Quasi-1d Frustrated Antiferromagnets

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Outline

- Frustration in quasi-1d systems
- Excitations: magnons versus spinons
  - Neutron scattering from Cs$_2$CuCl$_4$ and spinons in two dimensions
- Low energy properties of quasi-1d antiferromagnets and Cs$_2$CuCl$_4$ 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$_9$Ga$_3$O$_{19}$
- Pyrochlore lattice
- Spinel (AB$_2$O$_4$) $\text{Fe}_3\text{O}_4 = \text{FeFe}_2\text{O}_4$
- Checkerboard lattice
Quasi-1d systems

- Weakly coupled chains

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

- 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
  - Broadened domain of \( J'/J \) expansion

Zero net exchange field from one chain upon another
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Magnons

- Basic excitation: spin flip
  - Carries "S²"=± 1

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

\[ \varepsilon = \hbar \omega(k) \]

Image: B. Keimer
Inelastic neutron scattering

- Neutron can absorb or emit magnon

\[ S(k, \omega) \propto \text{Re} \left\langle S^\ast_k \delta(\omega - H) S^+_{-k} \right\rangle \sim Z(k) \delta(\omega - \epsilon(k)) \]

Line shape in Rb$_2$MnF$_4$

La$_2$CuO$_4$
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
  \[ \varepsilon_s(k) = \frac{\pi J}{2} |\sin k_x| \]
- Spin-1 states
  \[ k_x = k_{x1} + k_{x2} \]
  \[ \epsilon = \varepsilon_s(k_{x1}) + \varepsilon_s(k_{x2}) \]

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

\[ |\psi\rangle = \begin{array}{c}
\text{Diagram with two states}
\end{array} + \begin{array}{c}
\text{Diagram with two states}
\end{array} + \ldots \]

- Broken singlet “releases” 2 spinons

- Many phenomenological theories
  - No solid connection to experiment
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Cs$_2$CuCl$_4$: a 2d spin liquid?

Couplings:

- $J' \approx 0.3$ J
- $D \approx 0.05$ J
- $J \approx 0.37$ meV

Hamiltonian:

$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j - \sum_{ij} D_{ij} \cdot \vec{S}_i \times \vec{S}_j - \hbar \cdot \sum_i \vec{S}_i$$
Inelastic Neutron Results


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

Note asymmetry.

Fit of “peak” dispersion to spin wave theory requires adjustment of $J, J'$ by $\approx 40\%$ - in opposite directions!
2d theories

- **Arguments for 2d:**
  - \( J'/J = 0.3 \) not very small
  - Transverse dispersion

- **Exotic theories:**


- **Spin waves:**

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”

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

\[ |k_x, k_y; \epsilon \rangle = \sum_y e^{ik_y y} |k_x, \epsilon \rangle_y \otimes \chi_{y \neq y'} |0\rangle_{y'} \]

- Momentum conservation: 1d Schrödinger equation in \( \epsilon \) space

\[ \epsilon \psi_k(\epsilon) + \int d\bar{\epsilon} D_{k_x}(\bar{\epsilon}) \mathcal{J}'(k) A^*_k(\epsilon) A_{k,x}(\bar{\epsilon}) \psi_k(\bar{\epsilon}) = E \psi_k(\epsilon) \]

- Crucial matrix elements known exactly

\[ A_{k,x}(\epsilon) = \frac{1}{\sqrt{2}} \langle 0 | S_{-k,x,y}^- | k_x, \epsilon \rangle_{y} \]

Bougourzi et al, 1996
Structure Factor

- **Spectral Representation**

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

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

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

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

**References**
Bougourzi et al, J.S. Caux et al
Types of behavior

- Behavior depends upon spinon interaction

$J^*(k_x, k_y) < 0$

$J^*(k_x, k_y) = 0$

$J^*(k_x, k_y) > 0$

| Bound “triplon” | Identical to 1D | Upward shift of spectral weight. Broad resonance in continuum or antibound state (small k) |

Bound “triplon”

Identical to 1D

Upward shift of spectral weight. Broad resonance in continuum or antibound state (small k)
Broad lineshape: “free spinons”

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

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

  - Curves: 2-spinon theory with experimental resolution
  - Curves: 4-spinon RPA with experimental resolution

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- Curves: 2-spinon theory with 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$_2$CuCl$_4$ 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

- $\text{Cs}_2\text{CuCl}_4$ 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

- $\text{Cs}_2\text{CuCl}_4$ 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

![Diagram](relevant vs. irrelevant couplings)

- $\text{relevant relevant} \rightarrow \text{decoupled chain fixed point}$
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 $\varepsilon$

- Can order these by range and relevance

\[ H_1' = \sum_y g_1 \mathcal{O}_1(y)\mathcal{O}_1(y + 1) \]
\[ H_2' = \sum_y g_2 \mathcal{O}_2(y)\mathcal{O}_2(y + 2) \]

Further chain couplings just as relevant but smaller
Example: Zero field $J-J'$ model

- Allowed operators strongly restricted by reflections

\[ \tilde{N}(y) \sim \tilde{N}(y + 1) \]
RG Subtleties (1)

- “Accidentally” zero couplings
  - E.g. staggered magnetization coupling $g_N = 0$

$$g_2(g_N)$$

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

\[
\frac{dg_1}{d\ell} = -\lambda_1 g_1 \\
\frac{dg_2}{d\ell} = \lambda_2 g_2 - g_1^2
\]
RG Subtleties (2)

- Competing Relevant Operators
  - Fluctuations generate several relevant couplings that compete \((g_N, g_\varepsilon)\)

\[ g_1(g_N) \quad g_2(g_\varepsilon) \]

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

\[ \frac{dg_i}{d\ell} = \lambda_i g_i \quad \lambda_1 > \lambda_2 \]

- Two factors:
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**

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

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

  \[ \frac{D}{J} \sim 0.05 \gg \left( \frac{J'}{J} \right)^4 \sim (0.3)^4 \sim 0.01 \]

- **Result: non-collinear spiral state**

  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 $h_{\text{sat}}$ 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. 
  - Cycloid ? Commensurate AF state
  - AF state differs from theory ($J_2$?)

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Longitudinal Field

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Naïve theoretical phase diagram

Expt.
- Cycloid ? Commensurate AF state
- AF state differs from theory ($J_2$?)
```

\[ h/h_{sat} \]

\[ \sim 0.1 \]

\[ 0 \]

\[ T \]

\[ 0.9 \]

\[ 1 \]

\[ h/h_{sat} \]

Weak “collinear” SDW

“cone”

Polarized
Magnetization Plateau

"Umklapp" (dangerously irrelevant operator): commensurate SDW state unstable to plateau formation

- Strongest locking at \( M = M_{\text{sat}}/3 \)
- Gives \( \text{"uud"} \) state which also occurs in spin wave theory (Chubukov)

Magnetization plateau observed in \( \text{Cs}_2\text{CuBr}_4 \)
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