Orbital-selective Mott transitions

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Krunoslav Požgajčić, Univ. Frankfurt

Outline

Introduction: orbital/flavor-selective Mott transitions in correlated materials/ultracold atoms on optical lattices

Orbital-selective Mott transitions in 2-band Hubbard model

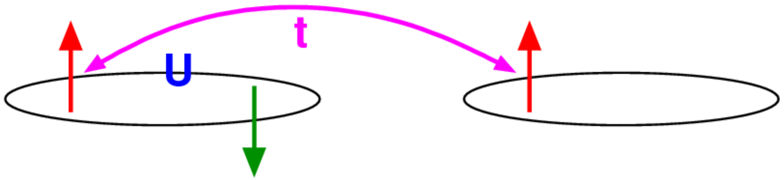
Order of wide-band transition at $T > 0$ and $T = 0$

Summary

Introduction

Reminder: Mott transition in frustrated 1-band Hubbard model

$$H = -t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



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transition at $U_c(T)$ (within DMFT)?

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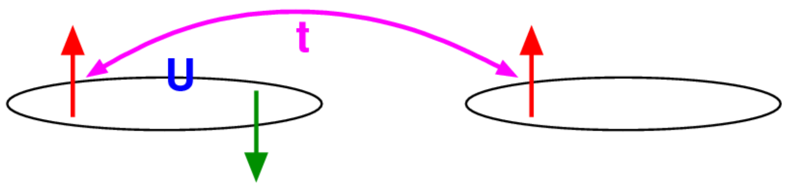

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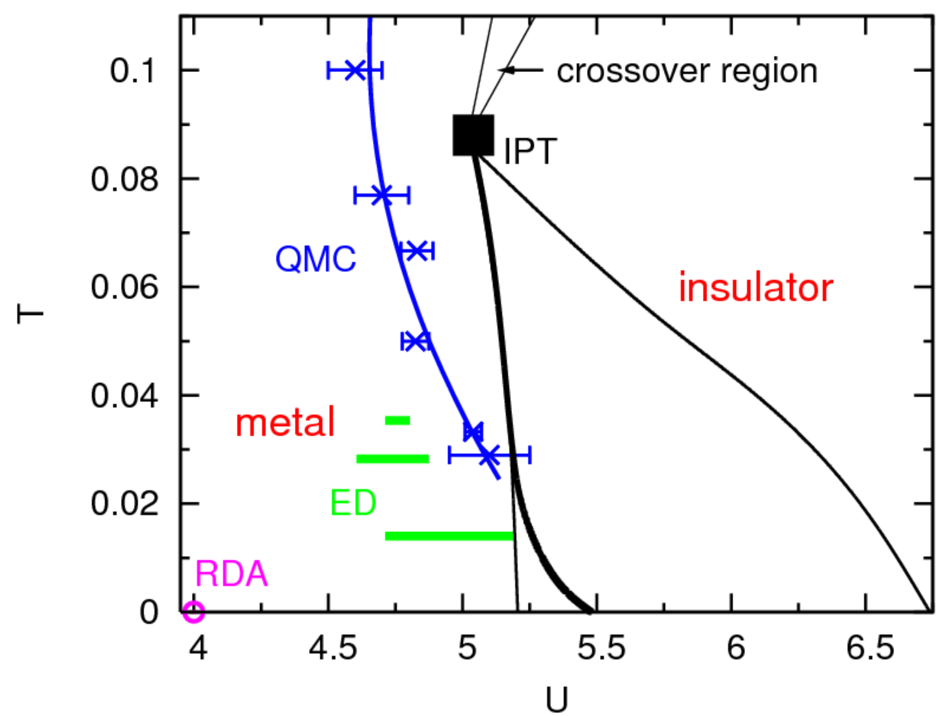

No conclusive answer up to 1999

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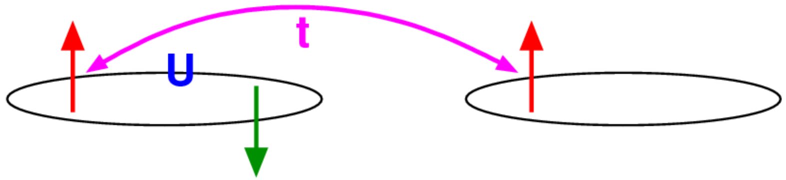

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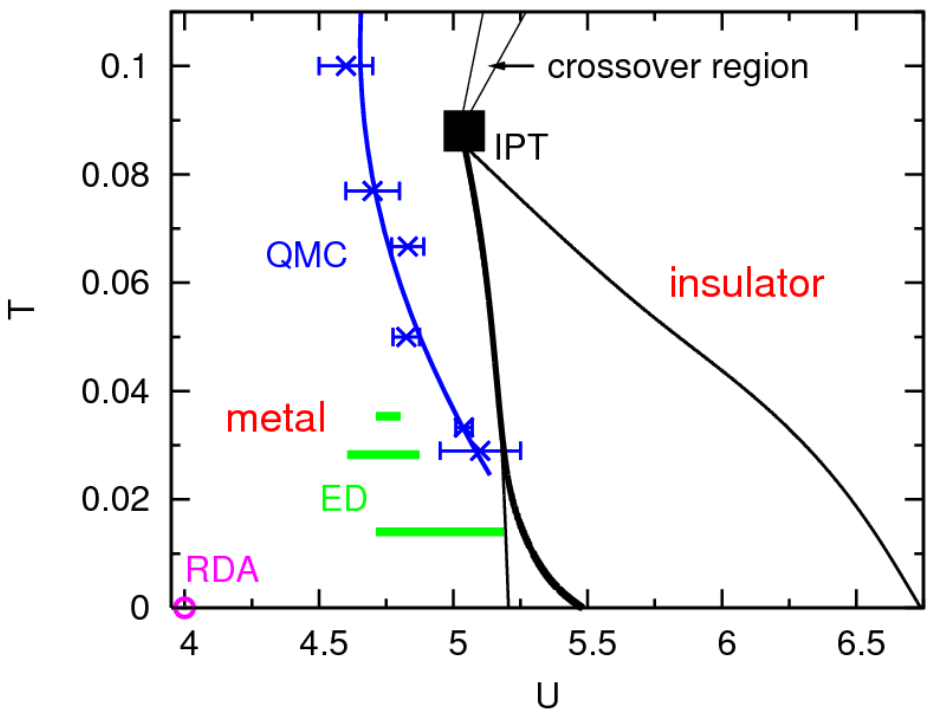

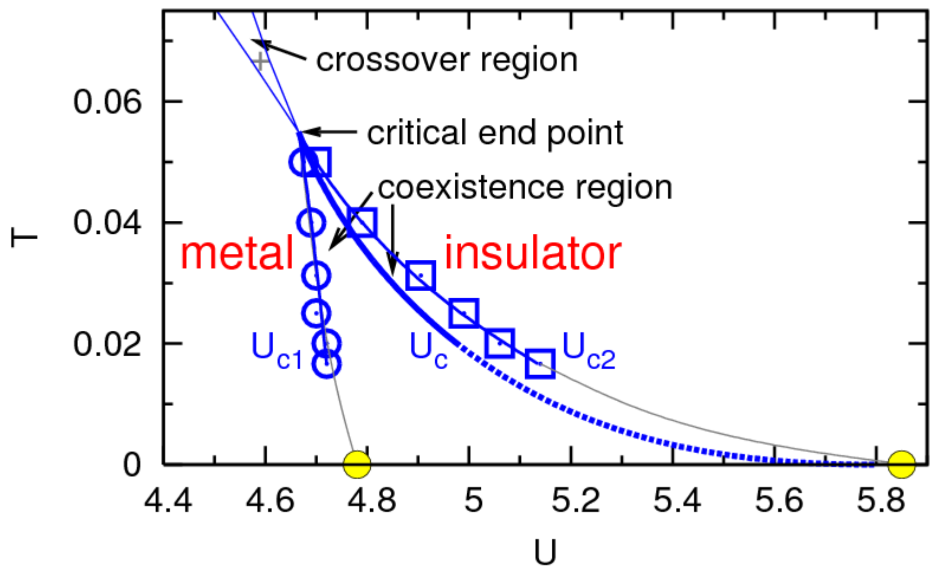

Now accepted: 1^{st} order transition for $0 < T < T^*$ (QMC + ePT, 2000-2005)

Multiorbital case ($M > 1$ orbitals, half filling $n = M$)?

Extension without additional parameters: SU(2M) symmetric case:

$$H = -t \sum_{\langle i,j \rangle, m, \sigma} c^\dagger_{im\sigma} c_{jm\sigma} + \frac{U}{2} \sum_i \sum_{(m,\sigma) \neq (m'\sigma')} n_{im\sigma} n_{im\sigma'}$$

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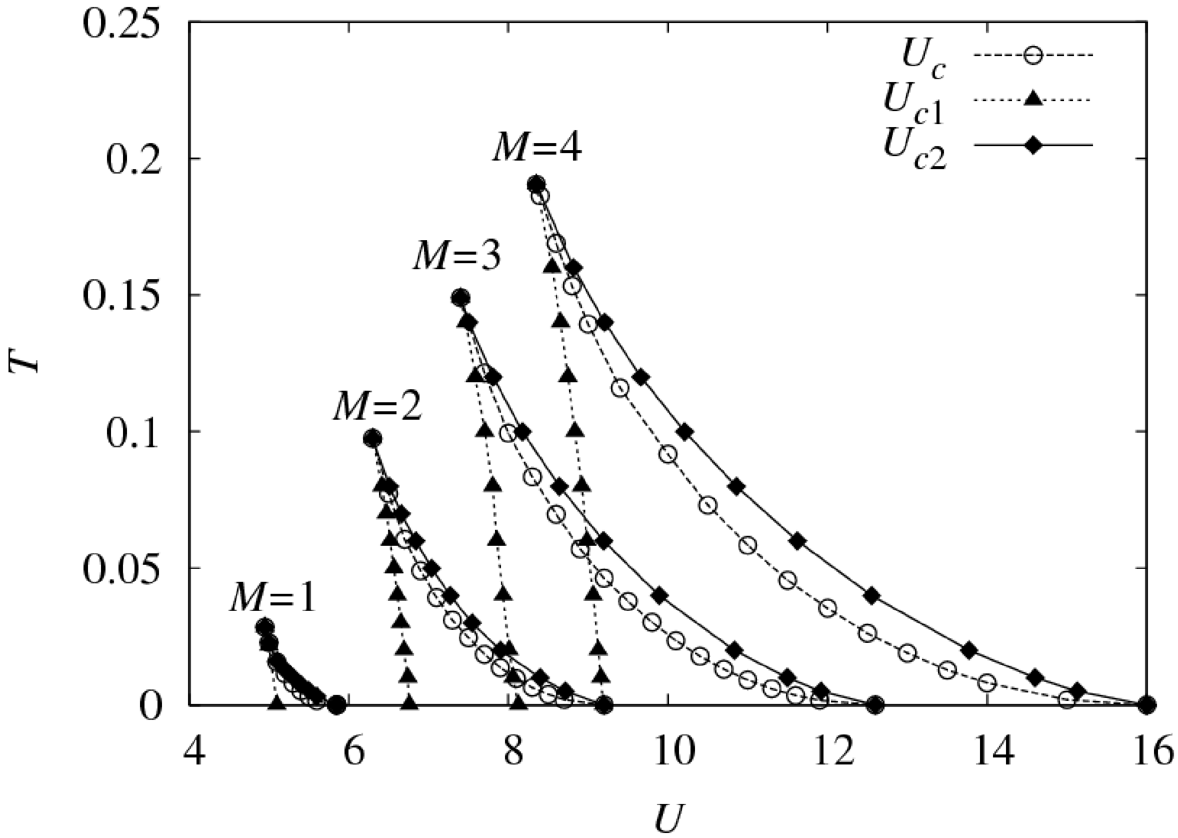

[Inaba, Koga, Suga, Kawakami, PRB **72**, 085112 (2005)]

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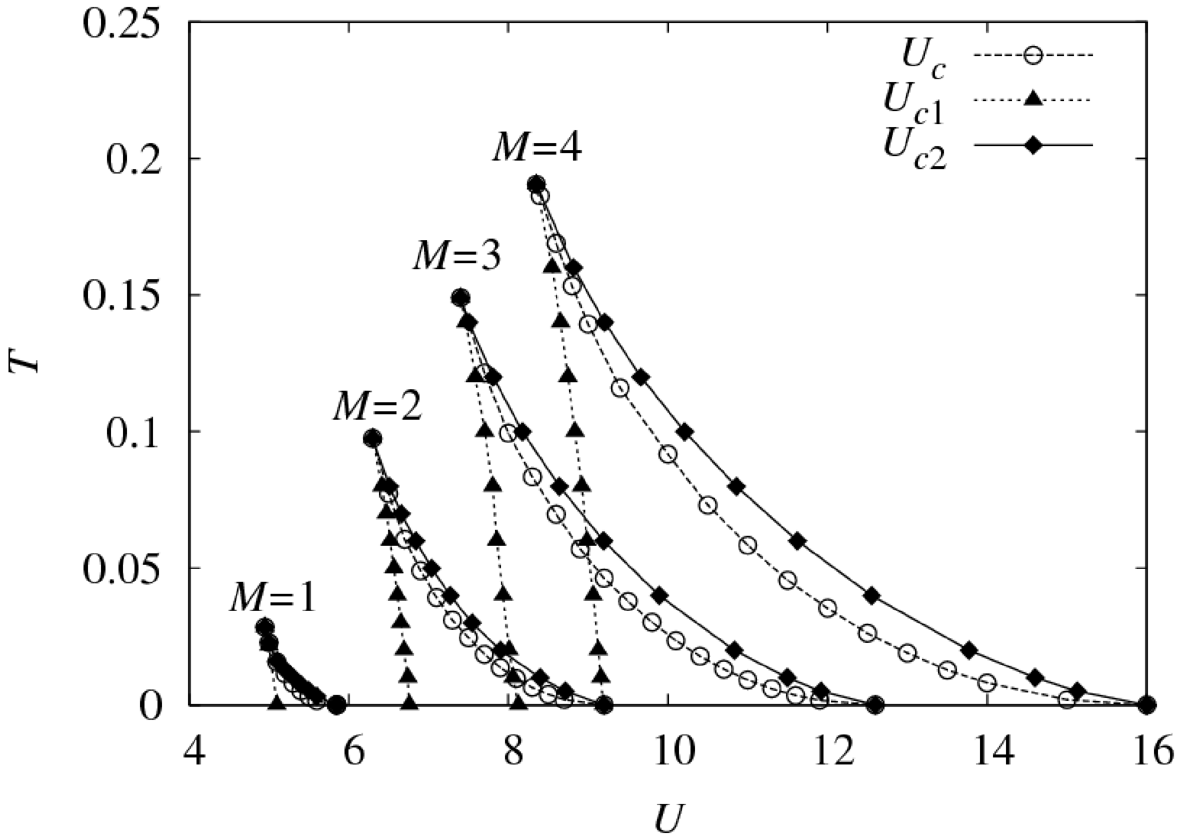

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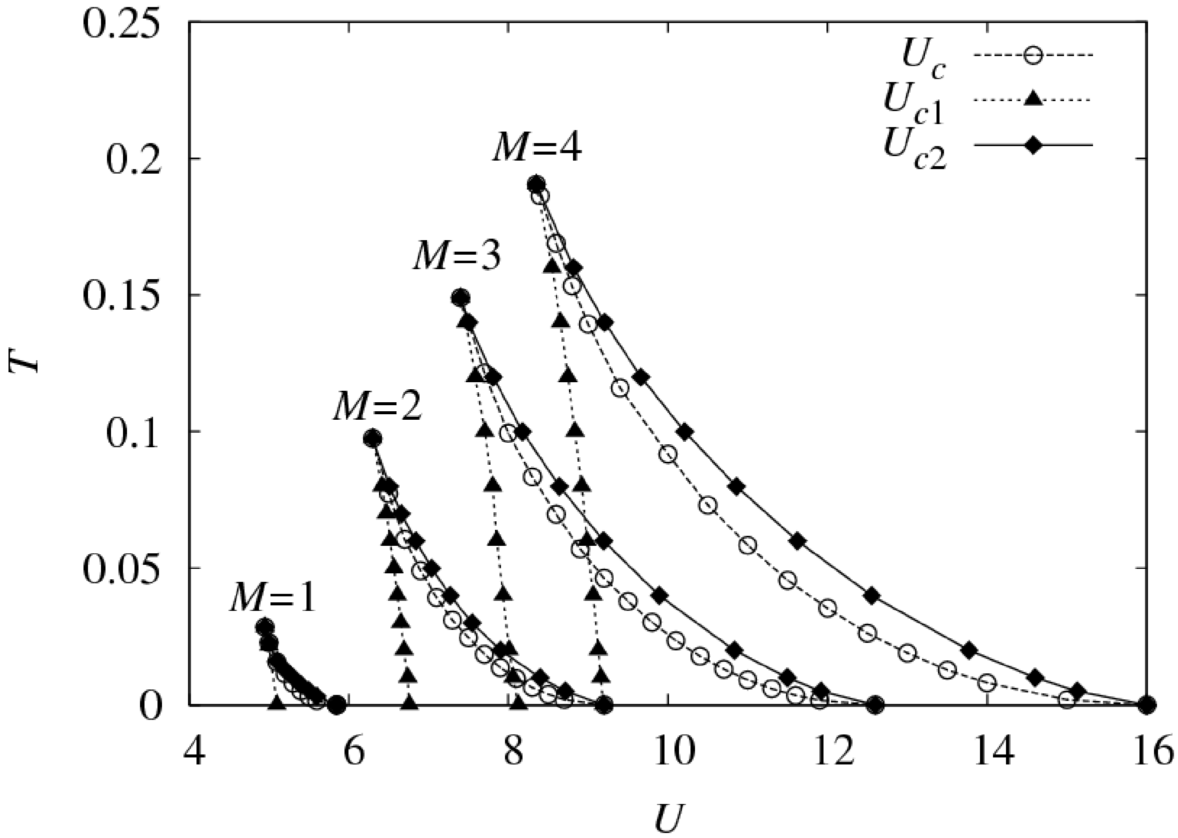

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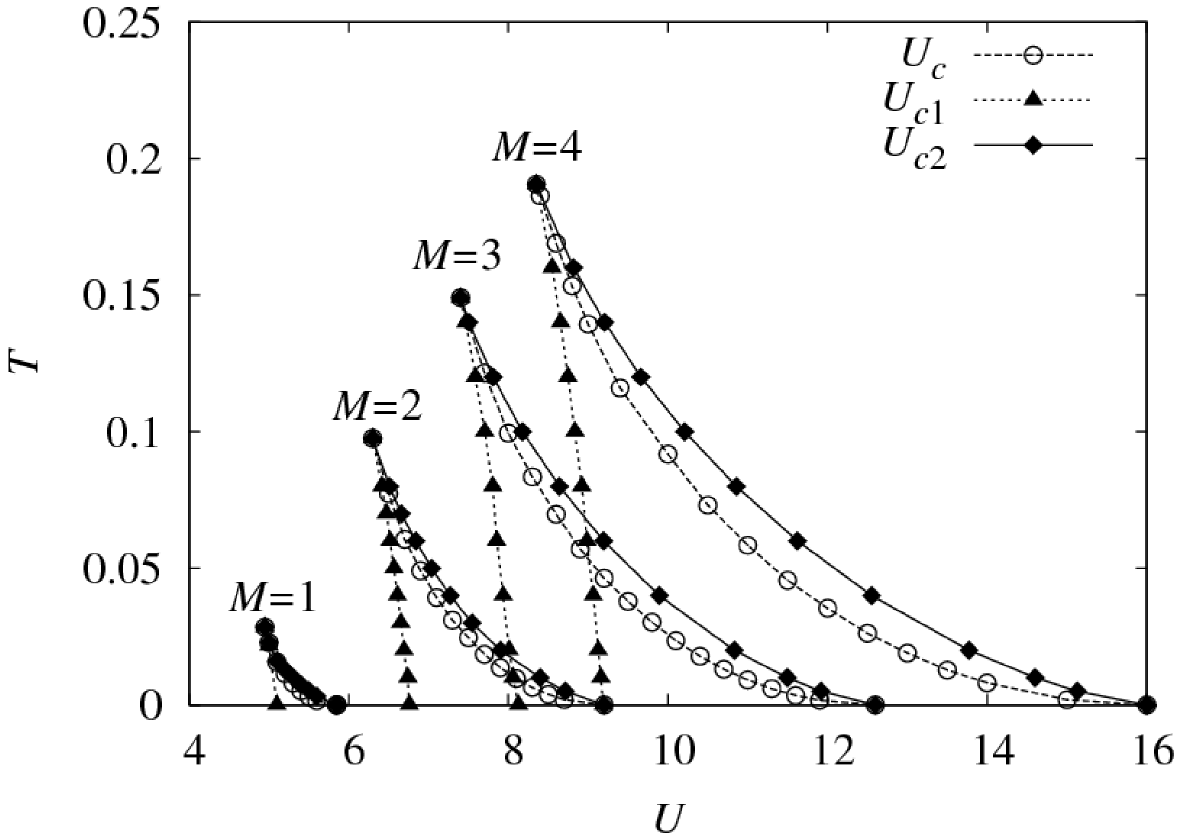

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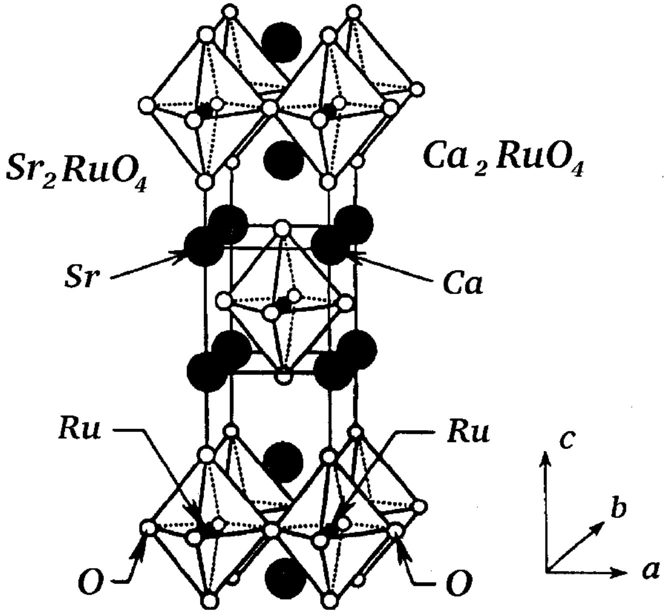
Inclusion of $J \rightsquigarrow 1^{\text{st}}$ order
[Bünemann, Weber, PRB (1997),
Ono, Potthoff, Bulla, PRB (2003)]

but still single Mott transition

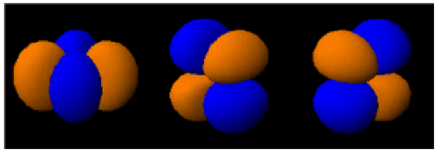
[Inaba, Koga, Suga, Kawakami, PRB **72**, 085112 (2005)]

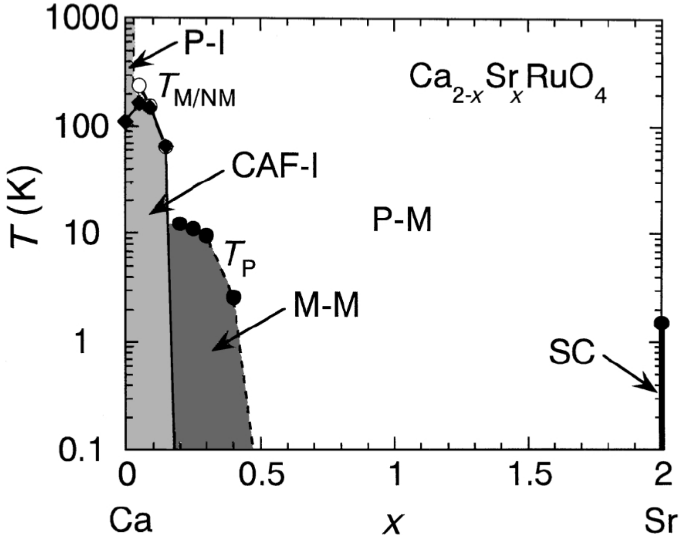
OSMTs in $Ca_{2-x}Sr_xRuO_4$



isostructural to $La_{2-x}Sr_xCuO_4$

4 valence electrons in 3 Ru t_{2g} orbitals





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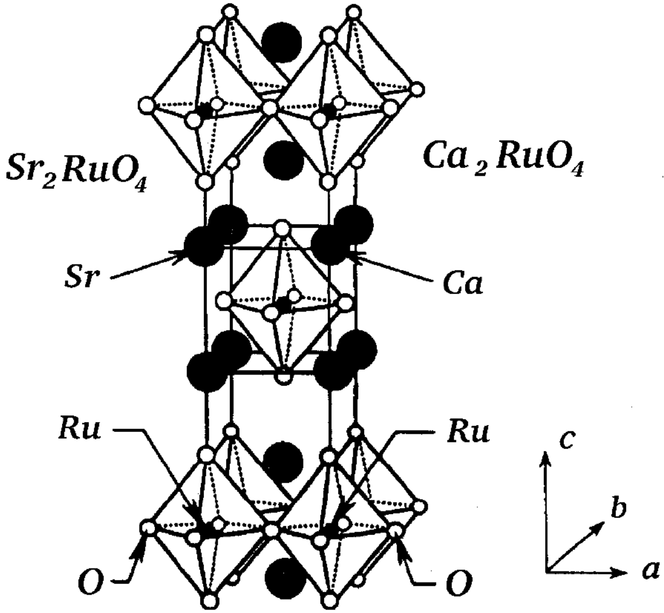

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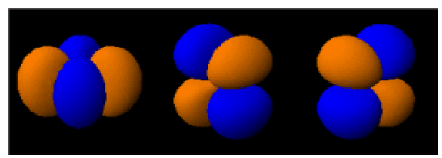

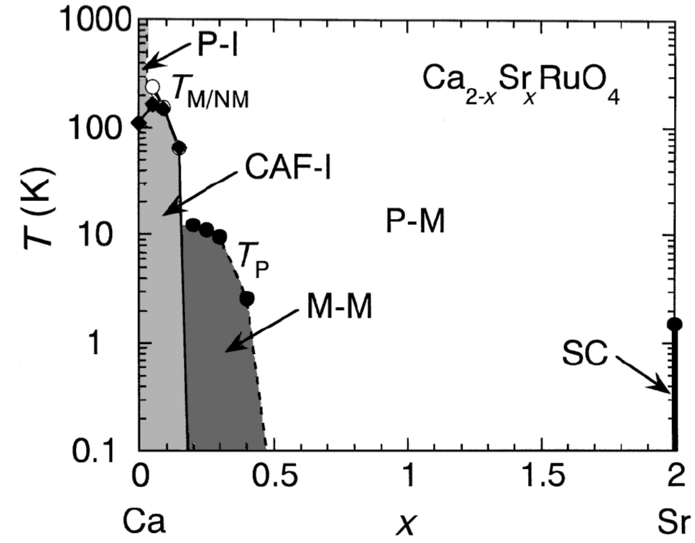

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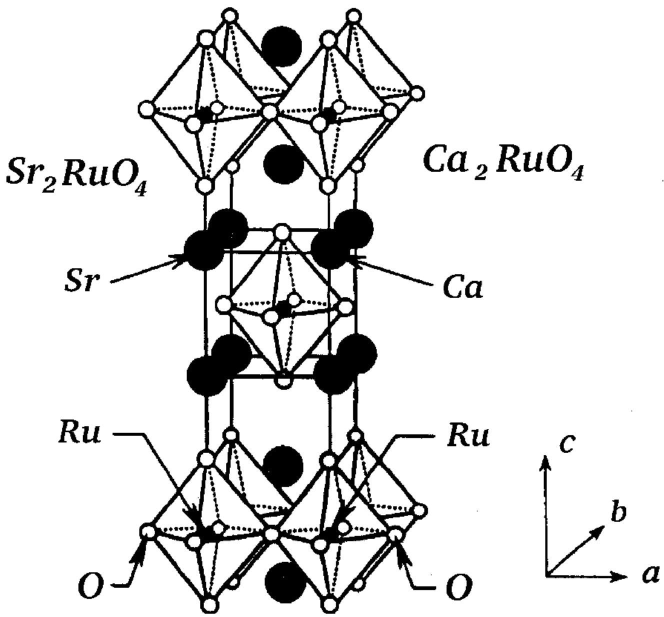

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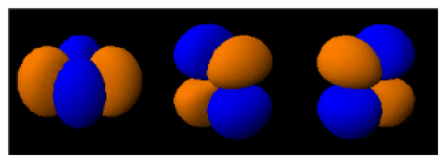

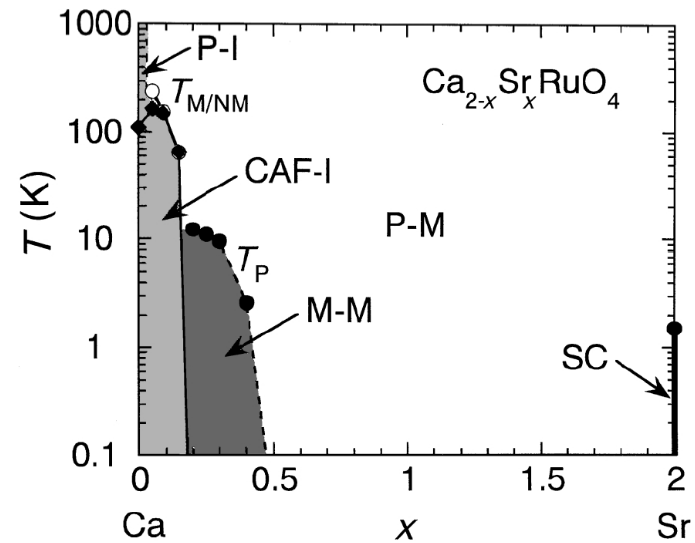

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Possible mechanism: different effective hopping amplitudes for in-plane and out-of-plane orbitals [Anisimov et al., EPJB (2002)]

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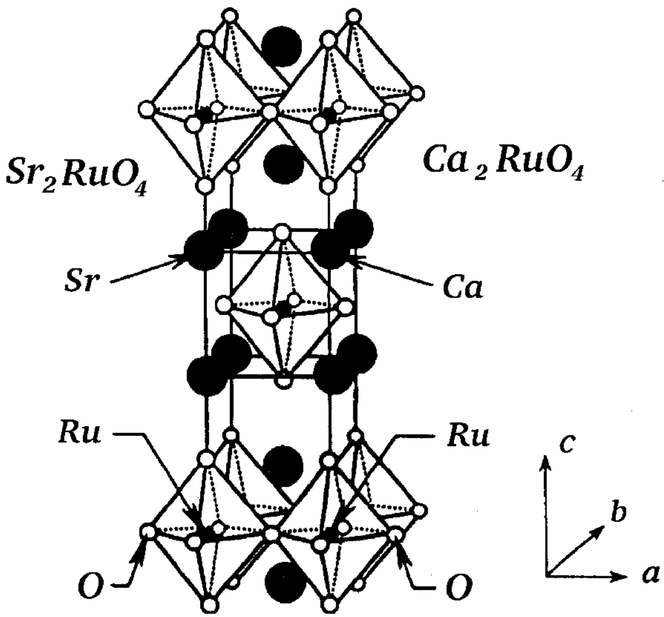

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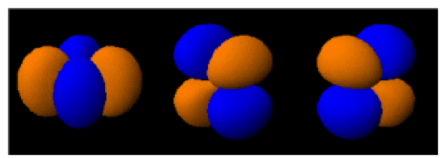

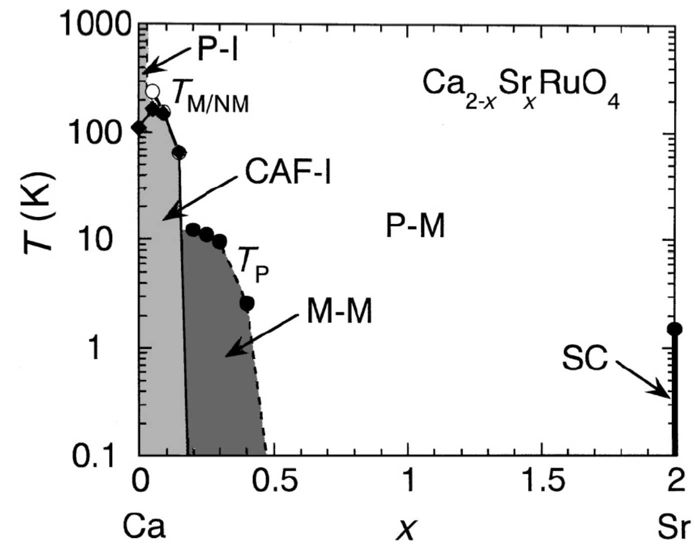

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Related: Dual nature of 5f electrons in UPt_3 [Zwicknagl, Yaresko, Fulde, PRB (2002)]

Ultracold fermionic atoms on optical lattices

Electronic case ($B = 0$): exact 2-fold spin degeneracy
in cubic system: orbital degeneracy ($2 \times e_g$, $3 \times t_{2g}$, ...)
neglected: core states, long-range Coulomb, phonons ...

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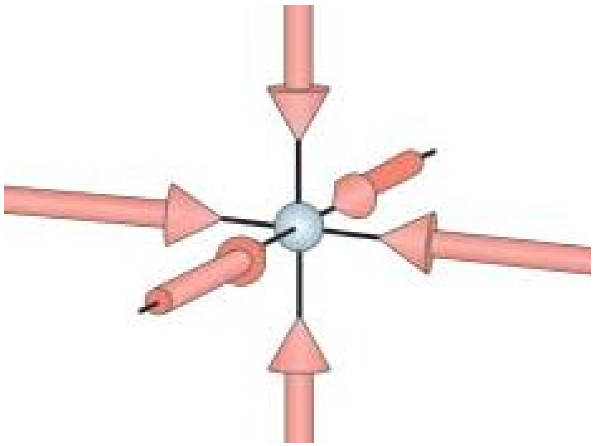

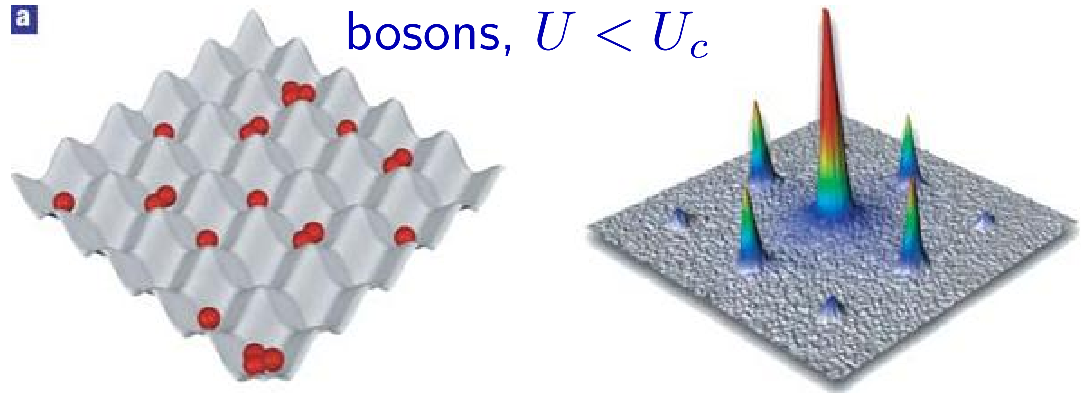

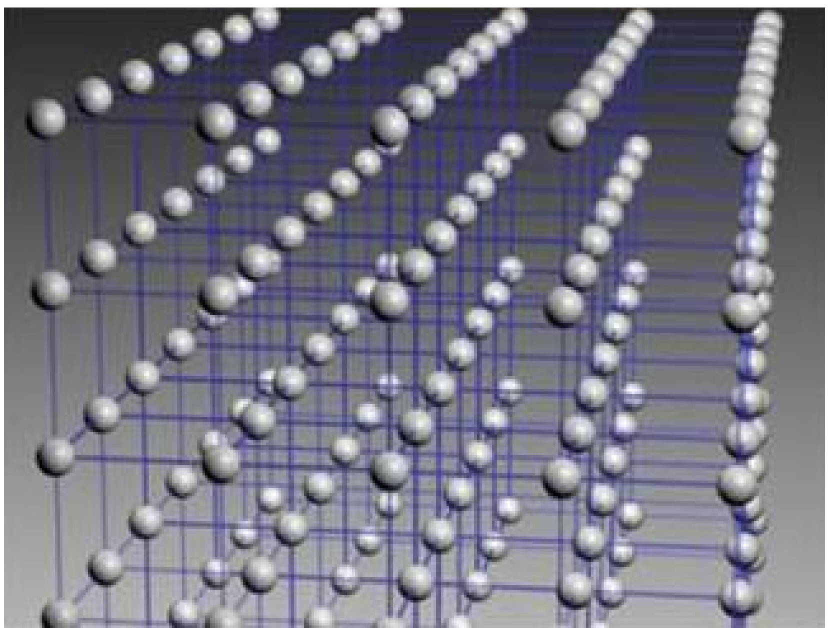

Alternative quantum systems with strong correlations: ultracold atoms on optical lattices

[Bloch, Nature Physics (2005)]

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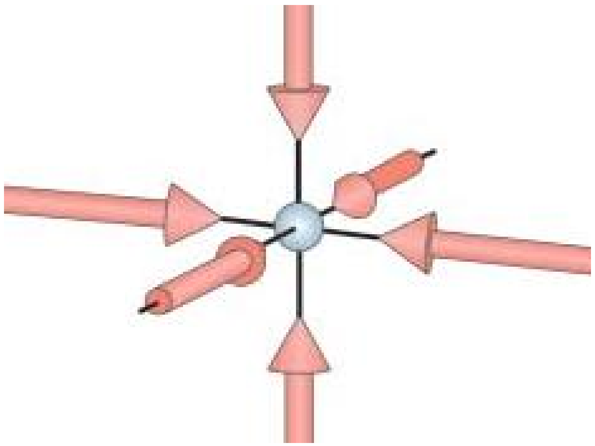
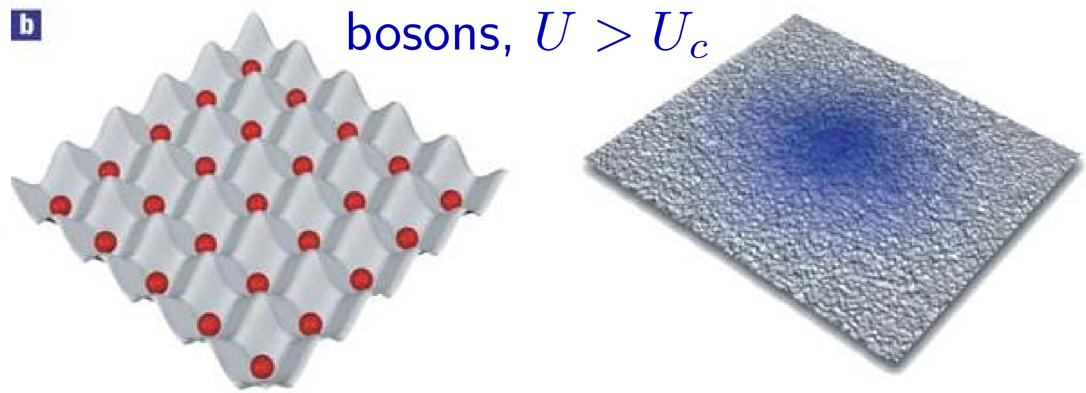
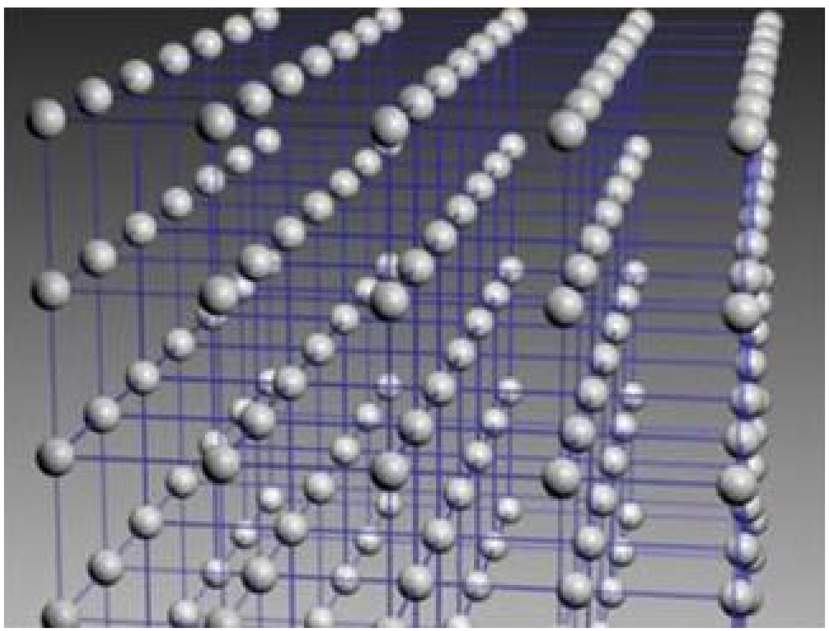




bosons, $U > U_c$



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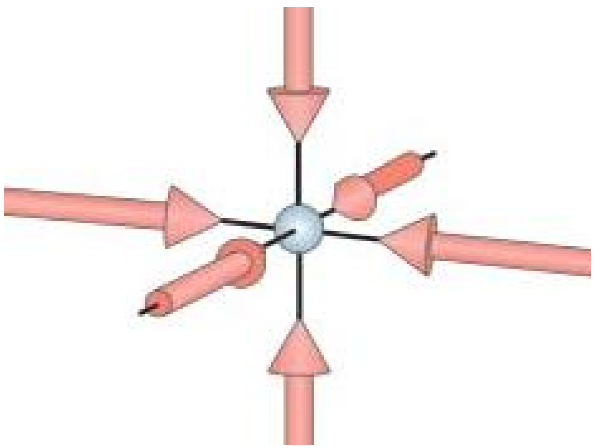

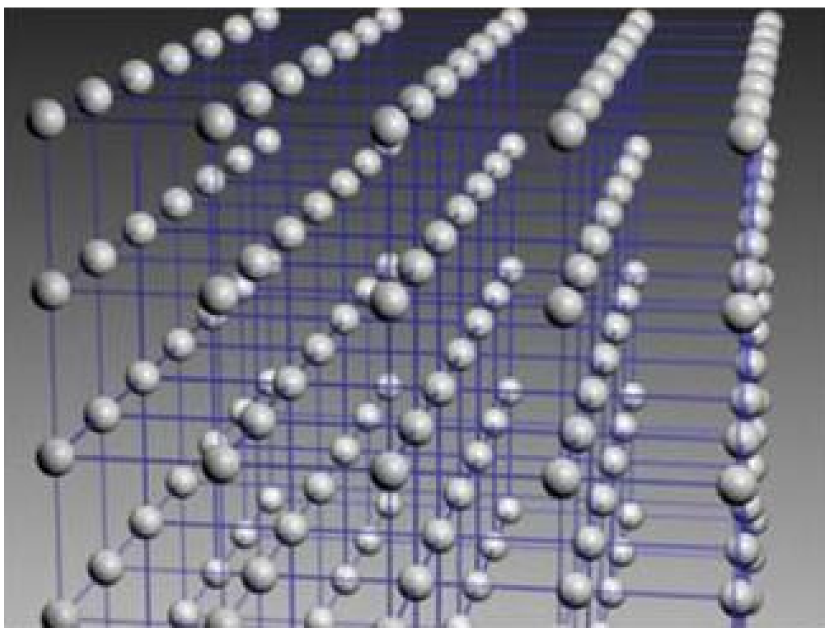

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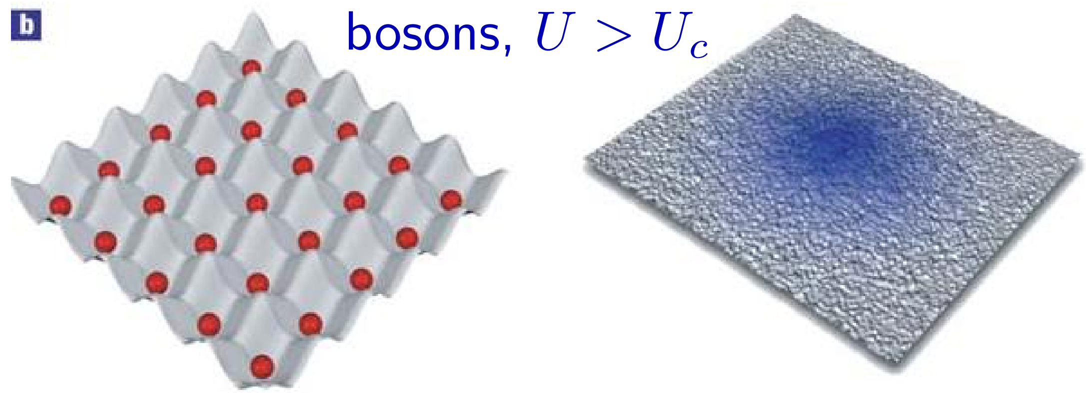
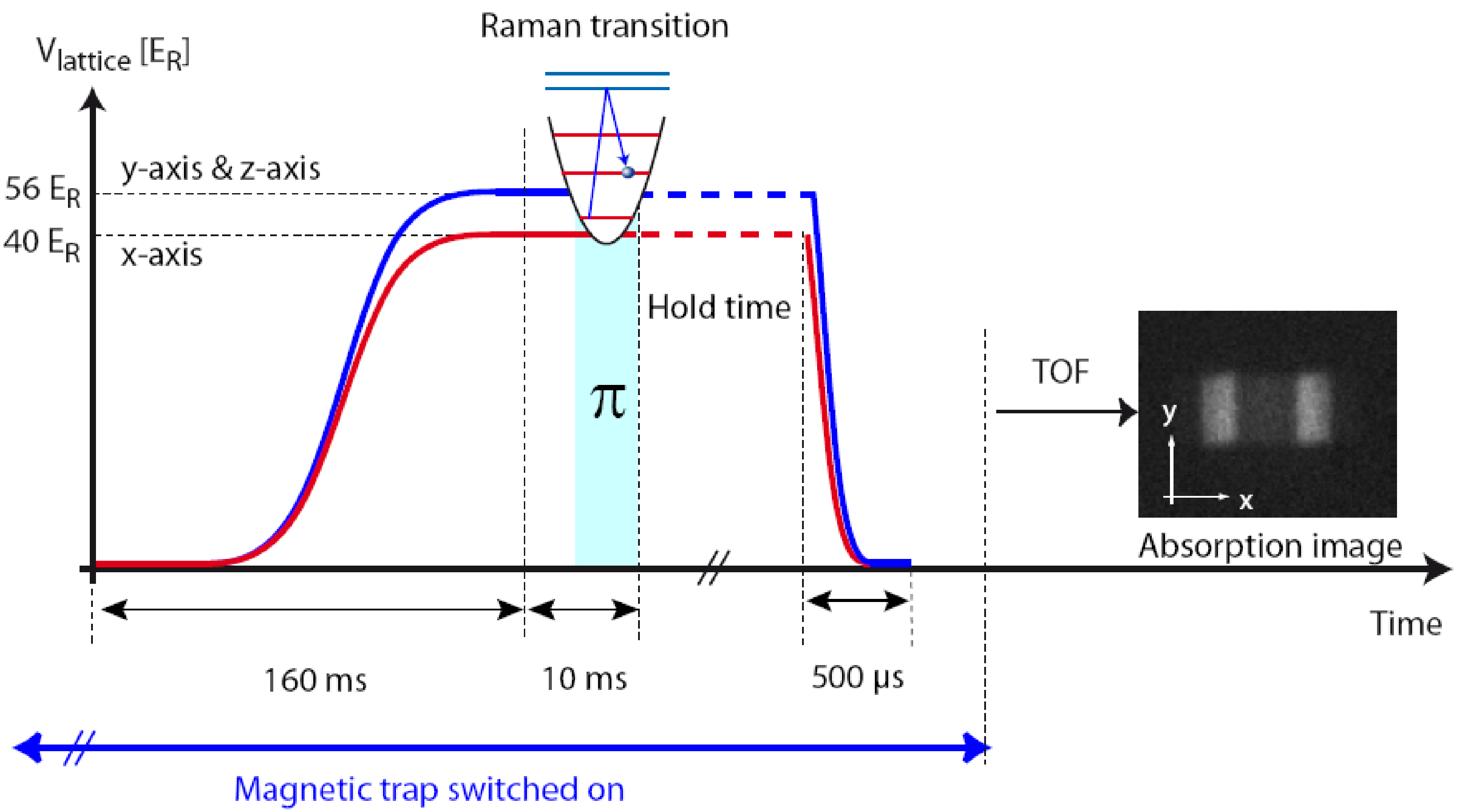


Alternative quantum systems with strong correlations: ultracold atoms on optical lattices

Flavors: species: ^{6}Li, ^{40}K
hyperfine states (spin and projections)
vibrational levels ($\sim$ Raman pulses)

Note: hopping and interactions are generically flavor-specific!

Raman excited higher vibrational states [T. Müller, diploma thesis, Mainz (2006)]



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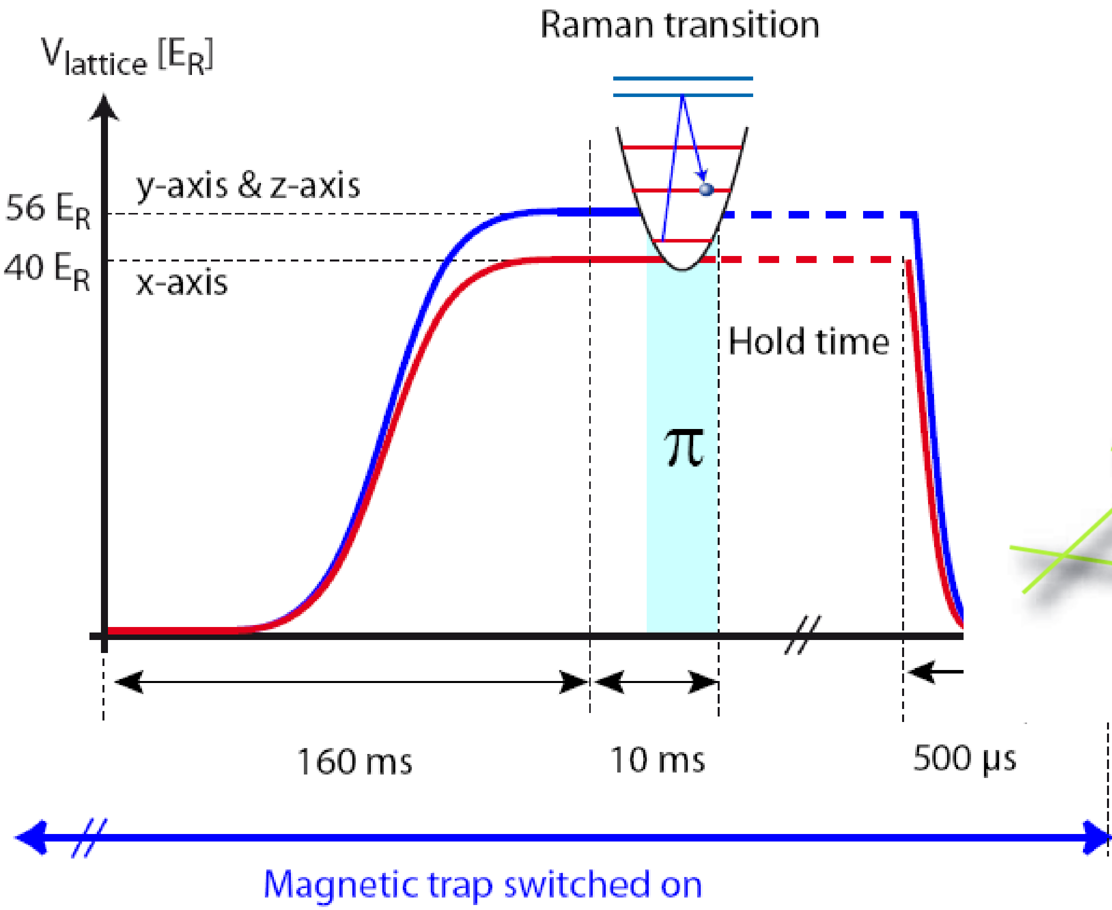

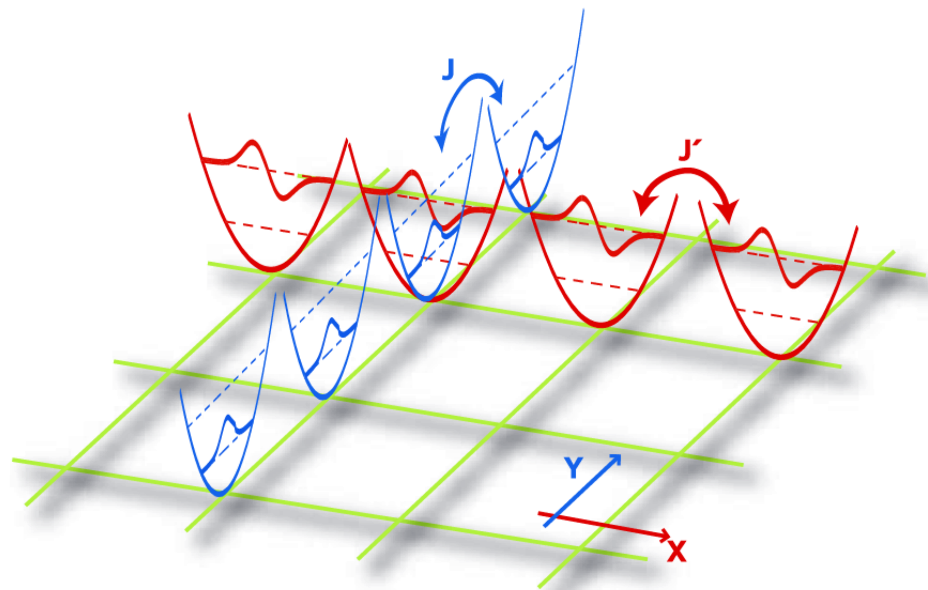

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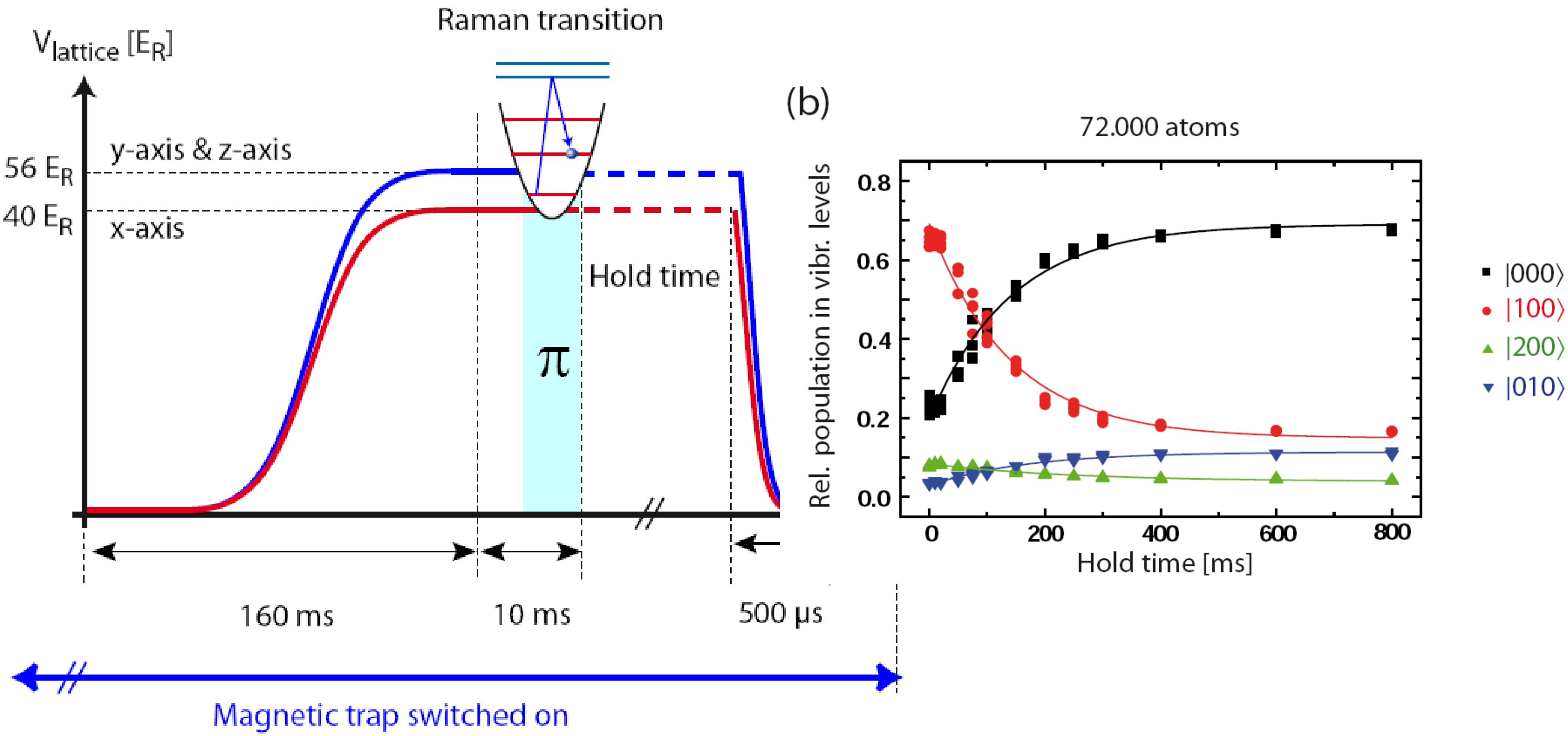
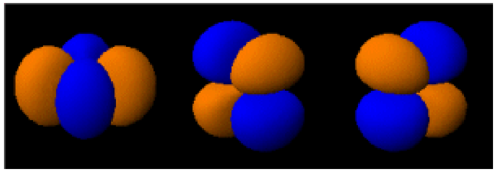
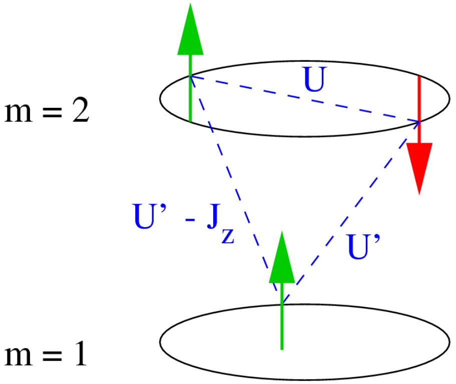


Many realizations of systems of ultracold atoms on optical lattices with flavor-specific hopping amplitudes (and interactions)!

OSMTs in 2-band Hubbard model

Minimal OSMT model: 2-band Hubbard model with
with orbital-dependent hopping





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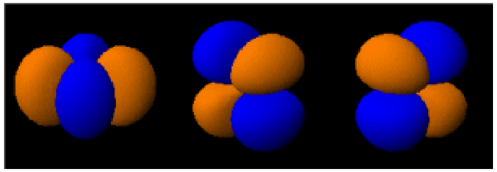

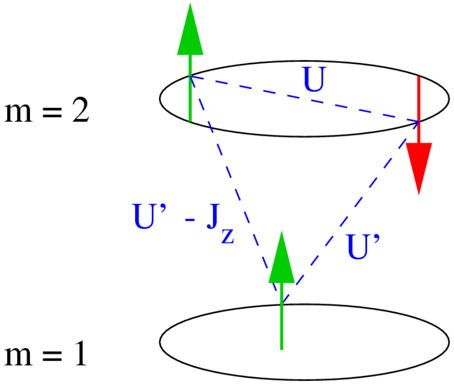

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Note: $J_\perp$ causes sign problem in (Hirsch-Fye) QMC
lattice, hopping anisotropic in $Ca_{2-x}Sr_xRuO_4$ $\rightsquigarrow$ coupling anisotropy?
quantum gas: no "spin-flip" terms for different atomic species

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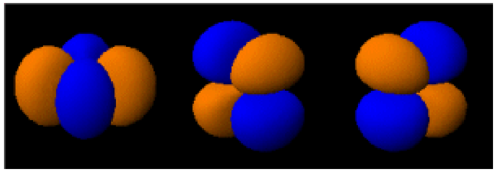

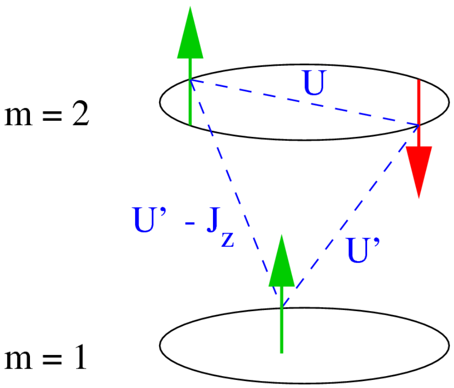

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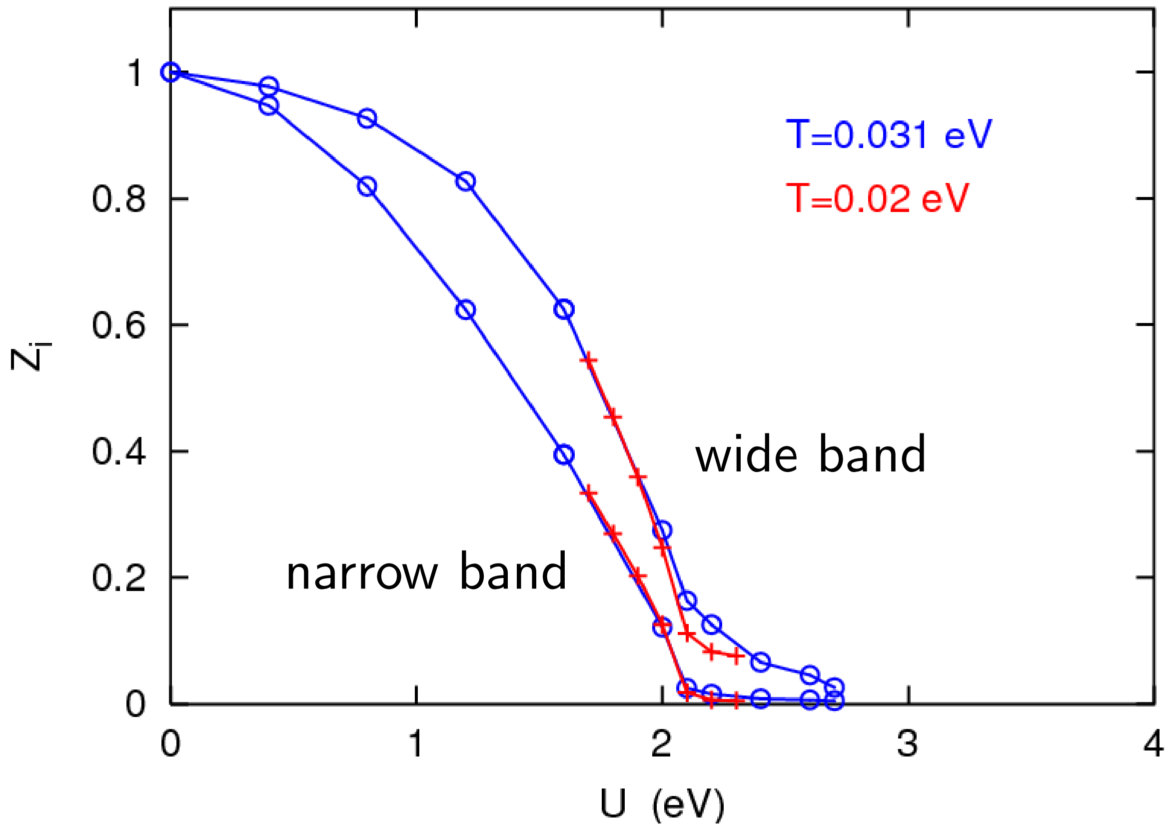
Bethe DOS, $t_2 = 2\,t_1$: two distinct MITs for $J_z = J_\perp = U/4$ [Koga *et al.*, PRL (2004)]
single MIT or **two OSMTs** for J_z model $(J_\perp = 0)$ **?**

Early DMFT-QMC results: single Mott transition in J_z model

Choice: $J_z = U/4,\ U' = U/2$

Metallicity $\sim$ qp weight

$Z_i = \frac{m}{m^*} \approx \left[1 - \mathrm{Im}\Sigma(i\pi T)/\pi T\right]^{-1}$



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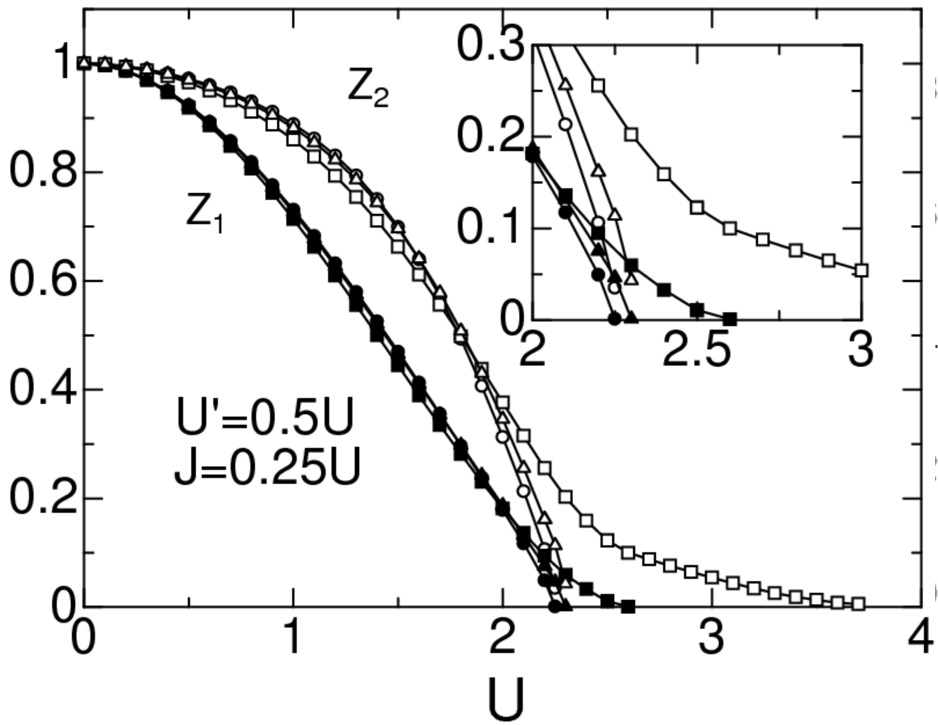
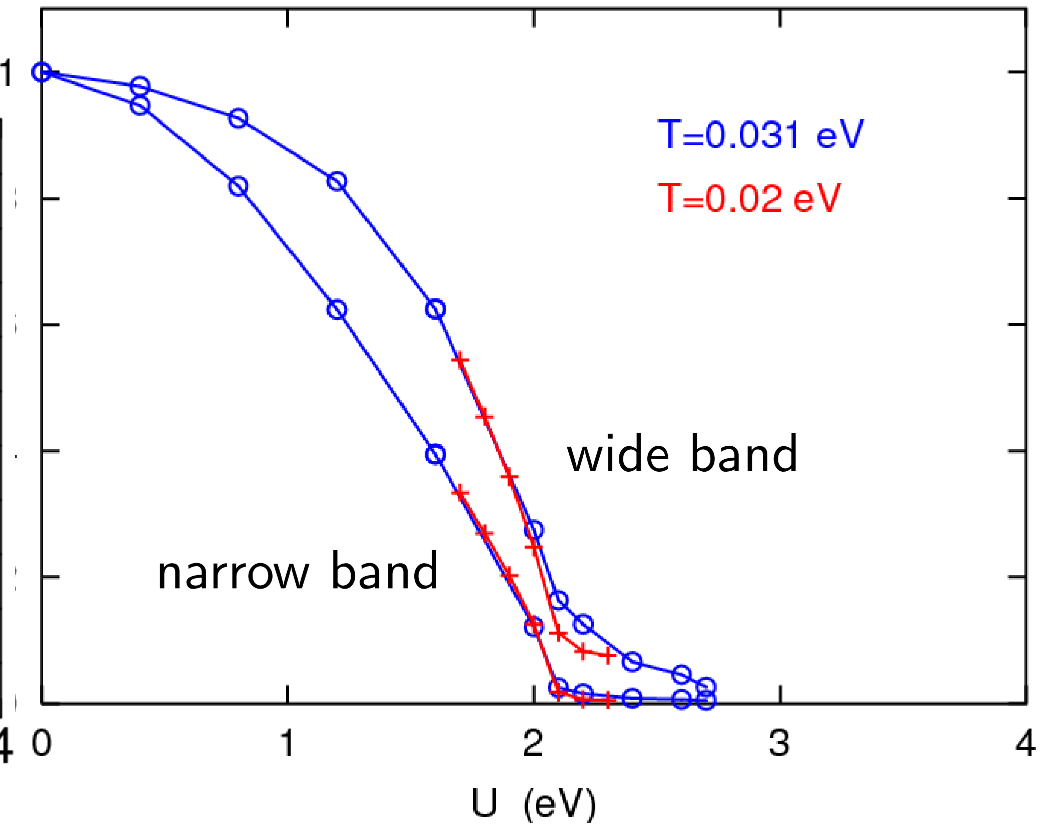




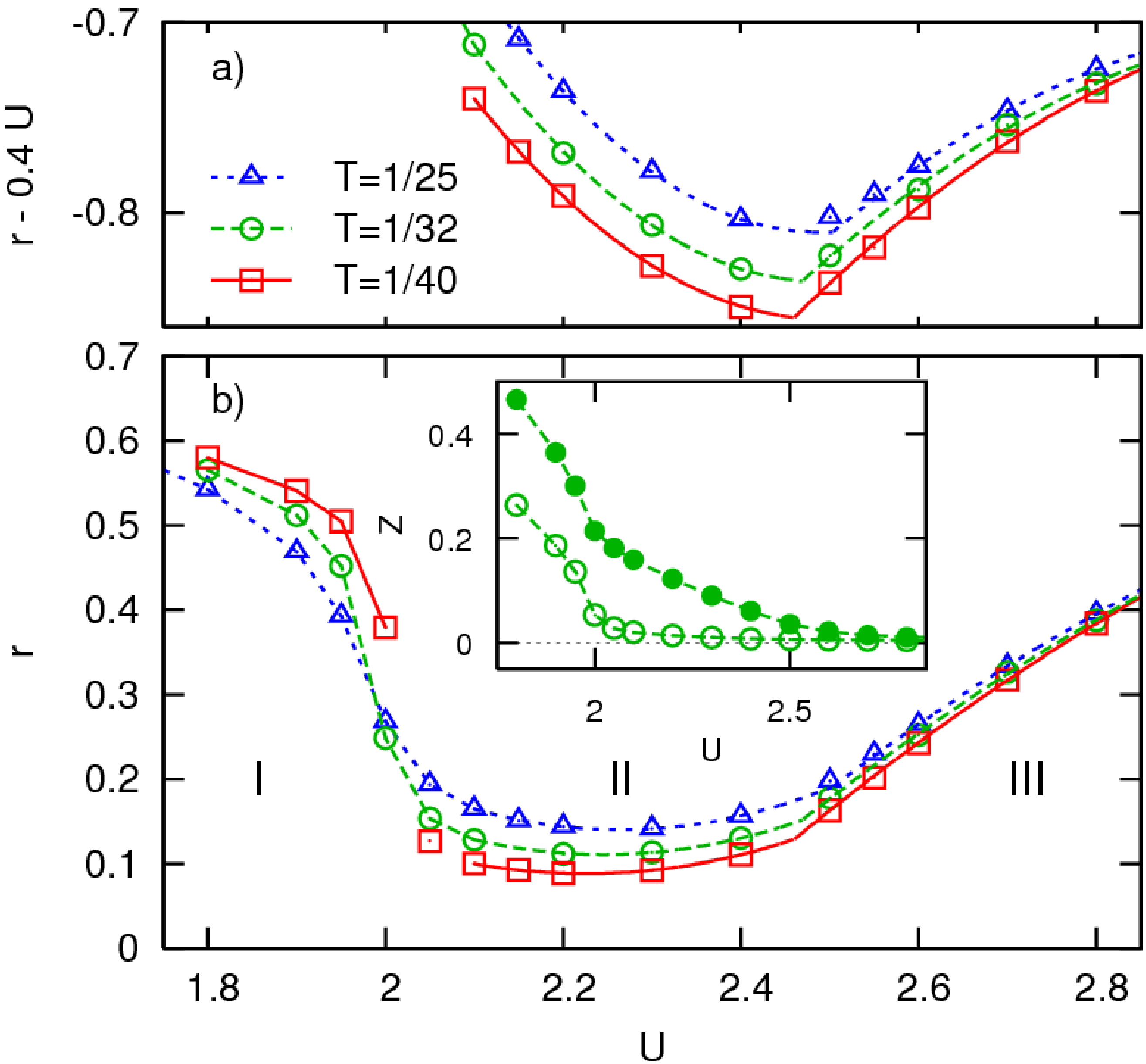
[Koga, Kawakami, Rice, Sigrist, Physica B (2005)]

[Liebsch, PRB **70**, 165103 (2004)]

Conclusion as of 03/2005: OSMT scenario in 2-band Hubbard model only for SU(2)-invariant Hund's exchange $(J_\perp = J_z)$!

Check using high-precision QMC algorithm . . .

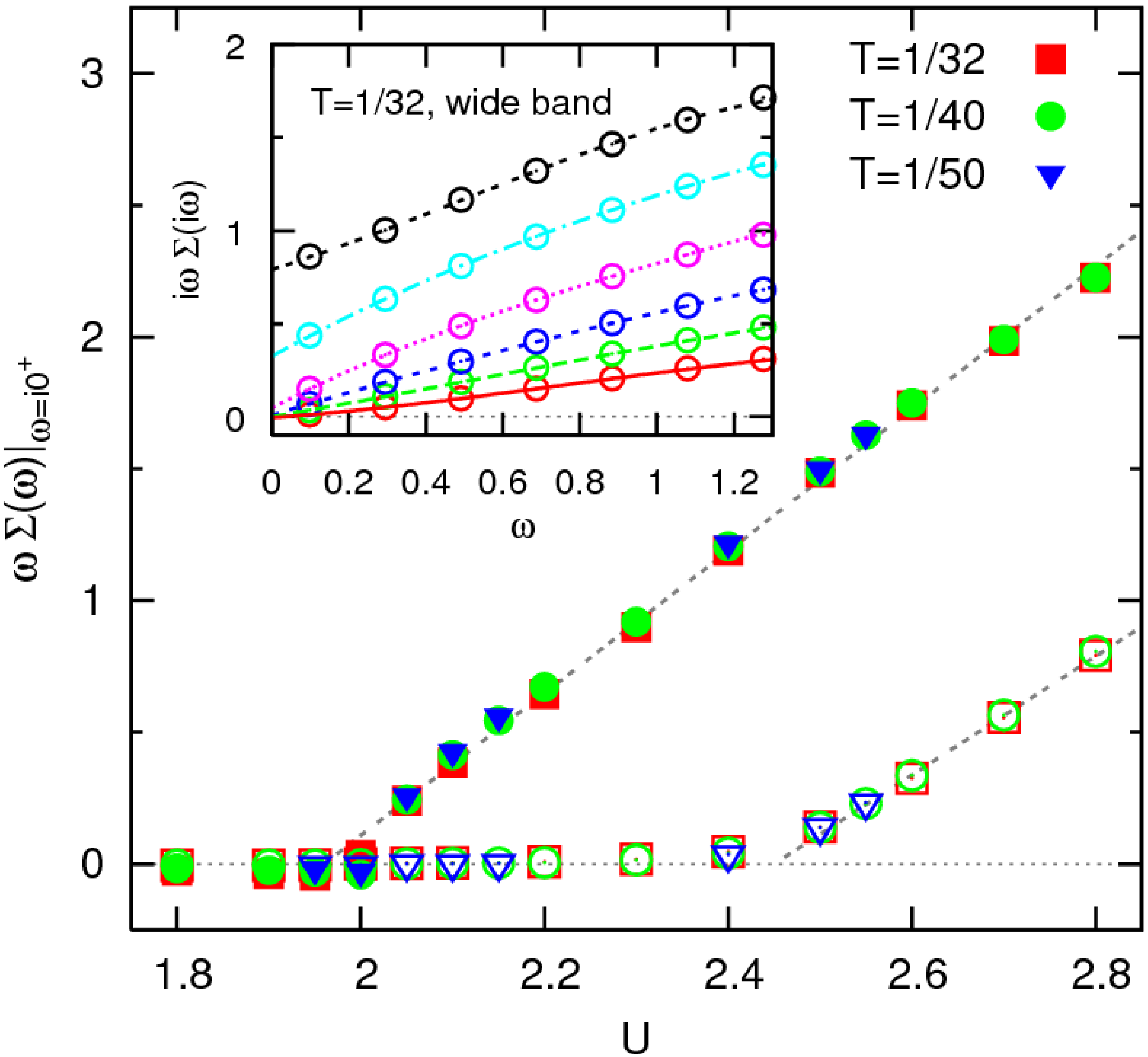
Ratio of quasiparticle weights $r = Z_{\text{narrow}}/Z_{\text{wide}}$



3 regions of different character

kinks indicate 2^{nd} transition at $U \approx 2.5$

Low-frequency analysis of self-energy



for regular self-energy:

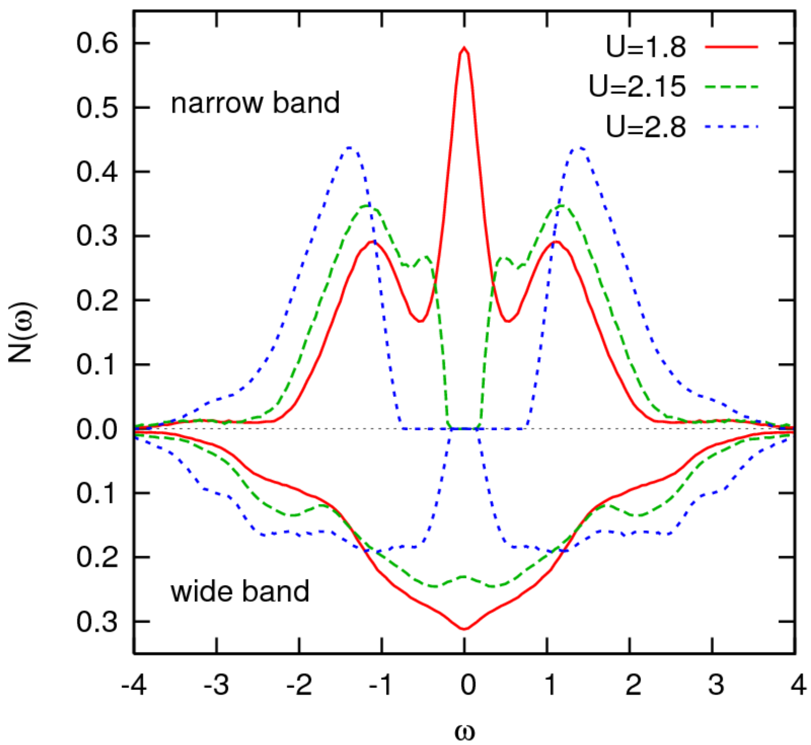
$\omega\Sigma(\omega) \stackrel{\omega\to 0}{\longrightarrow} 0$

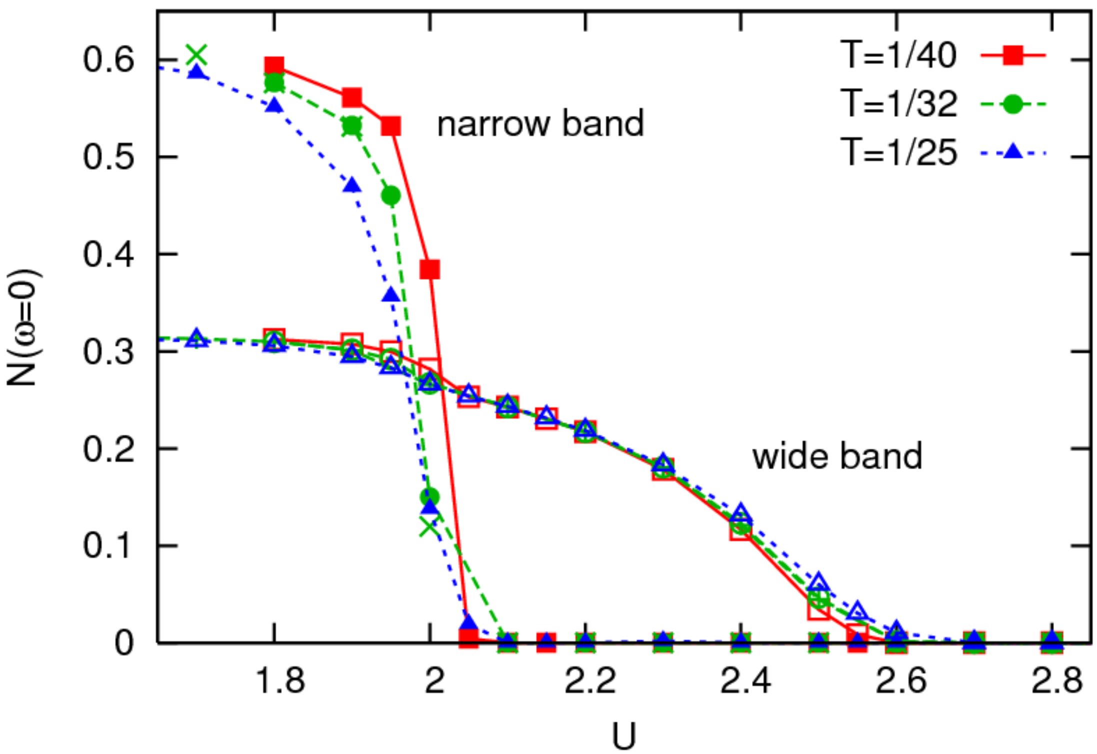
singularities ($\sim$ gap) for

$U \gtrsim 2$ in narrow band

$U \gtrsim 2.5$ in wide band

Spectral function (interacting DOS)





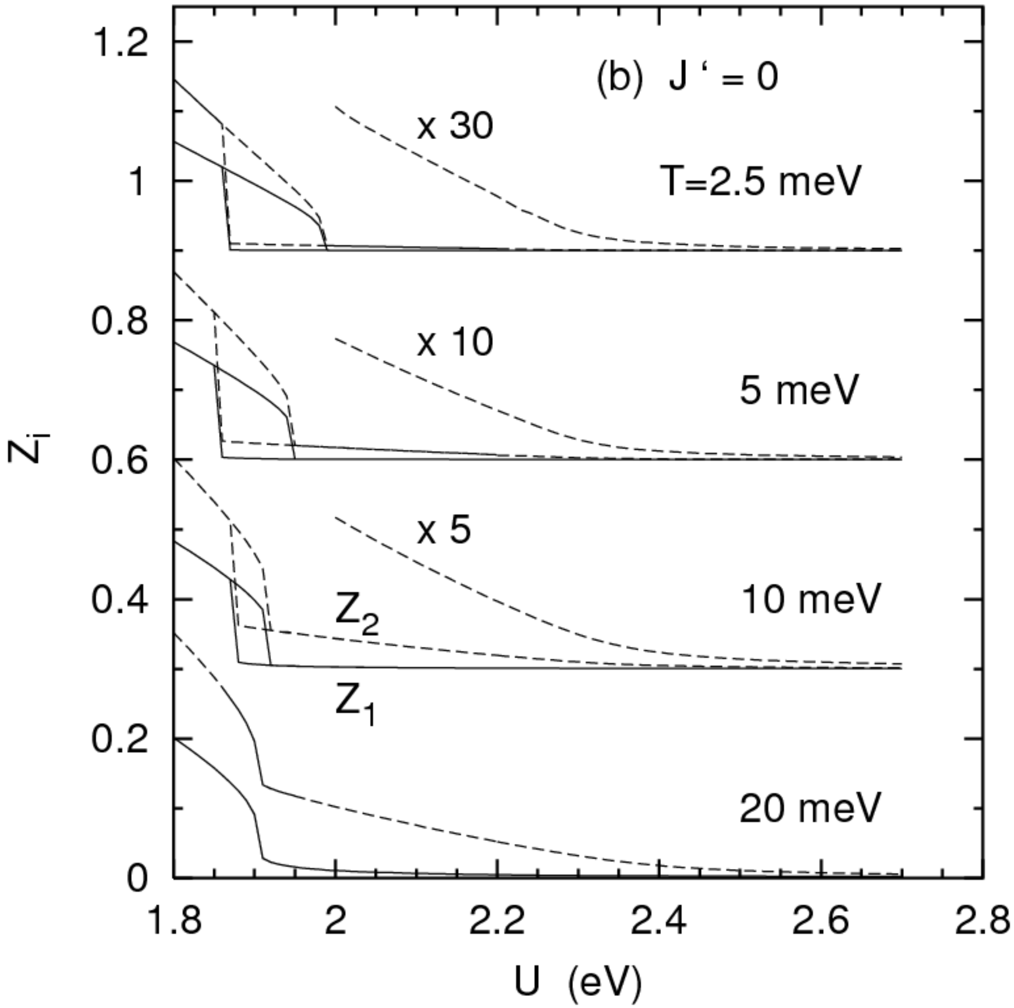
Clear indications for second singularity, wide band remains metallic at $U \approx 2.0$

$\rightsquigarrow$ **two orbital-selective Mott transitions** [Knecht, NB, van Dongen, PRB (2005)]

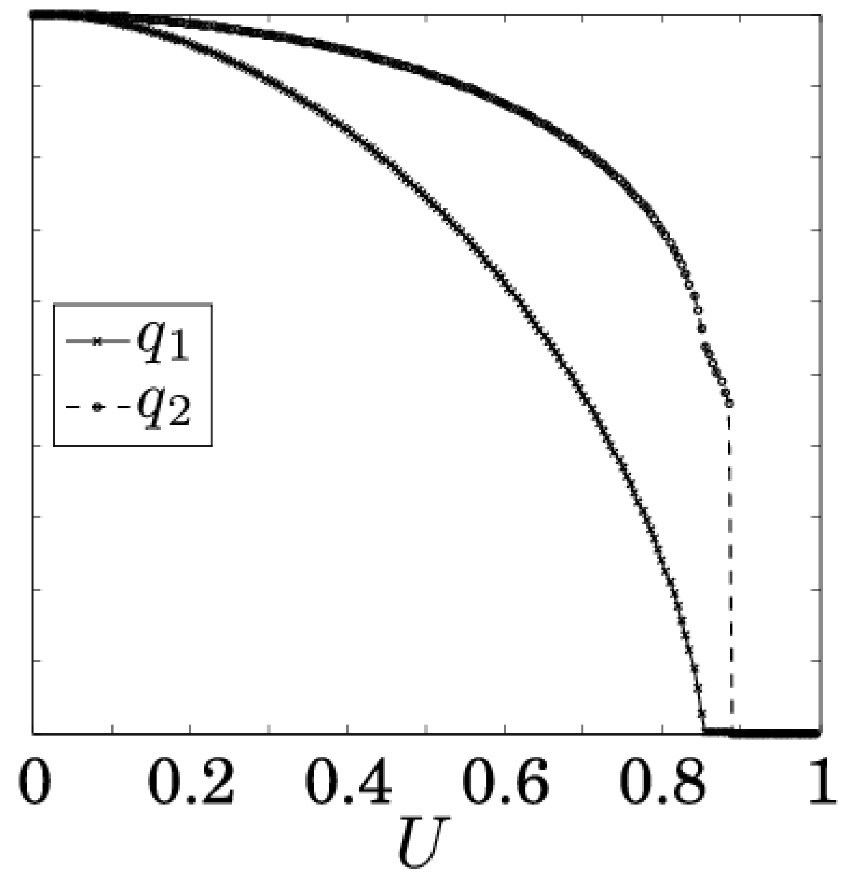
same conclusions from slave-spin approx. [de' Medici, Georges, Biermann, PRB (2005)]

and slave-boson MF [Rüegg, Indergand, Pilgram, Sigrist, EPJB (2005)]

Order of wide-band transition at $T > 0$ and $T = 0$



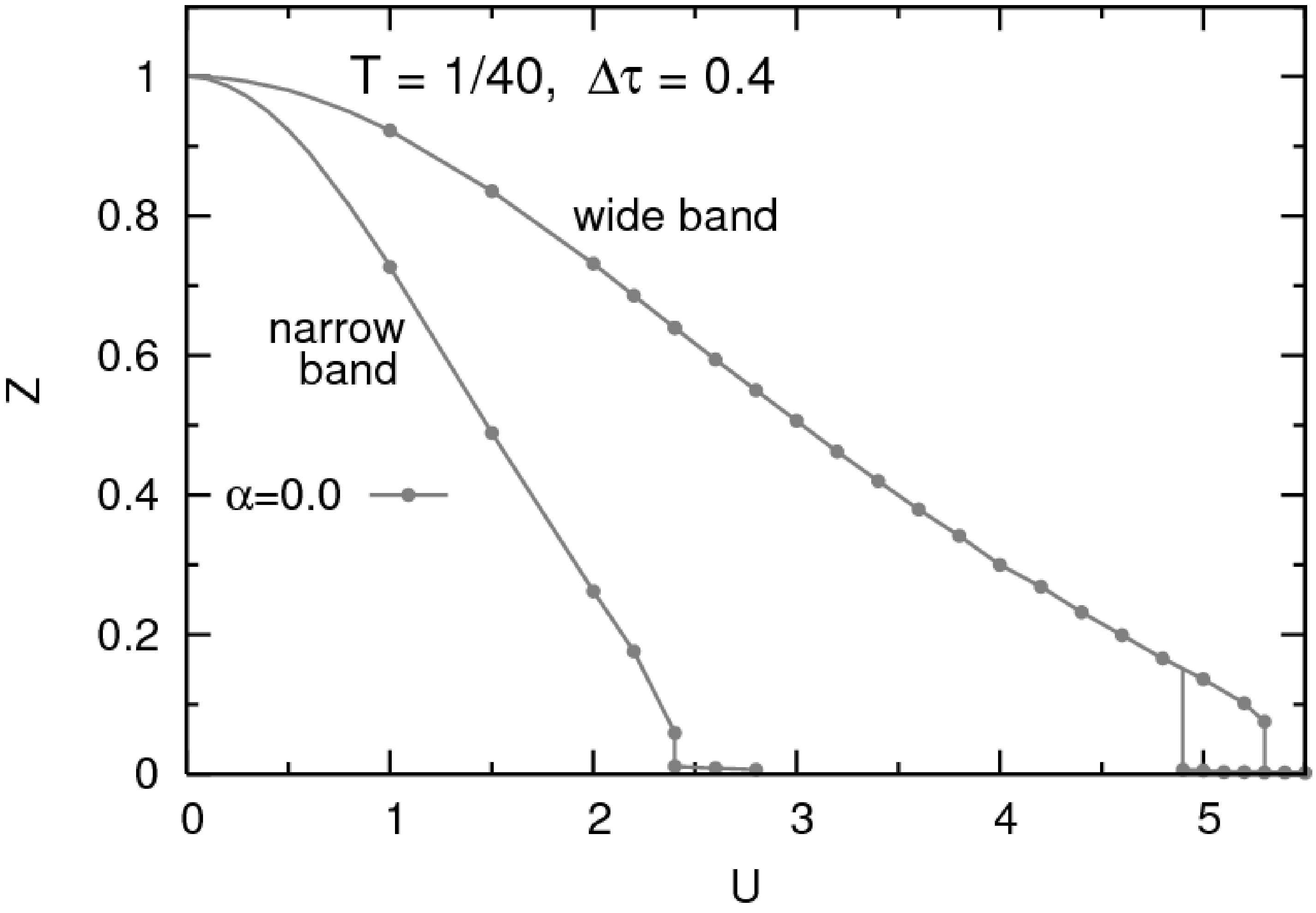
ED ⇝ no hysteresis at low T for wide-band transition [Liebsch, PRL (2005)]



Slave-boson MF ⇝ 1^{st} order wide-band transition (at $T = 0$) [Rüegg, Indergand, Pilgram, Sigrist, EPJB (2005)]

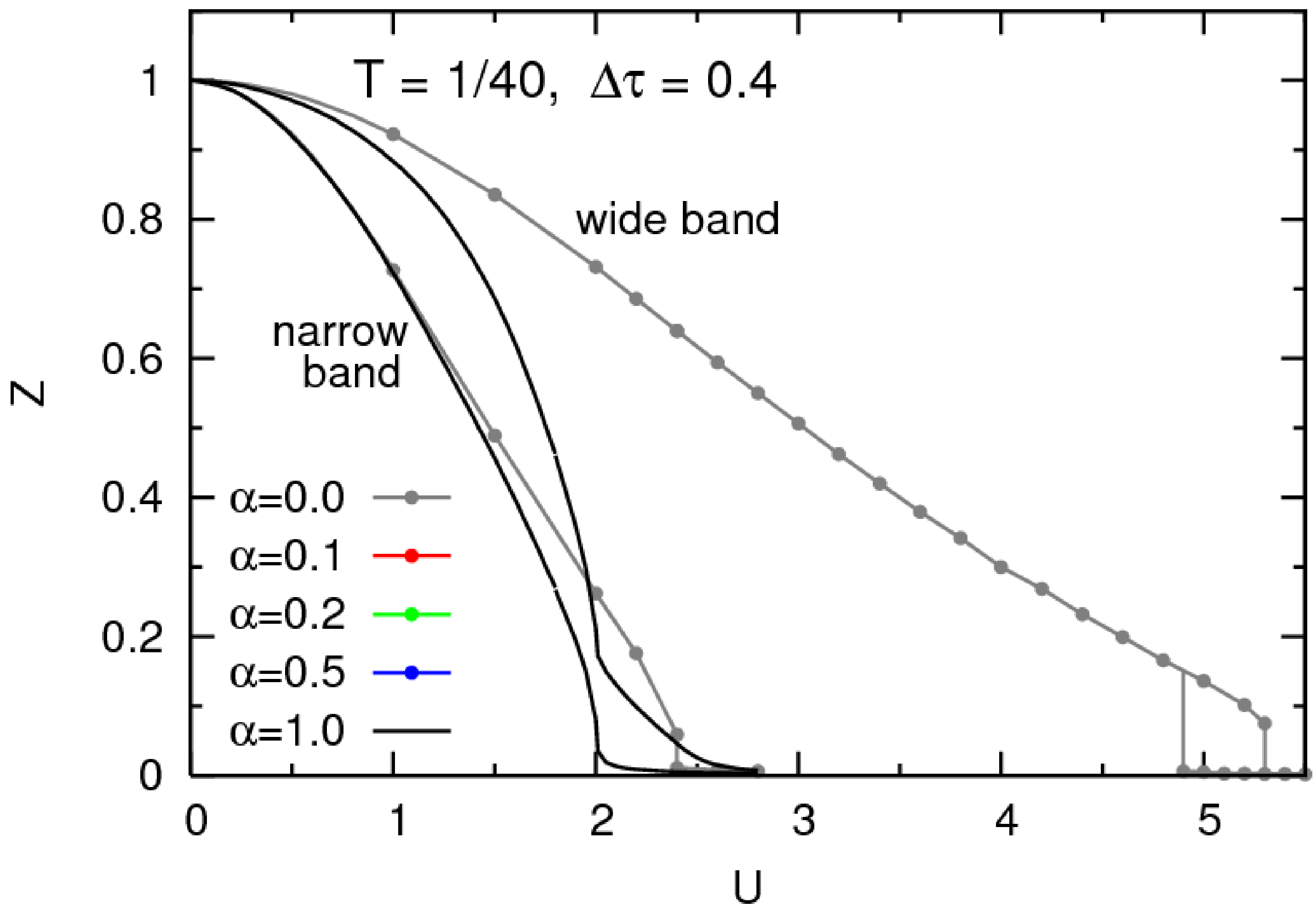
Systematic study: effect of inter-orbital coupling

$$H = \sum_{m=1}^{2} \left[-\sum_{\langle ij \rangle \sigma} t_m c^\dagger_{im\sigma} c_{jm\sigma} + U \sum_i n_{im\uparrow} n_{im\downarrow} \right] + \alpha \sum_{i\sigma\sigma'} (U/2 - \delta_{\sigma\sigma'} U/4)\, n_{i1\sigma}\, n_{i2\sigma'}$$



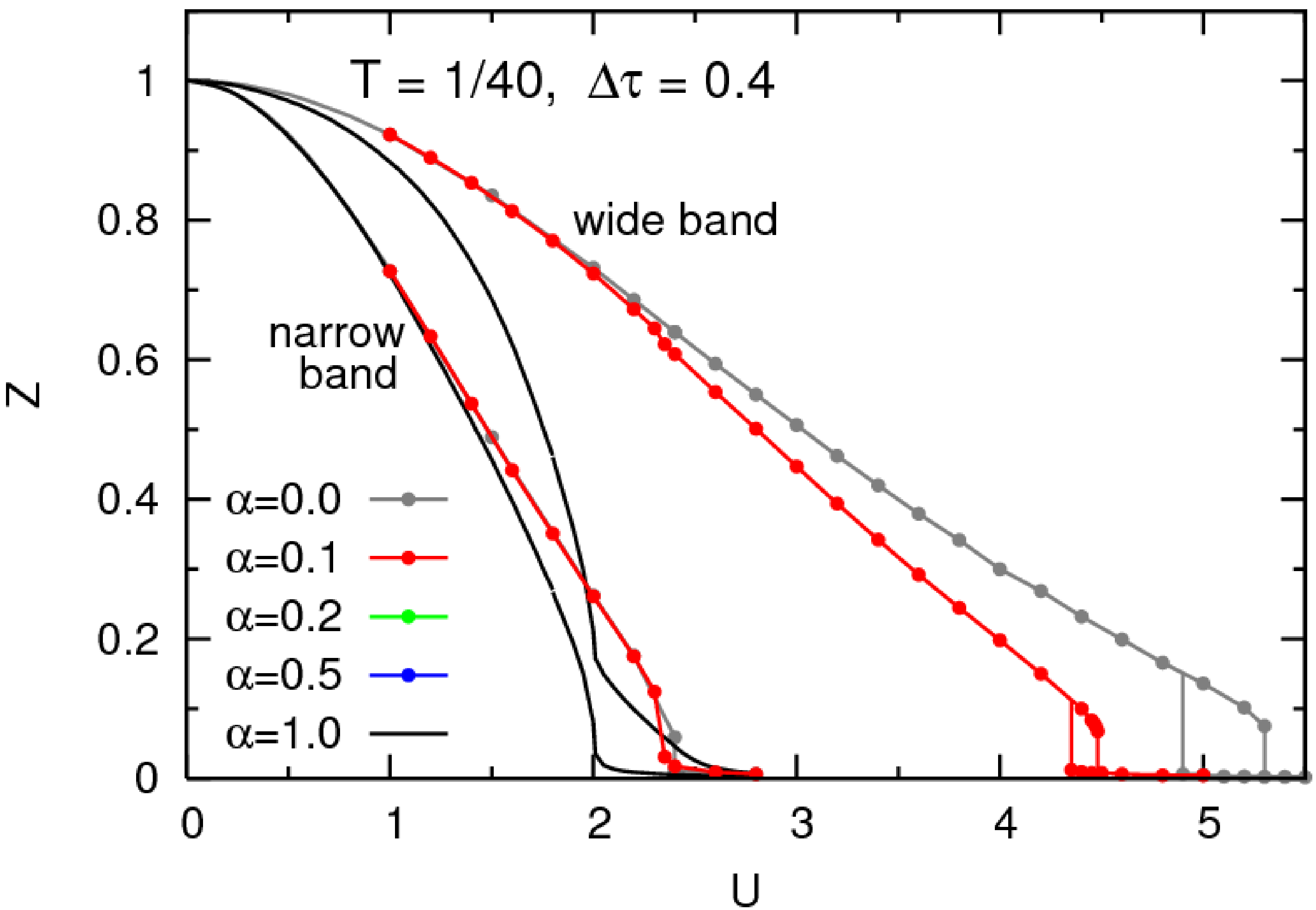
Systematic study: effect of inter-orbital coupling

$$H = \sum_{m=1}^{2} \left[-\sum_{\langle ij \rangle \sigma} t_m c^\dagger_{im\sigma} c_{jm\sigma} + U \sum_i n_{im\uparrow} n_{im\downarrow} \right] + \alpha \sum_{i\sigma\sigma'} (U/2 - \delta_{\sigma\sigma'} U/4)\, n_{i1\sigma}\, n_{i2\sigma'}$$



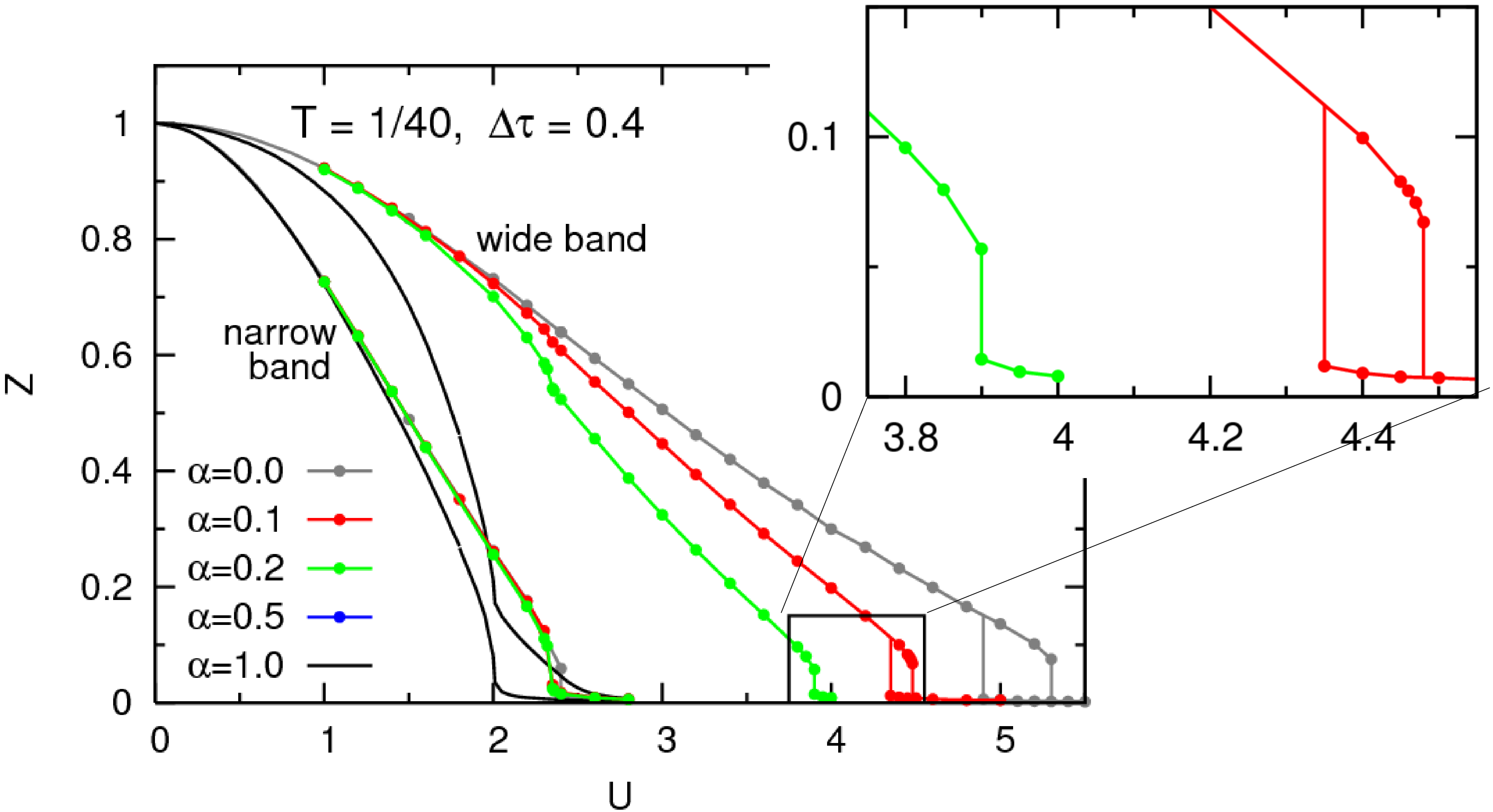
Systematic study: effect of inter-orbital coupling

$$H = \sum_{m=1}^{2} \Big[-\sum_{\langle ij \rangle \sigma} t_m c^\dagger_{im\sigma} c_{jm\sigma} + U \sum_i n_{im\uparrow} n_{im\downarrow} \Big] + \alpha \sum_{i\sigma\sigma'} (U/2 - \delta_{\sigma\sigma'} U/4)\, n_{i1\sigma}\, n_{i2\sigma'}$$



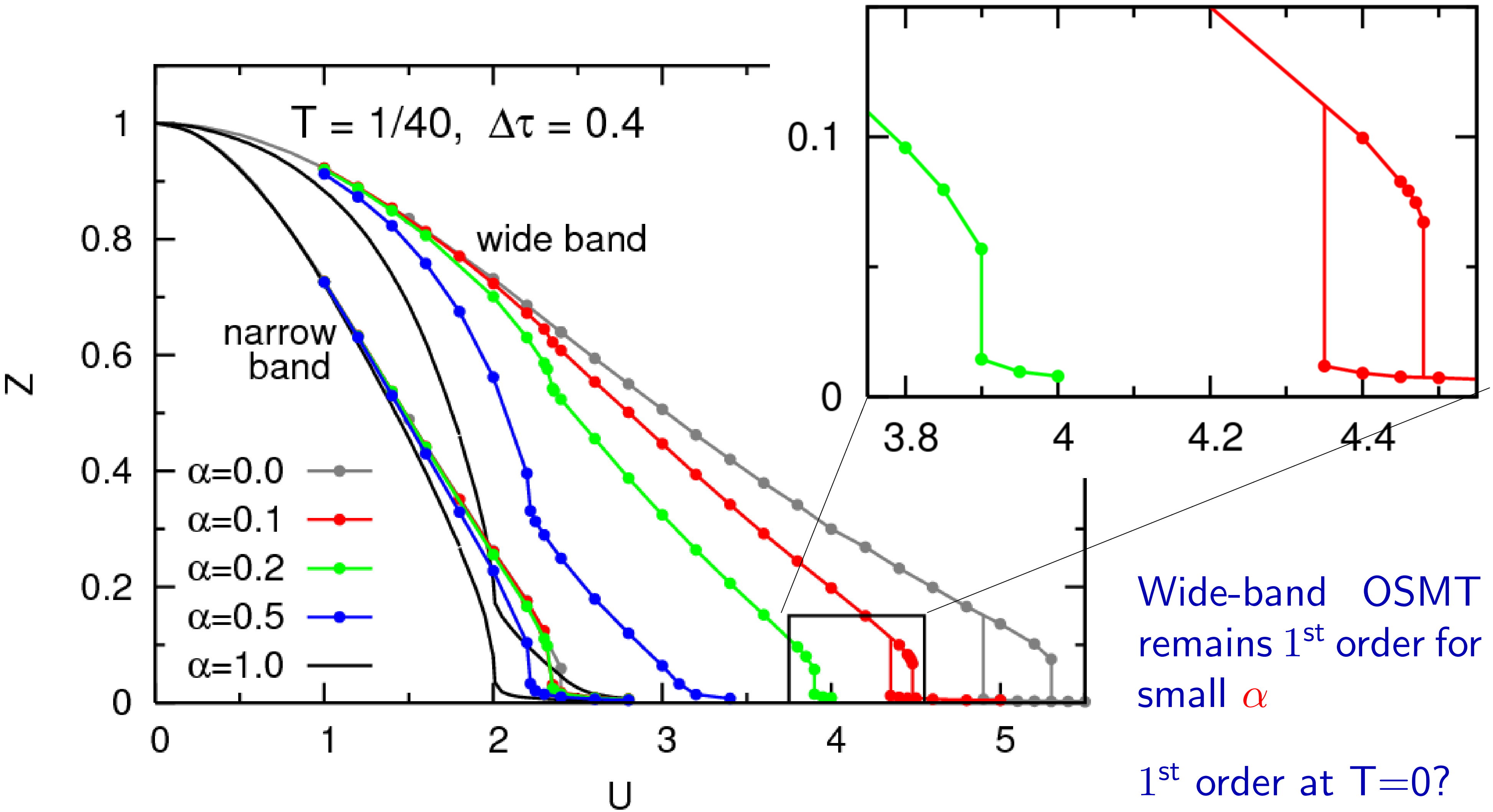
Systematic study: effect of inter-orbital coupling

$$H = \sum_{m=1}^{2}\left[-\sum_{\langle ij\rangle\sigma} t_m c^\dagger_{im\sigma} c_{jm\sigma} + U\sum_i n_{im\uparrow} n_{im\downarrow}\right] + \alpha \sum (U/2 - \delta_{\sigma\sigma'} U/4)\, n_{i1\sigma}\, n_{i2\sigma'}$$



Systematic study: effect of inter-orbital coupling

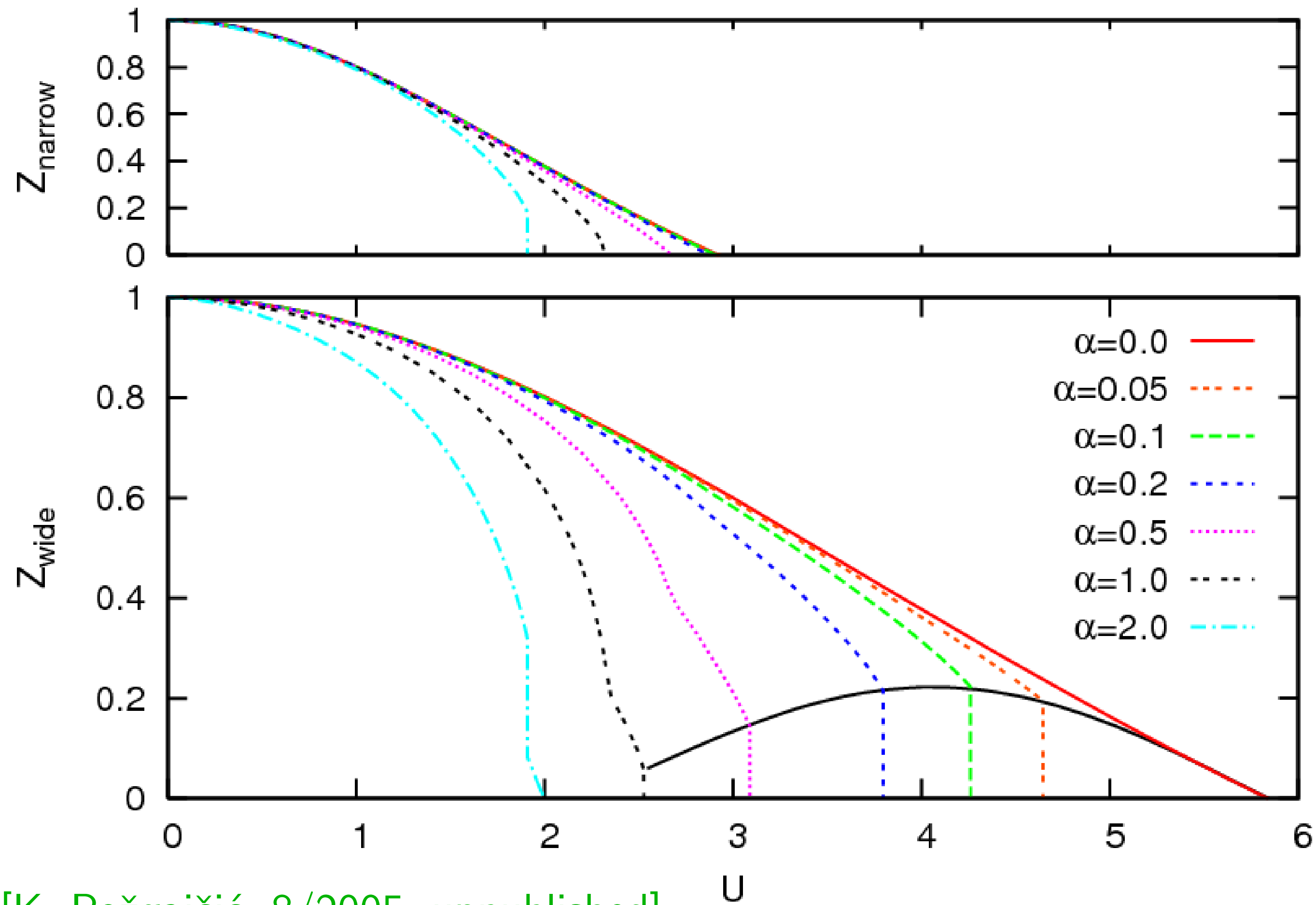
$$H = \sum_{m=1}^{2} \left[-\sum_{\langle ij \rangle \sigma} t_m c^\dagger_{im\sigma} c_{jm\sigma} + U \sum_i n_{im\uparrow} n_{im\downarrow} \right] + \alpha \sum (U/2 - \delta_{\sigma\sigma'} U/4)\, n_{i1\sigma}\, n_{i2\sigma'}$$



Wide-band OSMT remains 1^{st} order for small α

1^{st} order at $T=0$?

Self-energy functional theory (SFT+ED) with 1 bath site per orbital



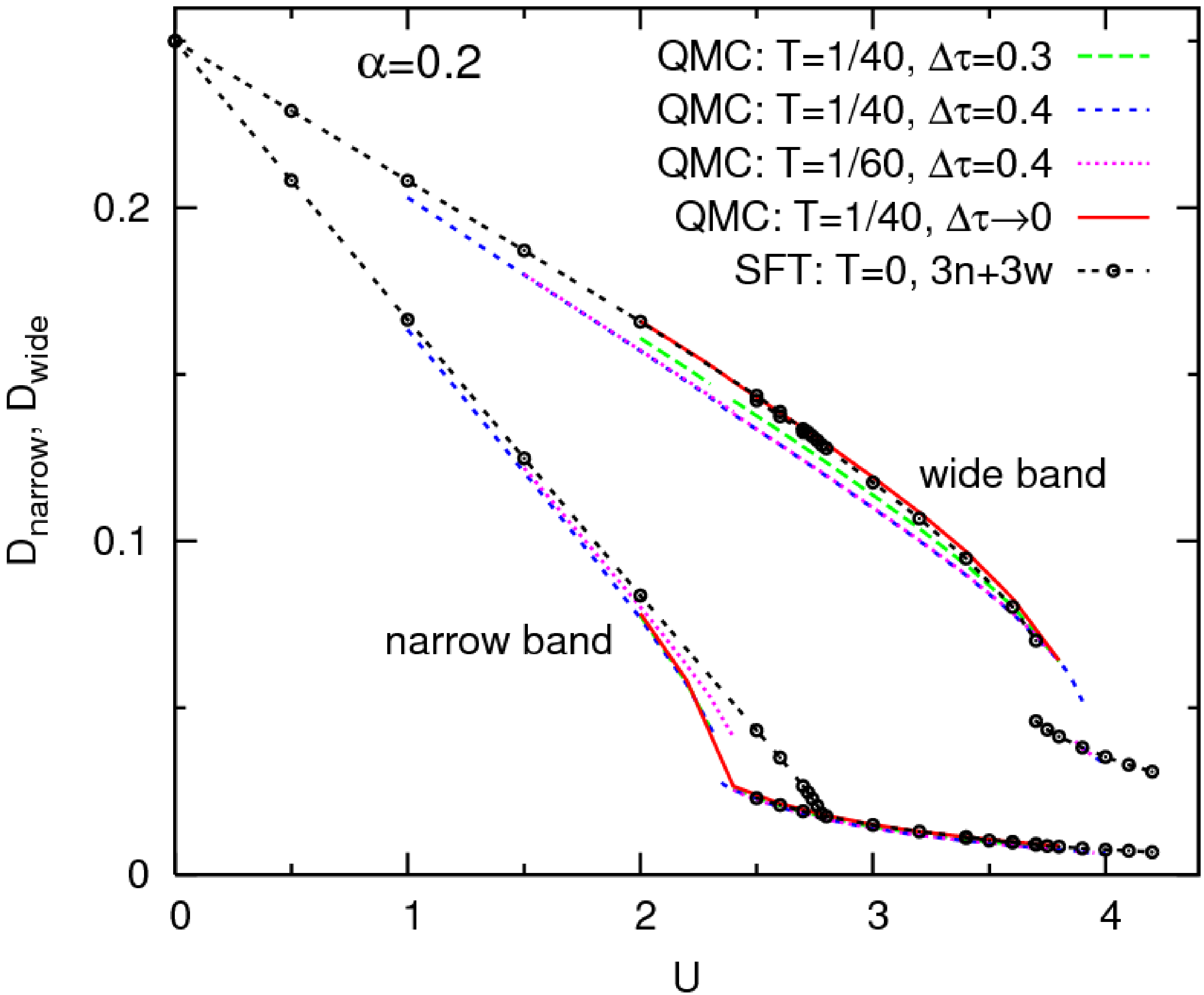
[K. Požgajčić, 8/2005, unpublished]

Problems: Low-frequency part of $\Sigma(\omega)$ inconsistent with QMC

Z problemetic in OSM phase $\rightsquigarrow$ search for kinks in Ω

massive finite-size effects with increasing number of bath sites!

Double occupancy (1^{st} order derivative of Ω)



Excellent agreement between SFT and QMC

1^{st} order at $T = 0$ (at least) for $0 < \alpha < 0.2$!?

Summary

Orbital-selective Mott transitions in 2-band Hubbard model ($J_z > J_\perp$)

transition at $U \approx 2.0$ is orbital-selective

clear indications for second singularity at $U \approx 2.5$

[C. Knecht, NB, P.G.J. van Dongen, Phys. Rev. B **72**, 081103(R) (2005)]

Systematic study: effect of inter-orbital coupling

wide-band OSMT 1^{st} order for small α for $T > 0$ and $T = 0$ (?)

[NB, C. Knecht, K. Požgajčić, P.G.J. van Dongen, JMMM **310**, 922 (2007)]

Not shown: Self-energy and quasiparticle weight Z in OSM phase
antiferromagnetic order, Falicov-Kimball model

[P.G.J. van Dongen, C. Knecht, NB, to appear in phys. stat. sol. (b)]

Not shown: many recent results - in particular on SU(2)-invariant Hund coupling and non-FL behavior - by Liebsch+Costi, Arita+Held, Koga/Inaba *et al.*, de'Medici +Biermann+Georges, Ferrero+Becca+Fabrizio+Capone, . . .

More OSMT physics: FeSi, (V_2O_3), fermions on optical lattices . . .