Momentum differentiation enhanced by Hund's coupling: A multi-orbital cluster DMFT study

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Outline

- Effect of local *U* and *J* in correlated electron systems

	Onsite correlation	Intersite correlation
U	DMFT	Cluster DMFT
J	Multi-orbital DMFT	multi-orbital cluster DMFT

- Efficient CTQMC algorithm for multi-orbital DCA

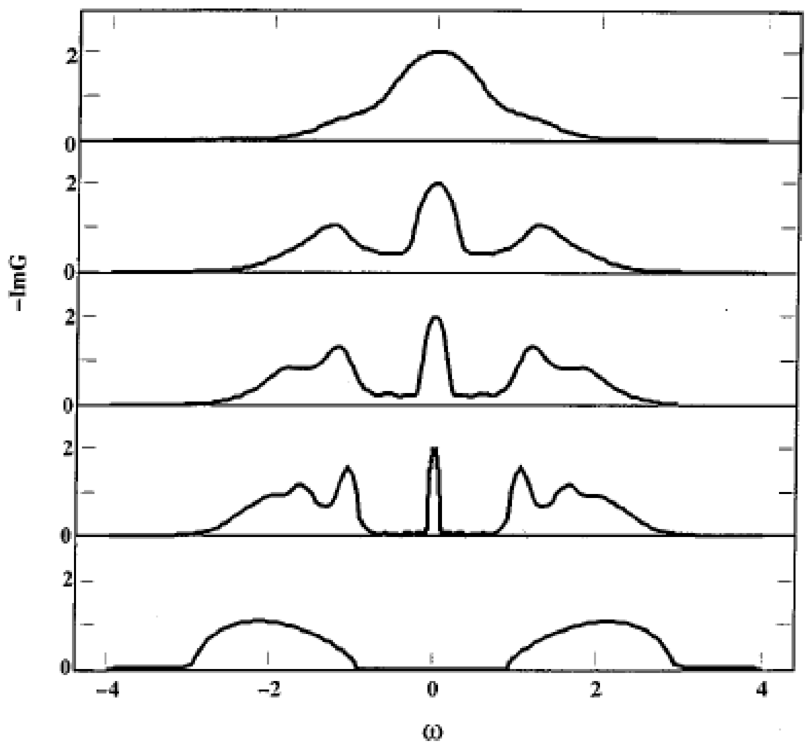
Y. Nomura, S. Sakai, and RA, Phys. Rev. B **89**, 195146 (2014)

- How local *J* enhances intersite correlations

DMFT study on the on-site correlation due to *U*

	Onsite correlation	Intersite correlation
U	DMFT	Cluster DMFT
J	Multi-orbital DMFT	multi-orbital cluster DMFT

Mott-Hubbard transition



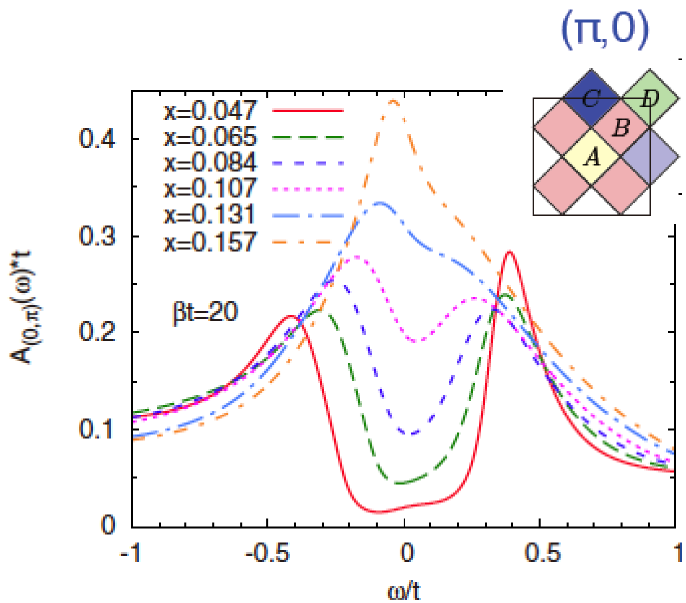
A. Georges et al., RMP 68 13 (1996)

Cluster DMFT study on the intersite correlation due to *U*

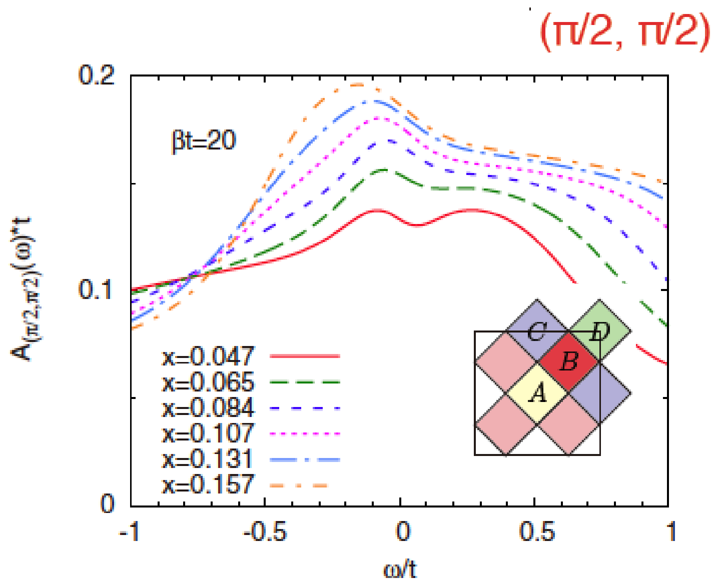
	Onsite correlation	Intersite correlation
U	DMFT	Cluster DMFT
J	Multi-orbital DMFT	multi-orbital cluster DMFT

Analytically continued spectral function A(ω): U = 7t, t'/t=0.15, βt=20

for the antinodal sector.



for the nodal sector.

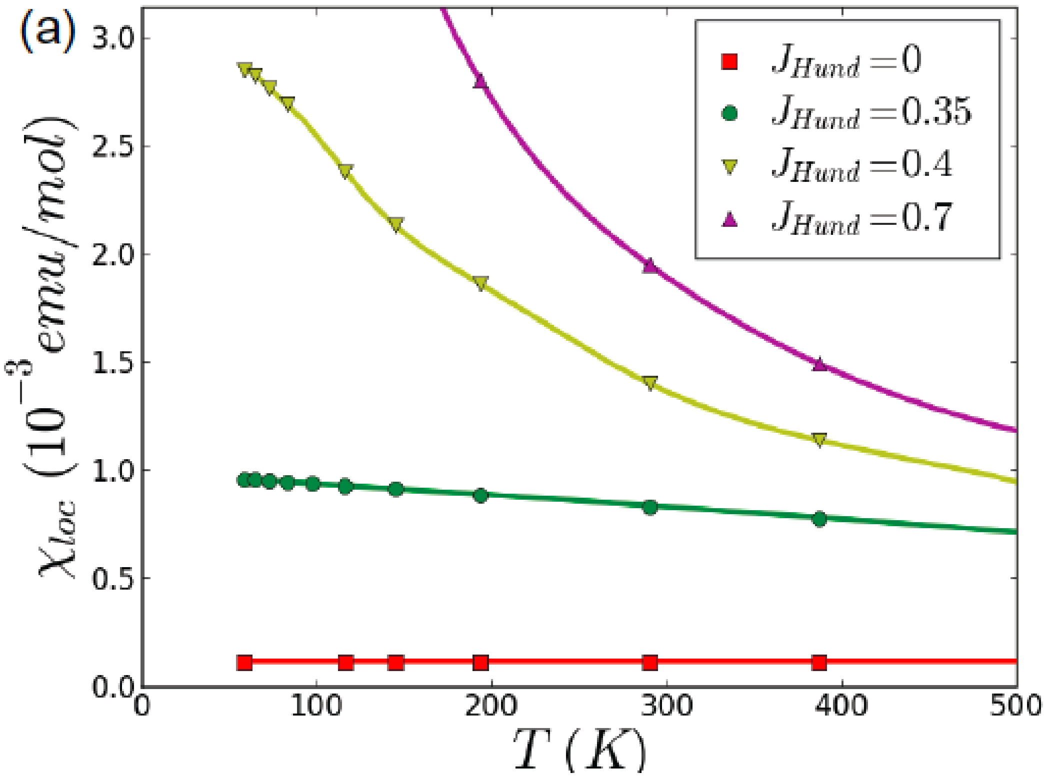


N. Lin, E. Gull, and A.J. Millis, Phys. Rev. B 82, 045104 (2010)

DMFT study on the on-site correlation due to *J*

	Onsite correlation	Intersite correlation
U	DMFT	Cluster DMFT
J	Multi-orbital DMFT	multi-orbital cluster DMFT

"Hund's metal" (Strong correlation induced by *J*)

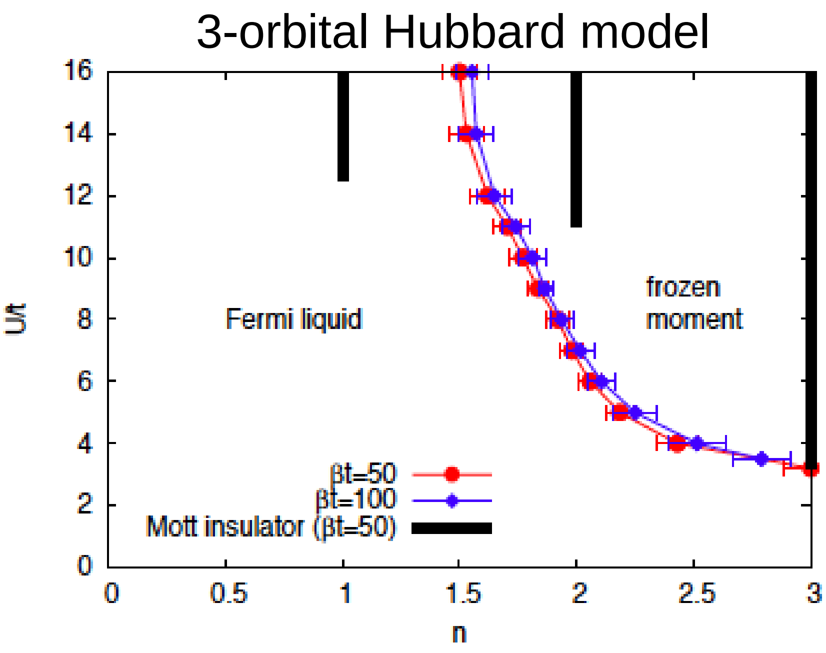


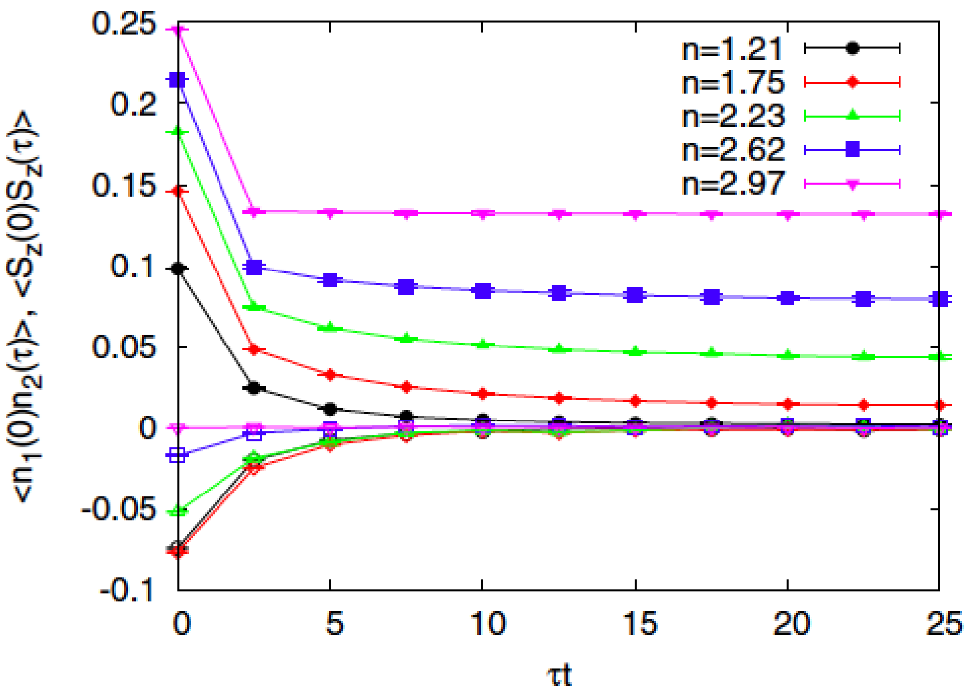
Haule and Kotliar, New J. Phys. 11, 025021 (2009)

DMFT study on the on-site correlation due to *J*

	Onsite correlation	Intersite correlation
U	DMFT	Cluster DMFT
J	Multi-orbital DMFT	multi-orbital cluster DMFT

"spin-freezing" transition





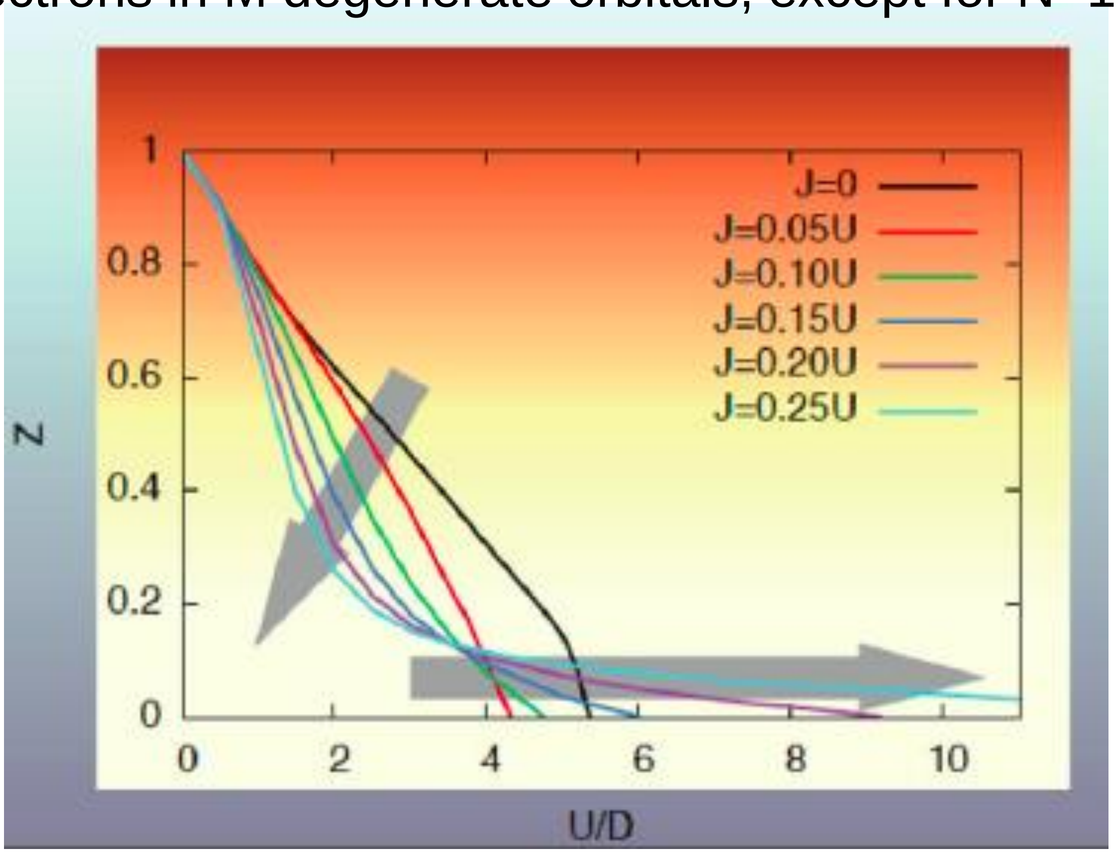
Werner *et al.*, PRL 101, 166405 (2008)

DMFT study on the on-site correlation due to *J*

	Onsite correlation	Intersite correlation
U	DMFT	Cluster DMFT
J	Multi-orbital DMFT	multi-orbital cluster DMFT

"Janus-Faced" effect

for N electrons in M degenerate orbitals, except for N=1 or N=M



Medici *et al*., PRL 107, 256401 (2011)

Purpose of the present study

	Onsite correlation	Intersite correlation
U	DMFT	Cluster DMFT
J	Multi-orbital DMFT	multi-orbital cluster DMFT

First multi-orbital cluster DMFT calculation using CTQMC with including spin-flip and pair-hopping terms

Y. Nomura, S. Sakai, and RA, Phys. Rev. B **89**, 195146 (2014)

CTQMC: weak coupling expansion

A. N. Rubtsov et al., Phys. Rev. B 72, 035122 (2005)
F. F. Assaad and T. C. Lang, Phys. Rev. B 76, 035116 (2007)
E. Gull et al., Rev. Mod. Phys. 83 349 (2011)

Diagrammatic expansion of the partition function of an impurity model
→ sampling of the series stochastically up to infinite order

$$Z = \mathrm{Tr}\left[e^{-\beta H_0} T_\tau \exp\left(- \int_0^\beta d\tau\, H_1(\tau) \right) \right]$$

Non-interacting part ($e^{-\beta H_0}$) Interacting part ($H_1(\tau)$)

$$\frac{Z}{Z_0} = \sum_{k=0}^{\infty} \int_k d\tau\, P(q_k)\,, \quad P(q_k) = (-1)^k \langle T_\tau H_1(\tau_k) \cdots H_1(\tau_2) H_1(\tau_1) \rangle_0$$

$$\langle A \rangle_0 \equiv \frac{1}{Z_0} \mathrm{Tr}\left[e^{-\beta H_0} A \right]$$

We used the sub-matrix update method originally developed for the Hirsch-Fye algorithm (Nukula et al., PRB09) and the Continuous-Time Auxiliary Field algorithm (Gull et al., PRB11)

CTQMC: weak coupling expansion

E. Gorelov et al., Phys. Rev. B 80, 155132 (2009)

Action for the multi-orbital model

$$S_0 = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_{ij,\sigma} [\tilde{\mathcal{G}}_{0\sigma}^{-1}(\tau-\tau')]_{ij} c_{i\sigma}^\dagger(\tau) c_{j\sigma}(\tau')$$

$$\begin{aligned} S_{\rm int} = \int_0^\beta d\tau \sum_{s=\pm 1} \Bigg[& \sum_i \frac{U}{2} [n_{i\uparrow}(\tau) - \underline{\alpha_{1\uparrow}}(s)][n_{i\downarrow}(\tau) - \underline{\alpha_{1\downarrow}}(s)] + \sum_{i<j,\sigma} \frac{U'}{2} [n_{i\sigma}(\tau) - \underline{\alpha_{1\sigma}}(s)][n_{j\bar{\sigma}}(\tau) - \underline{\alpha_{1\bar{\sigma}}}(s)] \\ & + \sum_{i<j,\sigma} \frac{U' - J_{\rm H}}{2} [n_{i\sigma}(\tau) - \underline{\alpha_{1\sigma}}(s)][n_{j\sigma}(\tau) - \underline{\alpha_{1\sigma}}(s)] + \sum_{i\neq j} \frac{J_{\rm H}}{2} [c_{i\uparrow}^\dagger(\tau) c_{j\uparrow}(\tau) - \underline{\alpha_{2\uparrow}}(s)][c_{j\downarrow}^\dagger(\tau) c_{i\downarrow}(\tau) - \underline{\alpha_{2\downarrow}}(s)] \\ & + \sum_{i\neq j} \frac{J_{\rm H}}{2} [c_{i\uparrow}^\dagger(\tau) c_{j\uparrow}(\tau) - \underline{\alpha_{2\uparrow}}(s)][c_{i\downarrow}^\dagger(\tau) c_{j\downarrow}(\tau) - \underline{\alpha_{2\downarrow}}(s)] \Bigg]. \end{aligned}$$

We introduce additional parameters

$$\begin{cases} \alpha_{1\uparrow}(s) = 1/2 + s\delta_1 \\ \alpha_{1\downarrow}(s) = 1/2 - s\delta_1 \end{cases} \qquad \delta_1 = 1/2 + 0^+$$

→ To reduce sign problem

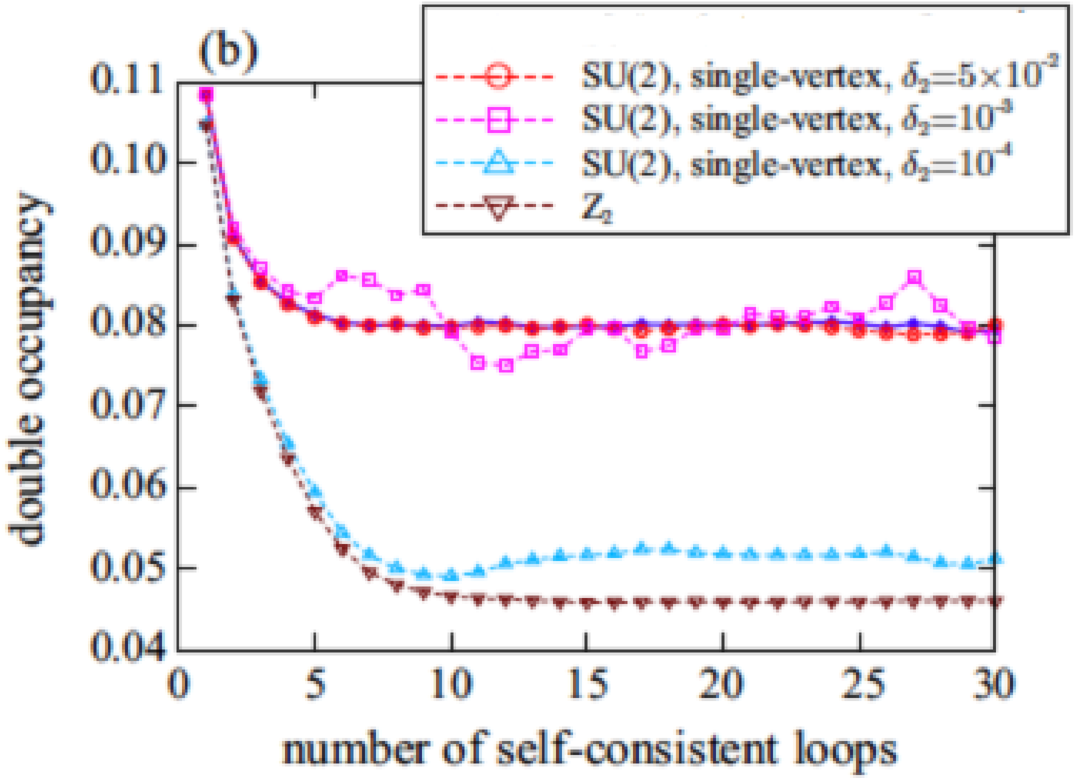
$$\begin{cases} \alpha_{2\uparrow}(s) = +s\delta_2 \\ \alpha_{2\downarrow}(s) = -s\delta_2 \end{cases}$$

δ_2: small positive number

→ To ensure the ergodicity (if $[G_0]_{ij} = 0$)
large δ_2 → sign problem

Two-orbital Hubbard model

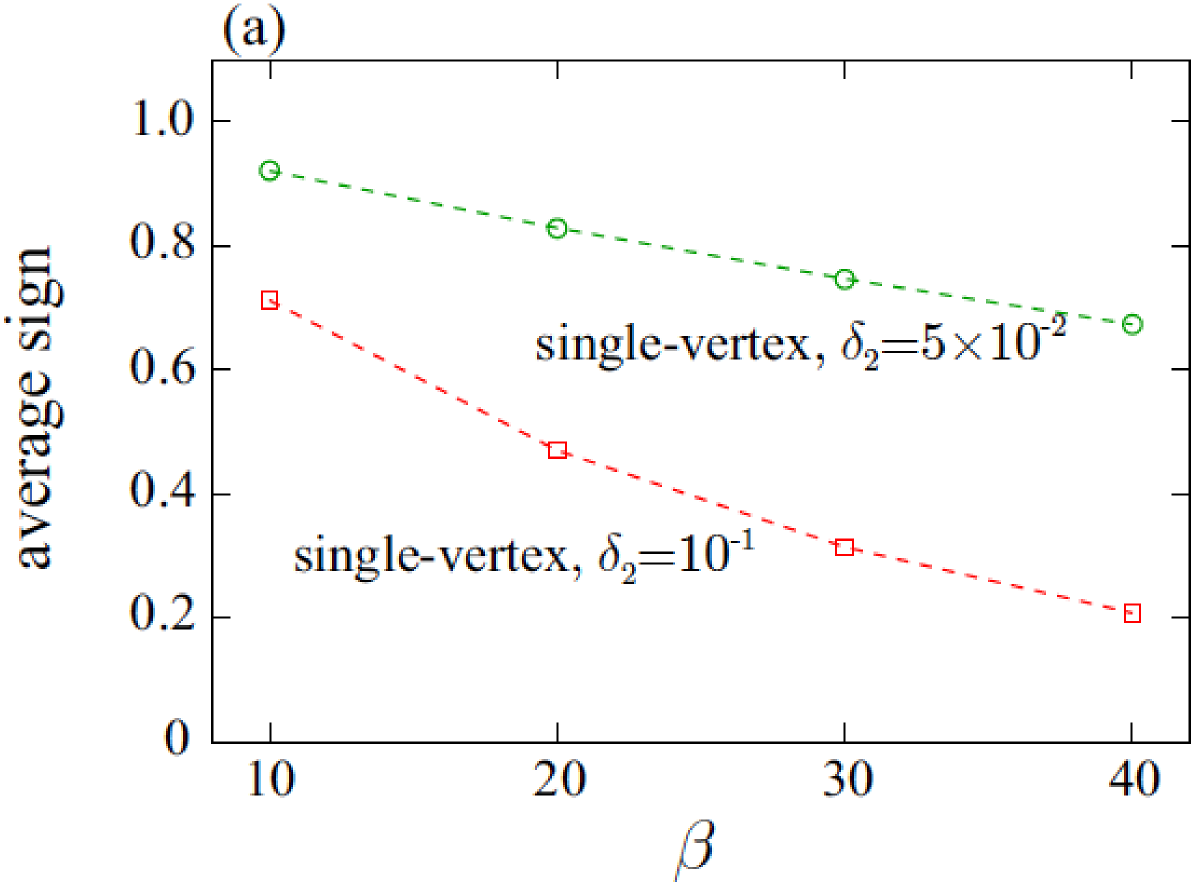
half-filling, t=1
T=0.05, U=6, J=1.5



We need sufficiently large δ_2 to guarantee the ergodicity

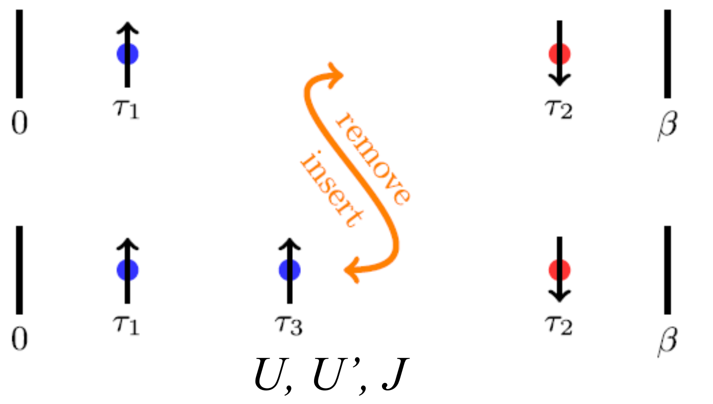
Two-orbital Hubbard model

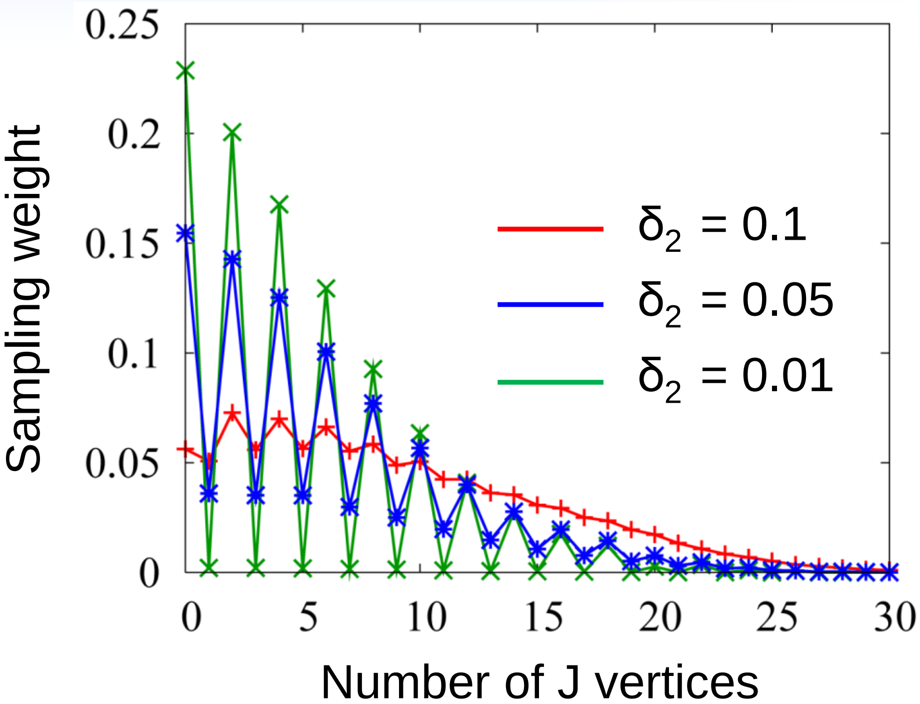
half-filling, t=1
T=0.05, U=6, J=1.5



Large δ_2 → Severer sign problem

Efficient sampling for spin-flip & pair-hopping terms





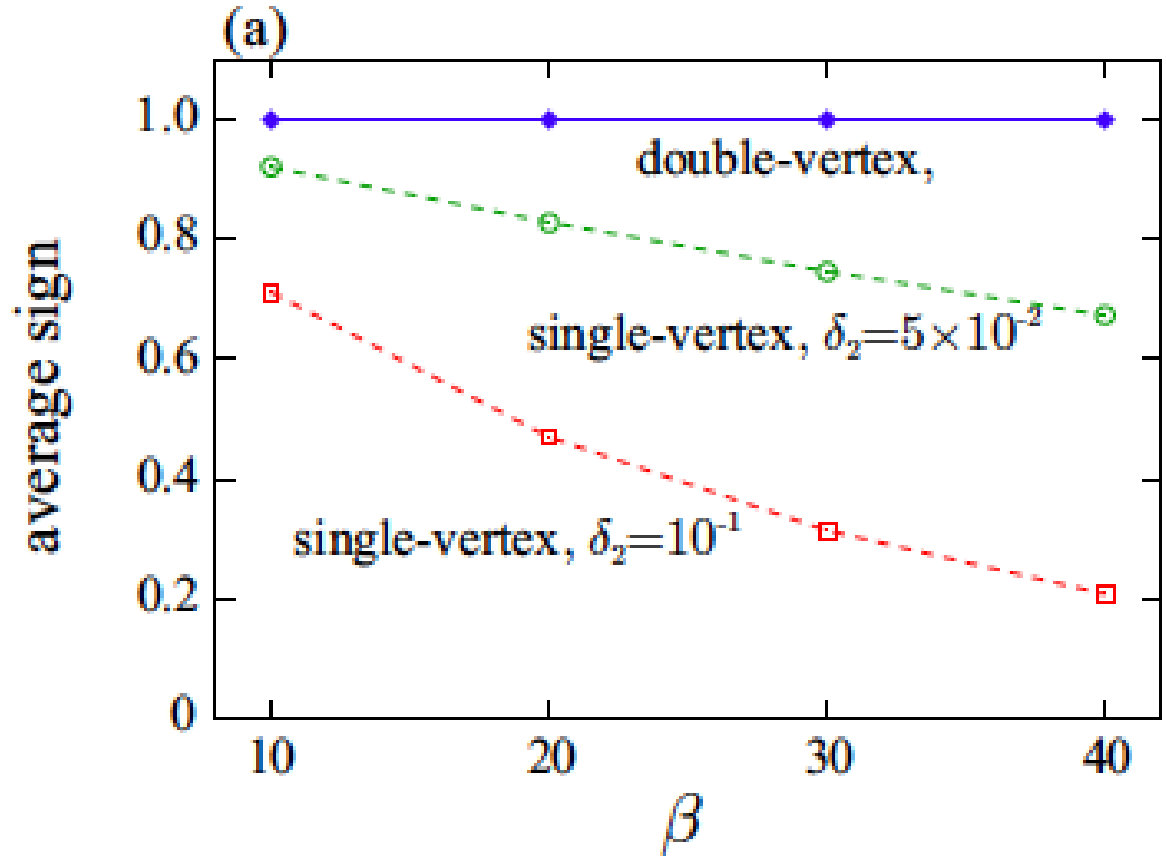
Weight of configurations with odd number of J vertices is zero for $\delta_2 \to 0$.

The odd-order terms are artificial but necessary, since the number of non-density J vertices can not be changed without passing through the odd-order terms.

➡ We only need to insert/remove two J vertices simultaneously (double vertex update)
We do not need to introduce δ_2

Double vertex update

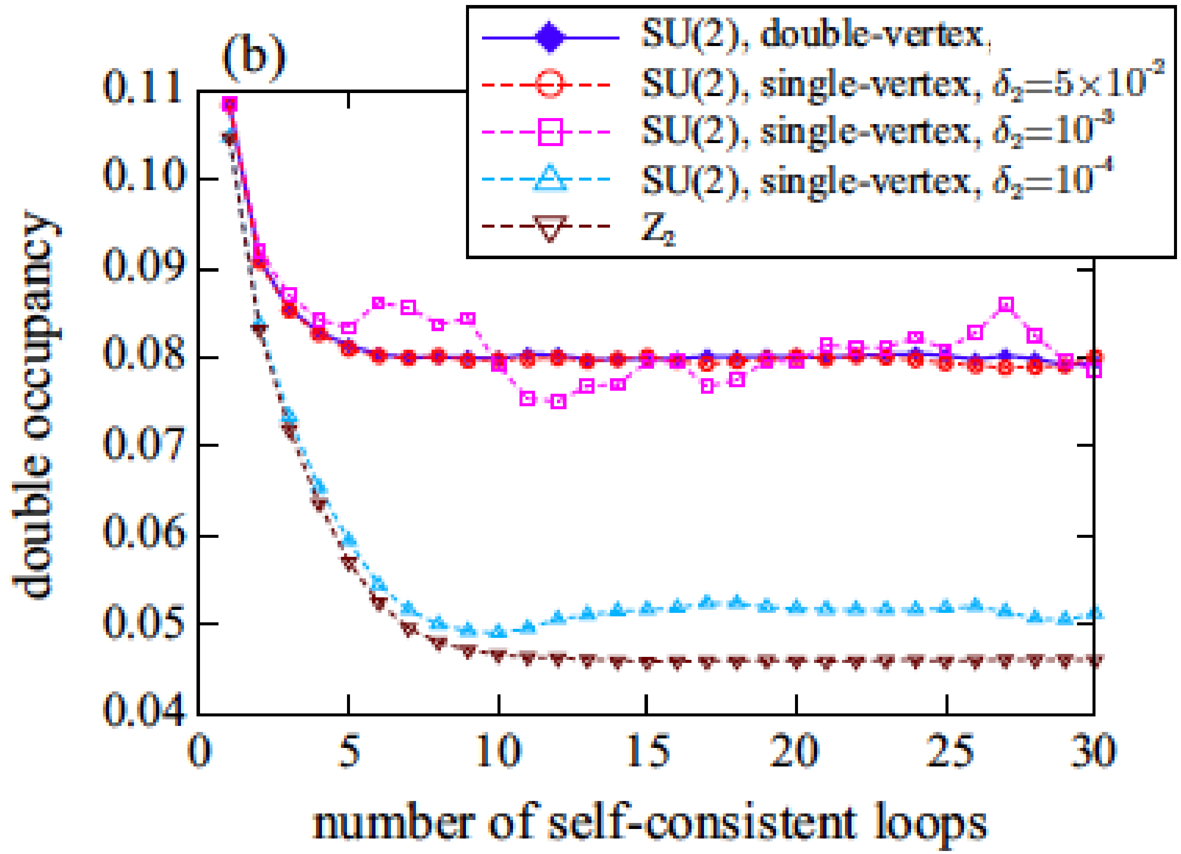
half-filling, t=1
T=0.05, U=6, J=1.5



No sign problem

Double vertex update

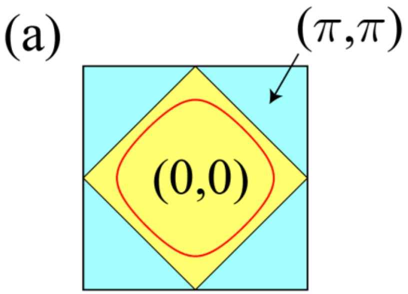
half-filling, t=1
T=0.05, U=6, J=1.5

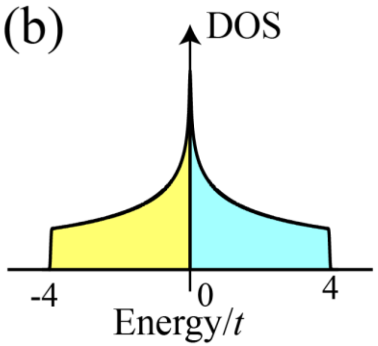


Three-orbital Hubbard model

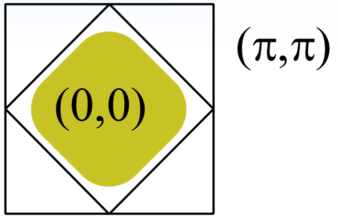
Calculation conditions:

- 2D square lattice, t = 1, t'=0
- Three-orbital Hubbard model with 2 electrons/site
- $J = U/4$
- cluster DMFT with 2 site cluster (DCA)
- Paramagnetic and para-orbital solution

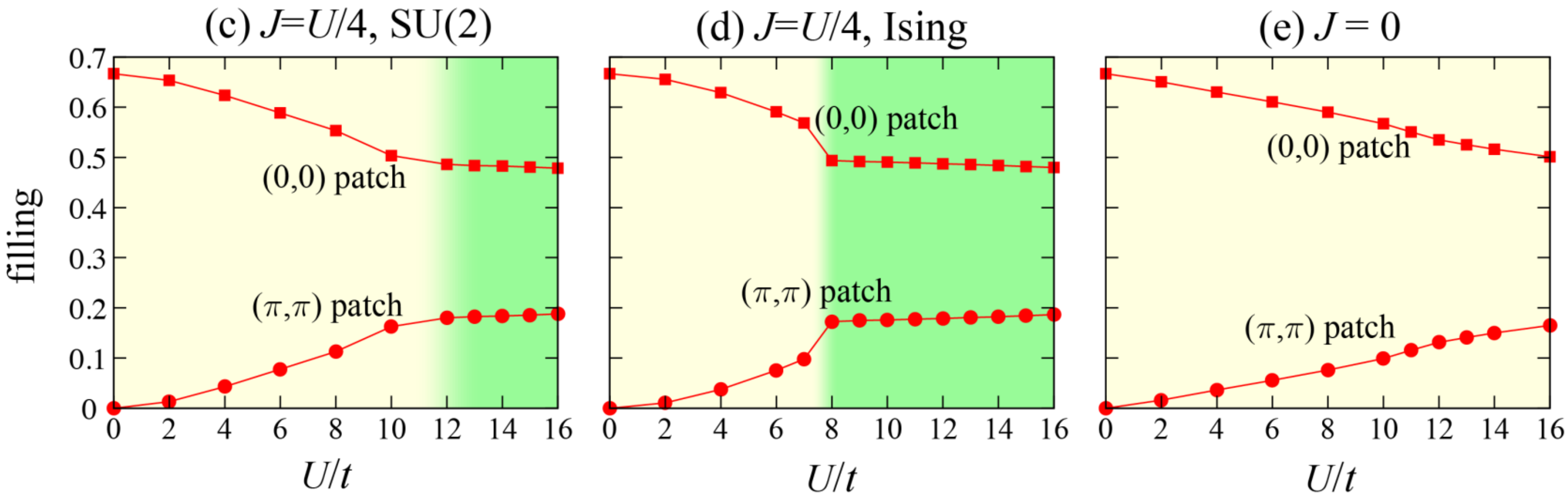




Three-orbital Hubbard model: one-particle quantity (1)

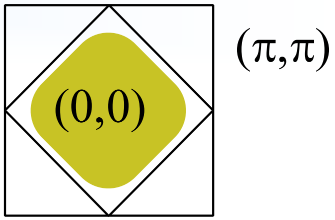


In the presence of *J*
filling redistribution within BZ: (0,0) patch tends to be half-filling

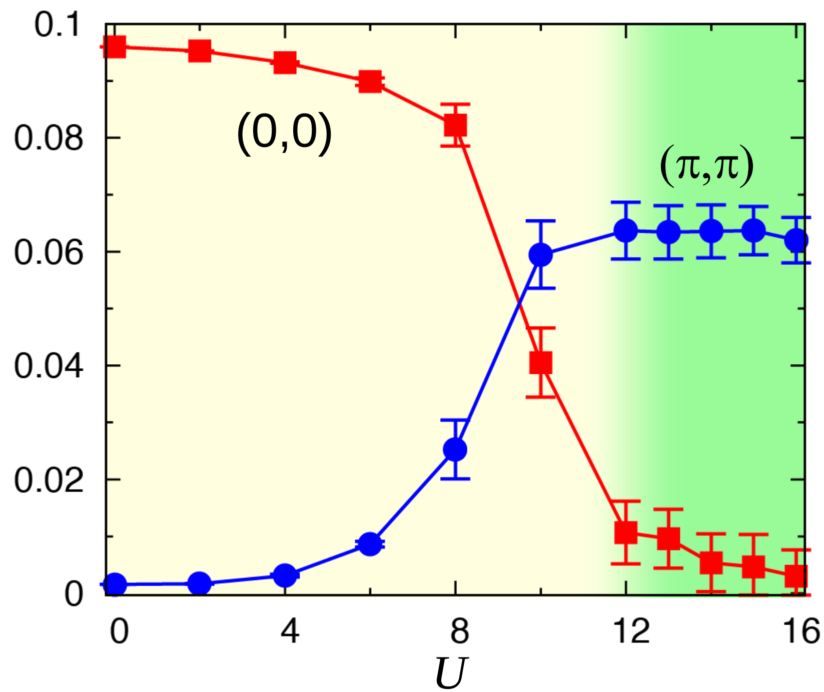


Three-orbital Hubbard model: one-particle quantity (2)

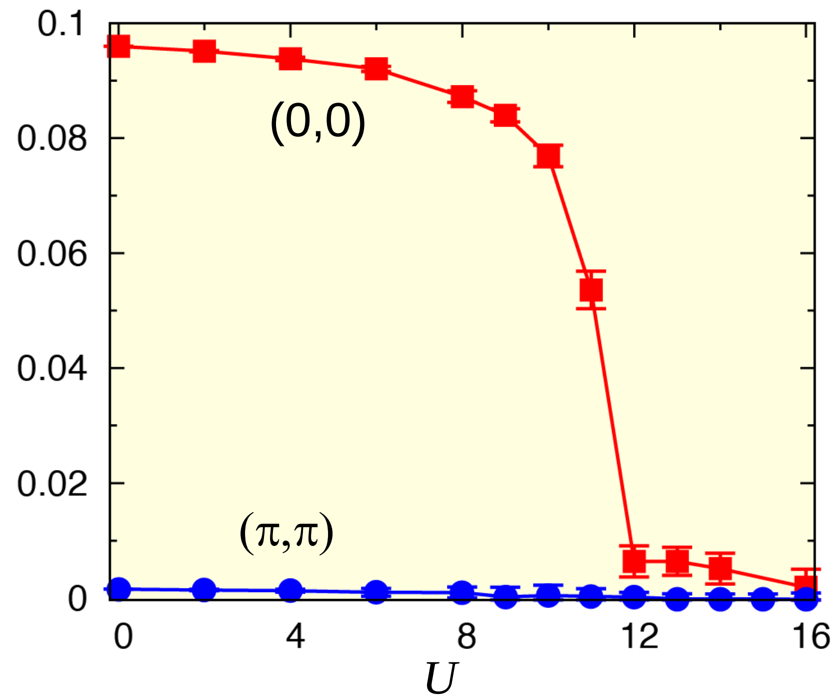
$$G(\tau = \beta/2)$$



J=*U*/4 (SU(2) symmetric)

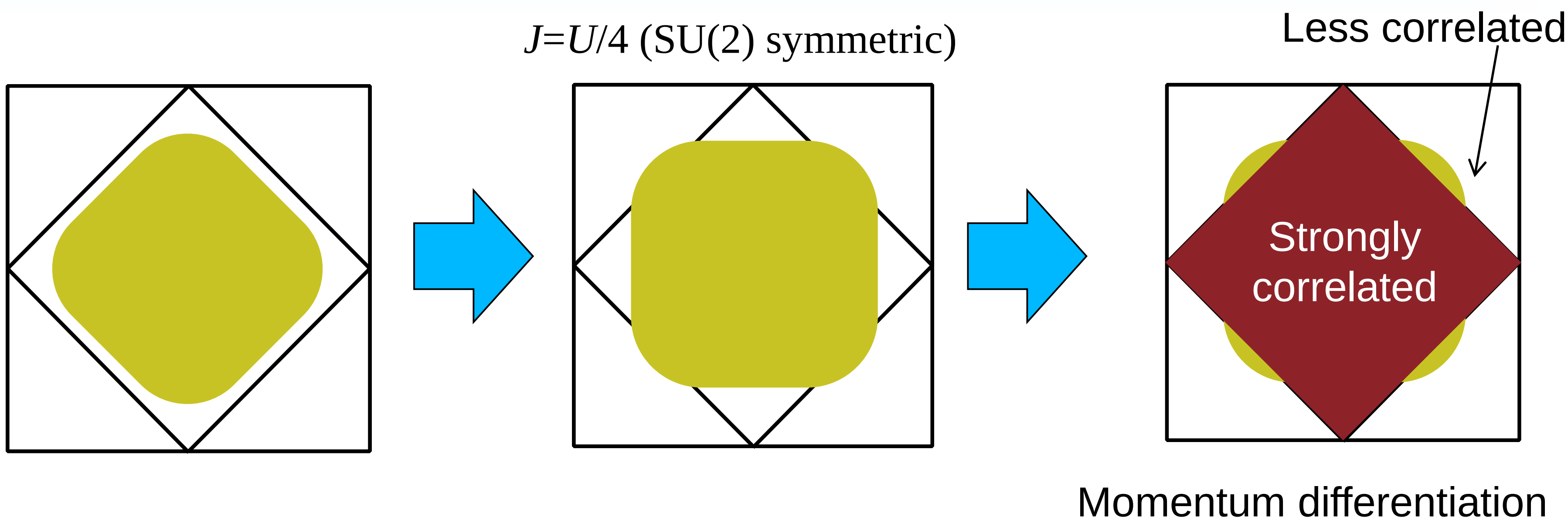


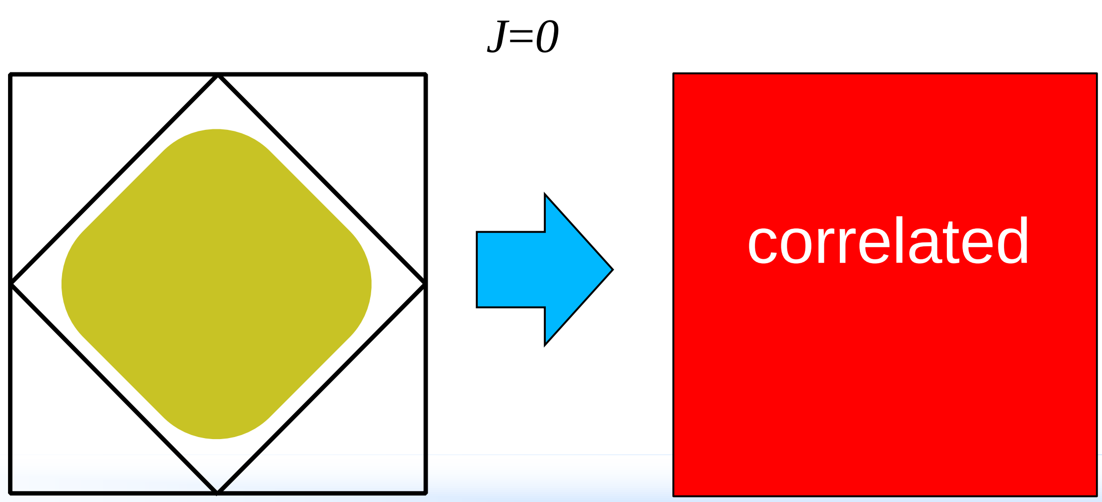
J=*0*



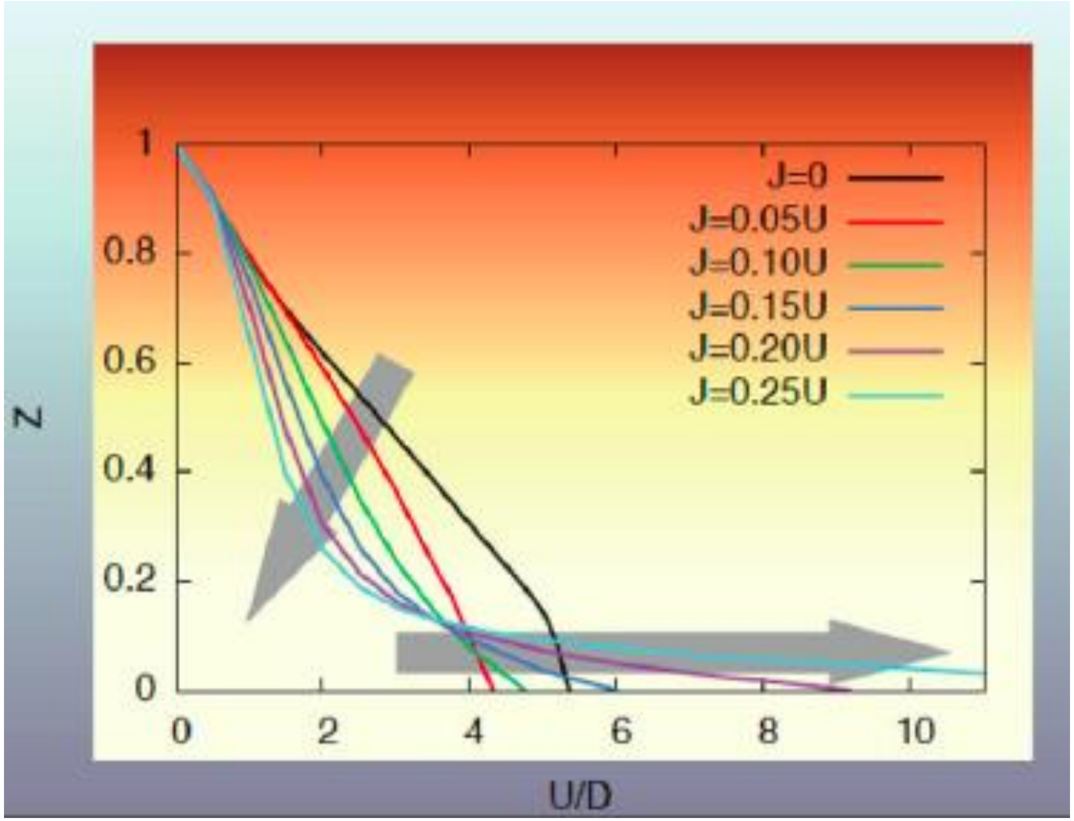
Low energy spectrum appears in (π,π) patch

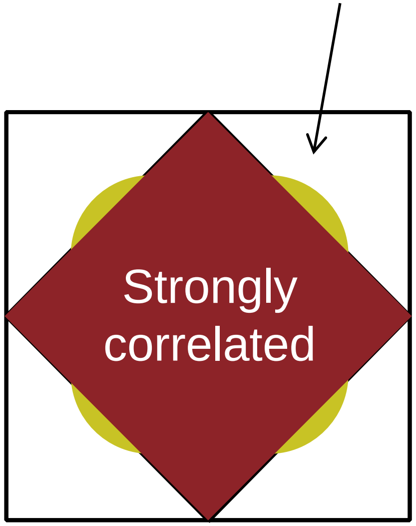
Three-orbital Hubbard model: one-particle quantity (3)





Janus-faced effect of *J*

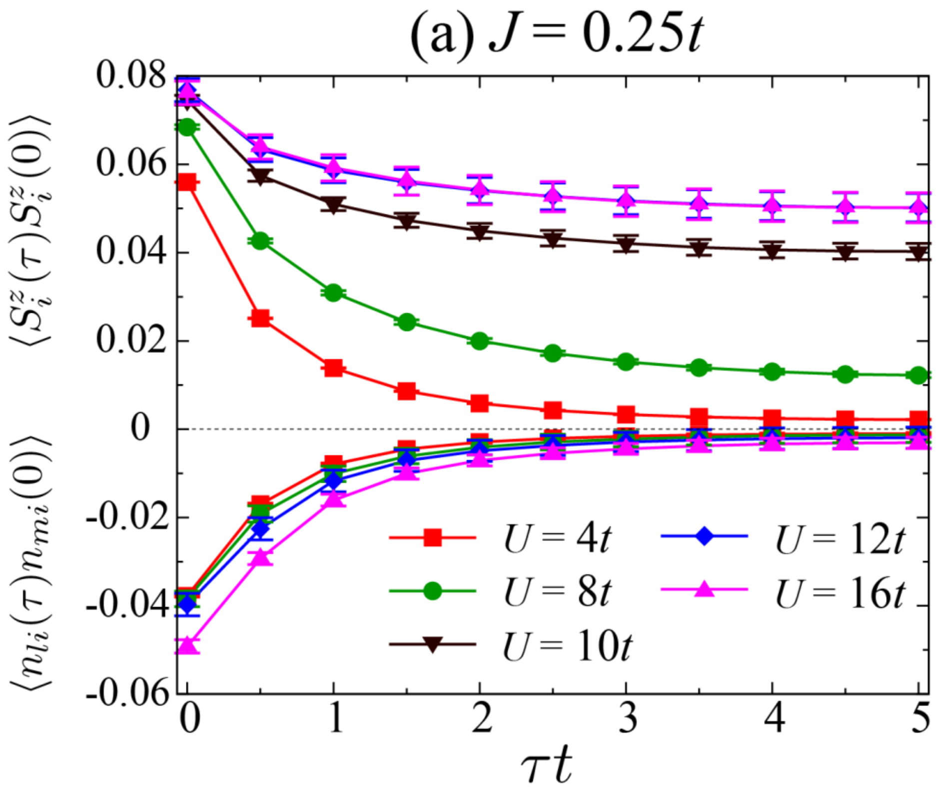


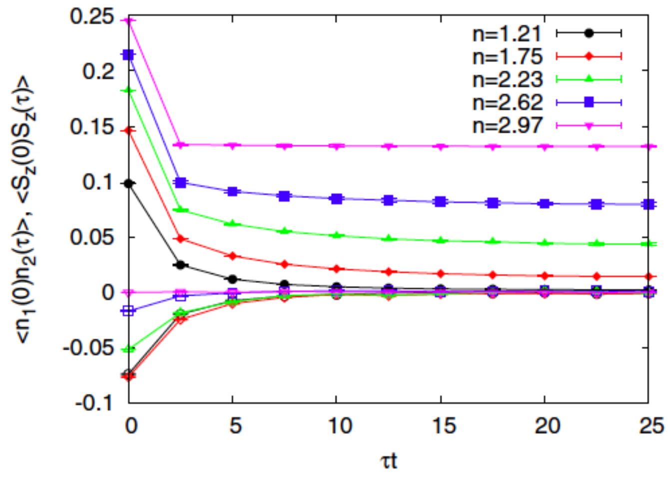


Medici *et al*., PRL 107, 256401 (2011)

Three-orbital Hubbard model: two-particle quantity (1)

Onsite correlation





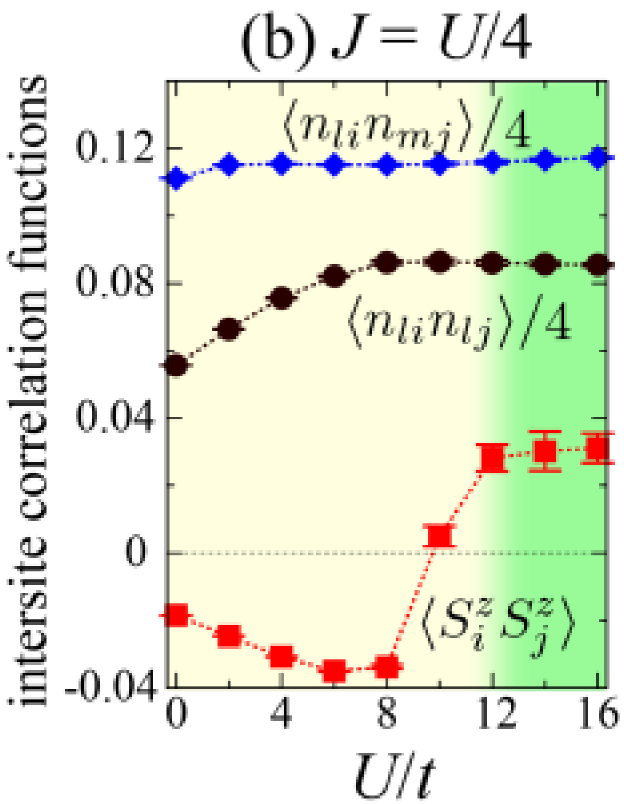
Werner *et al.*, PRL 101, 166405 (2008)

i,*j*: site
l, *m*: orbital

"Spin freezing" behavior for large *U*

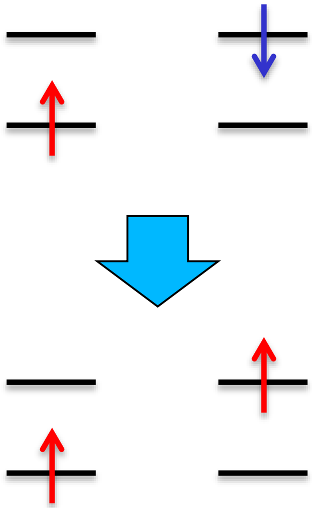
Three-orbital Hubbard model: two-particle quantity (2)

Intersite correlation



i,*j*: site
l, *m*: orbital

Ferromagnetic ground state
for 1D 2-orbital Hubbard model

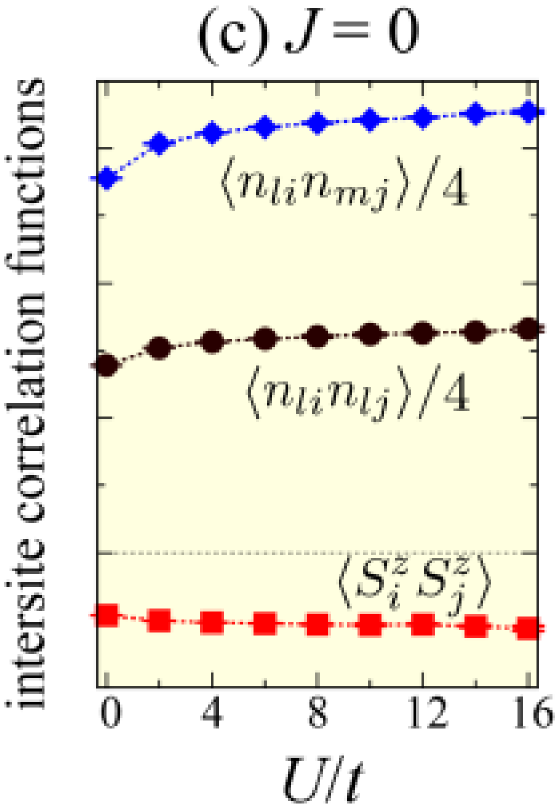


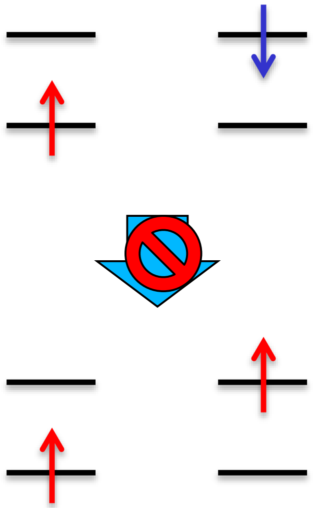
K. Kubo, JPSJ 1982
K. Kusakabe & H. Aoki, Physica 1994

DMFT
T. Momoi & K. Kubo, PRB 1998
K. Held & D. Vollhardt EPJ 1998
C-K. Chan et al., PRB2009

Three-orbital Hubbard model: two-particle quantity (2)

Intersite correlation





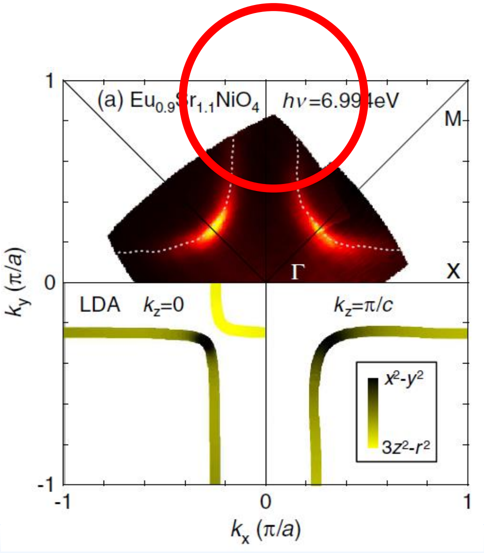
i,*j*: site
l, *m*: orbital

Conclusion

- Efficient CTQMC algorithm for multi-orbital DCA
- Effect of local *J* in correlated electron systems
  - *J* enhances spatial correlations
- Future problem: LDA+cDMFT calculation for multi-orbital systems

$LnSrNiO_4$

Uchida, RA *et al.*, PRL **106**, 027001(2011)

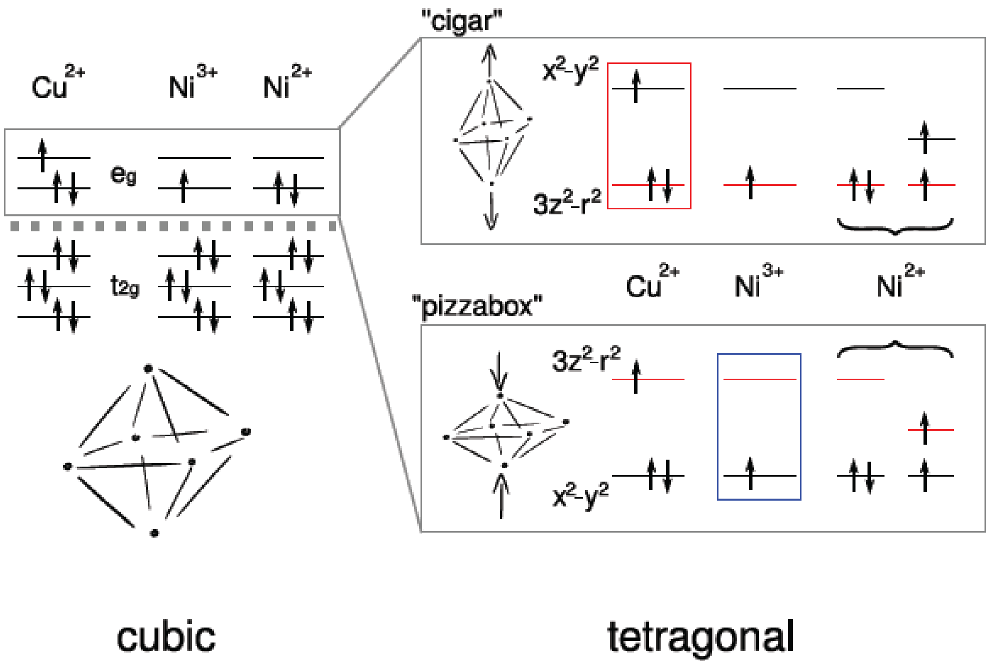


Intersite correlation due to *J*

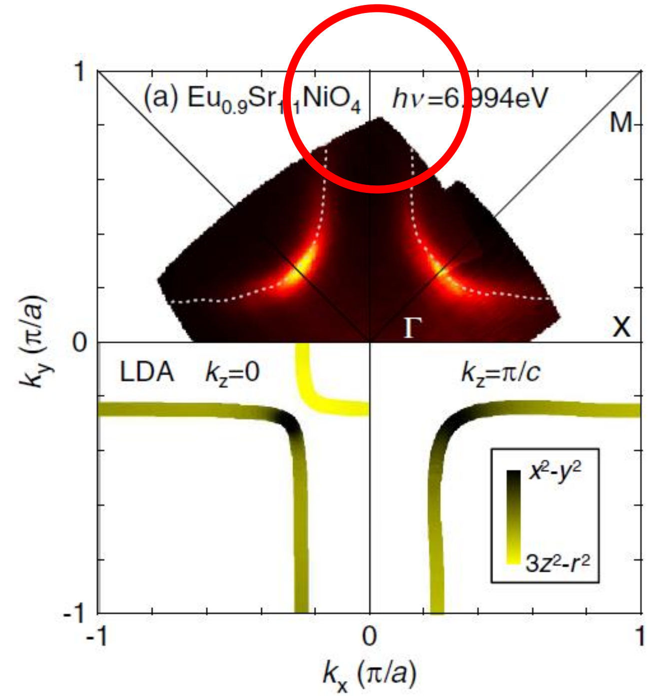
$LnSrNiO_4$: Layered perovskite $3d^7$ system

(Same crystal structure as La_2CuO_4)

	Onsite correlation	Intersite correlation
U	DMFT	Cluster DMFT
J	Multi-orbital DMFT	multi-orbital cluster DMFT



Pseudogap ?

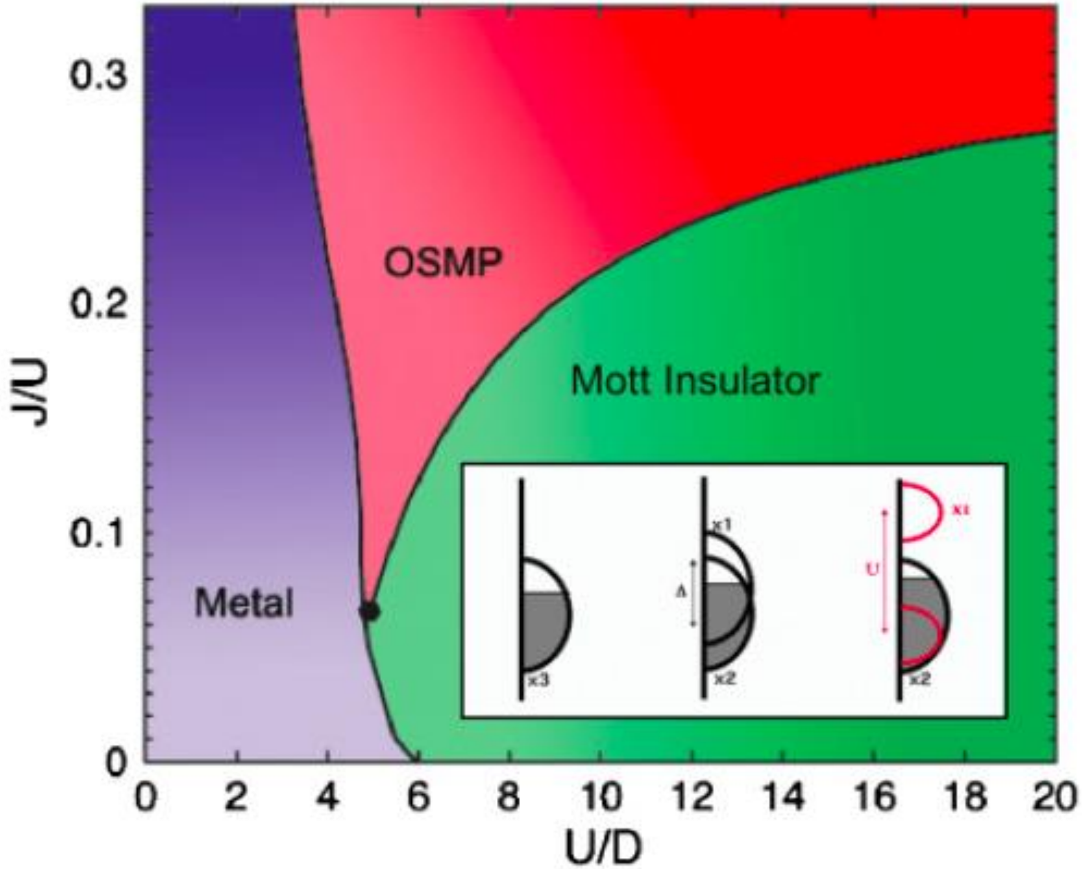


Uchida, RA *et al.*, PRL **106**, 027001(2011)

Motivation: effect of *J*

	Onsite correlation	Intersite correlation
U	DMFT	Cluster DMFT
J	Multi-orbital DMFT	multi-orbital cluster DMFT

“band decoupler” and orbital selective Mott transition

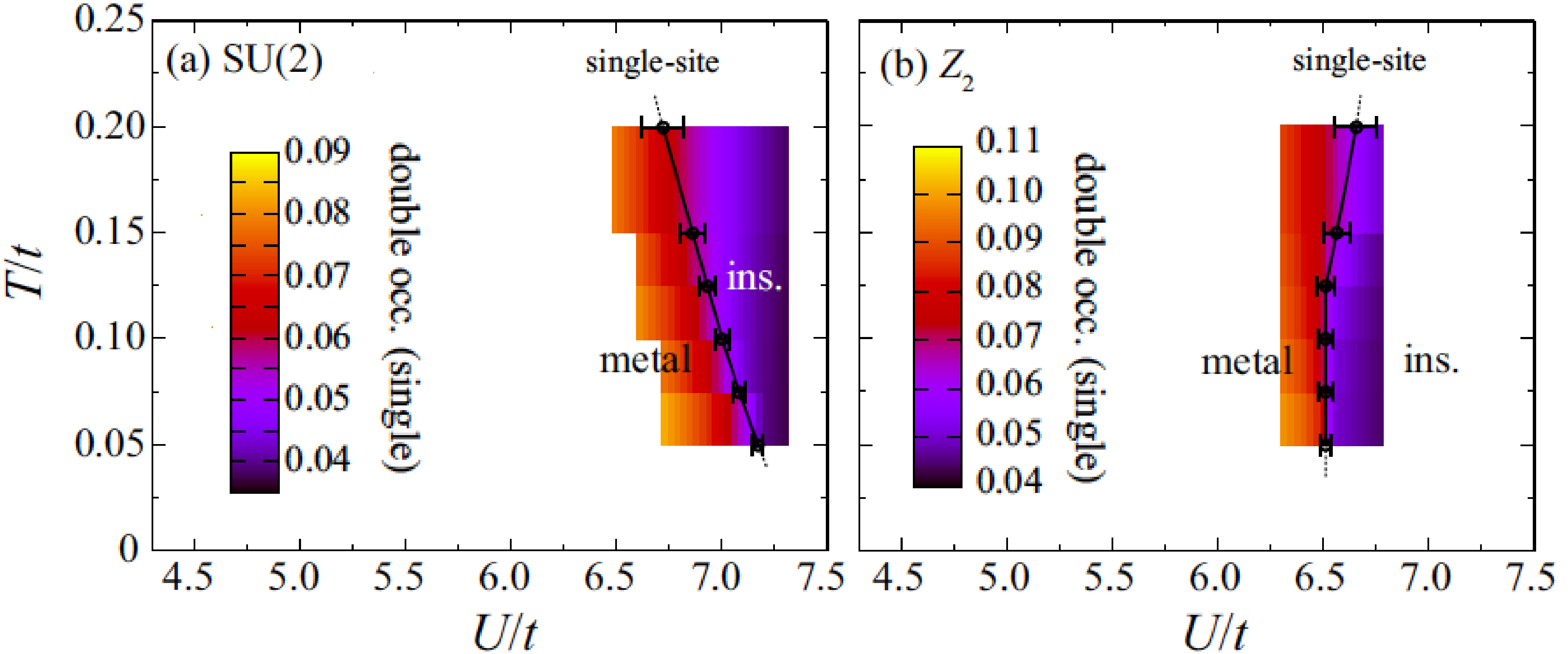


Medici *et al*., PRL 102, 126401 (2009);
Medici, PRB 83 205112 (2011)

Two-orbital Hubbard model: Mott transition

U=6J

(DMFT self-consistent loop starts with a metallic solution)

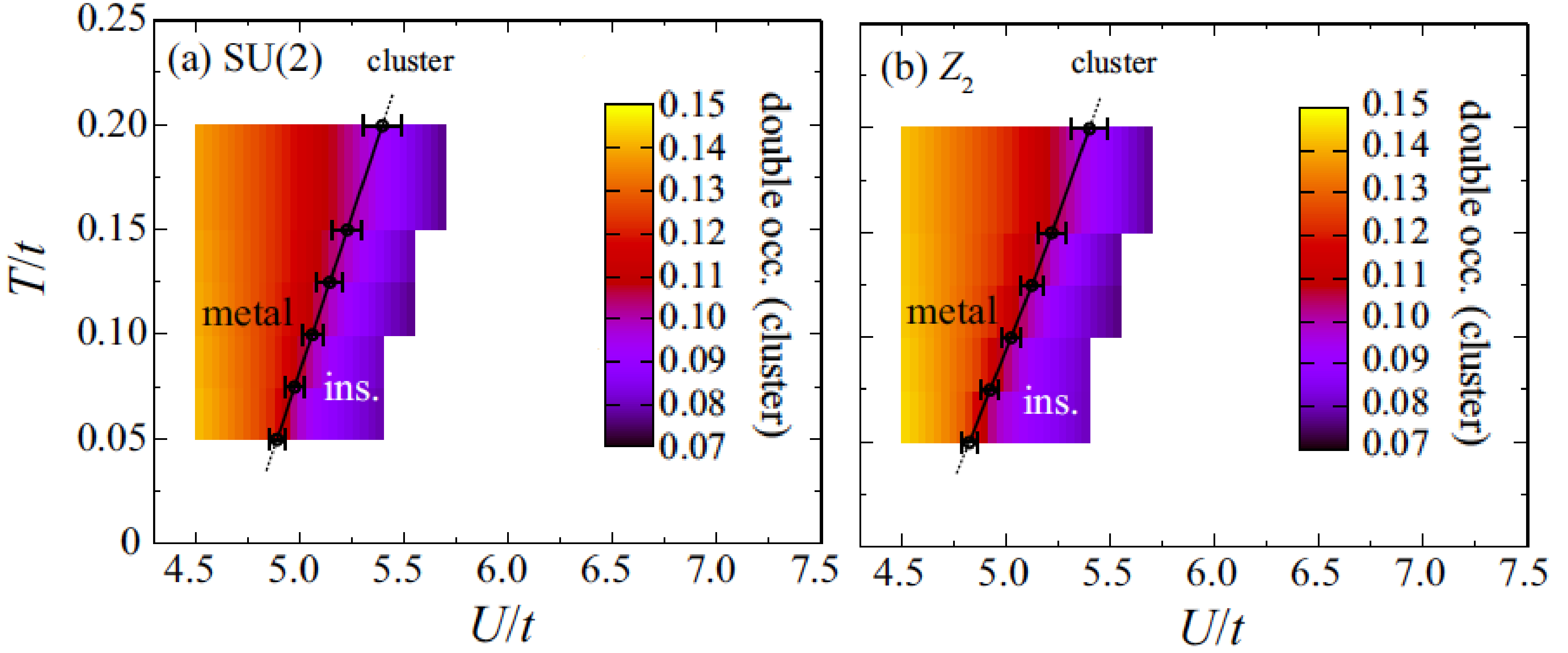


Entropy(ins,SU(2)) ~ ln(3) (S=1, Sz = 1,0,-1)
Entropy(ins,Ising) ~ ln(2) (S=1, Sz=±1)

Two-orbital Hubbard model: Mott transition

U=6*J*

(DMFT self-consistent loop starts with a metallic solution)



Entropy(metal) > Entropy(ins)