

# Orbital-selective Mott transitions in two-band Hubbard models

Nils Blümer, Carsten Knecht, Krunoslav Požgajčić,  
and Peter van Dongen, Univ. Mainz

## Outline

Motivation: OSMTs in  $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$

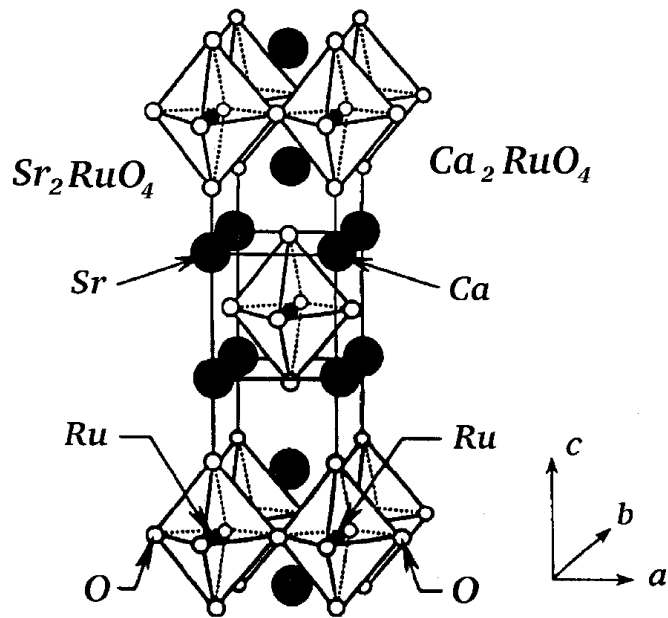
Orbital-selective Mott transitions in 2-band Hubbard model

Systematic study: effect of inter-orbital coupling

Self-energy and quasiparticle weight  $Z$  in OSM phase

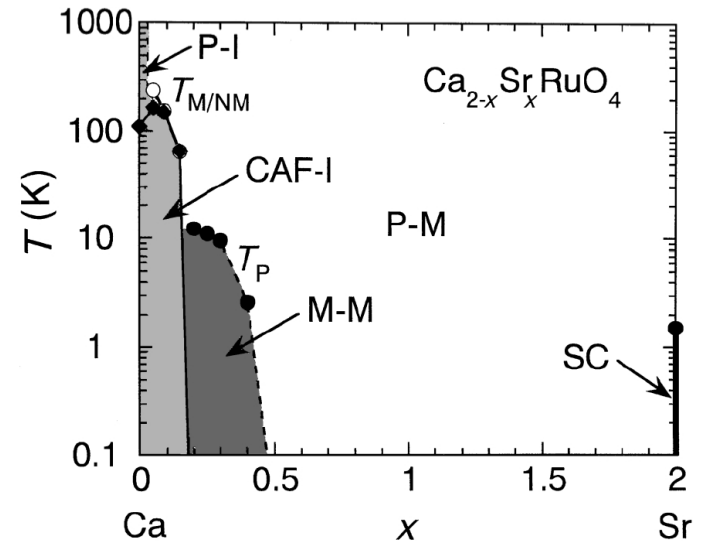
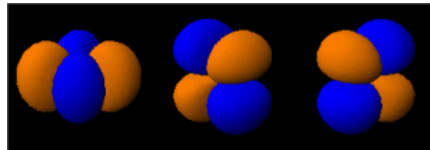
Summary

# Motivation: OSMTs in $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$



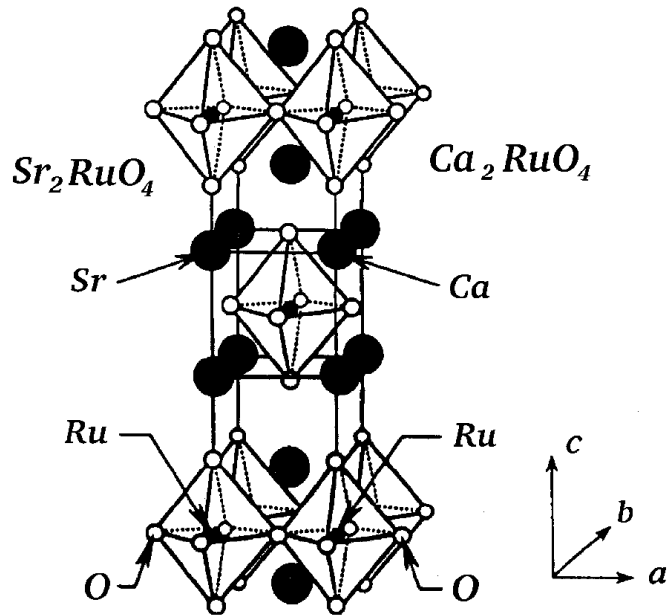
isostructural to  
 $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$

valence states:  
Ru  $t_{2g}$  orbitals



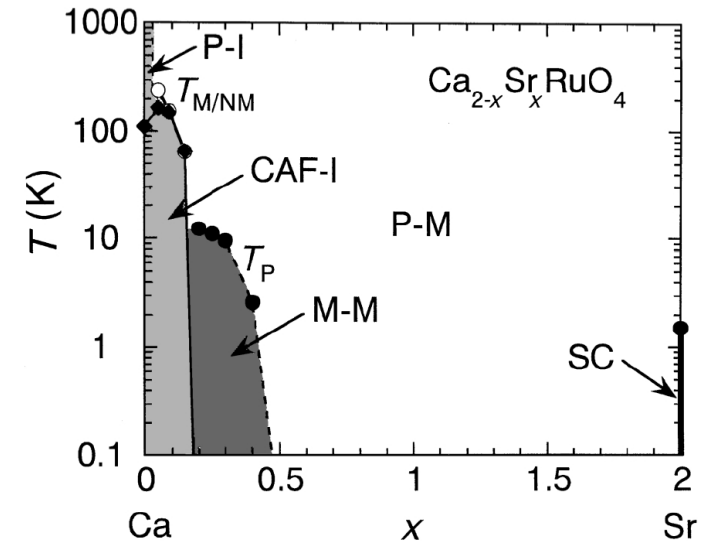
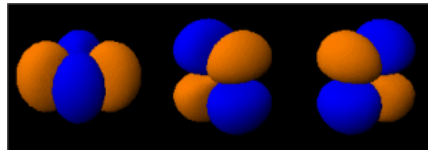
[Nakatsuji, Maeno, PRL (2000)]

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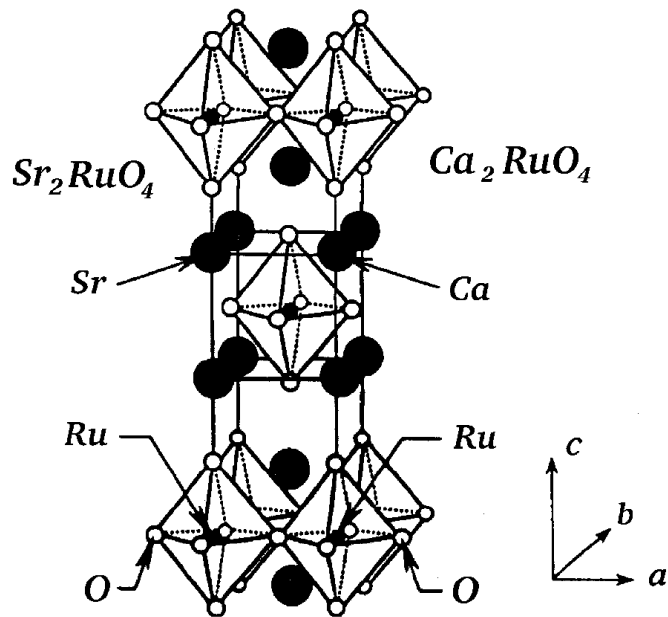


[Nakatsuji, Maeno, PRL (2000)]

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

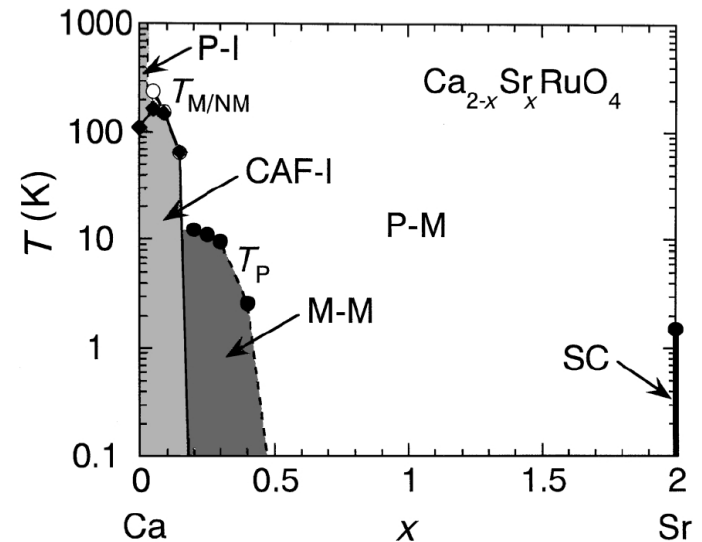
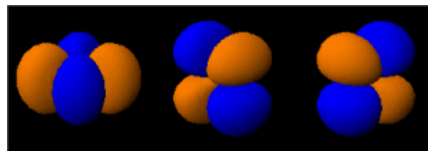
orbital-selective Mott metal-insulator transitions for  $x \approx 0.5$ ,  $x \approx 0.2$  ?

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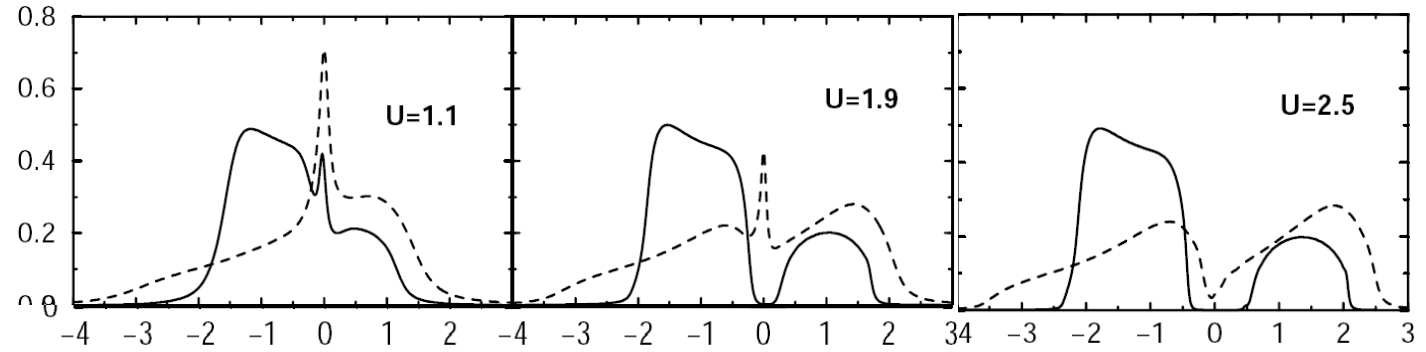
orbital-selective Mott metal-insulator transitions for  $x \approx 0.5$ ,  $x \approx 0.2$  ?

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

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

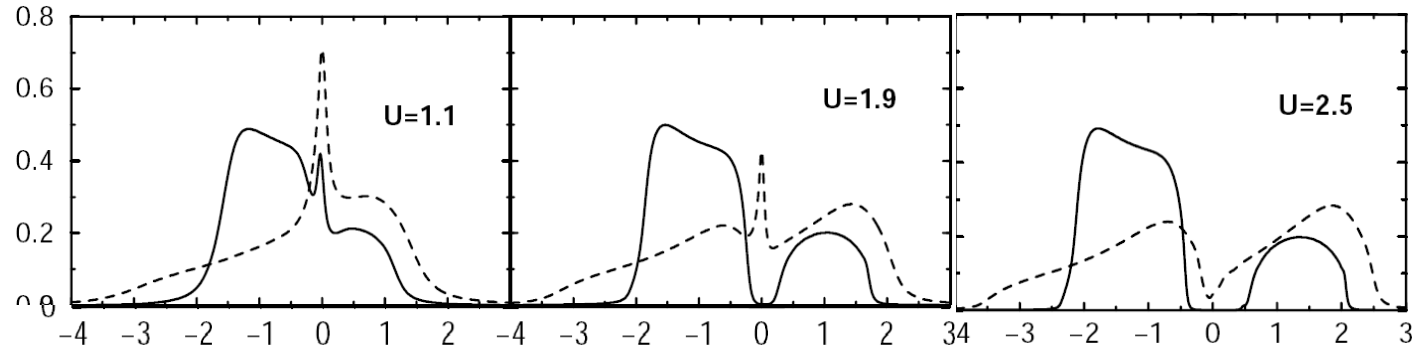
# OSMTs in 2-band Hubbard model

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



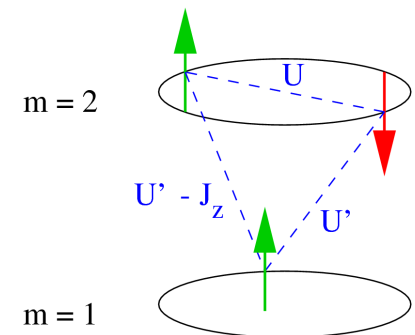
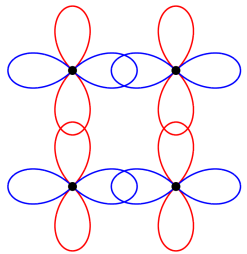
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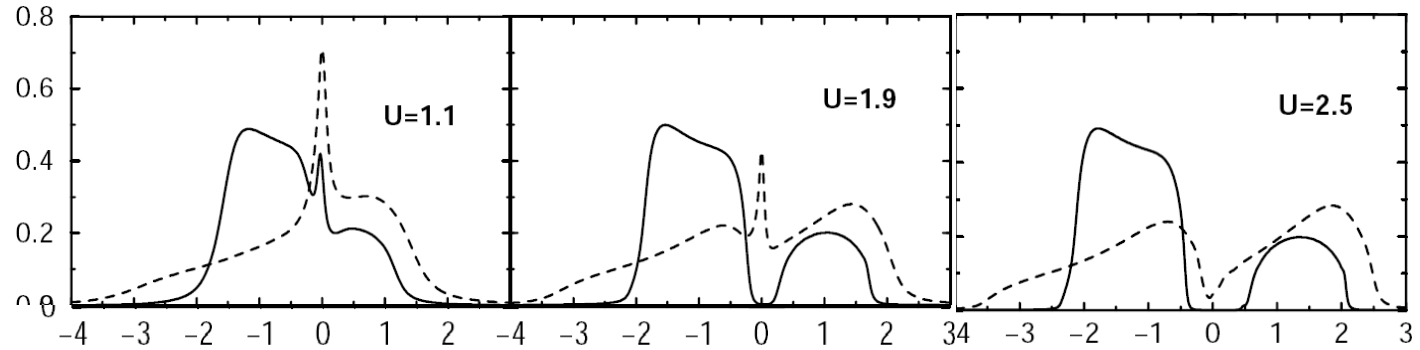
Minimal OSMT model: 2-band Hubbard model with orbital-dependent hopping

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

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

Bethe DOS,  $t_2 = 2t_1$ : 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

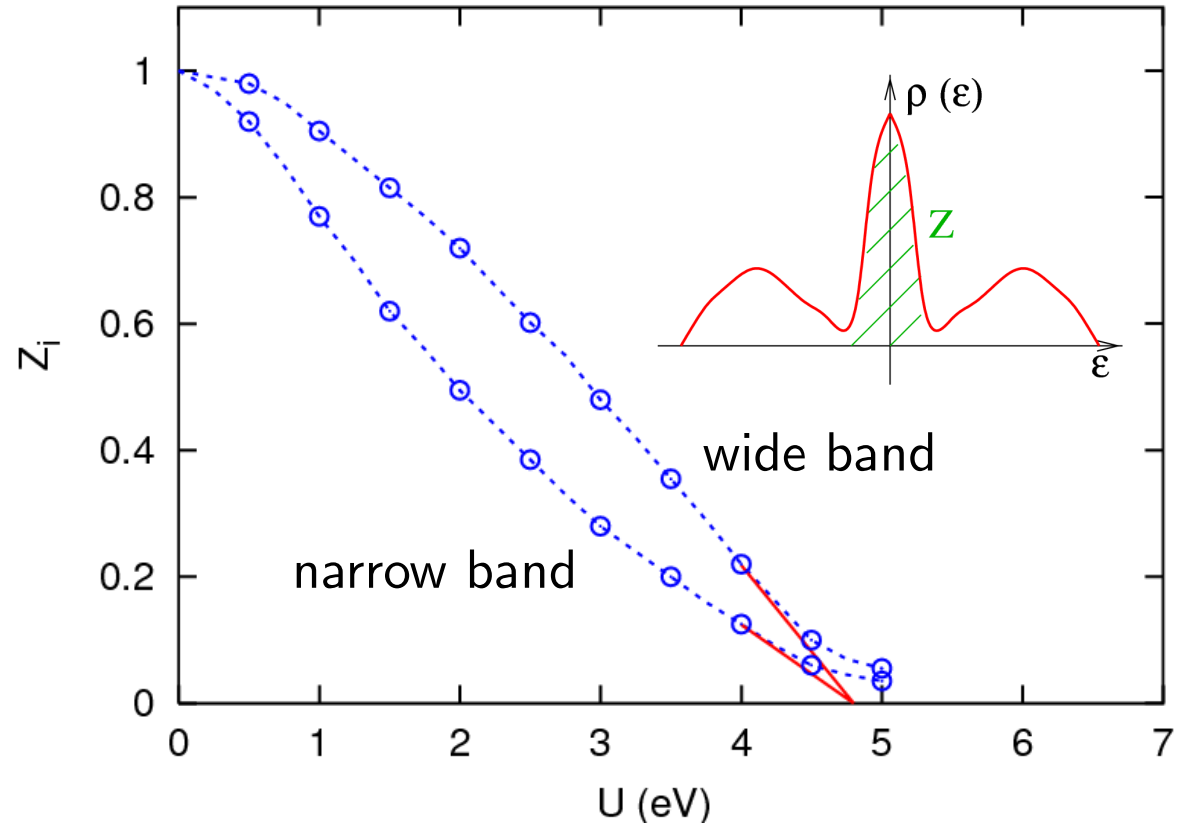
quasiparticle weight  $Z_i = m/m_i^*$

discrete QMC estimate:

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

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

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



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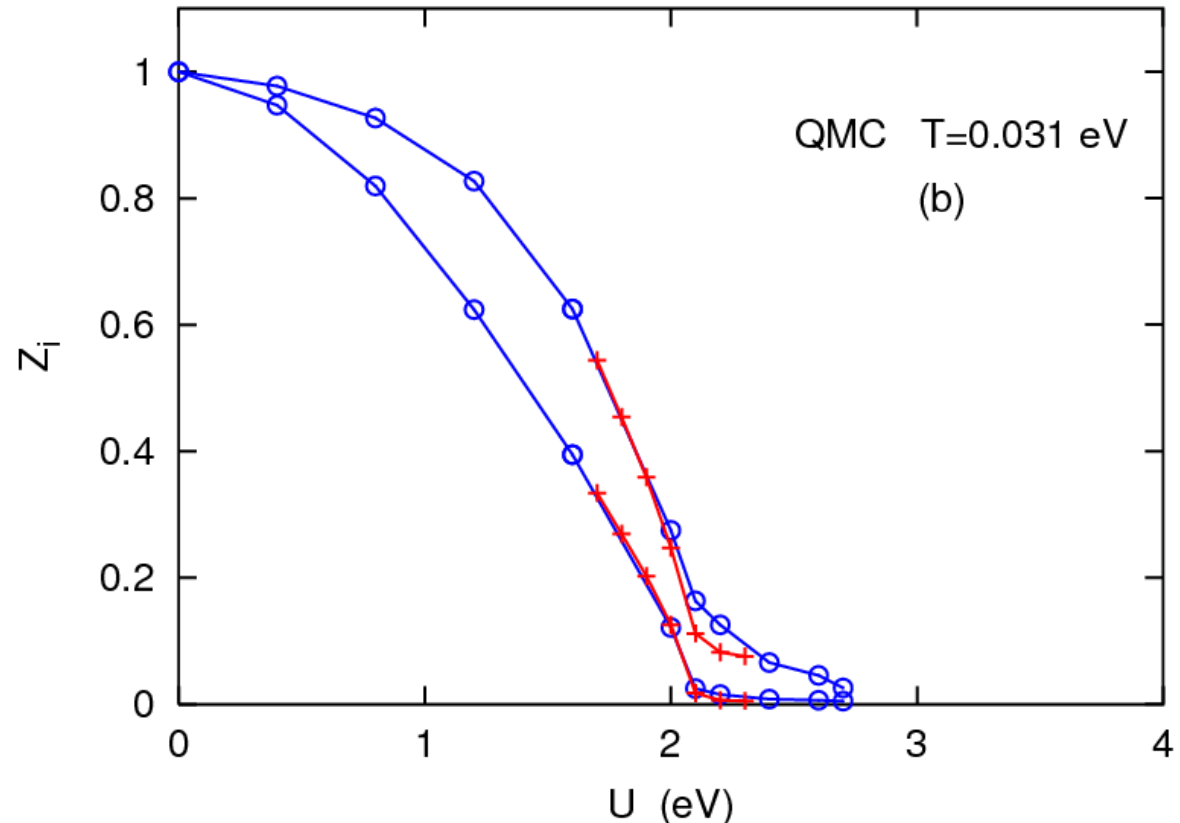
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$$J_z = 0.2, \quad U' = U - 0.4$$

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

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

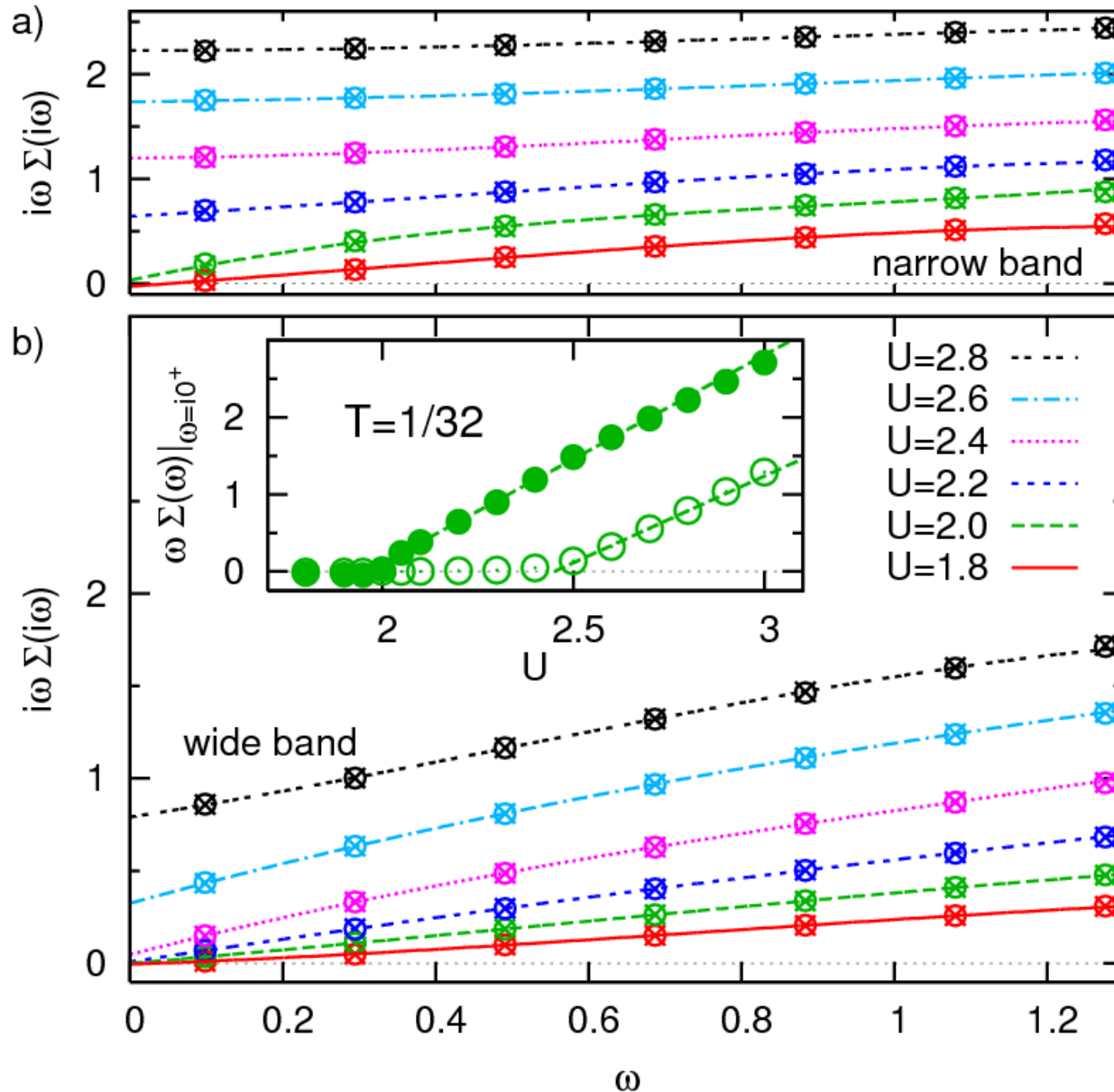
[Liebsch, PRB **70**, 165103 (2004)]



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:

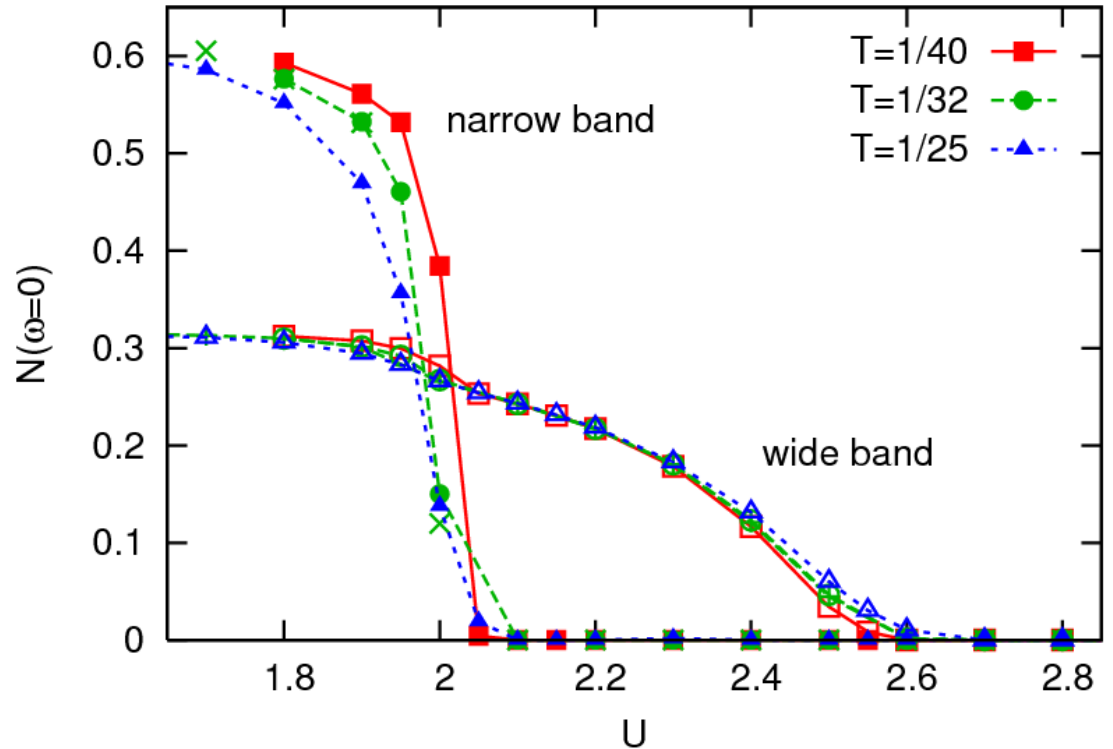
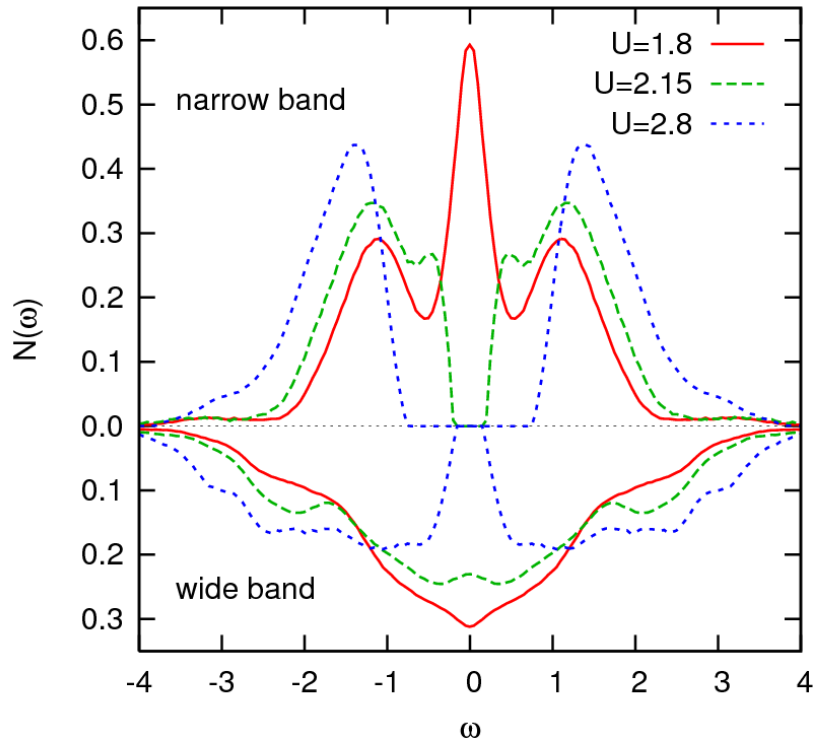
$$\omega \Sigma(\omega) \xrightarrow{\omega \rightarrow 0} 0$$

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

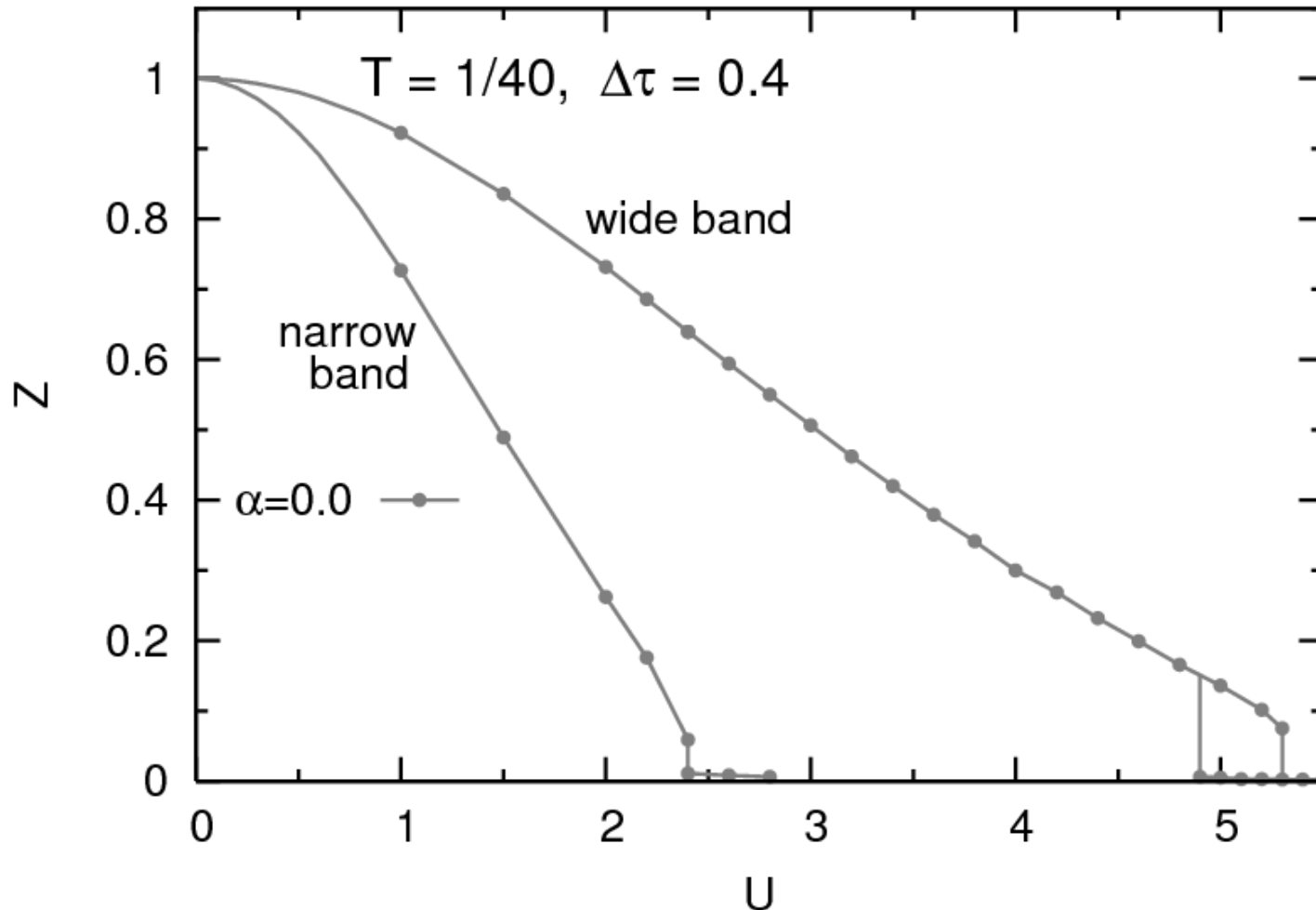
Wide band remains metallic at  $U \approx 2.0$

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

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

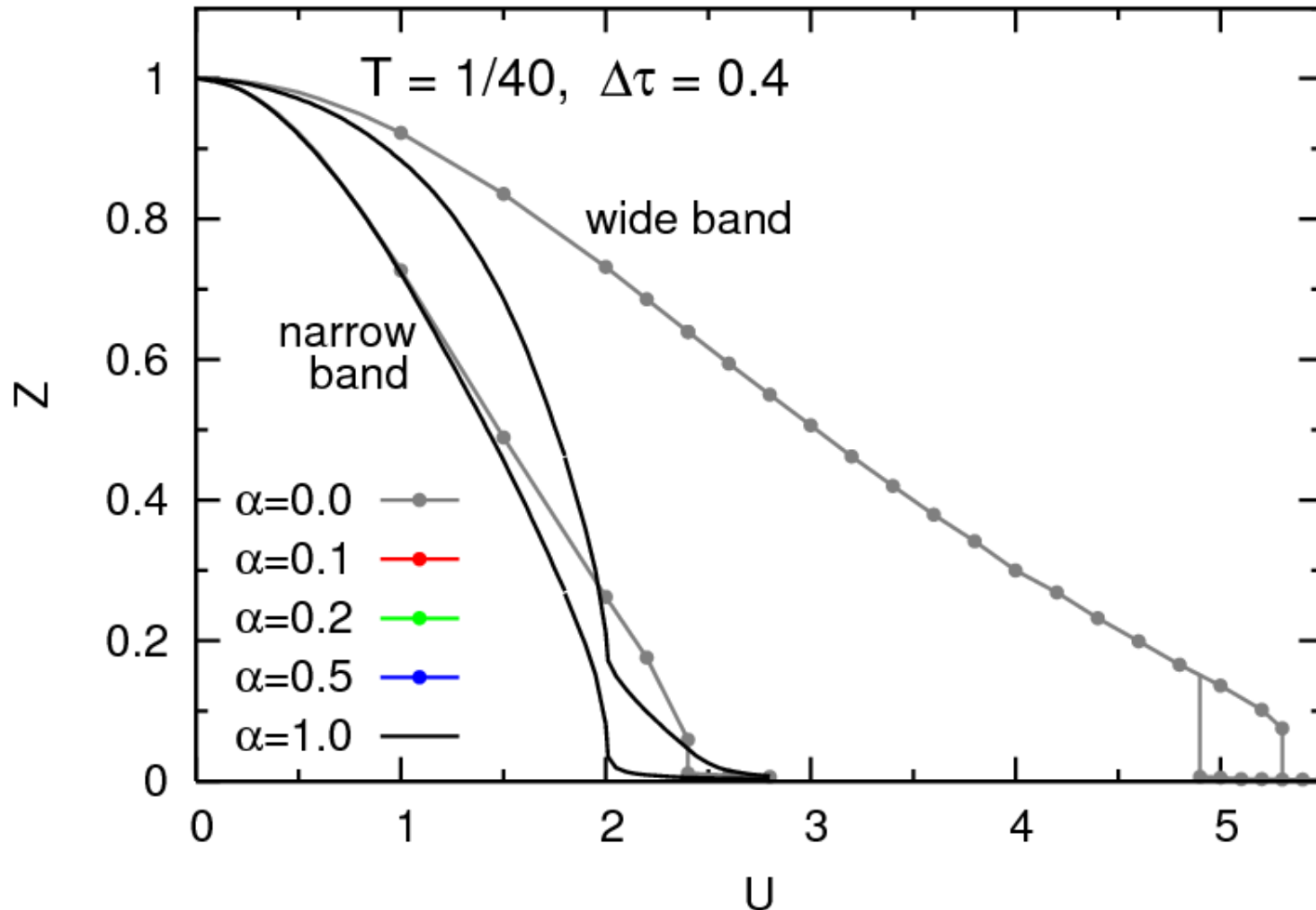
# Systematic study: effect of inter-orbital coupling

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



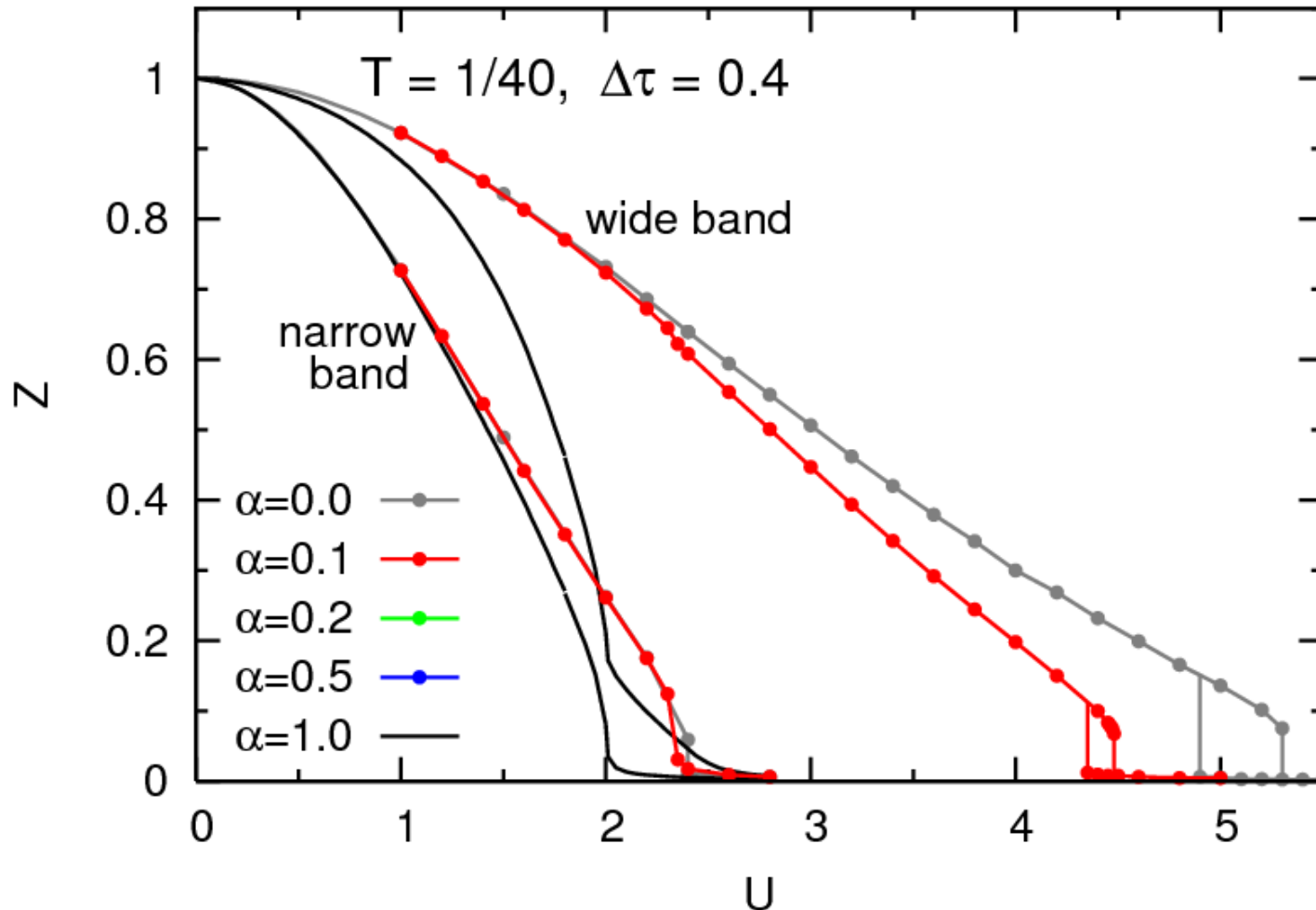
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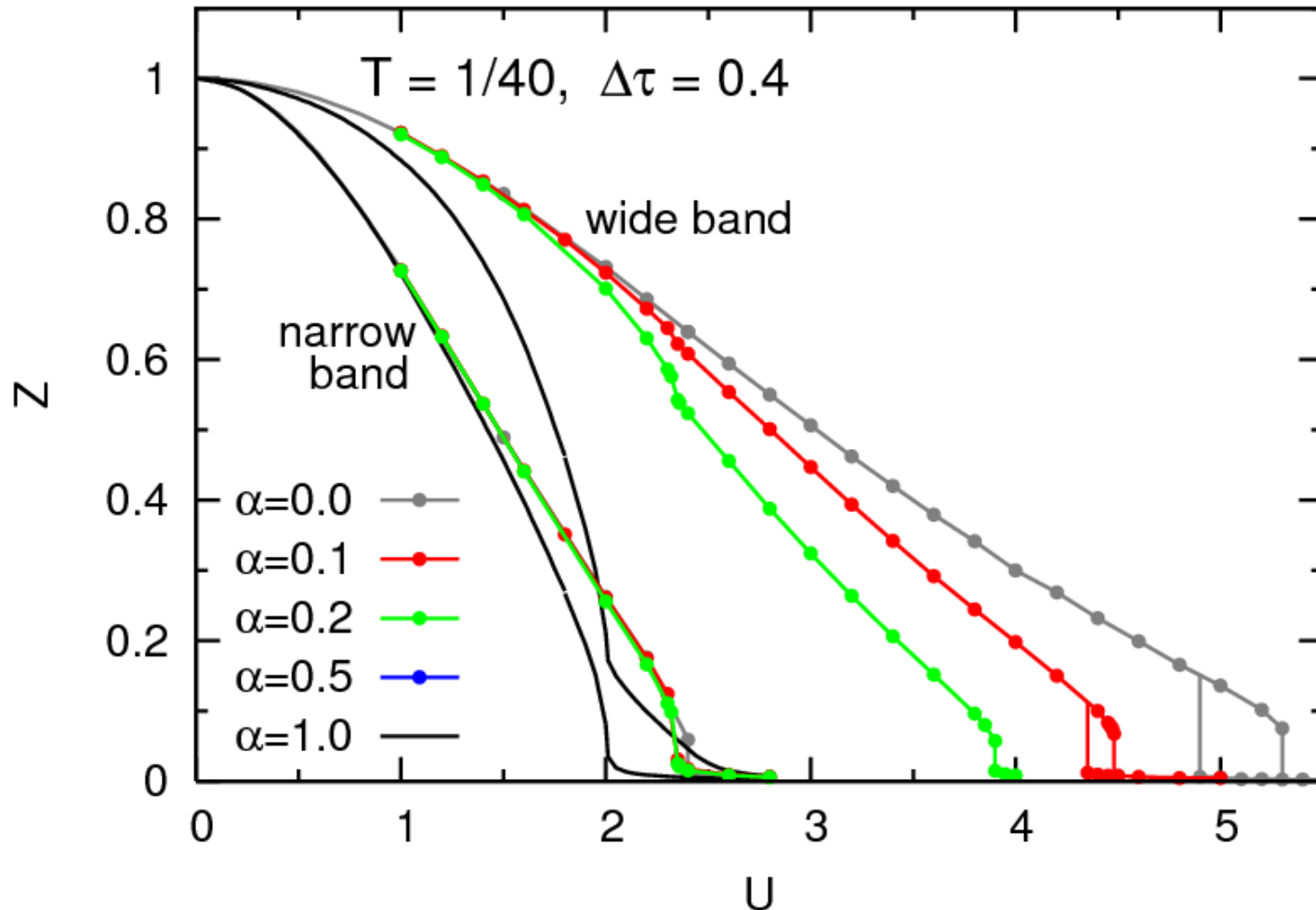
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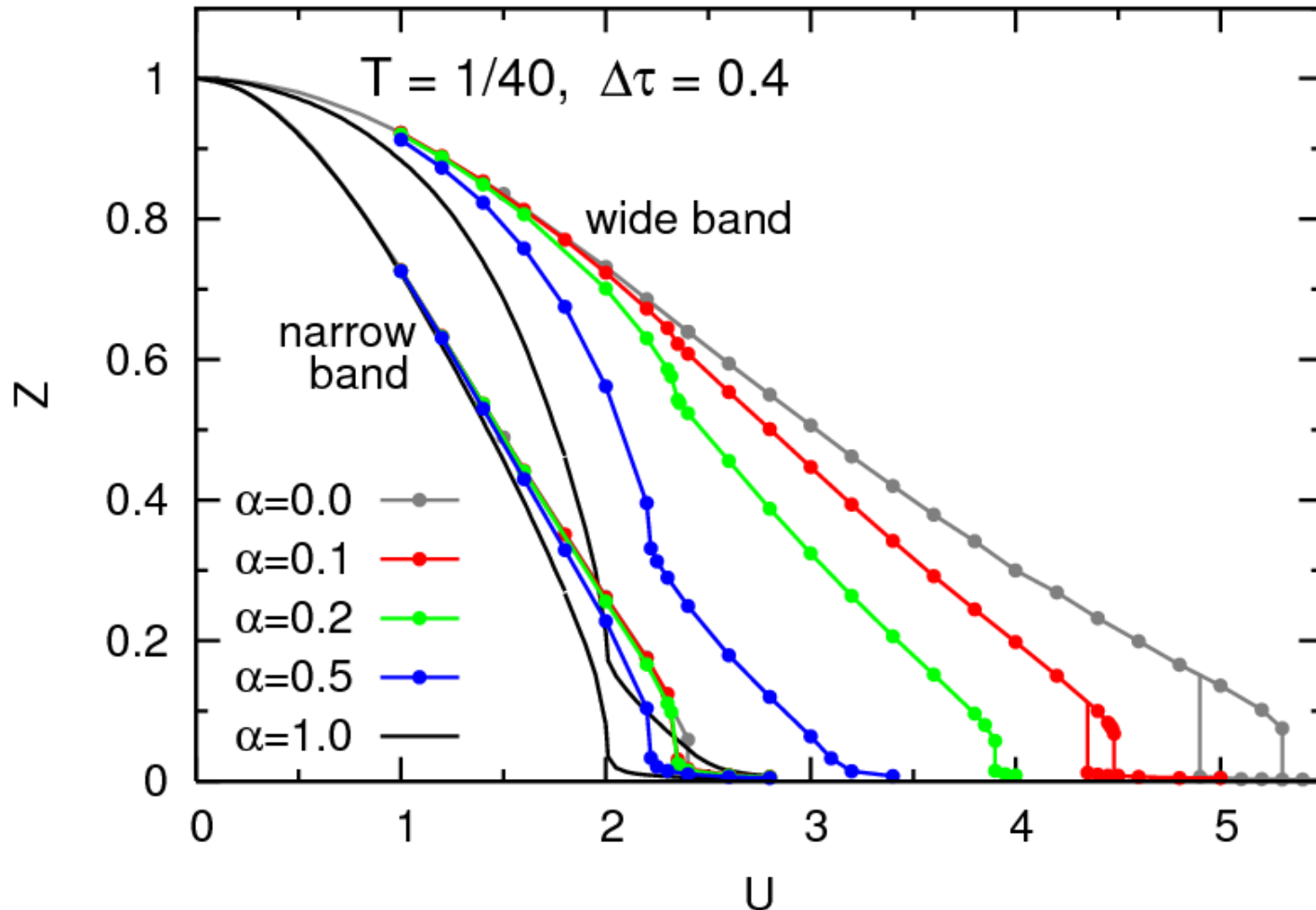
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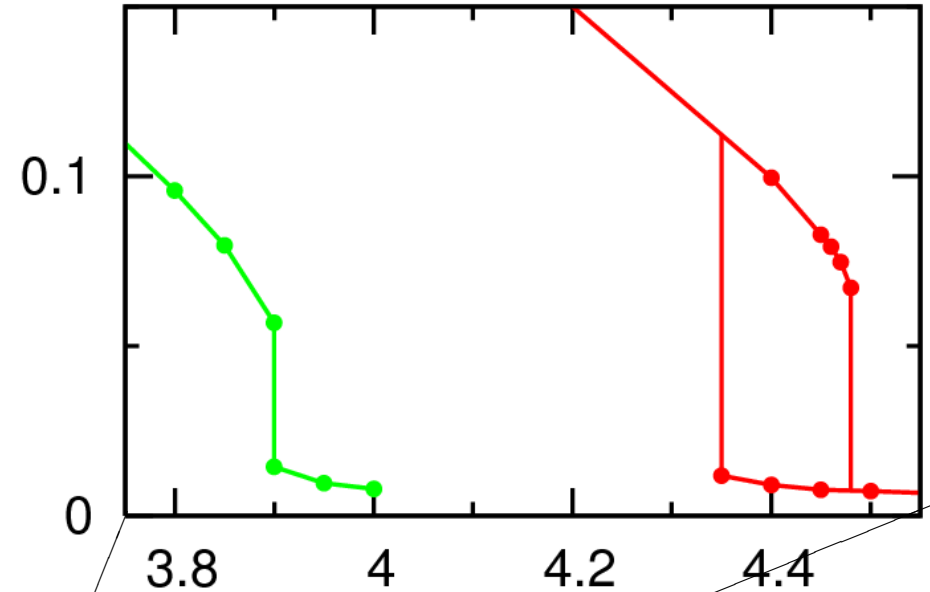
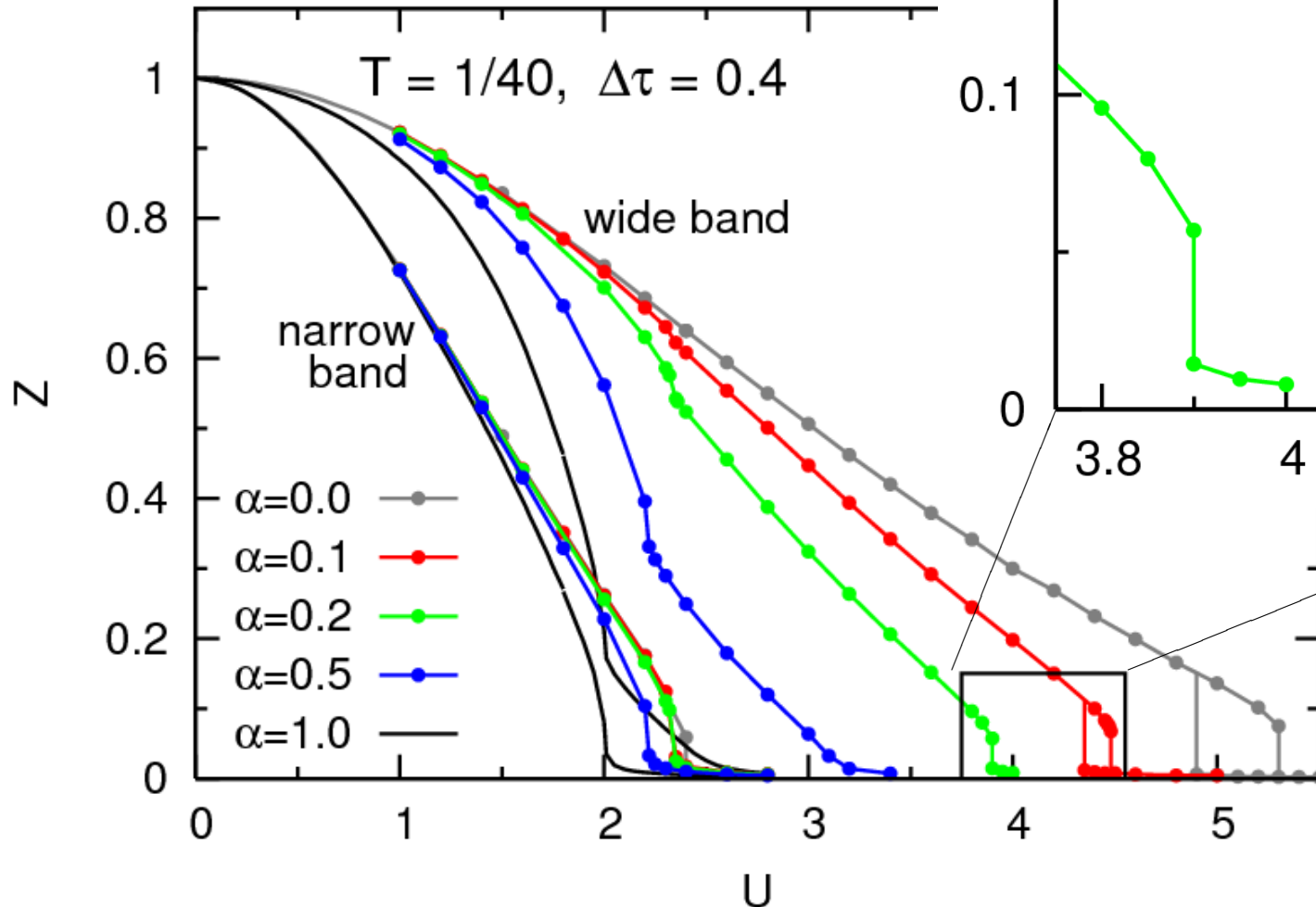
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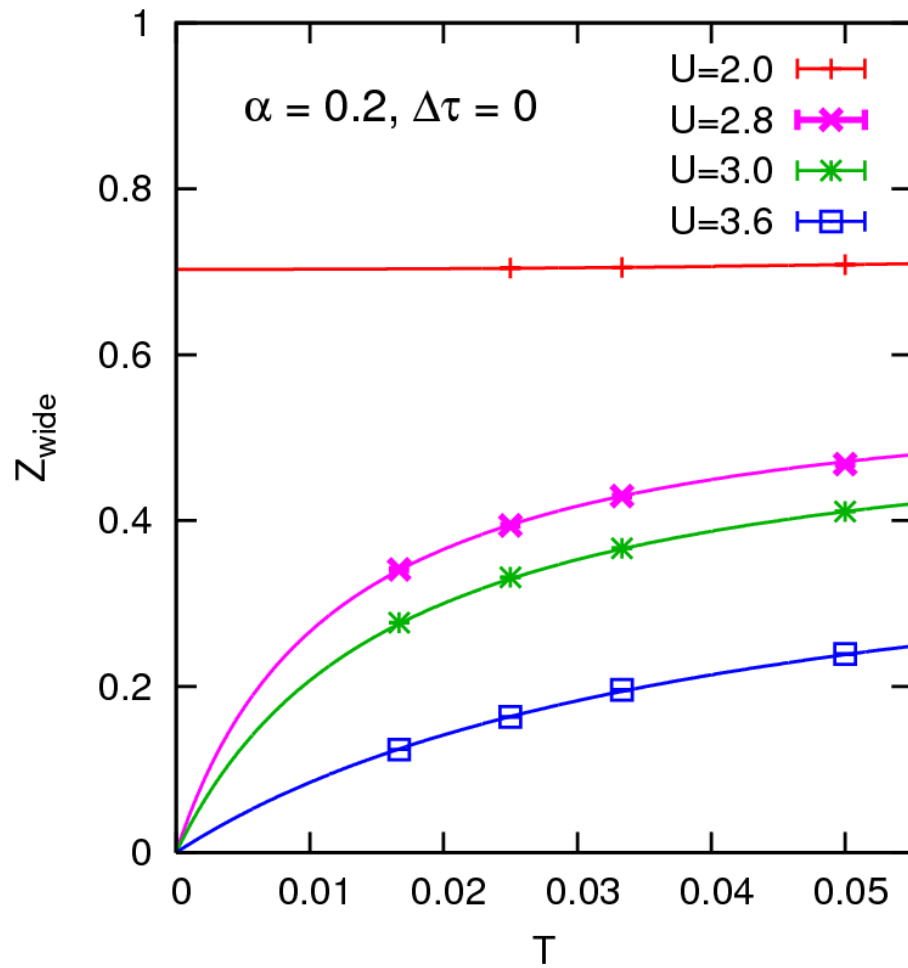
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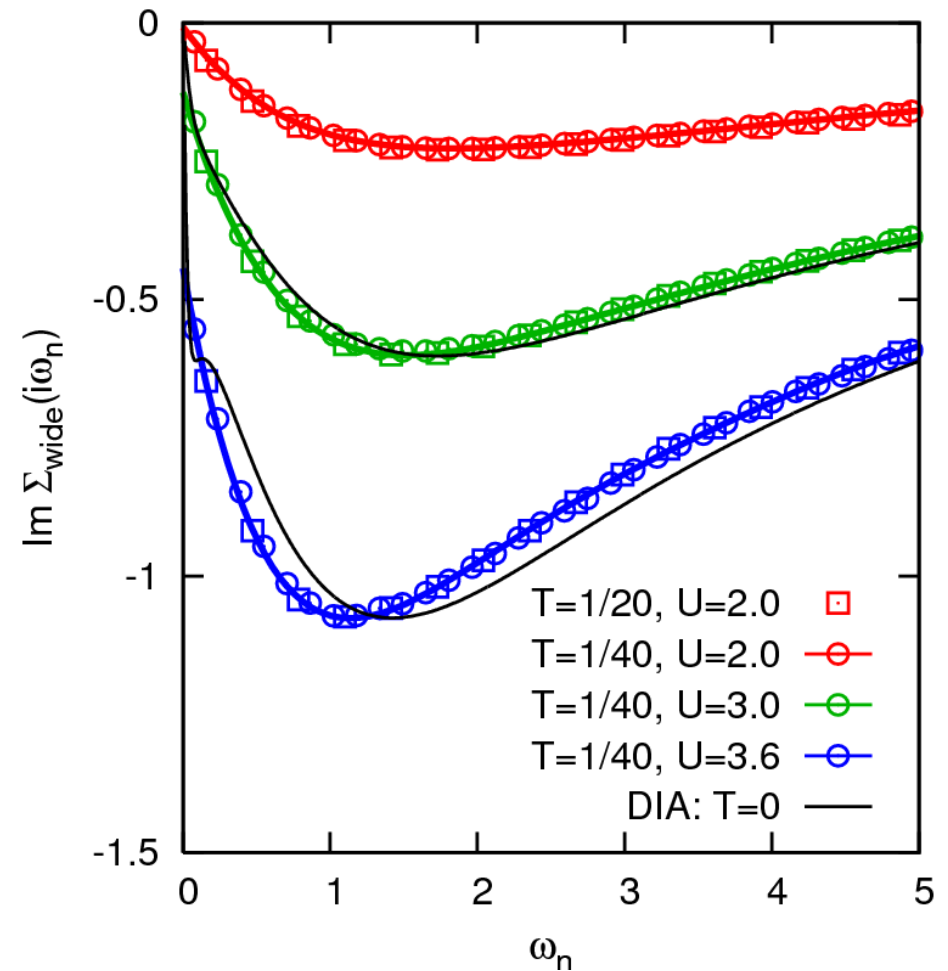
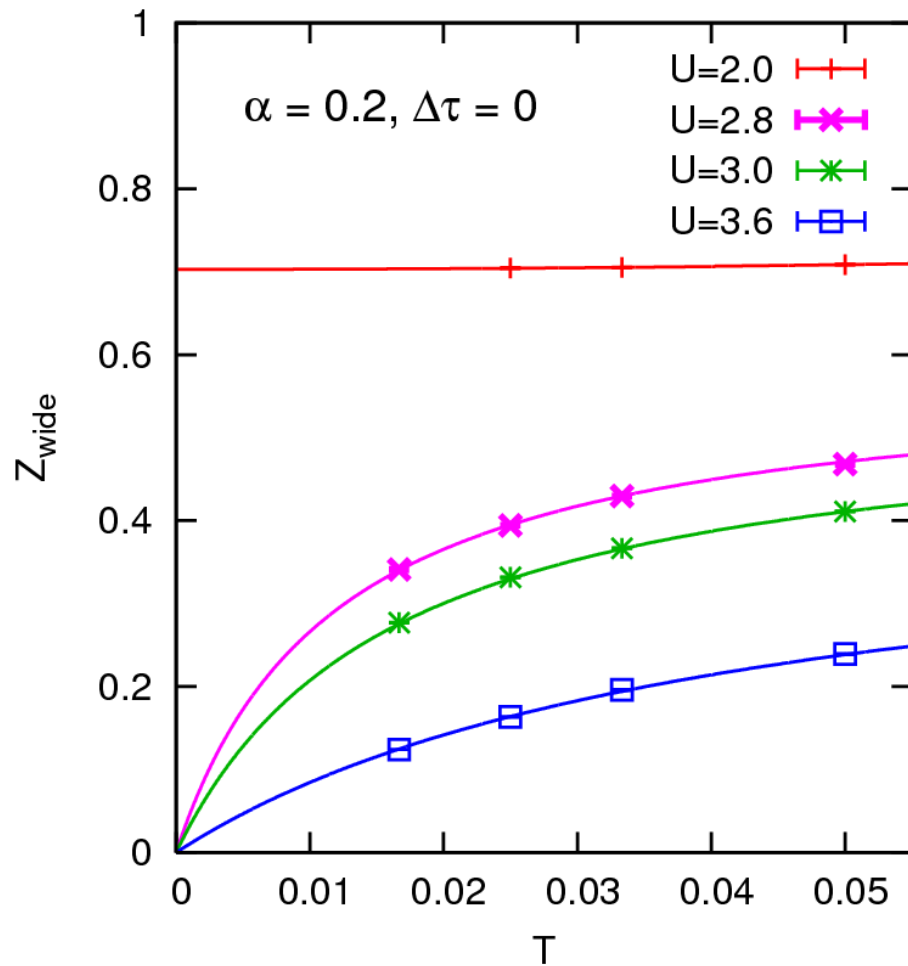
Wide-band OSMT remains 1<sup>st</sup> order for small  $\alpha$

$\rightsquigarrow$  quantum critical point?

# Self-energy and quasiparticle weight $Z$ in OSM phase



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

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

# Summary

Motivation: OSMTs in  $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$

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<sup>st</sup> order for small  $\alpha \rightsquigarrow$  qcp

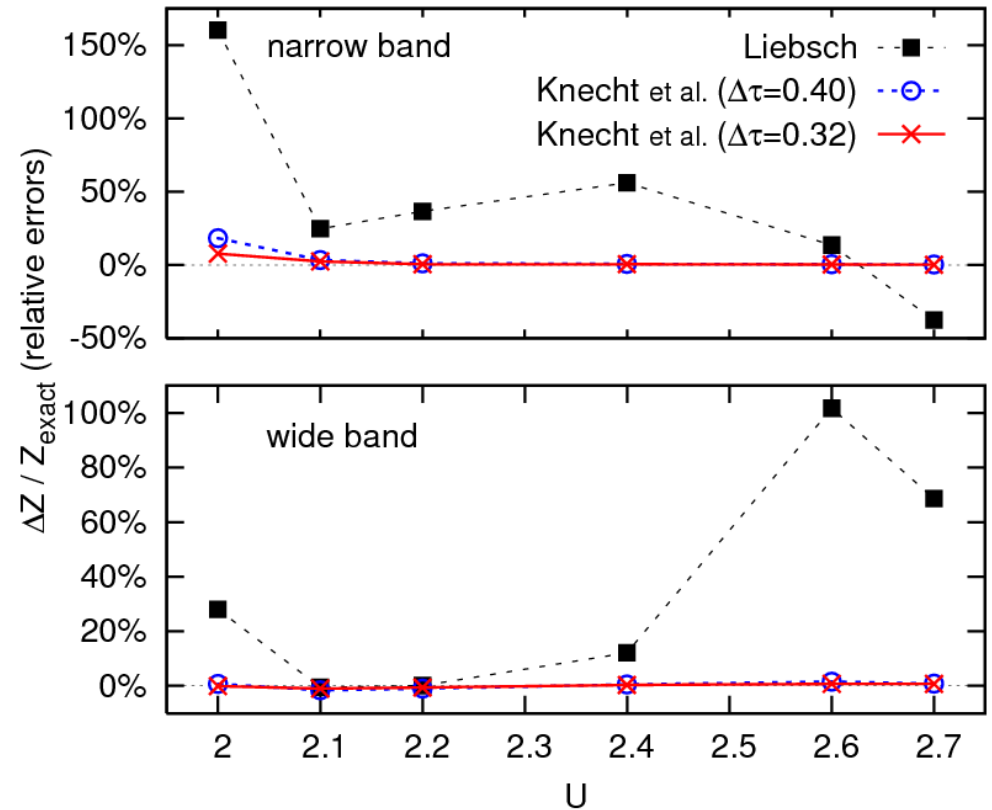
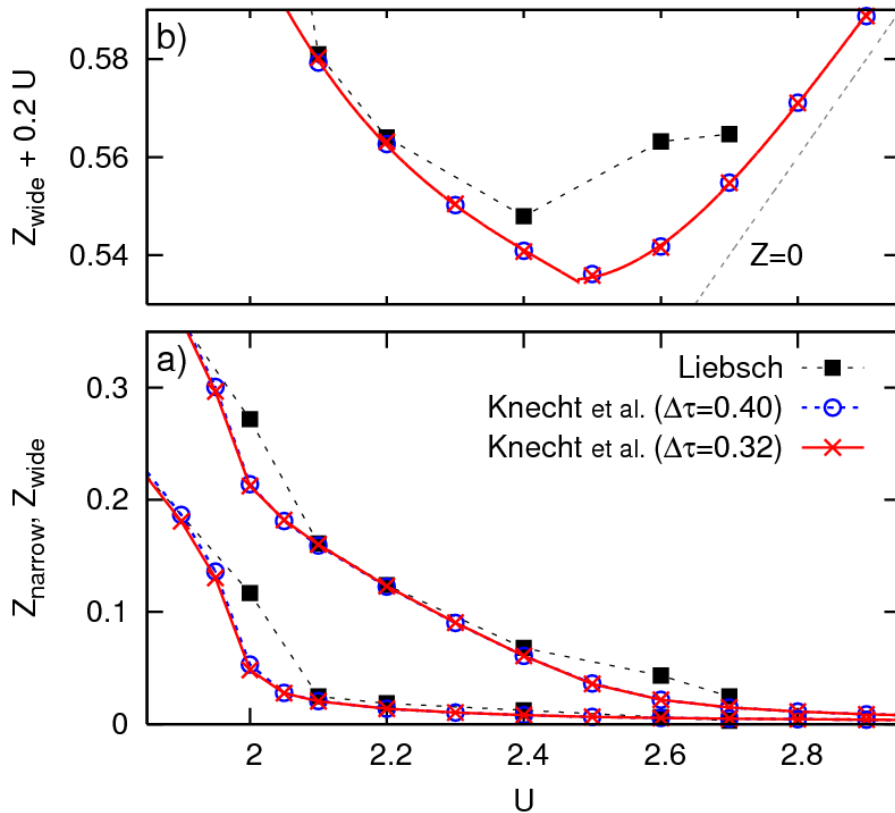
Self-energy and quasiparticle weight  $Z$  in OSM phase

$T$ -dependence of  $Z_{\text{wide}}$  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

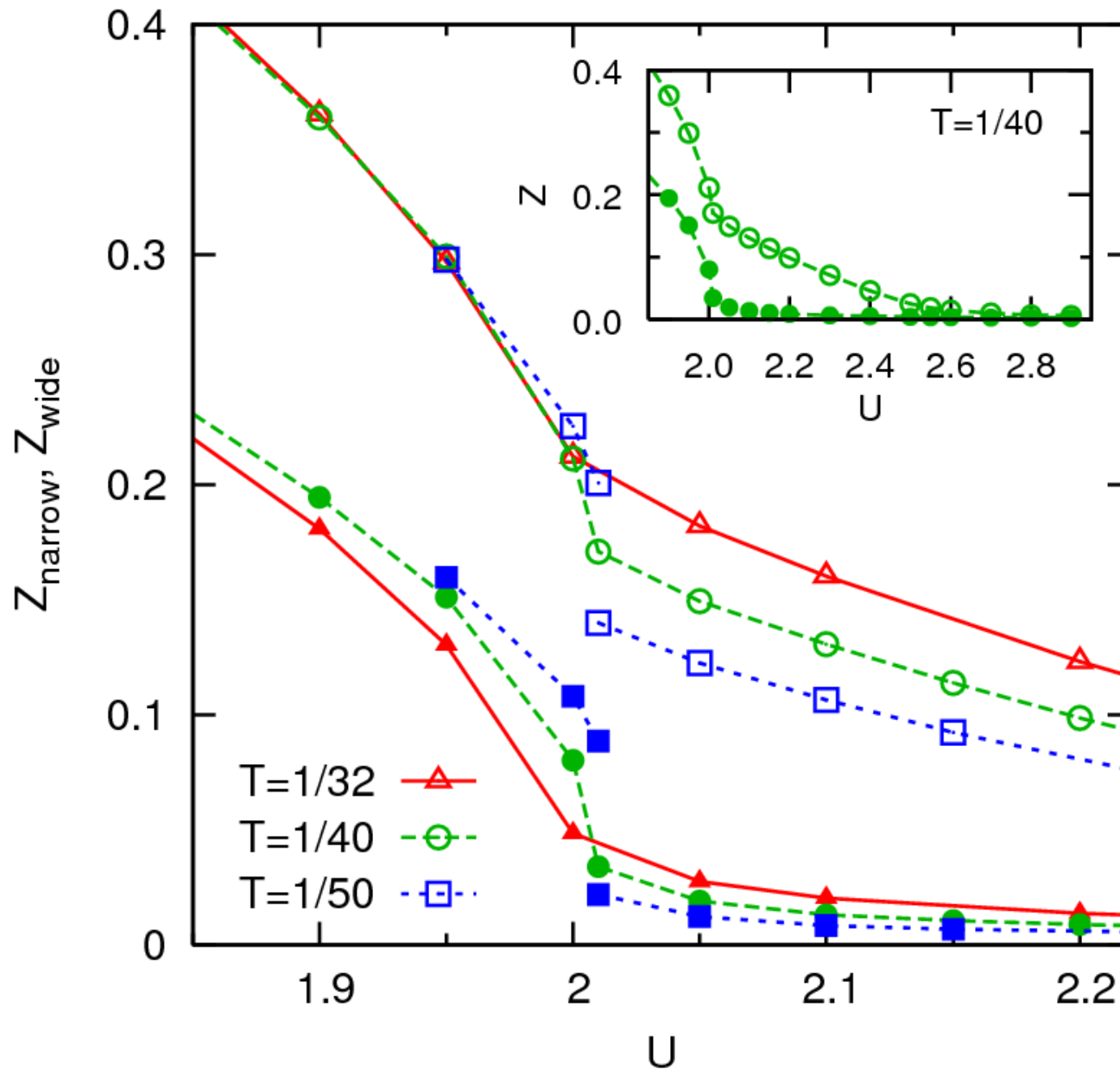


Numerical noise in Liebsch's QMC data obscures second transition

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]