Exploring spin-orbital models with cold gases loaded in p-bands of zig-zag optical lattice

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Spin-orbit couplings in solids

• Relativistic spin-orbit coupling (e.g. compounds with strong Rashba or Dresselhaus coupling):
Dirac equation for electron in external potential $V$ expanded to lowest order in $v^2/c^2$ leads to a Schrödinger equation with additional spin-orbit coupling term:

$$\frac{[\vec{\nabla}V \times \vec{p}] \vec{S}}{2m_e^2c^2} \rightarrow \frac{1}{2m_e^2c^2r} \frac{\partial V}{\partial r} (\vec{S} \vec{L})$$

• Non-relativistic spin-orbit coupling (Kugel-Khomskii):
If relevant electrons are from p, d, or f-bands and angular momentum is not quenched there is orbital degeneracy.

Spin-orbit coupling can give nontrivial topology to band insulators, with helical gapless edge modes or can induce topological superconductivity with Majorana particles.
Solid with zig-zag structure

In Mott insulators orbital degrees enhance thermal as well as quantum fluctuations, suppress Néel order, and lead to spin/orbital liquid states.

Mott insulating transition-metal compounds having structures of weakly coupled zig-zag chains:

• with strong relativistic coupling: $\text{Sr}_2\text{VO}_4$, the role of spins is played by an isospin variable discerning the Kramers partners, while the pseudo-orbital variables distinguishes two lowest Kramers doublets of $\text{V}^{4+}$ ion.

• with negligible relativistic coupling: Pyroxene titanium oxides $\text{ATiSi}_2\text{O}_6$ ($A = \text{Na}, \text{Li}$) with active $d_{xy}$ and $d_{yz}$ orbitals, and spin one-half from $\text{Ti}^{3+}$ ions.
Advantages of ultra-cold gases

- In many solid-state systems, the orbital dynamics is often quenched, due to the coupling of the orbitals to Jahn-Teller phonons, and the quantum nature of orbitals is lost.
- In real materials, the coupling strengths are fixed by nature, being very difficult to modify (e.g. by pressure), thus the experimental access to a potentially rich phase diagram is limited.

Ultra-cold dipolar spinor fermions in zig-zag type optical lattices can mimic spin-orbital models relevant in solid-state systems with the interesting advantage of reviving the quantum nature of orbital fluctuations and exploring vast phase diagram.
Zig-zag chains of optical lattice

Incoherent superposition between a triangular lattice

\[ V_1(\vec{r}) \equiv (x, y) = V_{10} \left[ \sin^2 \left( \vec{b}_1 \cdot \vec{r}/2 \right) + \sin^2 \left( \vec{b}_2 \cdot \vec{r}/2 \right) + \sin^2 \left( (\vec{b}_1 - \vec{b}_2) \cdot \vec{r}/2 \right) \right] , \]

with \( k \) the laser wavenumber

\( \vec{b}_1 = \sqrt{3}k \vec{e}_y \) and \( \vec{b}_2 = \sqrt{3}k (\sqrt{3}\vec{e}_x/2 - \vec{e}_y/2) \)

and an additional lattice \( V_2(\vec{r}) = V_{20} \sin^2(\sqrt{3}ky/4 - \pi/4) \).

On Figure \( V_{20}/V_{10} = 2 \).
P-bands of optical lattice

$P_z$ band is energetically higher due to tight confinement in $z$ direction.

$\sigma^x = +1 \rightarrow P_x$ orbital,
$\sigma^x = -1 \rightarrow P_y$ orbital.
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$U, V$ are on-site interaction energies, $t (>0)$ and $\lambda$ are hoppings. $\lambda \neq 0$ e.g. due to elongating confining potential in x-y plane along $\vec{e}_x + \vec{e}_y$ direction.
Dipolar Fermions

Magnetic dipoles, like Chromium atoms from ground state F=9/2 manifold in strong magnetic field. Polar fermionic molecules with strong electric dipole moment e.g., $^{40}\text{K}^{87}\text{Rb}$ or $^{7}\text{Li}^{40}\text{K}$. Spins $\uparrow$ and $\downarrow$ are provided by two internal states of fermion that are distinguished by nuclear spin, which in the lowest energy states decouples from electrons, and hence the interactions (which are due to electronic degrees of freedom) are spin independent, $SU(2)$: $V(\mathbf{r}_1 - \mathbf{r}_2)n(\mathbf{r}_1)n(\mathbf{r}_2)$, $n = n_\uparrow + n_\downarrow$.

Total interparticle potential includes dipolar and contact terms:

$$V(\mathbf{r}_1 - \mathbf{r}_2) = V_{\alpha,\beta}(\mathbf{r}_1 - \mathbf{r}_2) = \frac{\mu_0 d_\alpha d_\beta}{4\pi |\mathbf{r}_1 - \mathbf{r}_2|^3} + g\delta(\mathbf{r}_1 - \mathbf{r}_2)$$

For magnetic dipoles, in weak fields, the interparticle potential will depend on the hyperfine state, as different hyperfine components have different magnetic moments $d_\uparrow \neq d_\downarrow$. 
Fermionic chromium $^{53}\text{Cr}$: I=3/2, J=S=3 (Hund), F=9/2,...3/2. For strong magnetic fields, the magnetic dipole moment of 4 lowest energy states $|\frac{9}{2}, -\frac{9}{2}\rangle$, $|\frac{9}{2}, -\frac{7}{2}\rangle$, $|\frac{9}{2}, -\frac{5}{2}\rangle$, and $|\frac{9}{2}, -\frac{3}{2}\rangle$, are equal $d_\alpha \simeq d_\beta \simeq -2\mu_B m_J/\hbar = 6\mu_B$.

$$d^2 = 36\mu_B^2$$ for $^{53}\text{Cr}$, compare to $d^2 = \mu_B^2$ for alkali metals with $J = S = 1/2$ in the ground state. Erbium $d^2 = 49\mu_B^2$ and dysprosium $d^2 = 100\mu_B^2$. 
Dipolar Fermions

The interaction energy of two fermions occupying the same orbital of a given lattice site (necessarily in spin singlet state) is $U$,

$$U = \int dr_1 dr_2 P^2_{x(y)}(r_1) V(r_1 - r_2) P^2_{x(y)}(r_2),$$

when two fermions occupy different orbitals of the same lattice site they can be either in spin triplet or spin singlet state. Define ’average’ interaction energy $V$,

$$V = \int dr_1 dr_2 P^2_x(r_1) V(r_1 - r_2) P^2_y(r_2),$$

$P_x$ and $P_y$ are orbital wavefunctions at the same well.
Dipolar fermions in P-bands

Interaction in spin-triplet state is \[ V_t = V - J_H \]
Interaction in spin-singlet state is, \[ V_s = V + J_H. \]

\[ J_H = \int \! \! \int dr_1 dr_2 P_x(r_1) P_y(r_1) V(r_1 - r_2) P_x(r_2) P_y(r_2) \]

For the spin-triplet state, the contact s-wave interaction does not play any role, \( V(r_1 - r_2) \sim \delta(r_1 - r_2) \), \( V = J_H \) and scattering in the spin-triplet channel vanishes \( V_t = 0 \).

In general for Coulomb, dipolar, contact, other potential one can show \( V_t < V_s \rightarrow \) Hunds rule: by maximizing spin of two fermions on orthogonal orbitals, the energy (of Coulomb, dipolar or contact repulsion) is reduced, since fermions minimize their overlap in coordinate antisymmetric state (that has a node at vanishing relative distance).
Dipolar fermions in P-bands
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In strong coupling $U, V \pm J_H \gg t, \lambda$ and for one fermion per lattice site → spin-orbit model.
Dipolar fermions in P-bands

In strong coupling $U, V \pm J_H \gg t, \lambda$ and for one fermion per lattice site $\to$ spin-orbit model.

$$H = \frac{t^2}{2U} \sum_i (2S_i S_{i+1} + \alpha - \frac{1}{2})(1 + (-1)^i \sigma^x_i)(1 + (-1)^i \sigma^x_{i+1})$$

$$- \Delta \sum_i 2S_i S_{i+1}(1 - \sigma^x_i \sigma^x_{i+1}) - \lambda \sum_i \sigma^z_i$$

$$\alpha = \frac{U(V + J_H/2)}{V^2 - J_H^2} \simeq U/V \text{ and } \Delta = J_H U/(V^2 - J_H^2).$$

Possibility of $\lambda \neq 0$ gives to orbitals quantum character.

Note, despite that we restrict interactions within the same lattice site, dipolar (long-range) interaction is crucial for the stability of the Mott $1$ state. For contact potentials one would get metallic ferromagnetism, since $\Delta \to \infty$. Observe $SU(2)$ symmetry in spins, due to $V(r_1 - r_2)$ being independent of spin projection.
Ground state phases for $\alpha < 2$
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(a) $\Delta = 0$, (b) $\alpha = 1$

for $\alpha = \frac{U(V+J_H/2)}{V^2-J_H^2} < 2$ the similar topology of phase diagram.

Ground state is spin singlet, $S^T = 0$ or fully polarized $S^T = 1/2$ in Ferro phase.
Ground state phases for $\alpha > 2$
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For $\alpha > 2$ the similar topology of phase diagram. Ground state is global spin singlet, in iH states and fully polarized in Ferro phases.

In Ferrimagnetic phase total spin of the ground state changes smoothly and takes all values from $S^T = 0$ till $S^T = 1/2$. Interplay between $\lambda$ (singlet formation) and $\Delta$ (Hund triplet formation) produces Ferrimagnetic state.
2 fermions per site

The case of 2 fermions per site does not need dipolar interactions. Due to Hunds rule on-site triplet states $S^T = 1$ will be favoured (interaction energy in spin-triplet state vanishes for local interactions) and low energy effective model is Haldane $S = 1$ spin chain:

$$H = J \sum_{i} S_i S_{i+1}.\]

Ground state is that of AKLT type.
Spin exchange scale
Spin exchange scale

2-component Hubbard model:

For $U \gg t$, retain one particle per site.

Second order perturbation theory in tunneling,

$$H_{\text{Heisenberg}} = \pm JS_1 S_2, \quad S_i = \frac{1}{2} b_{i,\alpha}^\dagger \sigma_{\alpha,\beta} b_{i,\beta}$$

+ sign for fermions $\rightarrow$ antiferromagnetism, opposite to Hund rule, gain is due to delocalization energy

- sign for bosons $\rightarrow$ ferromagnetism.

$J = \frac{4t^2}{U} \rightarrow$ strength of spin exchange.

In cold gases currently $U > T > J$. 
Resolving spin degeneracy

For $U \gg T \gg J$, probability that spin looks up or down is 50%, independent of its neighbors, $s = k_B \ln 2$.

To resolve spin coherence for 3D antiferromagnets on cubic lattice, $T < T_N \simeq J$, $s(T_N) \simeq 0.5 \ln 2 k_B$ (QMC).

To observe AFM spin order $s < 0.5 \ln 2 k_B$.

Current experiments $s \simeq \ln 2 k_B$ (spin incoherent Mott state).

- How to get so small entropy per site?
- Start from Band insulator state with practically zero entropy (boundary defects and uncertainty of double occupancy will give some residual but small entropy).
- Use spin-changing collisions and orbital degeneracy.
Towards the spin degeneracy

Use internal degrees of freedom (hyperfine spin components) and spin-changing collisions. \(^{40}K \rightarrow \) has 10 states in the lowest hyperfine multiplet.

Initially \(|F = \frac{9}{2}, m_F = \frac{9}{2}\rangle\) and \(|\frac{9}{2}, \frac{1}{2}\rangle\) both in s-orbital

\(\rightarrow\) finaly \(|\frac{9}{2}, \frac{7}{2}\rangle\) and \(|\frac{9}{2}, \frac{3}{2}\rangle\) in p-orbital.

In experiments currently \(\lambda \gg t\).
Topological Haldane state

- Take multi-component fermions and initially select 2 components by magnetic field in band insulator state.
- Quench magnetic field to resonant value (to allow production of other two components) and after one cycle, $t = t^*$, quench it again away of the resonant value.
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One can load with high efficiency p-bands and allow to time evolve the system. Since effective Hamiltonian is of Haldane spin-1 chain one can arrive at Haldane state.

Adiabatic change of field → talk by Juan Jaramillo.
Vielen Dank!