Orbital-selective Mott transitions in Hubbard models with orbital-dependent hopping

Nils Blümer, Carsten Knecht, Krunoslav Požgajčić,

and Peter van Dongen, Univ. Mainz

Outline

Motivation: OSMTs in $Ca_{2-x}Sr_xRuO_4$

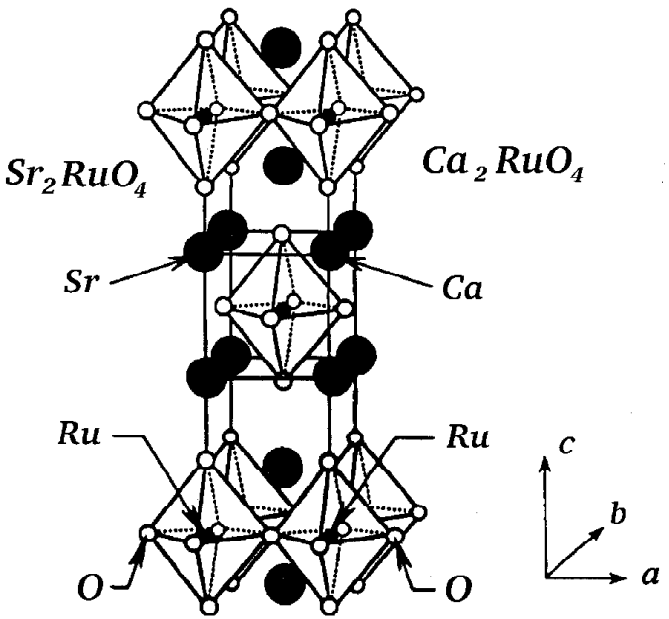
Orbital-selective Mott transitions in 2-band Hubbard model

Systematic study: effect of inter-orbital coupling

Self-energy and quasiparticle weight Z in OSM phase

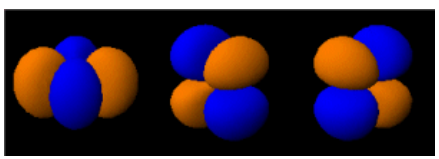
Summary

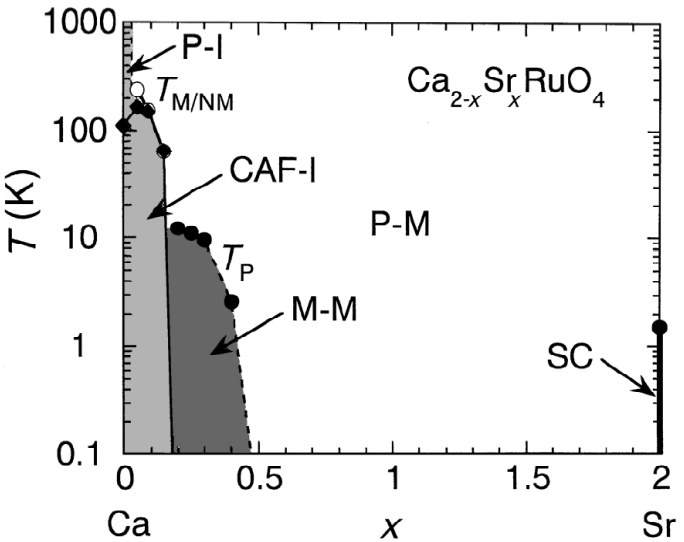
Motivation: OSMTs in $Ca_{2-x}Sr_xRuO_4$



isostructural to $La_{2-x}Sr_xCuO_4$

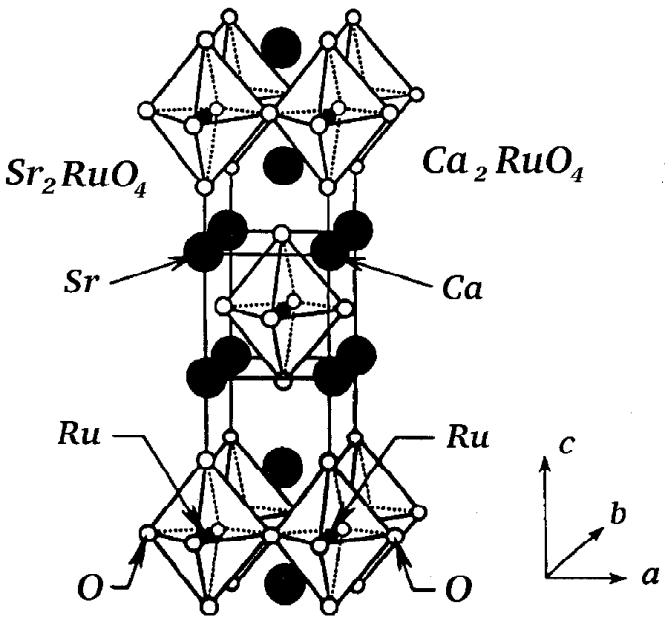
valence states: Ru t_{2g} orbitals





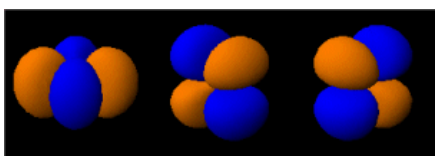
[Nakatsuji, Maeno, PRL (2000)]

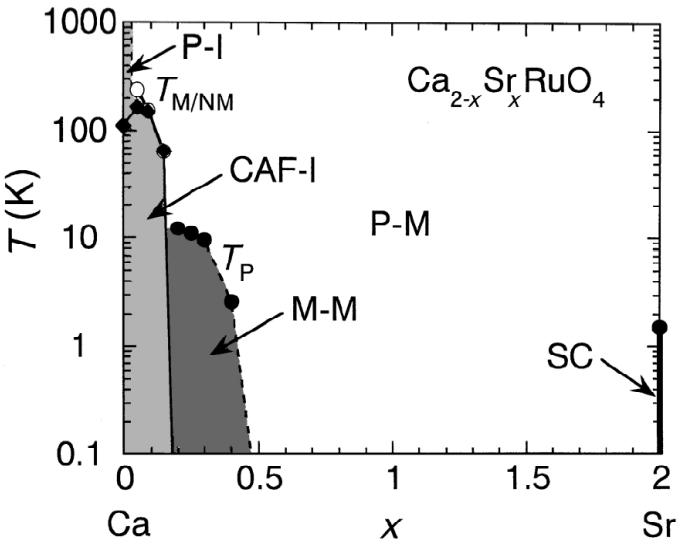
Motivation: OSMTs in $Ca_{2-x}Sr_xRuO_4$



isostructural to $La_{2-x}Sr_xCuO_4$

valence states:
Ru t_{2g} orbitals



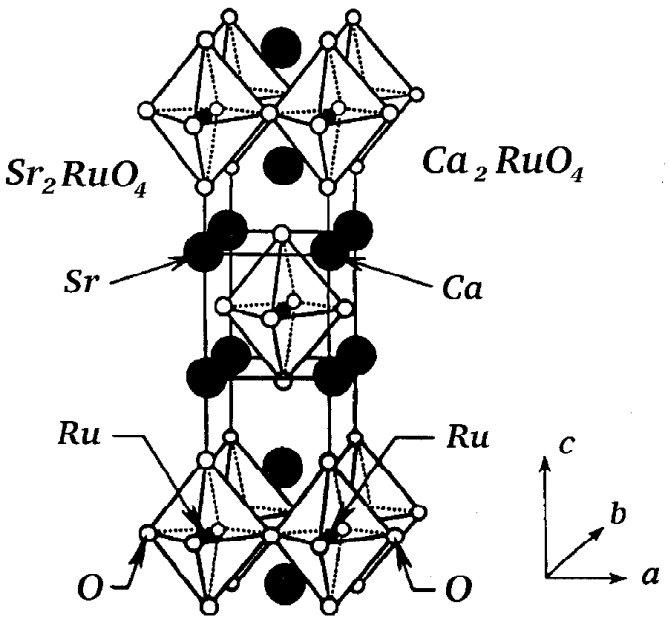


[Nakatsuji, Maeno, PRL (2000)]

saturation moment, susceptibility, MR $\rightsquigarrow$ $S = 1/2$ system for $x \gtrsim 0.2$ (not $S = 1$)

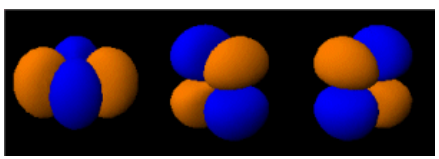
orbital-selective Mott metal-insulator transitions for $x \approx 0.5$, $x \approx 0.2$?

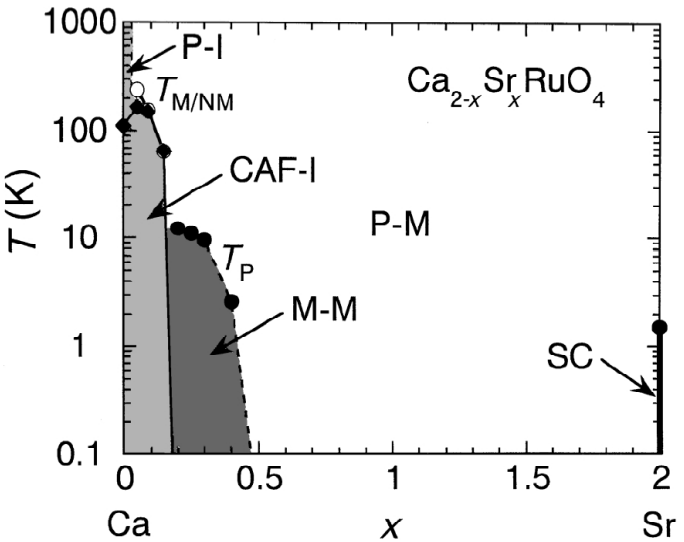
Motivation: OSMTs in $Ca_{2-x}Sr_xRuO_4$



isostructural to $La_{2-x}Sr_xCuO_4$

valence states: Ru t_{2g} orbitals





[Nakatsuji, Maeno, PRL (2000)]

saturation moment, susceptibility, MR $\rightsquigarrow$ $S = 1/2$ system for $x \gtrsim 0.2$ (not $S = 1$)

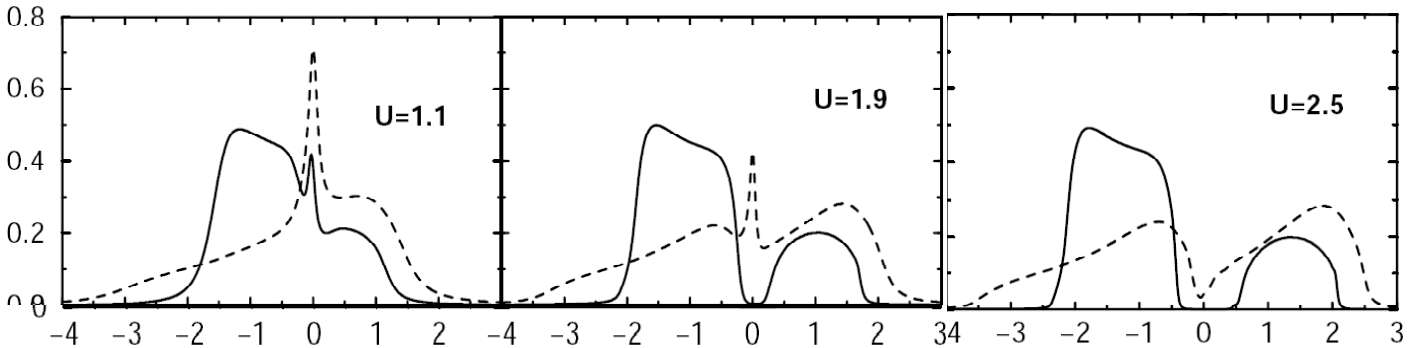
orbital-selective Mott metal-insulator transitions for $x \approx 0.5$, $x \approx 0.2$?

Anisimov, Nekrasov, Kondakov, Rice, Sigrist (EPJB 2002): yes!

Liebsch (EPL 2003, PRL 2003, PRB 2004): no!

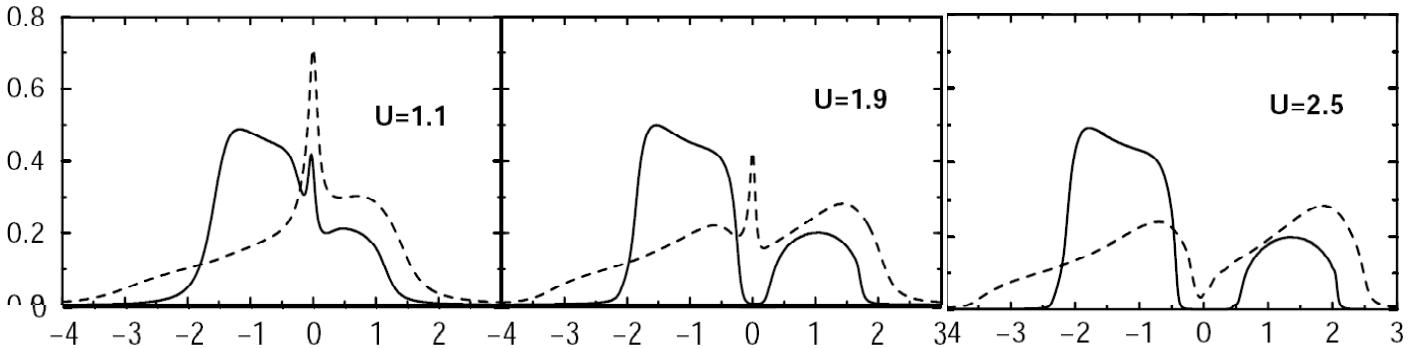
OSMTs in 2-band Hubbard model

LDA+DMFT(NCA)
for 2+1 bands
$\rightsquigarrow$ 2 OSMTs
[Anisimov et al. (2002)]



OSMTs in 2-band Hubbard model

LDA+DMFT(NCA)
for 2+1 bands
$\rightsquigarrow$ 2 OSMTs
[Anisimov et al. (2002)]

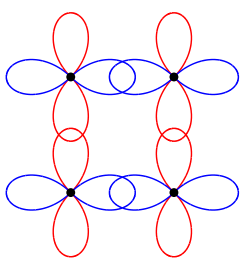


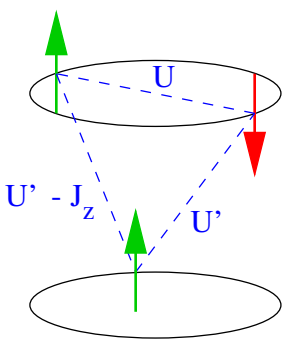
Minimal OSMT model: 2-band Hubbard model with orbital-dependent hopping

$$H = \sum_{m=1}^{2} \Big[- \sum_{\langle ij \rangle \sigma} t_m c^\dagger_{im\sigma} c_{jm\sigma} + U \sum_i n_{im\uparrow} n_{im\downarrow} \Big]$$

$$+ \sum_{i\sigma\sigma'} (U' - \delta_{\sigma\sigma'} J_z)\, n_{i1\sigma}\, n_{i2\sigma'}$$

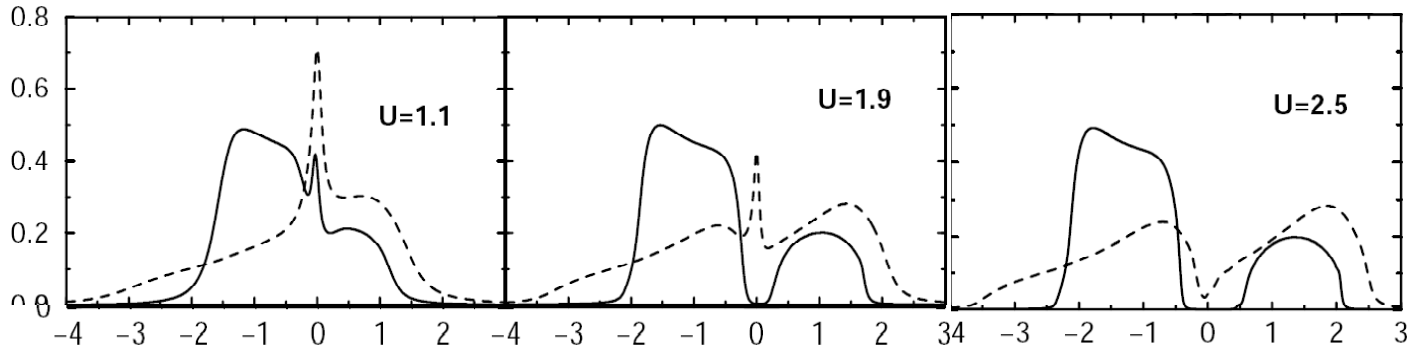
$$+ \tfrac{1}{2} J_\perp \sum_{i\sigma} \Big[c^\dagger_{i1\sigma} \left(c^\dagger_{i2\bar{\sigma}} c_{i1\bar{\sigma}} + c^\dagger_{i1\bar{\sigma}} c_{i2\bar{\sigma}} \right) c_{i2\sigma} + \text{h.c.} \Big]$$





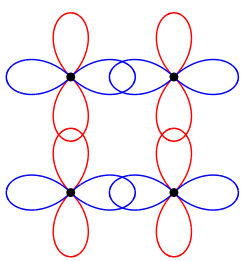
OSMTs in 2-band Hubbard model

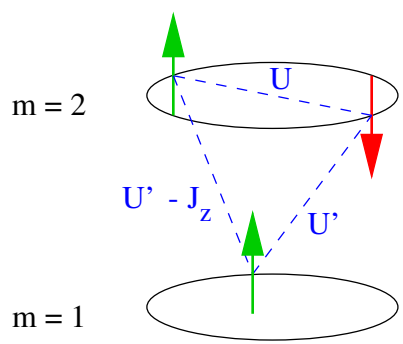
LDA+DMFT(NCA)
for 2+1 bands
$\rightsquigarrow$ 2 OSMTs
[Anisimov et al. (2002)]



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

$$H = \sum_{m=1}^{2}\Big[-\sum_{\langle ij\rangle\sigma} t_m c^\dagger_{im\sigma} c_{jm\sigma} + U\sum_i n_{im\uparrow} n_{im\downarrow}\Big]$$
$$+ \sum_{i\sigma\sigma'} (U' - \delta_{\sigma\sigma'} J_z)\, n_{i1\sigma}\, n_{i2\sigma'}$$
$$+ \tfrac{1}{2} J_\perp \sum_{i\sigma}\Big[c^\dagger_{i1\sigma}\left(c^\dagger_{i2\bar\sigma} c_{i1\bar\sigma} + c^\dagger_{i1\bar\sigma} c_{i2\bar\sigma}\right) c_{i2\sigma} + \text{h.c.}\Big]$$





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

Measure metallicity by

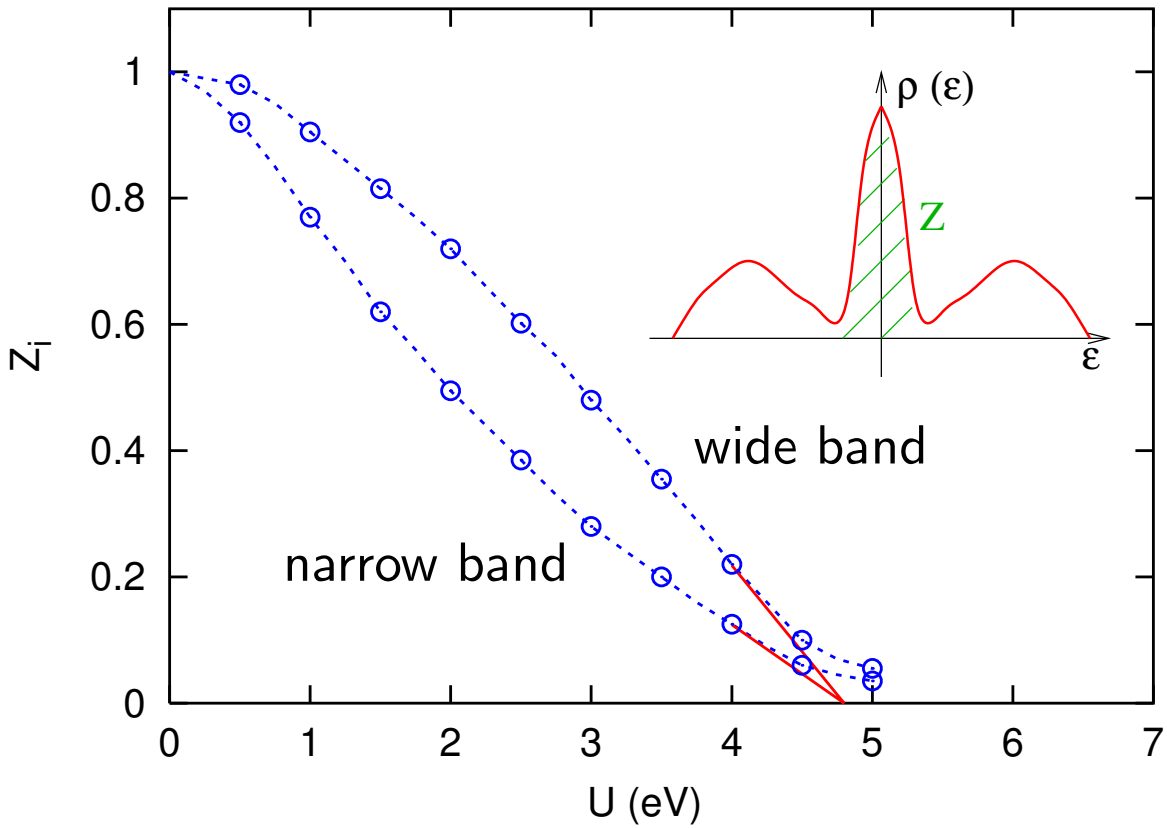
quasiparticle weight $Z_i = m/m_i^*$

discrete QMC estimate:

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

$J_z = 0.2,\ U' = U - 0.4$

[Liebsch, PRL **90**, 226401 (2003)]



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

Measure metallicity by

quasiparticle weight $Z_i = m/m_i^*$

discrete QMC estimate:

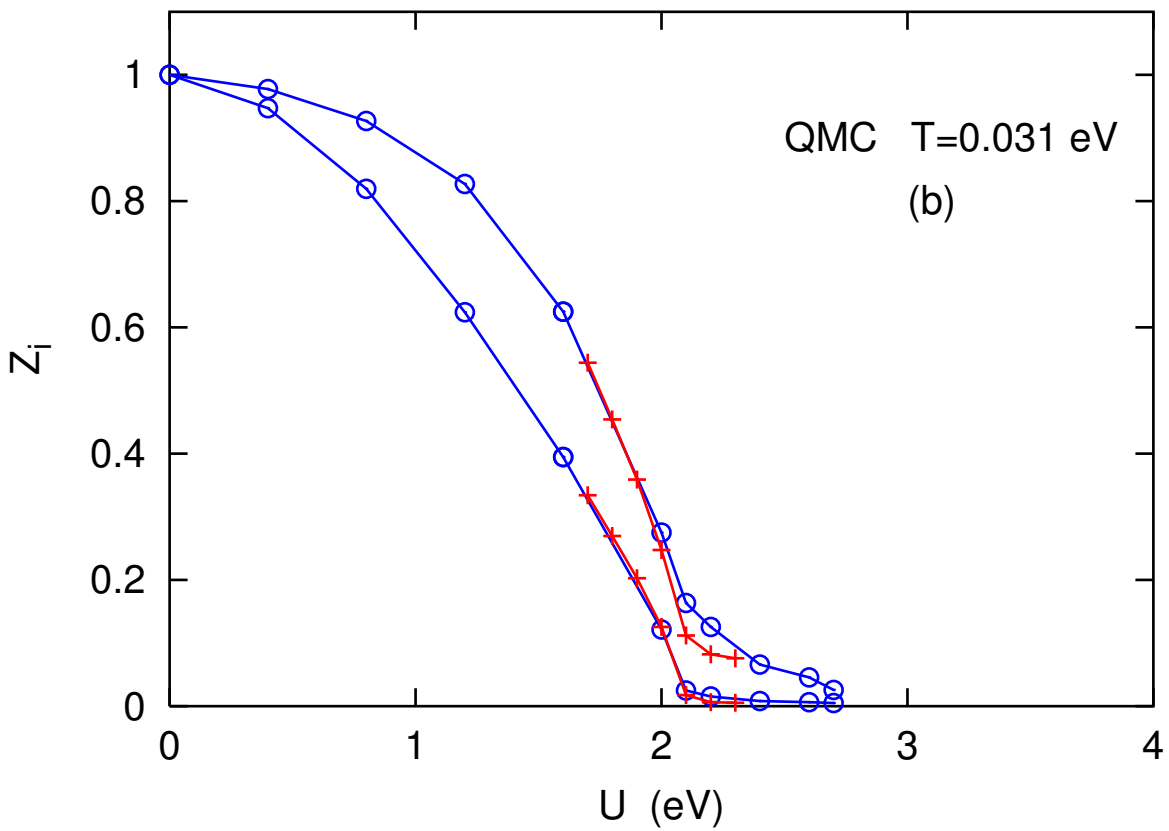
$Z_i \approx \left[1 - \mathrm{Im}\Sigma(i\pi T)/\pi T\right]^{-1}$

$J_z = 0.2,\ U' = U - 0.4$

[Liebsch, PRL **90**, 226401 (2003)]

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

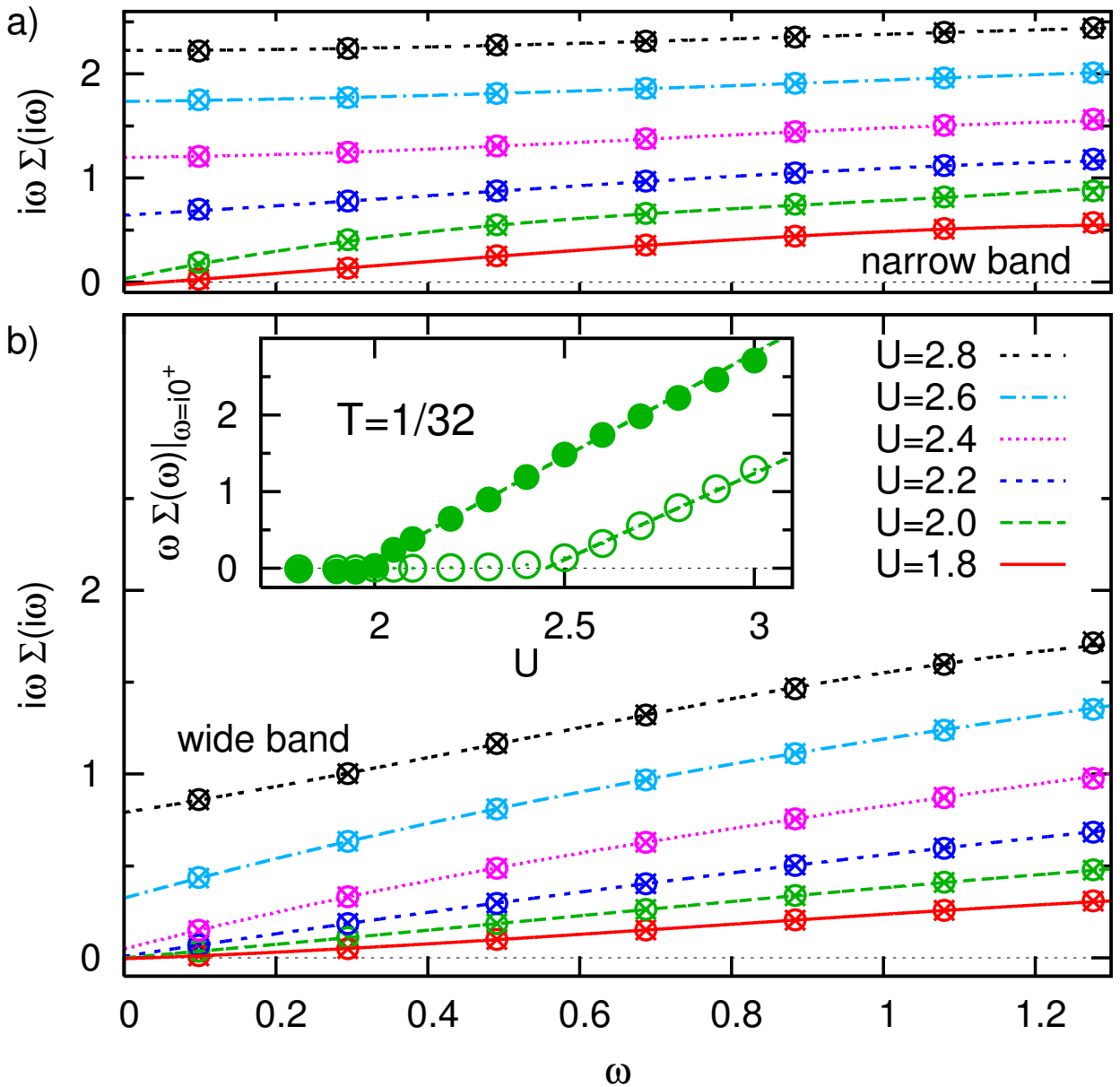
[Liebsch, PRB **70**, 165103 (2004)]



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 . . .

Low-frequency analysis of self-energy



for regular self-energy:

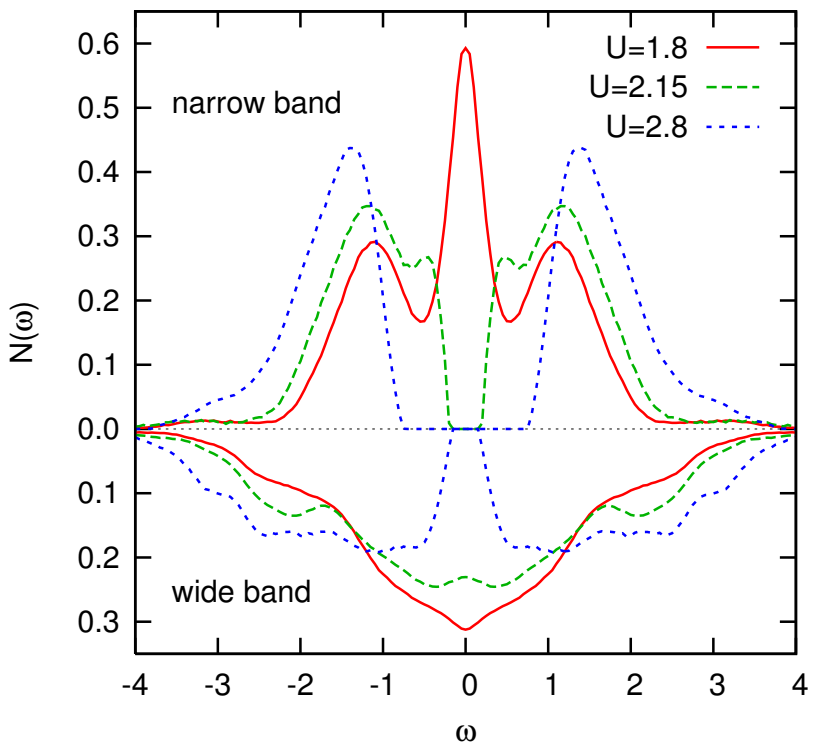
$\omega\Sigma(\omega) \stackrel{\omega\to 0}{\longrightarrow} 0$

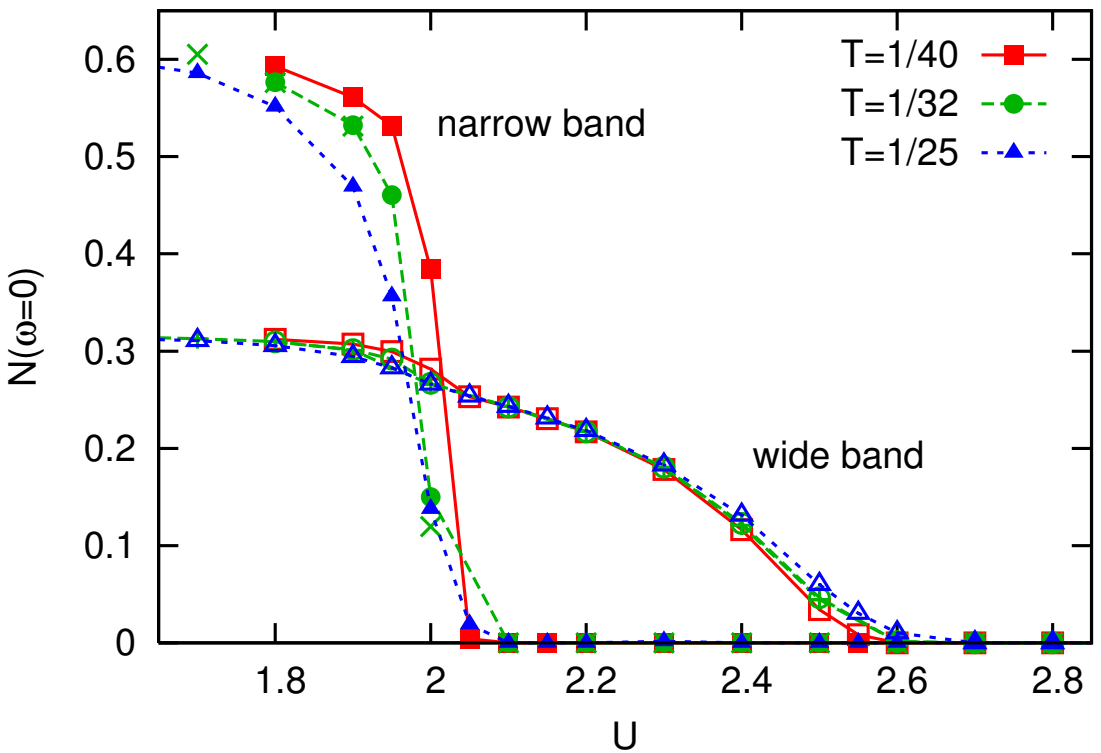
singularities ($\sim$ gap) for

$U \gtrsim 2$ in narrow band

$U \gtrsim 2.5$ in wide band

Spectral function (interacting DOS)





Clear indications for second singularity

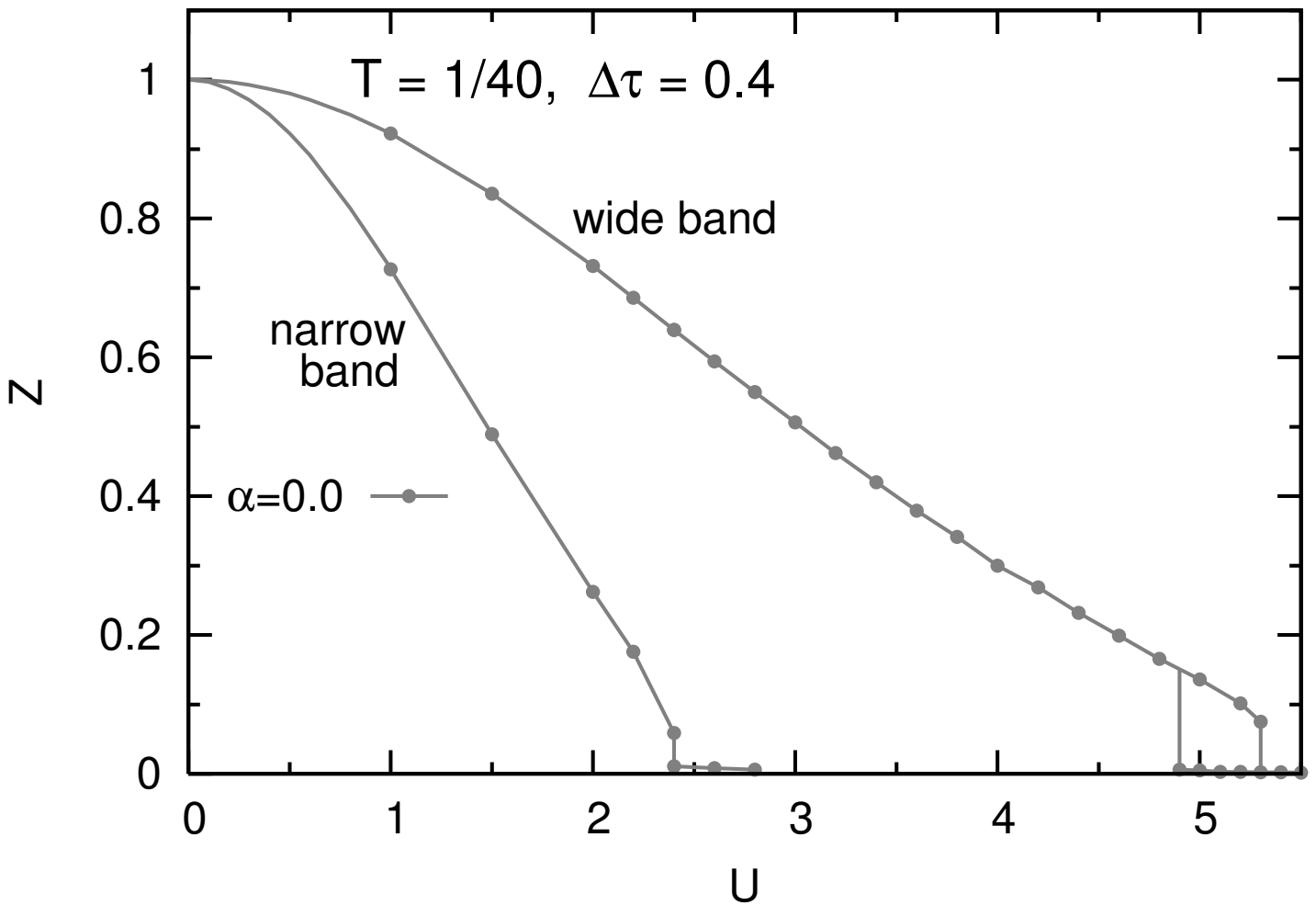
Wide band remains metallic at $U \approx 2.0$

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

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

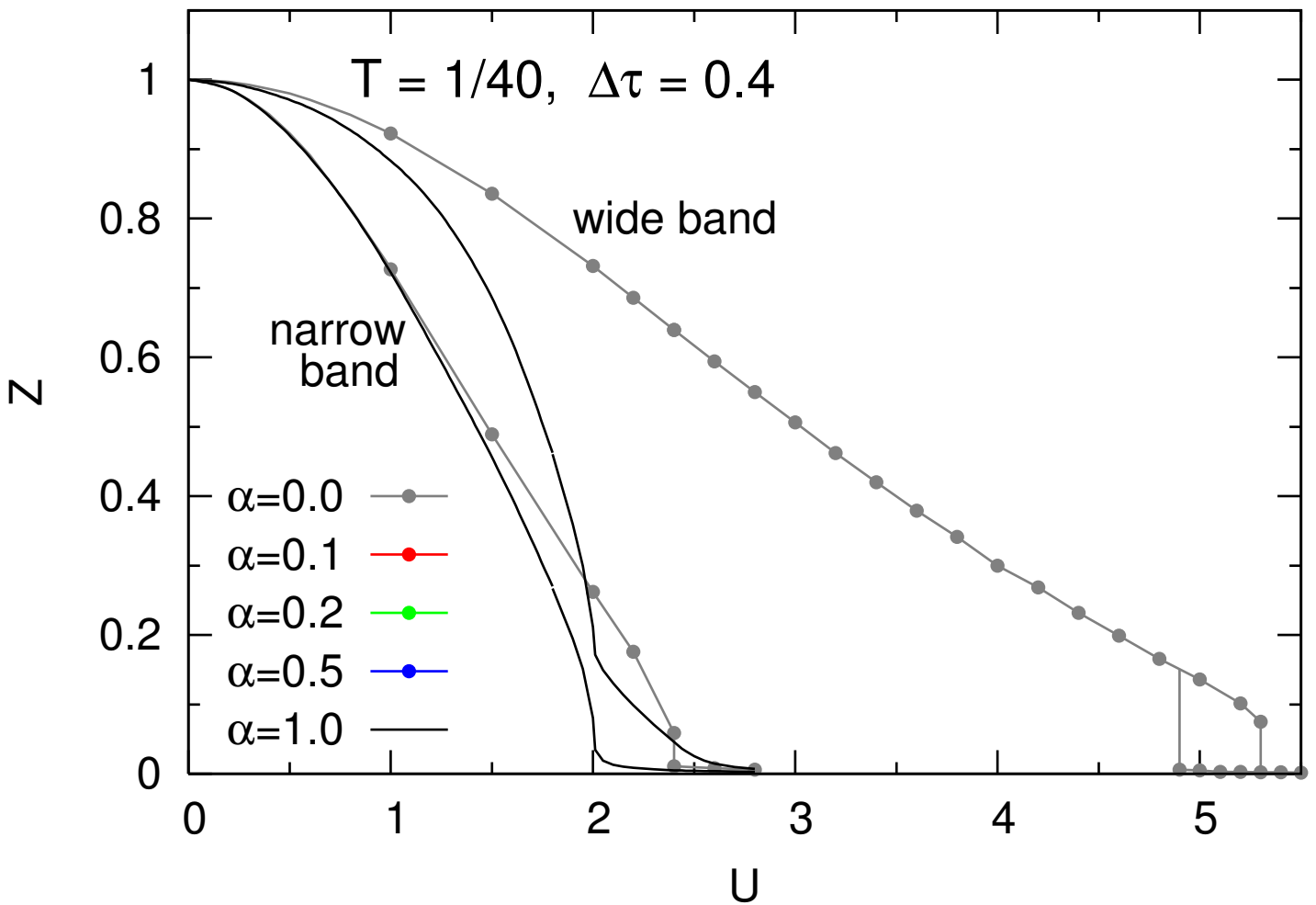
Systematic study: effect of inter-orbital coupling

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



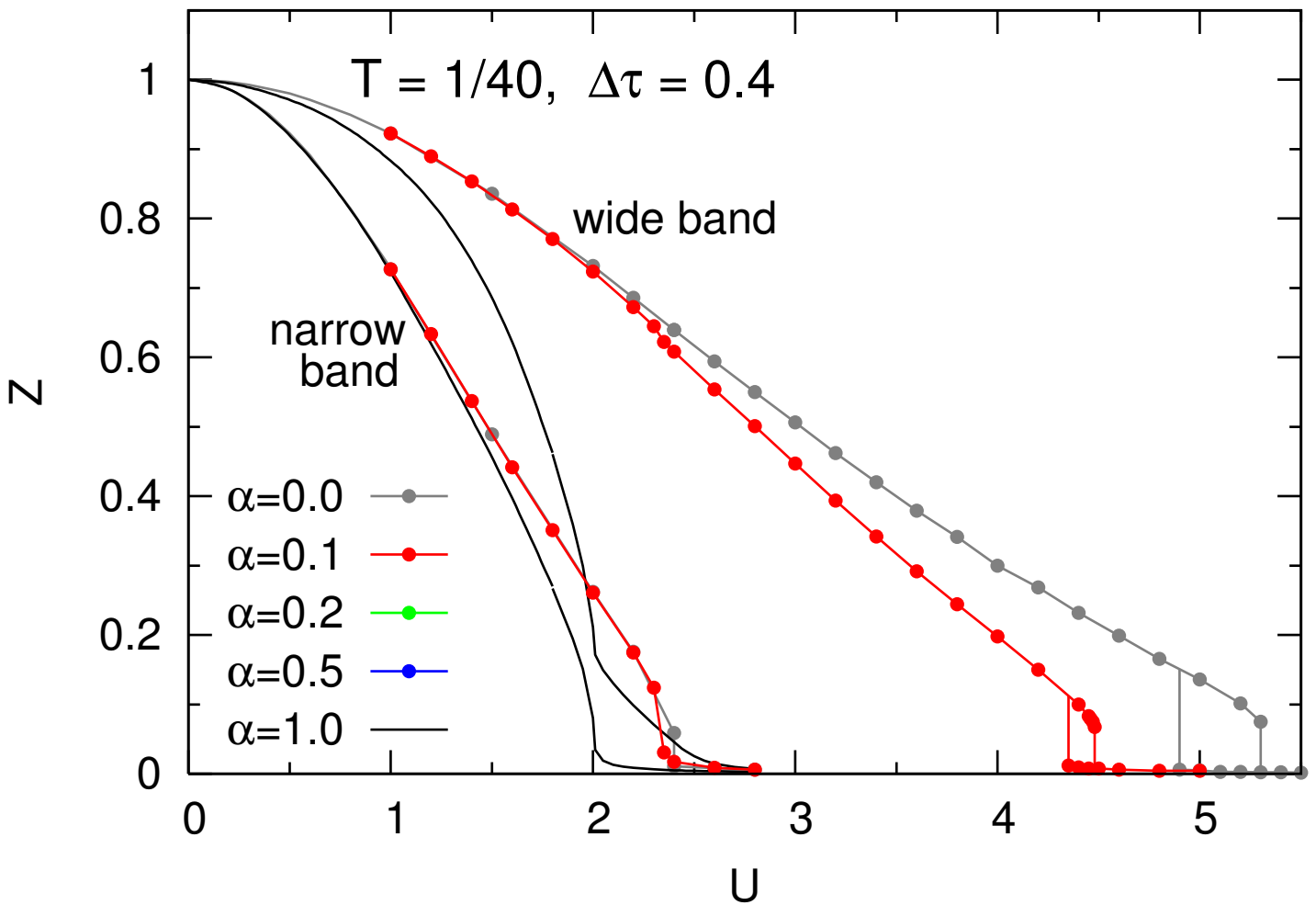
Systematic study: effect of inter-orbital coupling

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



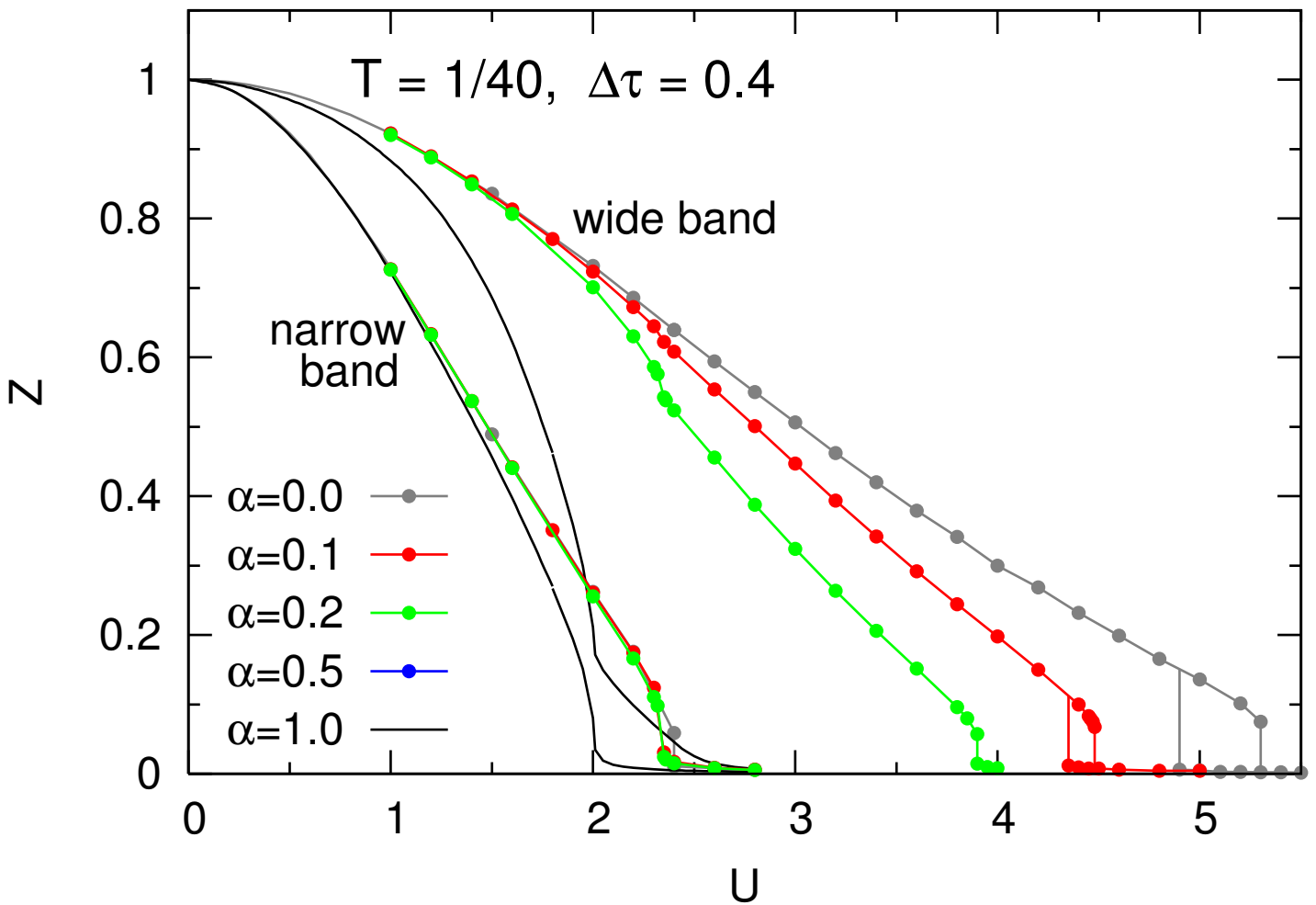
Systematic study: effect of inter-orbital coupling

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



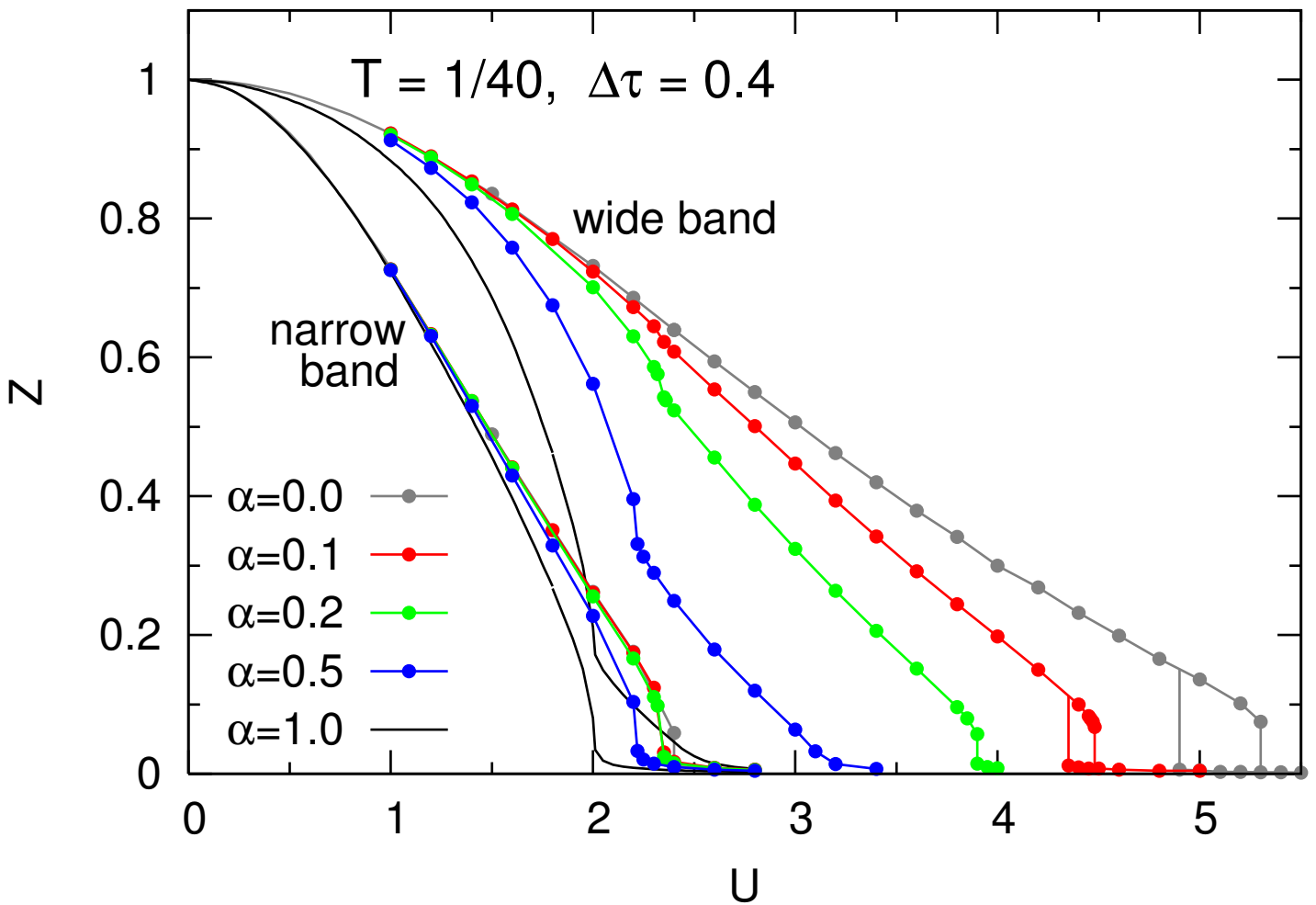
Systematic study: effect of inter-orbital coupling

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



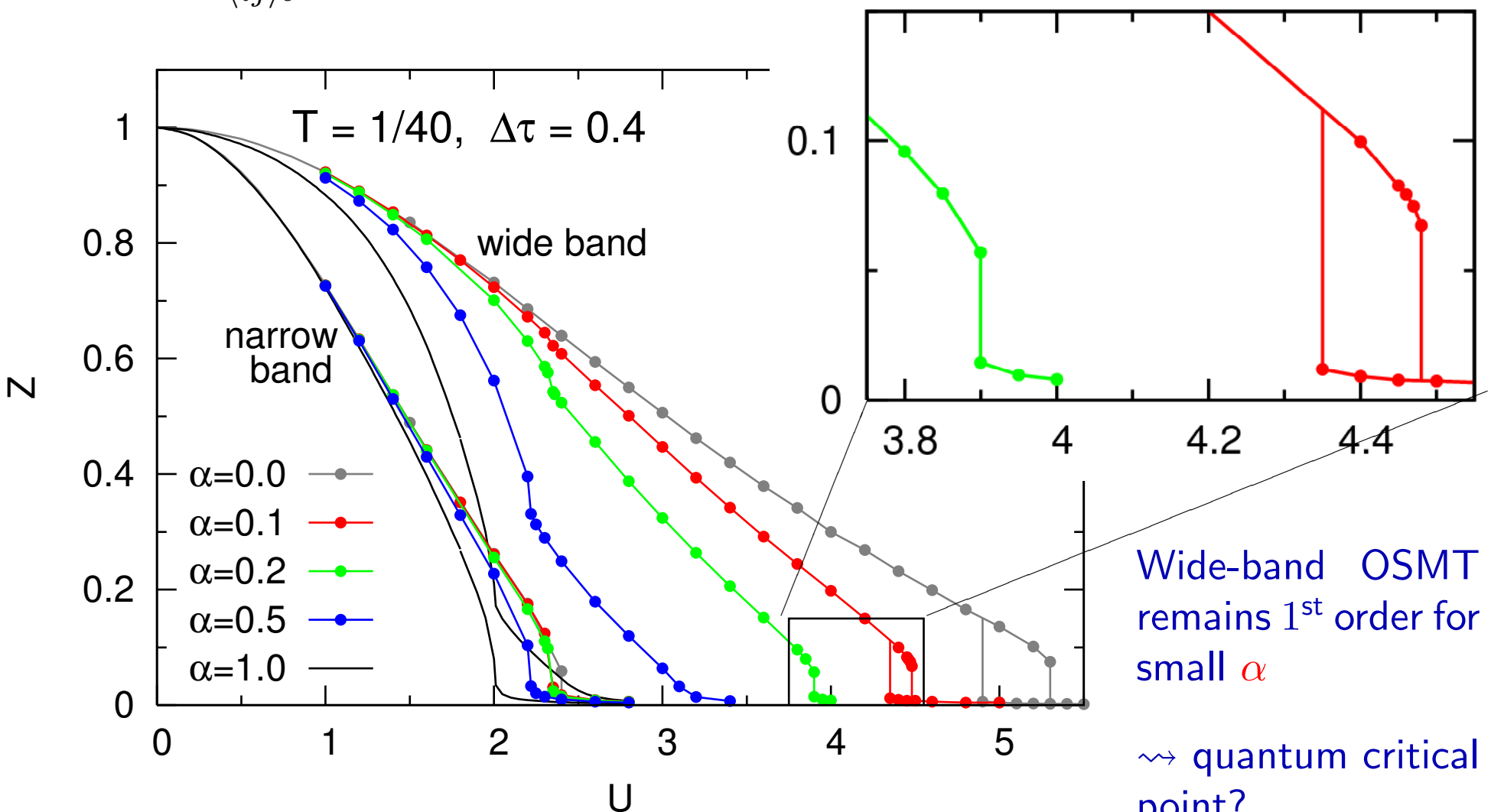
Systematic study: effect of inter-orbital coupling

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



Systematic study: effect of inter-orbital coupling

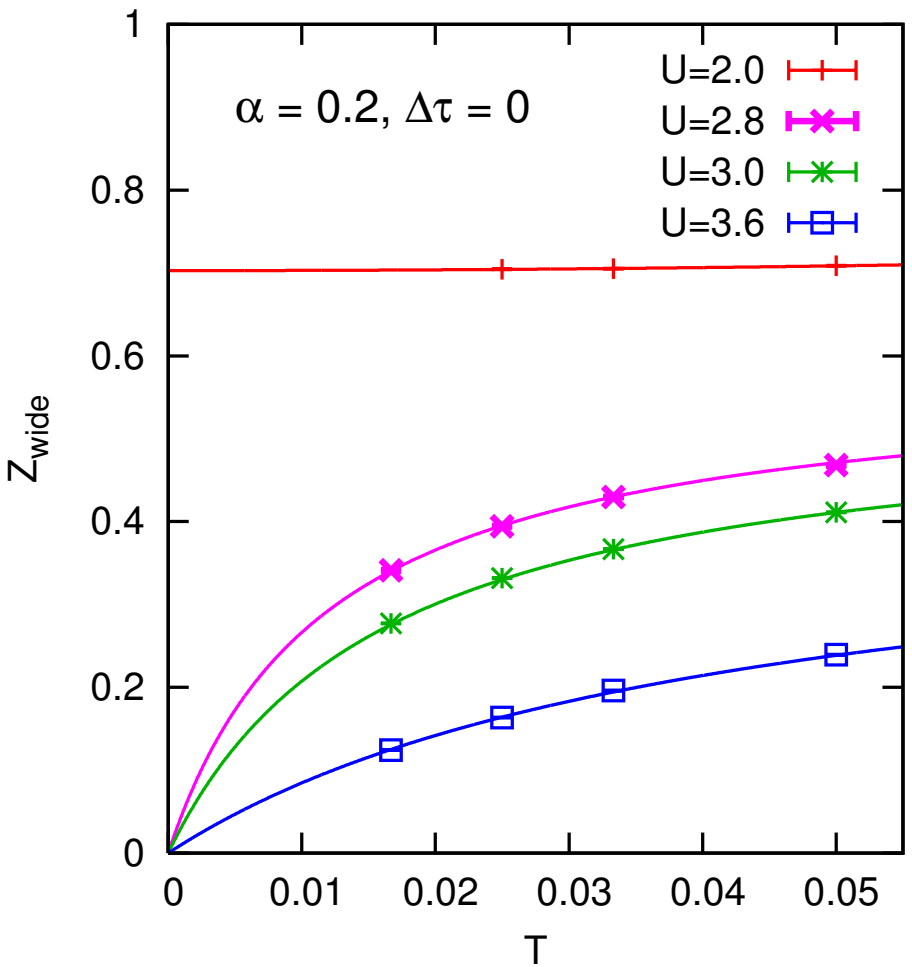
$$H = \sum_{m=1}^{2} \left[-\sum_{\langle ij \rangle \sigma} t_m c^\dagger_{im\sigma} c_{jm\sigma} + U \sum_i n_{im\uparrow} n_{im\downarrow} \right] + \alpha \sum (U/2 - \delta_{\sigma\sigma'} U/4)\, n_{i1\sigma}\, n_{i2\sigma'}$$



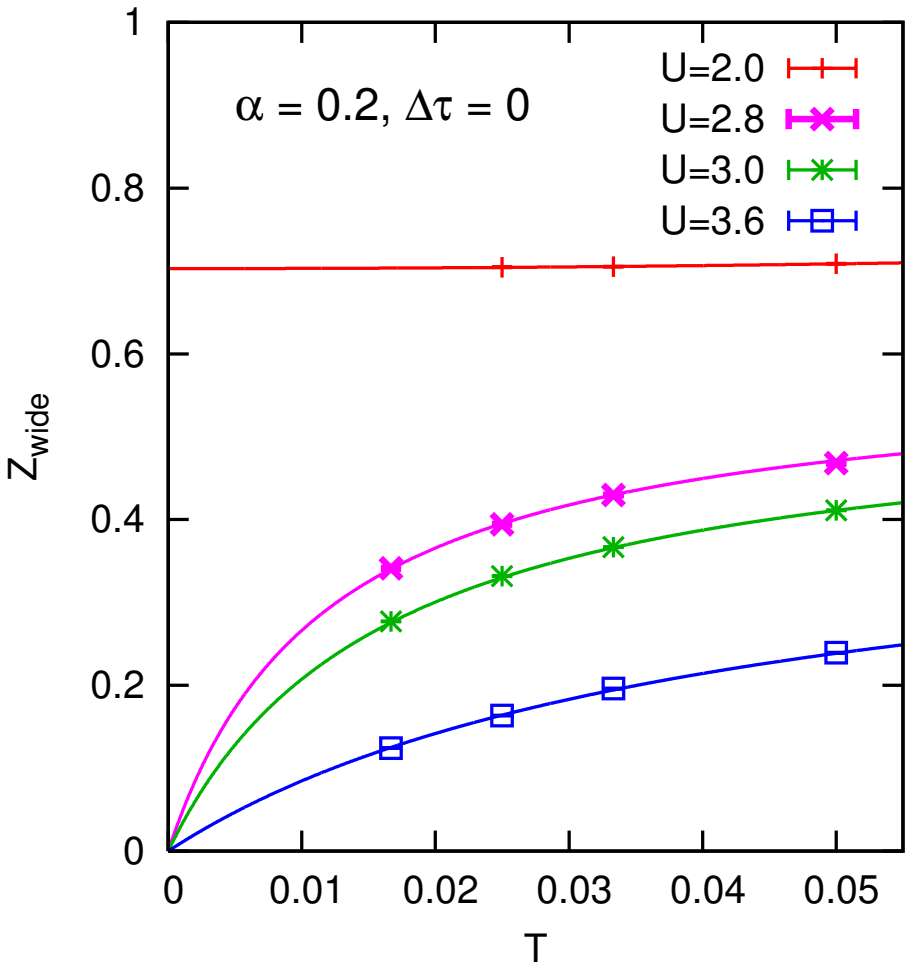
Wide-band OSMT remains 1st order for small α

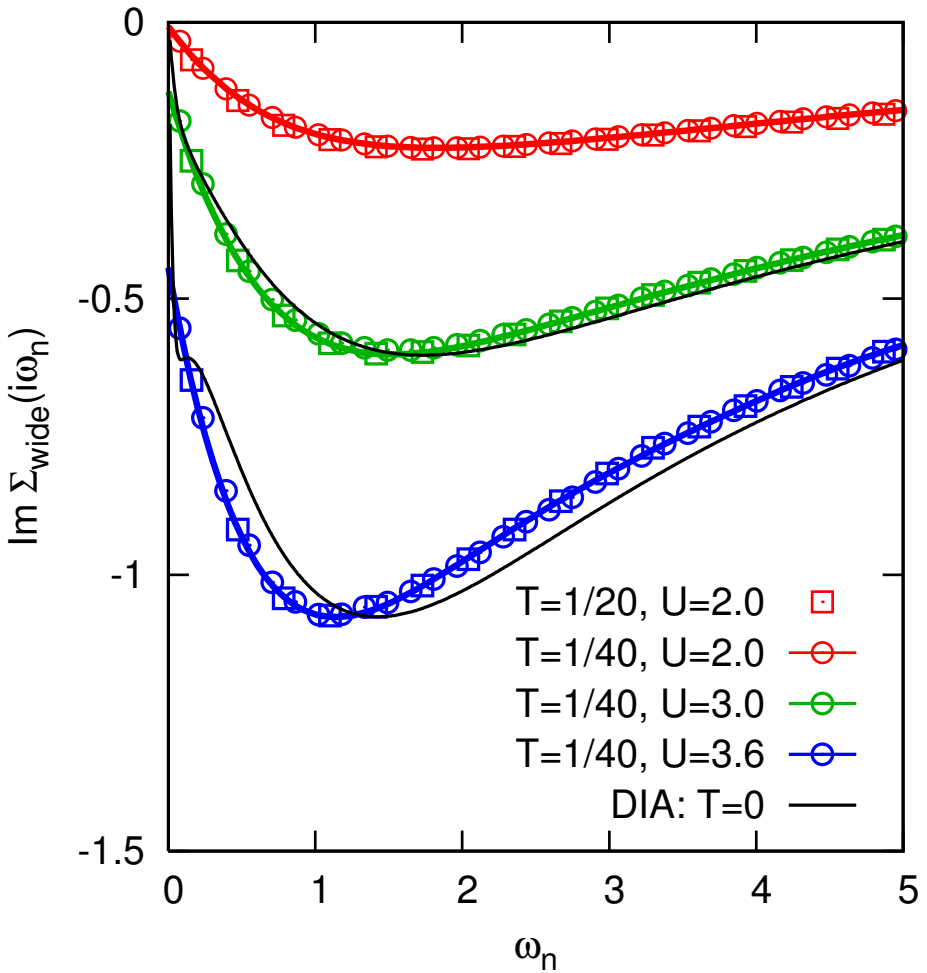
$\rightsquigarrow$ quantum critical point?

Self-energy and quasiparticle weight Z in OSM phase



Self-energy and quasiparticle weight Z in OSM phase





T-dependence of Z_{wide} in non-FL OSM phase:

artifact of QMC estimate $Z = \left[1 - \dfrac{\text{Im}\Sigma(i\pi T)}{\pi T}\right]^{-1}$

Summary

Motivation: OSMTs in $Ca_{2-x}Sr_xRuO_4$

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 $U \approx 2.6$

Systematic study: effect of inter-orbital coupling

wide-band OSMT 1^{st} order for small α $\rightsquigarrow$ qcp

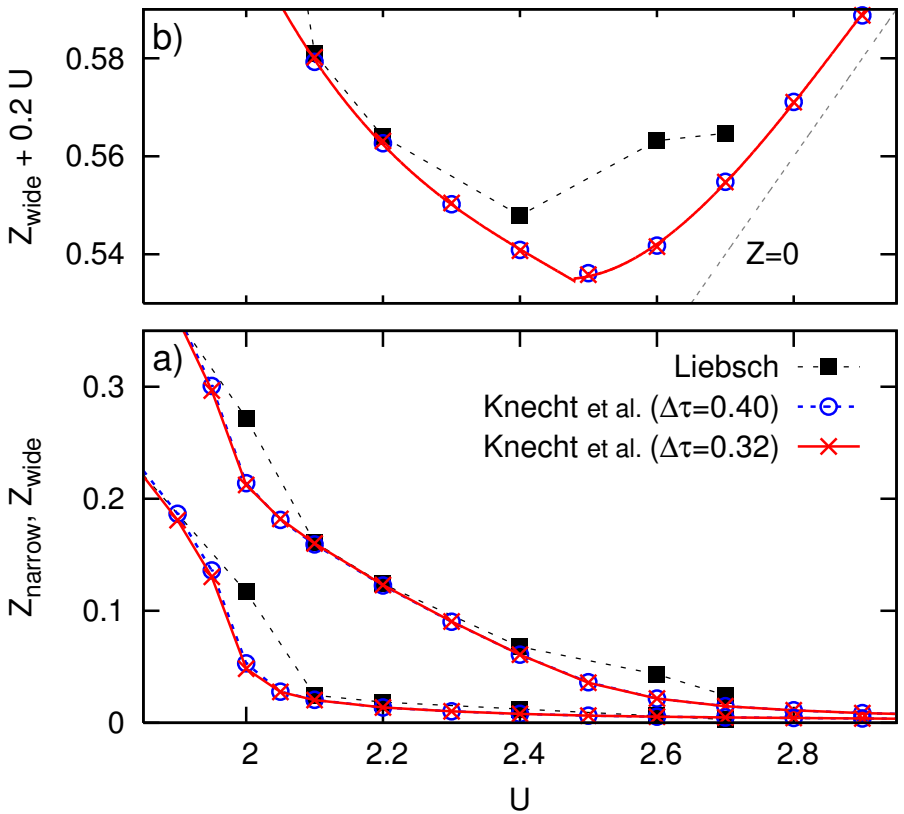
Self-energy and quasiparticle weight Z in OSM phase

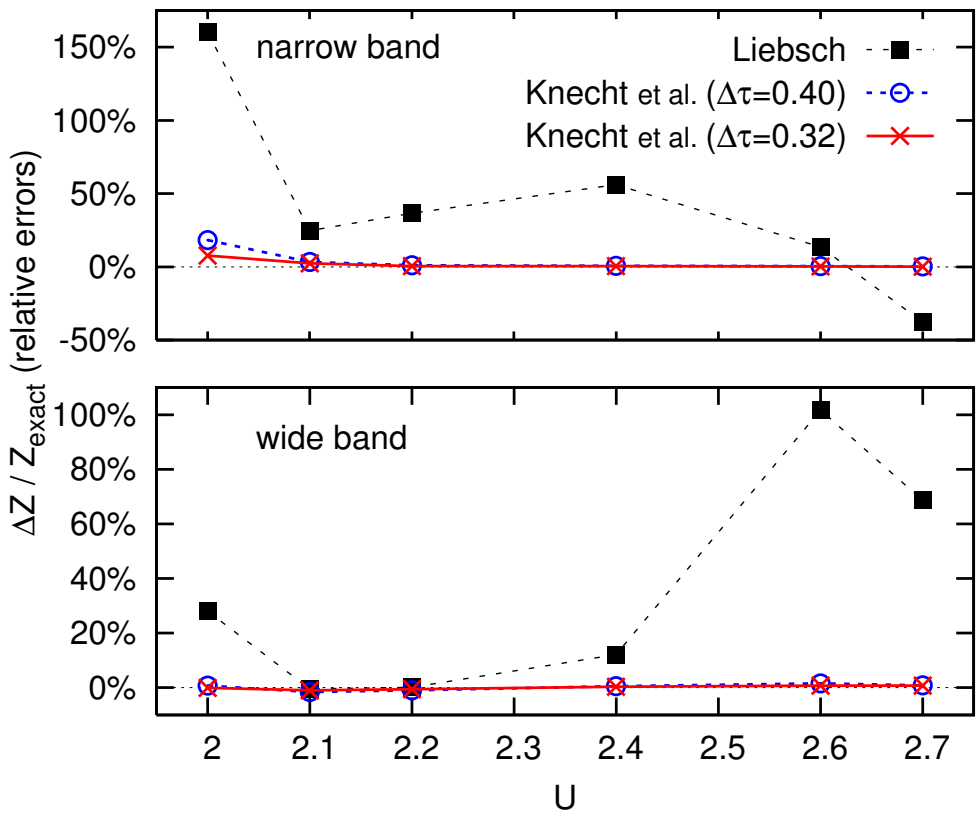
T-dependence of Z_{wide} in OSMP artifact of QMC estimate

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, . . .

Comparison at $T = 1/32$ with Liebsch, PRB **70**, 165103 (2004)

triggered by Comment [Liebsch, cond-mat/0506138] on our preprint



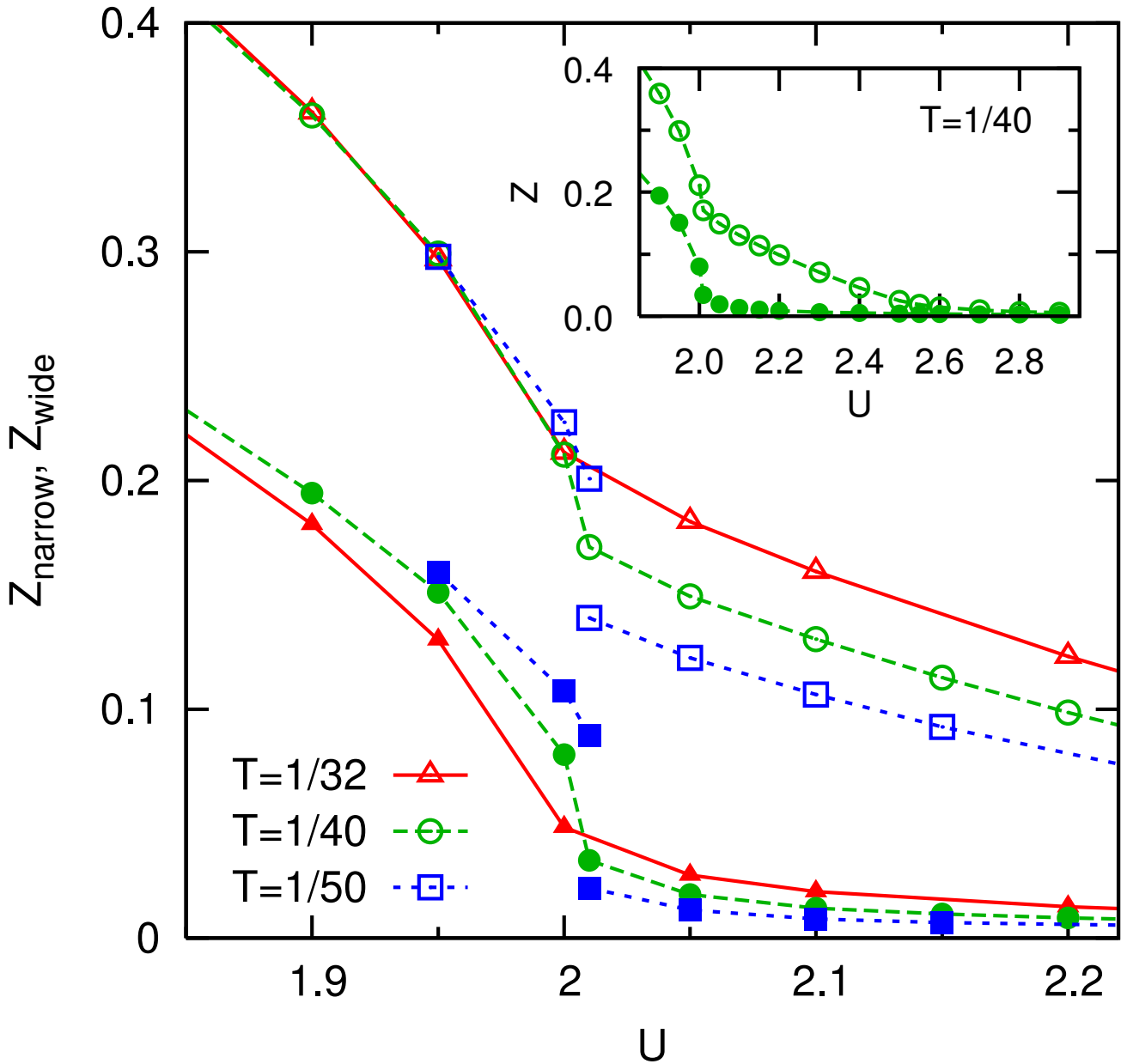


Numerical noise in Liebsch's QMC data obscures second transition

Liebsch's relative errors $>100\%$ at both transitions [our error: $\mathcal{O}(1\%)$]

[Knecht, NB, van Dongen, cond-mat/0506450]

Determination of critical temperature for narrow-band transition



Coexistence only for
$T \lesssim 0.02 = 1/50$
[van Dongen, Knecht, NB, cond-mat/0507682]