Quantum Phases in Bose-Hubbard Models with Spin-orbit Interactions

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The plan

1. Introduction to Bose-Hubbard model (BHM)

2. BHM with spin-orbit coupling
   - Weak interaction superfluid
   - Strong coupling Mott insulator; 1D & 2D magnetic models
   - Phase diagram - magnetic structure in strongly interacting superfluid

3. Slave boson theory
   - Construction
   - Some consequences

4. Conclusions and outlook
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Optical lattice: Bose-Hubbard model

\[
H = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + U \sum_i \frac{n_i(n_i - 1)}{2} - \mu \sum_i n_i
\]

**Theory:** M. Fisher et al, PRB 40 546 (1989)

**Experiment:** M. Greiner et al., Nature 415 39 (2002)
Bose-Hubbard Model: mean field theory

\[ a_i ^\dagger a_j \rightarrow \langle a_i ^\dagger \rangle a_j + a_i ^\dagger \langle a_j \rangle - \langle a_i ^\dagger \rangle \langle a_j \rangle \]

Order parameter

\[ H^{\text{mft}} = U \frac{n_i (n_i - 1)}{2} - \mu n_i - t \sum_{j \in \text{nn}} (\langle a_j \rangle a_i ^\dagger + \langle a_j ^\dagger \rangle a_i) \]

Credit: Bloch@Munich

Bose-Hubbard Model: excitations, RPA

## Bose-Hubbard Model: summary

<table>
<thead>
<tr>
<th></th>
<th>Mott</th>
<th>Superfluid</th>
<th>Normal</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Order Parameters</strong></td>
<td>zero</td>
<td>nonzero (uniform)</td>
<td>zero</td>
</tr>
<tr>
<td><strong>Compressibility</strong></td>
<td>zero</td>
<td>nonzero</td>
<td>nonzero</td>
</tr>
<tr>
<td><strong>Excitations</strong></td>
<td>gapped</td>
<td>gapless</td>
<td>gapless (?)</td>
</tr>
<tr>
<td><strong>Charge Transport</strong></td>
<td>zero</td>
<td>nonzero + superfluid</td>
<td>nonzero</td>
</tr>
</tbody>
</table>

Considerations in terms of **many-body wave functions** and **density matrices** can be carried out for these different phases (Yang, Kohn, Bloch, Leggett).
What are the effects of spin-orbit couplings in Bose-Hubbard model?


William Cole

Arun Paramekanti

Nandini Trivedi
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Bose-Hubbard Model: with spin-orbit interactions

\[ H_{\text{hop}} = -t a_{i\sigma}^\dagger \mathcal{R}_{\hat{\nu}}^{\sigma\sigma'} a_{i+\hat{\nu}\sigma'} \]

\[ \sigma, \sigma' = \uparrow, \downarrow \]

\[ \hat{\nu} = \hat{x}, \hat{y} \]
Bose-Hubbard Model: non-interacting band structure

- Two internal states
- Hopping:
  - $t \cos \alpha$
- On-site interaction:
  - $U$
- $\pm t \sin \alpha$
  - $\lambda U$
- Lattice version of the Rashba spin-orbit coupling

$\alpha = \pi / 4$
Non-interacting band structure

Non-trivial winding (Chern number) around the $\Gamma$ point due to existence of Dirac points:

$$\alpha = \frac{\pi}{4}$$

Lattice version of the Rashba spin-orbit coupling
Weak coupling superfluid

Four degenerate states: \((\pm k_0, \pm k_0)\)

\[ \sqrt{2} \tan k_0 = \tan \alpha \]

Spins lie in the x-y plane.

\[ U_{\text{int}} \propto \frac{1 + \lambda}{2} (n_\uparrow + n_\downarrow)^2 + \frac{1 - \lambda}{2} (n_\uparrow - n_\downarrow)^2 \]

\( \lambda < 1 \)  
no polarization
only one state is occupied; uniform spin and number density

\( \lambda > 1 \)  
polarization
two opposite states are occupied; strip spin and uniform number density

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Strong coupling Mott insulator

Consider the case in which on average, there is one boson per site. Standard perturbation theory gives low energy effective magnetic Hamiltonian

**x-direction:**

\[-\frac{\cos(2\alpha)}{\lambda} S_i^x S_l^x - \frac{1}{\lambda} S_i^y S_l^y - \frac{2\lambda - 1}{\lambda} \cos(2\alpha) S_i^z S_l^z \]

\[-\sin(2\alpha) \hat{y} \cdot (S_i \times S_l) \]

**y-direction:**

\[-\frac{1}{\lambda} S_i^x S_j^x - \frac{\cos(2\alpha)}{\lambda} S_i^y S_j^y - \frac{2\lambda - 1}{\lambda} \cos(2\alpha) S_i^z S_j^z \]

\[+ \sin(2\alpha) \hat{x} \cdot (S_i \times S_j) \]

Dzyaloshinskii-Moriya coupling

Cf. DM term in superfluid, X. Xu and J.Han PRL 108 185301 (2012)
J.Radic et al. PRL 109 085303 (2012)
Z.Cai et al. PRA 85 061606R (2012)
M.Gong et al, arXiv:1205.6211
1D magnetic Hamiltonian

For example, 1D Hamiltonian along x-direction. Rotate spins around x by $\pi/2$, such that DM vector is along z

$$
-\frac{\cos(2\alpha)}{\lambda} S_i^x S_l^x - \frac{\cos(2\alpha)}{\lambda} (2\lambda - 1) S_i^y S_l^y - \frac{1}{\lambda} S_i^z S_l^z - \sin(2\alpha)(S_i^y S_l^x - S_i^x S_l^y)
$$

Some 1D AFM system with DM

<table>
<thead>
<tr>
<th>System</th>
<th>DM/Exchange</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cooper Benzoate</td>
<td>0.05</td>
</tr>
<tr>
<td>Yb$_4$As$_3$</td>
<td>?</td>
</tr>
<tr>
<td>BaCu$_2$Si$_2$O$_7$</td>
<td>0.02?</td>
</tr>
<tr>
<td>CsCuCl$_3$</td>
<td>0.18</td>
</tr>
</tbody>
</table>

XY-exchange and DM couplings can be tuned by changing $\alpha$ and $\lambda$, in particular, DM can be made as large as exchange coupling;

Various limits of the model can be solved exactly.
1D magnetic Hamiltonian: special cases

**Case I** \( \lambda \to 0 \) rotation around x by \( \pi \) every other site

\[
-\frac{1}{\lambda} \left( \cos(2\alpha) S_i^x S_l^x + \cos(2\alpha) S_i^y S_l^y - S_i^z S_l^z \right)
\]

**Z-ferromagnetic**

\( 0 < \alpha < \pi/2; \quad |\cos(2\alpha)| < 1 \)

**critical points:**

\( \alpha = 0, \pi/2; \quad |\cos(2\alpha)| = 1 \)
1D magnetic Hamiltonian: special cases

Case II \( \lambda = 1 \) XXZ+DM

\[-S_i^x S_l^x - S_i^y S_l^y - \frac{1}{\cos(2\alpha)} S_i^z S_l^z - \tan(2\alpha)(S_i^y S_l^x - S_i^x S_l^y)\]

Rotate each spin around z by \( \phi = 2\alpha \).

Can be mapped to XXZ model with a new twisted boundary condition. It can be solved with Bethe ansatz and turns out to be always critical in bulk.

\[-(\tilde{S}_i^x \tilde{S}_l^x + \tilde{S}_i^y \tilde{S}_l^y + \tilde{S}_i^z \tilde{S}_l^z)\]
1D magnetic Hamiltonian: special cases

Case III $\lambda \to \infty$

$$-2 \cos(2\alpha) S_i^y S_l^y - \sin(2\alpha) (S_i^y S_l^x - S_i^x S_l^y)$$

Can be solved using Jordan-Wigner.

$$E_\pm(k) = \sin(2\alpha) \sin k \pm |\cos(2\alpha)|$$

Critical points: $\alpha = \pi/8; 3\pi/8$

[Diagram showing the energy $E(k)$ as a function of $k$ with special cases and critical points labeled]
1D magnetic Hamiltonian: special cases

**Case IV** \( \alpha = \pi/4 \)

\[-\frac{1}{\lambda} S^z_i S^z_l - (S^y_i S^x_l - S^x_i S^y_l) \]

Ising+DM, can be mapped to XXZ model

- \( \lambda > 1 \) XY-chiral
- \( \lambda < 1 \) Z-Ferromagnetism

**Case V** XXZ model

\[-\frac{1}{\lambda} (\pm S^x_i S^x_l \pm (2\lambda - 1) S^y_i S^y_l + S^z_i S^z_l) \]

- \( \alpha = 0 \) \( \alpha = \pi/2 \)

- \( \lambda < 1 \) Para Para
- \( \lambda > 1 \) Y-Ferro Y-Antiferro
Schematic Phase diagram

What needs to be done:

Exact Diagonalization (12 sites) suggests phase diagram as shown left. It confirms the part for $\lambda > 1$; but for $\lambda < 1$, not very clear;

Calculate phase diagram with DMRG technique;

Calculate correlation functions and investigate experimental signatures.
2D classical magnetic phases

Magnetic structure factors:

\[ S_q = \left| \sum_i S_i \exp(iq \cdot r_i) \right|^2 \]

Calculated with classical Monte Carlo annealing procedure + variational ansatz
What are the implications of magnetic ordering for the superfluid states?
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Mean field theory

\begin{align*}
H_{\text{hop}} &= -ta_{i\sigma}^\dagger \mathcal{R}_{\hat{\nu}}^{\sigma\sigma'} a_{i+\hat{\nu}\sigma'} \\
H_{\text{int}} &= \frac{U}{2} \left( n_{i\uparrow}^2 + n_{i\downarrow}^2 + 2\lambda n_{i\uparrow} n_{i\downarrow} \right) \\
H_{\text{hop}}^{\text{mft}} &= -t \left( \langle a_{i\sigma}^\dagger \rangle \mathcal{R}_{\hat{\nu}}^{\sigma\sigma'} \right) a_{i+\hat{\nu}\sigma'} - ta_{i\sigma}^\dagger (\mathcal{R}_{\hat{\nu}}^{\sigma\sigma'} \langle a_{i+\hat{\nu}\sigma'} \rangle)
\end{align*}

Due to complicated magnetic ordering, we carry out calculations on a finite cluster (8\times8) with periodic boundary conditions to attain self-consistency.

Local magnetization:

\[ m_i = \langle a_{i\sigma}^\dagger \tau_{\sigma\sigma'} a_{i\sigma'} \rangle \]

Bond current:

\[ \kappa_{\hat{\nu}}^{\sigma\sigma'} = -it \left( \mathcal{R}_{\hat{\nu}}^{\sigma\sigma'} \langle a_{i\sigma}^\dagger a_{i+\hat{\nu}\sigma'} \rangle - \text{c.c.} \right) \]
Phase diagram

Smooth evolution of magnetic order from Mott insulator to superfluid!
How are the current patterns related to magnetic ordering?
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Slave boson theory: construction

To describe the interplay between magnetism and superfluidity, introduce

\[ a_{\sigma}^{\dagger} = \frac{1}{\sqrt{n_b}} b^{\dagger} f_{\sigma}^{\dagger}, \quad n_b = b^{\dagger} b \]

Both \( b \) and \( f_{\sigma} \) are bosons operators, satisfying commutation relations

\[ [b, b^{\dagger}] = 1; \quad [f_{\sigma}, f_{\sigma'}^{\dagger}] = \delta_{\sigma \sigma'} \]

Single site Hilbert space: \( |m \uparrow, n \downarrow\rangle \)

\[ |m + n\rangle_b \otimes |m \uparrow, n \downarrow\rangle_f \]

The canonical commutation relations of a-operators are preserved in the physical Hilbert space.

\[ H_{\text{hop}} = -t a_{i \sigma}^{\dagger} R_{i \sigma, \sigma'}^{\sigma \sigma'} a_{i+\hat{\nu} \sigma'} + \text{c.c.} \]

\[ H_{\text{hop}} = -t \frac{1}{\sqrt{n_{ib}}} f_{i \sigma}^{\dagger} R_{i \sigma, \sigma'}^{\sigma \sigma'} f_{i+\hat{\nu} \sigma'} + \frac{1}{\sqrt{n_{i+\hat{\nu}, b}}} b_{i}^{\dagger} b_{i+\hat{\nu}} + \text{c.c.} \]
Slave boson mean field theory

Assuming that the magnetic moments are ordered in the ground state, we can then make the classical field approximation and define:

$$z_\sigma = \eta^{-1} \left\langle \frac{f_\sigma}{\sqrt{n_b}} \right\rangle \quad z^\dagger = (z^*_\uparrow, z^*_\downarrow) \quad z^\dagger z = 1$$

Hopping Hamiltonian within mean field becomes:

$$H_{\text{hop}}^{\text{mft}} = -t \left| \eta \right|^2 z^*_i \hat{R}^{\sigma \sigma'}_{i+\hat{\nu}} z_{i+\hat{\nu} \sigma'} b_i^\dagger b_{i+\hat{\nu}}$$

Thus, the original spin-orbit couplings for a-bosons become abelian gauge fields for the charge degrees of freedom b, **within slave boson mean field and if spinons (f) are condensed**.

The constraint is implemented with U(1) gauge fields, which will be gapped through Higgs mechanism, **if spinons are condensed**. The suppressed gauge fluctuations may ensure the validity of the slave boson mean field theory.
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Slave boson theory: understand current patterns

**Case I: Ferromagnetic background**

\[ \mathbf{z}_i = (1, 0), \quad \forall \ i \]

\[ H_{\text{hop}}^{\text{mf}} = -(t \cos \alpha) b_i^\dagger b_{i+\hat{y}} \]

renormalized hopping.

\[ U_c^{\text{fm}} = U_c \cos \alpha \]

**Case II: Anti-ferromagnetic background**

\[ \mathbf{z}_i = (1, 0); \quad \text{Sublattice A} \]

\[ \mathbf{z}_i = (0, 1); \quad \text{Sublattice B} \]

\[ \prod t_{12} t_{23} t_{34} t_{41} = -t^4 \sin^4 \alpha < 0 \]

π-flux lattice, Dirac points at \((0, \pm \pi/2)\)

Two-fold degeneracy of current patterns!
Slave boson theory: understand current patterns

**Case III:** Spin crystal background

\[ \prod t_{12} t_{23} t_{34} t_{41} = -\frac{1}{4} (\cos \alpha - i \sqrt{2} \sin \alpha)^4 \]

Alternating flux \( \Phi \) in each plaquette.

**Fixed current patterns!**

**What needs to be done:**

Self-consistent determination of the spinon fields \( z \) (full slave boson mean field theory);

Possibility of an “exotic” Mott insulator in BHM with spin-orbit coupling;

![Diagram showing the relationship between flux and angle \( \alpha \).]
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Conclusions and outlook

We have studied Bose-Hubbard Model with spin-orbit interactions and established its weak coupling superfluid states, magnetic structure in the Mott insulating states and determined the phase diagram using mean field theory.

We proposed a new slave boson theory and argued that it was helpful for us to understand certain features of the strongly interacting superfluids close to the Mott transition.

Magnetic models in either 1D or 2D are worth investigating in detail. In particular, for 1D, the complete phase diagram with exact diagonalization or density matrix renormalization group calculation; possibility of experimental implementation. For 2D, collective excitations and order from disorder calculations.

Understand the phase diagram with slave boson theory. In particular, investigate the possibility of “exotic” Mott insulating states (e.g. disordered magnetic states close to the Mott boundary).
Thank you!