Orbital-selective Mott transitions in the anisotropic 2-band Hubbard model at finite temperatures

Nils Blümer

Outline

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

Complementing QMC with high-frequency expansions

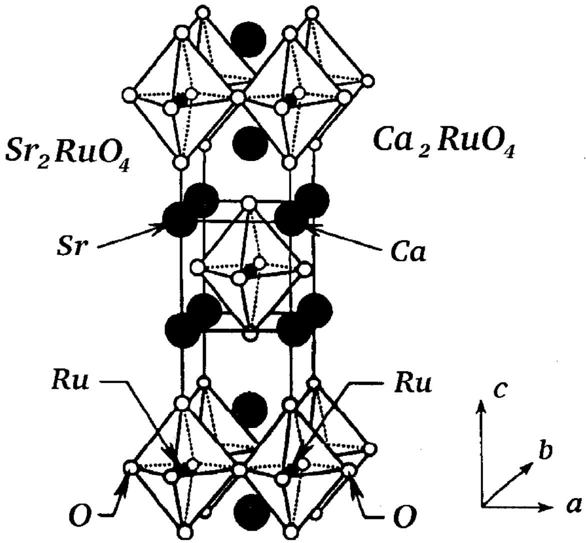
Mott transition in frustrated 1-band Hubbard model

High-precision ground state estimates from QMC

Orbital-selective Mott transitions in 2-band Hubbard model

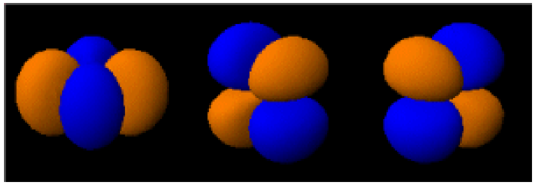
Summary

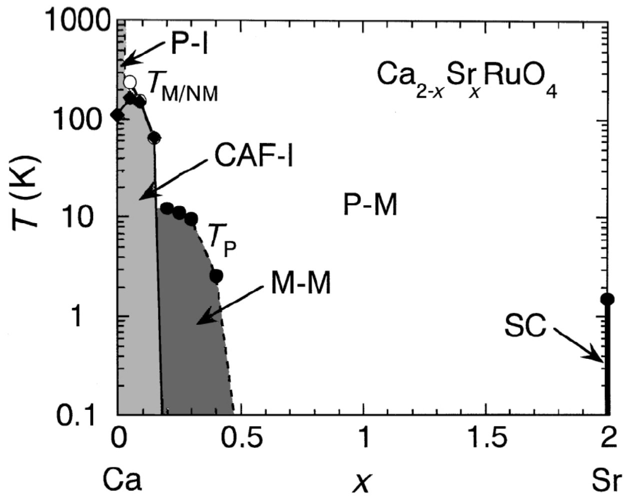
Motivation: OSMTs in $Ca_{2-x}Sr_xRuO_4$



$Ca_{2-x}Sr_xRuO_4$:
isostructural to $La_{2-x}Sr_xCuO_4$

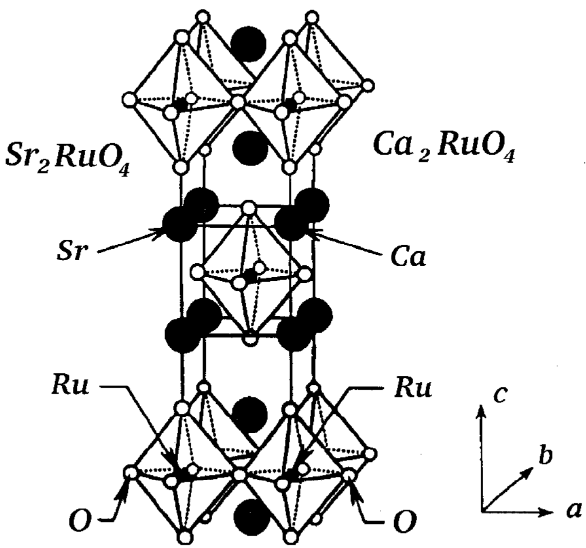
Sr_2RuO_4: quasi-2d FL,
spin-triplet superconductor





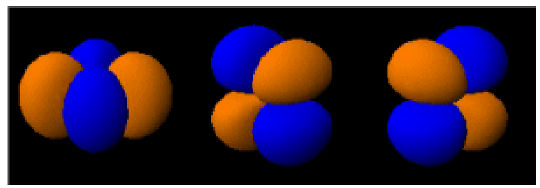
[Nakatsuji, Maeno, PRL **84**, 2666 (2000)]

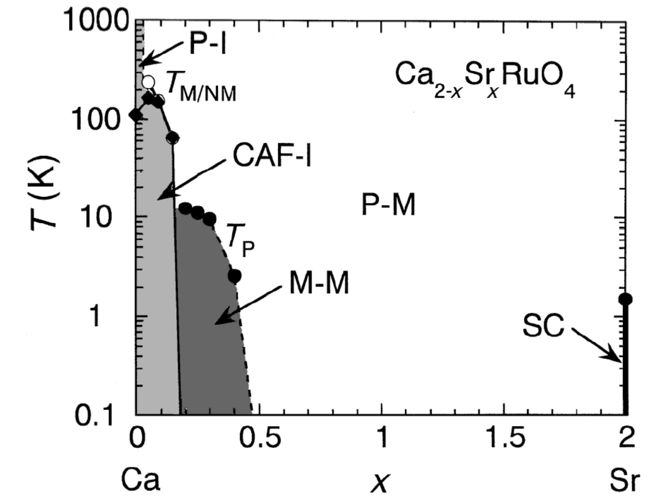
Motivation: OSMTs in $Ca_{2-x}Sr_xRuO_4$



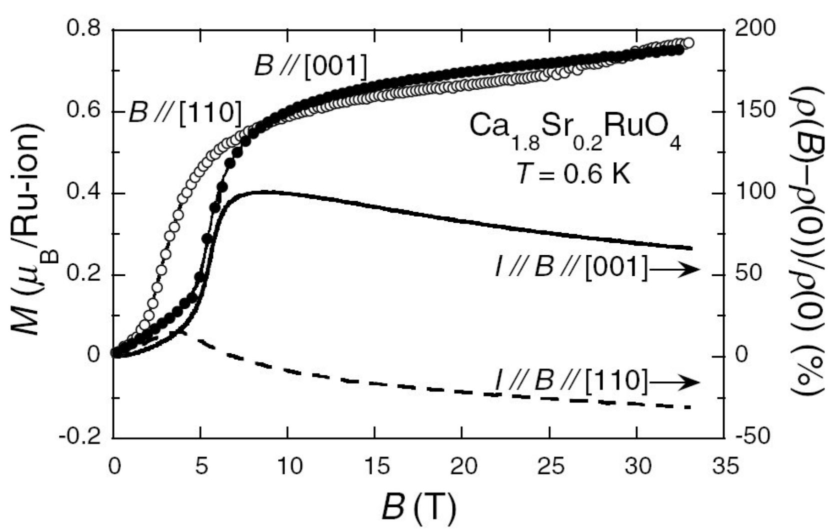
$Ca_{2-x}Sr_xRuO_4$:
isostructural to $La_{2-x}Sr_xCuO_4$

Sr_2RuO_4: quasi-2d FL,
spin-triplet superconductor





[Nakatsuji, Maeno, PRL **84**, 2666 (2000)]



[Nakatsuji *et al.*, PRL **90**, 137202 (2003)]

saturation moment, susceptibility

$\rightsquigarrow S = 1/2$ system for $x \gtrsim 0.2$ (not $S = 1$)

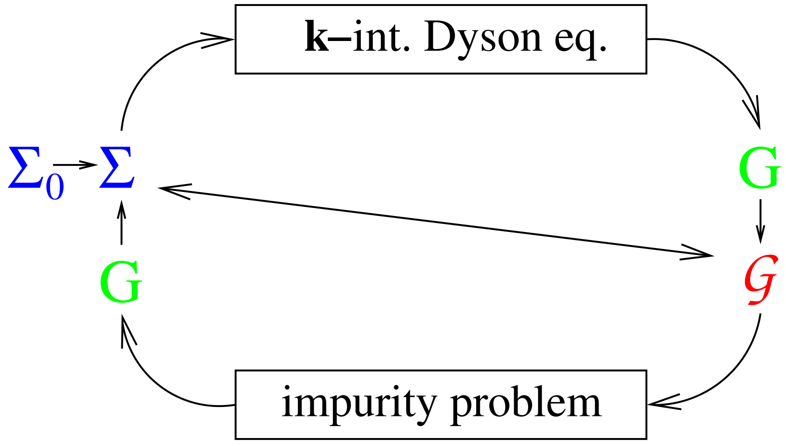
strongly anisotropic magnetoresistance

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

high-precision methods needed!

Complementing QMC with high-frequency expansions

Iterative solution of DMFT equations



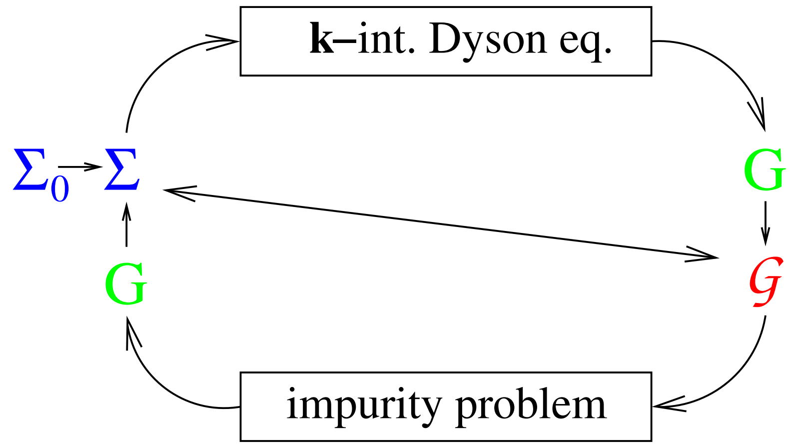
$\longleftarrow$ DOS / t_{ij} / $\epsilon_{\nu \boldsymbol{k}}$

Fourier transformations

$\longleftarrow$ local interactions

Complementing QMC with high-frequency expansions

Iterative solution of DMFT equations

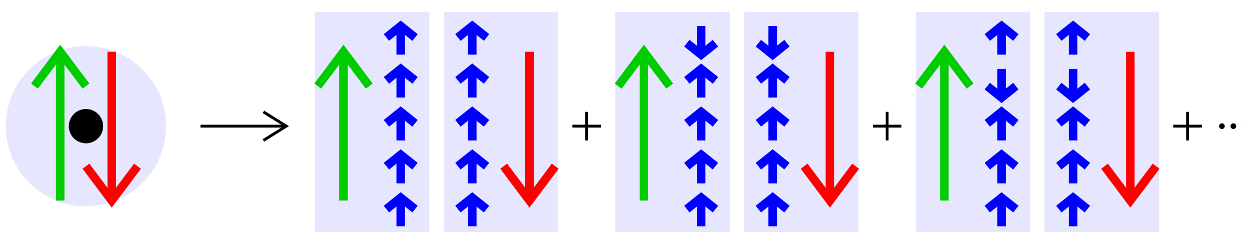


$\longleftarrow$ DOS / t_{ij} / $\epsilon_{\nu \boldsymbol{k}}$

Fourier transformations

$\longleftarrow$ local interactions

QMC: discretization $\beta = \Lambda\,\Delta\tau$, Trotter decoupling, discrete Hubbard-Stratonovich transformation



Wick theorem:

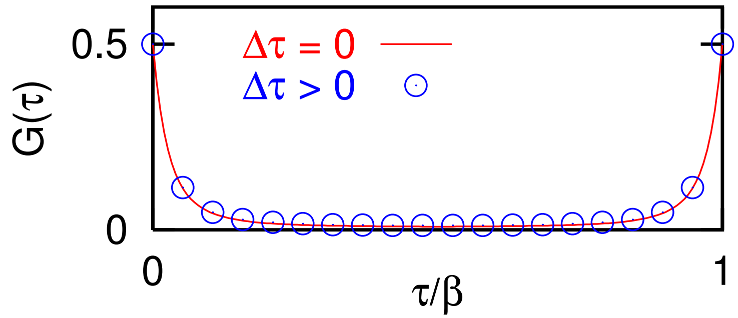
$$G = \frac{\sum M \det\{M\}}{\sum \det\{M\}}$$

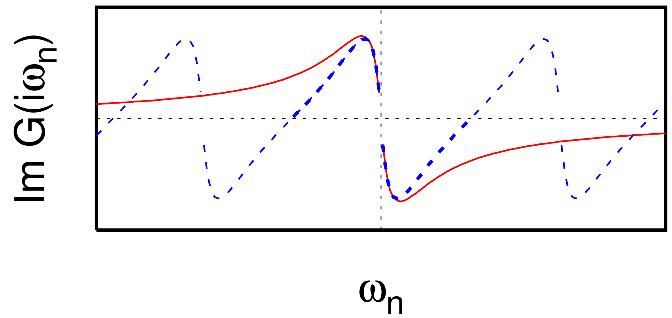
Metropolis MC importance sampling over auxiliary Ising field, 2^{Λ} configurations, $50 \lesssim \Lambda \lesssim 400$

+ numerically exact   – effort scales as T^{-3}

– no info for $\omega \gtrsim \omega_{\text{Nyquist}}$ $\rightsquigarrow$ problems with Fourier transforms

naive discrete FT
$\rightsquigarrow$ oscillations
(instead of
$G(\omega) \xrightarrow{\omega\to\infty} 1/\omega$)





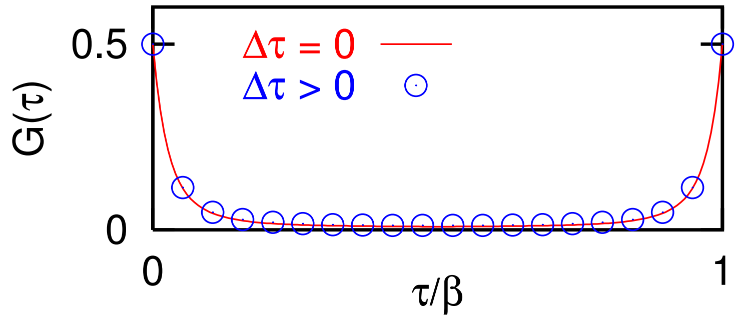
1^{st} solution: correct unphysical behavior for $|\omega| \lesssim \omega_{\text{Nyquist}}$ by transformation [Ulmke]

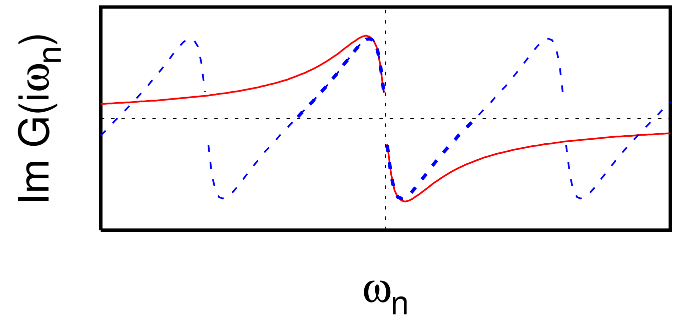
2^{nd} solution: interpolate $G_{\text{QMC}}(\tau)$
by cubic splines [Jarrell, Krauth, . . .]

but: natural boundary conditions not appropriate for $G(\tau)$:

- adjust bc's [Oudovenko]
- spline-fit only difference w.r.t. reference problem:
  - IPT [Jarrell]

naive discrete FT
⇝ oscillations
(instead of
$G(\omega) \overset{\omega\to\infty}{\longrightarrow} 1/\omega$)



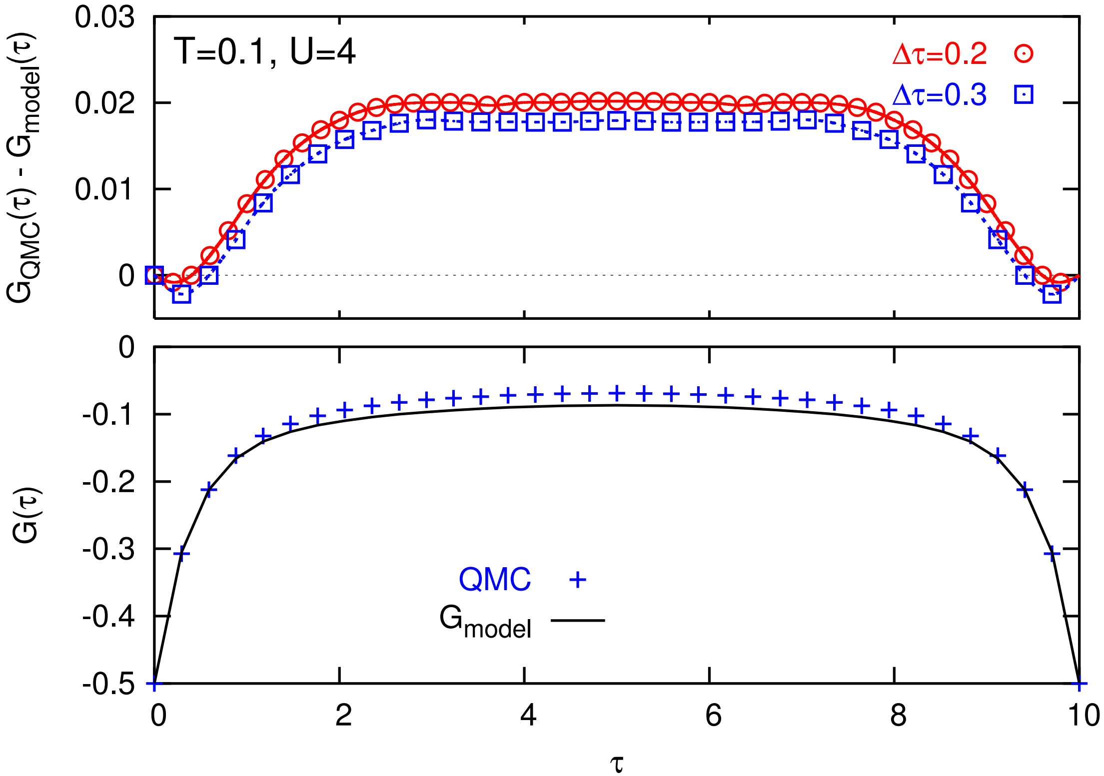


1^{st} solution: correct unphysical behavior for $|\omega| \lesssim \omega_{\text{Nyquist}}$ by transformation [Ulmke]

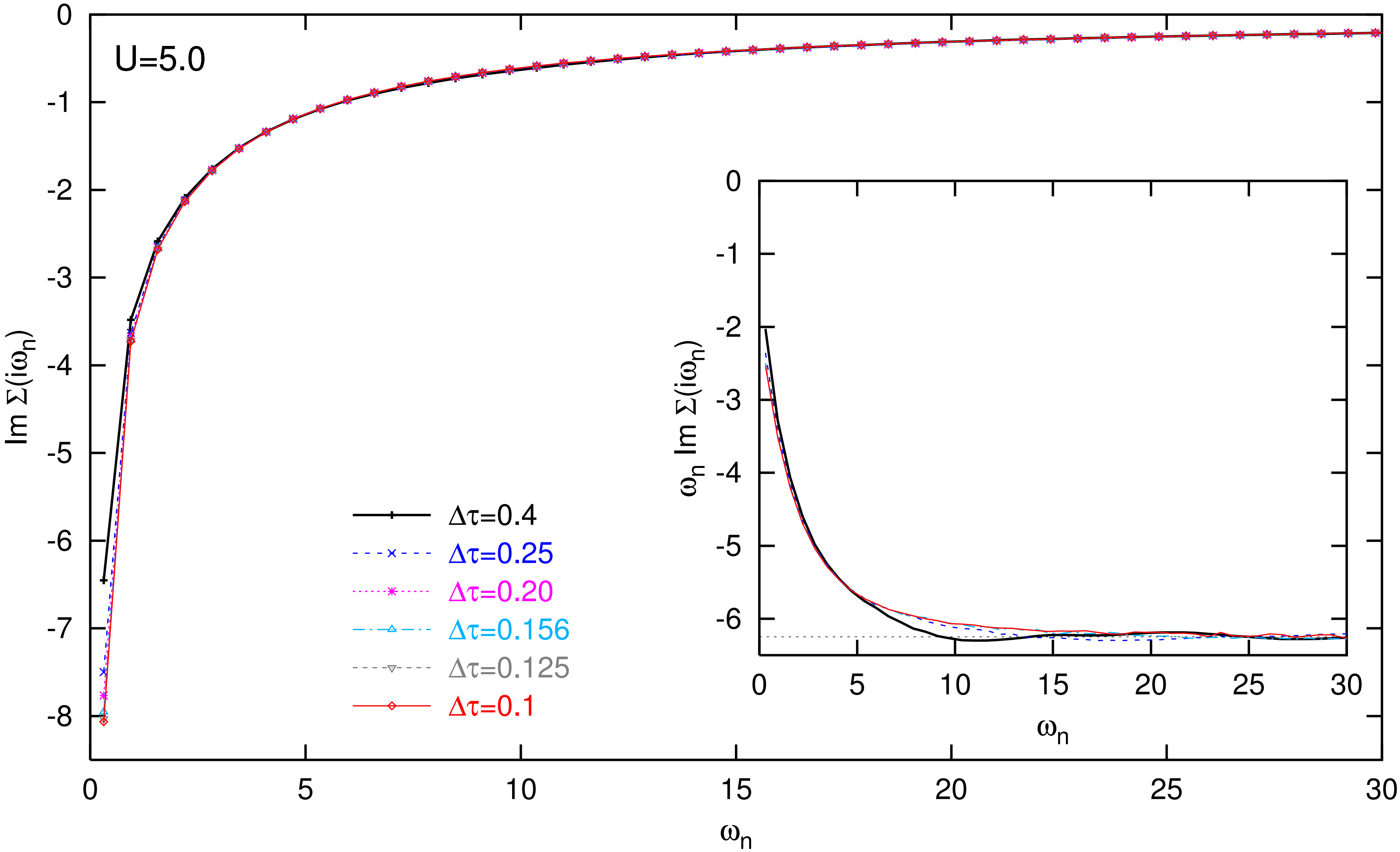
2^{nd} solution: interpolate $G_{\text{QMC}}(\tau)$ by cubic splines [Jarrell, Krauth, . . .]

but: natural boundary conditions not appropriate for $G(\tau)$:

- adjust bc's [Oudovenko]
- spline-fit only difference w.r.t. reference problem:
  - IPT [Jarrell]
  - high-frequency expansion for Σ + fit-param. [Knecht, NB]

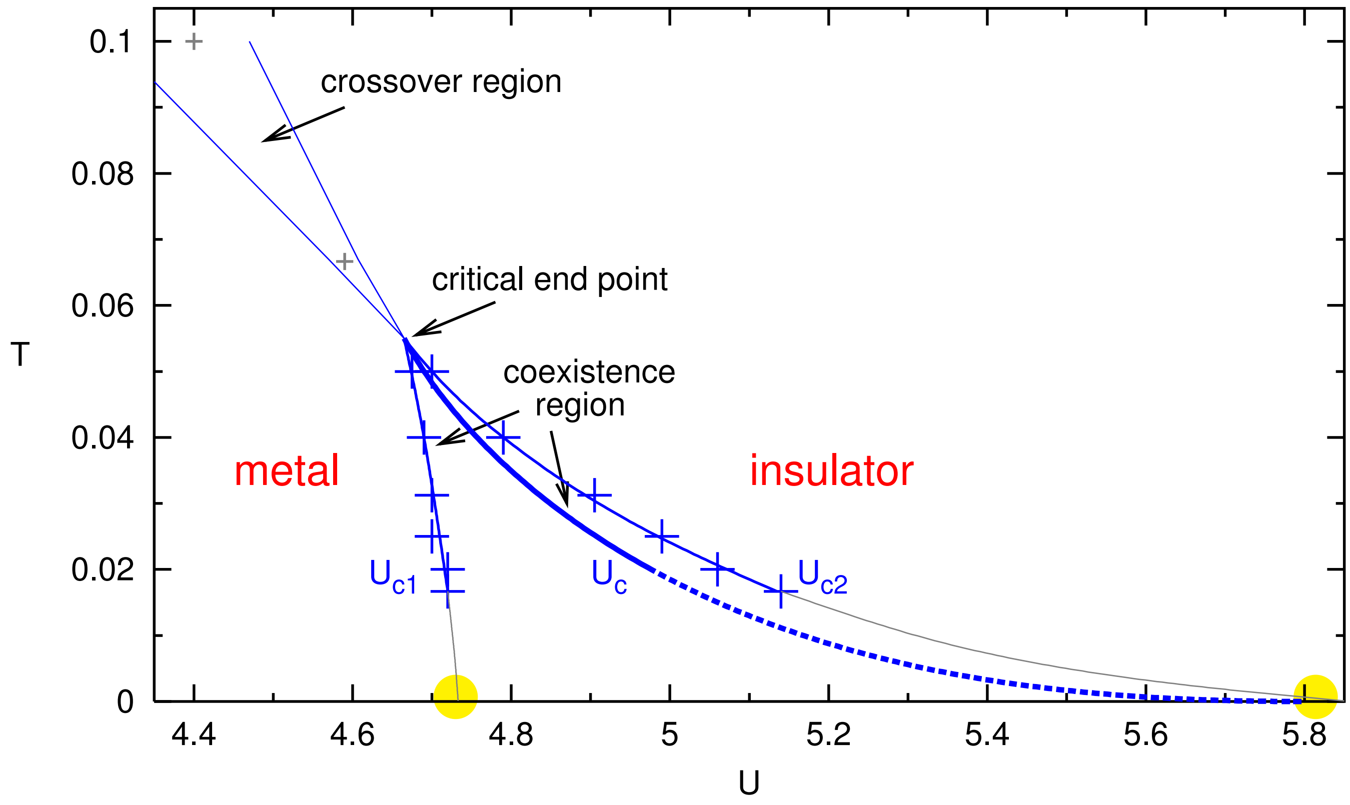


Sensitive test: self-energy $\Sigma(i\omega_n)$ for insulating phase ($T = 0.1$, $U = 5.0$)



Rapid convergence at all frequencies for "QMC + $1/\omega$" DMFT solver

Mott transition in frustrated 1-band Hubbard model



Georges and Krauth (1993)

Rozenberg, Kotliar, Zhang (1994)

Georges *et al.* (RMP, 1996)

Schlipf *et al.* (1999)

Rozenberg, Chitra, Kotliar (1999)

Krauth (2000)

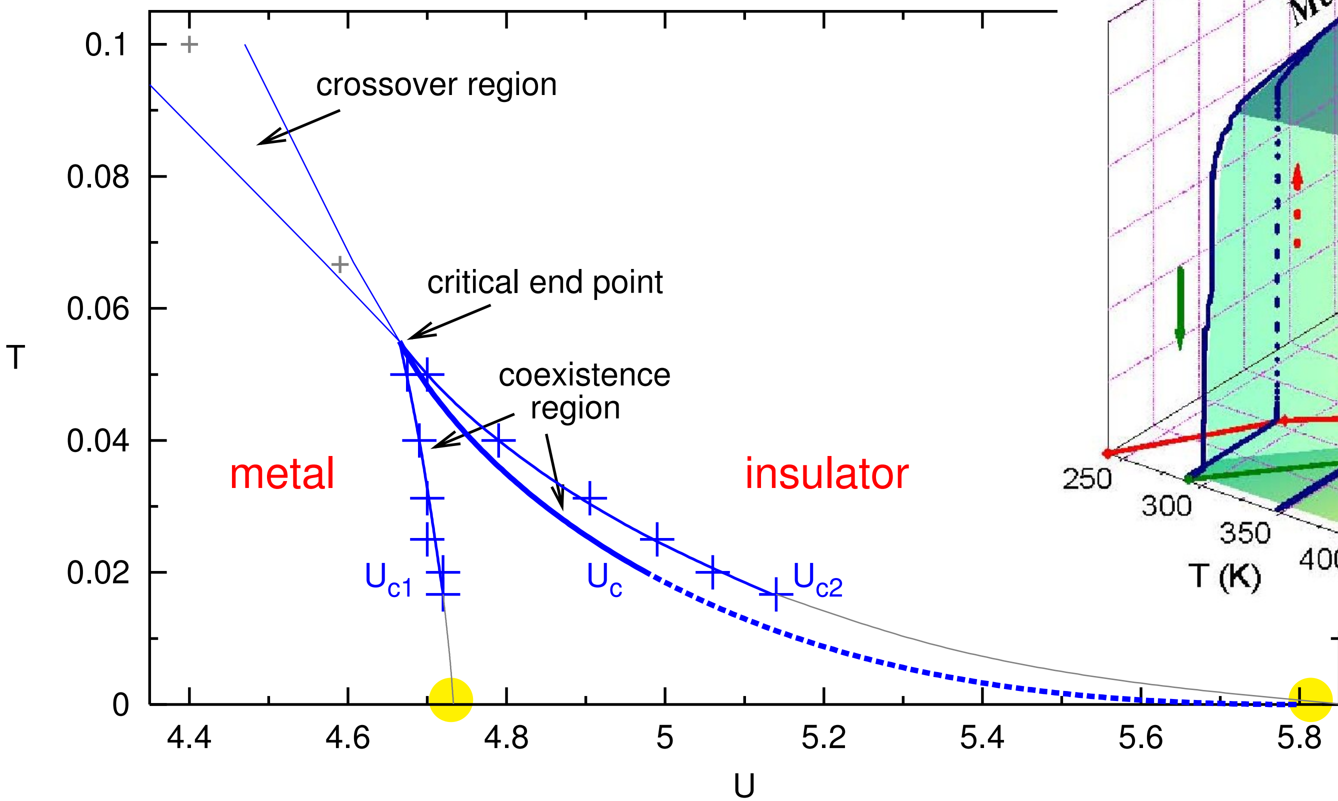
Bulla (1999, 2001)

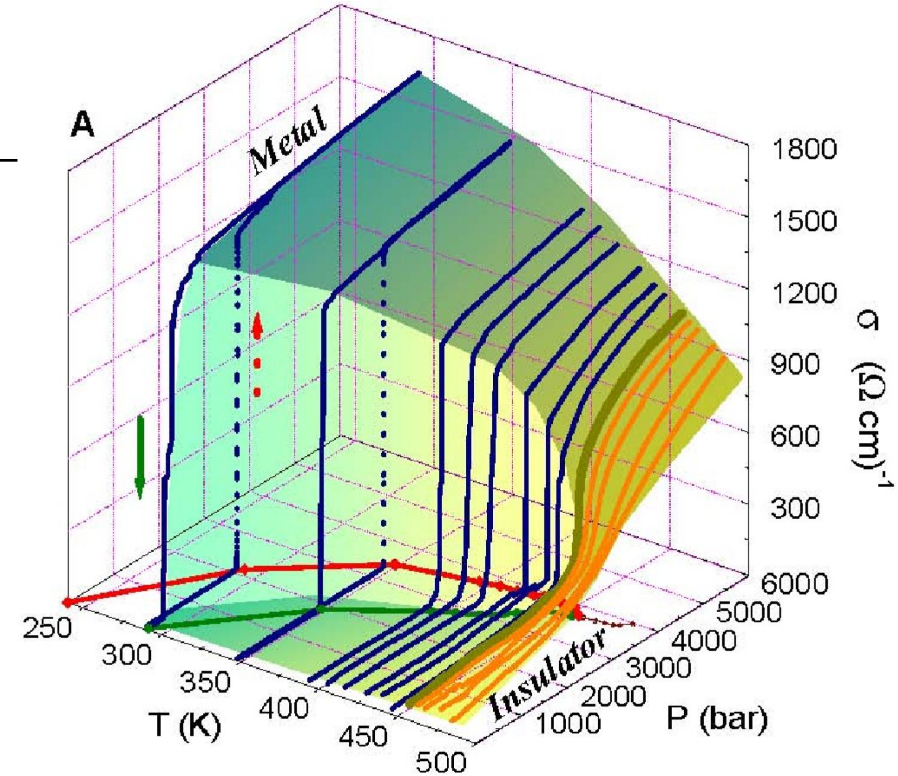
Joo, Oudovenko (2001)

Tong (2001)

Blümer (2000, 2002)

Mott transition in frustrated





Blümer (2000, 2002)

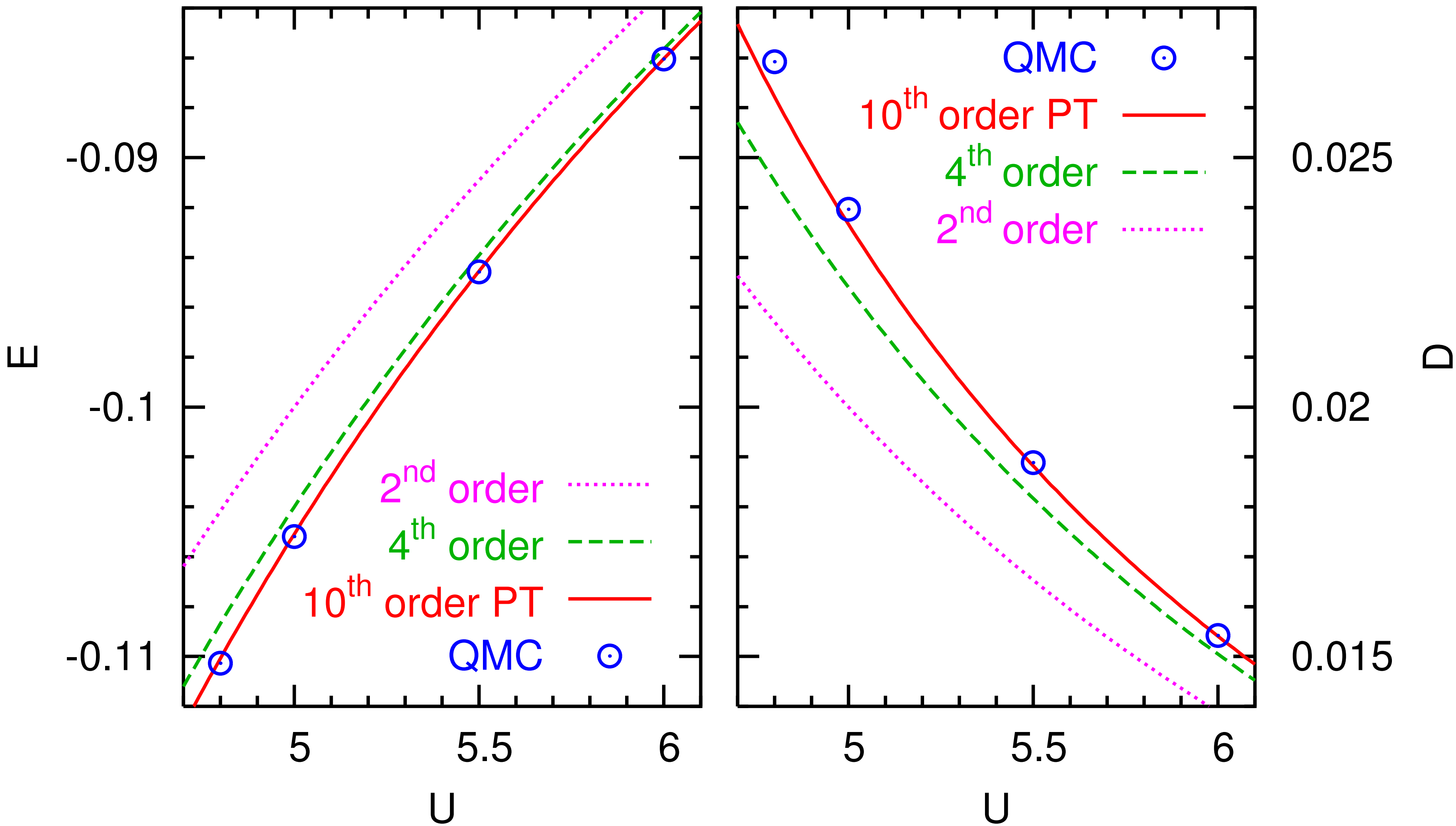
1st order line from $\dfrac{\mathrm{d}U_c(T)}{\mathrm{d}T} = f(T, U_c(T));\ \ f(T,U) := \dfrac{\Delta E(T,U)}{T\,\Delta D(T,U)}$

low-T asymptotics from $U_c(T) = U_c^0 - \sqrt{\dfrac{2S_oT}{a}} + \dfrac{\gamma_0}{4S_0}T + \mathcal{O}(T^{3/2})$

High-precision energetics needed, even for $T \longrightarrow 0$

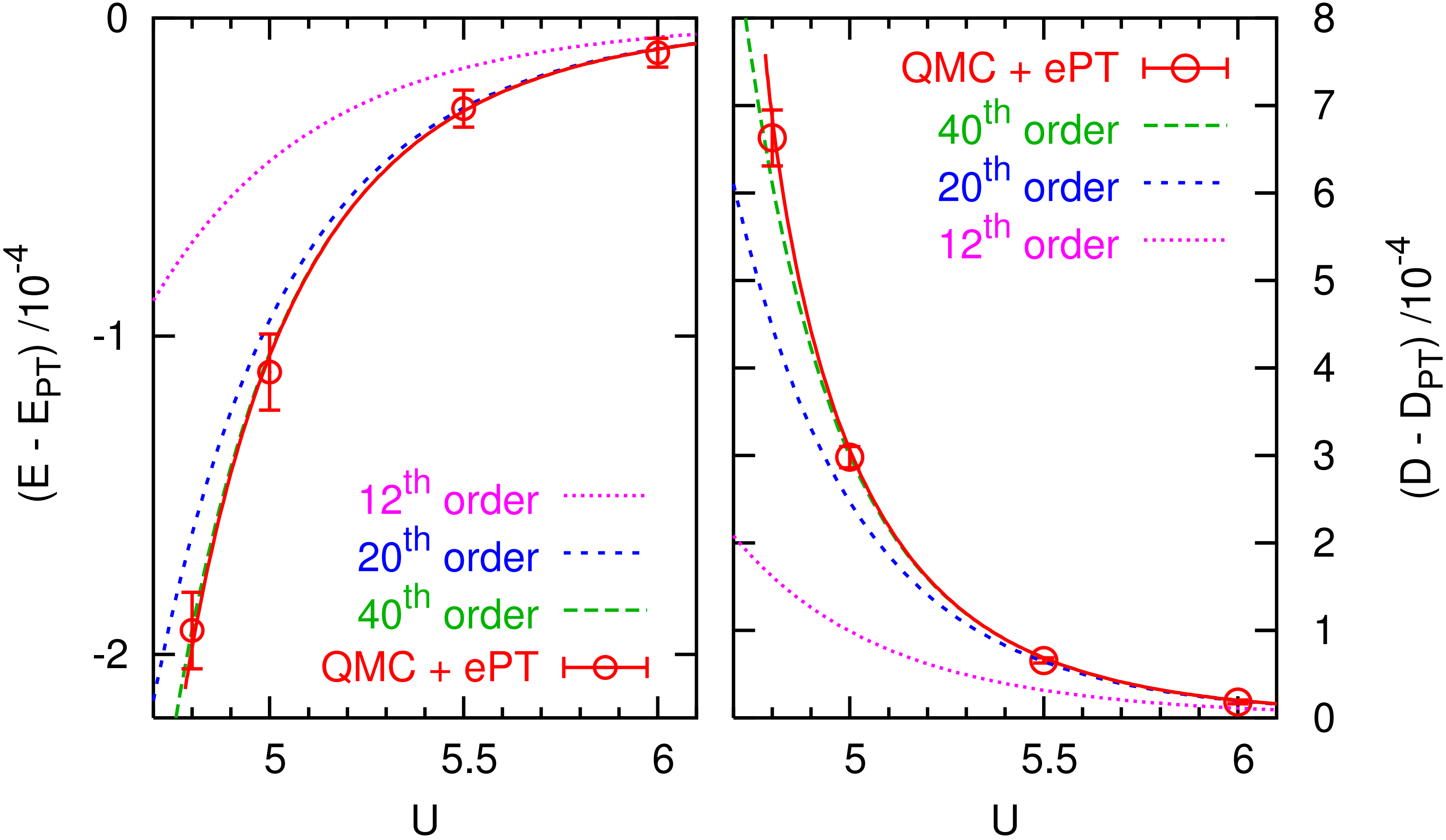
High-precision ground state estimates from QMC

QMC (+ high-frequency expansion) vs. strong-coupling PT for insulating phase



Excellent agreement at $U = 6.0$, deviations below.

Higher resolution plots: differences w.r.t. 10^{th} order PT

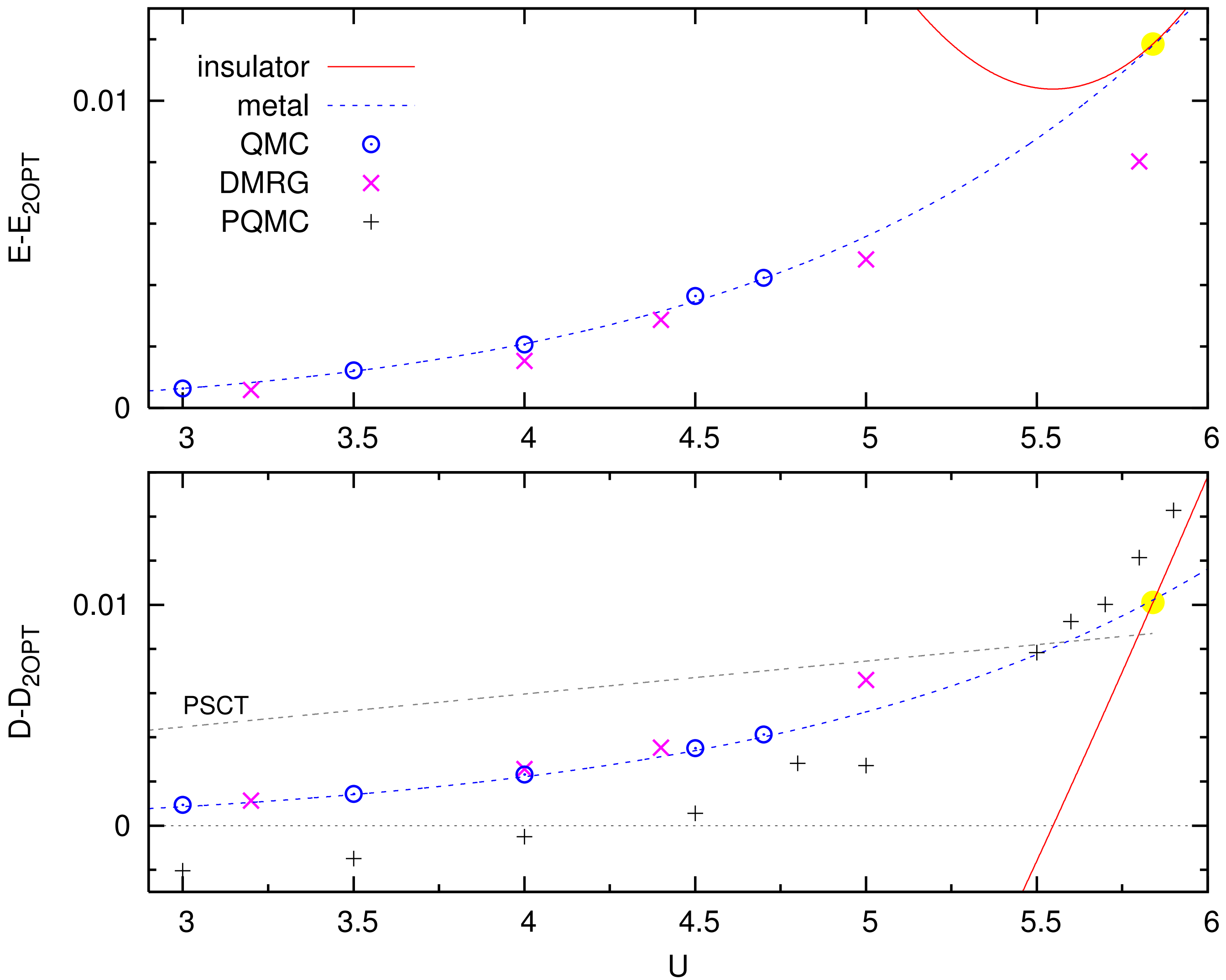


ePT: extrapolation of PT to infinite order [NB, Kalinowski, Phys. Rev B **71**, 195102 (2005)]

$\rightsquigarrow$ critical interaction U_{c1}, critical exponents, benchmark ($\Delta E \lesssim 10^{-6}$)

QMC algorithm has passed only available authoritative (1-band) test!

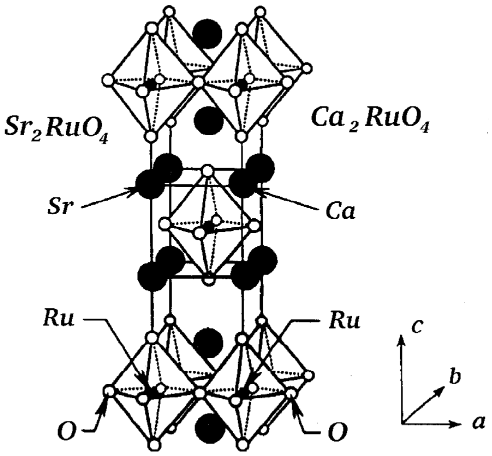
Metallic phase: differences w.r.t. 2^{nd} order weak-coupling PT for E and D

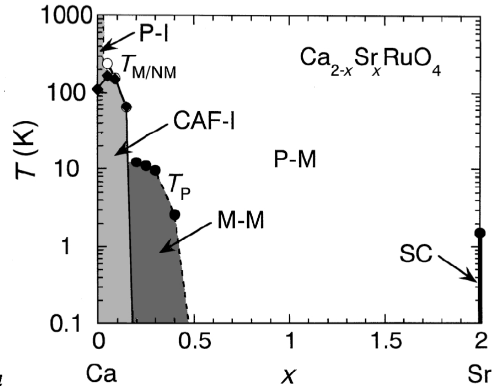


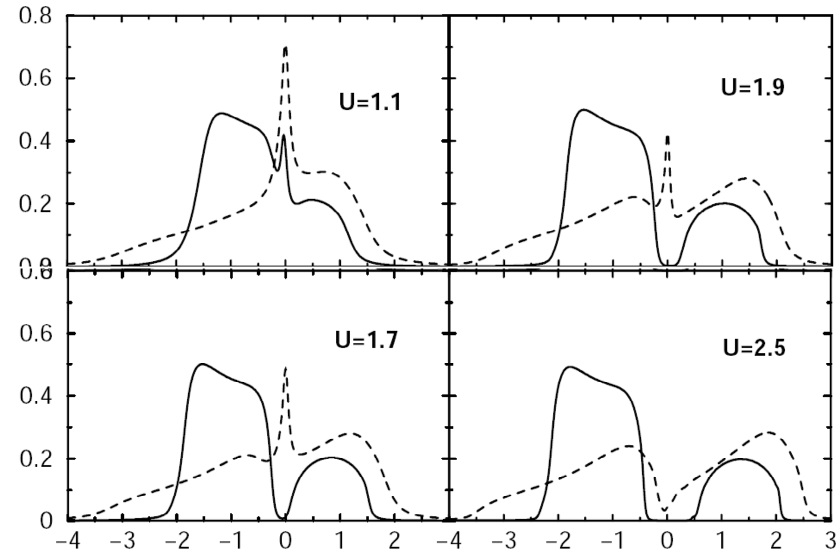
QMC-fit consistent with ePT for insulator; larger deviations of PSCT, DMRG, and PQMC.

4^{th} order PT coefficient corrected by QMC $(-62 \longrightarrow +5)$

Orbital-selective Mott transitions in 2-band Hubbard model

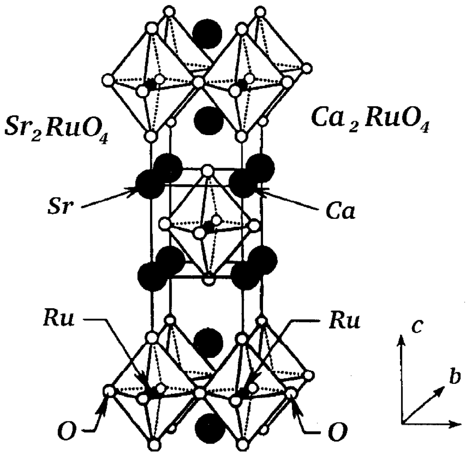


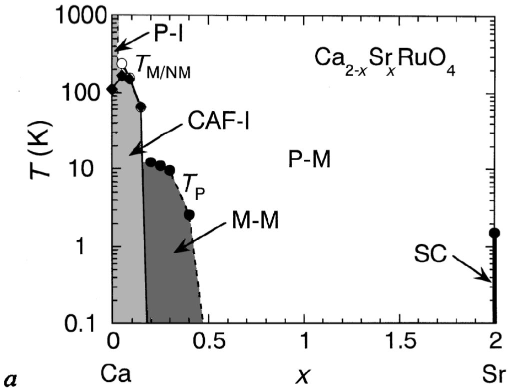


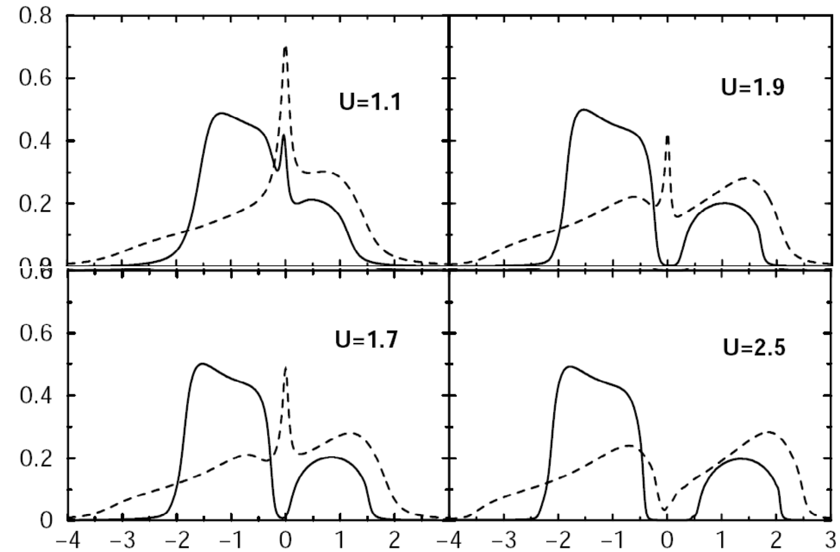


[LDA+DMFT(NCA): Anisimov *et al.* (2002)]

Orbital-selective Mott transitions in 2-band Hubbard model

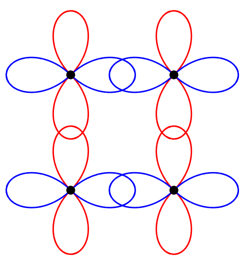






[LDA+DMFT(NCA): Anisimov *et al.* (2002)]

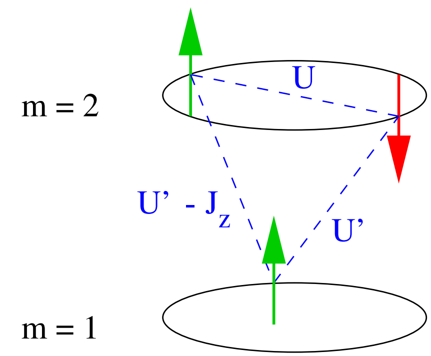
Minimal model: 2-band Hubbard model
with orbital-dependent hopping



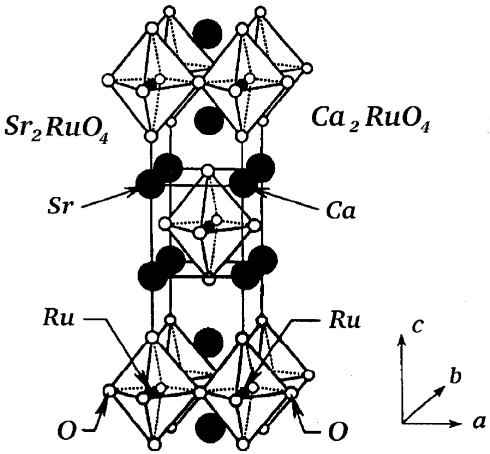
$$H = \sum_{m=1}^{2} \Big[-\sum_{\langle ij\rangle\sigma} t_m c^\dagger_{im\sigma} c_{jm\sigma} + U \sum_i n_{im\uparrow} n_{im\downarrow} \Big]$$

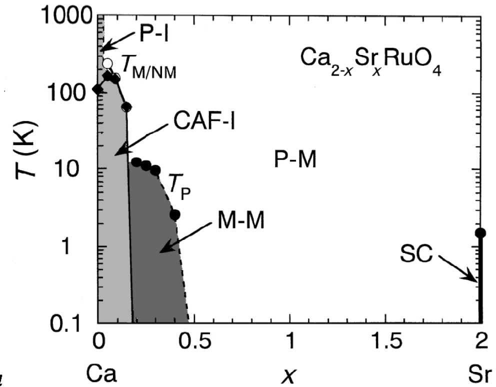
$$+ \sum_{i\sigma\sigma'} (U' - \delta_{\sigma\sigma'} J_z)\, n_{i1\sigma}\, n_{i2\sigma'}$$

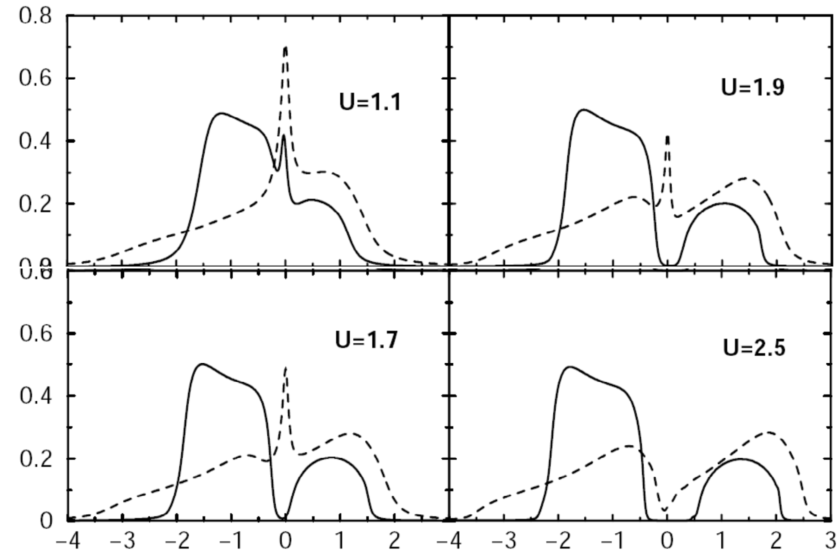
$$+ \tfrac{1}{2} J_\perp \sum_{i\sigma} \Big[c^\dagger_{i1\sigma} \Big(c^\dagger_{i2\bar\sigma} c_{i1\bar\sigma} + c^\dagger_{i1\bar\sigma} c_{i2\bar\sigma} \Big) c_{i2\sigma} + \text{h.c.} \Big]$$



Orbital-selective Mott transitions in 2-band Hubbard model

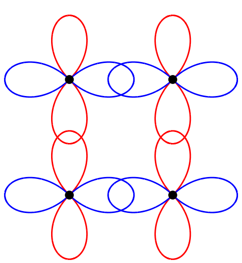




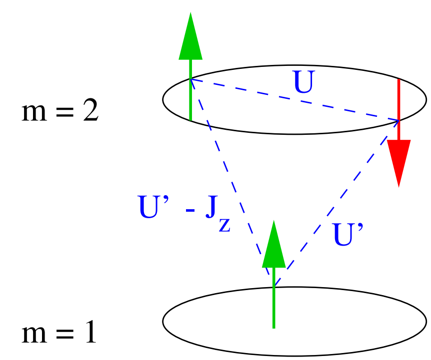


[LDA+DMFT(NCA): Anisimov *et al.* (2002)]

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



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



For Bethe DOS, $t_2 = 2\,t_1$: two 1^{st} order MITs for $U' = J_z = J_\perp = 0$ (trivial)

two distinct MITs for $J_z = J_\perp = U/4$ [Koga *et al.*, PRL **92**, 216402 (2004)]

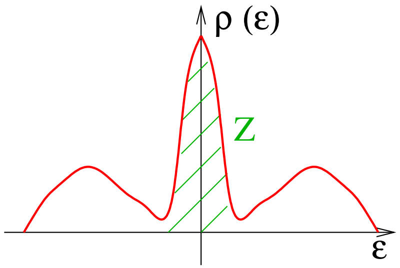
single MIT or **two OSMTs** for $J_\perp = 0,\ J_z = U/4$ **?**

Earlier DMFT-QMC results: single Mott transition in J_z model ($J_\perp = 0$)

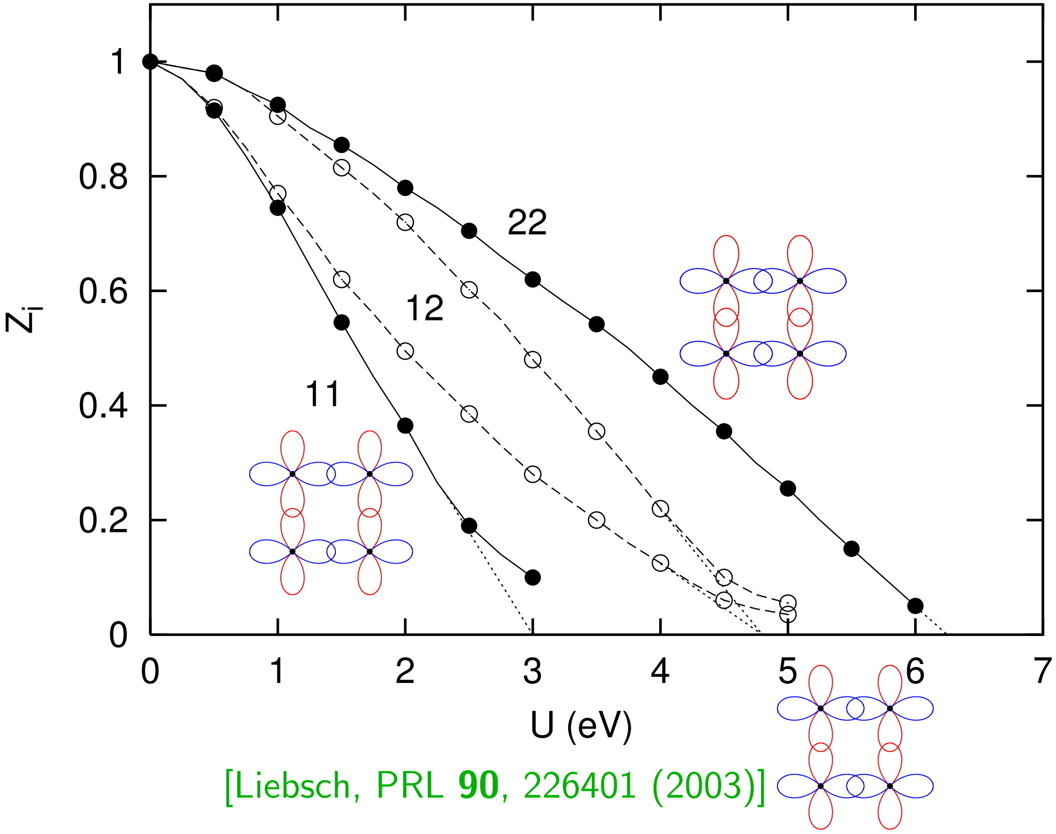
quasiparticle weight $Z_i = m/m_i^*$

discrete QMC estimate:

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



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



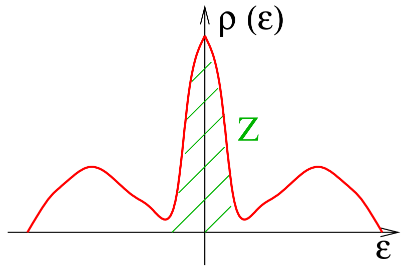
[Liebsch, PRL **90**, 226401 (2003)]

Earlier DMFT-QMC results: single Mott transition in J_z model ($J_\perp = 0$)

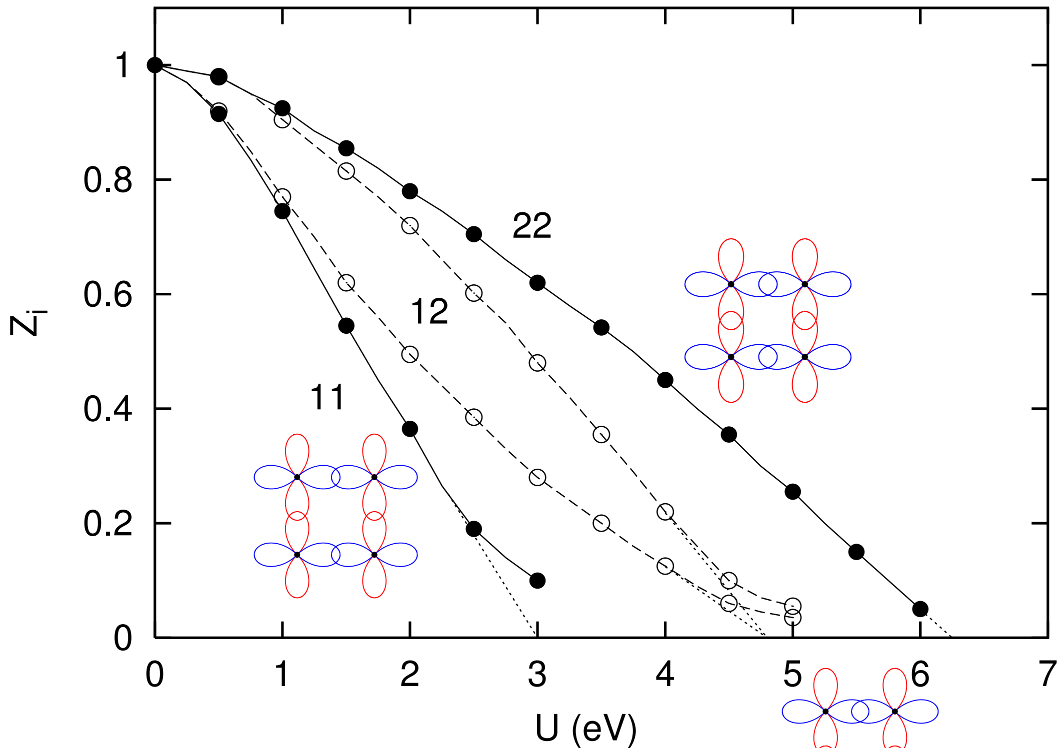
quasiparticle weight $Z_i = m/m_i^*$

discrete QMC estimate:

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

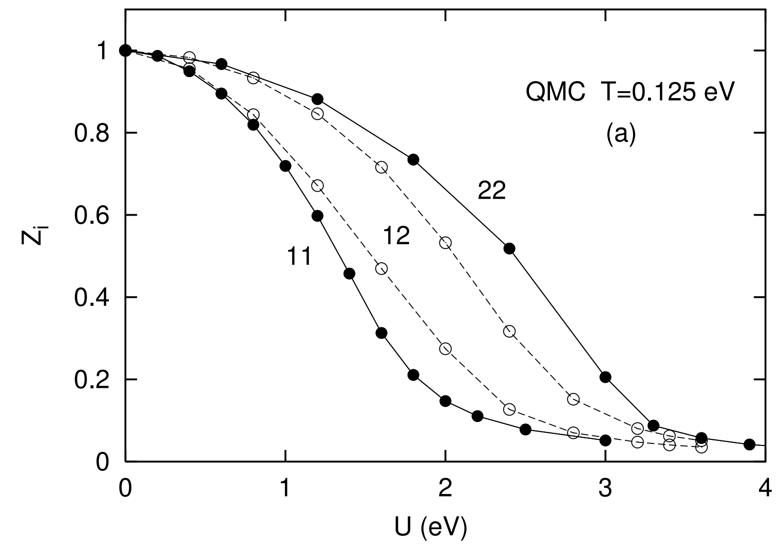


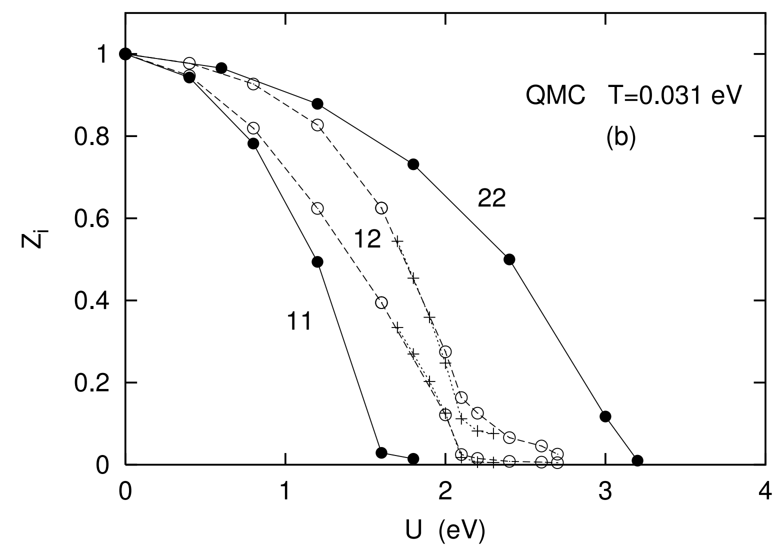
$J_z = 0.2,\ U' = U - 0.4$



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

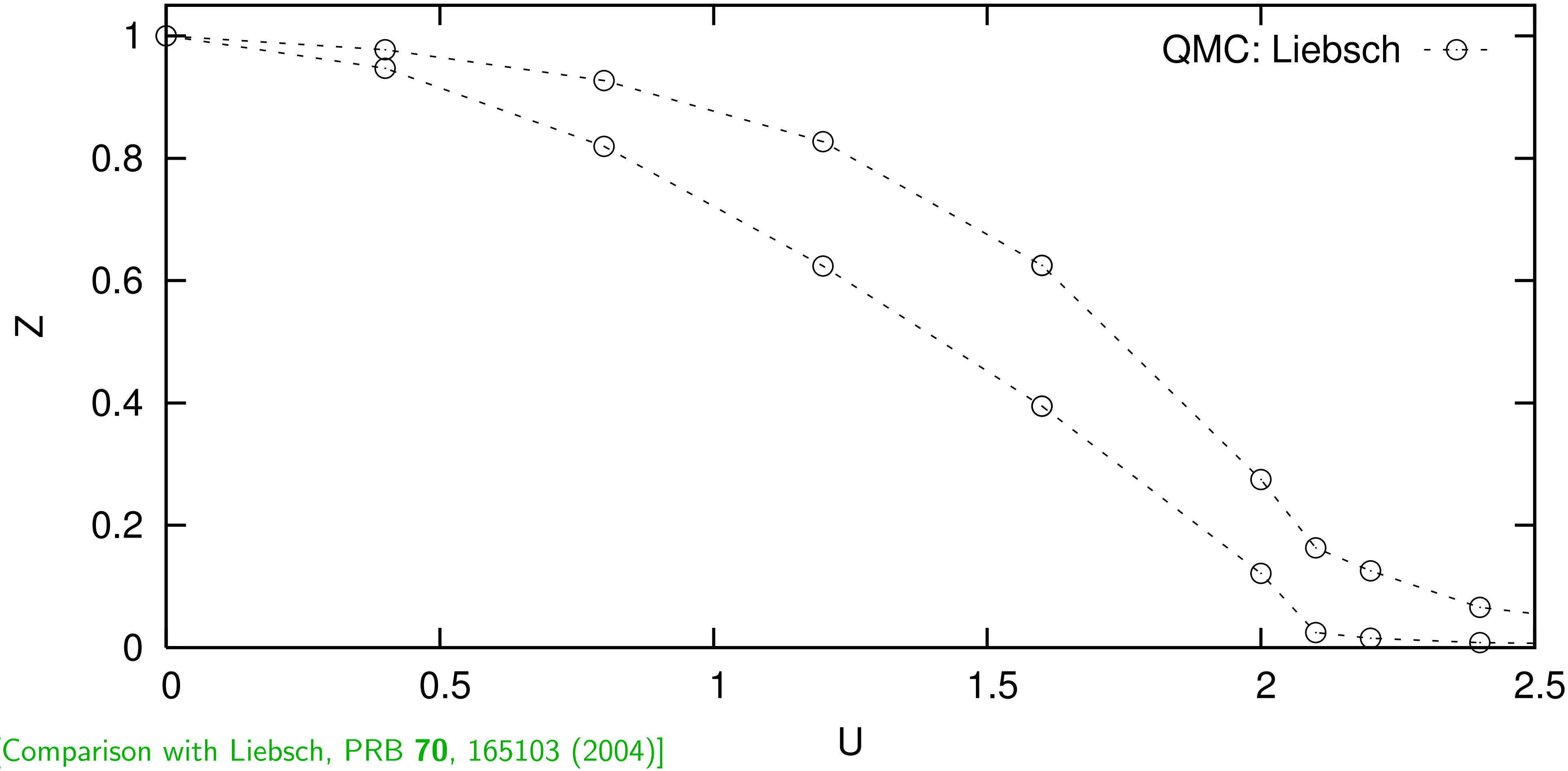
$J_z = U/4,\ U' = U/2$





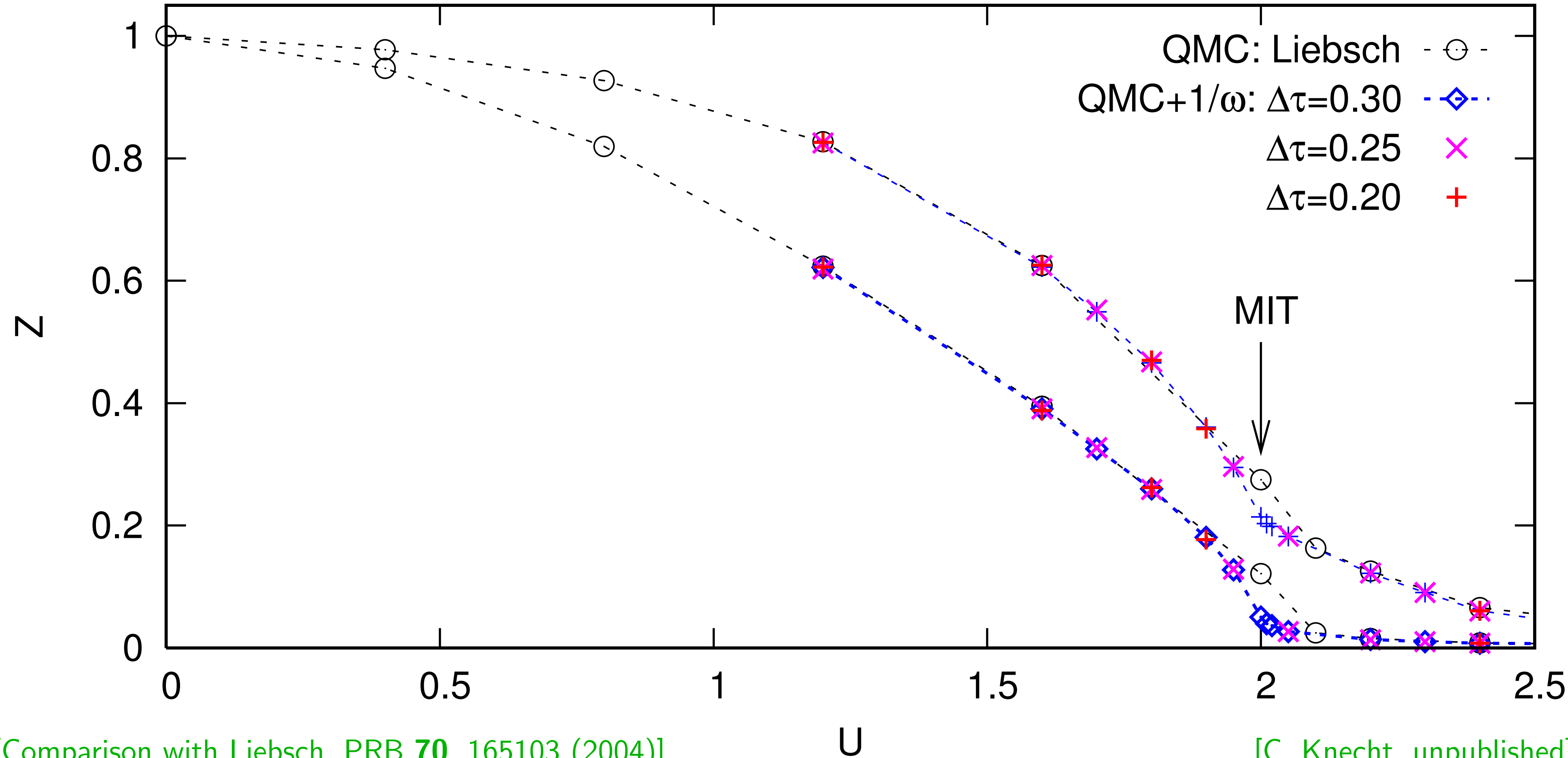
[Liebsch, PRB **70**, 165103 (2004)]

Test for multiband-QMC: quasiparticle weights $Z = m/m^*$ in 2-band model



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

Test for multiband-QMC: quasiparticle weights $Z = m/m^*$ in 2-band model



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

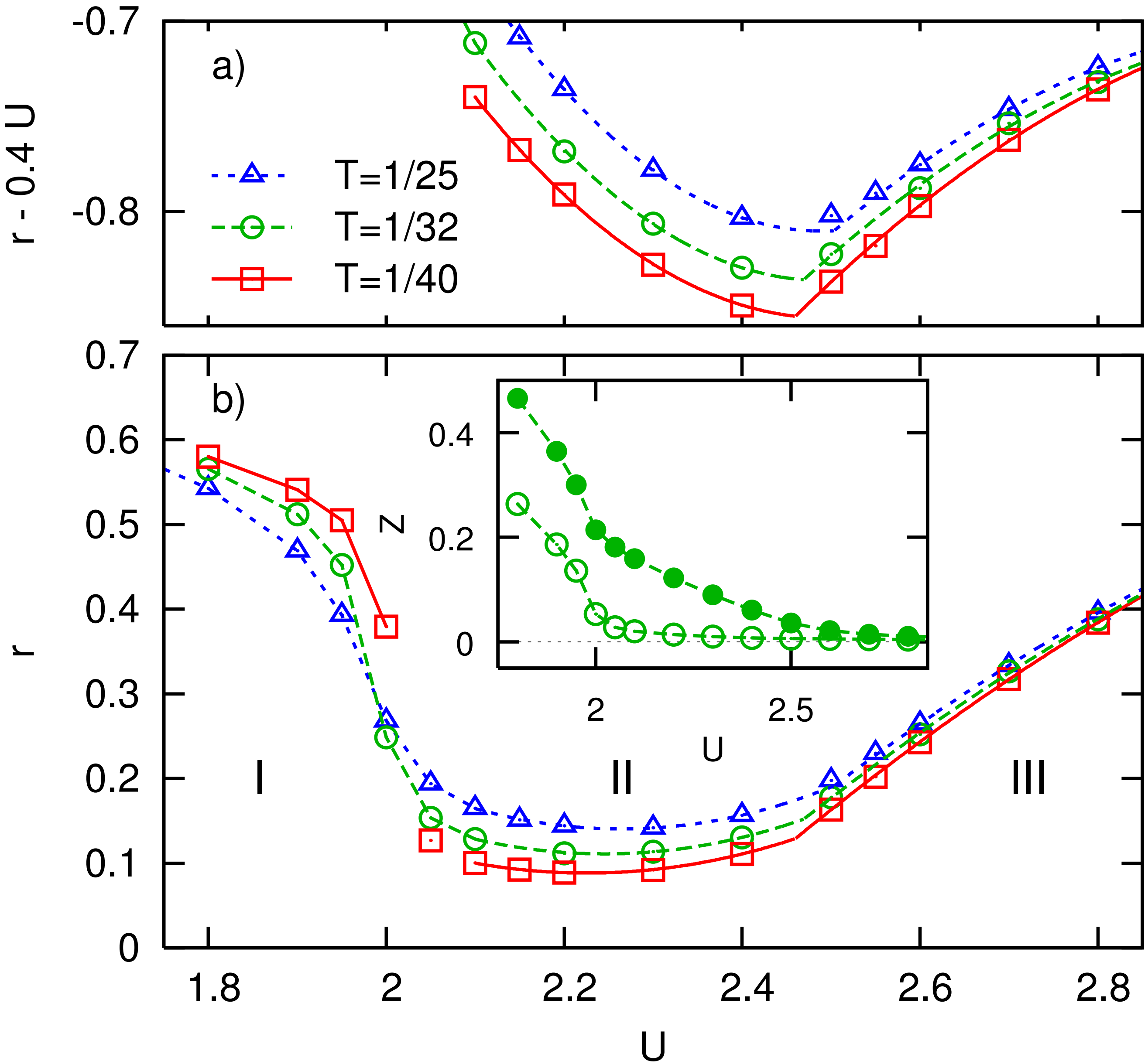
[C. Knecht, unpublished]

Very small dependence on discretization $\Delta\tau$ (here for $T = 1/32$).

Conclusion in 3/2005: New algorithm clearly exposes (single) metal-insulator transition (MIT)

But: wide band still "quite metallic" for $U > 2.0$ – 2^{nd} transition?

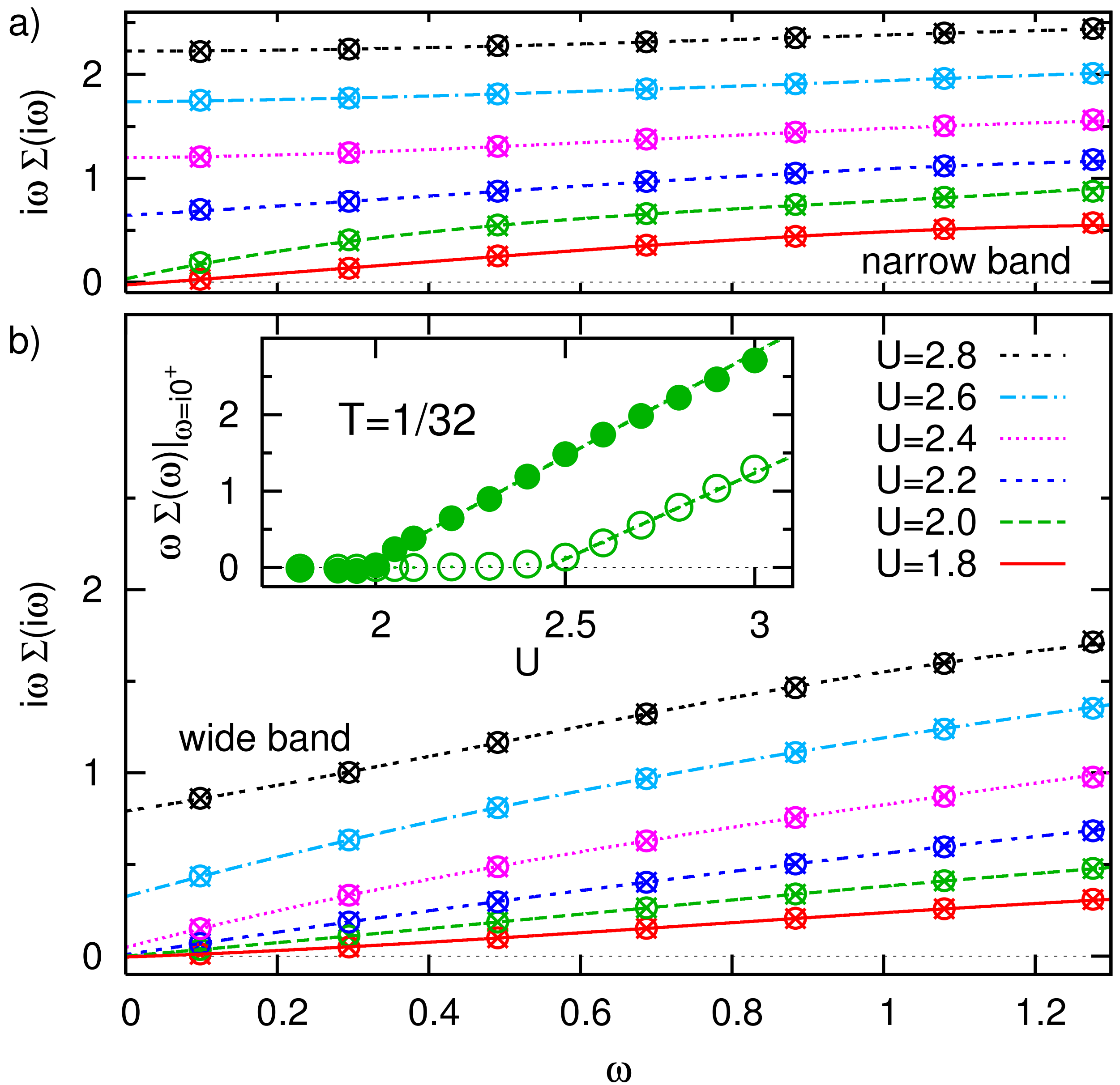
Ratio of quasiparticle weights $r = Z_{\text{narrow}}/Z_{\text{wide}}$



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:

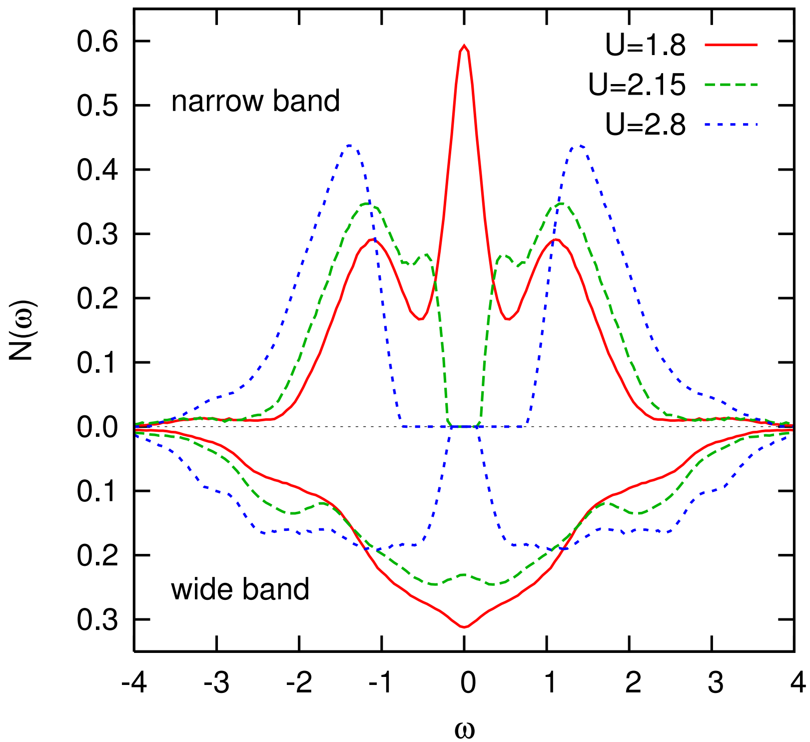
$$\omega\Sigma(\omega) \xrightarrow{\omega\to 0} 0$$

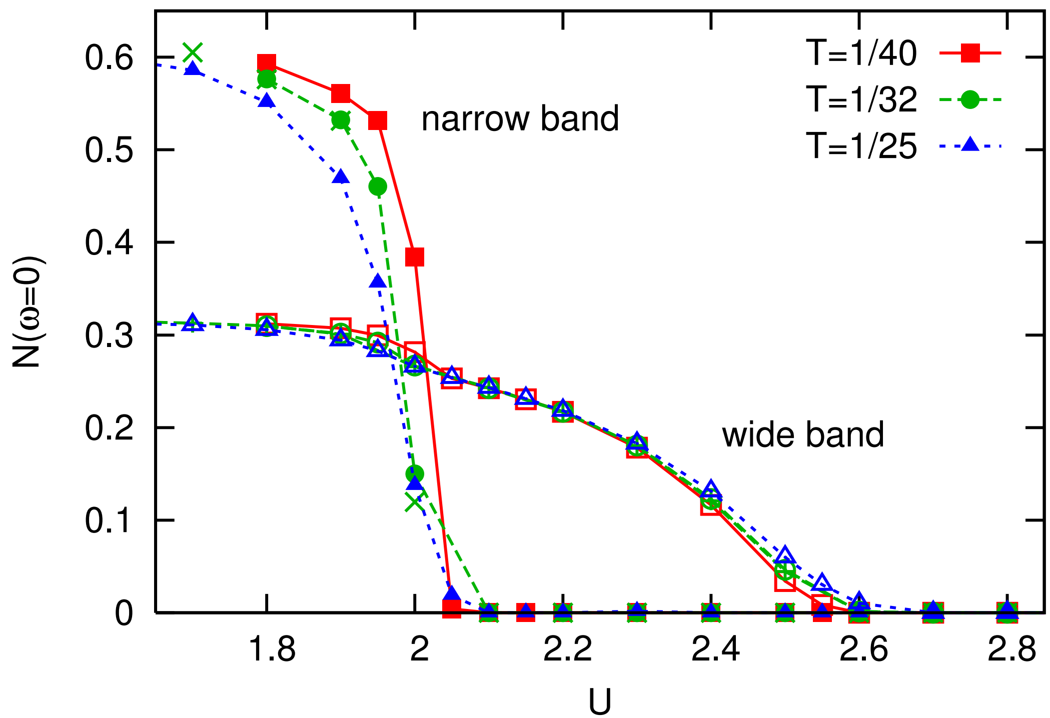
singularities ($\sim$ gap) for

$U \gtrsim 2$ in narrow band

$U \gtrsim 2.5$ in wide band

Spectral function (interacting DOS)





Clear indications for second singularity

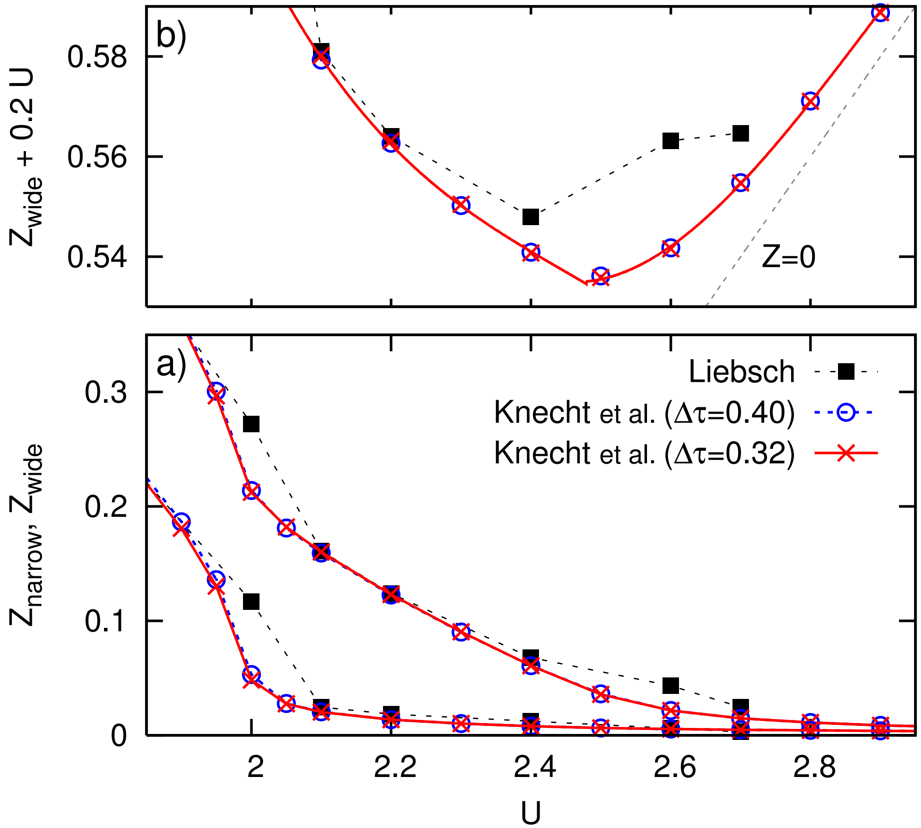
Wide band remains metallic at $U \approx 2.0$

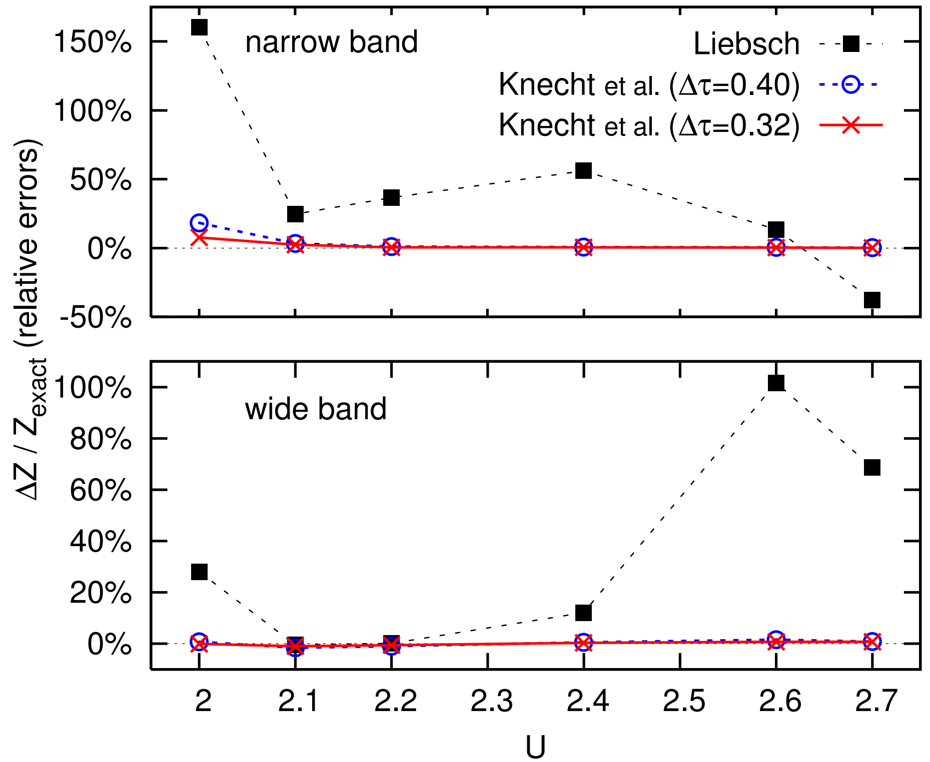
⇝ **two orbital-selective Mott transitions** [Knecht, NB, van Dongen, cond-mat/0505106, to appear in PRB RC]

same conclusions from slave-spin approximation [de' Medici, Georges, Biermann, cond-mat/0503764]

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

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



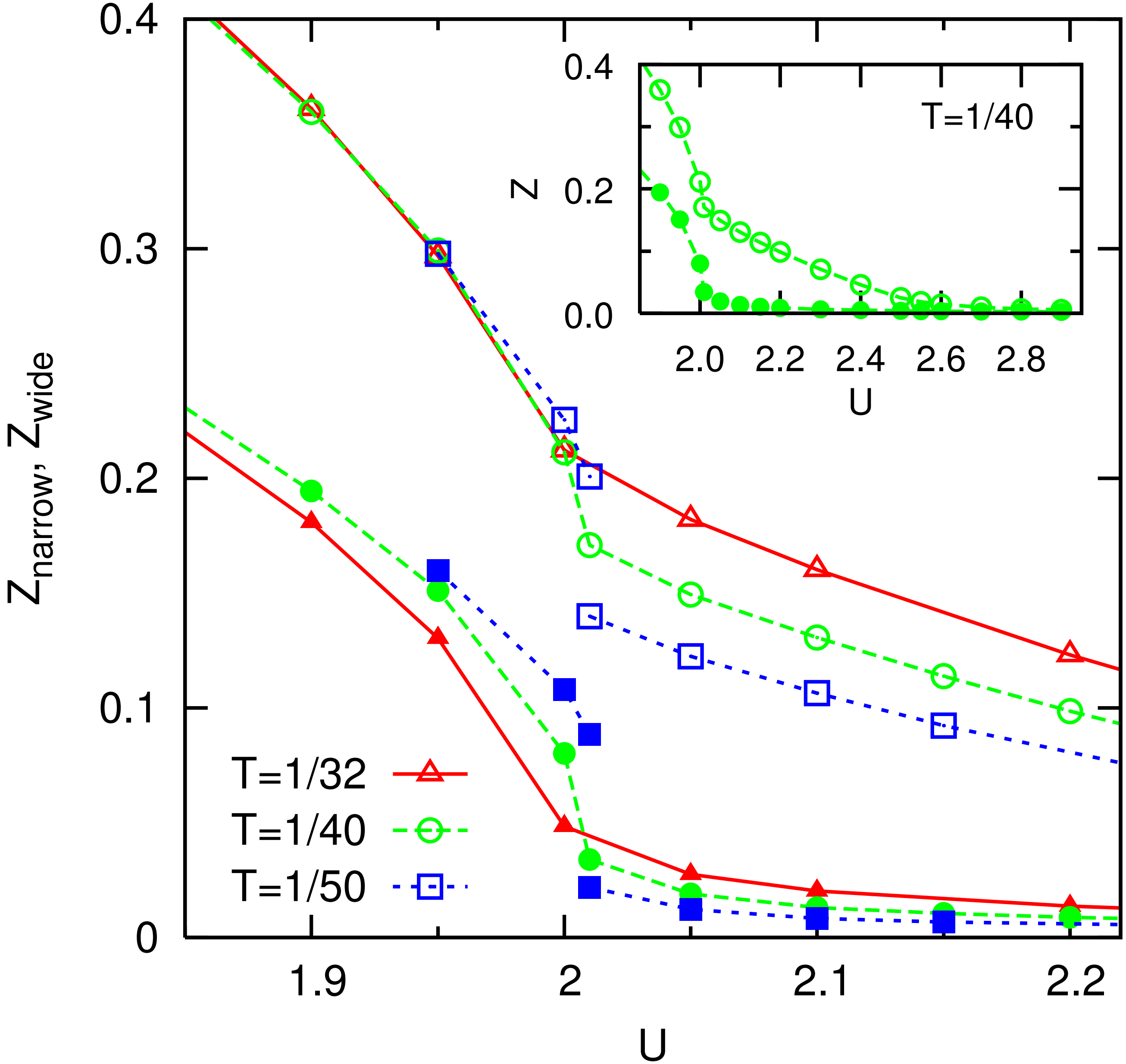


Numerical noise in Liebsch's QMC data obscures second transition

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

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

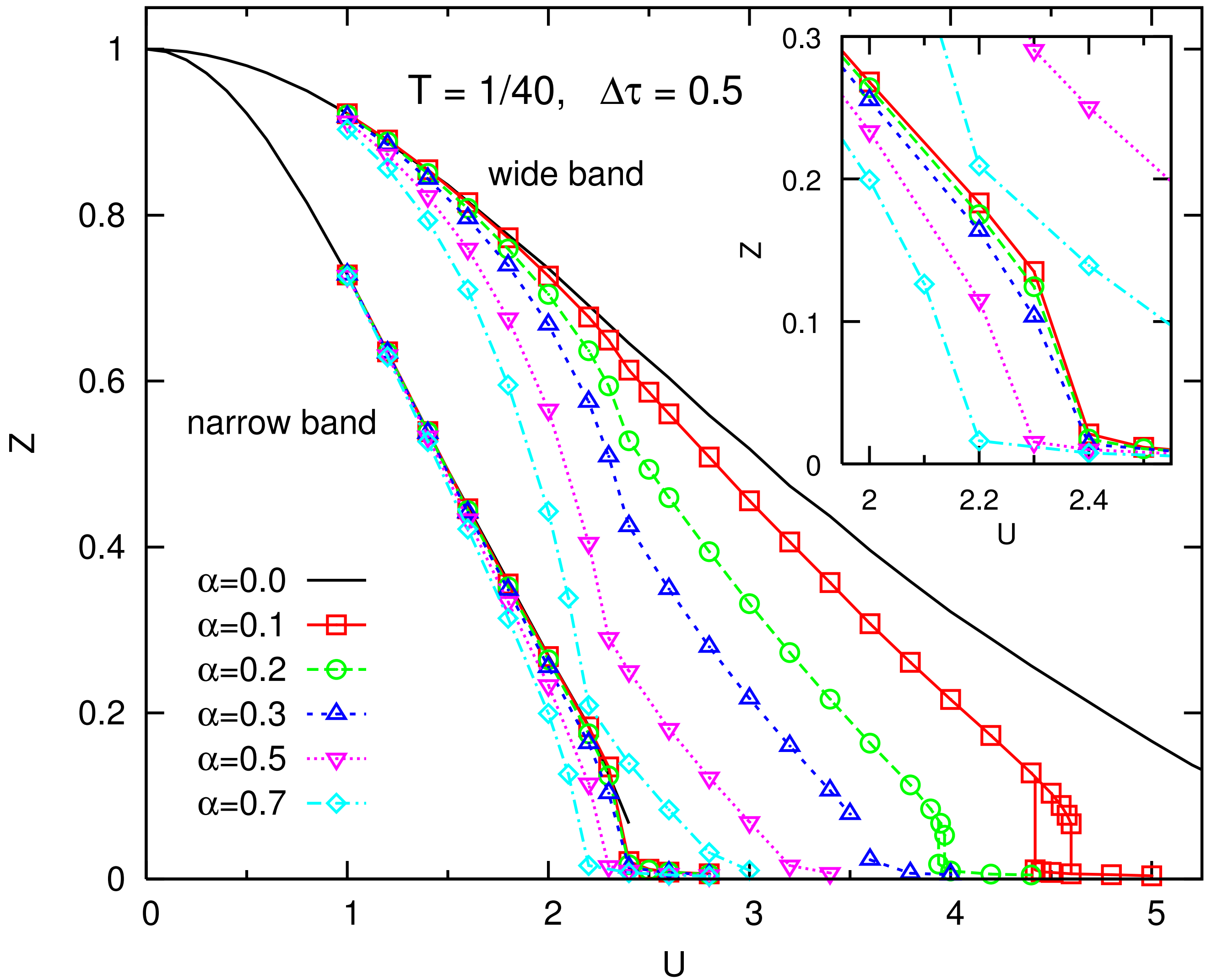
Determination of critical temperature for narrow-band transition



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

Systematic study: effect of inter-orbital coupling (preliminary results)

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



Both orbital-selective Mott transitions remain first order (at least) for small α

Summary

Improved DMFT-QMC scheme using high-frequency expansion of $\Sigma(\omega)$

Mott transition in frustrated 1-band Hubbard model

High-precision ground state estimates from QMC

Critical exponents from (infinite-order) ePT

Orbital-selective Mott transition in 2-band Hubbard model

J_z model: minimal model for OSMTs in $Ca_{2-x}Sr_xRuO_4$

narrow-band transition 1^{st} order for $T \lesssim 0.02$

wide-band transition 1^{st} order for small J_z, U'

Thanks to: D. Vollhardt, E. Kalinowski, C. Knecht, P. van Dongen

NIC Jülich, DFG (Bl775/1)