Quantum Monte Carlo Studies of Mott Metal-Insulator Transitions within Dynamical Mean-field Theory

Nils Blümer

Outline

Motivation: Mott transition in V_2O_3

Introduction: Hubbard Model, DMFT, QMC

Mott transition in frustrated 1-band Hubbard model

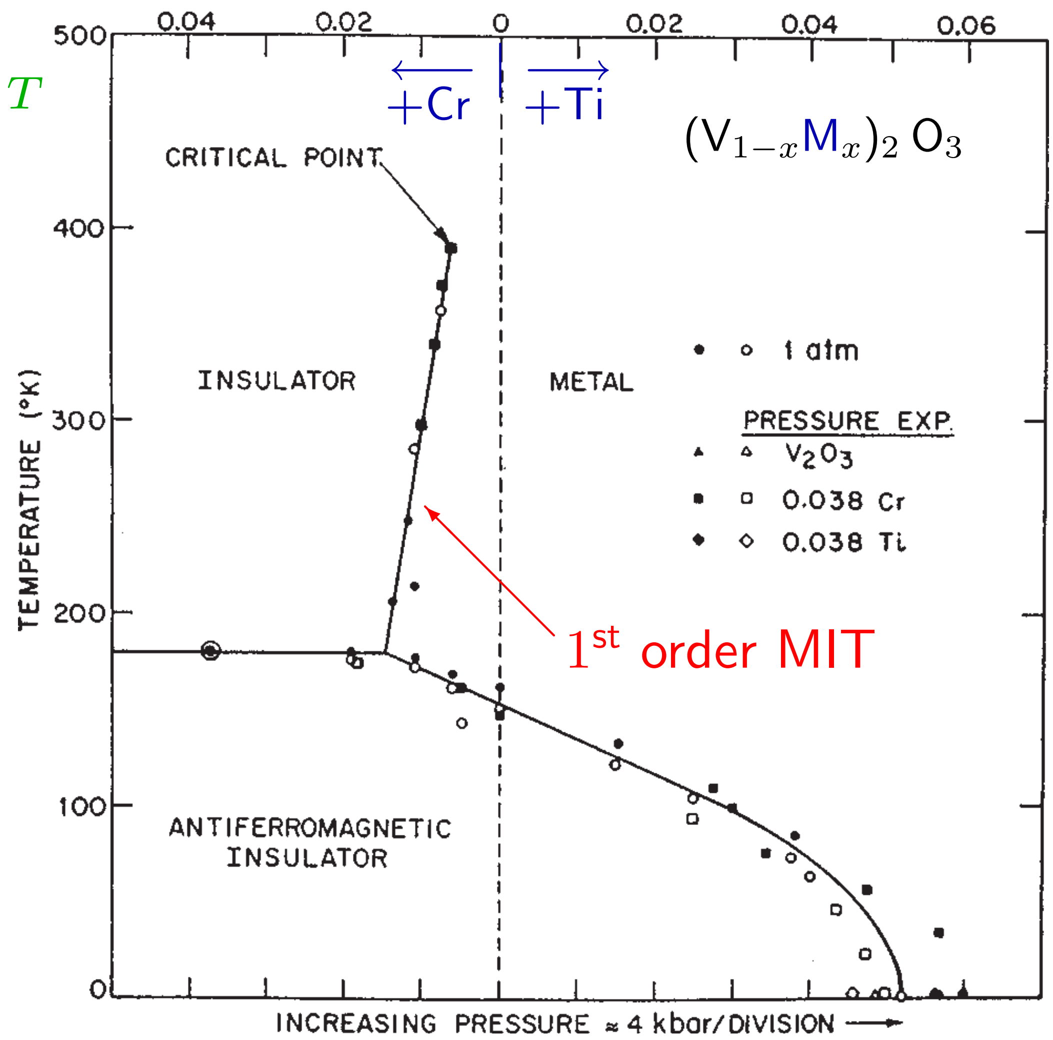
High-precision ground state estimates from QMC

Orbital-selective Mott transition in 2-band Hubbard model

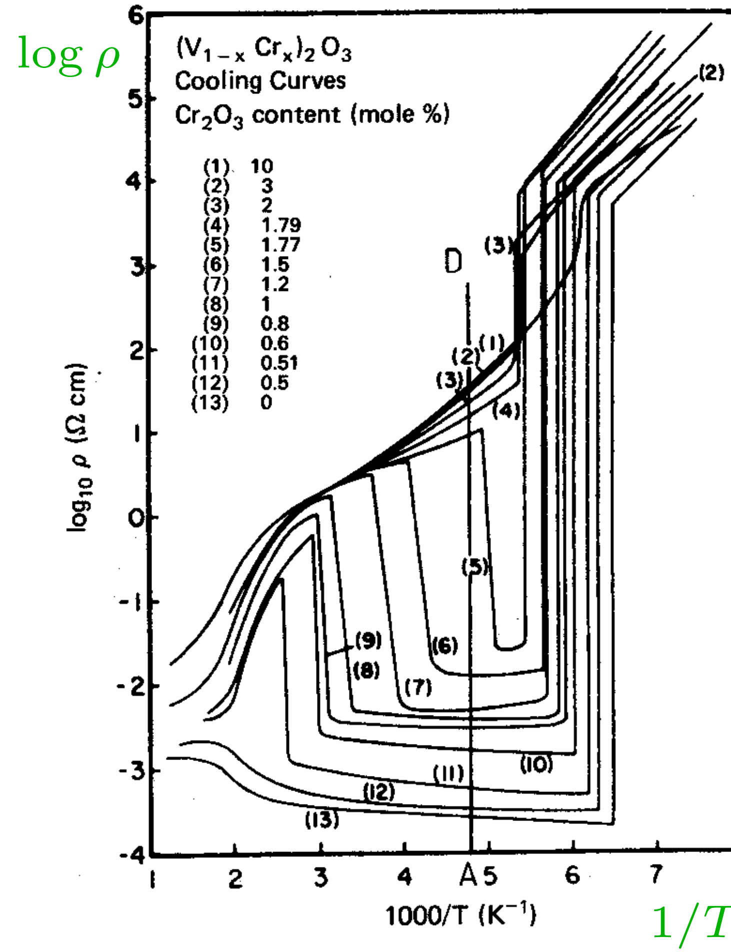
Summary and Outlook

Motivation

Prototype correlated system: V_2O_3

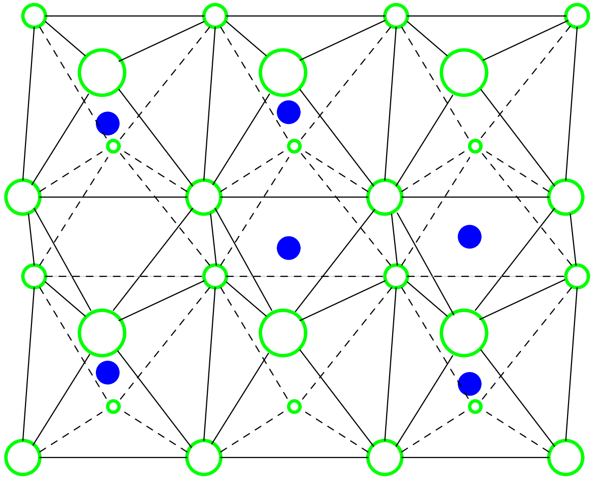


McWhan et al, 1971



Kawamoto et al, 1980

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



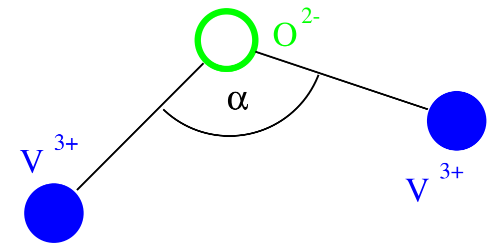
Corundum structure

Corundum structure:

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

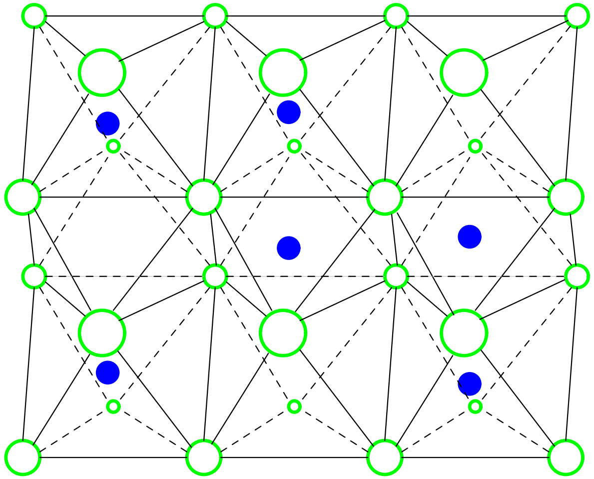
doping with Ti, Cr:

- (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?



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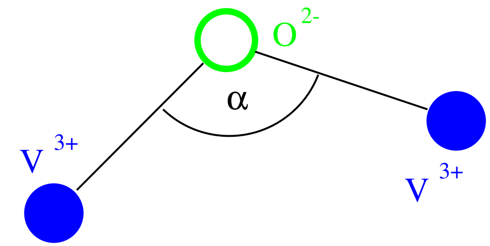

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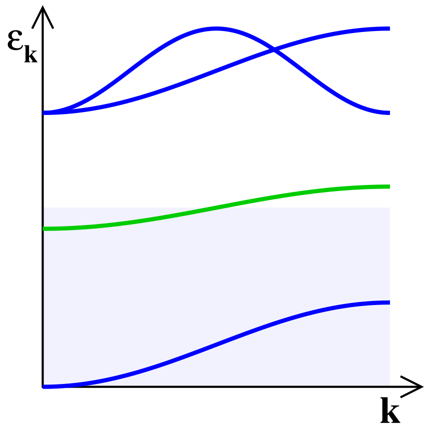
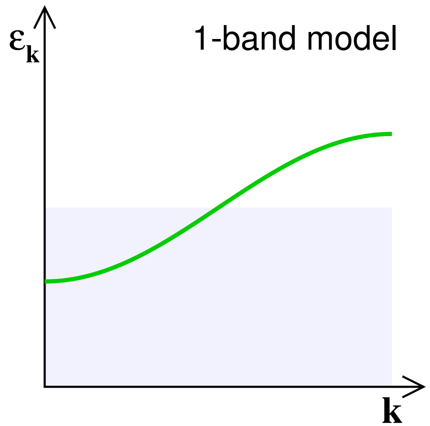
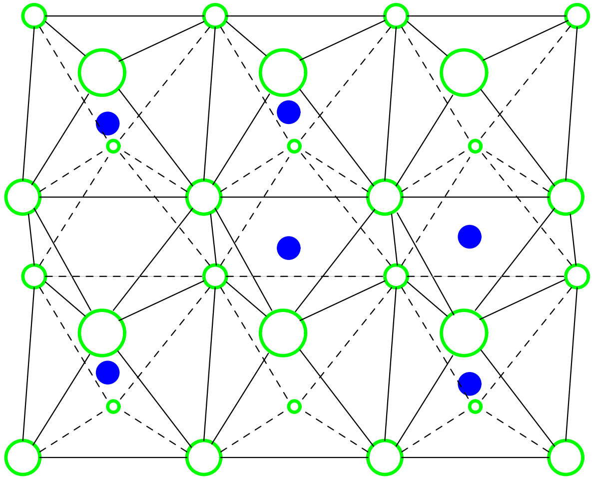
Bloch states near Fermi energy,







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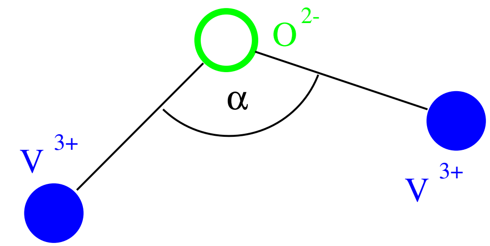

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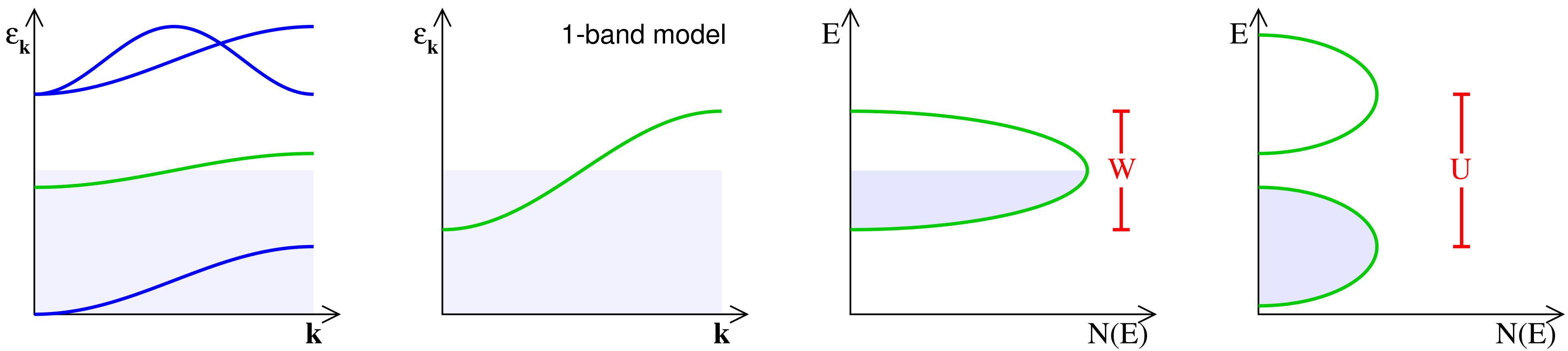
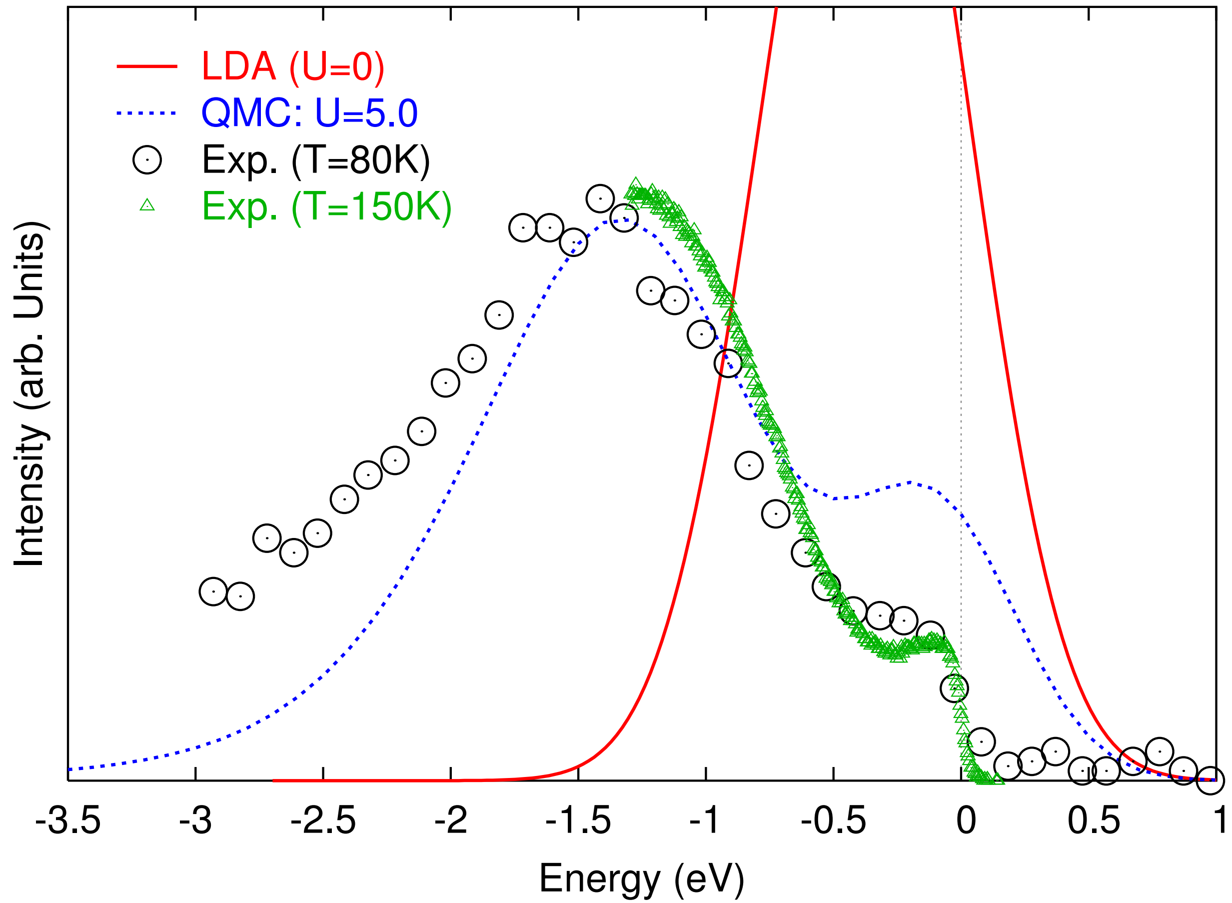
Bloch states near Fermi energy, band-splitting by Coulomb correlations ($\sim U$)



Paramagnetic Mott transition not captured by LDA band structure calculations!

System near Mott transition: $La_{1-x}Sr_xTiO_3$ (x=0.06) – photoemission spectra



[Nekrasov, Held, NB, Poteryaev, Anisimov, Vollhardt (2000)]

LDA fails to capture low-energy features

LDA+DMFT(QMC): Reasonable accuracy, drastic improvement over LDA

Introduction: Hubbard model, DMFT, QMC

$$H = \sum_{i=1}^{N_e} \frac{\boldsymbol{p}_i^{\,2}}{2m} + \sum_{k=1}^{L} \frac{\boldsymbol{P}_k^{\,2}}{2M_k} + \sum_{k<l} \frac{Z_k Z_l\, e^2}{|\boldsymbol{R}_k - \boldsymbol{R}_l|} - \sum_{i,k} \frac{Z_k\, e^2}{|\boldsymbol{r}_i - \boldsymbol{R}_k|} + \sum_{i<j} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$$

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Born-Oppenheimer approximation ↓

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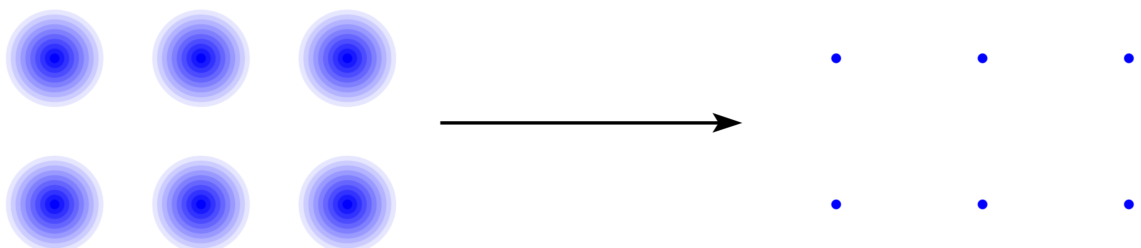

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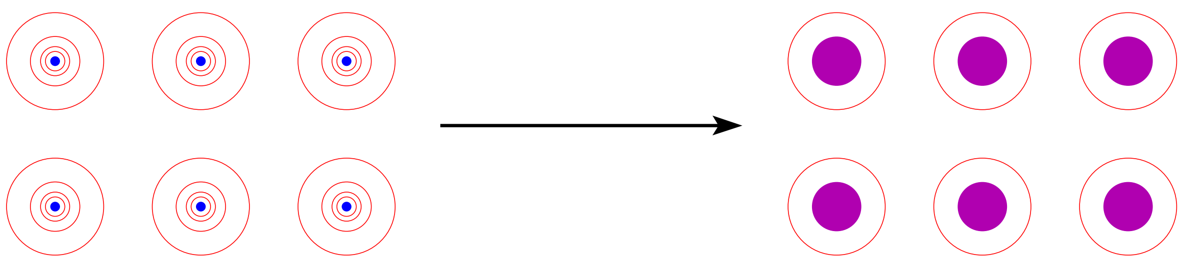
$$H = \sum_{i=1}^{N_v} \frac{\boldsymbol{p}_i^2}{2m} + \sum_{i=1}^{N_v} V^{\text{ion}}(\boldsymbol{r}_i) + \sum_{i=1}^{N_v-1} \sum_{j=i+1}^{N_v} V^{ee}(\boldsymbol{r}_i, \boldsymbol{r}_j)$$



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occupation number formalism, Wannier orbitals ↓

$$\hat{H} = \sum_{i\nu j\sigma} t_{ij}^{\nu}\, \hat{c}_{i\nu\sigma}^{\dagger}\, \hat{c}_{j\nu\sigma} + \frac{1}{2} \sum_{\nu\nu'\mu\mu'} \sum_{ijmn} \sum_{\sigma\sigma'} \mathcal{V}_{ijmn}^{\nu\nu'\mu\mu'}\, \hat{c}_{i\nu\sigma}^{\dagger}\, \hat{c}_{j\nu'\sigma'}^{\dagger}\, \hat{c}_{n\mu'\sigma'}\, \hat{c}_{m\mu\sigma}$$

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← **density functional theory (DFT)**

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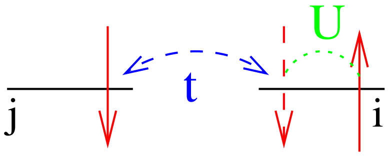
Hubbard model

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



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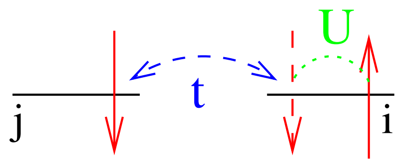

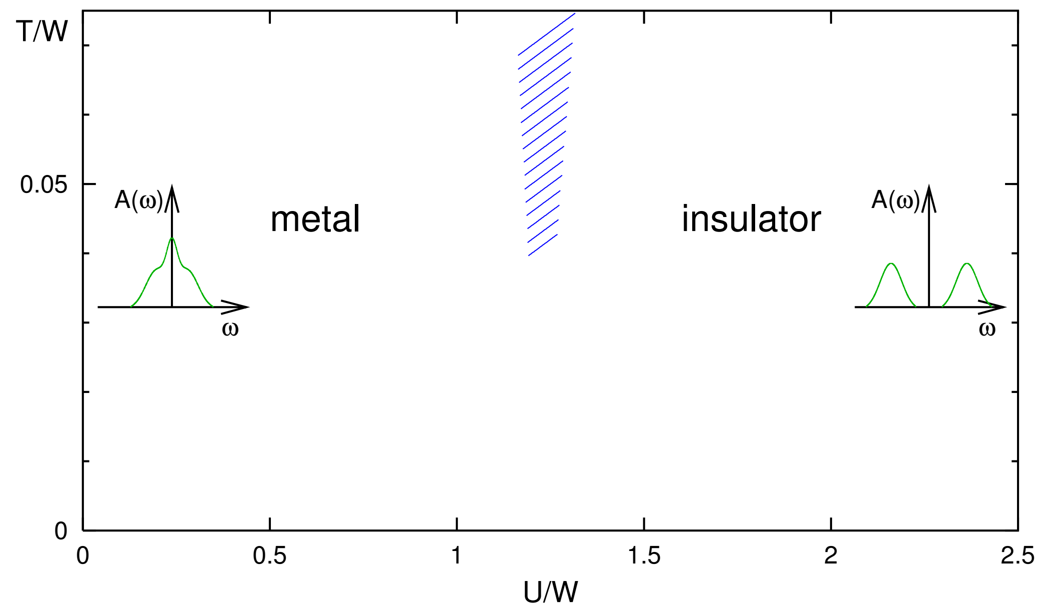

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Minimal model for correlated electrons

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

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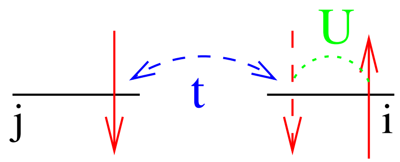

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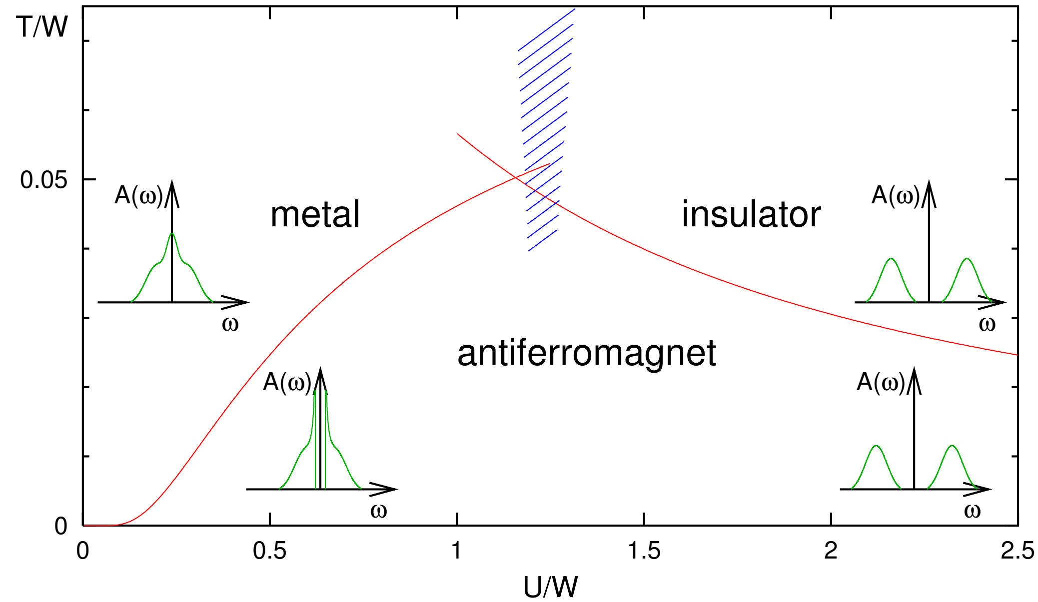
But: generically antiferromagnetism at low T



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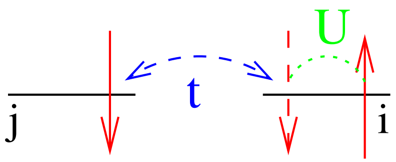

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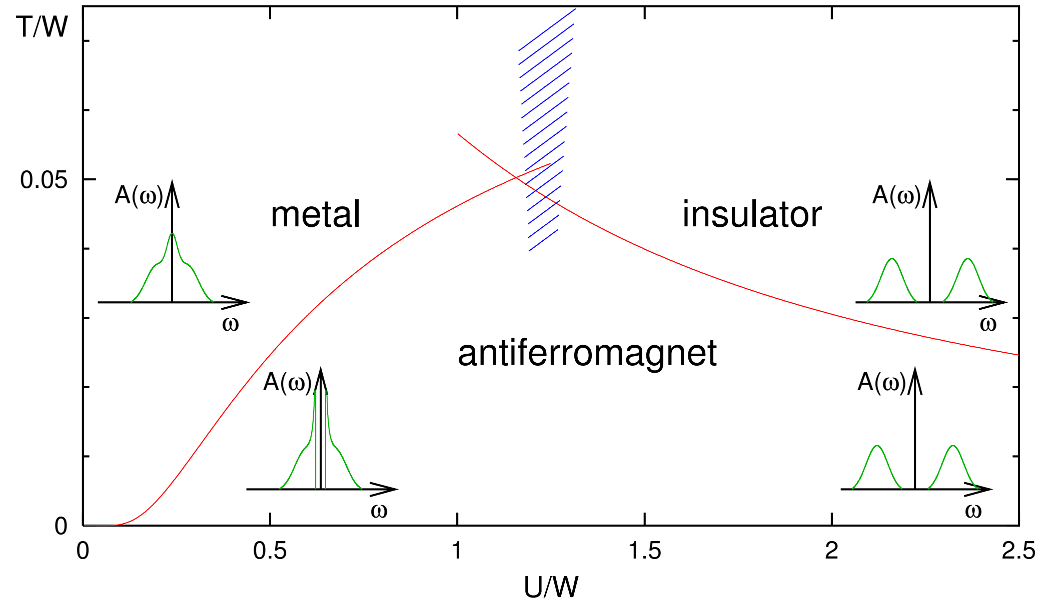

How to solve (frustrated) Hubbard model in regime of $W \sim U$?

Approaches for Hubbard-type models

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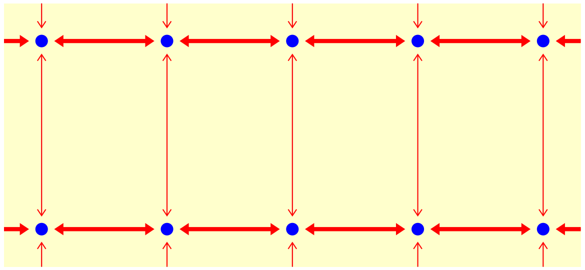
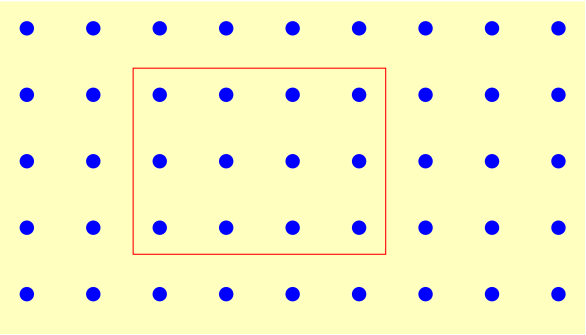
Perturbation theory, e.g.

- $U \longrightarrow 0$: Hartree-Fock (uncorrelated)
- $t/U \longrightarrow 0$: half filling $(n = 1)$ $\rightsquigarrow$ Heisenberg model
- $T \longrightarrow \infty$, $n \longrightarrow 0$
- ($V_{\text{ion}} \longrightarrow 0$ $\rightsquigarrow$ jellium model $\rightsquigarrow$ LDA)

$d = 1$: Bethe ansatz, DMRG



finite clusters: ED, QMC



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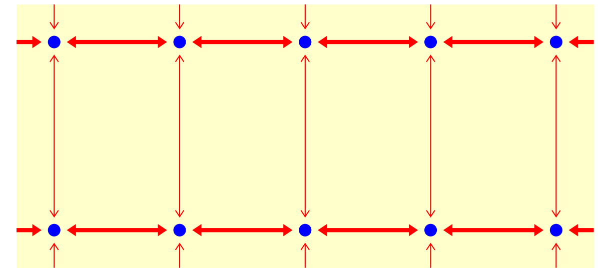

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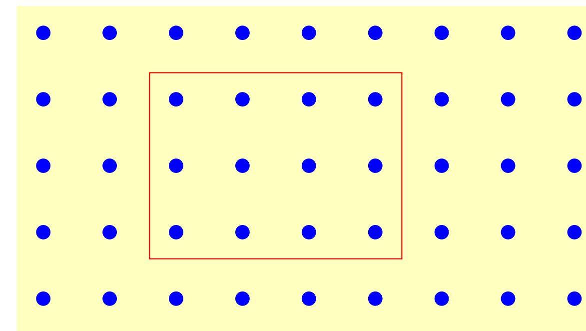
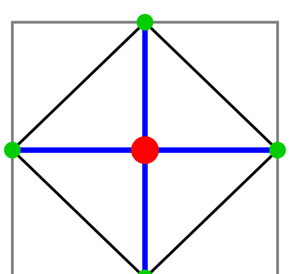
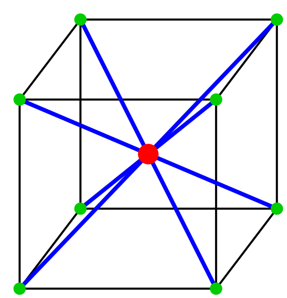


Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$

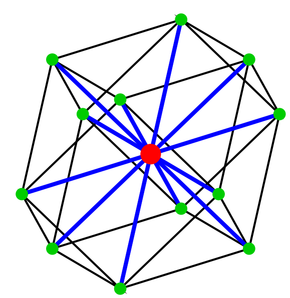
+ non-perturbative $\rightsquigarrow$ valid at MIT
+ dynamical on-site correlations preserved
+ in thermodynamic limit
+ exact for $Z \rightarrow \infty$



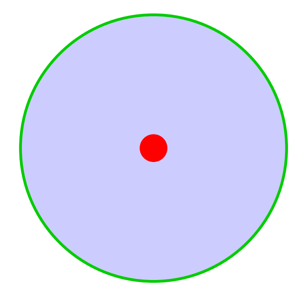
d=2: $Z = 4$



bcc: $Z = 8$



fcc: $Z = 12$



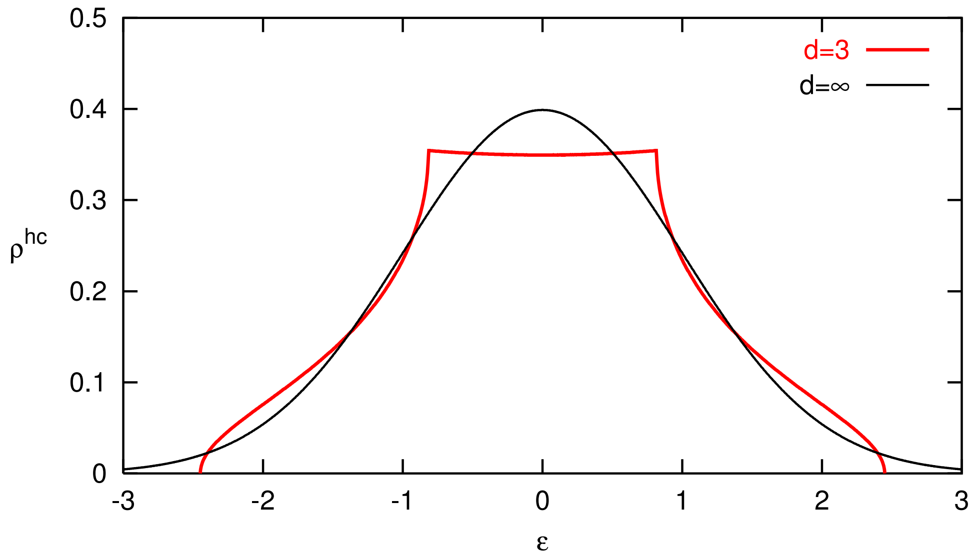
DMFT: $Z = \infty$

Brief History of DMFT

1989 Metzner, Vollhardt: **limit $\mathbf{d} \to \infty$**: Gutzwiller approximation exact

Müller-Hartmann: local self-energy: $\Sigma(\boldsymbol{q}, \omega) \to \Sigma(\omega)$

Brandt, Mielsch: exact solution of Falicov-Kimball model



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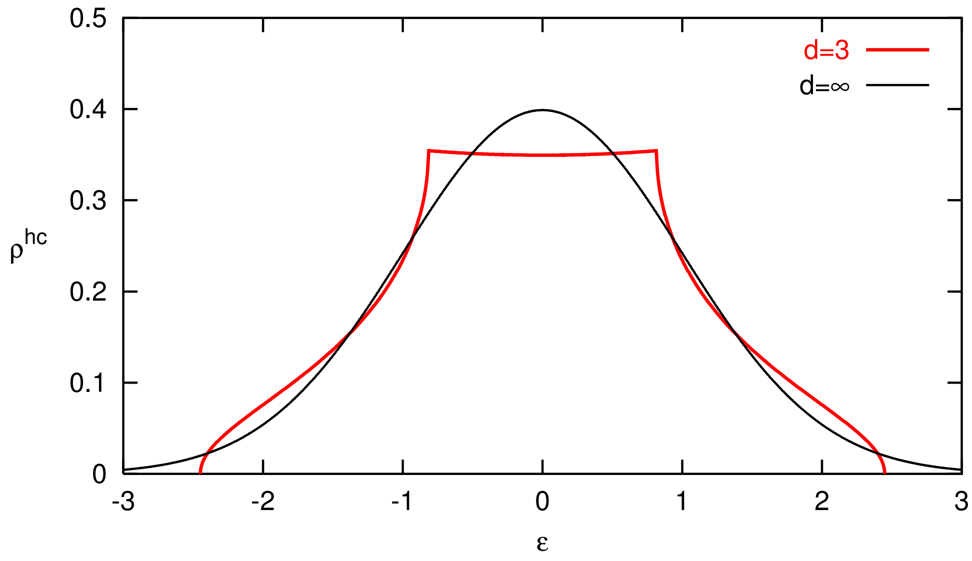
Jarrell: Quantum Monte-Carlo $\rightsquigarrow$ antiferromagnetism, Mott-Hubbard behavior



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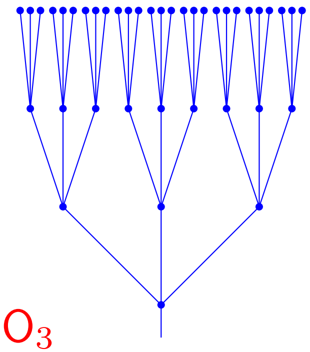

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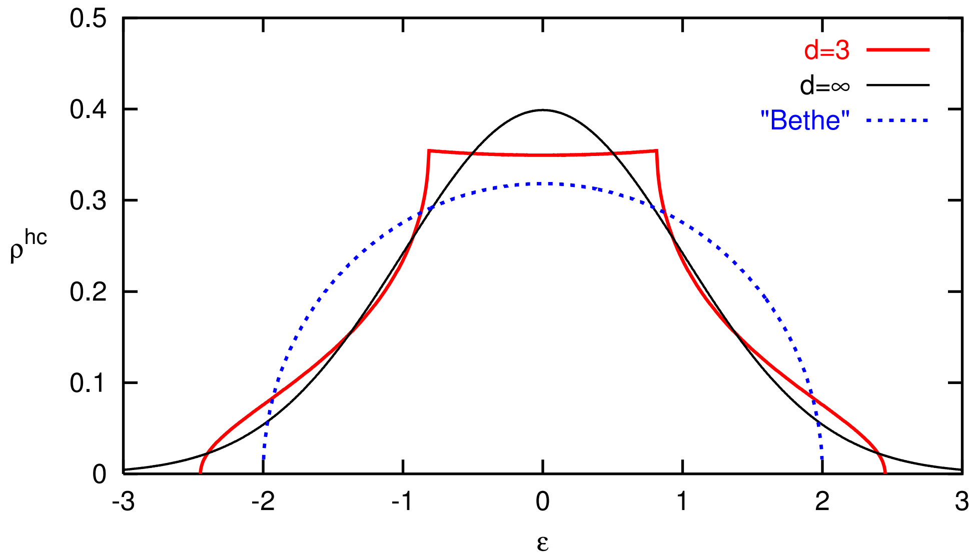
Vollhardt group: ferro/metamagnetism (NN exchange, asymmetric DOS, multi-band)



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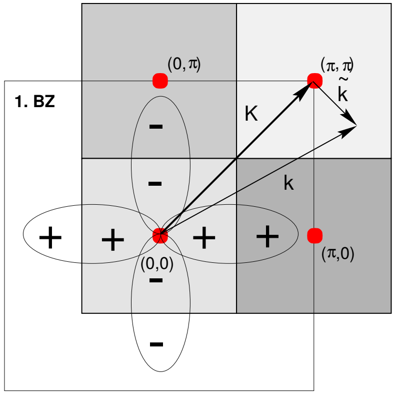
Jarrell group: dynamical cluster approximation (DCA) $\rightsquigarrow$ d-wave superconductivity

Brief History of DMFT



1989 Metzner, Vollhardt: **limit d** $\rightarrow \infty$: Gutzwiller approximation exact

Müller-Hartmann: local self-energy: $\Sigma(\boldsymbol{q}, \omega) \longrightarrow \Sigma(\omega)$

Brandt, Mielsch: exact solution of Falicov-Kimball model

1992 Georges, Kotliar: mapping to Anderson impurity model + self consistency

Jarrell: Quantum Monte-Carlo $\rightsquigarrow$ antiferromagnetism, Mott-Hubbard behavior

1993 Georges et al., Kotliar et al.: frustrated Bethe lattice (IPT/QMC) $\rightsquigarrow$ MIT of V_2O_3

1996 Georges, Kotliar, Krauth, Rozenberg: **Rev. Mod. Phys.** article

Vollhardt group: ferro/metamagnetism (NN exchange, asymmetric DOS, multi-band)

1997 Anisimov, Kotliar: LDA+DMFT(IPT) $\rightsquigarrow$ PES for $La_{1-x}Sr_xTiO_3$

2000 Katsnelson, Lichtenstein: LDA+DMFT(QMC) $\rightsquigarrow$ $T_C, M(T), \chi(T)$ for iron

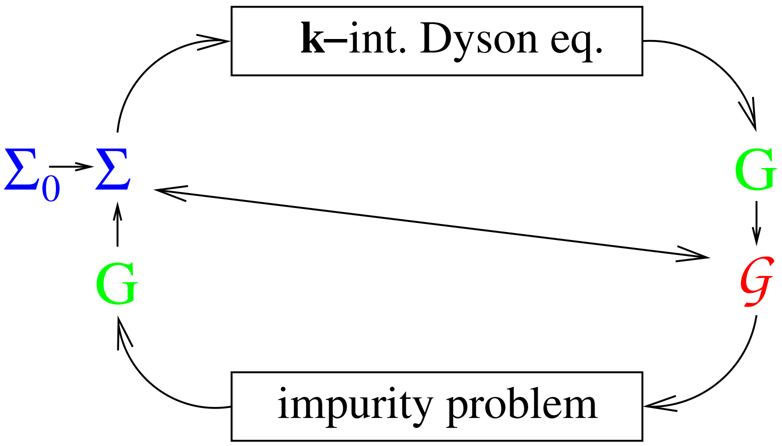
Vollhardt+Anisimov groups: LDA+DMFT(QMC) $\rightsquigarrow$ PES for $La_{1-x}Sr_xTiO_3$

Jarrell group: dynamical cluster approximation (DCA) $\rightsquigarrow$ d-wave superconductivity

2004 **Physics Today** article; lecture notes; conferences "beyond LDA",. . .

Future: complete understanding of phenomena and abstract models (within DMFT)
realistic calculations (LDA+DMFT), cluster methods (DCA, CDMFT)

Iterative solution of DMFT equations

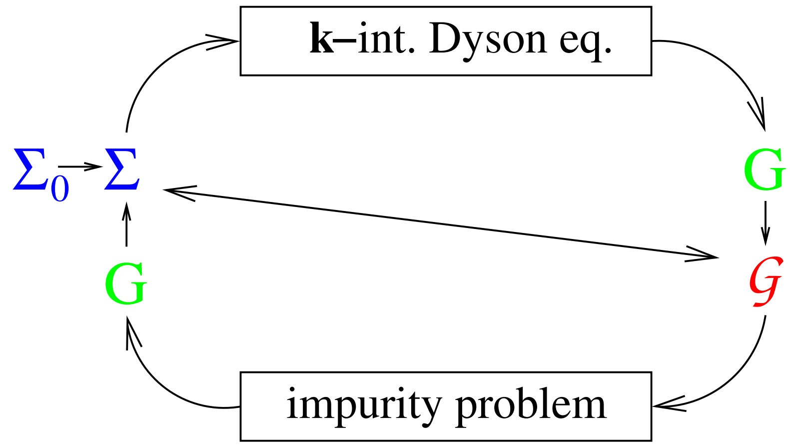


⟵ DOS / t_{ij} / $\epsilon_{\nu \boldsymbol{k}}$

Fourier transformations

⟵ local interactions

Iterative solution of DMFT equations

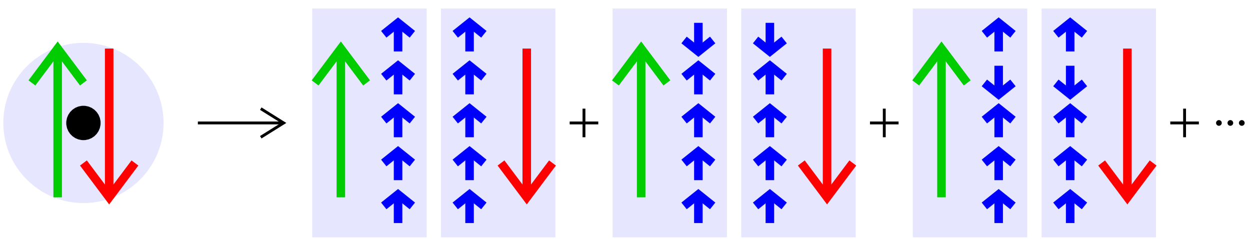


$\longleftarrow$ DOS / t_{ij} / $\epsilon_{\nu \boldsymbol{k}}$

Fourier transformations

$\longleftarrow$ local interactions

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



Wick theorem:

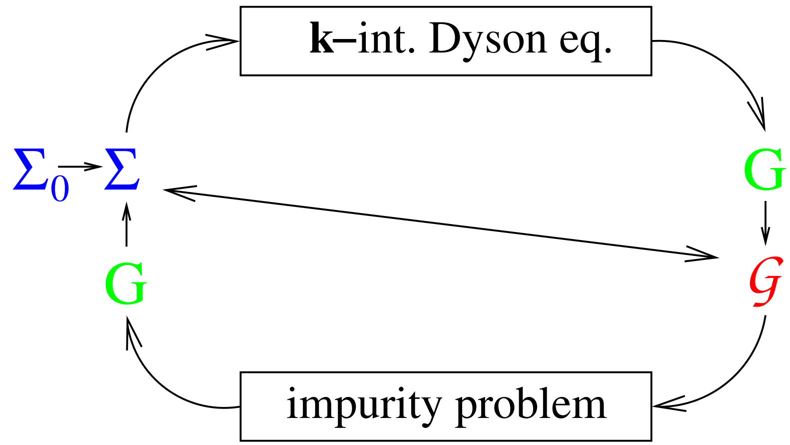
$$G = \frac{\sum M \det\{M\}}{\sum \det\{M\}}$$

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

$+$ numerically exact

$-$ effort scales as T^{-3}

Iterative solution of DMFT equations

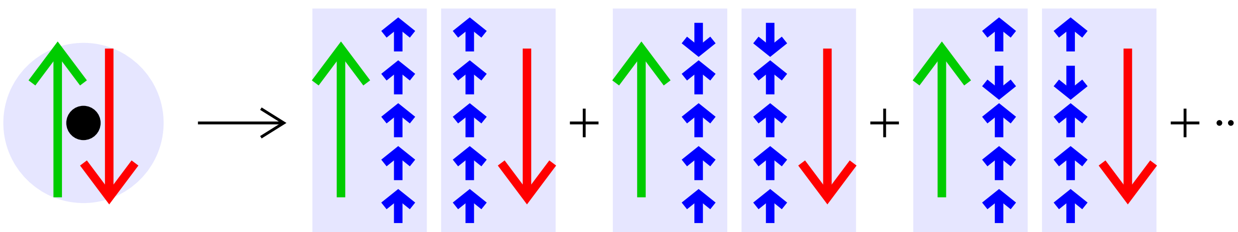


$\longleftarrow$ DOS / t_{ij} / $\epsilon_{\nu \boldsymbol{k}}$

Fourier transformations

$\longleftarrow$ local interactions

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



Wick theorem:

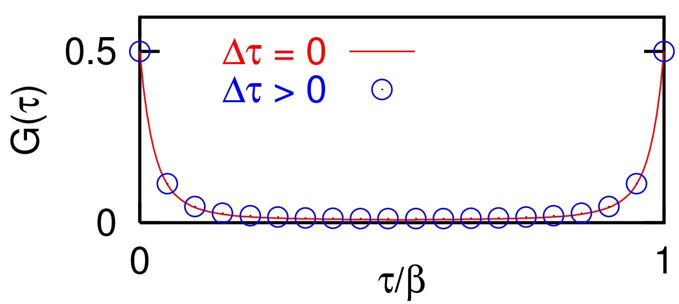
$$G = \frac{\sum M \det\{M\}}{\sum \det\{M\}}$$

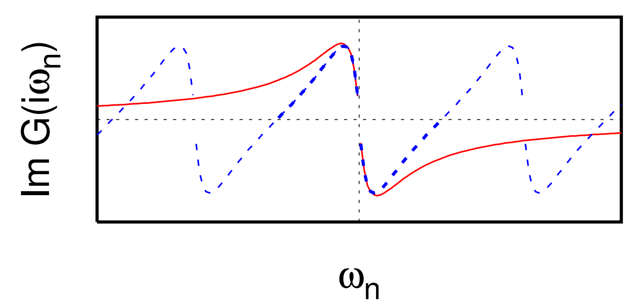
Metropolis MC importance sampling over auxiliary Ising field, 2^{Λ} configurations, $50 \lesssim \Lambda \lesssim 400$

+ numerically exact

– effort scales as T^{-3}

– no info for $\omega \gtrsim \omega_{\text{Nyquist}}$





Mott transition in frustrated 1-band Hubbard model

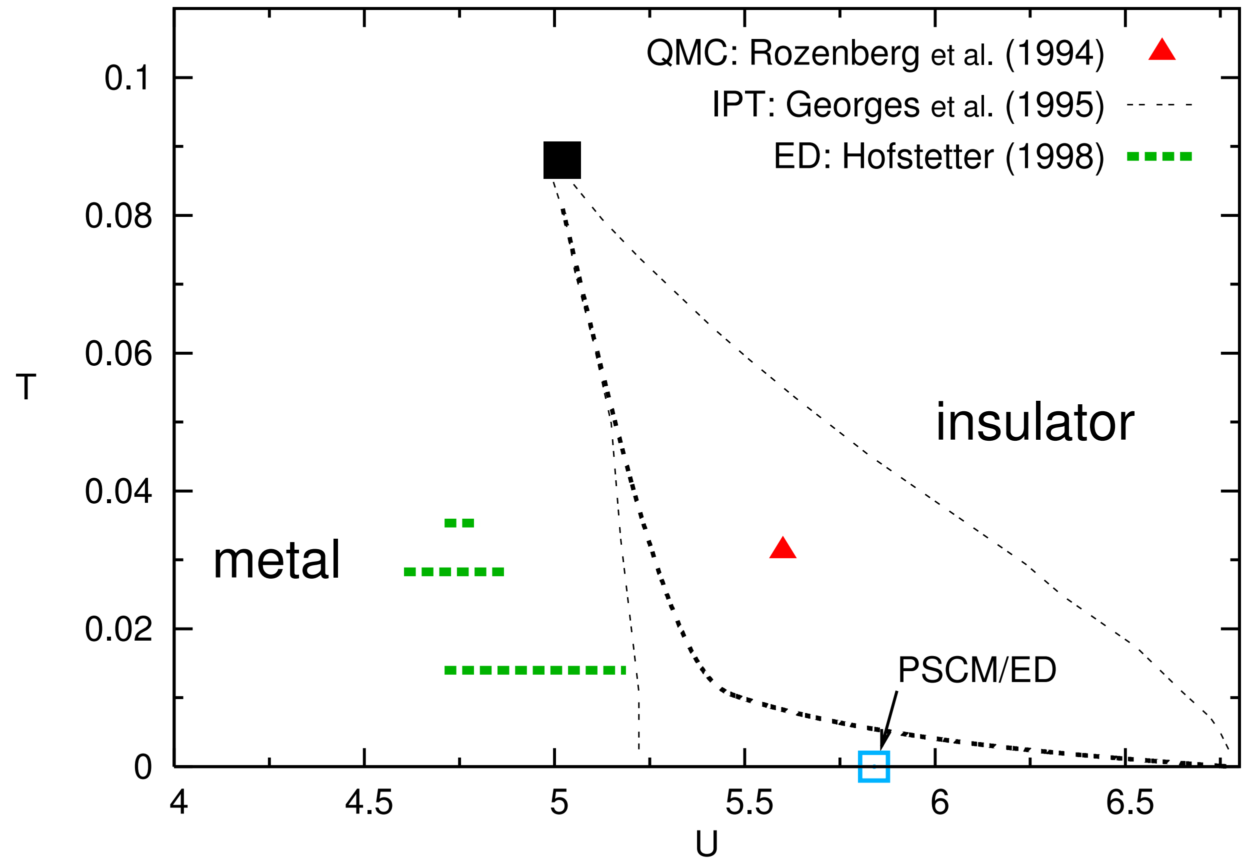
Controversy in 1999:

1st order MIT ("Bethe" DOS)?

Hysteresis in DMFT cycle?

Coexistence of metal + insulator?

- IPT, ED: yes!



Mott transition in frustrated 1-band Hubbard model

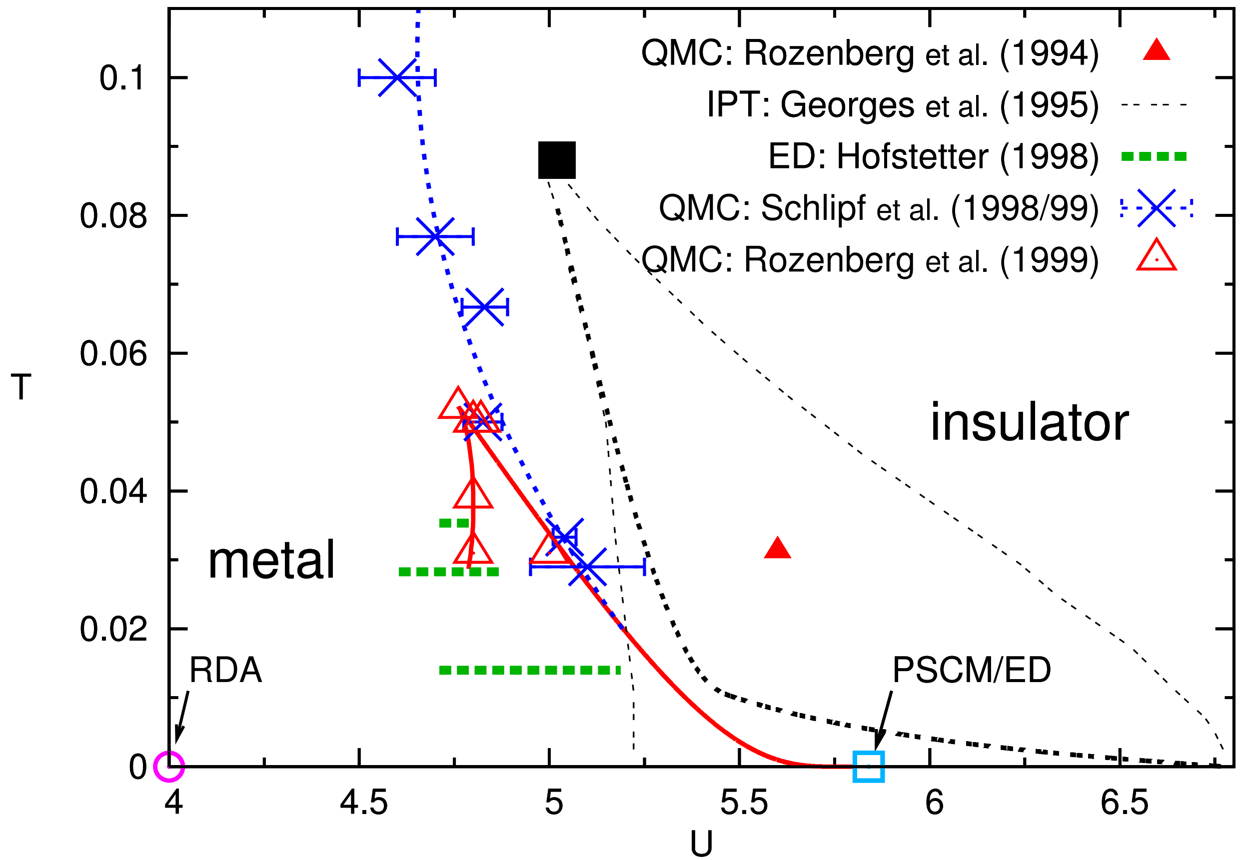
Controversy in 1999:

1st order MIT ("Bethe" DOS)?

Hysteresis in DMFT cycle?

Coexistence of metal + insulator?

- IPT, ED: yes!
- QMC (Schlipf et al.): no!
- RDA: no! (much lower U_c)
- QMC (Rozenberg et al.): yes!



- Who is right / What went wrong?
- Precise coexistence phase diagram?
- Thermodynamic first order phase transition line?

Fourier transformation schemes: self-energy Σ $(T = 0.1, U = 5.0)$

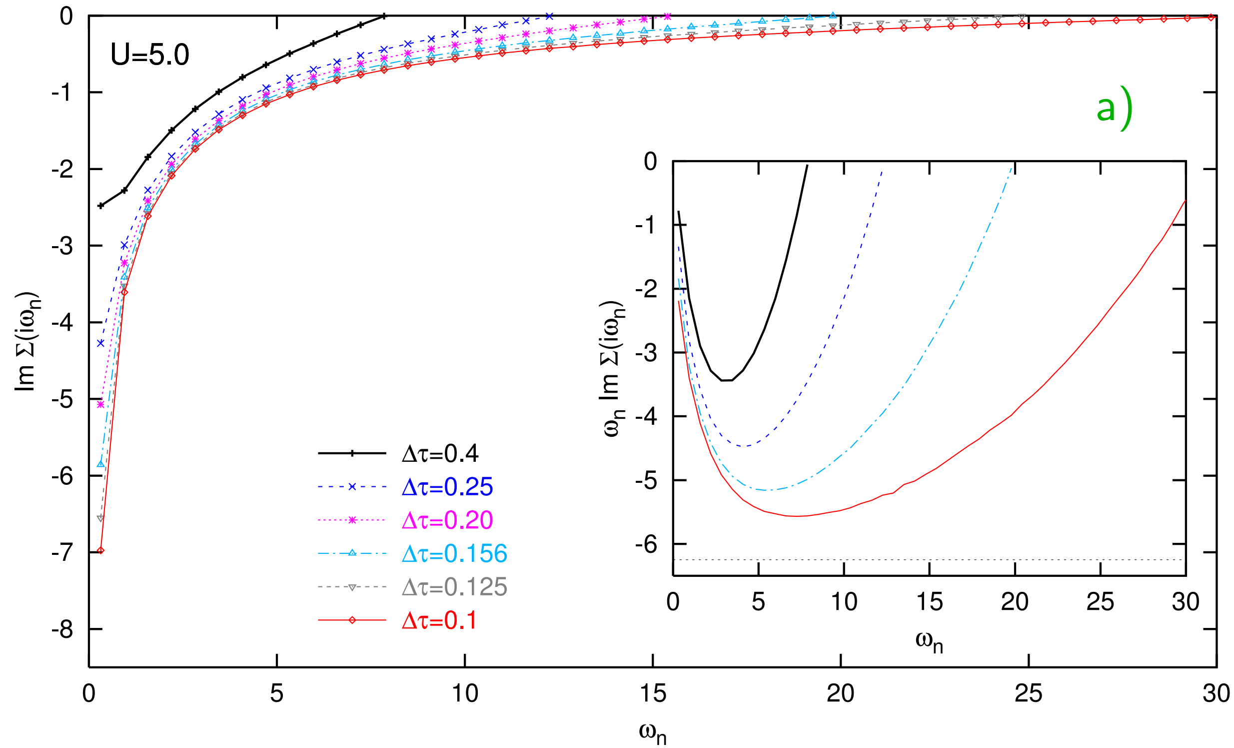
a) "Ulmke smoothing",

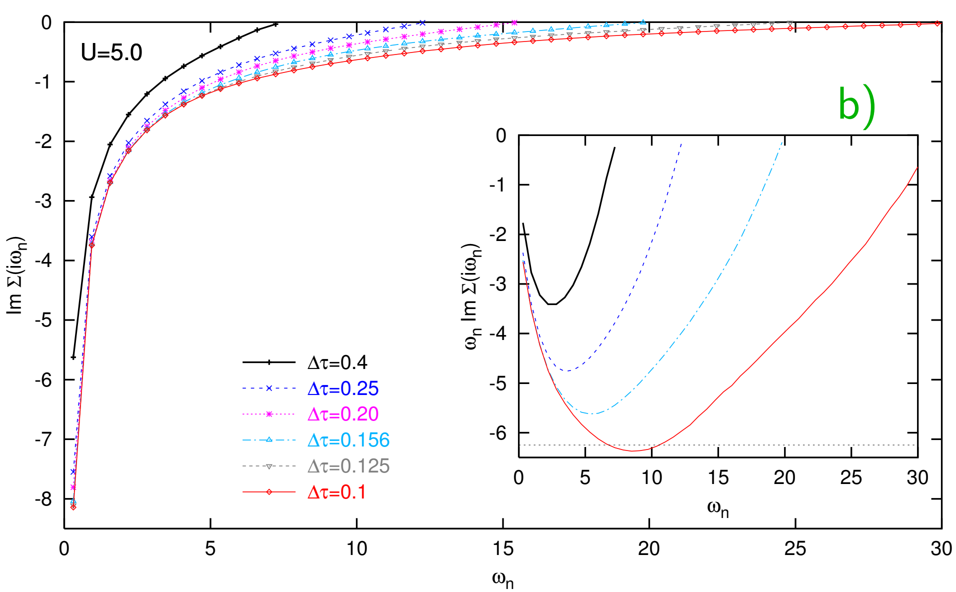
b) improved "Smoothing",

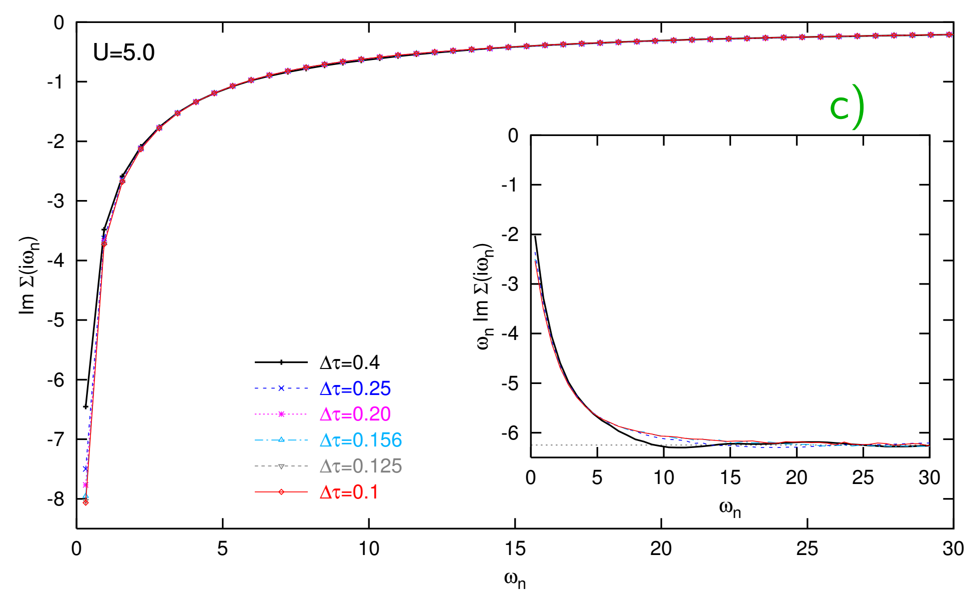
c) cubic spline + analytic high-frequency corrections

large errors even for $\omega \longrightarrow 0$ in a)

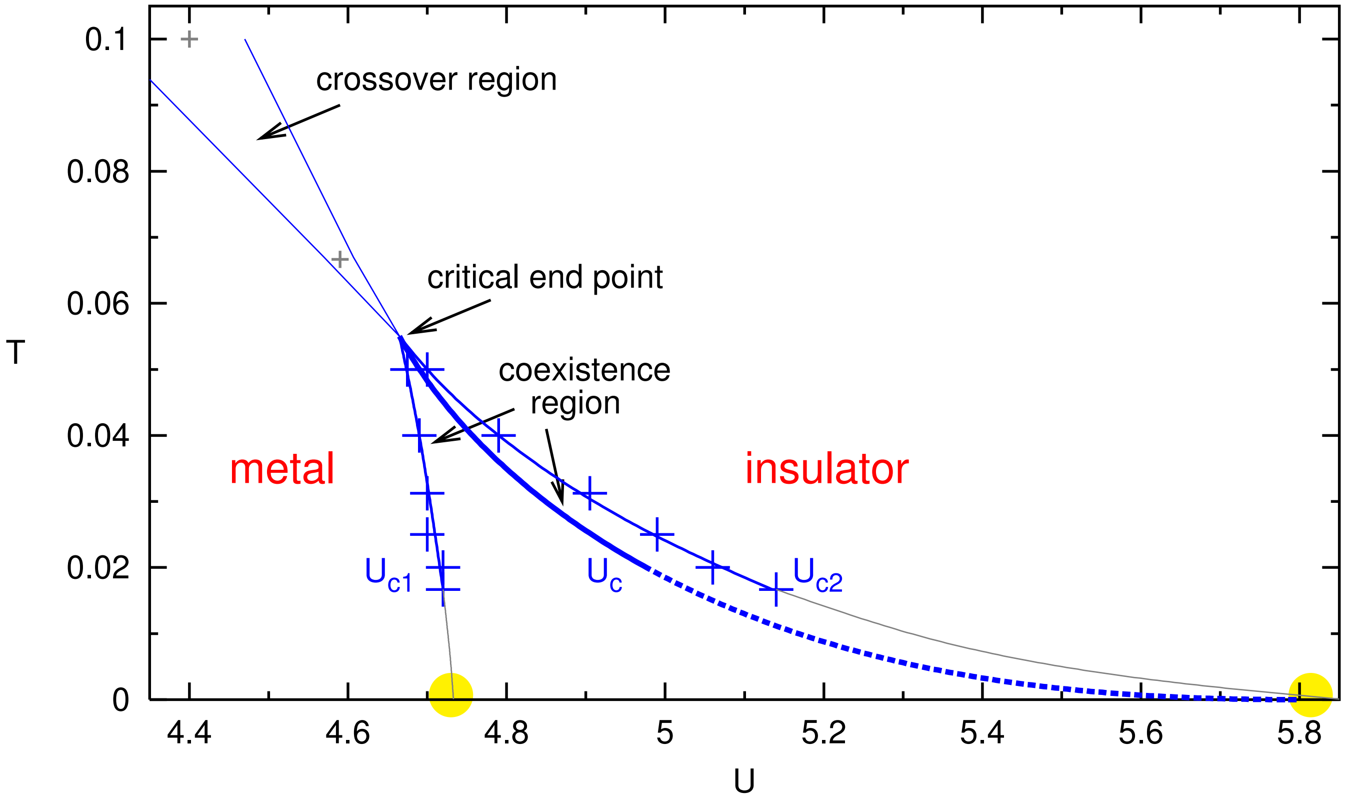
low-frequency errors of $\Sigma(\omega)$ small in b) and c)







Frustrated 1-band Hubbard model: 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)

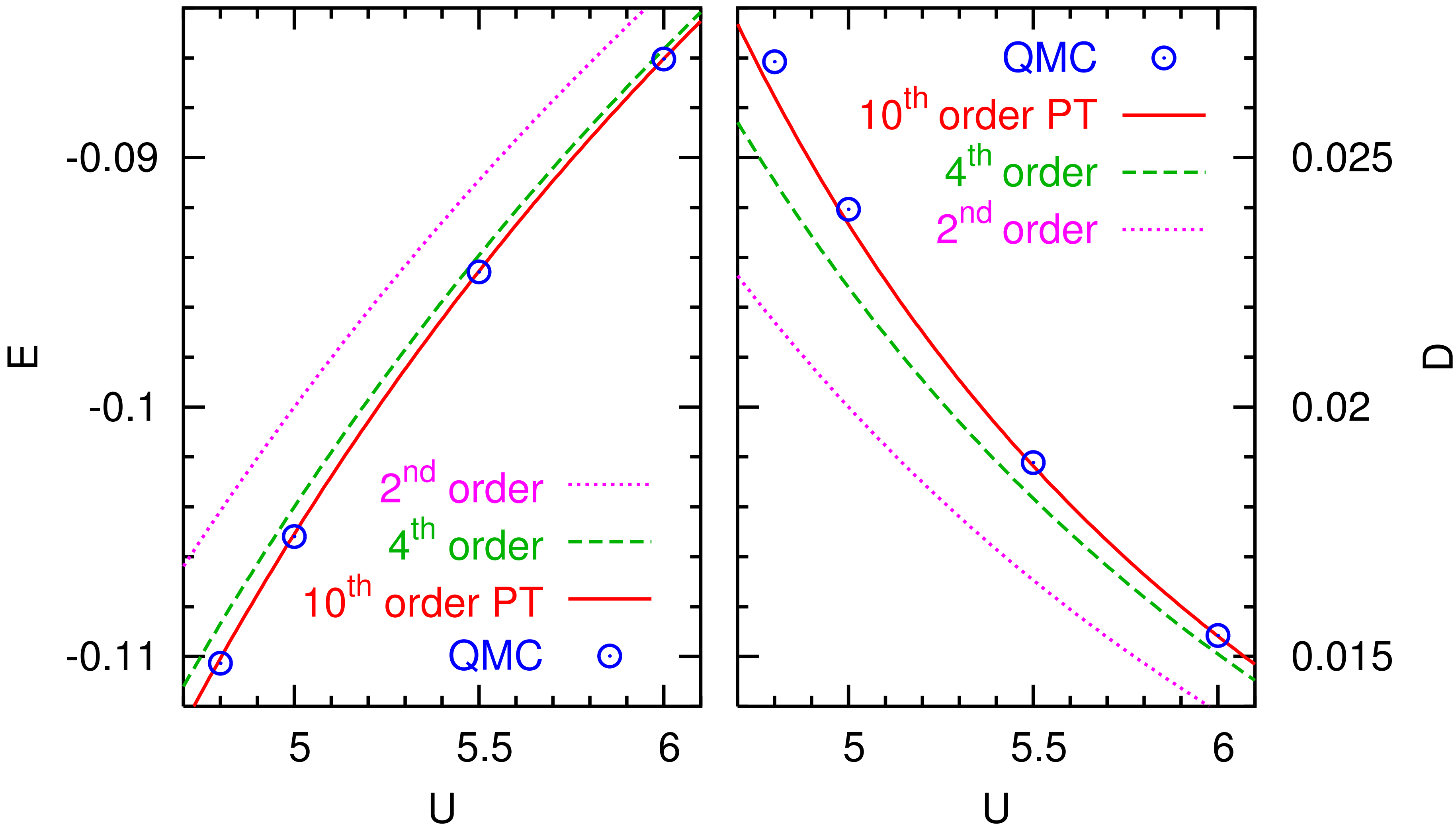
1^{st} order line from $$\frac{\mathrm{d}U_{\mathrm{c}}(T)}{\mathrm{d}T} = f(T, U_{\mathrm{c}}(T)); \;\; f(T,U) := \frac{\Delta E(T,U)}{T\,\Delta D(T,U)}$$

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 needed, even for $T \rightarrow 0$

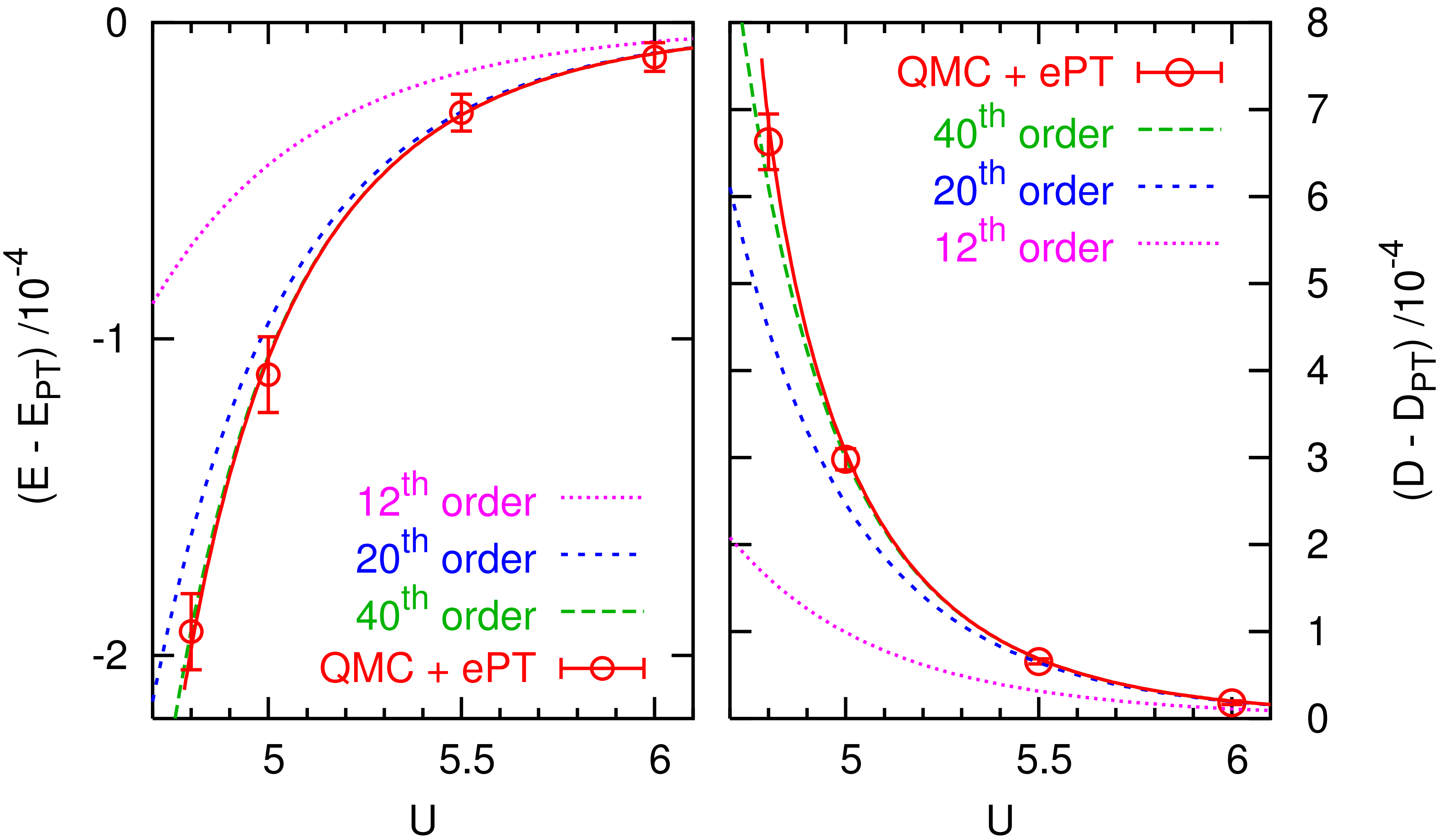
High-precision ground state estimates from QMC

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

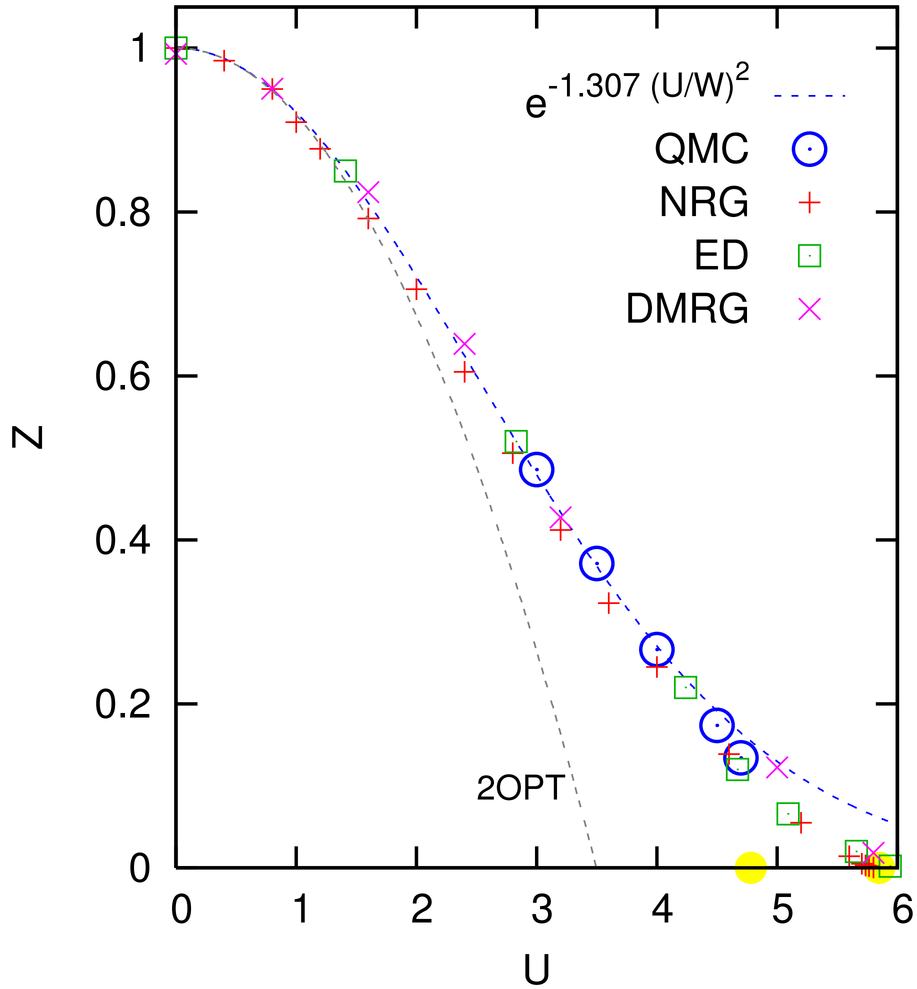


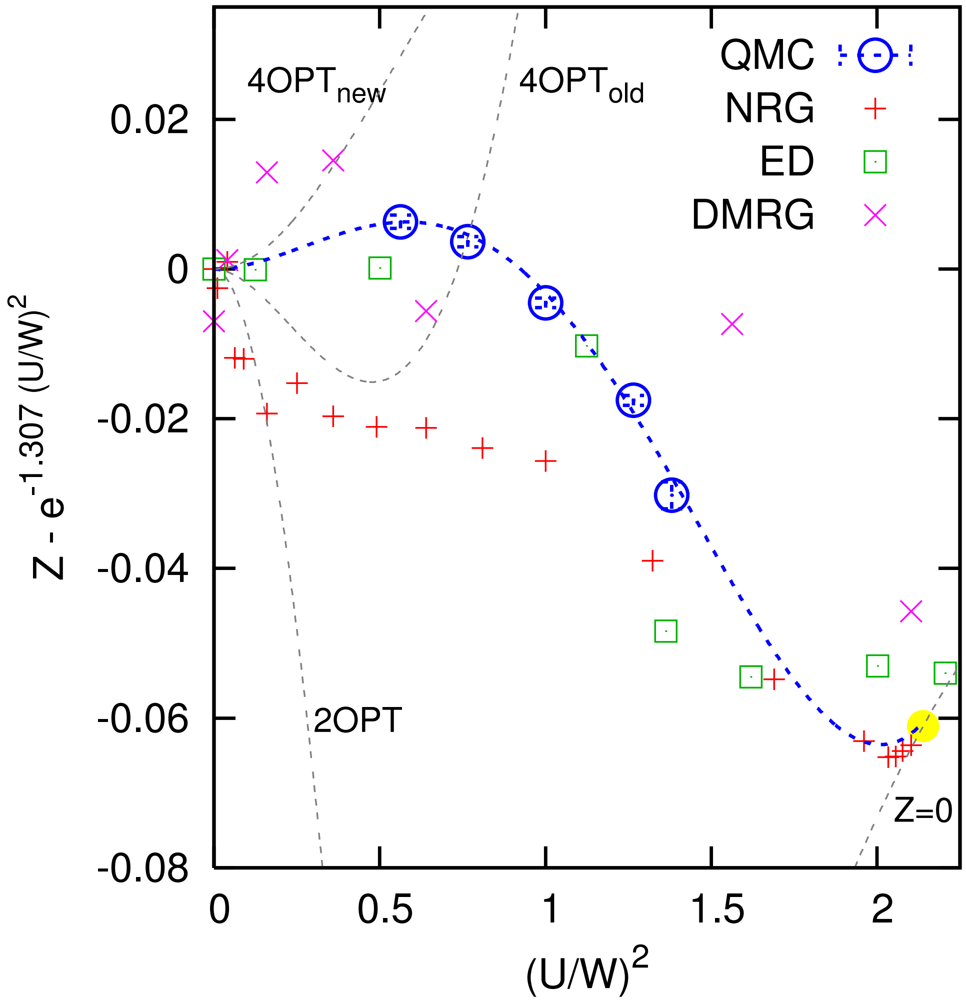
ePT: extrapolation of PT to infinite order [NB, Kalinowski, Phys. Rev B **71**, 195102 (2005)]

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

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

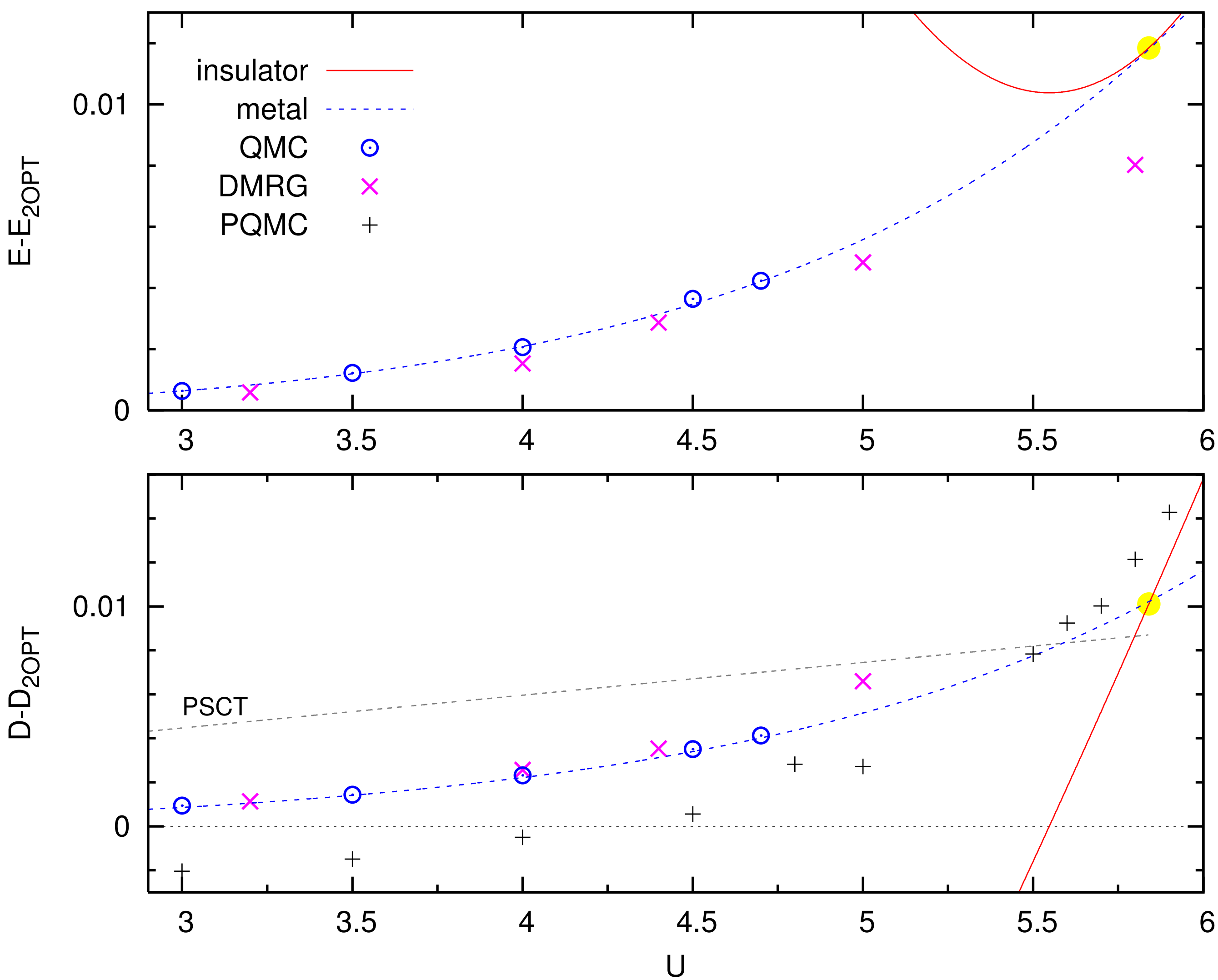
Quasiparticle weight/mass enhancement $Z = m/m^*$ in metal at $T = 0$





T-extrapolated QMC even beats all ground state methods!

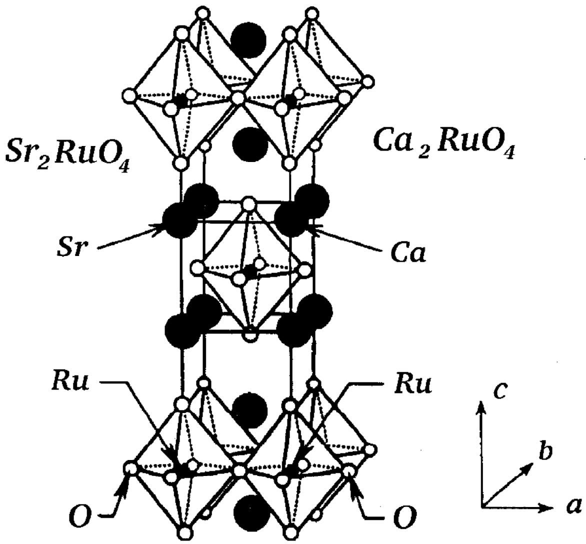
Energetics: differences w.r.t. 2^{nd} order weak-coupling PT for E and D



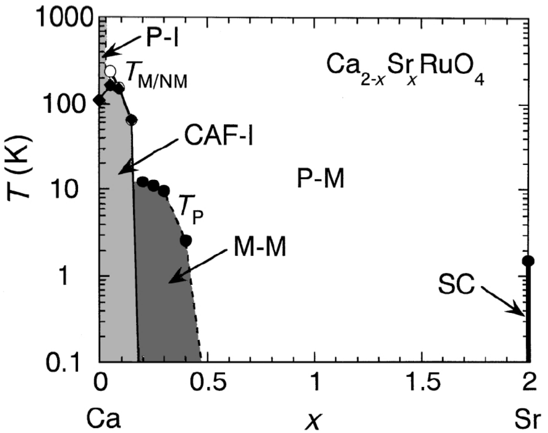
QMC-fit consistent with ePT for insulator; large deviations of PQMC, PSCT.

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

Orbital-selective Mott transition in 2-band Hubbard model

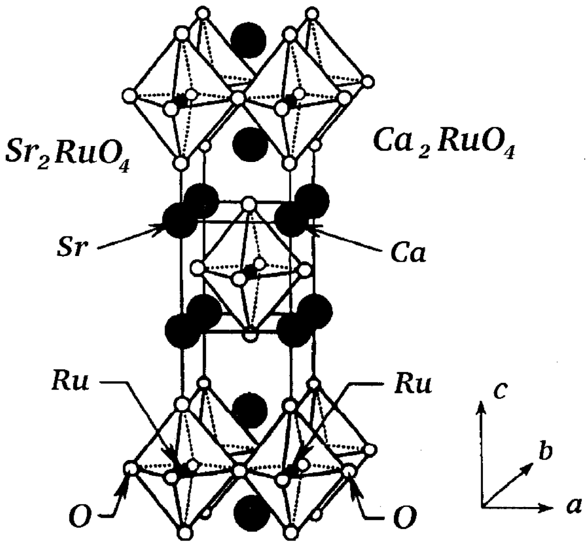


Motivation: $Ca_{2-x}Sr_xRuO_4$



[Nakatsuj, Maeno (2002)]

Orbital-selective Mott transition in 2-band Hubbard model



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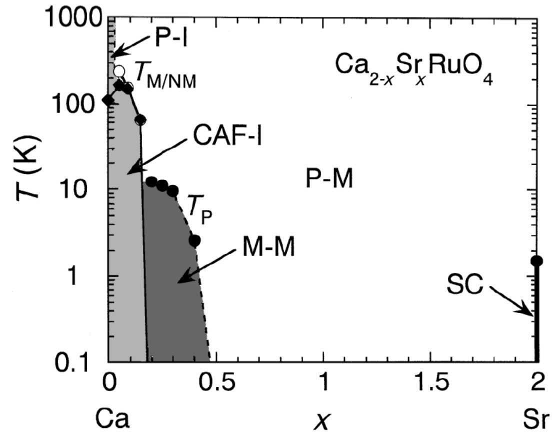

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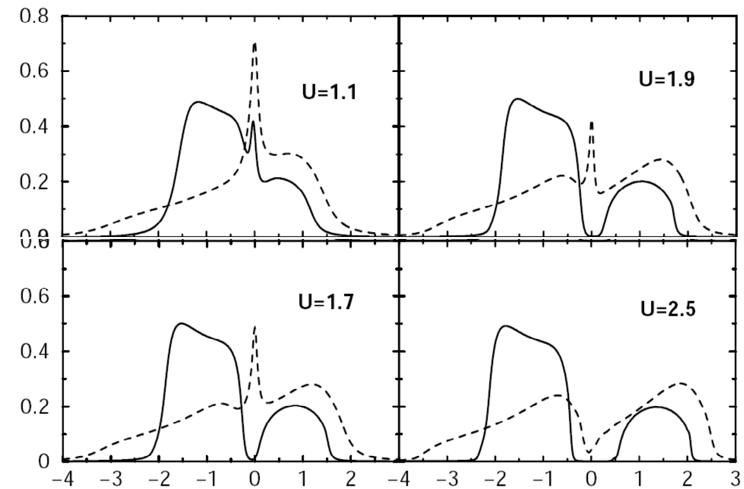
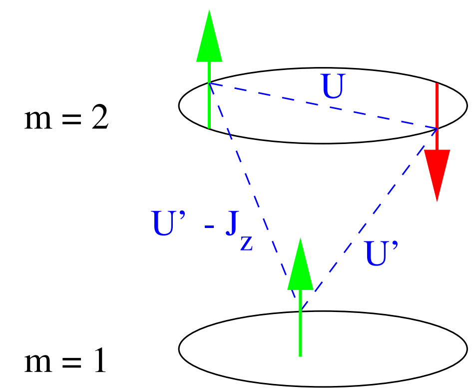


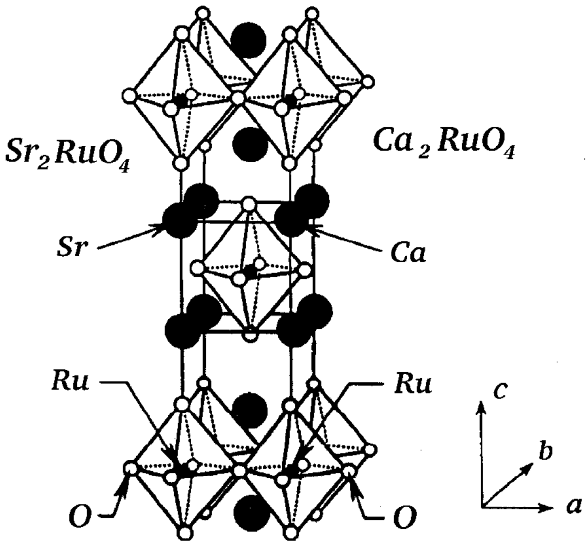
[Anisimov et al. (2002)]

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



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

Orbital-selective Mott transition in 2-band Hubbard model



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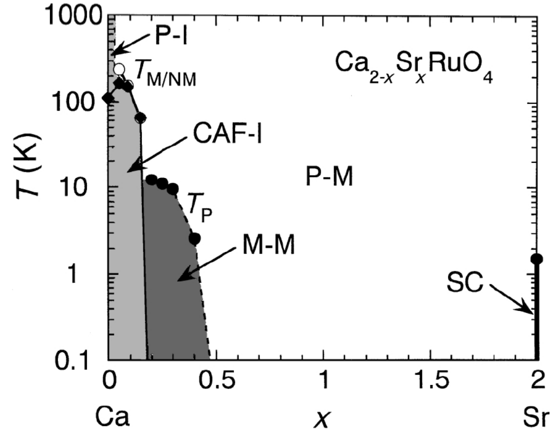

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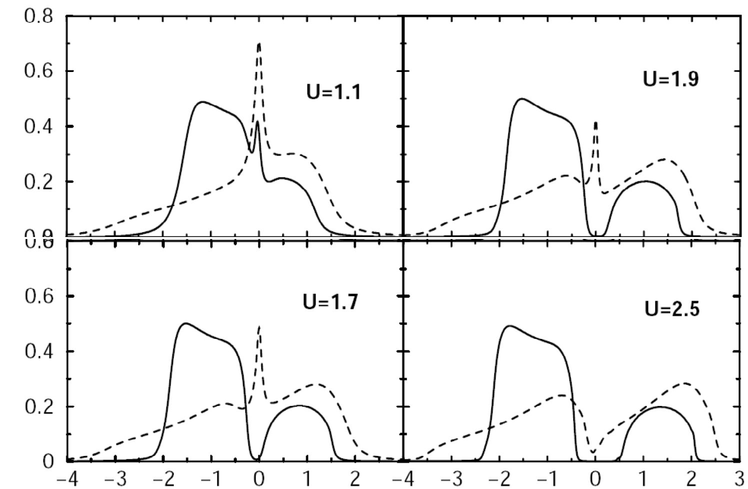
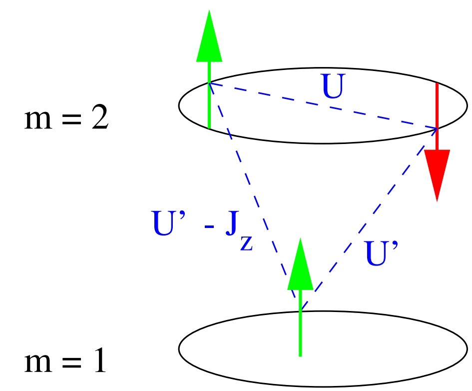


[Anisimov et al. (2002)]

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

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

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

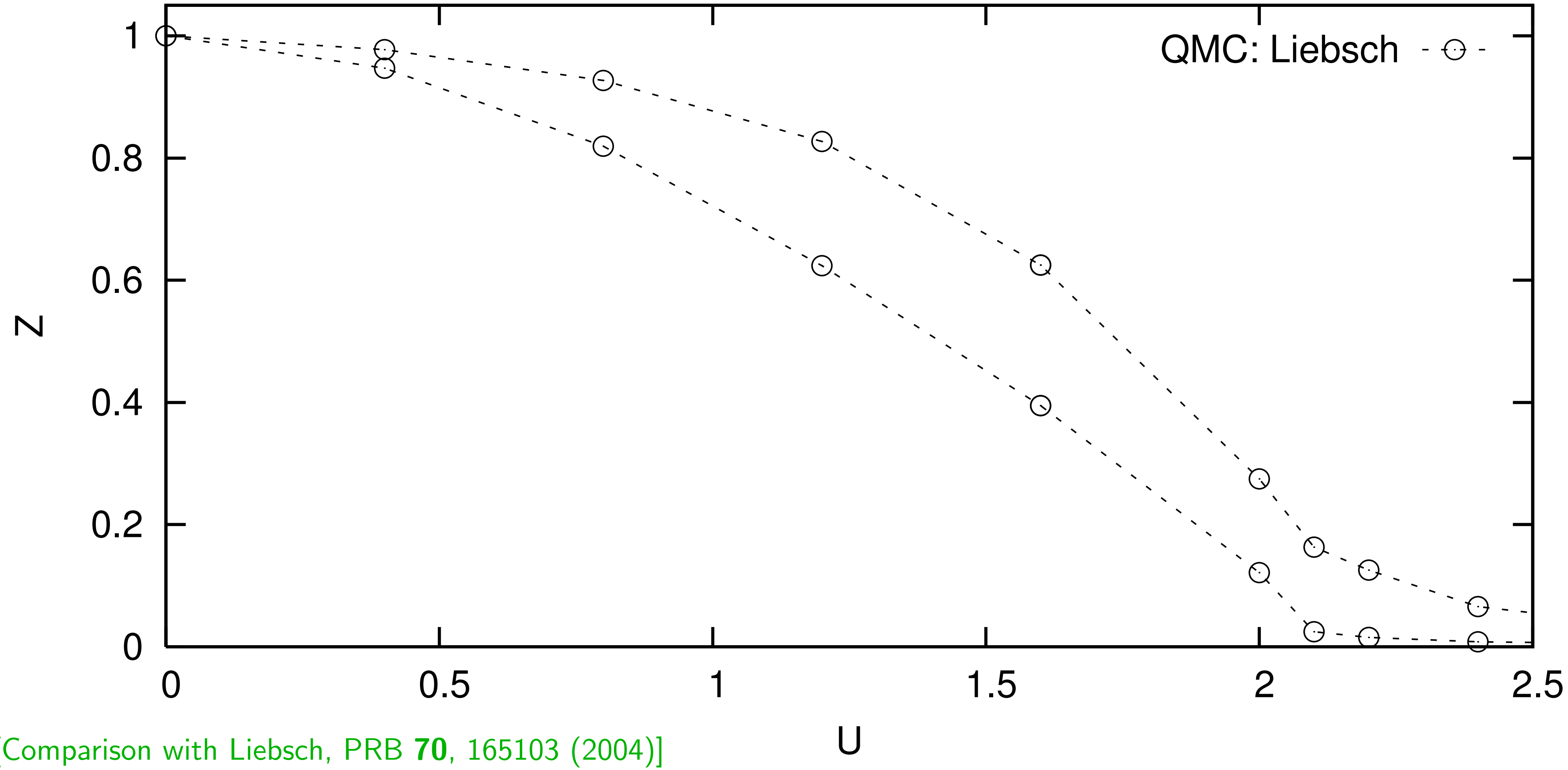


For Bethe DOS, $t_2 = 2\, t_1$: two 1^{st} order MITs for $U' = J_z = J_\perp = 0$

two distinct MITs for $J_z = J_\perp = U/4$

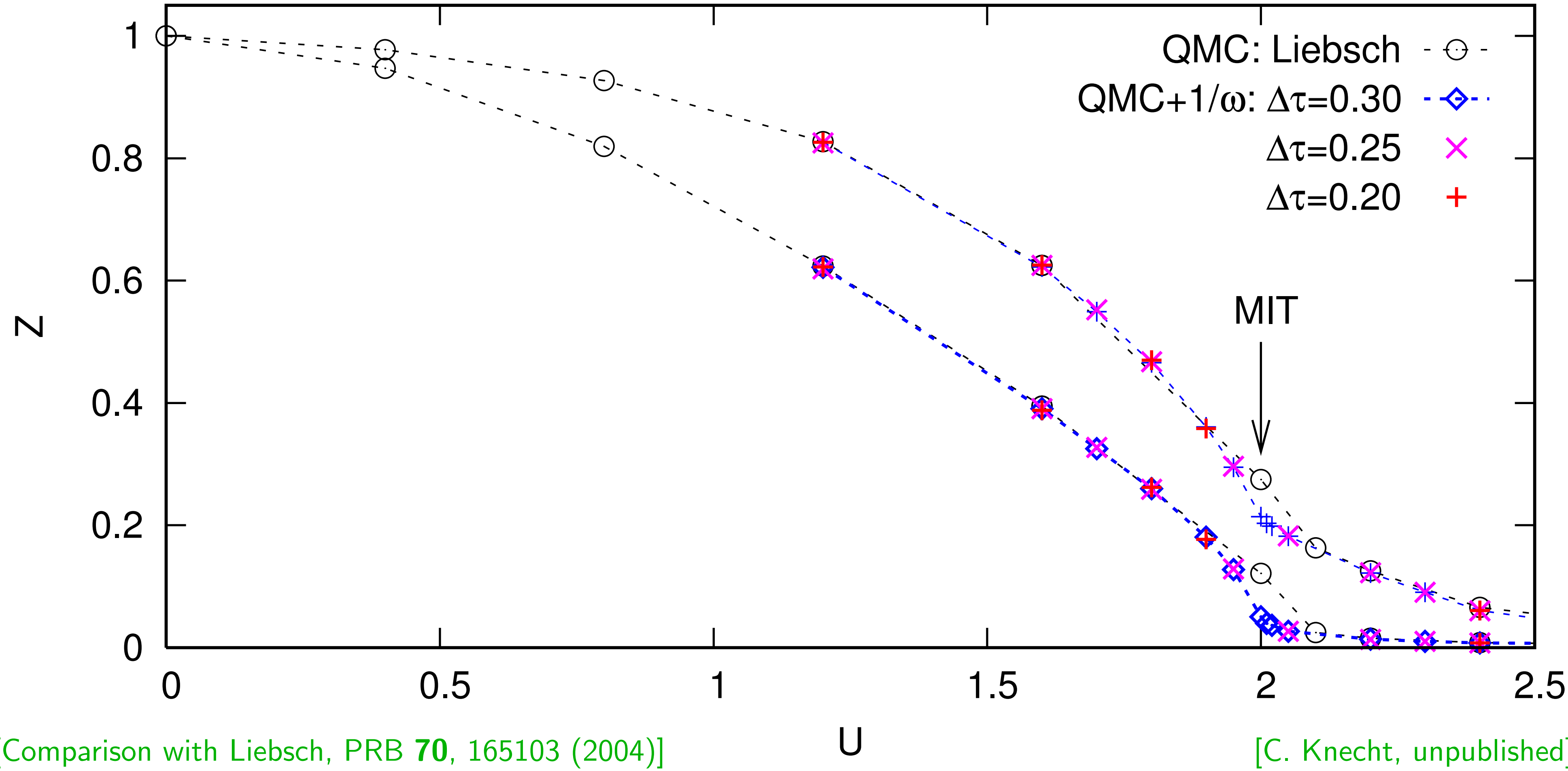
single MIT or **OSMTs** for $J_\perp = 0,\ J_z = U/4$ **?**

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



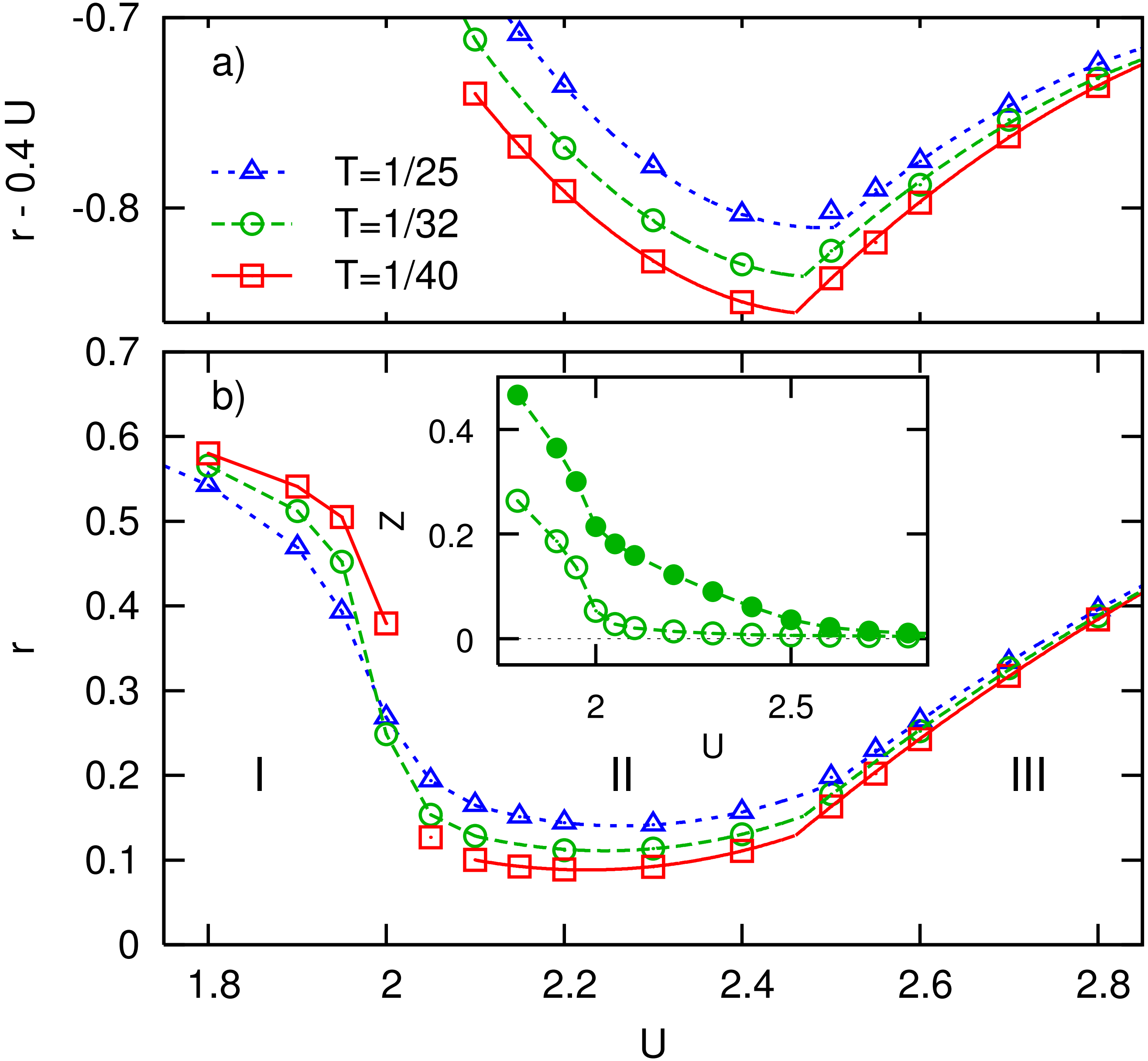
[Comparison with Liebsch, PRB **70**, 165103 (2004)] [C. Knecht, unpublished]

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?

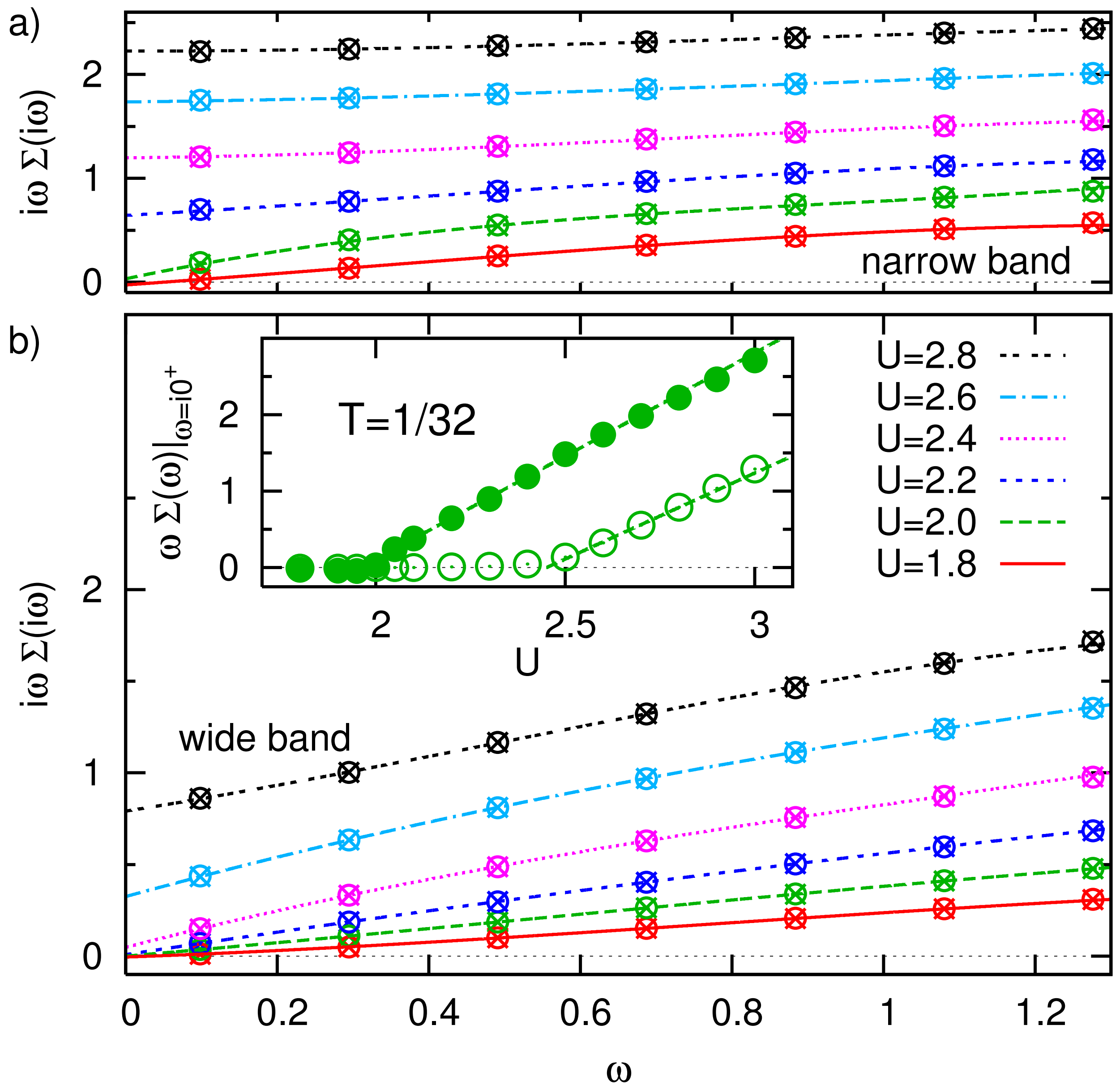
Ratio of quasiparticle weights $r = Z_{\text{narrow}}/Z_{\text{wide}}$



3 regions of different character

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

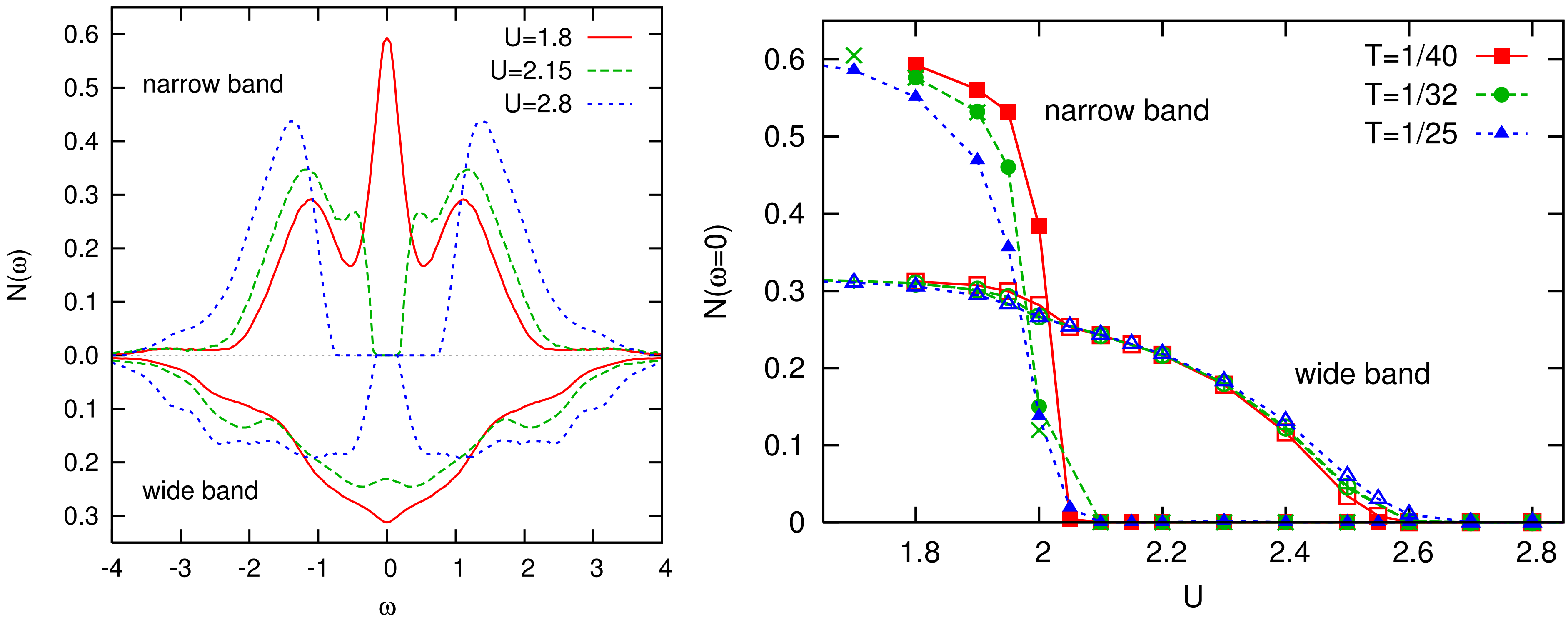
Low-frequency analysis of self-energy



for regular self-energy: $\omega\Sigma(\omega) \xrightarrow{\omega\to 0} 0$

singularities ($\sim$ gap) for $U > 2$, $U > 2.5$

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]

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

– Fourier transformation scheme crucial for reliability and efficiency

Mott transition in frustrated 1-band Hubbard model

High-precision ground state estimates from QMC

Orbital-selective Mott transition in 2-band Hubbard model

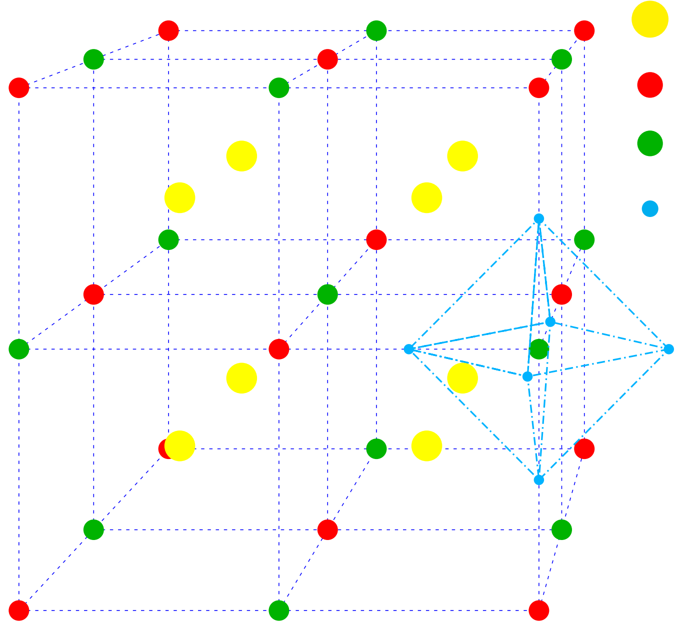
Outlook: realistic material-specific calculations with LDA+DMFT . . .

Thanks to: Carsten Knecht, Krunoslav Pozgajcic, Peter van Dongen

NIC Jülich, DFG (Bl775/1)

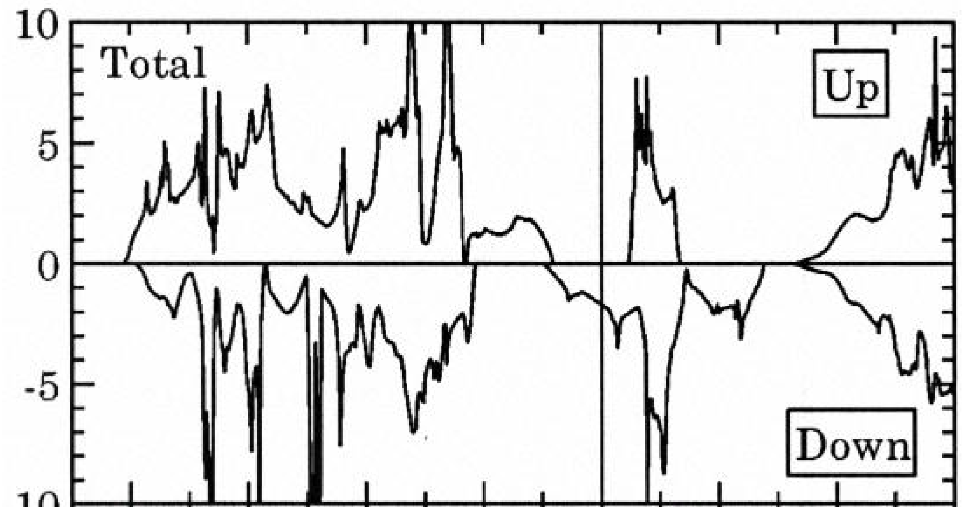
Outlook: theory of half-metallic double perovskites

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)]

$$H = \epsilon^f \sum_{i\alpha} n^f_{i\alpha} + \epsilon^m \sum_{i\alpha} n^m_{i\alpha} + \sum_{i,\,\alpha\neq\alpha'} U^f_{\alpha\alpha'}\, n^f_{i\alpha} n^f_{i\alpha'} + \sum_{j,\,\alpha\neq\alpha'} U^m_{\alpha\alpha'}\, n^m_{j\alpha} n^m_{j\alpha'}$$
$$+ \sum_{\langle ij\rangle\,\alpha} t^{fm} \left(f^\dagger_{i\alpha} m_{j\alpha} + \mathrm{hc}\right) + \sum_{\langle jj'\rangle\,\alpha} t^{mm}\, m^\dagger_{j\alpha} m_{j'\alpha} + \sum_{\langle ii'\rangle\,\alpha} t^{ff}\, f^\dagger_{i\alpha} f_{i'\alpha}$$

DPG research group 559 on "New materials with high spin polarization"

Speakers: Felser (Mainz), Hillebrands (Kaiserslautern)

List of projects

1	Felser	Synthesis: Heusler compounds
2	Jacob, Adrian	Thin films
3	Jourdan, Jacob, Adrian	Tunnel spectroscopy
4	Tremel	Synthesis: double perovskites
5	Elmers	Surface magnetization
6	Blümer, van Dongen	Theory of double perovskites: LDA+DMFT(QMC)
7	Schönhense, Felser	Spin resolved photoemission and DFT(LDA)
8	Ksenofontov, Felser	Mößbauer spectroscopy
9	Demokritov, Hillebrands	Brillouin light scattering spectroscopy
10	Aeschlimann, Bauer	Spectroscopy of unoccupied states (2PPE)

Additional material for discussions

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