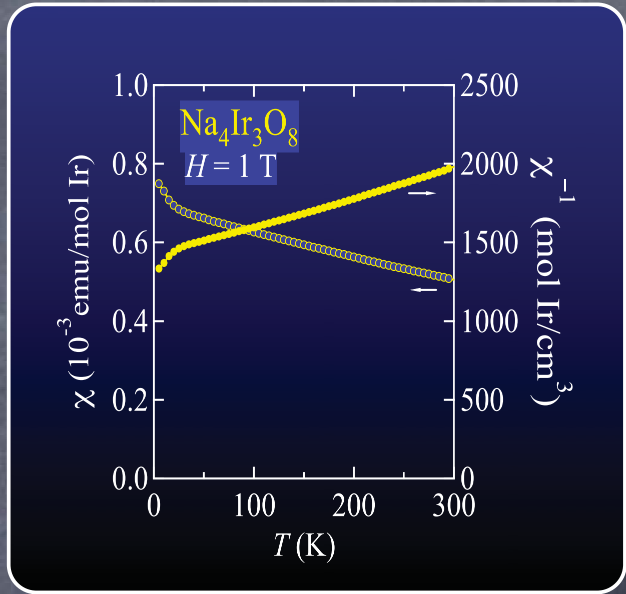
- Approximate Heisenberg description
  - Low "coherence" scale expected
  - Spin-liquid ground state plausible
- Recent proposals of QSLs with fermionic spinons

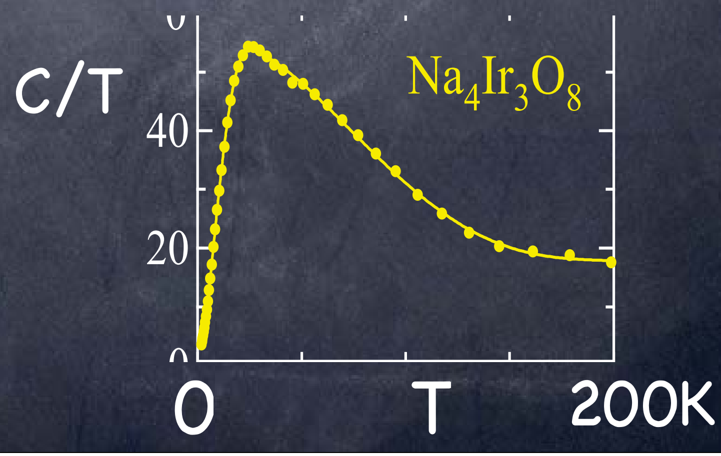
  Yi Zhou, Patrick A. Lee, Tai-Kai Ng, Fu-Chun Zhang, arXiv:0806.3323

  M. Lawler, A. Paramekanti, Y.-B. Kim, LB arXiv:0806.4395
  - "U(1)" Fermi surface state somewhat consistent with $C_v(T)$
  - Spinon pairing might also be involved, but there are difficulties

SO and Susceptibility

- $Na_4Ir_3O_8$ shows large low-T susceptibility
- Nevertheless C_v/T suppressed below 30K
  - Large R_W inconsistent?
- Resolution: DM interactions lead to non-zero $\chi(T=0)$ even when DOS vanishes





$Na_4Ir_3O_8$

- A seemingly consistent picture of $Na_4Ir_3O_8$ emerges including strong spin-orbit
- Heisenberg-like behavior in this material may be a happy accident!
- But we should keep an open mind:
  - itinerancy might be important near Mott transition