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

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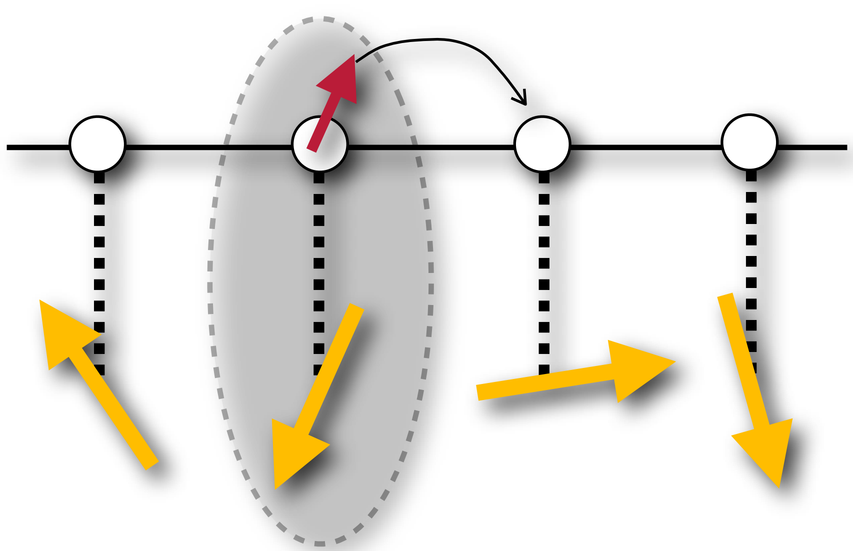
- Introduction
  - heavy *d* electrons: Kondo or correlation + frustration?
- Model and Method
- Results
  - energy hierarchy among charge, spin, and chirality
  - heavy-mass behavior due to the degeneracy associated with chirality
- Summary

Heavy mass: Conventional Kondo physics

- heavy-fermion *f*-electron systems:

  hybrid of <u>conduction electrons</u> and <u>localized moments</u>



- large mass renormalization due to

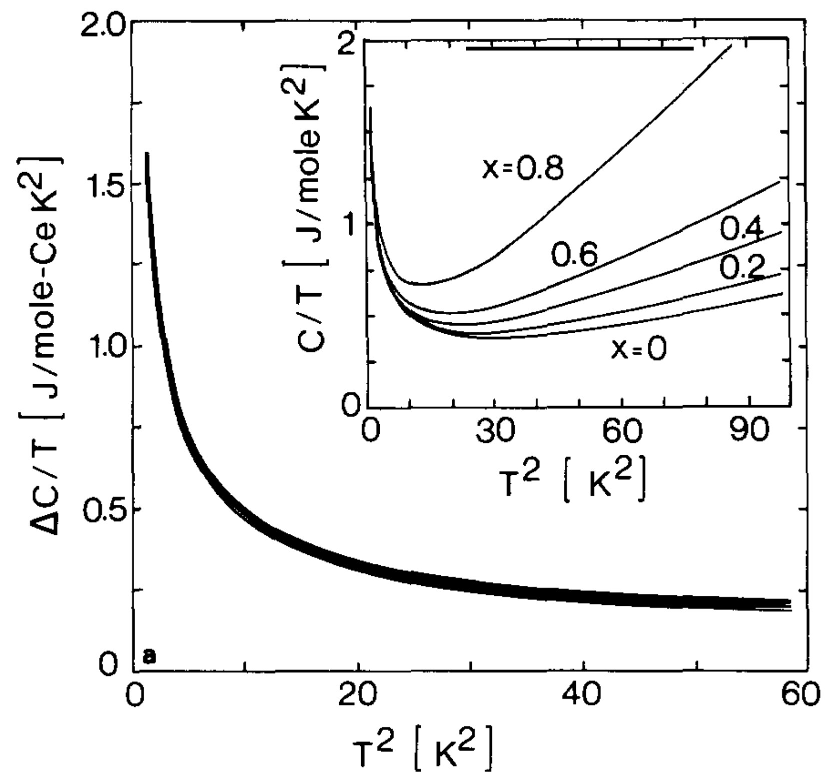
  screening of localized spins by conduction electrons at Kondo temperature $T \sim T_K$

  ➡ release of the spin entropy below T_K

  ➡ specific-heat coefficient:

  $$\gamma \sim \log 2/T_K$$

✓ localized moments = entropy reservoir

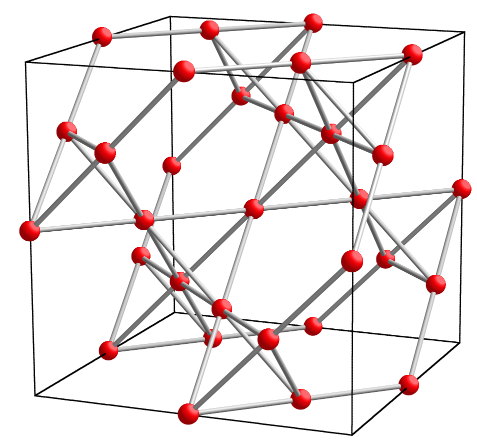


P. Schlottmann, 1989

Heavy mass in transition metal oxides: Unconventional mass enhancement?

- several examples of heavy *d* electrons

  LiV_2O_4, $(Y_{1-x}Sc_x)Mn_2$, β-Mn, ...



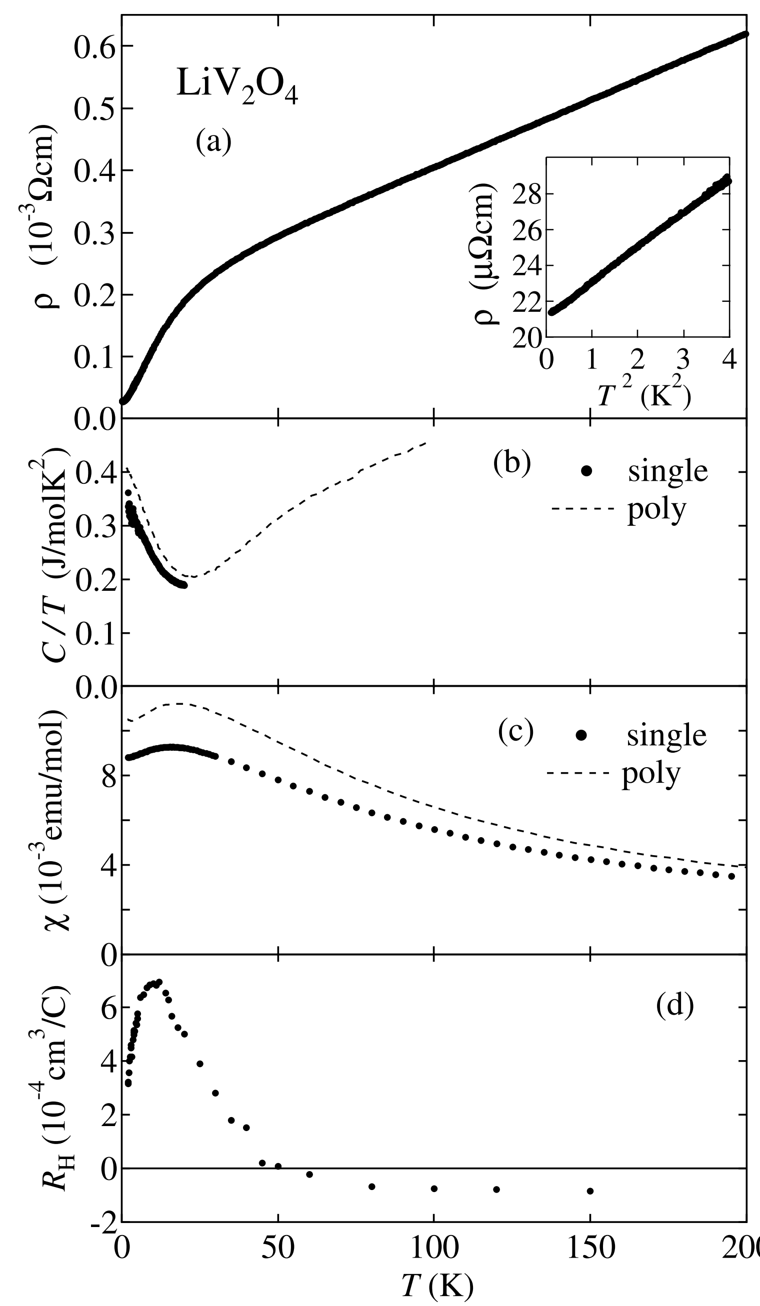
- typical: spinel oxide LiV_2O_4
  - frustrated pyrochlore lattice of V
  - no clear sign of phase transition
  - characteristic temperature T^*~20-30K: heavy mass behavior at lower T

- controversial on the mechanism of heavy mass behavior: no obvious entropy reservoir

  Kondo ? V. I. Anisimov *et al.*, 1999

  electron correlation + frustration ?

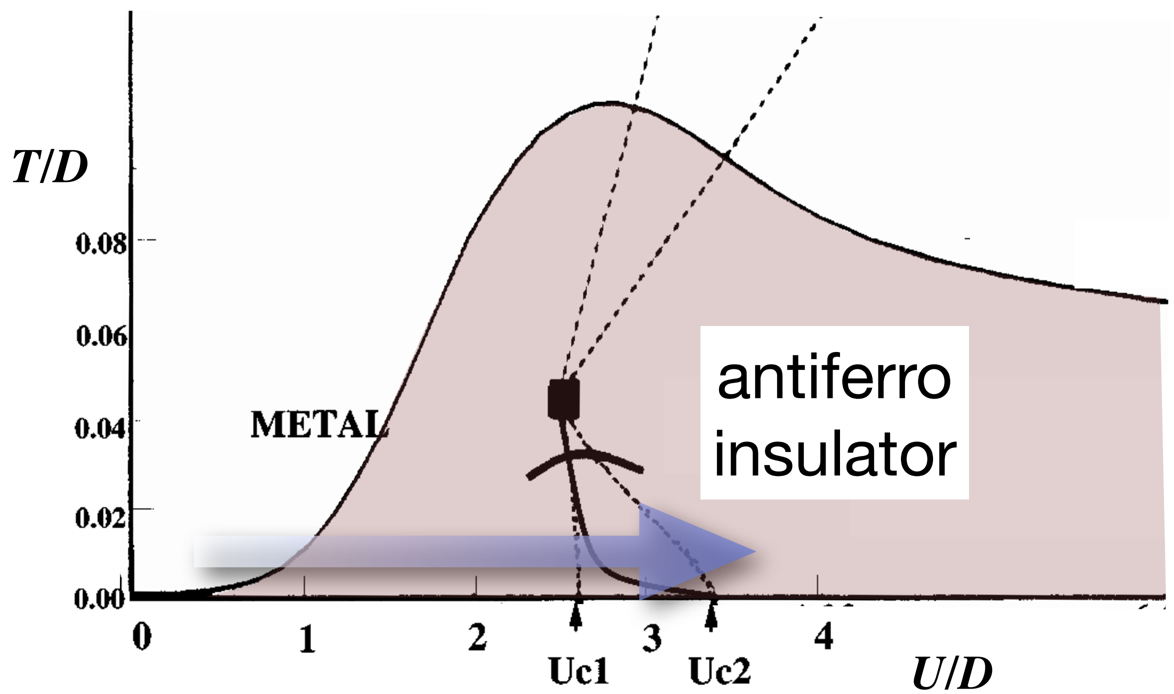
  V. Eyert *et al.*, 1999; H. Tsunetsugu, 2002; Y. Yamashita and K. Ueda, 2003, etc.



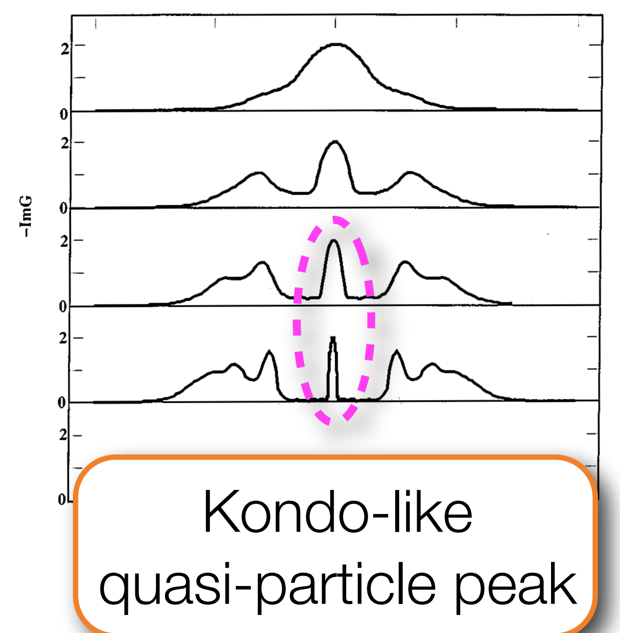
J. Kondo *et al.*, 1999
C. Urano *et al.*, 2000

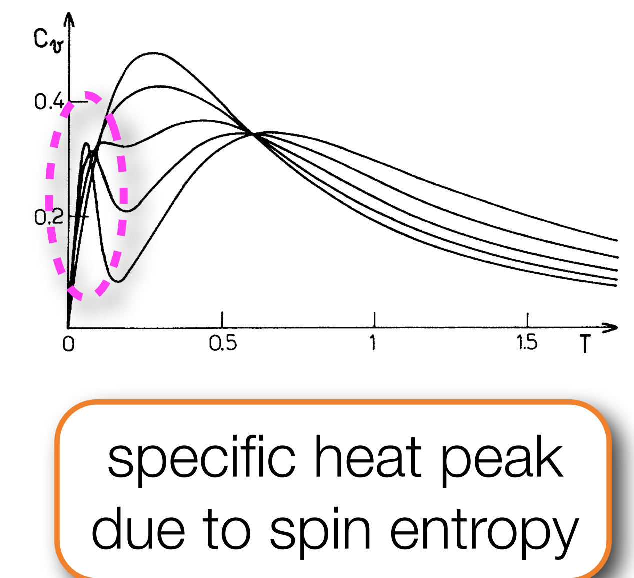
Electron correlation + Frustration: A “folklore”

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



A. Georges *et al.*, 1993, 1996
M. J. Rozenberg *et al.*, 1994





✓ critical mass enhancement in the paramagnetic solution

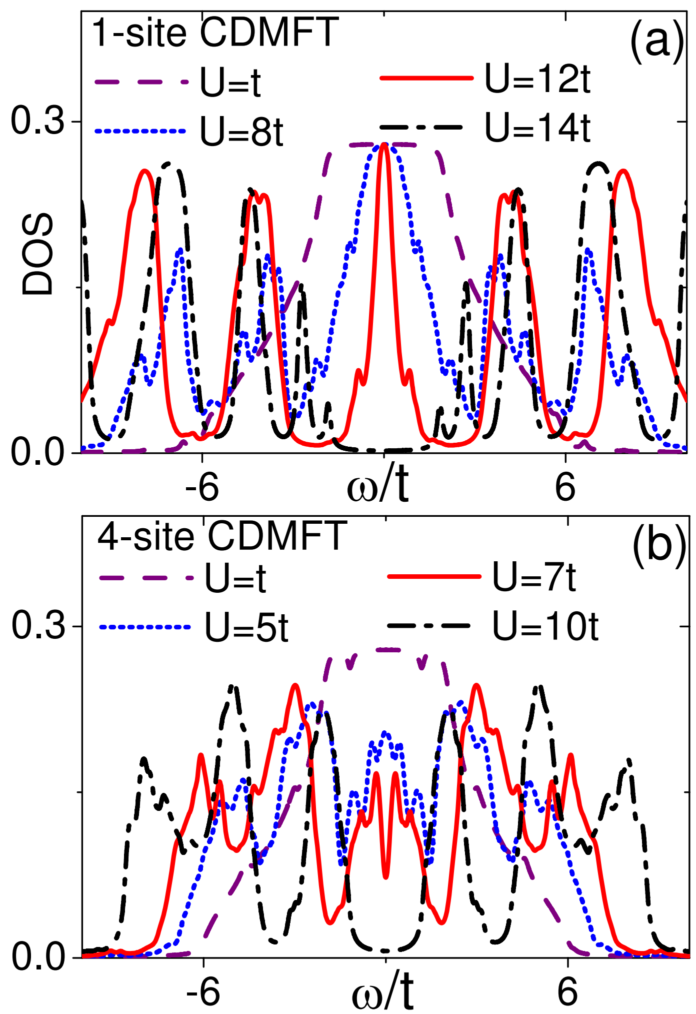
✓ local spin fluctuation under strong correlation = entropy reservoir

✓ 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...

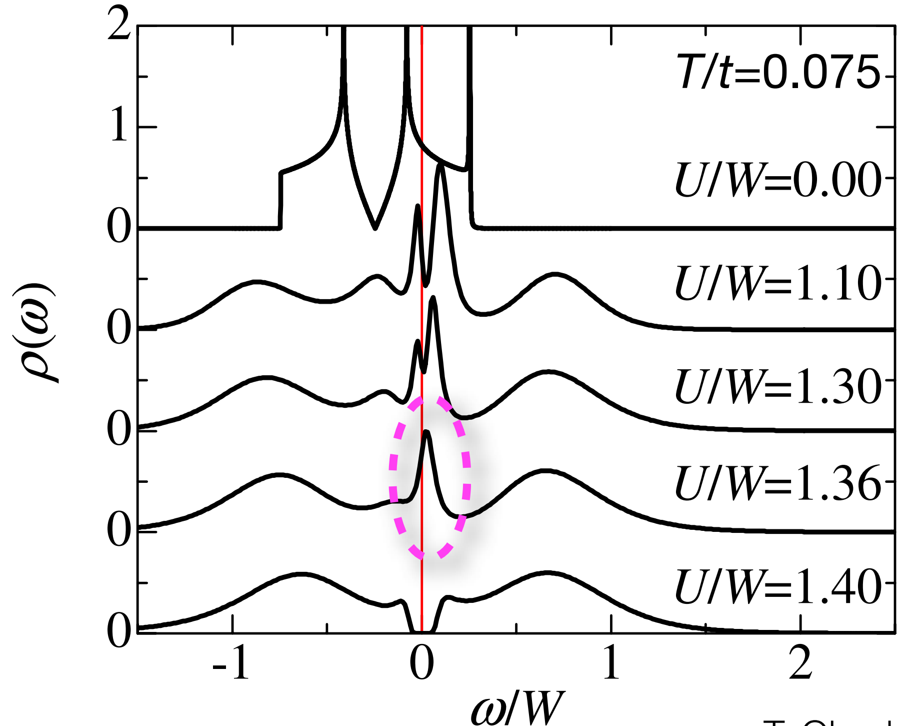
- Even in the paramagnetic solution, the quasi-particle peak is fragile against spatial correlations.



Y. Z. Zhang and M. Imada, 2007

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

3-site CDMFT for kagome Hubbard model



T. Ohashi *et al.*, 2006

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 ~ 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

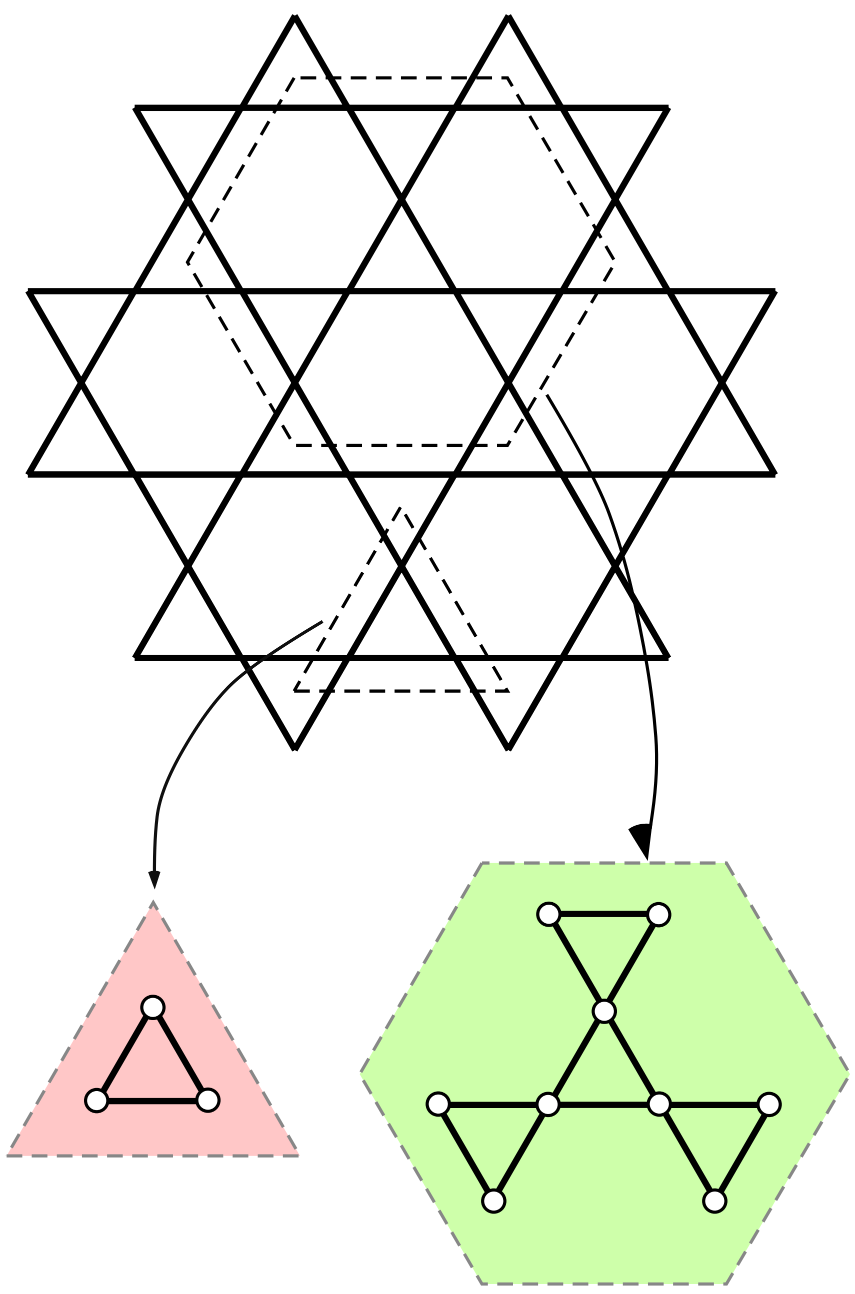
Model and Method

- Hubbard model on the kagome lattice at half filling

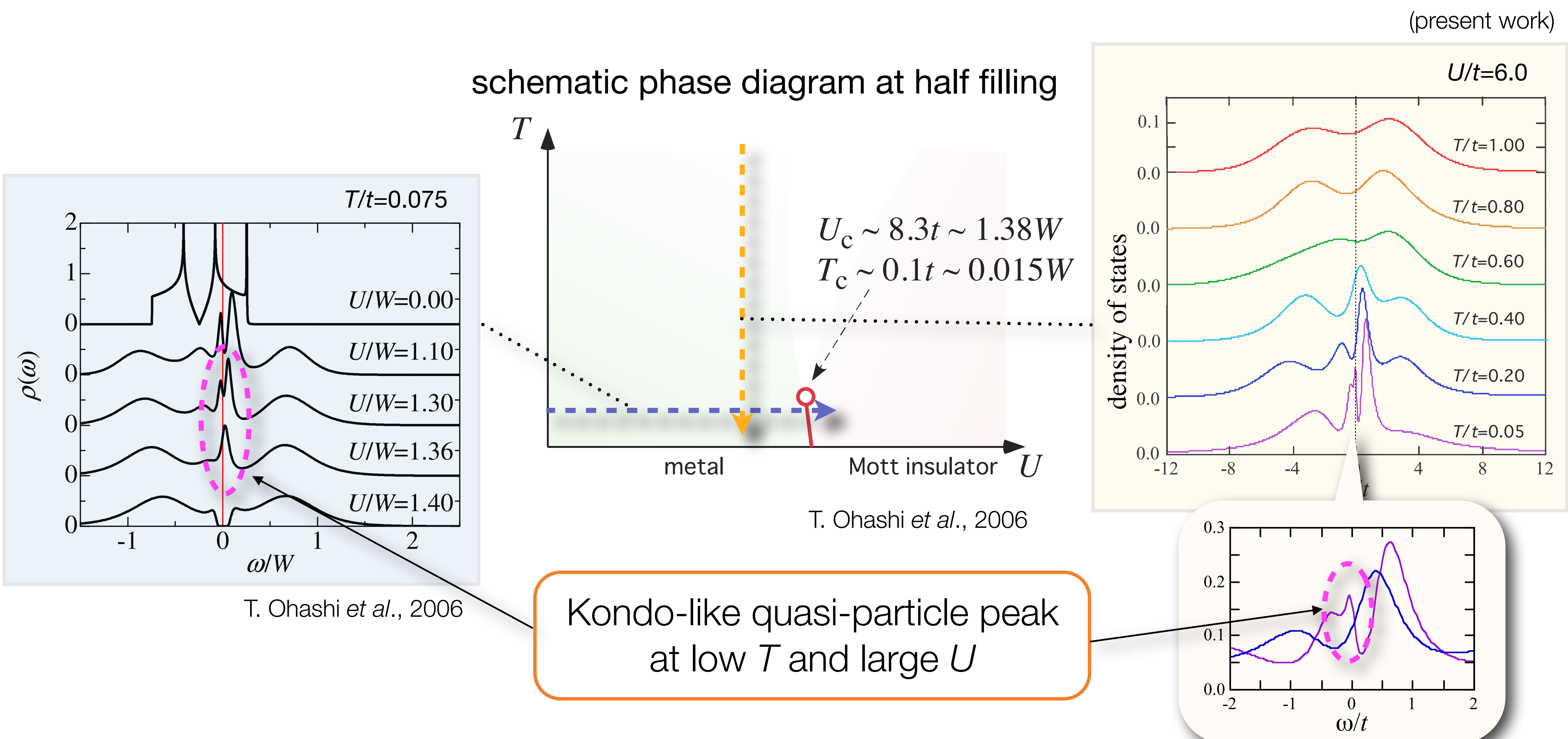
$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + \mathrm{h.c.}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

  - 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~$8.3t$ (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

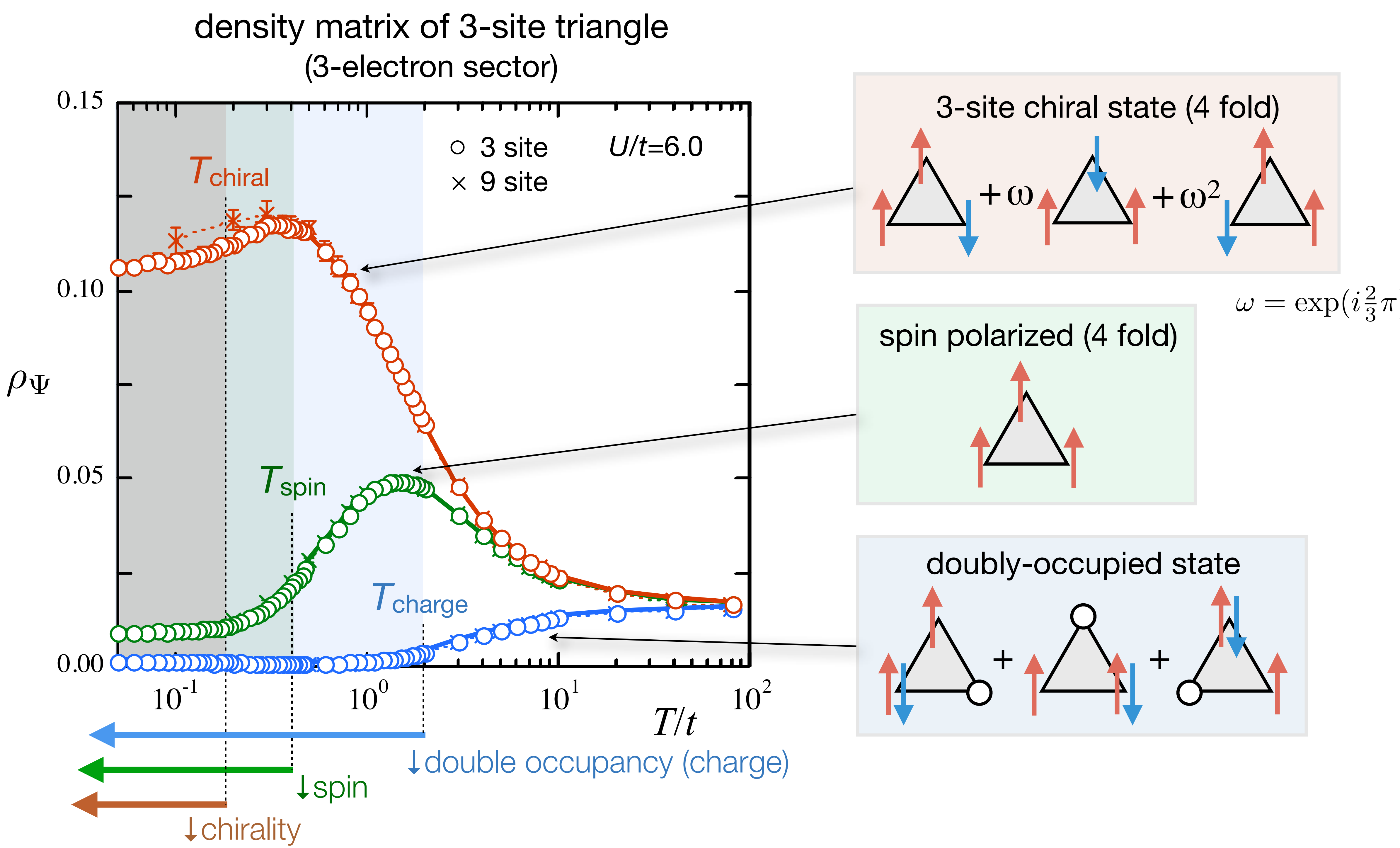


- To identify the relevant degree of freedom, we calculate

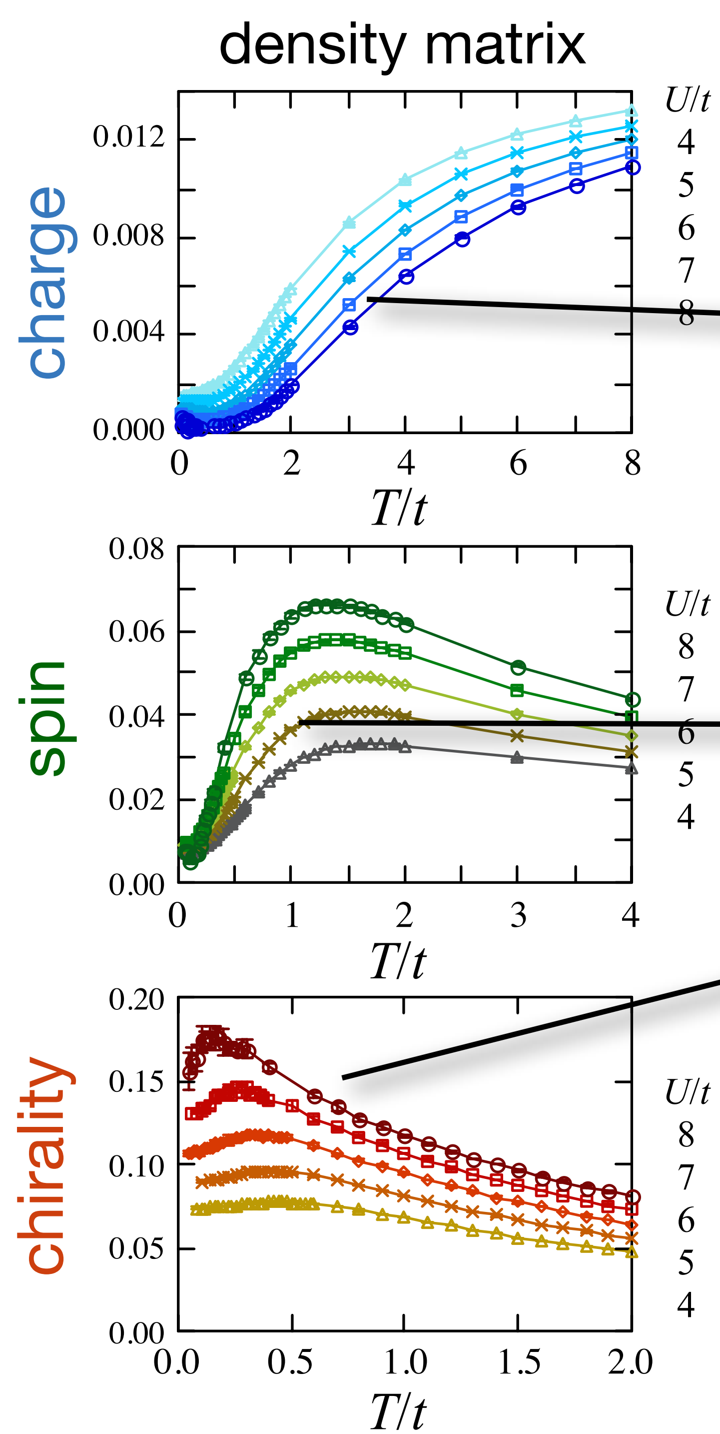
  density matrix = prob. distribution of quantum mechanical states

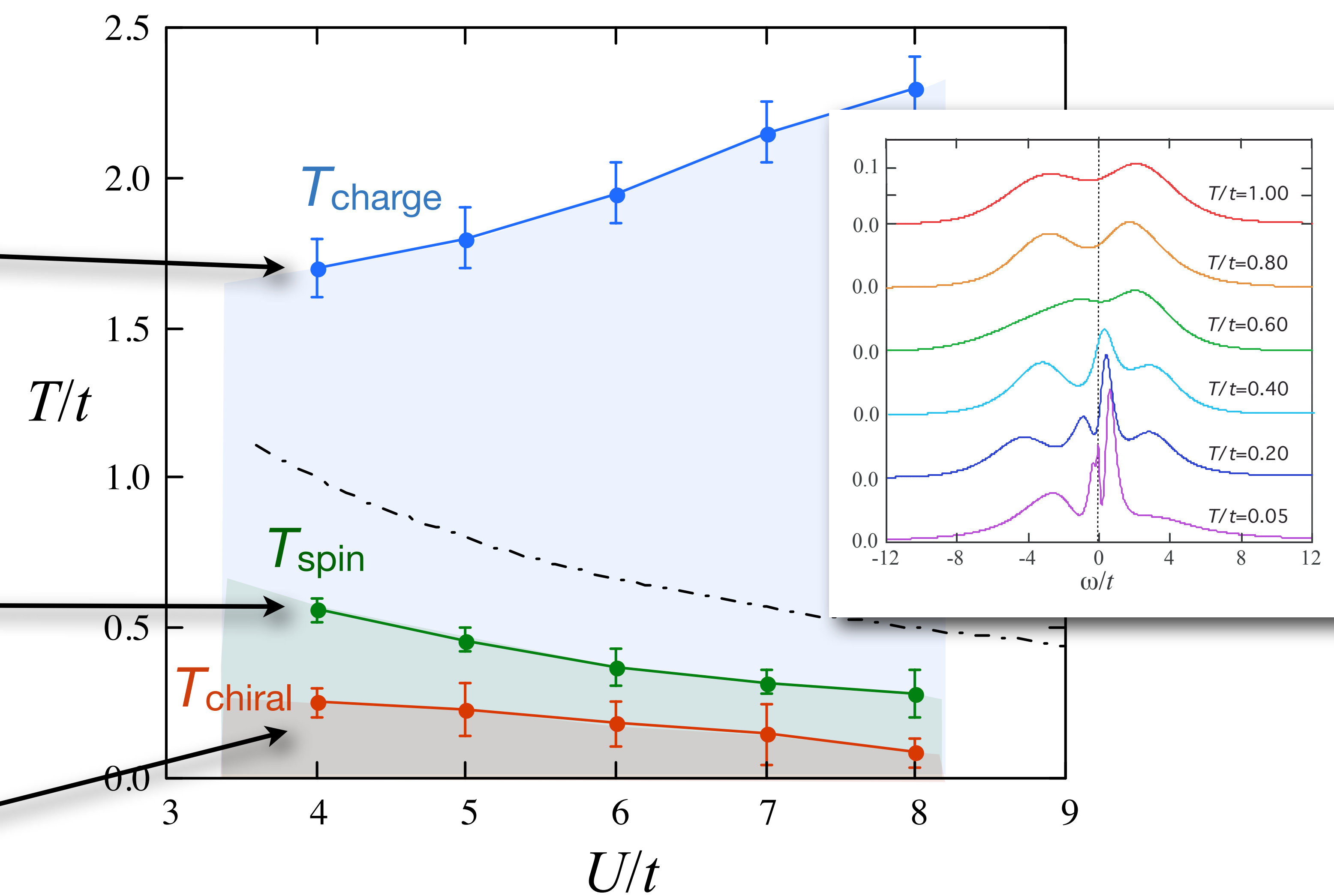
$$\rho_\Psi = \frac{1}{Z}\mathrm{Tr}|\Psi\rangle\langle\Psi|e^{-\beta\mathcal{H}}$$

Result: Spin chirality degree of freedom



Result: Crossover temperatures





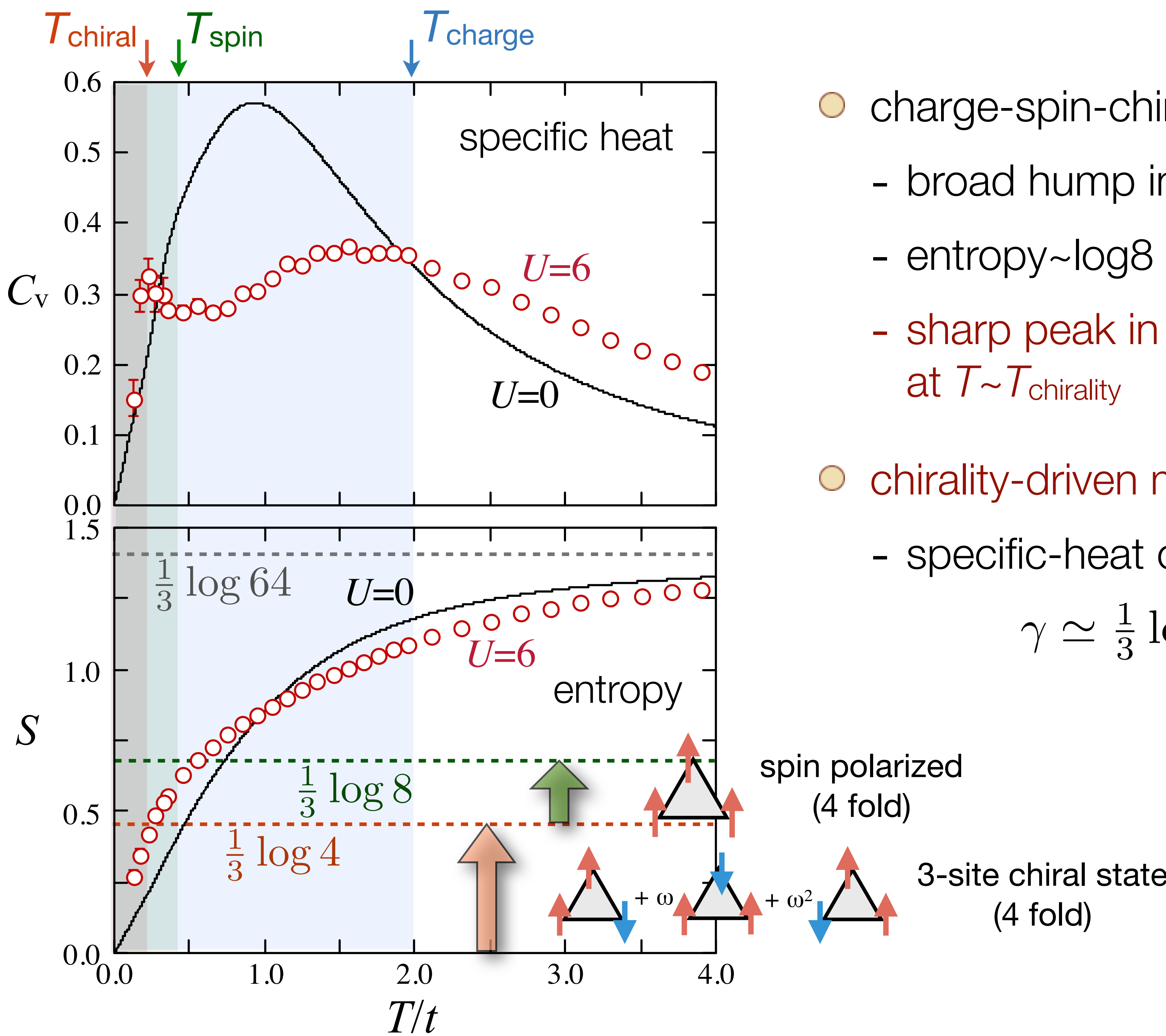
- energy hierarchy among charge, spin, and chirality

$$T_{\text{charge}} \sim U - W^* > T_{\text{spin}} \sim \alpha J > T_{\text{chiral}}$$

- quasi-particle peak in DOS develops below T_{chiral}

➡ chirality-driven heavy fermion state

Result: Specific heat and entropy



- charge-spin-chirality separation
  - broad hump in C_v at $T \sim T_{charge}$
  - entropy~log8 at $T \sim T_{spin}$
  - sharp peak in C_v and entropy~log4 at $T \sim T_{chirality}$
- chirality-driven mass enhancement
  - specific-heat coefficient:

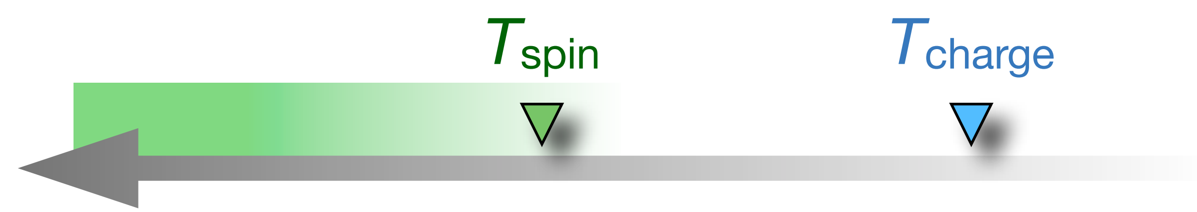
$$\gamma \simeq \frac{1}{3}\log 4/T_{\mathrm{chiral}}$$

Discussion

- "Folklore" scenario

  Frustration just suppresses magnetic LRO

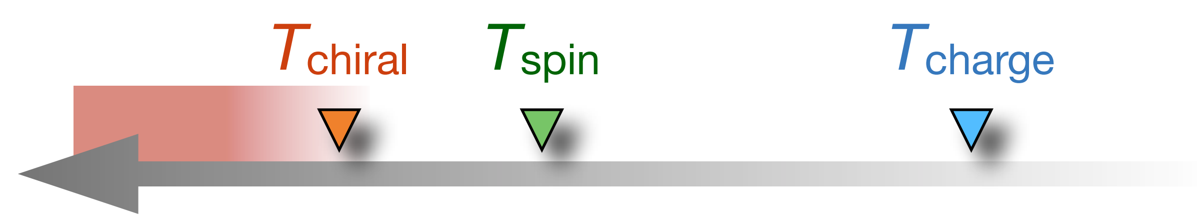
  ➡ heavy mass due to spin entropy



- Present mechanism

  Frustration brings about an emergent degree of freedom, chirality

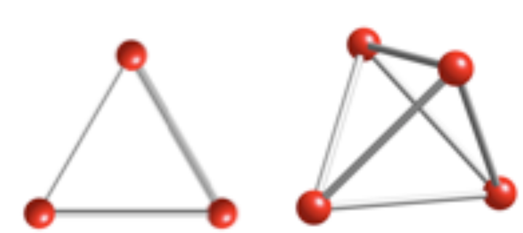
  ➡ heavy mass due to spin chirality



- heavy-mass behavior:

  crossover from highly-symmetric local state to renormalized Fermi liquid

emergent composite objects
with high local symmetry



chirality, multipole, etc.

Summary

M. Udagawa and YM, Phys. Rev. Lett. **102**, 106409 (2010)

- 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).