Two studies of frustration on the triangular lattice:

1. Bose Mott transitions on the Triangular Lattice

2. Is there room for exotica in Cs$_2$CuCl$_4$? Investigating the 1d-2d crossover

Frustrating Mott Transitions on the Triangular Lattice

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cond-mat/0505258

cond-mat/0506457
Outline (1)

• XXZ Model
  – persistent superfluidity at strong interactions
  – supersolid

• Dual vortex theory of Mott transition
  – Field theory
  – Mott phases in (dual) mean field theory
  – Supersolid as melted Mott state, and a candidate for deconfined Mott criticality
Bose Mott Transitions

• Superfluid-Insulator transition of bosons in a periodic lattice: now probed in atomic traps

Filling $f=1$: Unique Mott state w/o order, and LGW works

$f \neq 1$: localized bosons must order

Interesting interplay between superfluidity and charge order!

Triangular Lattice

- "Hard-core": no double occupancy
  \[ \mathcal{P} = \text{hard-core projector} \]

\[ H = -t \sum_{\langle ij \rangle} \mathcal{P} (b_i^\dagger b_j + \text{h.c.}) \mathcal{P} + V \sum_{\langle ij \rangle} n_i n_j \]

- S=1/2 XXZ model with FM XY and AF Ising exchange

\[ H = \sum_{\langle ij \rangle} -\frac{J_{\perp}}{2} (S_i^+ S_j^- + \text{h.c.}) + J_z S_i^z S_j^z \]

- Frustration: Cannot satisfy all \( J_z \) interactions
  - no simple "crystalline" states near half-filling

Ising particle-hole symmetric

any solid order determined by kinetic energy
Supersolid Phase

• Recent papers on XXZ model find *supersolid* phase near $\frac{1}{2}$-filling

  - D. Heidarian, K. Damle, cond-mat/0505257
  - R. G. Melko *et al*, cond-mat/0505258
  - M. Troyer and S. Wessel, cond-mat/0505298

T=0

½ filling

from M. Troyer and S. Wessel

from Melko *et al*
Supersolid Phases

**“ferrimagnetic”**

spontaneous magnetization = phase separation

superfluid on \( \approx \frac{1}{4} \)-filled honeycomb

“interstitial lattice” of 1/3-triangular solid

particle-hole transform not identical

**“antiferromagnetic”**

superfluid on 1/2 -filled triangular

“interstitial lattice“ of honeycomb

“antiferromagnetic” solid

expect stabilized by 2\(^{nd}\) neighbor hopping
Surprises

- Superfluidity survives even when $V = J_z \to \infty$!

Symptomatic of frustration: superfluid exists within extensively degenerate classical antiferromagnetic ground state Hilbert space.

- Persistent superfluidity is exceedingly weak.

- Energy difference between 2 supersolid states is nearly unobservable.

$$\rho_s(J_z = \infty) \approx 0.04\rho_s(J_z = 0)$$ close to Mott insulator.
Mott Transition

- Goal: continuum quantum field theory
  - describes “particles” condensing at QCP

- Conventional approach: use extra/missing bosons
  - Leads to LGW theory of bose condensation
  - Built in diagonal order, the same in both Mott and SF state

- Dual approach: use vortices/antivortices of superfluid
  - non-LGW theory, since vortices are non-local objects
  - focuses on Mott physics, diagonal order is secondary
  - theory predicts set of possible diagonal orders
Duality


• Exact mapping from boson to vortex variables

\[ n = \frac{1}{2\pi} \vec{\nabla} \times \vec{A} \]

\[ \vec{\nabla} \phi = 2\pi \hat{z} \times \vec{E}, \]

\[ \vec{\nabla} \cdot \vec{E} = N \]

\[ \oint \vec{\nabla} \phi \cdot d\vec{l} = 2\pi \]

\[ \int d^2 x B = 2\pi \]

• Dual magnetic field

\[ B = 2\pi n \]

• Vortex carries dual U(1) gauge charge

\[ n = 1 \]

\[ \vec{v}_{sf} \propto \vec{\nabla} \phi \]

\[ \vec{E} \]

\[ N = 1 \]

• All non-locality is accounted for by dual U(1) gauge force
Dual Theory of QCP for f=1

- Two completely equivalent descriptions
  - really one critical theory (fixed point) with 2 descriptions

C. Dasgupta and B.I. Halperin,
*Phys. Rev. Lett.* 47, 1556 (1981);

\[ S = \int d^3x \left[ |\partial_\mu \psi|^2 + s|\psi|^2 + u|\psi|^4 \right] \]

\[ \tilde{S} = \int d^3x \left[ |(\partial_\mu - iA_\mu)\varphi|^2 + \tilde{s}|\varphi|^2 + u|\varphi|^4 + \frac{1}{2e^2}(\epsilon_{\mu\nu\lambda}\partial_\nu A_\lambda)^2 \right] \]

- N.B.: vortex field \( \varphi \) is not gauge invariant
  - not an order parameter in Landau sense

- Real significance: "Higgs" mass \( |\langle \varphi \rangle|^2 A^2 \)
  indicates insulating dielectric constant \( \epsilon_d \sim 1/|\langle \varphi \rangle|^2 \)
Non-integer filling $f \neq 1$

- Vortex approach now superior to Landau one
  - need not postulate unphysical disordered phase

- Vortices experience average dual magnetic field
  - physics: phase winding


- Vortex field operator transforms under a *projective* representation of lattice space group

Aharonov-Bohm phase in vortex wavefunction encircling dual flux

$2\pi$ winding of boson wavefunction on encircling vortex
Vortex Degeneracy

- Non-interacting spectrum = honeycomb Hofstadter problem
- Physics: magnetic space group

\[ T_1 T_2^{-1} T_3 T_1^{-1} T_2 T_3^{-1} = e^{2\pi i f} \]

and other PSG operations

- For \( f = p/q \) (relatively prime) and \( q \) even (odd), all representations are at least \( 2q \) \((q)\)-dimensional

- This degeneracy of vortex states is a robust property of a superfluid (a “quantum order”)
1/3 Filling

• There are 3 vortex “flavors” $\xi_1, \xi_2, \xi_3$ with the Lagrangian

$$\mathcal{L} = \sum_{\ell} \left[ |(\partial_{\mu} - iA_{\mu})\xi_{\ell}|^2 + s|\xi_{\ell}|^2 \right] + \frac{1}{2e^2} (\epsilon_{\mu\nu\lambda} \partial_{\nu}A_{\lambda})^2 + u(\sum_{\ell} |\xi_{\ell}|^2)^2 + \sum_{\ell \neq \ell'} \{v|\xi_{\ell}|^2|\xi_{\ell'}|^2 + w \text{ Re } [(\xi_{\ell}^*\xi_{\ell'})^3]\}$$

• Dual mean-field analysis predicts 3 possible Mott phases

v>0:

1/3 solid of XXZ model

v<0:

Expect “deconfined” Mott QCP with fluctuations included
½-Filling

• $2 \times 2 = 4$ vortex flavors with pseudo-spinor structure $z_{\pm\sigma}$
  - Space group operations appear as “rotations”

\[ T_1, T_2, T_3, R_{2\pi/3} \]

• Order parameters

\[ \tilde{S}_\alpha = z_\alpha^* \vec{\tau} z_\alpha \]

\[ \psi = e^{i\pi/4} z_+^* \vec{\tau} z_- \]

\[ \vec{d} = z_+^* \vec{\tau} z_- \]

XXZ supersolid diagonal order parameter

ordering wavevectors
Dual $\frac{1}{2}$-Filling Lagrangian

\[
\mathcal{L} = \mathcal{L}_0 + u \left( |S_+| + |S_-| \right)^2 + v |S_+||S_-| + w_1 \vec{S}_+ \cdot \vec{S}_- + w_2 \sum_{\alpha} \left( (S_{x\alpha}^\alpha)^4 + (S_{y\alpha}^\alpha)^4 + (S_{z\alpha}^\alpha)^4 \right) - w_3 \text{Re} \left( \psi^6 \right) \]

- Emergent symmetry:
  - Quartic Lagrangian has SU(2)×U(1)×U(1)\_g invariance
  - SU(2)×U(1) symmetry is approximate near Mott transition
  - Leads to “skyrmion” and “vortex” excitations of SU(2) and U(1) order parameters

- Mean field analysis predicts 10 Mott phases
  - e.g. $v,w_1<0$

Note similarity to XXZ supersolids
Hard-Spin Limit: Beyond MF analysis

• Example: $v, w_1 < 0$: $\vec{s}_+ = \vec{s}_- \quad |S_+| = |S_-| = \text{const.}$

  - Solution: $z_{\pm \sigma} = z_\sigma e^{\pm i\theta/2}$  
    $z_\sigma^* z_\sigma = 1$

  - $\mathbb{Z}_2$ gauge redundancy:  \[
  \begin{align*}
  & z_\sigma \rightarrow -z_\sigma \\
  & \theta \rightarrow \theta + 2\pi
  \end{align*}
  \]

• Hard-spin (space-time) lattice model:

\[
\mathcal{L}_{\text{eff}} = -t z_i \sigma_{i\mu} e^{-iA_{i\mu}} z_{i\sigma}^* z_{i+\mu\sigma} - t \theta \sigma_{i\mu} \cos(\Delta_{\mu \theta i}/2) + \frac{1}{2e^2} (\epsilon_{\mu\nu\lambda} \Delta_{\nu A_i \lambda})^2
\]

• $\mathbb{Z}_2$ gauge field  
• $\mathbb{C}P^1$ field  
• XY field  
• $U(1)$ gauge field

Phase Diagram

- Blue lines: LGW “roton condensation” transitions
- Red lines: non-LGW transitions
  - Diagonal order parameters change simultaneously with the superfluid-insulator transition
- Should be able to understand supersolids as “partially melted” Mott insulators
Physical Picture

- Superfluid to columnar VBS transition of $\frac{1}{4}$-filled honeycomb lattice!
Skyrmion

• VBS Order parameter: pseudo-spin vector $\langle \vec{S} \rangle = S_0 \hat{n}$

$\hat{n} = (100)$ $(00-1)$ $(001)$ $(0-10)$ $(010)$ $(-100)$

• Skyrmion:
  - integer topological index
  - finite size set by irrelevant “cubic anisotropy”

\[ Q = \frac{1}{4\pi} \int d^2r \hat{n} \cdot \partial_x \hat{n} \times \partial_y \hat{n} \]

• Boson charge is bound to skyrmion!

$N_b = Q$
Mott-SS3 Criticality

• SS3-Mott transition is *deconfined quantum critical point*
  - Non-compact CP¹ universality class
  - Equivalent to hedgehog-free O(3) transition

• Disordering of pseudospin

• Hedgehogs = skyrmion number changing events

Motrunich+Vishwanath

skyrmions condense: superfluid
Conclusions (1)

• Frustration in strongly interacting bose systems seems to open up a window through to observe a variety of exotic phenomena
• The simplest XXZ model exhibits a robust supersolid, and seems already quite close to non-trivial Mott state
• It will be interesting to try to observe Mott states and deconfined transitions by perturbing the XXZ model slightly (Chromium condensate?)
  – Cartoon pictures of the supersolid and Mott phases may be useful in suggesting how this should be done
Is there room for exotica in Cs$_2$CuCl$_4$? Checking the consistency of a “prosaic” 1d-2d crossover.

L.B.
O. Starykh, University of Utah
Cs$_2$CuCl$_4$: magnetic structure

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

• (Very good) approximate conservation of total $S^a$
2d Spin Liquid Physics?

- Broad inelastic neutron spectra have been interpreted as evidence for “exotic” physics.
  - Scenario: some “exotic” effective field theory governs intermediate energy behavior

\[ E \sim J \]
Decoupled chains

\[ E \sim J', D? \]
exotic

\[ E \sim T_N \]
ordered

- Is there room?
  - investigate possibility of direct crossover
  - i.e. assume most relevant perturbations of decoupled chains drive ordering, and study resulting phase diagram (can be done by RG+”chain mean field theory”)

Measurement of Couplings


- Single-magnon energies of fully-polarized state (in a-direction) exactly related to Hamiltonian parameters

- Fit gives

\[ J \approx 0.37 \text{ meV} \]
\[ J' \approx 0.3 \text{ J} \]
\[ D \approx 0.05 \text{ J} \]

- Spatially anisotropic S=1/2 antiferromagnet with non-negligible DM interaction
Low-T phase diagram

• Very different behavior for two field orientations indicates importance of DM interaction

• Phase diagram in transverse field roughly agrees with classical analysis

• How well can we understand this phase diagram from a quasi-1d approach?

**S=1/2 AF Chain: a primer**

\[ \mathcal{H} = J \sum_x \vec{S}(x) \cdot \vec{S}(x+1) - h \sum_x S^z(x) \]

- **Exact solution:**
  - Power-law spin (and dimerization) correlations

  \[ h = 0 \quad h \rightarrow h_{\text{sat}} \quad \delta = \pi M \]

- XY AF correlations grow with h and remain commensurate
- Ising “SDW” correlations decrease with h and shift in k
- Even all amplitudes of these correlations are known (Hikihara+Furusaki, 2004)
An Academic Problem

- **D=h=0, J’ \ll J**: Spatially anisotropic triangular lattice AF
  
  - problem: J’ is frustrated: $S_\pi$ doesn’t couple on neighboring chains
  
  - naïve answer: spiral state with exponentially small gap due to “twist” term $\vec{S}_\pi \cdot \partial_x \vec{S}_\pi$
  
  - True answer: effective 2nd–neighbor chain couplings generated $\sim (J')^4/J^3$

- Probable GS: four-fold degenerate “diagonal dimer” state
Why it’s academic

• Even $D=0.05J \gg (J')^4/J^3$ (with constants)
• DM allows *relevant* coupling of $S^b_{\pi}$ and $S^c_{\pi}$ on neighboring chains
  – immediately stabilizes spiral state
  – small $J'$ *perturbatively* makes spiral weakly incommensurate

\[
\mathcal{H}_{\text{eff}} \sim \sum_{y \in 2\mathbb{Z}} \left[ D \left( S^b_{\pi}(y) S^c_{\pi}(y + 1) - S^c_{\pi}(y) S^b_{\pi}(y + 1) \right) + J' \vec{S}_{\pi}(y) \cdot \partial_x \vec{S}_{\pi}(y + 1) \right]
\]

relevant: dim = 1  marginal: dim = 2
Transverse Field

- 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

- DM term: $S^b S^c \sim S^z S^{\pm}$
  - wavevector mis-match for $h>0$: DM “irrelevant” for $h \gtrsim D$
- With DM killed, sub-dominant instabilities take hold
- Two important couplings for $h>0$:
  \[ \mathcal{H}_{\text{eff}} \sim \sum_{y \in 2\mathbb{Z}} \left[ J' \sin(\delta) S_{\pi-2\delta}(y) S_{\pi+2\delta}(y+1) + J' \left( S^+_{\pi}(y) \partial_x S^-_{\pi}(y+1) + \text{h.c.} \right) \right] \]
  \[ \begin{array}{l}
  \text{dim } 1/2\pi R^2 \\
  \text{“collinear” SDW}
  \end{array} \]
  \[ \begin{array}{l}
  \text{dim } 1+2\pi R^2 \\
  \text{spiral “cone” state}
  \end{array} \]
- “Critical point”: $2\pi R^2 = (\sqrt{5} - 1)/2 \approx 0.62$

Predicts spiral state for $h > h_c \approx 0.9 h_{\text{sat}} \approx 7.2 \text{ T}$

observed for $h > 7.1 \text{T}$
• **Guess:** “spin liquid” region is really SDW with low ordering temperature

  - expected since amplitude of SDW interaction vanishes at $h=0$, and relevance (in RG sense) decreases with $h$. 
Beyond the naïve

• Collinear state is not truly collinear:
  - “irrelevant” DM involves $\sim D S_y^b S_{y+1}^c$
  - effective oscillating field in c-direction with $\langle S^b \rangle \neq 0$:
    result is very elongated cycloid

• “Collinear” SDW state locks to the lattice at low-T
  - “irrelevant” (1d) umklapp terms become relevant once
    SDW order is present (when commensurate)
  - strongest locking is at $M=1/3 M_{sat}$

• Same “uud” state predicted by large-S expansion (Chubukov…)

• coincidentally uud state seems to occur near maximum $T_c$ of collinear region
Cs$_2$CuBr$_4$

- Isostructural to Cs$_2$CuCl$_4$ but believed to be less quasi-1d

T. Ono et al, 2004

- Magnetization plateau at $M=1/3\, M_{\text{sat}}$ observed for longitudinal but not transverse fields

(additional feature at $2/3\, M_{\text{sat}}$)

- “Commensurate Collinear” order of some sort has apparently been observed in Cs$_2$CuCl$_4$ recently (Coldea, private communication)
Conclusions (Cs$_2$CuCl$_4$)

• A quasi-1d approach based on direct decoupled chain → ordered crossover is quite successful in explaining low-energy behavior
• Work in progress to calculate ordering temperature, wavevector, spin stiffness, etc. quantitatively
• Appears likely the “spin liquid” state is just another ordered (quasi-collinear) phase with low $T_c$
  – perhaps can observe “uud” commensurate state?
• “Exotic” scenario with intervening non-trivial fixed point seems rather unlikely

• A proper theoretical calculation (open problem!) of the inelastic spectrum in a 1d-2d crossover is sorely needed.