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

Nils Blümer

Outline

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

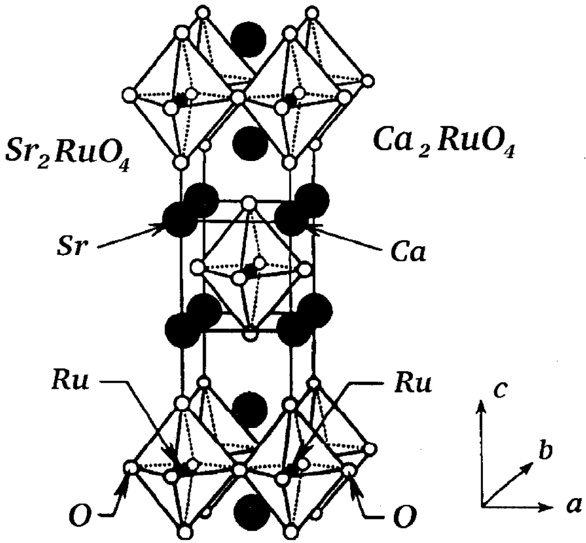
Mott metal-insulator transition in doped V_2O_3

DMFT-QMC calculations for frustrated 1-band Hubbard model

Orbital-selective Mott transitions in 2-band Hubbard model

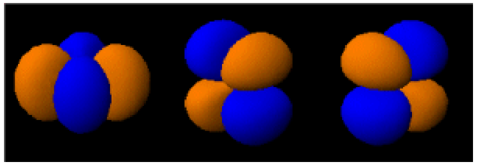
Summary and Outlook

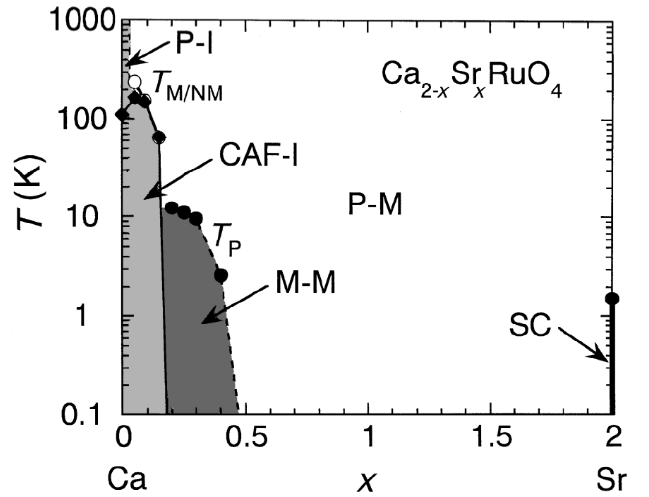
Motivation: OSMTs in $Ca_{2-x}Sr_xRuO_4$



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

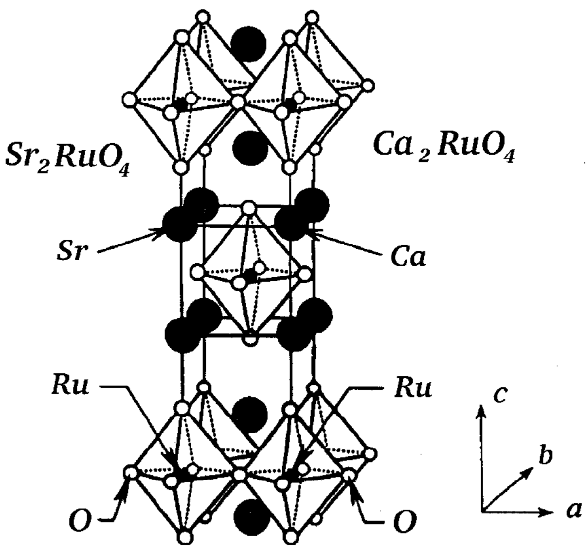
Sr_2RuO_4: quasi-2d FL,
spin-triplet superconductor





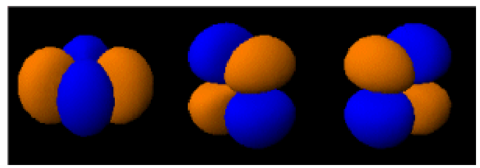
[Nakatsuji, Maeno, PRL **84**, 2666 (2000)]

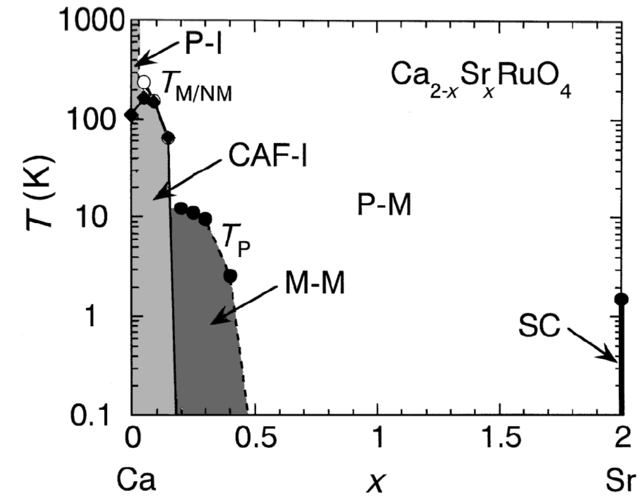
Motivation: OSMTs in $Ca_{2-x}Sr_xRuO_4$



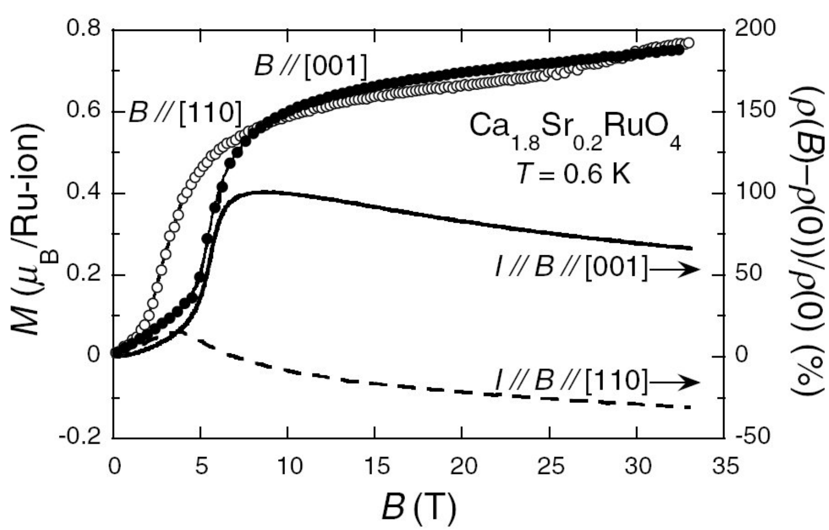
$Ca_{2-x}Sr_xRuO_4$:
isostructural to $La_{2-x}Sr_xCuO_4$

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

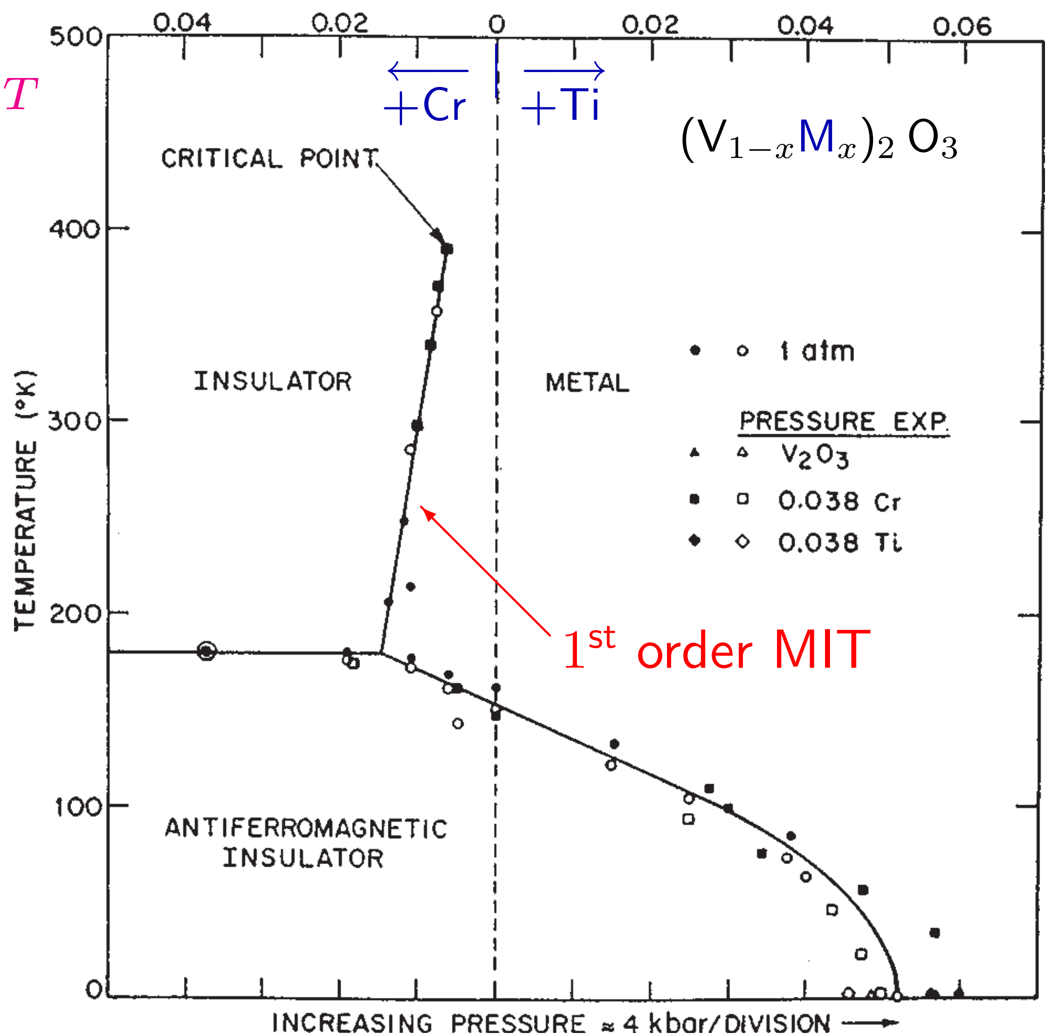
$\rightsquigarrow$ $S = 1/2$ system for $x \gtrsim 0.2$ (not $S = 1$)

strongly anisotropic magnetoresistance

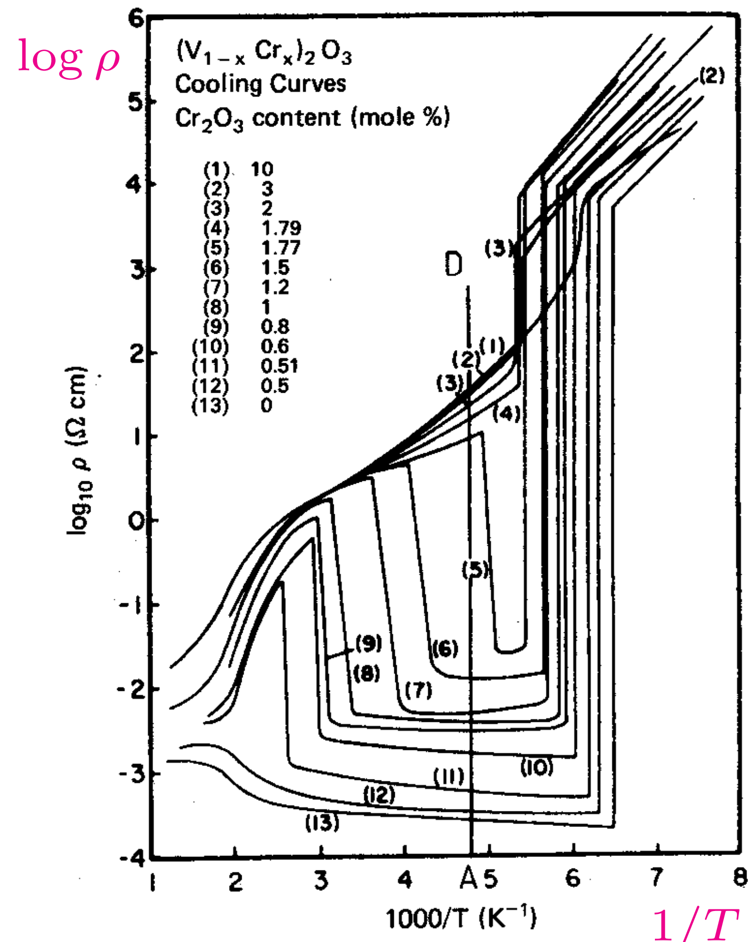
orbital-selective Mott metal-insulator transitions for $x \approx 0.5$, $x \approx 0.2$?

Mott metal-insulator transition in doped V_2O_3

Prototype correlated system: V_2O_3

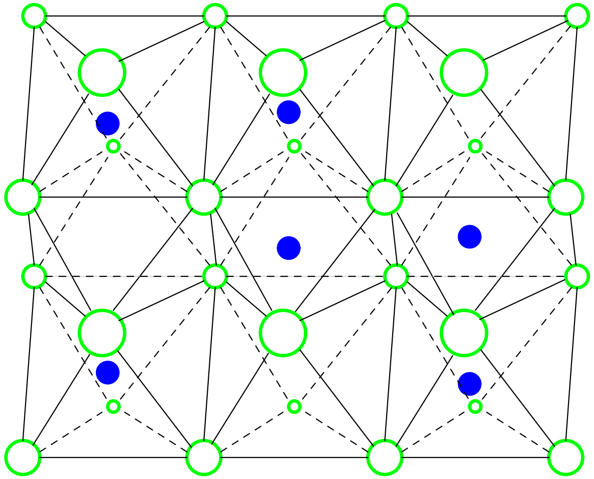


[McWhan *et al.*, PRL **27**, 941 (1971)] ⟵ U/W



[Kuwamoto, Honig, Appel, PRB **22**, 2626 (1980)]

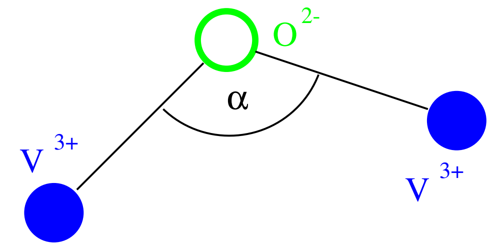
MIT without long-range order
resistivity ρ increases by factor 10^3
shift in lattice parameters



Corundum structure

Corundum structure:

- hcp O^{2-} lattice
- V^{3+} fill 2/3 of octahedra

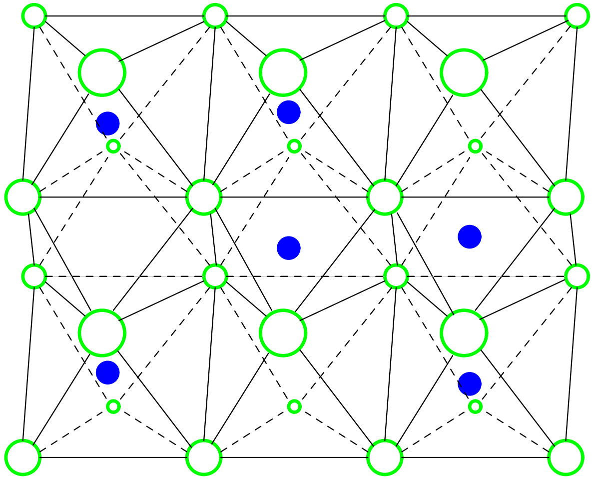


$\alpha_{\mathbf{Cr}} < \alpha_{\mathbf{V}} < \alpha_{\mathbf{Ti}}$

doping with Ti, Cr:

- (nearly) isovalent
- distorts lattice $\longrightarrow$ changes overlap
- drives MIT (like pressure)

Paramagnetic, bandwidth-controlled metal-insulator transition in V_2O_3 $\longrightarrow$ microscopic model?



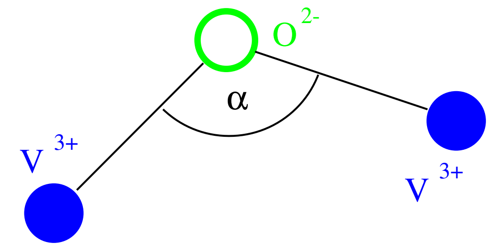
Corundum structure

Corundum structure:

- hcp O^{2-} lattice
- V^{3+} fill 2/3 of octahedra

doping with Ti, Cr:

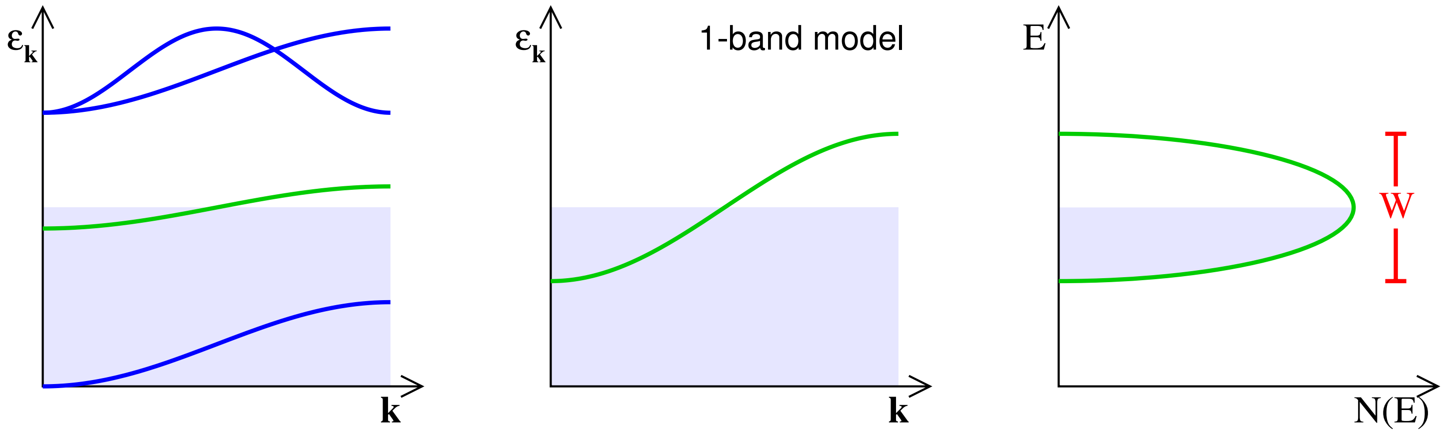
- (nearly) isovalent
- distorts lattice $\longrightarrow$ changes overlap
- drives MIT (like pressure)



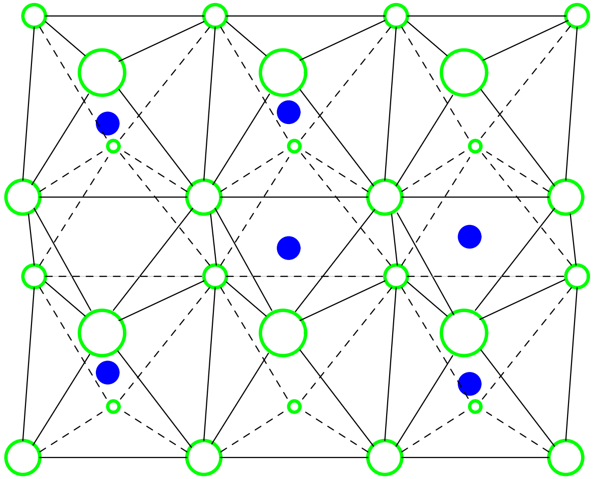
$\alpha_{\mathbf{Cr}} < \alpha_{\mathbf{V}} < \alpha_{\mathbf{Ti}}$

Paramagnetic, bandwidth-controlled metal-insulator transition in V_2O_3 $\longrightarrow$ microscopic model?

Bloch states near Fermi energy,



Paramagnetic Mott transition not captured by LDA band structure calculations!



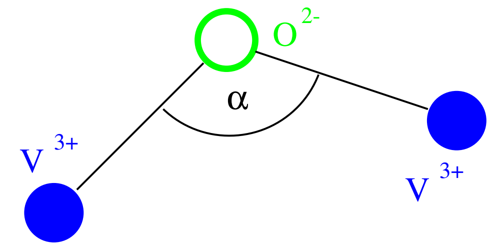
Corundum structure

Corundum structure:

- hcp O^{2-} lattice
- V^{3+} fill 2/3 of octahedra

doping with Ti, Cr:

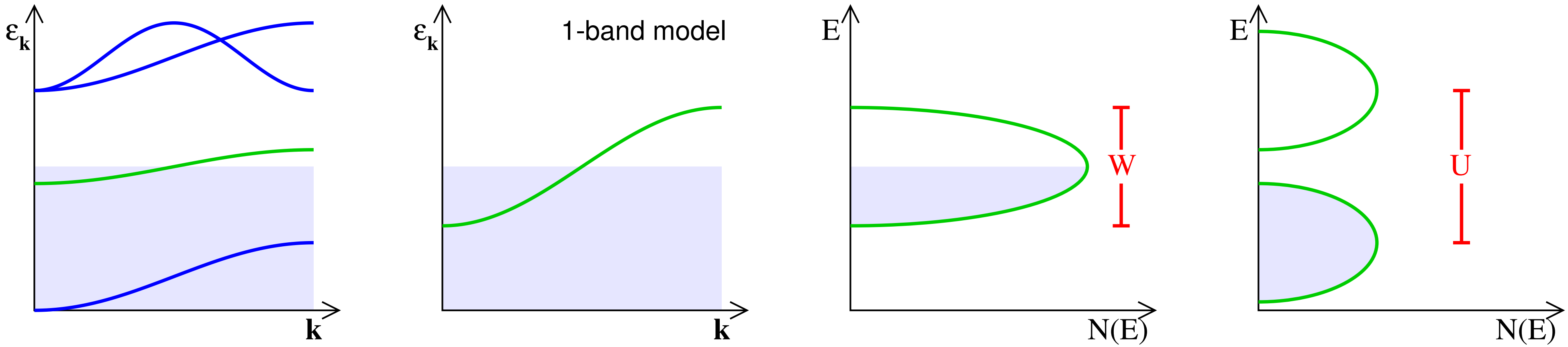
- (nearly) isovalent
- distorts lattice $\longrightarrow$ changes overlap
- drives MIT (like pressure)



$\alpha_{\mathbf{Cr}} < \alpha_{\mathbf{V}} < \alpha_{\mathbf{Ti}}$

Paramagnetic, bandwidth-controlled metal-insulator transition in V_2O_3 $\longrightarrow$ microscopic model?

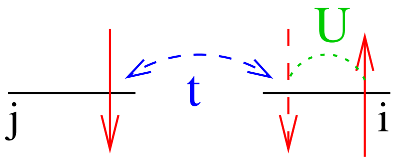
Bloch states near Fermi energy, band-splitting by Coulomb correlations ($\sim U$)



Paramagnetic Mott transition not captured by LDA band structure calculations!

Mott transition in frustrated 1-band Hubbard model

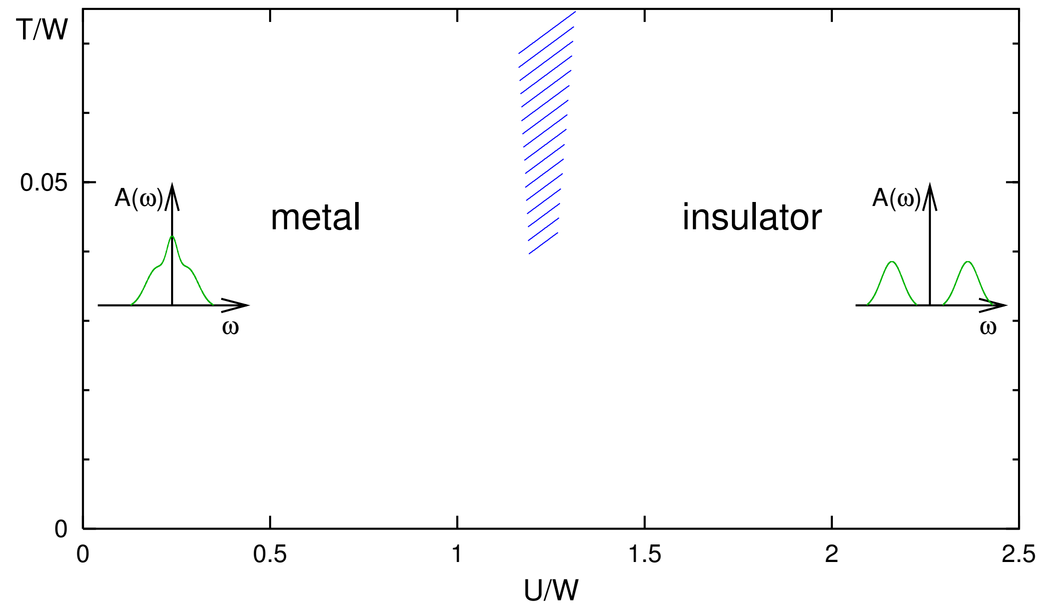
Hubbard model



$$\hat{H} = \sum_{(i,j),\sigma} t_{ij}(\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

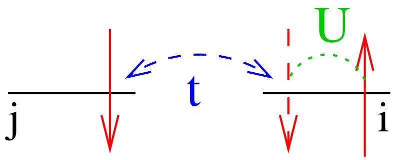
Minimal model for correlated electrons

MIT/crossover at $U/W \approx 1$ (and half filling)



Mott transition in frustrated 1-band Hubbard model

Hubbard model

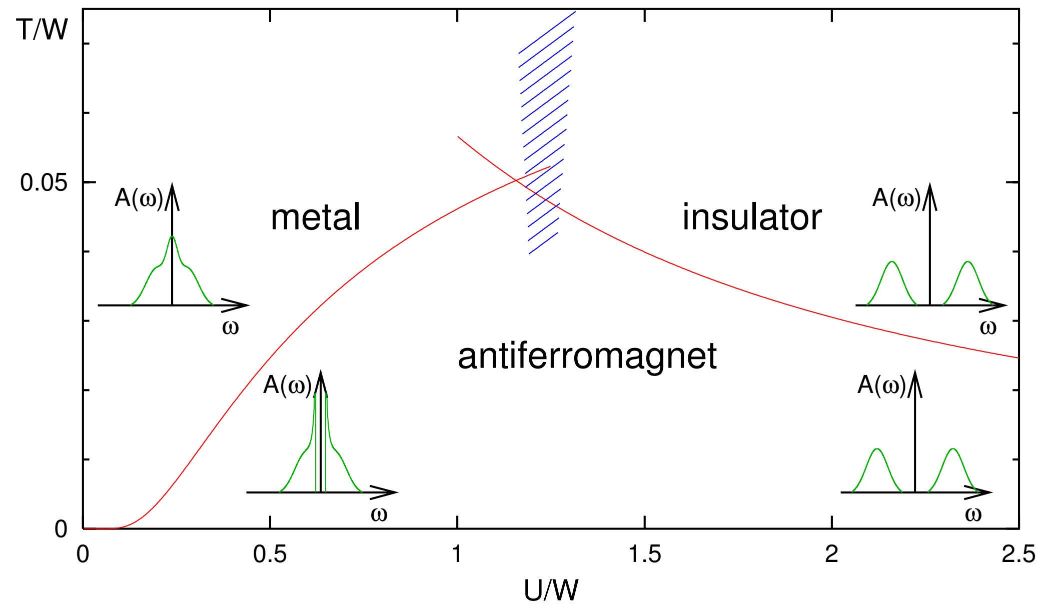


$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} (\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Minimal model for correlated electrons

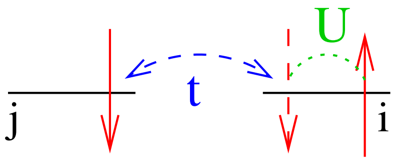
MIT/crossover at $U/W \approx 1$ (and half filling)

But: generically antiferromagnetism at low T



Mott transition in frustrated 1-band Hubbard model

Hubbard model

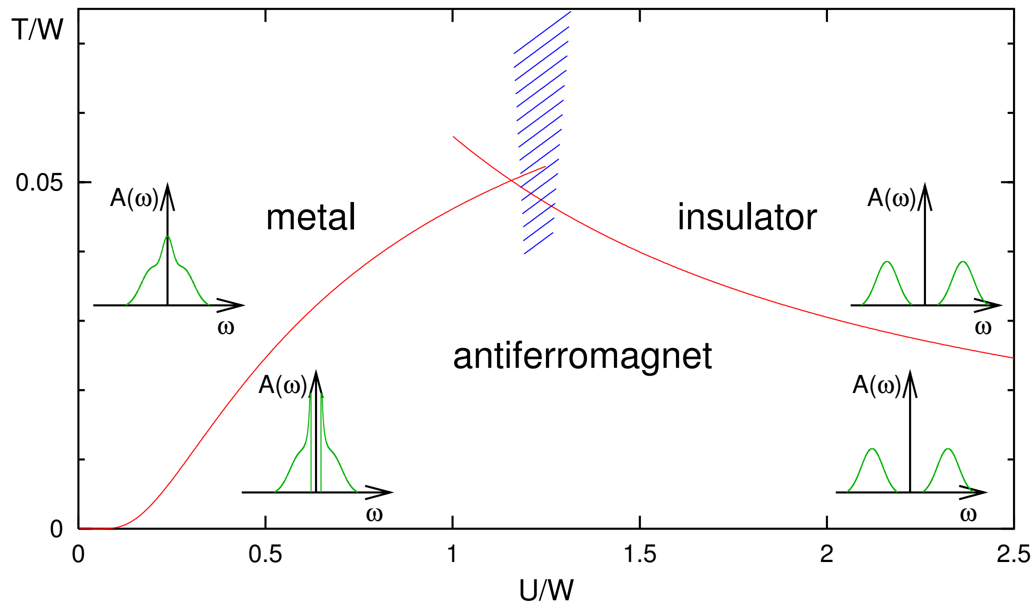


$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} (\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Minimal model for correlated electrons

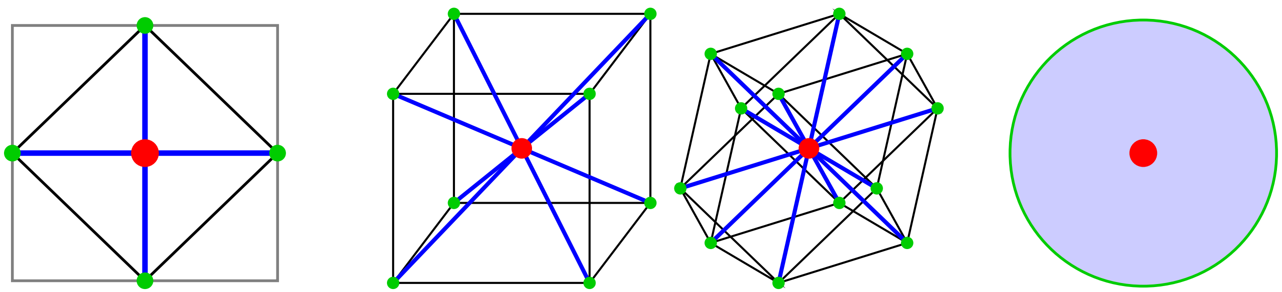
MIT/crossover at $U/W \approx 1$ (and half filling)

But: generically antiferromagnetism at low T



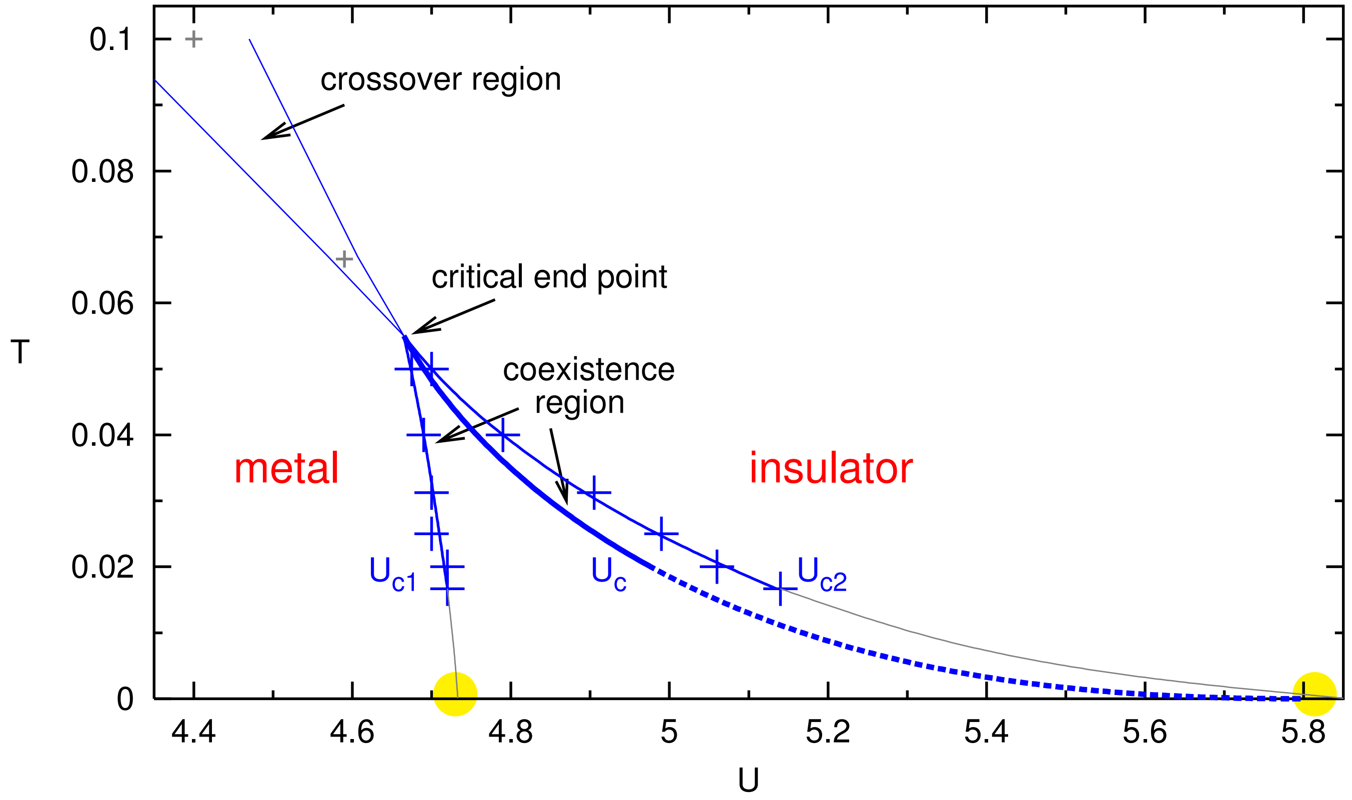
Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$

+ non-perturbative
  $\rightsquigarrow$ valid at MIT
+ dynamical on-site correlations preserved
+ in thermodynamic limit
+ exact for $Z \to \infty$



d=2: $Z = 4$ bcc: $Z = 8$ fcc: $Z = 12$ DMFT: $Z = \infty$

Frustrated 1-band Hubbard model (DMFT+QMC): 1^{st} order MIT + coexistence



Georges and Krauth (1993)

Rozenberg, Kotliar, Zhang (1994)

Georges *et al.* (RMP, 1996)

Schlipf *et al.* (1999)

Rozenberg, Chitra, Kotliar (1999)

Krauth (2000)

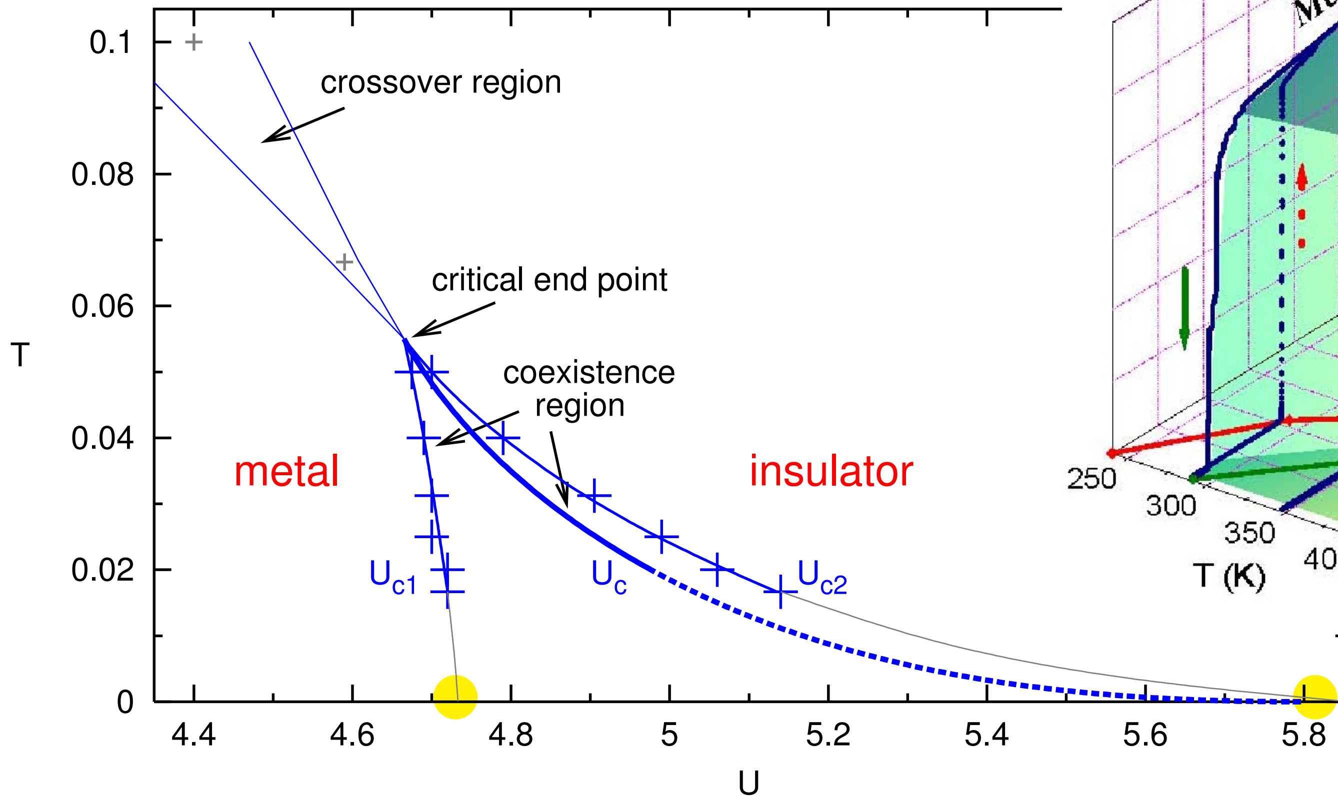
Bulla (1999, 2001)

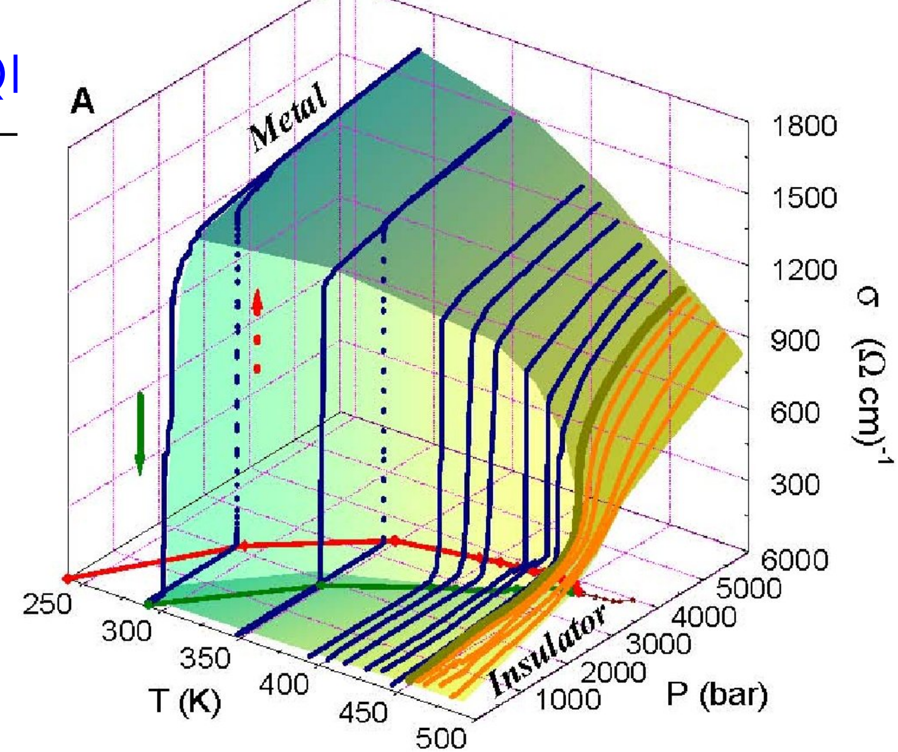
Joo, Oudovenko (2001)

Tong (2001)

Blümer (2000, 2002)

Frustrated 1-band Hubbard model (DMFT+QI





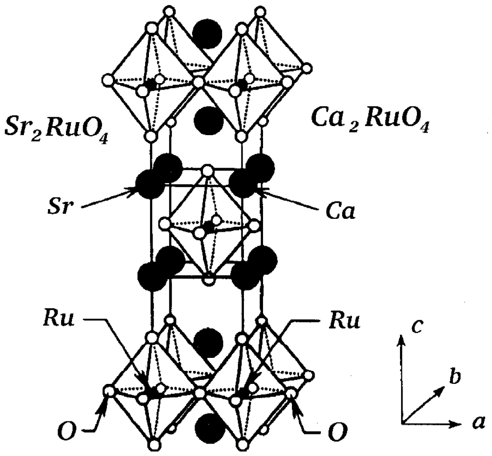
Blümer (2000, 2002)

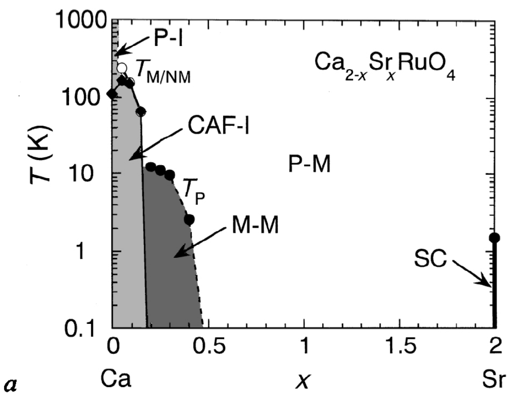
1^{st} order line from $$\frac{\mathrm{d}U_\mathrm{c}(T)}{\mathrm{d}T} = f(T, U_\mathrm{c}(T)); \;\; f(T,U) := \frac{\Delta E(T,U)}{T\,\Delta D(T,U)}$$

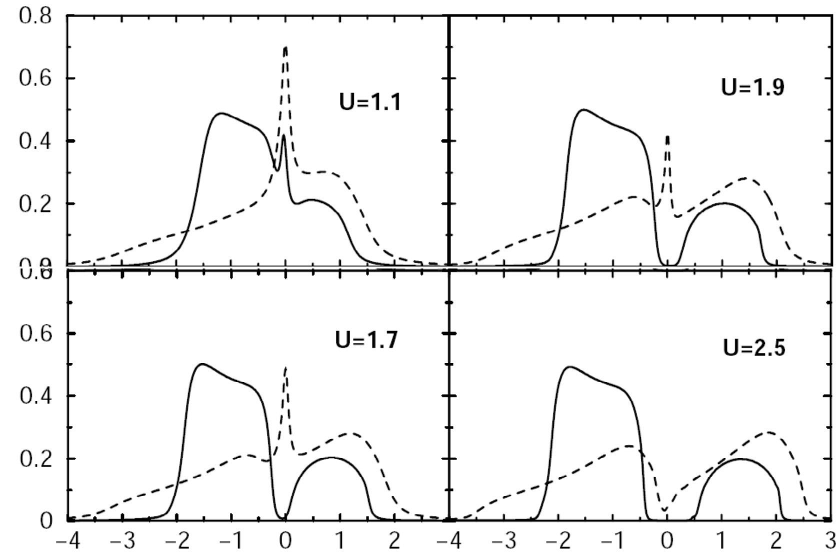
low-T asymptotics from $$U_\mathrm{c}(T) = U_\mathrm{c}^0 - \sqrt{\frac{2S_oT}{a}} + \frac{\gamma_0}{4S_0}T + \mathcal{O}(T^{3/2})$$

High-precision energetics from QMC (even for $T \longrightarrow 0$) [NB, Kalinowski, PRB **71**, 195102 (2005)]

Orbital-selective Mott transition in 2-band Hubbard model

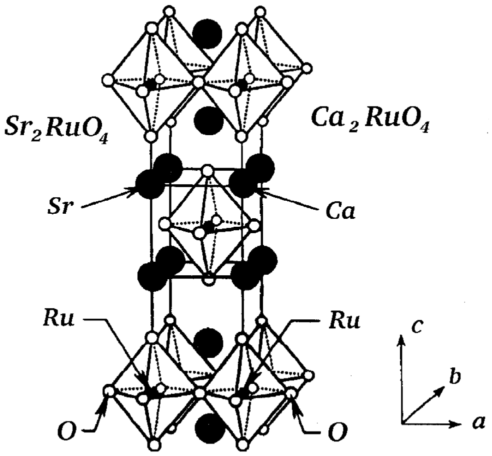


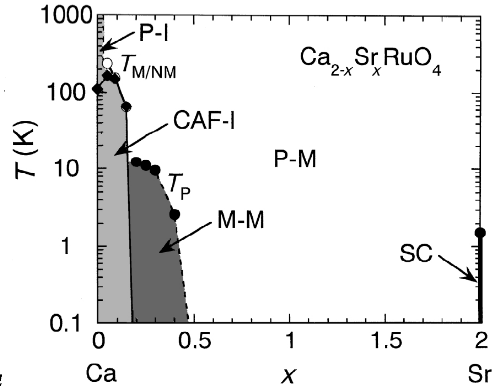


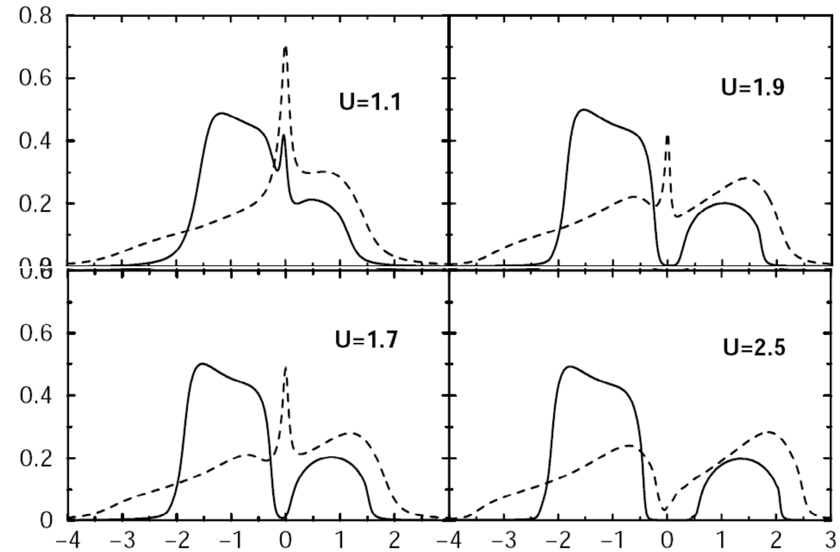


[LDA+DMFT(NCA): Anisimov *et al.* (2002)]

Orbital-selective Mott transition in 2-band Hubbard model

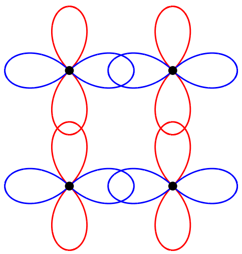






[LDA+DMFT(NCA): Anisimov *et al.* (2002)]

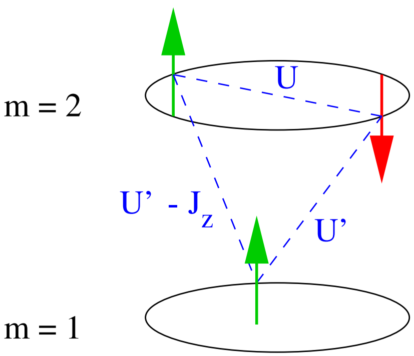
Minimal model: 2-band Hubbard model
with orbital-dependent hopping



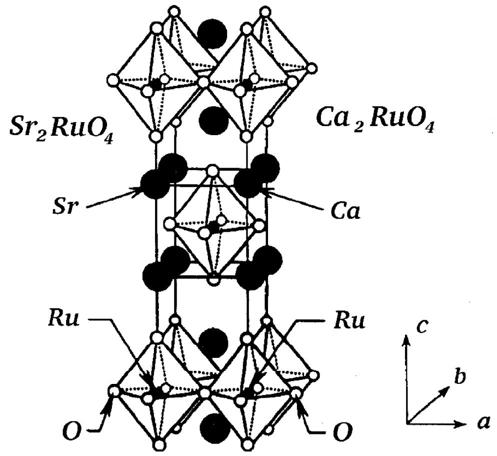
$$H = \sum_{m=1}^{2} \Big[-\sum_{\langle ij\rangle\sigma} t_m c^\dagger_{im\sigma} c_{jm\sigma} + U \sum_i n_{im\uparrow} n_{im\downarrow} \Big]$$

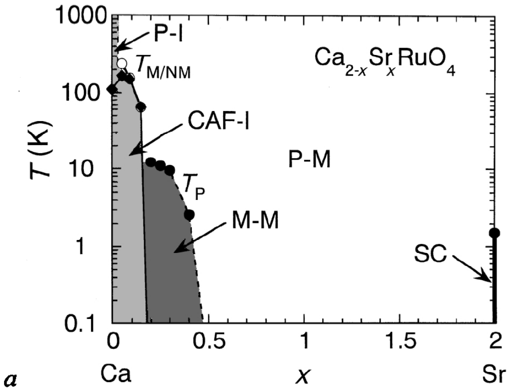
$$+ \sum\nolimits_{i\sigma\sigma'} (U' - \delta_{\sigma\sigma'} J_z)\, n_{i1\sigma}\, n_{i2\sigma'}$$

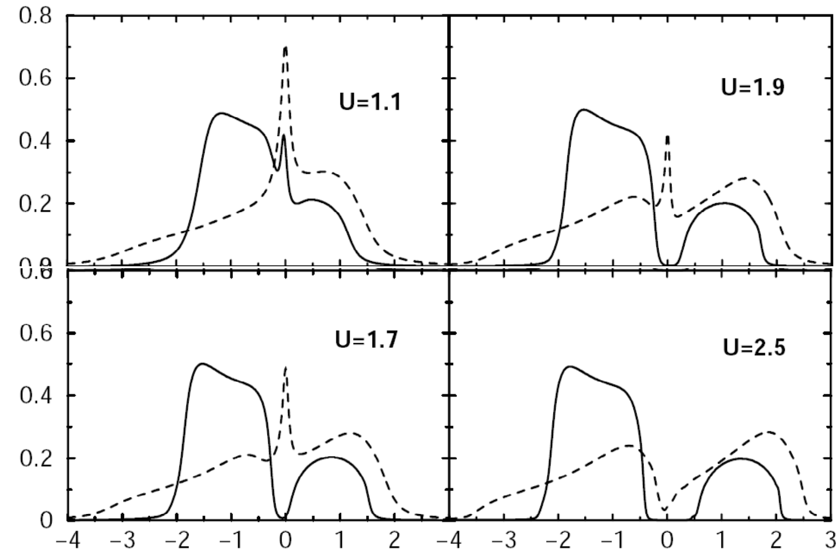
$$+ \tfrac{1}{2} J_\perp \sum\nolimits_{i\sigma} \Big[c^\dagger_{i1\sigma} \Big(c^\dagger_{i2\bar\sigma} c_{i1\bar\sigma} + c^\dagger_{i1\bar\sigma} c_{i2\bar\sigma} \Big) c_{i2\sigma} + \text{h.c.} \Big]$$



Orbital-selective Mott transition in 2-band Hubbard model

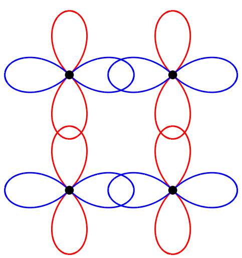






[LDA+DMFT(NCA): Anisimov *et al.* (2002)]

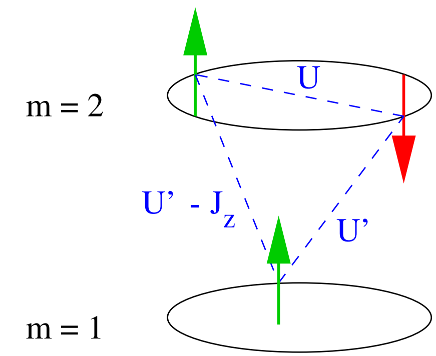
Minimal model: 2-band Hubbard model
with orbital-dependent hopping



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

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

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



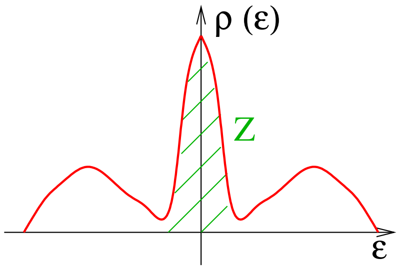
For Bethe DOS, $t_2 = 2\,t_1$: two 1^{st} order MITs for $U' = J_z = J_\perp = 0$ (trivial)

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

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

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

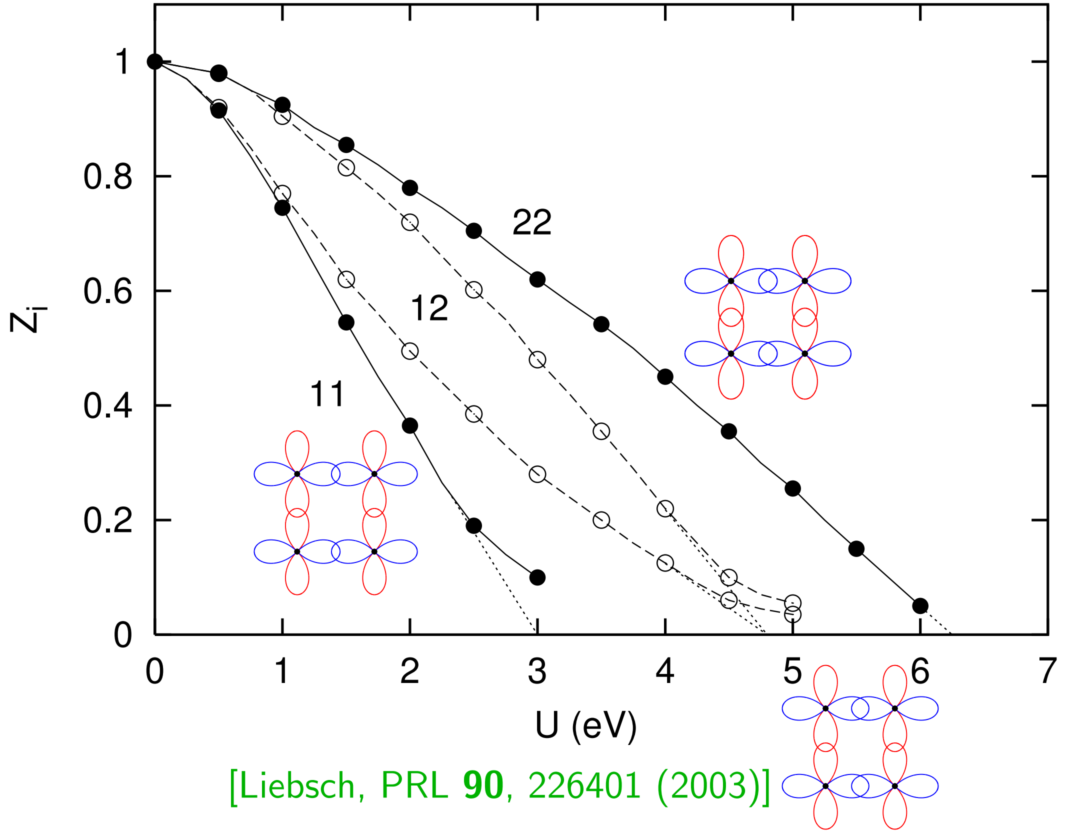
quasiparticle weight $Z_i = m/m_i^*$



discrete QMC estimate:

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

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



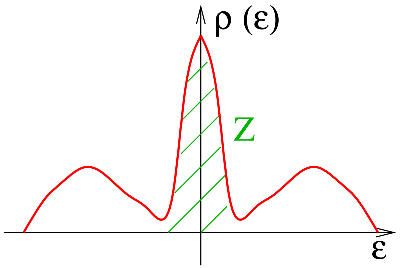
[Liebsch, PRL **90**, 226401 (2003)]

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

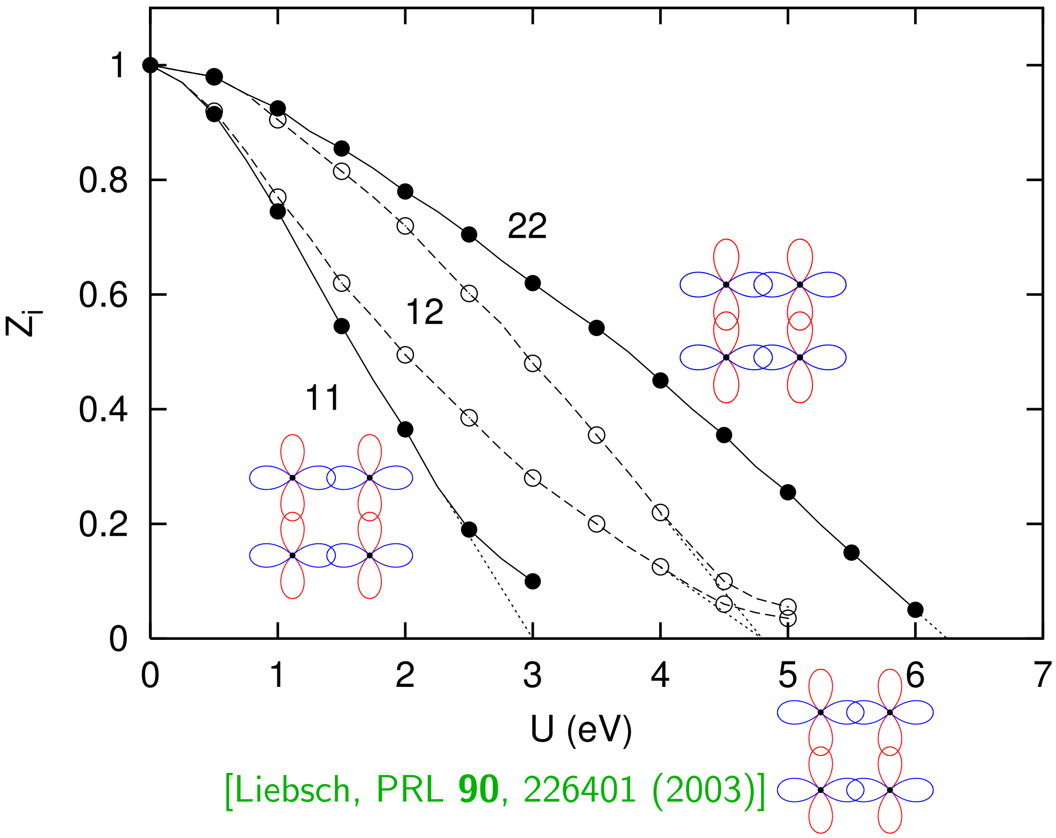
quasiparticle weight $Z_i = m/m_i^*$

discrete QMC estimate:

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

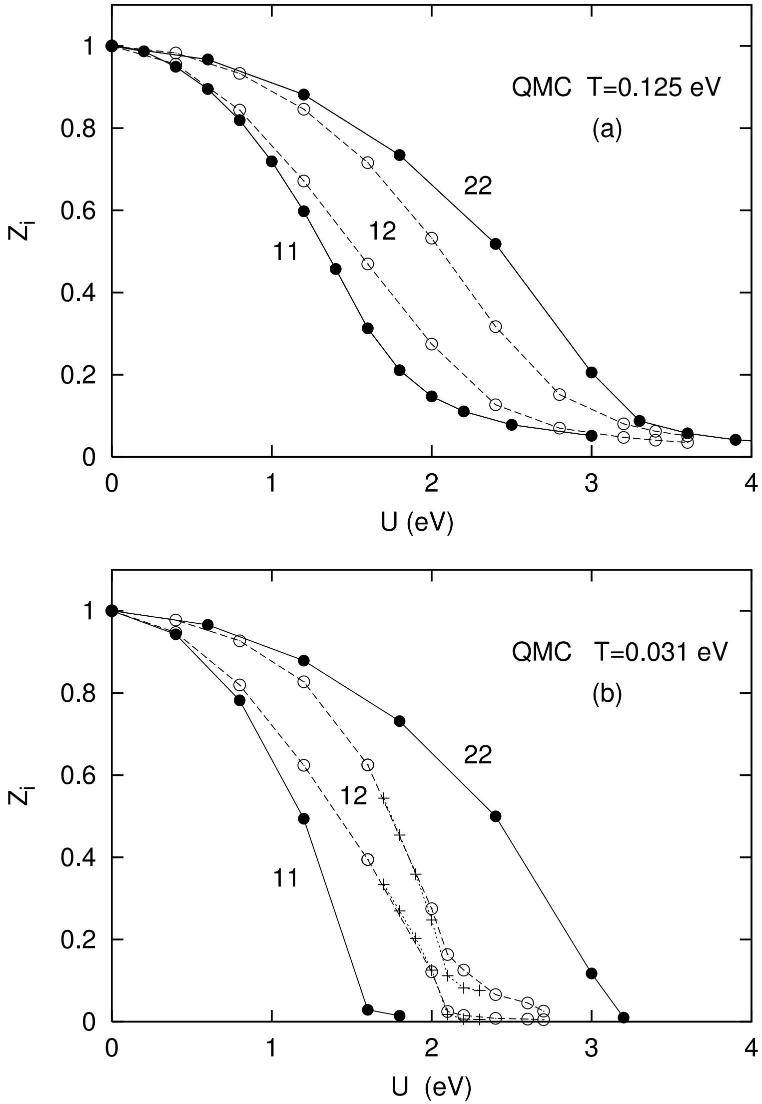


$J_z = 0.2,\ U' = U - 0.4$



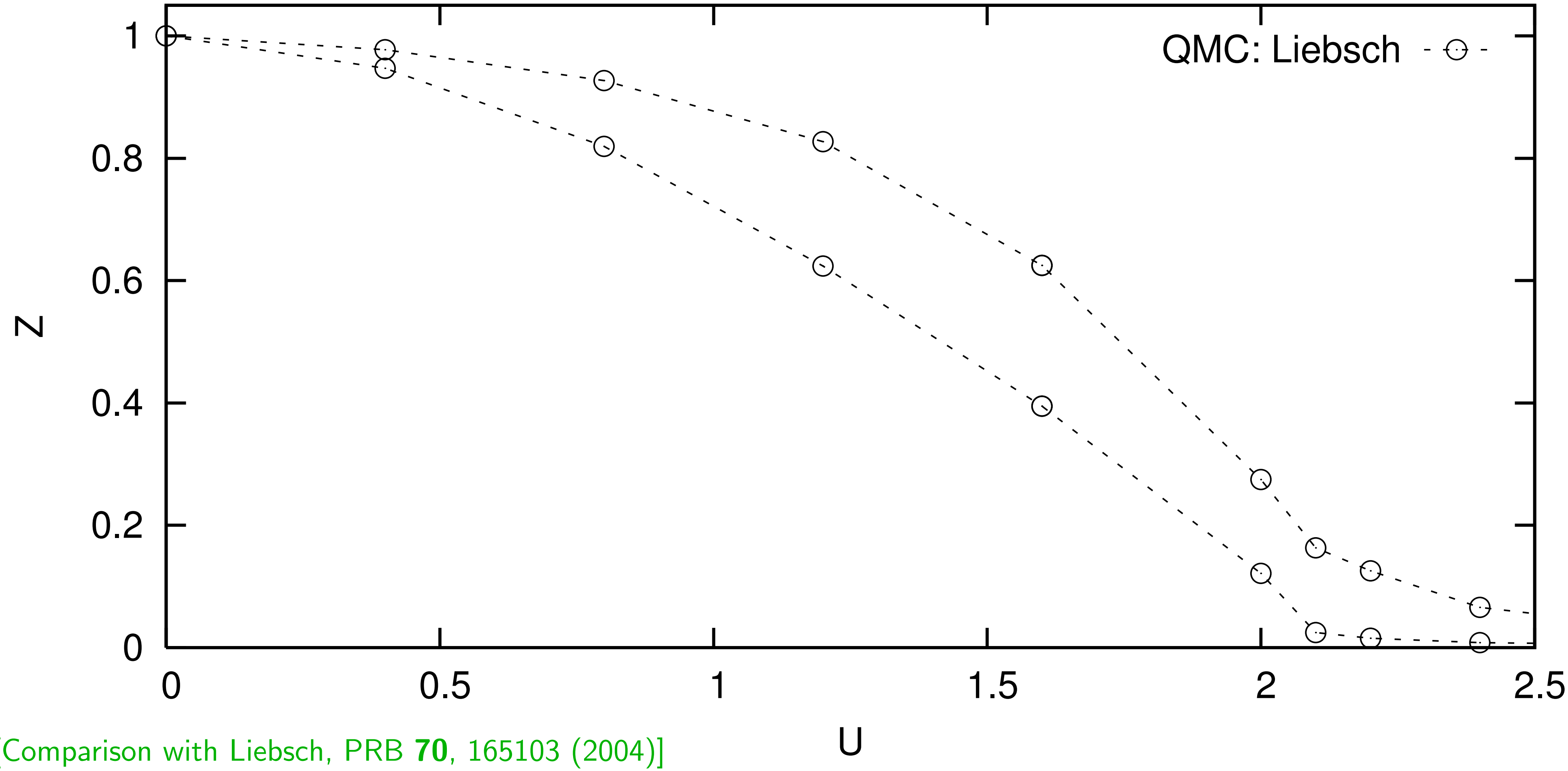
[Liebsch, PRL **90**, 226401 (2003)]

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



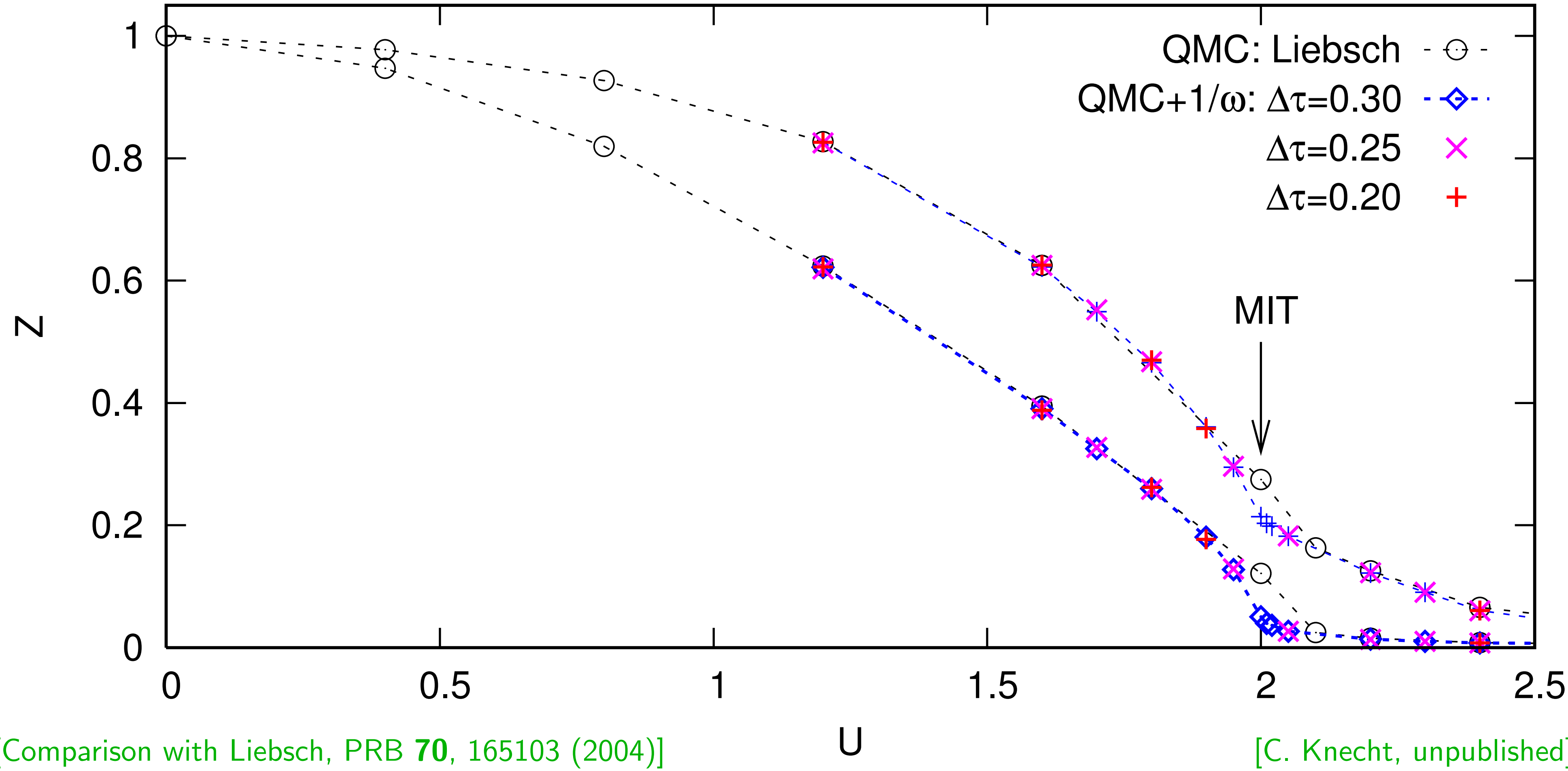
[Liebsch, PRB **70**, 165103 (2004)]

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



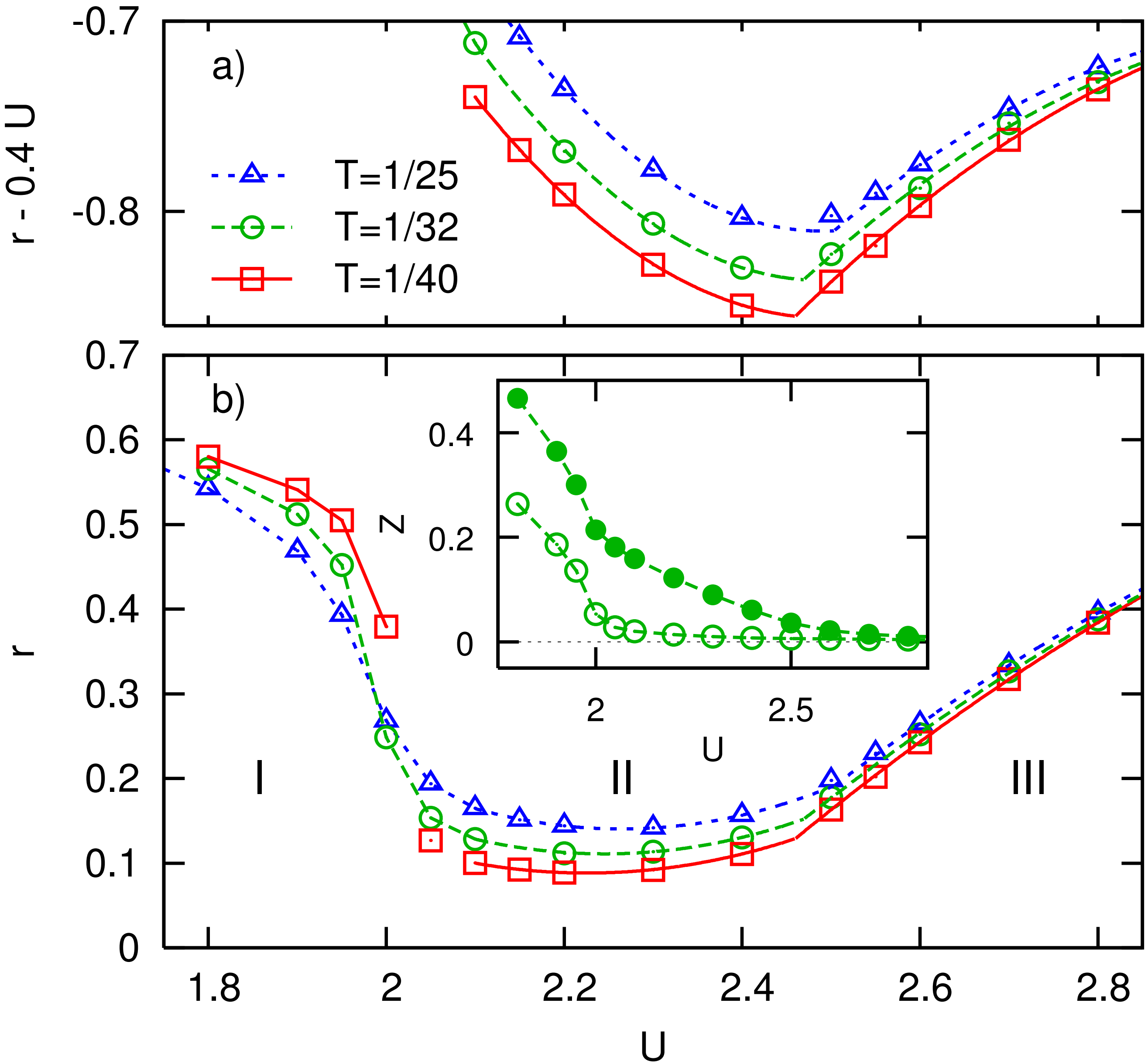
[Comparison with Liebsch, PRB **70**, 165103 (2004)] [C. Knecht, unpublished]

Very small dependence on discretization $\Delta\tau$.

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?

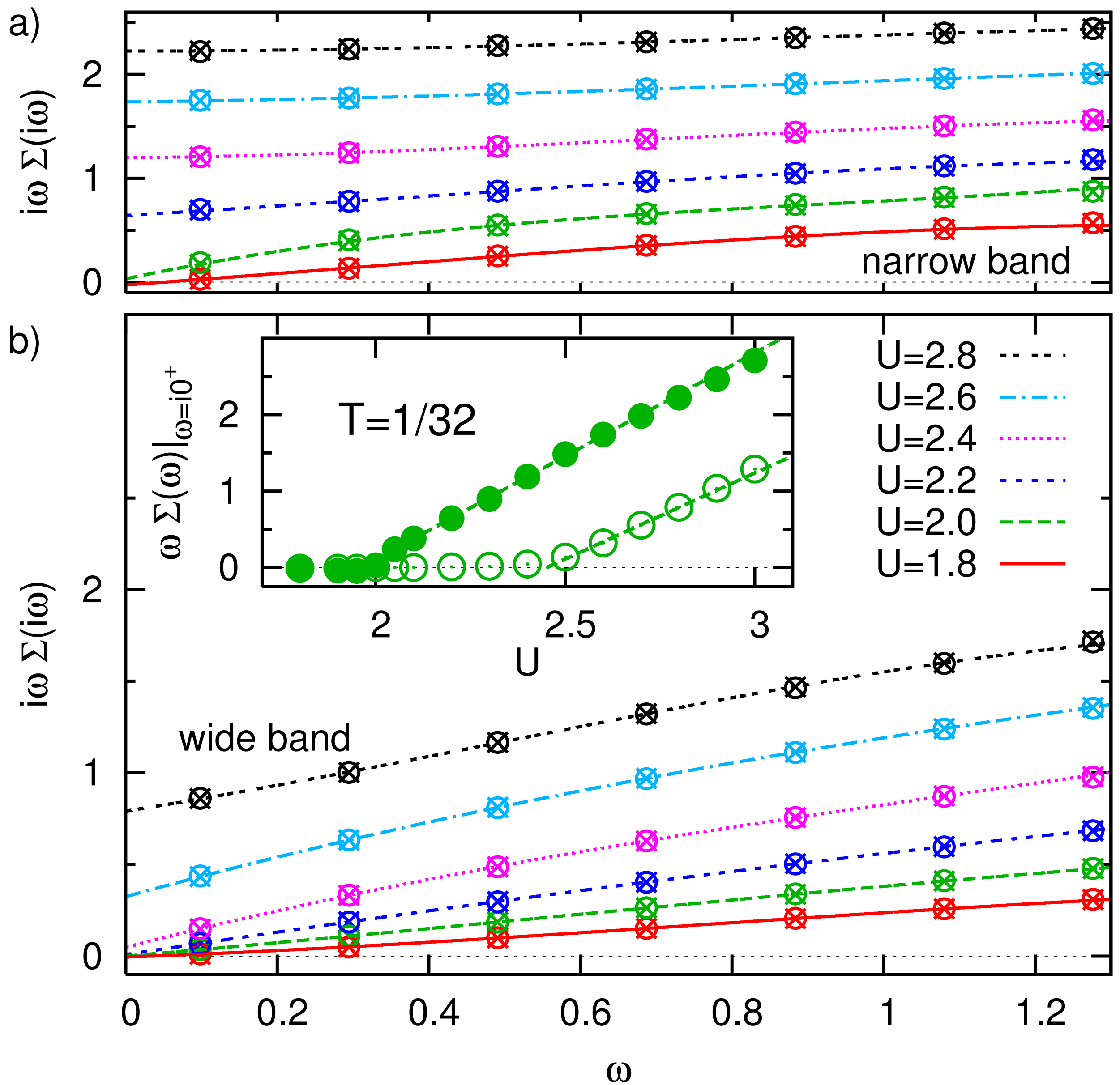
Ratio of quasiparticle weights $r = Z_{\text{narrow}}/Z_{\text{wide}}$



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:

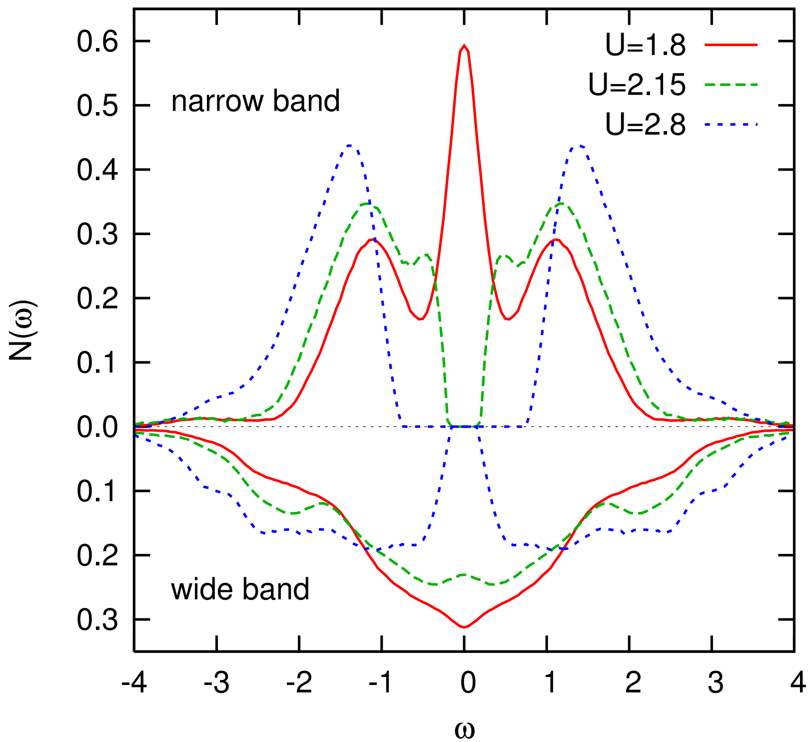
$\omega\Sigma(\omega) \xrightarrow{\omega\to 0} 0$

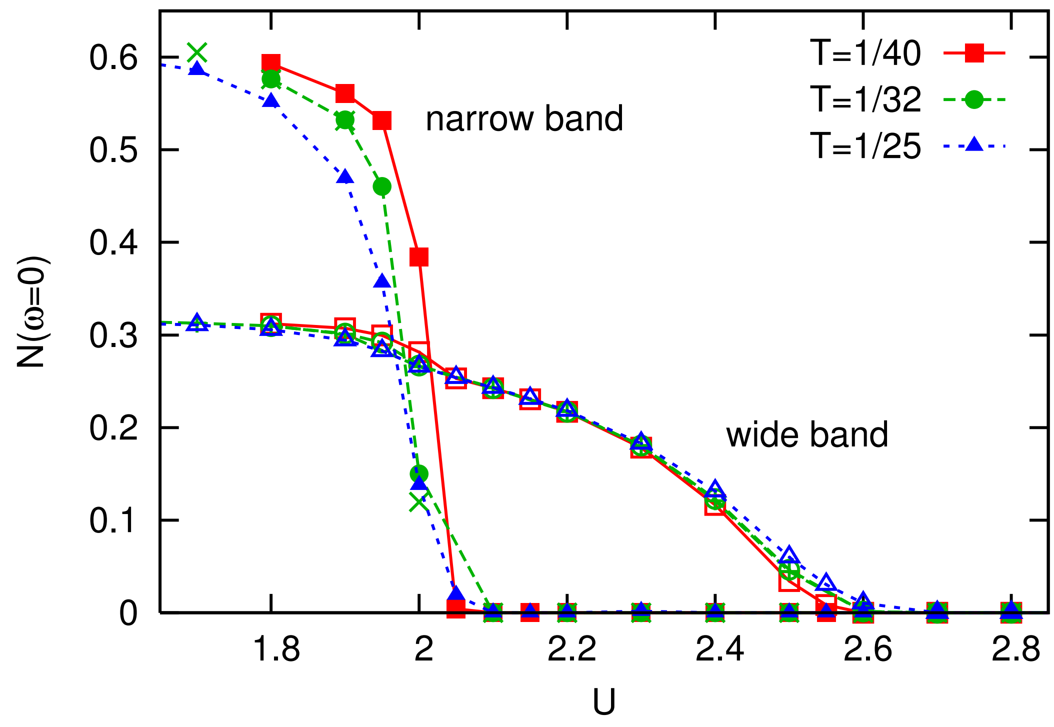
singularities (∼ gap) for

$U > 2$ in narrow band

$U > 2.5$ in wide band

Spectral function (interacting DOS)





Clear indications for second singularity

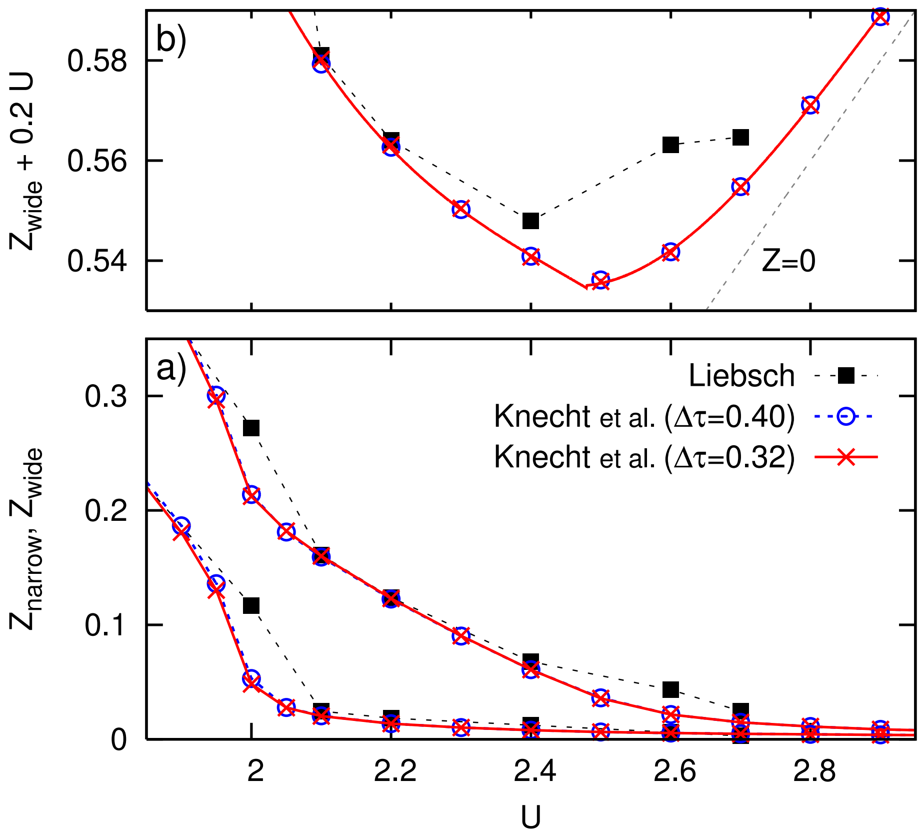
Wide band remains metallic at $U \approx 2.0$

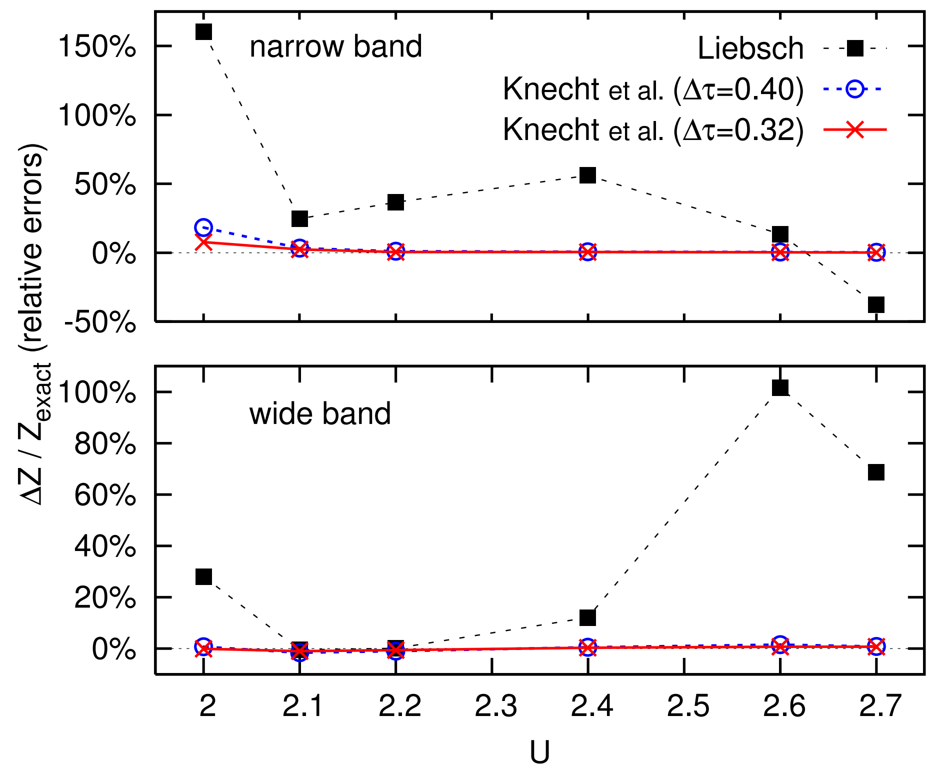
$\rightsquigarrow$ **two orbital-selective Mott transitions** [Knecht, NB, van Dongen, cond-mat/0505106, to appear in PRB RC]

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]

Summary and Outlook

DMFT+QMC: valuable numerical approach for correlated electron systems

– ab initio approach in combination with DFT(LDA)

– even broader applicability for cluster extensions

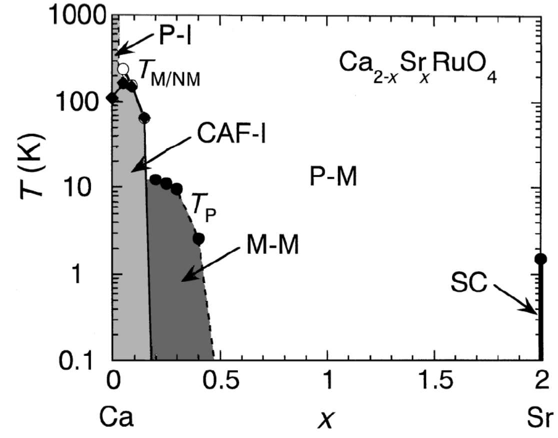
Mott transition in frustrated 1-band Hubbard model

Orbital-selective Mott transition in 2-band Hubbard model

J_z model: minimal model for OSMTs in $\mathrm{Ca}_{2-x}\mathrm{Sr}_x\mathrm{RuO}_4$

not shown: narrow-band transition 1^{st} order for $T \lesssim 0.02$

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

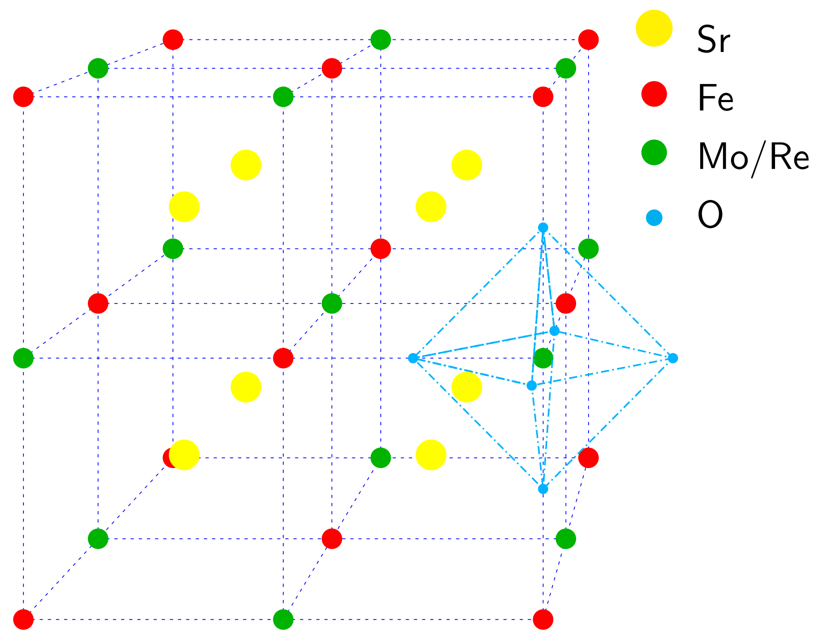


Outlook: realistic material-specific calculations with LDA+DMFT . . .

Thanks to: NIC Jülich, DFG (Bl775/1)

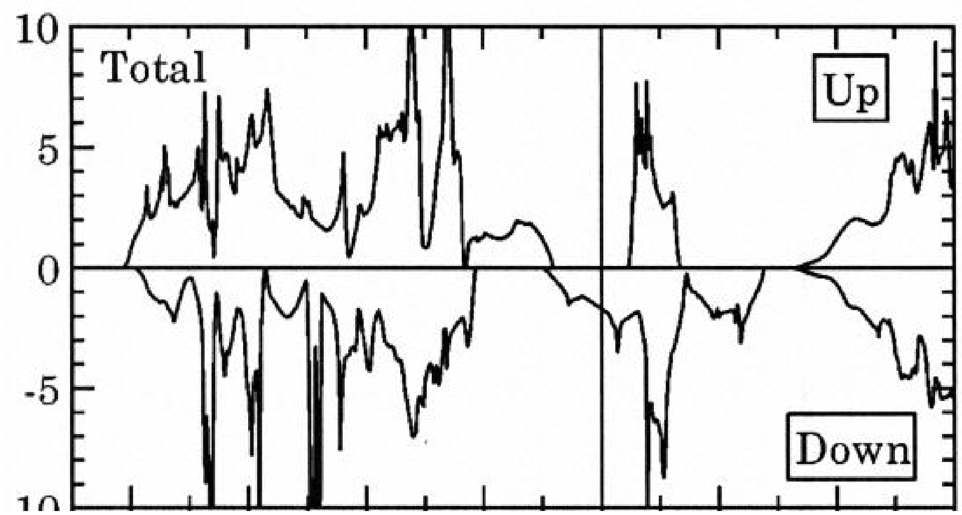
Outlook: theory of half-metallic double perovskites

Sr_2FeMoO_6 and Sr_2FeReO_6



Valences:

Sr^{2+}	[Kr]
Fe^{3+}	[Ar] $3d^5$
Mo^{5+}	[Kr] $4d^1$
O^{2-}	[Ne]



[LSDA+U for Sr_2FeMoO_6, Saitoh *et al.* (2002)]

$$H = \epsilon^f \sum_{i\alpha} n^f_{i\alpha} + \epsilon^m \sum_{i\alpha} n^m_{i\alpha} + \sum_{i,\,\alpha\neq\alpha'} U^f_{\alpha\alpha'}\, n^f_{i\alpha} n^f_{i\alpha'} + \sum_{j,\,\alpha\neq\alpha'} U^m_{\alpha\alpha'}\, n^m_{j\alpha} n^m_{j\alpha'}$$

$$+ \sum_{\langle ij\rangle\,\alpha} t^{fm} \left(f^\dagger_{i\alpha} m_{j\alpha} + \text{hc}\right) + \sum_{\langle jj'\rangle\,\alpha} t^{mm}\, m^\dagger_{j\alpha} m_{j'\alpha} + \sum_{\langle ii'\rangle\,\alpha} t^{ff}\, f^\dagger_{i\alpha} f_{i'\alpha}$$