Role of Hund Coupling in Two-Orbital Systems

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Mott-Hubbard Transition

\[ H = - \sum_{(ij), \sigma} t_{ij} (c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Weakly correlated

Intermediate regime:
hard to describe quantitatively

Strongly correlated

Kotliar, Vollhardt (2004)
Quasiparticle Weight (DMFT+NRG)

\[ Z = \frac{1}{1 - \frac{\partial \text{Re} \Sigma(\omega)}{\partial \omega} \mid_{\omega=0}} , \]

Bulla, PRL (1999)
Two-Orbital System

- **Degenerate bands with different bandwidths**
  - different $U_c$ for Mott transition
- **Orbital-Selective Mott Phase (OSMP)**
  - coexistence of localized and itinerant electrons
  - $Ca_{2-x}Sr_xRuO_4$ $(0.2 < x < 0.5)$

Multiband System

- inter-orbital Coulomb interaction $U'$, Hund coupling $J$

- Renormalization by the inter-orbital coupling may affect the transition behaviors.

from Sakai (2006)
Single Transition?

- large deviation of $Z_1$ and $Z_2$ from bare values

- claim for single Mott transition

- DMFT+QMC

$W_1 = 2\text{eV}, \ W_2 = 4\text{eV}$
$J = 0.2\text{eV}, \ U' = U - 2J$
$T = 0.125\text{meV}$

*Liebsch (2003)*
Orbital-Selective Transition?

- single transition for $J=0$
- orbital-selective transition for finite $J$
- DMFT+ED

Koga, Kawakami, Rice, Sigrist (2004)
Hamiltonian for Two-Orbital Systems

- Hamiltonian

\[
H_1 = - \sum_{(ij)\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_{im} n_{im\uparrow} n_{im\downarrow} \\
+ \sum_{i\sigma\sigma'} (U' - \delta_{\sigma\sigma'} J) n_{i\sigma} n_{i2\sigma'}
\]

\[
H_2 = \frac{1}{2} J' \sum_{im\sigma} c_{i\sigma}^\dagger (c_{i\sigma}^\dagger c_{im\sigma} + c_{im\sigma}^\dagger c_{i\bar{m}\sigma}) c_{im\sigma}
\]

- $J$: Ising type Hund coupling
- $J'$: including spin-flip and pairwise hopping
Resolution to this issue

- **Isotropic Hund coupling** \((J' = J)\)
  - Two successive first-order transition
  - near 2.0 eV,
    - narrow band: complete MIT
    - wide band: incomplete transition to new more correlated phase
  - near 3.0 eV
    - wide band: complete MIT

*Liebsch (2005)*
Resolution to this issue

- **Ising-type Hund coupling only (\( J' = 0 \))**
  - lower transition:
    - first-order for both bands
  - upper transition:
    - change of slope

Liebsch (2005)
NFL for Ising-type Hund Coupling

- In intermediate phase
  - \( \text{Im} \Sigma_2(i0^+) \neq 0 \): finite lifetime at Fermi level
  - non-Fermi liquid

- Fermi liquid
  - non-Fermi liquid → Mott insulator

\( \text{Biermann, de’Medici, Georges (2005); Liebsch, Costi (2006)} \)
Motivation

Aim to investigate the dependence of transition nature on Ising-type Hund coupling strength $J$

\[ \mathcal{H} = - \sum_{\langle ij \rangle_{\alpha \sigma}} t_{\alpha} (c_{i\alpha \sigma}^\dagger c_{j\alpha \sigma} + h.c.) + U \sum_{i\sigma} n_{i\alpha \uparrow} n_{i\alpha \downarrow} \]

\[ + U' \sum_{i\sigma} n_{i1\sigma} n_{i2\sigma} + (U' - J) \sum_{i\sigma} n_{i1\sigma} n_{i2\sigma} \]

- intra-orbital hopping, $t_{\alpha}$
- Intra- and inter-orbital Coulomb interaction, $(U, U')$
- Ising-type Hund’s coupling, $J$
- $U' = U - 2J$; $W_1=2$, $W_2=4$
- Bethe lattice in infinite dimensions
- half-filled case
- paramagnetic phase
Dynamical Mean-Field Theory + Continuous Time QMC

Mapping of lattice model onto two-impurity model

- two-impurity problem

\[ \mathcal{H}_{\text{impurity}} = \sum_{p,\alpha,\sigma} \epsilon_{p,\alpha} a_{p,\sigma}^{\dagger} a_{p,\sigma} + \sum_{p,\alpha,\sigma} \left( V_{p}^{\alpha,\sigma} d_{\alpha,\sigma}^{\dagger} a_{p,\sigma} + \text{h.c.} \right) - \mu \sum_{\alpha} n_{\alpha} \]

\[ + U \sum_{\alpha} n_{\alpha \uparrow} n_{\alpha \downarrow} + U' \sum_{\sigma} n_{1\sigma} n_{2\sigma} + (U' - J) \sum_{\sigma} n_{1\sigma} n_{2\sigma} \]

- impurity solver: continuous-time QMC
- hybridization expansion

Bethe lattice

Impurity model

Impurity solver

Inverse Fourier transform

Fourier transform

Self-consistency relation

Self-consistent Loop

DMFT

G(\tau)

G_{0}(\tau)

G_{0}(i\omega_{n})

G(i\omega_{n})

\Sigma(i\omega_{n})
ORBITAL-SELECTIVE MOTT TRANSITION FOR $J = U/4$
• Monotonic decrease as $U$ increases.
• First-order transition with hysteresis for both around $U_{c1} \approx 2.0$
• Long tail in $Z_2$ above $U_{c2}$
• Change in slope around $U_{c2} \approx 2.5$
Double Occupancy

- Monotonic decrease as $U$ increases.
- First-order transition with hysteresis for both around $U_{c_1} \approx 2.0$
- Change in the slope of $d_2$ around $U_{c_2} \approx 2.5$
- $d_1$ and $d_2$ are insensitive to temperature above $U_{c_1}$
- For $U_{c_1} < U < U_{c_2}$
  - $d_1$ far suppressed → narrow band is MI
  - $d_2$ is rather high and decreases gradually → wide band is not MI
Monotonic increase as $U$ increases.

First-order transition with hysteresis for both around $U_{c1} \approx 2.0$

Change in the slope for wide band around $U_{c2} \approx 2.5$

Both are insensitive to temperature above $U_{c1}$

For $U_{c1} < U < U_{c2}$

- narrow band: high moment $\rightarrow$ MI
- wide band: comparatively low and gradually increasing $\rightarrow$ not MI
Self-Energy for Wide Band

- For $U < U_{c1}$
  - $\text{Im} \Sigma_2(i\omega_n) \rightarrow 0$ linearly as $\omega_n \rightarrow 0$
  - Fermi liquid (FL)

- For $U > U_{c2}$
  - $\text{Im} \Sigma_2(i\omega_n) \rightarrow -\infty$ as $\omega_n \rightarrow 0$
  - Mott insulator (MI)

- For $U_{c1} < U < U_{c2}$
  - $\text{Im} \Sigma_2(i\omega_n) \rightarrow \text{finite as } \omega_n \rightarrow 0$
  - finite lifetime at Fermi level
  - non-Fermi liquid (NFL)
Determination of $U_{c2}$

- imaginary part of self-energy in wide band
- fitting low frequency part

$$\text{Im} \Sigma_2(i \omega_n) = \frac{c}{\omega_n - a} + b$$

- $a=0$: divergence to $-\infty$ at $\omega = 0$, MI
- $a<0$: convergence to finite negative value at $\omega = 0$, NFL
Phase Diagram

- $\text{DMFT+CT-QMC (□, ■, ◆): this work}$
- $\text{DMFT+ED (○, ---)}$
- $\text{DMFT+ED (T=0) (▲)}$
- $\text{DMFT+HF-QMC (▼)}$

- $\text{FL→NFL →MI}$
- $\text{FL-NFL: first-order transition with negative slope, conventional Mott transition}$
- $\text{NFL-MI: continuous transition with positive slope}$
EFFECTS OF \textit{HUND COUPLING} ON ORBITAL-SELECTIVE MOTT TRANSITION
Ising-type Hund coupling

Phase diagram in $U-U'$

Isotropic Hund coupling

- generally similar to that with isotropic Hund coupling
- $U_c$'s are slightly lower than isotropic case
- second transition change from continuous to first-order

Koga, Kawakami, Rice, Sigrist (2004)
VARIATION OF BANDWIDTH RATIO
Variation of bandwidth ratio

DMFT + ED

Gutzwiller

- When bandwidth ratio is far from unity, OSMP shows up even for $J=0$

de’Medici, Georges, Biermann (2005); Ferrero, Becca, Fabrizio, Capone (2005)
- A single first-order transition for small $W_2/W_1$
- Two separate transitions for large $W_2/W_1$
- $(W_2/W_1)_c = 1.5 \pm 0.1$
- OSMT appears above finite $(W_2/W_1)_c$
- slightly smaller NFL region for lower $T$

$de’Medici, Georges, Biermann$ (2005)
Summary

- We have investigated metal-insulator transitions in two-orbital system with Ising-type Hund coupling $J$.
- For large $J/U$, FL $\rightarrow$ NFL $\rightarrow$ MI as $U \uparrow$.
- Transition from FL to NFL is first-order.
- Transition from NFL to MI is
  - continuous for large $J/U$
  - first-order for small $J/U$
- We anticipate richer physics by the interplay of Hund coupling and bandwidth ratio.
Thank You!

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Ewha,
Where Change Begins