Spin-charge interplay in frustrated itinerant systems

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Partial list of recent activities...

Chirality-driven mass enhancement in the kagome Hubbard model
(M. Udagawa and YM, Phys. Rev. Lett. 104, 106409 (2010); Fig. 1 in Abstract)

Phase competition in the pyrochlore double-exchange model
(YM and N. Furukawa, Phys. Rev. Lett. 104, 106407 (2010); Fig. 2 in Abstract)

Partial Kondo screening in frustrated Kondo models [P15 K. Nakamikawa]
(K. Nakamikawa, Y. Yamaji, M. Udagawa, and YM, in preparation)

Non-coplanar order and anomalous Hall effect in the triangular-lattice
double-exchange model (Y. Akagi and YM, in preparation)

... and more!
[P16 H. Ishizuka; P17 J. Yoshitake; P22 M. Udagawa; P43 T. Misawa]
Chirality-driven mass enhancement in the kagome Hubbard model

Masafumi Udagawa and Yukitoshi Motome

Introduction
• heavy $d$ electrons: Kondo or correlation + frustration?

Model and Method

Results
• energy hierarchy among charge, spin, and chirality
• heavy-mass behavior due to the degeneracy associated with chirality

Summary
Heavy mass: Conventional Kondo physics

- heavy-fermion \( f \)-electron systems: hybrid of conduction electrons and localized moments

- large mass renormalization due to screening of localized spins by conduction electrons at Kondo temperature \( T \sim T_K \)
  - release of the spin entropy below \( T_K \)
  - specific-heat coefficient:
    \[ \gamma \sim \log 2/T_K \]

✓ localized moments = entropy reservoir
Heavy mass in transition metal oxides: Unconventional mass enhancement?

- several examples of heavy $d$ electrons
  - LiV$_2$O$_4$, (Y$_{1-x}$Sc$_x$)Mn$_2$, β-Mn, ...

- typical: spinel oxide LiV$_2$O$_4$
  - frustrated pyrochlore lattice of V
  - no clear sign of phase transition
  - characteristic temperature $T^* \sim 20$-30K: heavy mass behavior at lower $T$

- controversial on the mechanism of heavy mass behavior: no obvious entropy reservoir
  - Kondo? V. I. Anisimov et al., 1999
  - electron correlation + frustration? V. Eyert et al., 1999; H. Tsunetsugu, 2002; Y. Yamashita and K. Ueda, 2003, etc.
  - J. Kondo et al., 1999
  - C. Urano et al., 2000
Electron correlation + Frustration: A "folklore"

- Mott criticality (Brinkman-Rice, Gutzwiller, dynamical mean-field, ...)

- Critical mass enhancement in the paramagnetic solution
- Local spin fluctuation under strong correlation = entropy reservoir
- Usually, all of these are masked by the symmetry breaking

"Folklore": Frustration suppresses the symmetry breaking and rejuvenates the mass enhancement hidden in the ‘bare’ paramagnetic state.
Caveat...

- Even in the paramagnetic solution, the quasi-particle peak is fragile against spatial correlations.

- On the other hand, in the frustrated case...

3-site CDMFT for kagome Hubbard model

- What is the ‘true’ role of frustration?
Objectives

- to clarify the role of frustration in correlated metals
  - secondary role, just to suppress the spatial correlations?
    - If yes, mass enhancement occurs in the energy scale of spin $\sim J$
  - The answer is NO! (as we will see later)
    - mass enhancement occurs at much smaller energy scale
  - What determines the smaller new energy scale?
    - emergent degree of freedom under frustration + correlation

- to explore the new mechanism of quasi-particle mass enhancement
Model and Method

- Hubbard model on the kagome lattice at half filling

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

- a minimal model including both electron correlation and frustration (Y. Imai et al., 2003; N. Bulut et al., 2005; T. Ohashi et al., 2006; B. H. Bernhard et al., 2007)

- Mott transition at \( U_c \sim 8.3t \) (T. Ohashi et al., 2006)

- cluster extension of the dynamical mean-field theory

  - mapping to cluster impurity models (3 or 9 sites)

  - impurity problem solver: continuous-time quantum Monte Carlo method (E. Gull et al., 2008)
Result: Heavy-fermion behavior

![Schematic phase diagram at half filling](image)

- Kondo-like quasi-particle peak at low $T$ and large $U$

To identify the relevant degree of freedom, we calculate the density matrix as the probability distribution of quantum mechanical states:

$$\rho_\Psi = \frac{1}{Z} \text{Tr} |\Psi\rangle \langle \Psi| e^{-\beta \mathcal{H}}$$
Result: Spin chirality degree of freedom

$U/t = 6.0$

$\rho_{\psi}$

$T_{\text{chiral}}$

$T_{\text{spin}}$

$T_{\text{charge}}$

$\omega = \exp(i \frac{2}{3} \pi)$

3-site chiral state (4 fold)

Spin polarized (4 fold)

Doubly-occupied state

$\downarrow$ double occupancy (charge)

$\downarrow$ chirality

$\downarrow$ spin

$\downarrow$ spin

$\downarrow$ double occupancy (charge)

$\downarrow$ chirality

$\downarrow$ spin
Result: Crossover temperatures

- Energy hierarchy among charge, spin, and chirality:
  \[ T_{\text{charge}} \sim U - W^* > T_{\text{spin}} \sim \alpha J > T_{\text{chiral}} \]

- Quasi-particle peak in DOS develops below \( T_{\text{chiral}} \)

- Chirality-driven heavy fermion state
Result: Specific heat and entropy

- Charge-spin-chirality separation
  - Broad hump in $C_v$ at $T \sim T_{\text{charge}}$
  - Entropy $\sim \log 8$ at $T \sim T_{\text{spin}}$
  - Sharp peak in $C_v$ and entropy $\sim \log 4$ at $T \sim T_{\text{chirality}}$

- Chirality-driven mass enhancement
  - Specific-heat coefficient:
    \[ \gamma \sim \frac{1}{3} \log 4/T_{\text{chiral}} \]

![Diagram showing specific heat and entropy curves with annotations](image)
Discussion

- “Folklore” scenario
  Frustration just suppresses magnetic LRO
  ➡ heavy mass due to spin entropy

- Present mechanism
  Frustration brings about an emergent degree of freedom, chirality
  ➡ heavy mass due to spin chirality

- heavy-mass behavior:
  crossover from highly-symmetric local state to renormalized Fermi liquid

emergent composite objects with high local symmetry
chirality, multipole, etc.
Summary


cellular DMFT study of correlated metallic region in the kagome Hubbard model
✓ continuous-time QMC
✓ cluster-size dependence

Emergent degree of freedom, chirality, plays a decisive role at low $T$.
✓ energy hierarchy
✓ sharp peak in the specific heat
✓ mass enhancement

Our results uncover an intensive role of geometrical frustration in correlated metal (not secondary just to suppress LRO).