Quasi-1d Frustrated Antiferromagnets

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The David and Lucile Packard Foundation

Outline

- Frustration in quasi-1d systems
- Excitations: magnons versus spinons
  - Neutron scattering from Cs_2CuCl_4 and spinons in two dimensions
- Low energy properties of quasi-1d antiferromagnets and Cs_2CuCl_4 in particular
  - Renormalization group technique

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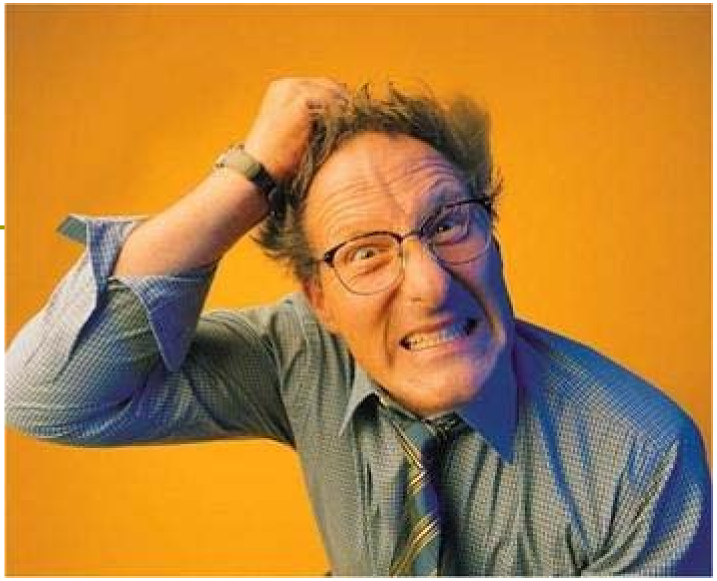
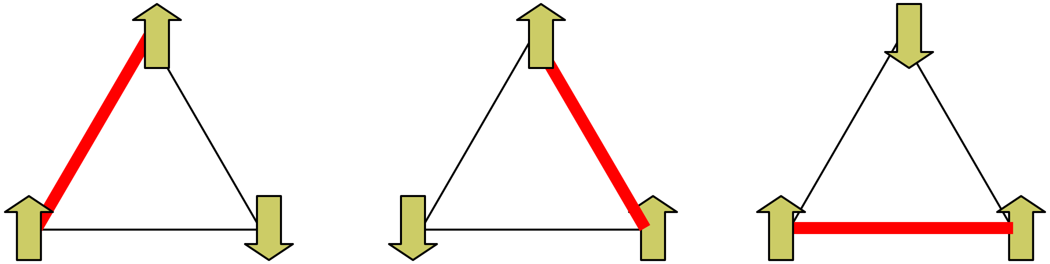
What is frustration?

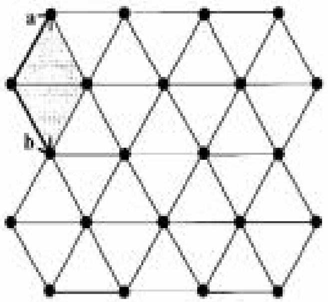


- Competing interactions
  - Can’t satisfy all interactions simultaneously
  - Optimization is “frustrating”

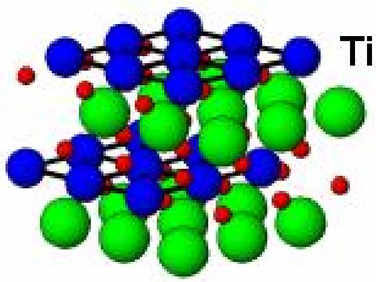


- “People need trouble – a little frustration to sharpen the spirit on, toughen it. Artists do; I don't mean you need to live in a rat hole or gutter, but you have to learn fortitude, endurance. Only vegetables are happy.” – William Faulkner

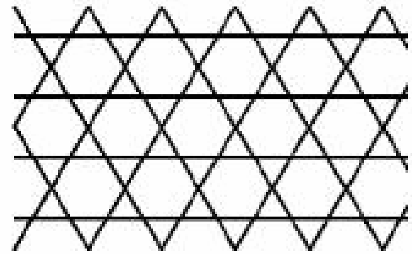
Geometrically Frustrated Lattices



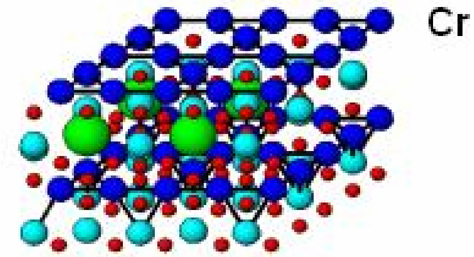
Triangular lattice



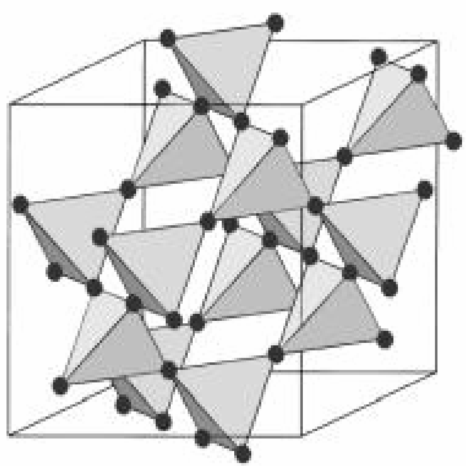
$NaTiO_2$, $LiVO_2$, ...



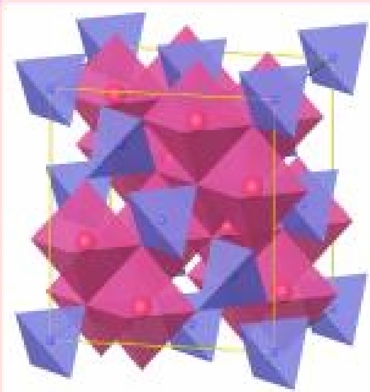
Kagome lattice



$SrCr_9Ga_3O_{19}$

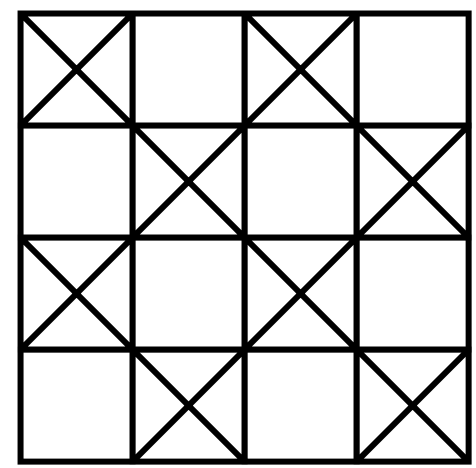


Pyrochlore lattice



Spinel (AB_2O_4)

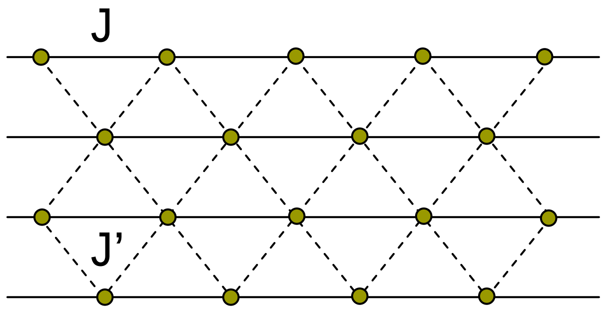
$Fe_3O_4=FeFe_2O_4$



Checkerboard lattice

Quasi-1d systems

- Weakly coupled chains



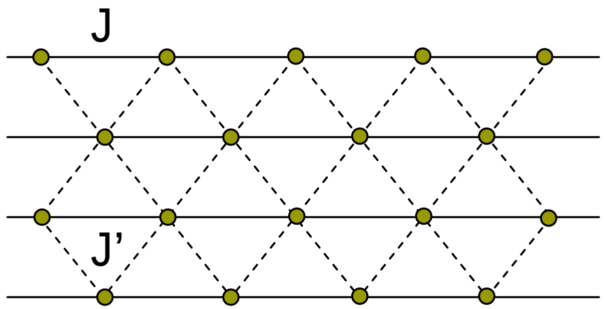
$$H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

J' $\ll$ J

- Single Heisenberg chain well understood
  - Exact solution (Bethe 1932...) gives energies, wavefunctions, some correlations
  - Low energy bosonization theory
- J'/J gives expansion parameter

Frustration in quasi-1D systems

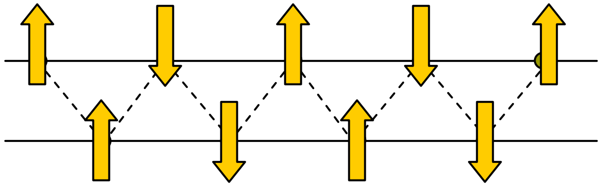
- Weakly coupled chains



$$H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

J' $\ll$ J

- Frustration
  - Dominant antiferromagnetic correlations incompatible between chains



Zero net exchange field from one chain upon another

  - Broadened domain of J'/J expansion

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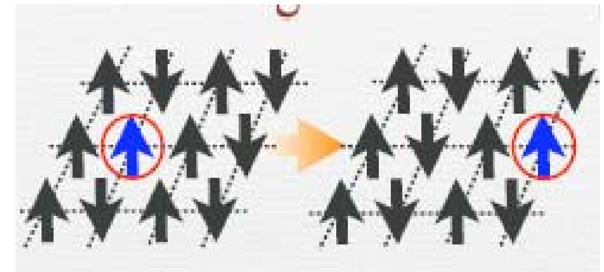
Magnons

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



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

MnF$_2$

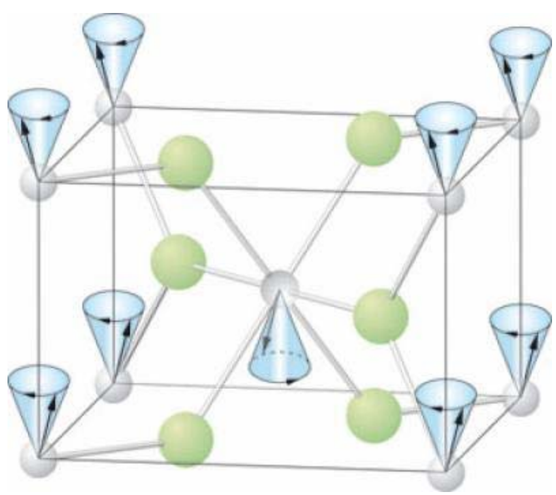
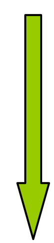


Image: B. Keimer



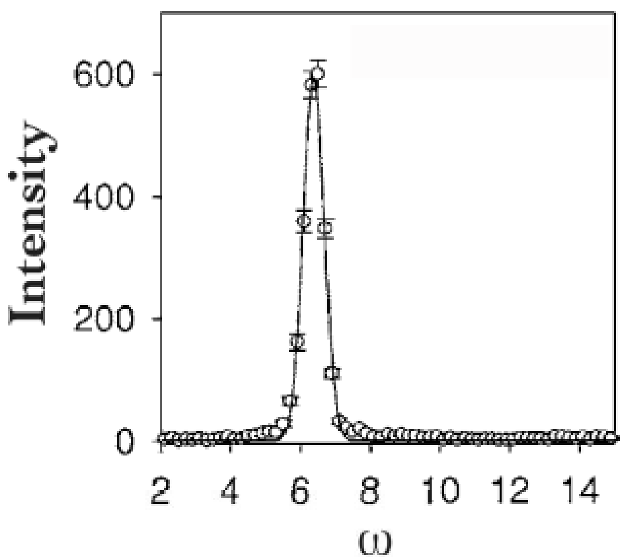
$\vec{k}$

$$\epsilon = \hbar\omega(k)$$

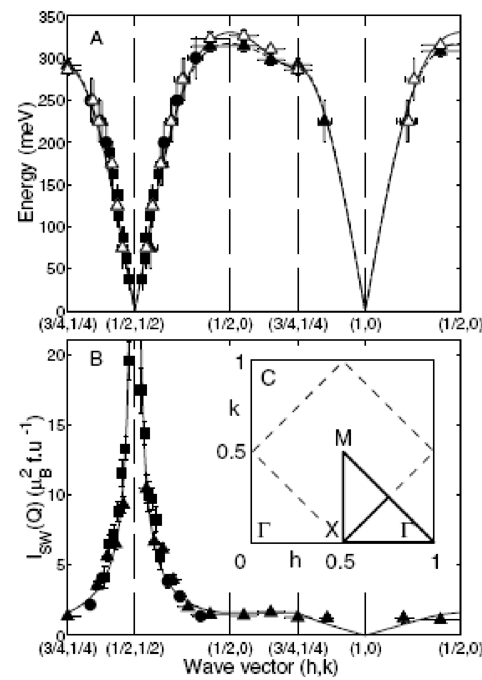
Inelastic neutron scattering

- Neutron can absorb or emit magnon

$$S(k,\omega) \propto \mathrm{Re}\left\langle S_k^- \delta(\omega - H) S_k^+ \right\rangle \sim Z(k)\delta(\omega - \epsilon(k))$$



Line shape in Rb_2MnF_4



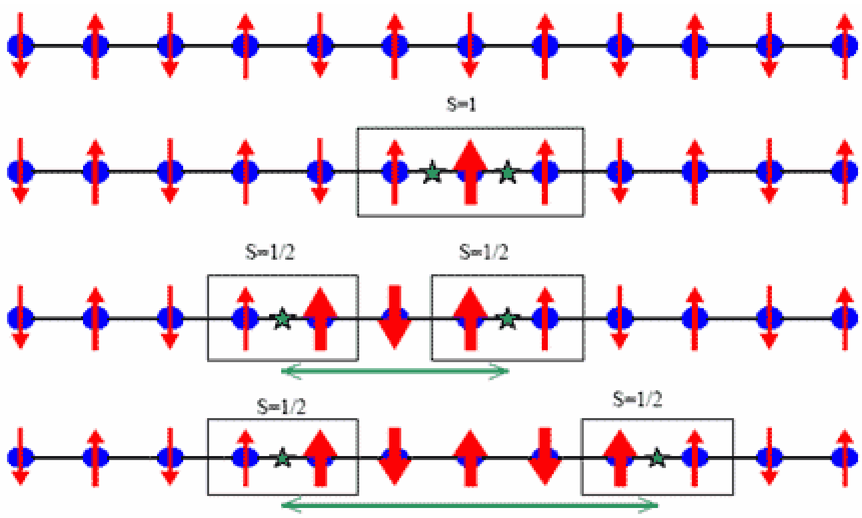
La_2CuO_4

One dimension

- Heisenberg model is a *spin liquid*
  - No magnetic order
  - Power law correlations of spins and dimers

$$\langle \vec{S}(x) \cdot \vec{S}(x') \rangle \sim \frac{(-1)^{x-x'}}{|x-x'|} + \cdots$$

- Excitations are s=1/2 *spinons*
  - General for 1d chains
  - Cartoon
    - Ising anisotropy



Spinons by neutrons

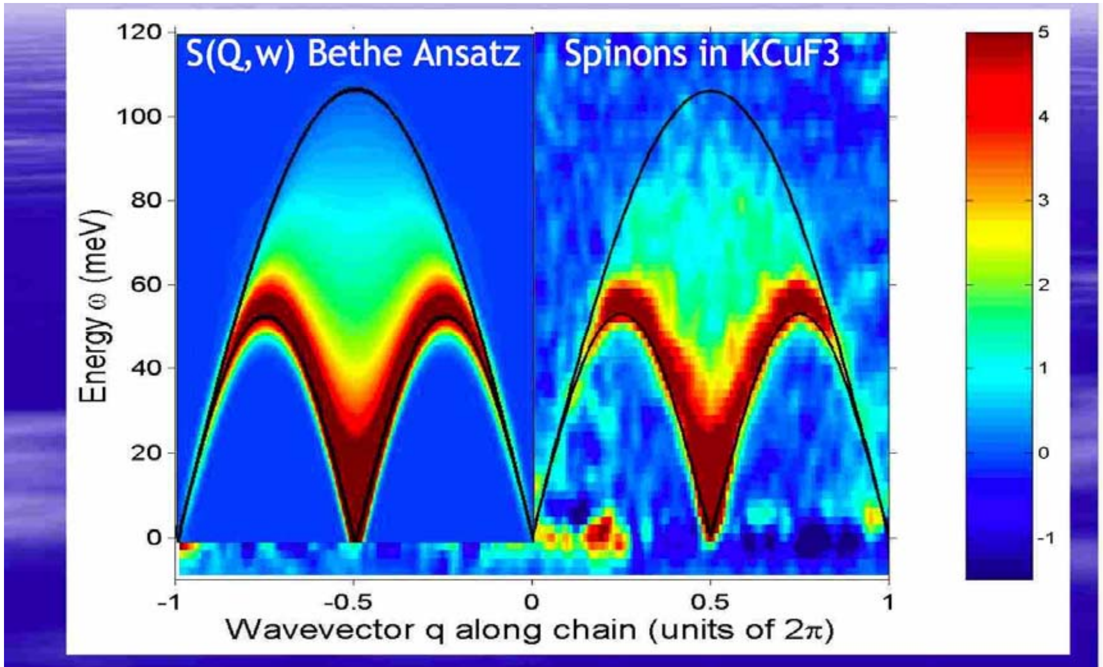
- Bethe ansatz:
  - Spinon energy $\epsilon_s(k) = \frac{\pi J}{2}|\sin k_x|$
  - Spin-1 states

$$k_x = k_{x1} + k_{x2}$$
$$\epsilon = \epsilon_s(k_{x1}) + \epsilon_s(k_{x2})$$

} 2-particle continuum

- Theory versus experiment for $KCuF_3$, with spatial exchange anisotropy of **30** (very 1d)

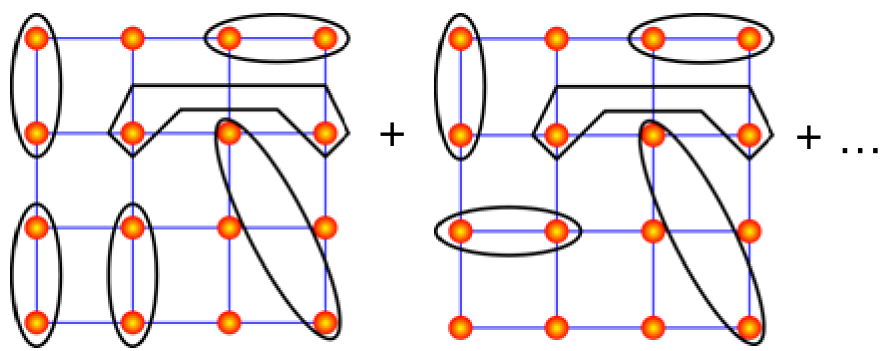
B. Lake *et al*, HMI



Spinons in d>1?

- Resonating Valence Bond theories (Anderson...)
  - Spin “liquid” of singlets

$$|\Psi\rangle =$$



  - Broken singlet “releases” 2 spinons
- Many phenomenological theories
  - No solid connection to experiment

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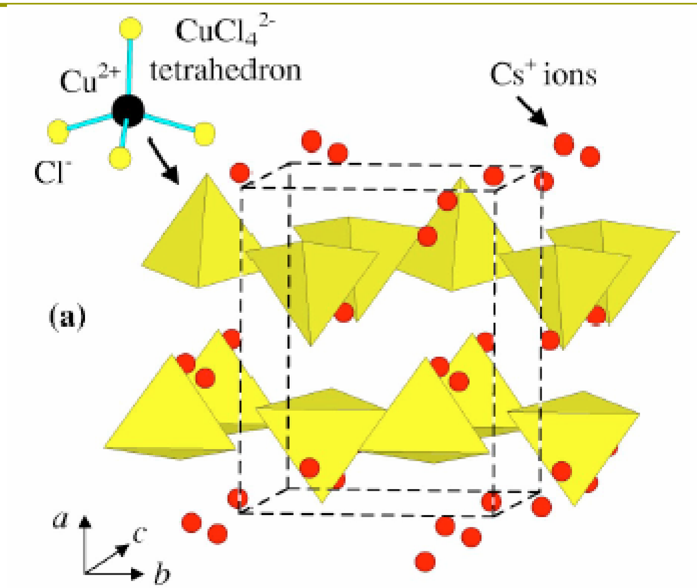
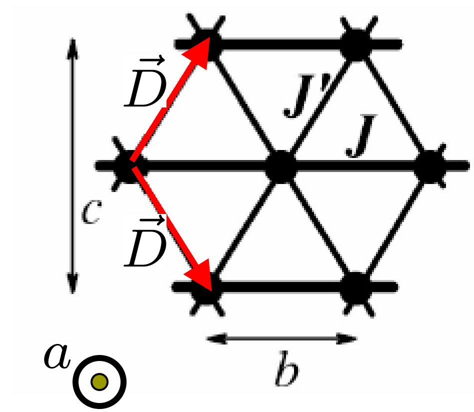
Cs_2CuCl_4: a 2d spin liquid?





J'/J ≈ 0.3

$\vec{D} = (D, 0, 0)$

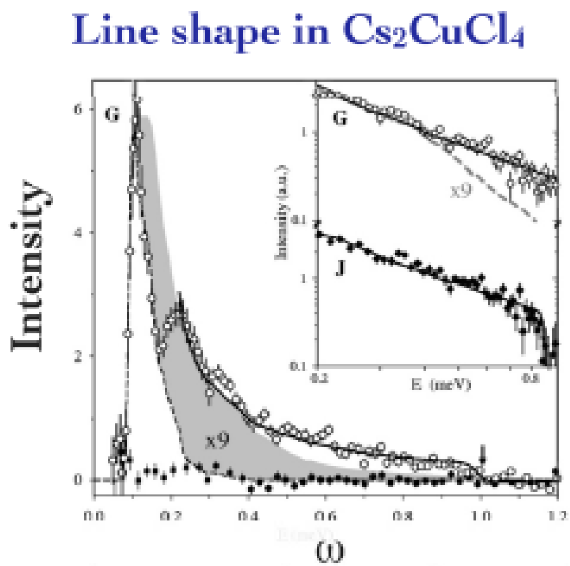
$$\mathcal{H} = \sum_{(ij)} J_{ij} \vec{S}_i \cdot \vec{S}_j - \sum_{(ij)} \vec{D}_{ij} \cdot \vec{S}_i \times \vec{S}_j - \vec{h} \cdot \sum_i \vec{S}_i$$

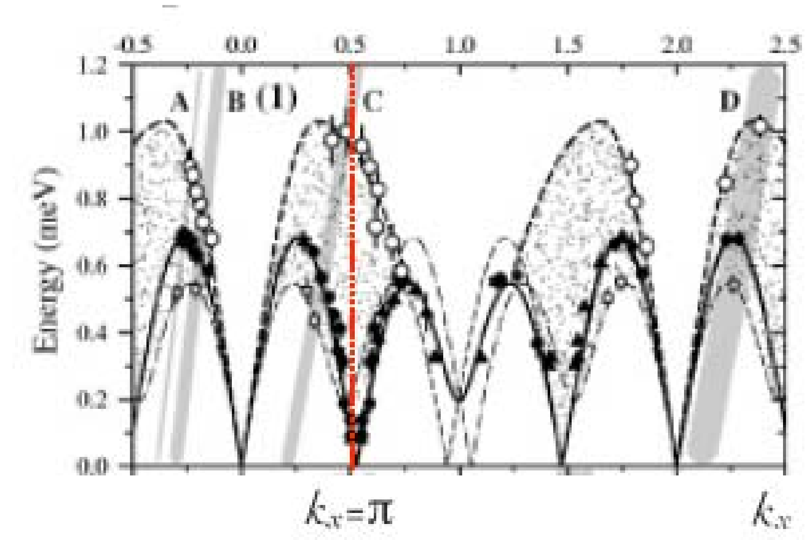
- Couplings: J ≈ 0.37 meV J' ≈ 0.3 J D ≈ 0.05 J

Inelastic Neutron Results

- Coldea *et al*, 2001,2003

Note asymmetry



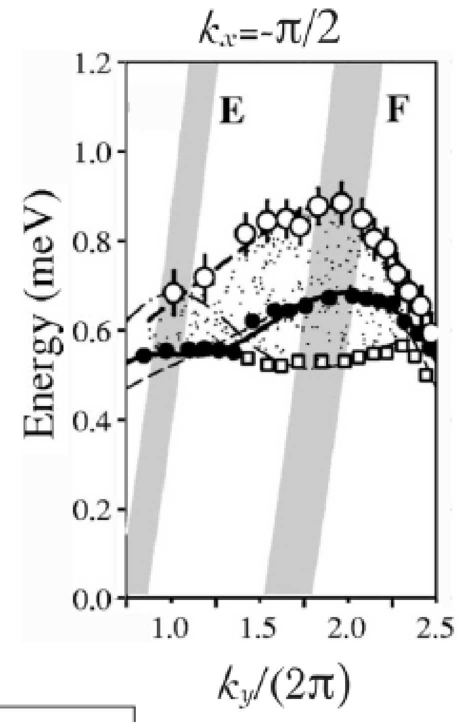


Very broad spectra similar to 1d (in some directions of k space). Roughly fits to power law

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:



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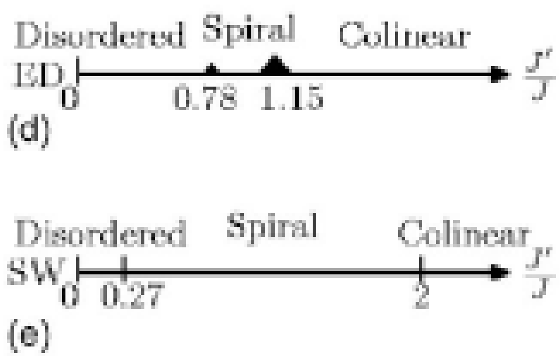
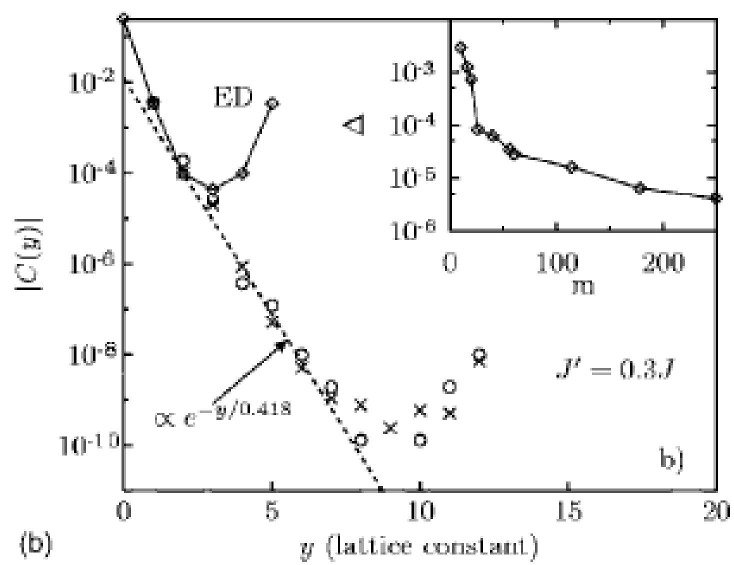
Back to 1d

- Frustration *enhances one-dimensionality*
  - First order energy correction vanishes due to cancellation of effective field
  - Numerical evidence: J'/J <0.7 is "weak"

Weng et al, 2006



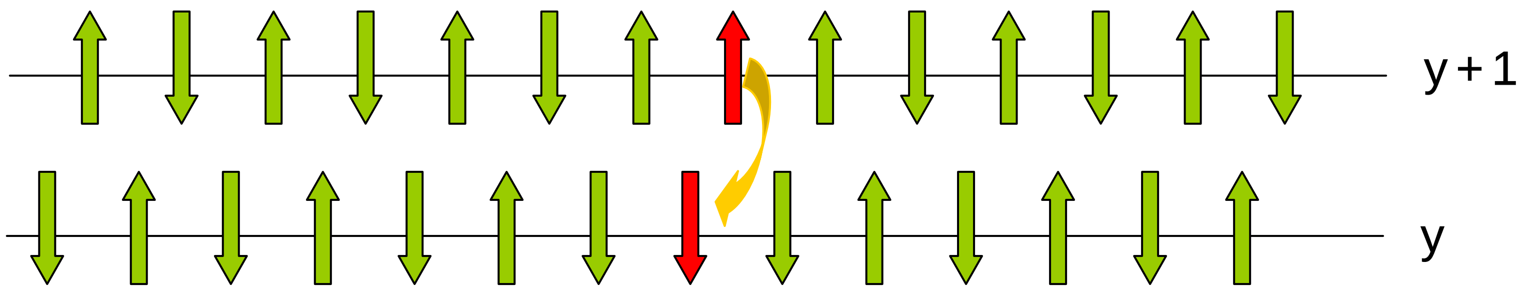
Numerical phase diagram contrasted with spin wave theory



Very small inter-chain correlations

Excitations for J'>0

- Coupling J' is *not* frustrated for excited states
- Physics: transfer of spin 1



  - Spinons can hop *in pairs*
  - Expect spinon binding to lower energy
  - Spin bound state="triplon" clearly disperses transverse to chains

Effective Schrödinger equation

- Study two spinon subspace

$$|k_x, k_y; \epsilon\rangle = \sum_y e^{ik_y y} |k_x, \epsilon\rangle_y \otimes_{y' \neq y} |0\rangle_{y'}$$

  - Momentum conservation: 1d Schrödinger equation in ε space

effective "potential"

$$\epsilon \psi_{\mathbf{k}}(\epsilon) + \int d\tilde{\epsilon} D_{k_x}(\tilde{\epsilon}) \, J'(\mathbf{k}) \, A^*_{k_x}(\epsilon) A_{k_x}(\tilde{\epsilon}) \, \psi_{\mathbf{k}}(\tilde{\epsilon}) = E \psi_{\mathbf{k}}(\epsilon)$$

- Crucial matrix elements known exactly

$$A_{k_x}(\epsilon) \equiv \frac{1}{\sqrt{2}} \langle 0 | S^-_{-k_x,y} | k_x, \epsilon \rangle_y$$

Bougourzi *et al*, 1996

Structure Factor

- Spectral Representation

Bougourzi *et al*,
J.S. Caux *et al*

$$S(k,\omega) \propto \sum_n \left|\langle n|S_k^+|0\rangle\right|^2 \delta(\omega - E_n)$$

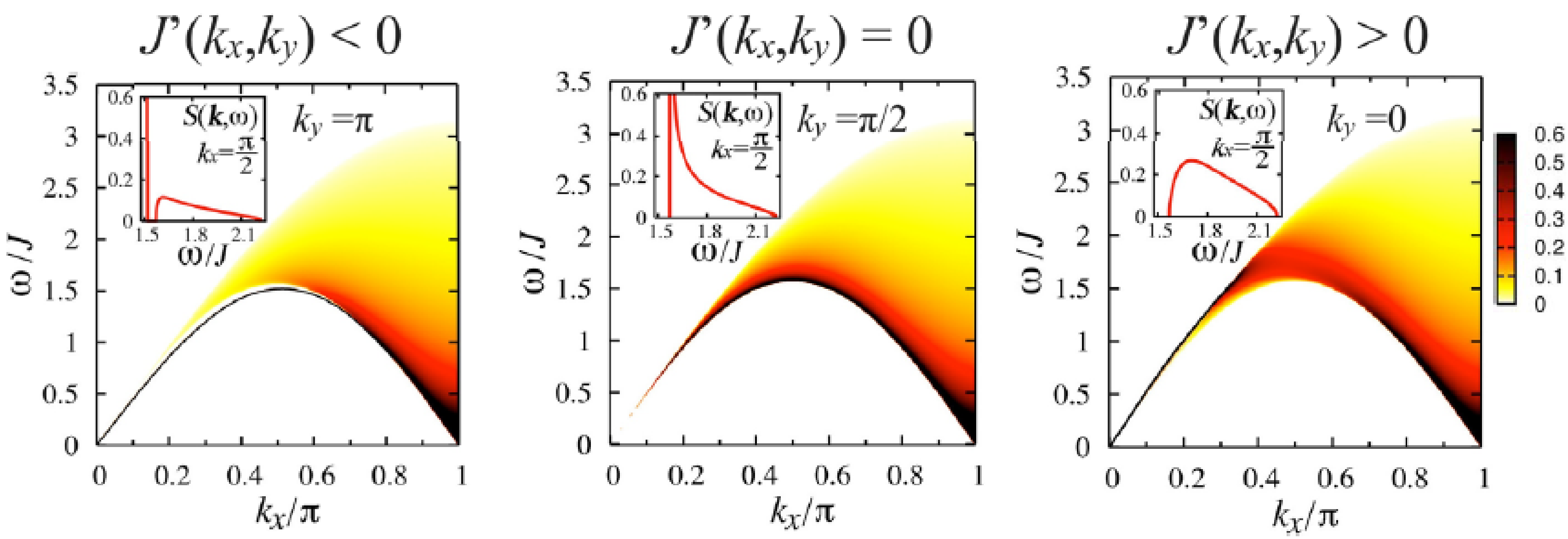
Weight in 1d:
73% in 2 spinon states
99% in 2+4 spinons

  - Can obtain closed-form “RPA-like” expression for 2d S(k,ω) in 2-spinon approximation

$$S(k,\omega) = \frac{S_{1d}(k,\omega)}{[1 + J'(k)\chi'_{1d}(k,\omega)]^2 + [\pi J'(k) S_{1d}(k,\omega)]^2}$$

Types of behavior

- Behavior depends upon spinon interaction



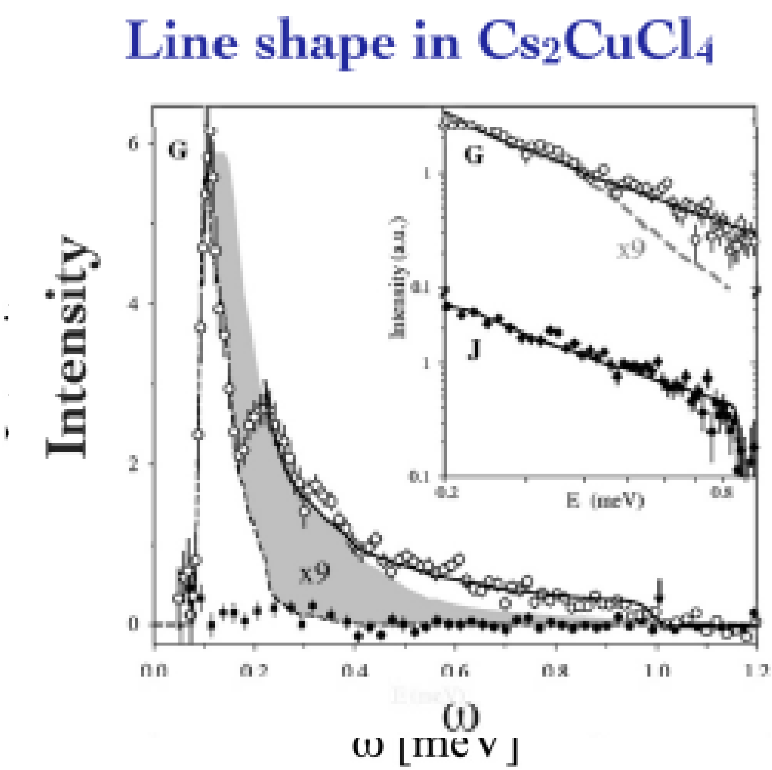
Bound "triplon"

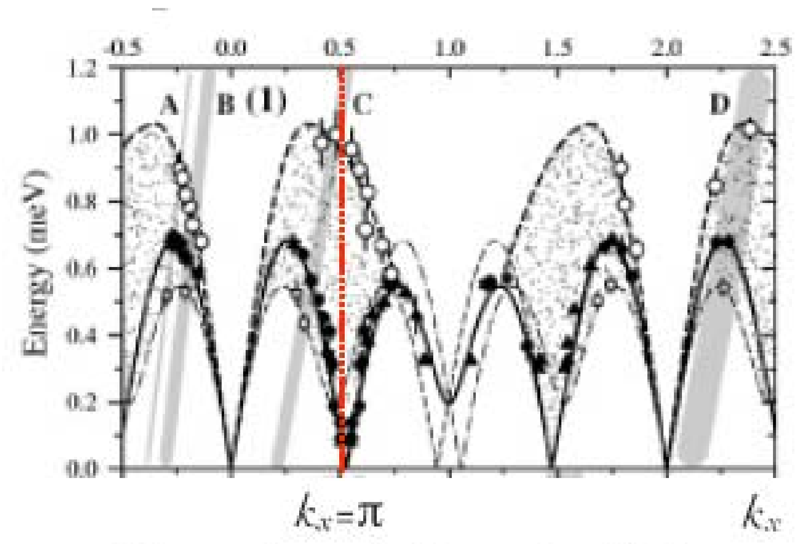
Identical to 1D

Upward shift of spectral weight. Broad resonance in continuum or anti-bound state (small k)

Broad lineshape: “free spinons”

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

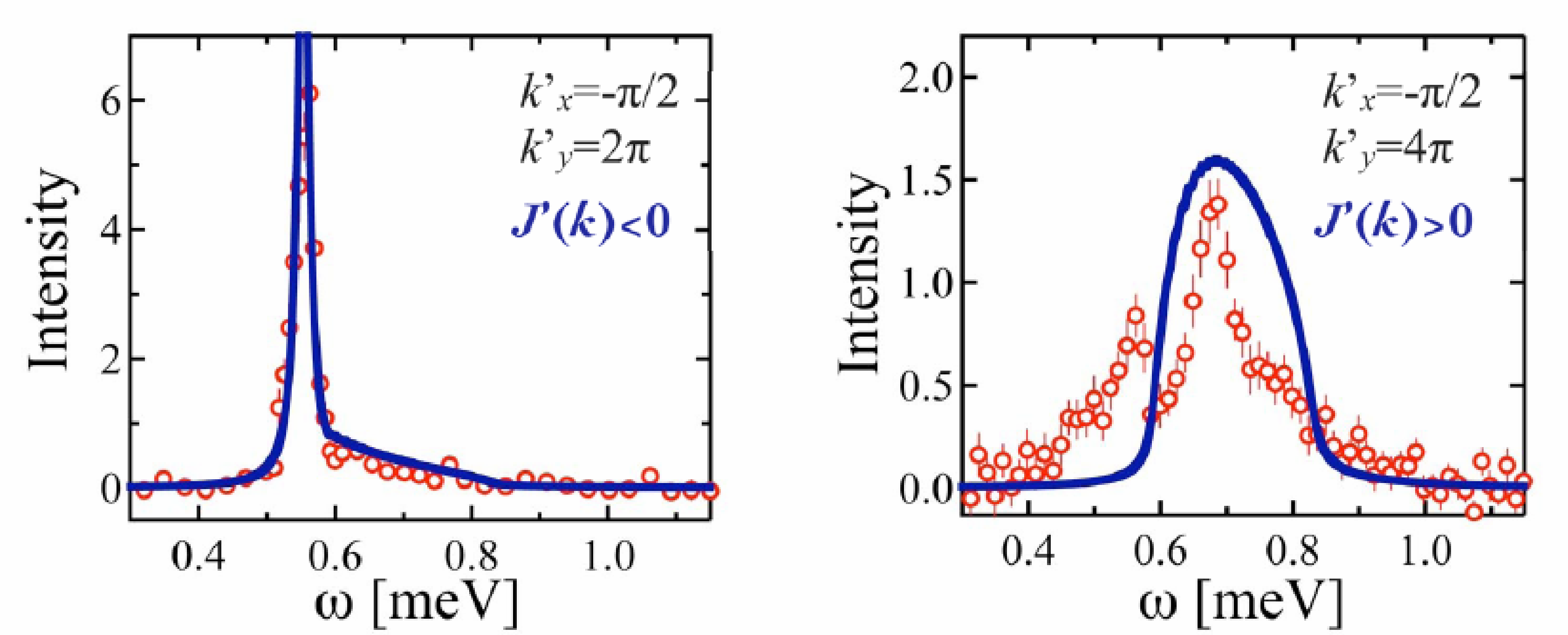




J’(k)=0 here

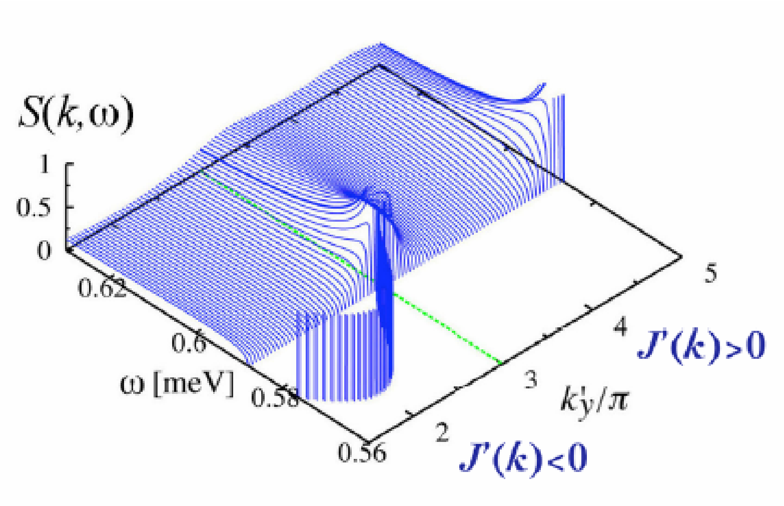
Bound state

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

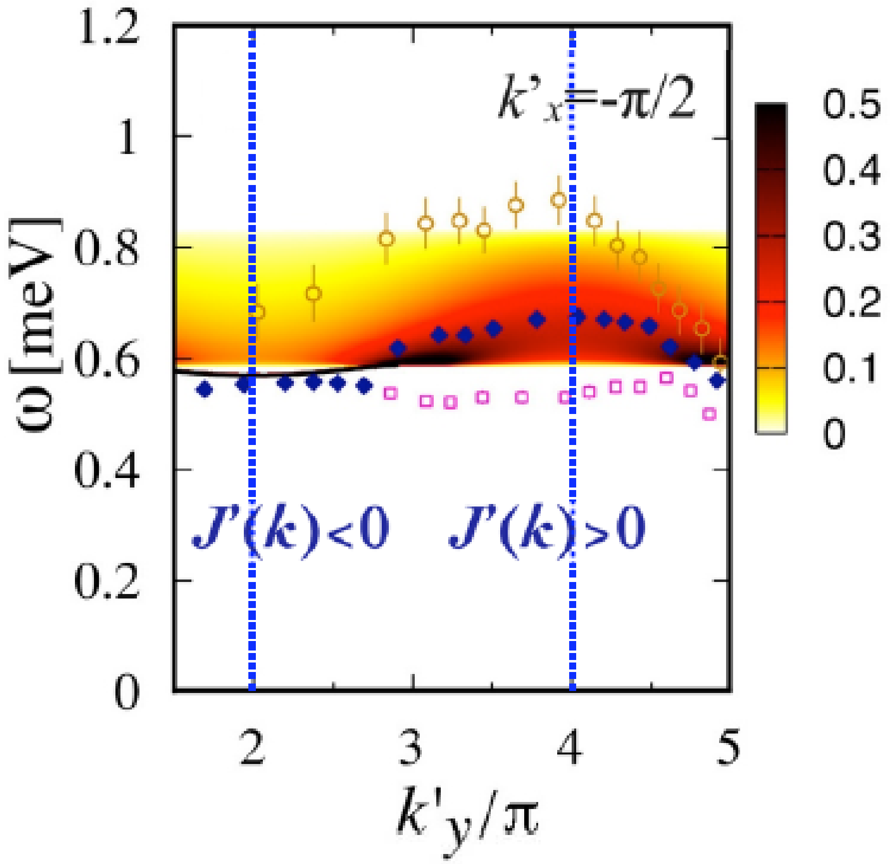


- Curves: 4-spinon theory w/ experimental resolution
- Curves: 2-spinon RPA w/ experimental resolution

Transverse dispersion



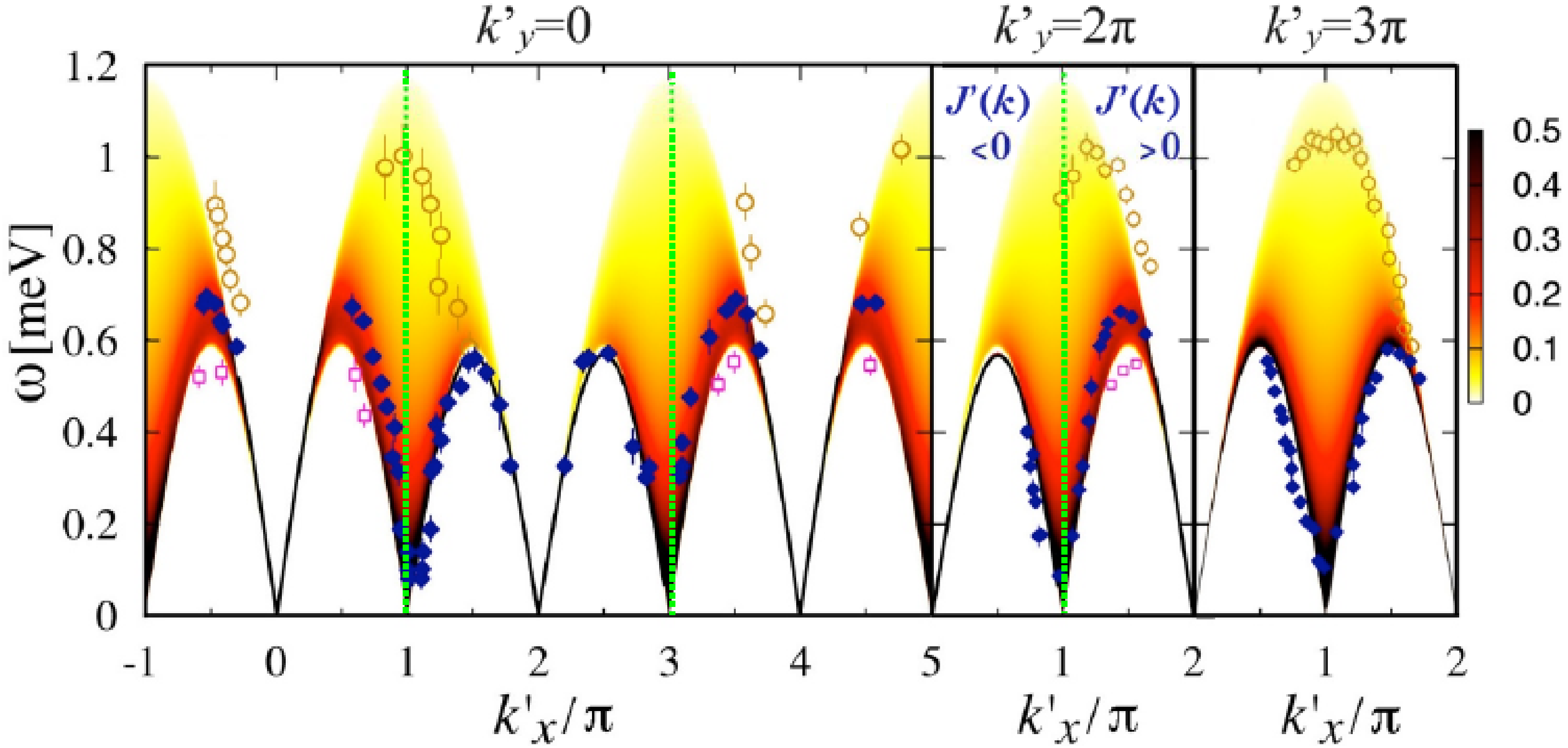
Bound state and resonance



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

Spectral asymmetry

- Comparison:



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

Conclusion (spectra)

- Simple theory works well for frustrated quasi-1d antiferromagnets
  - Frustration actually simplifies problem by enhancing one-dimensionality and reducing modifications *to the ground state*
- "Mystery" of Cs_2CuCl_4 solved
  - Need to look elsewhere for 2d spin liquids!

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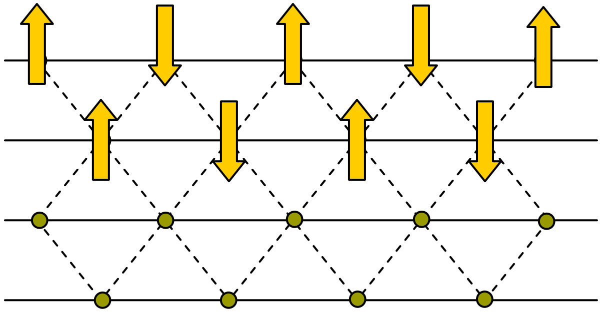
Frustration: Low energy physics

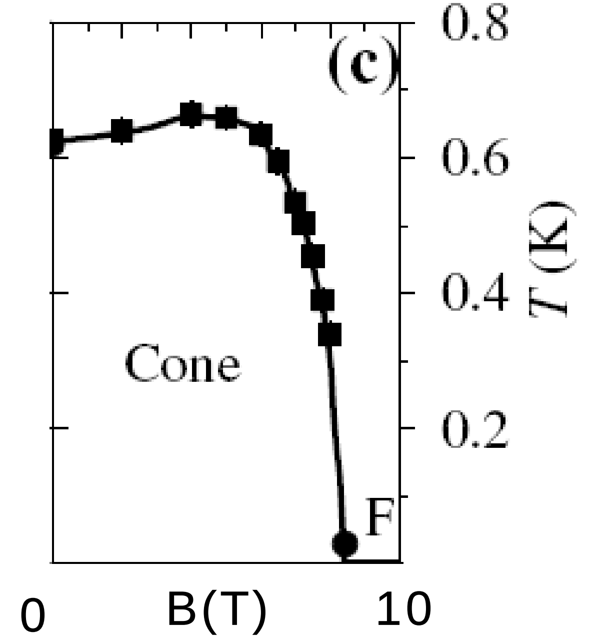
- Recall: no naïve (leading order) preference for inter-chain ordering



- Q: How is the degeneracy resolved in the ground state?
  - Magnetic order? What sort?
  - Dimerization?
  - Spin liquid?

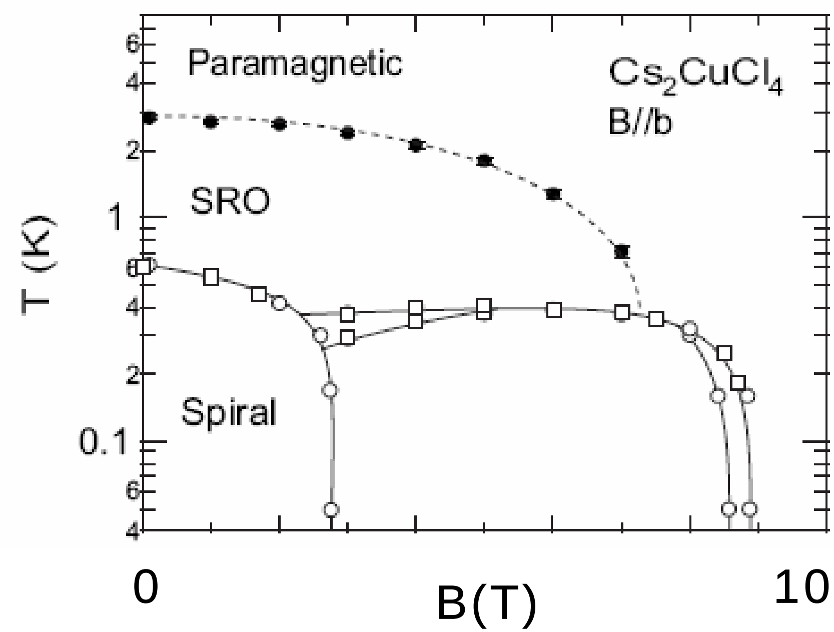
Experimental Behavior

- Cs_2CuCl_4 *orders* at 0.6K into weakly incommensurate coplanar spiral
- Order evolves in complex way in magnetic field
- Field normal to plane:
  - Only one phase
  - Order slightly enhanced in field



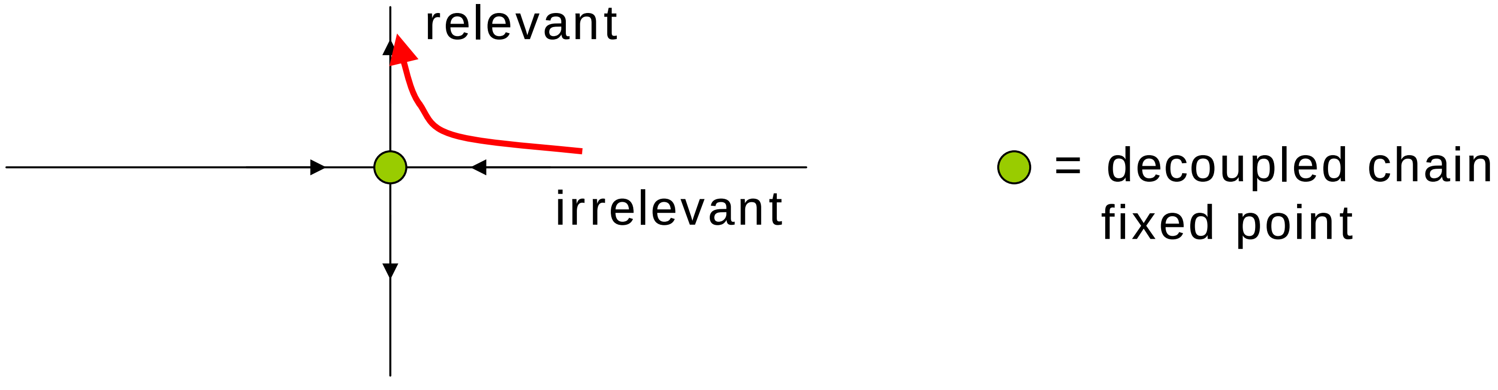
Experimental Behavior

- Cs_2CuCl_4 *orders* at 0.6K into weakly incommensurate coplanar spiral
- Order evolves in complex way in magnetic field
- Field parallel to plane:
  - Several phases
  - Zero field state weakened by field



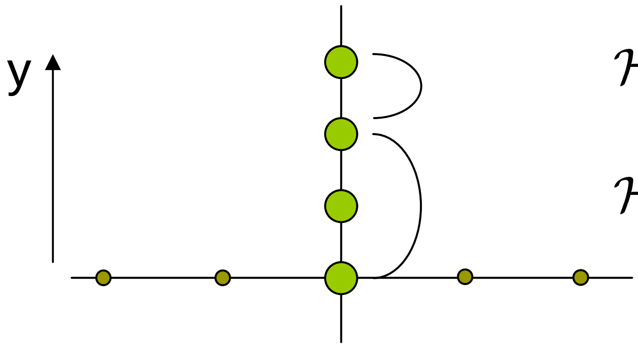
Renormalization Group theory

- Strategy:
  - Identify instability of weakly coupled chains (science)
  - Try to determine the outcome (art)
- Instabilities
  - Renormalization group view: relevant couplings



What are the couplings?

- Inter-chain couplings are composed from scaling operators of individual chain theory, e.g. in zero field:
  - Staggered magnetization $\vec{N}$
  - Staggered dimerization ε
- Can order these by range and relevance



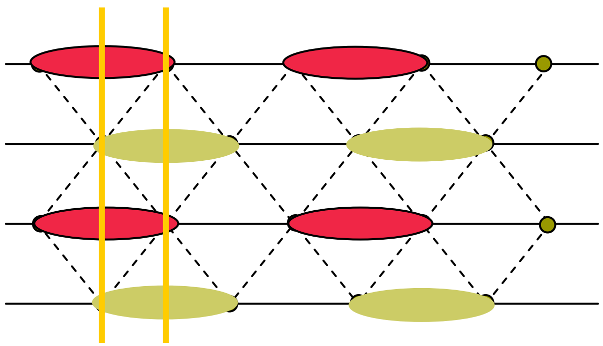
$$\mathcal{H}'_1 = \sum_y g_1 \mathcal{O}_1(y)\mathcal{O}_1(y+1)$$

$$\mathcal{H}'_2 = \sum_y g_2 \mathcal{O}_2(y)\mathcal{O}_2(y+2)$$

Further chain couplings just as relevant but smaller

Example: Zero field J-J' model

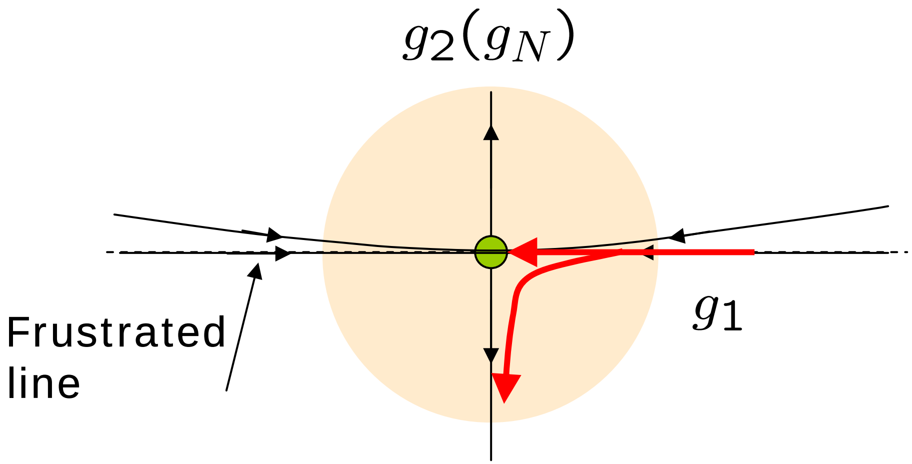
- Allowed operators strongly restricted by reflections



$$\vec{N}(y)\ \vec{N}(y+1)$$

RG Subtleties (1)

- "Accidentally" zero couplings
  - E.g. staggered magnetization coupling g_N=0

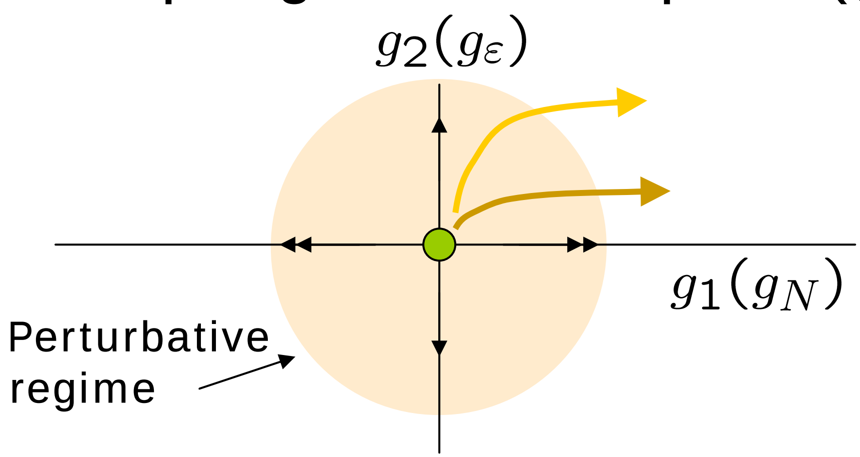


$$dg_1/d\ell = -\lambda_1 g_1$$
$$dg_2/d\ell = \lambda_2 g_2 \underline{-g_1^2}$$

- Fluctuations generate relevant operator
  - Non-linearities bend RG flow lines

RG Subtleties (2)

- Competing Relevant Operators
  - Fluctuations generate several relevant couplings that compete (g_N,g_ε)

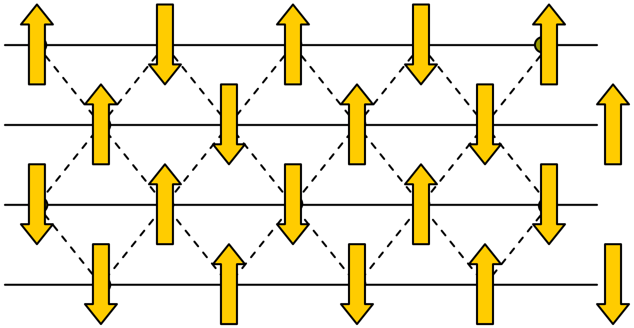


$dg_i/d\ell = \lambda_i g_i$ $\lambda_1 > \lambda_2$

- Two factors:
  - More relevant operators grow faster under RG
  - Larger bare values can compensate

Result in Zero Field

- Pure J-J' model:
  - Staggered magnetization coupling g_N dominates and induces *collinear magnetic order*



  - Very weak instability occurs only below energy scale $\sim (J')^4/J^3$

Result in Zero Field

- Dzyaloshinskii-Moriya interaction

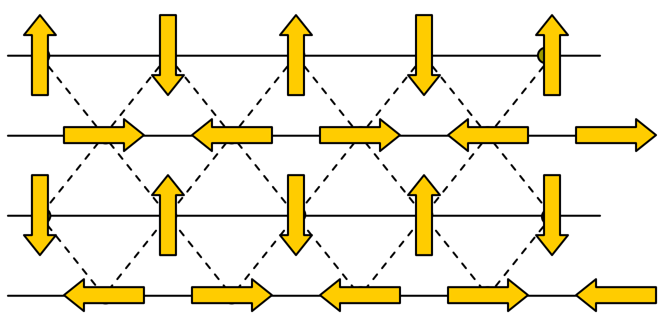
$$\mathcal{H}_{DM} = D \sum_y (-1)^y \hat{z} \cdot \vec{N}_y \times \vec{N}_{y+1}$$ relevant

  - Cannot be neglected since it is *large* compared to fluctuation-generated coupling

$$D/J \sim 0.05 \gg (J'/J)^4 \sim (0.3)^4 \sim 0.01$$

- Result: non-collinear spiral state

$\approx$



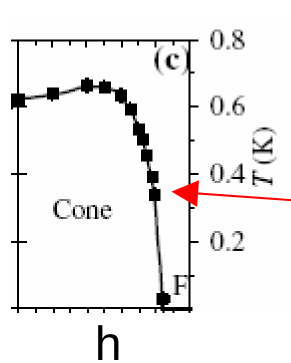
Agrees with neutron experiments

Transverse (to plane) Field

- XY spin symmetry preserved
  - DM term becomes *more relevant*
- b-c spin components remain commensurate: XY coupling of “staggered” magnetizations still cancels by frustration (reflection symmetry)
- Spiral (cone) state just persists for all fields.

Experiment:

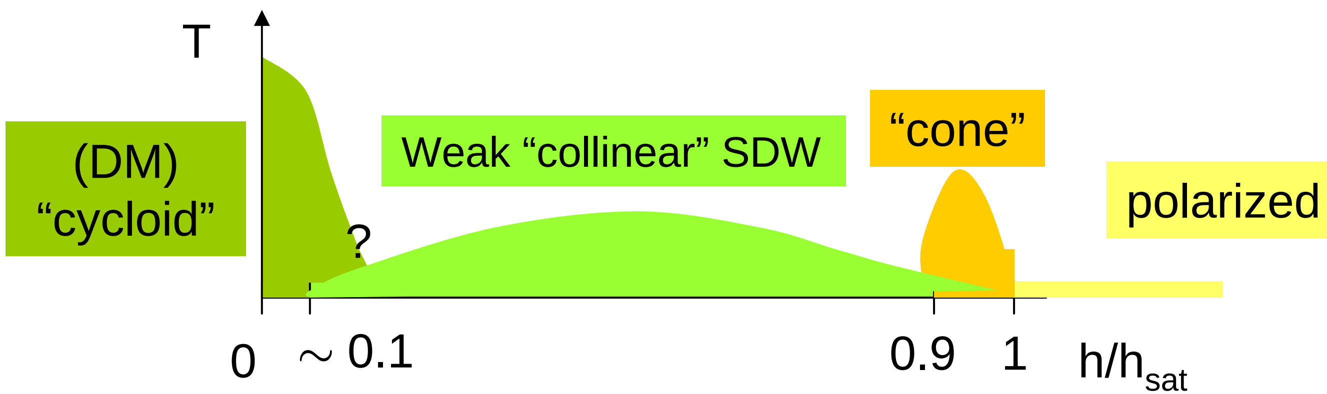
Order *increases* with h here due to increasing relevance of DM term



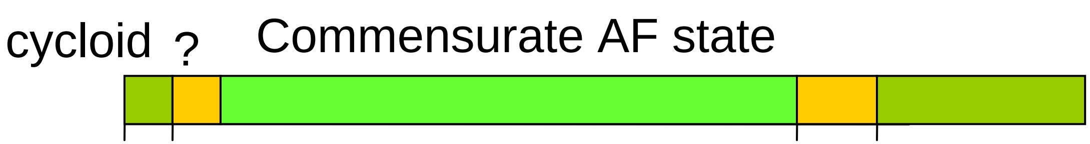
Order *decreases* with h here due to vanishing amplitude as h_{sat} is approached

Longitudinal Field

- Field breaks XY symmetry:
  - *Competes* with DM term and eliminates this instability for H $\gtrsim$ D
  - Other weaker instabilities take hold
- Naïve theoretical phase diagram



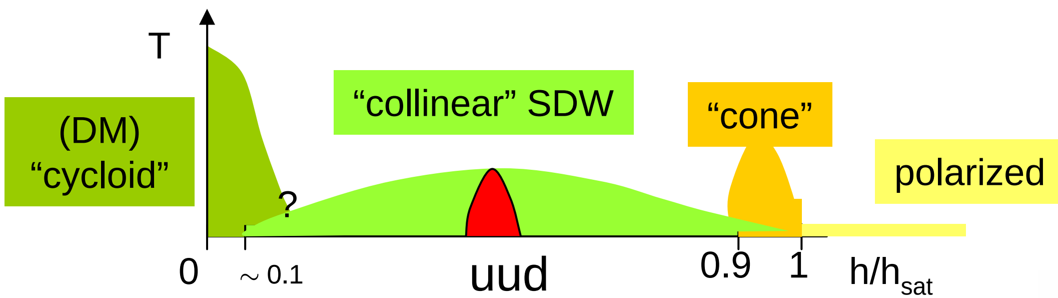
- Expt.

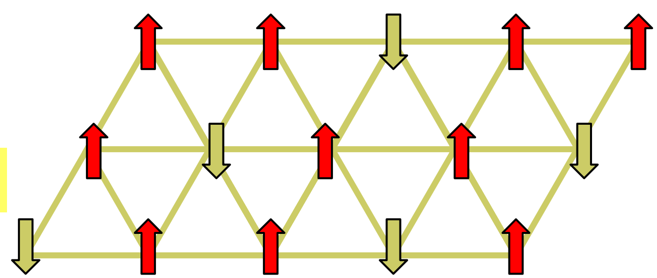


AF state differs from theory (J_2?)

Magnetization Plateau

- “Umklapp” (dangerously irrelevant operator): commensurate SDW state unstable to plateau formation
  - Strongest locking at $M=M_{sat}/3$
  - Gives “uud” state which also occurs in spin wave theory (Chubukov)





- Magnetization plateau observed in Cs_2CuBr_4

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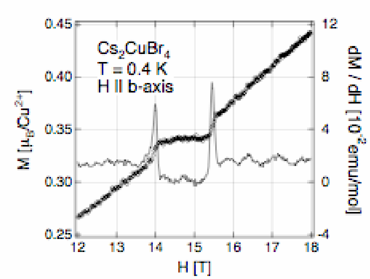

Fig. 8. The magnetization curve and dM/dH versus H for $H \parallel b$ measured at $T = 0.4$ K in magnetic fields up to 20 T.

Summary

- One-dimensional methods are very powerful for quasi-1d frustrated magnets, even when inter-chain coupling is not too small
- Integrability allows access to high energy spectral properties
- Systematic RG methods describe low energy physics for
  - Triangular lattice
  - Checkerboard lattice
  - Spatially anisotropic frustrated square lattice

For the Future

- Quasi-1d conductors
- Spectra in magnetic field
- Other geometries

Shojoshin-in
清浄心院

kagome basket, Shojoshin-in temple, Koyasan