Dynamical mean-field theory of Mott transitions and Mott insulators

Nils Blümer

Outline

Motivation: Mott transition in V_2O_3

Introduction: Hubbard Model, DMFT, QMC

Mott transition in frustrated 1-band Hubbard model

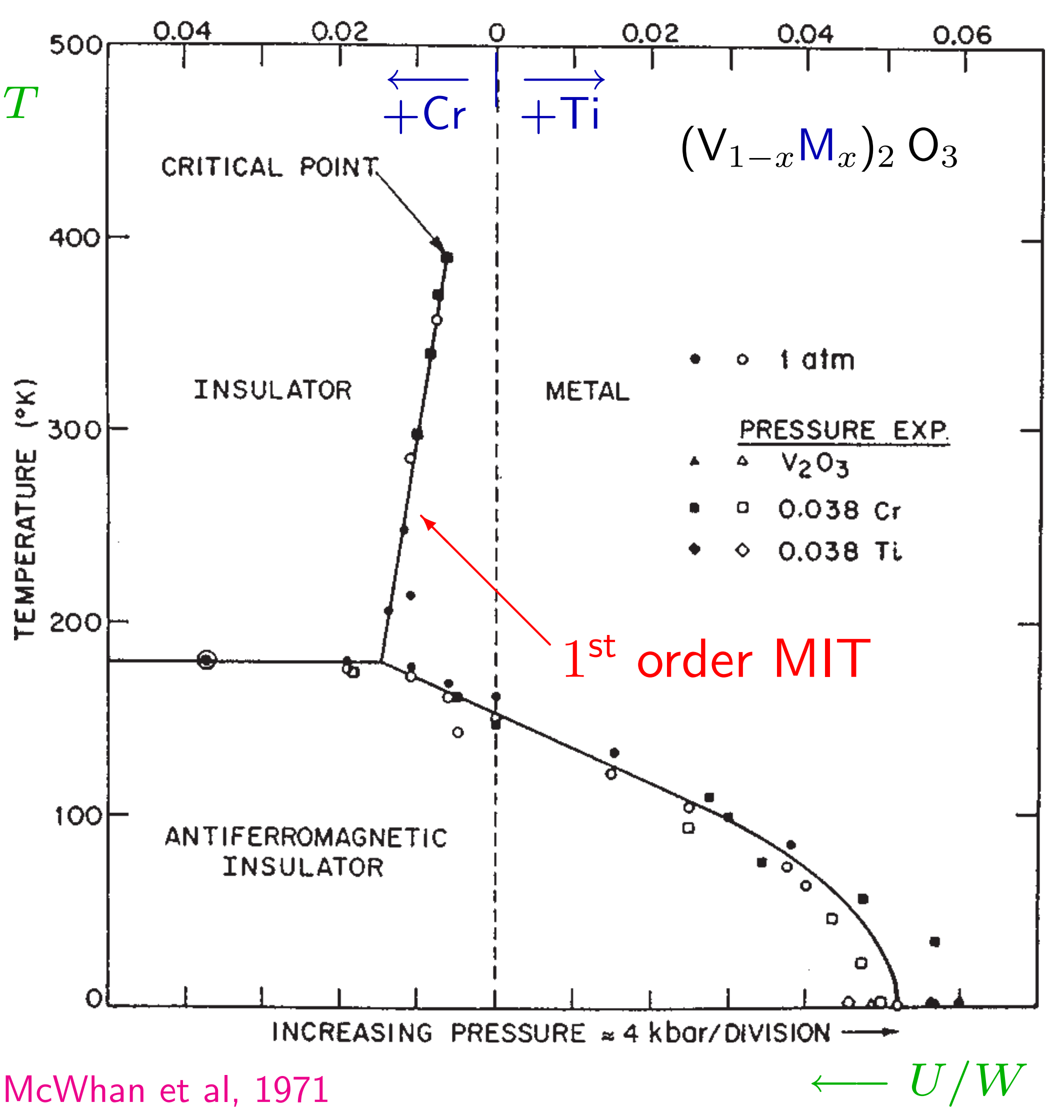
High-precision ground state estimates from QMC and ePT

Orbital-selective Mott transition in 2-band Hubbard model

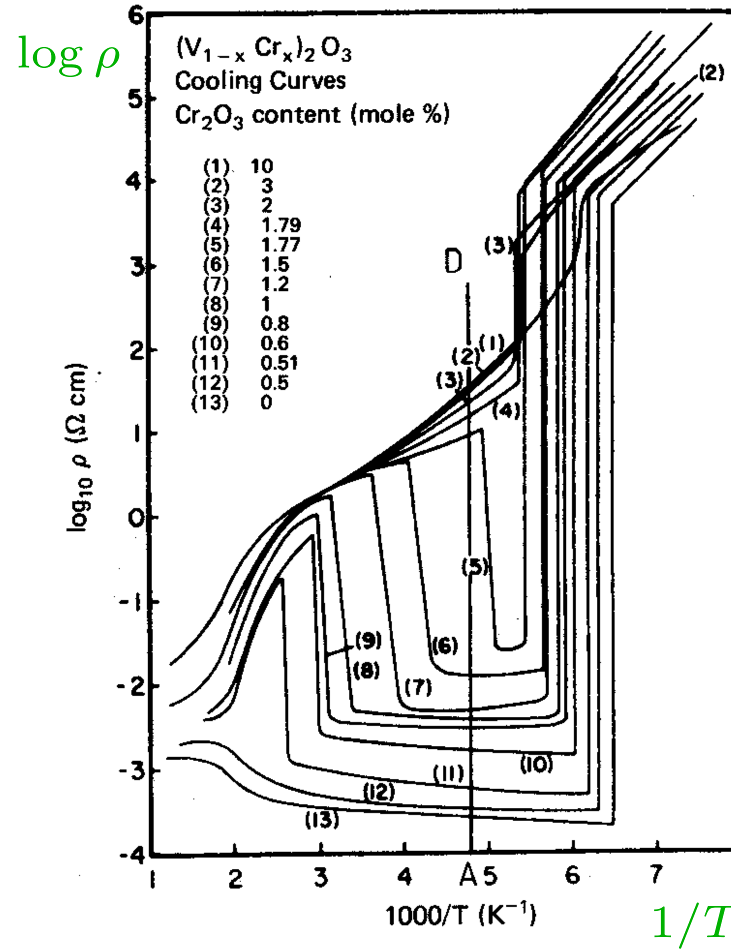
Summary and Outlook

Motivation

Prototype correlated system: V_2O_3

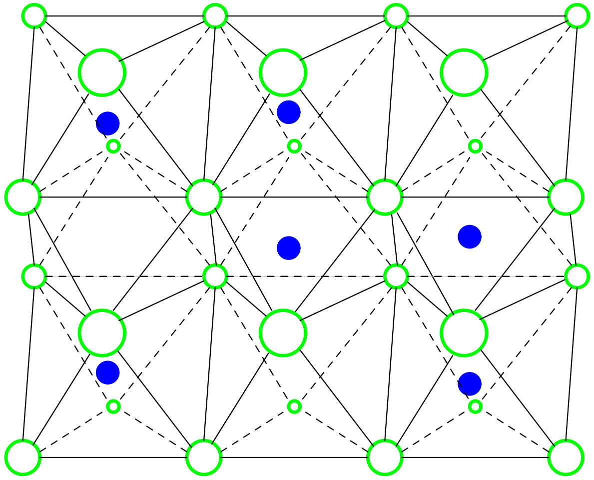


McWhan et al, 1971



Kawamoto et al, 1980

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



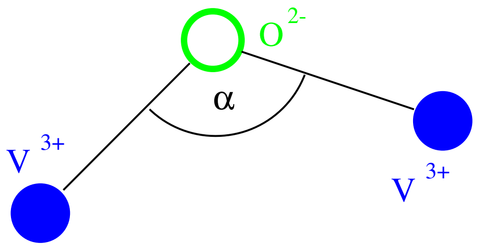
Corundum structure

Corundum structure:

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

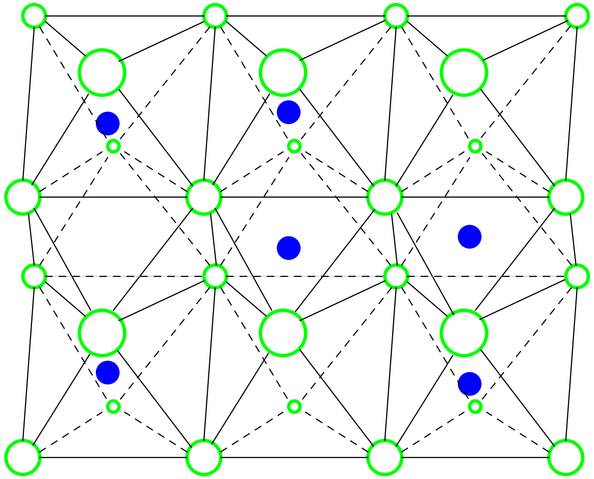
doping with Ti, Cr:

- (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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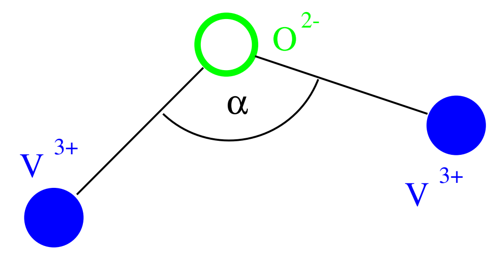

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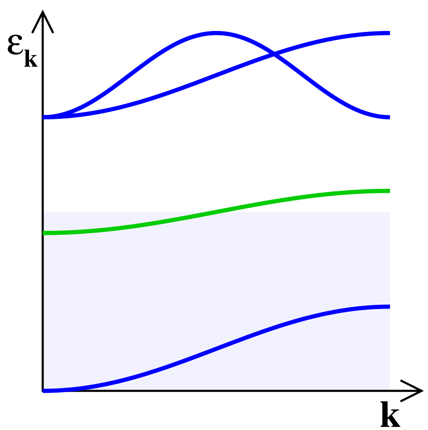
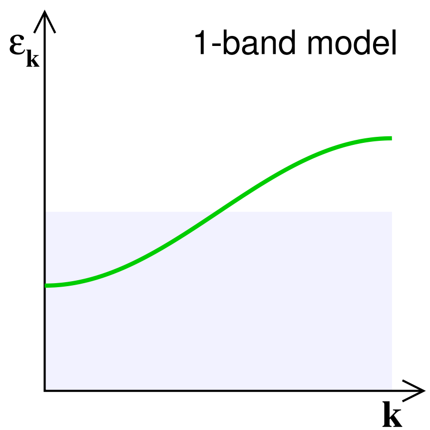
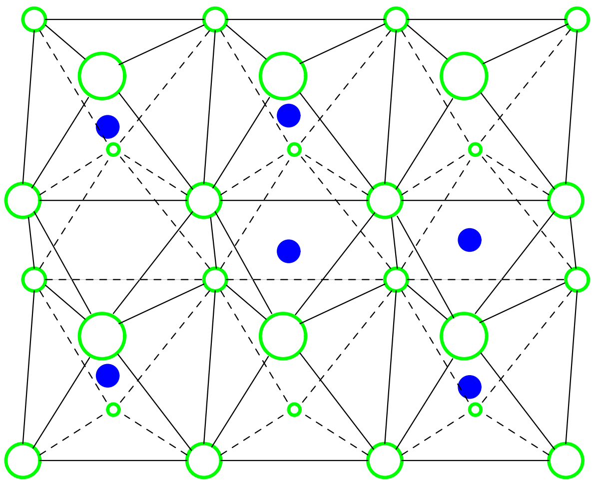
Paramagnetic, bandwidth-controlled metal-insulator transition in V_2O_3 $\longrightarrow$ microscopic model?

Bloch states near Fermi energy,







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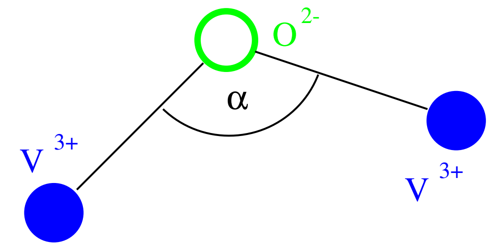

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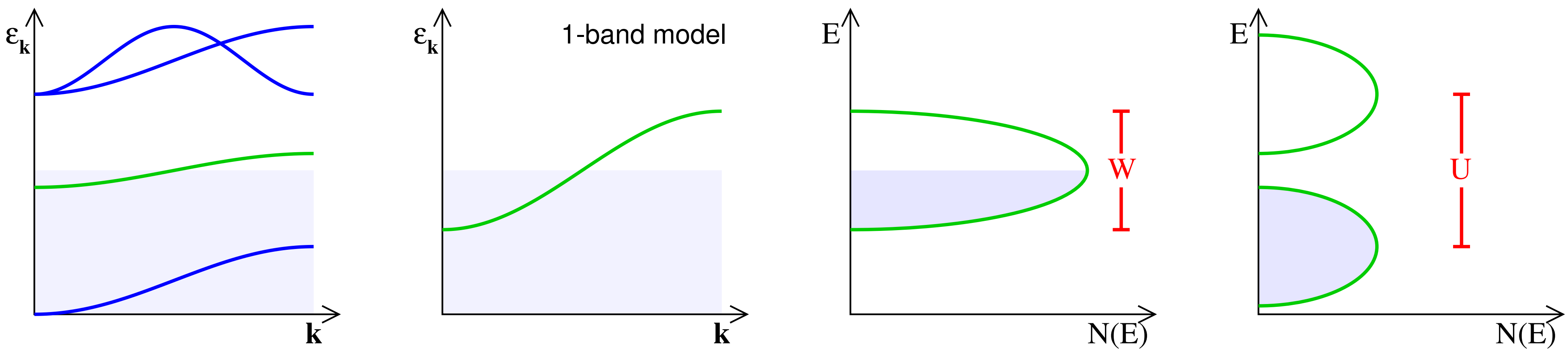
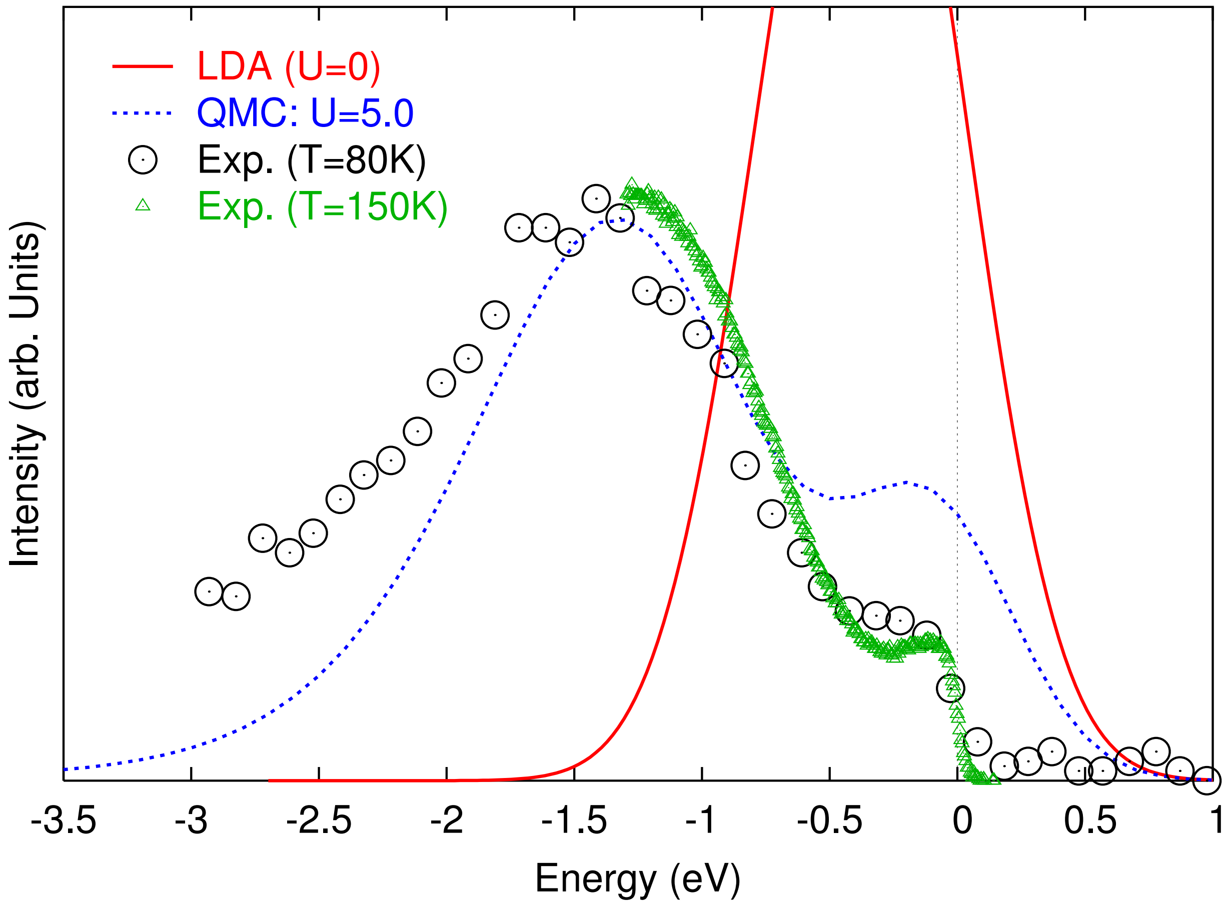
Paramagnetic, bandwidth-controlled metal-insulator transition in V_2O_3 $\longrightarrow$ microscopic model?

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



Paramagnetic Mott transition not captured by LDA band structure calculations!

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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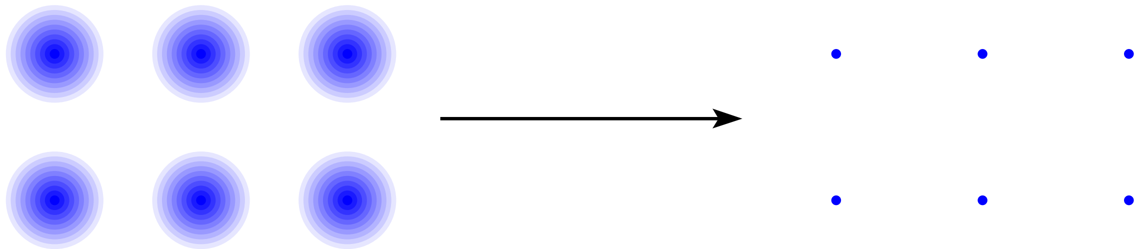
$$H = \sum_{i=1}^{N_e} \frac{\boldsymbol{p}_i^{\,2}}{2m} + \sum_{i} V(\boldsymbol{r}_i) + \sum_{i<j} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$$



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reduction to valence electrons ↓

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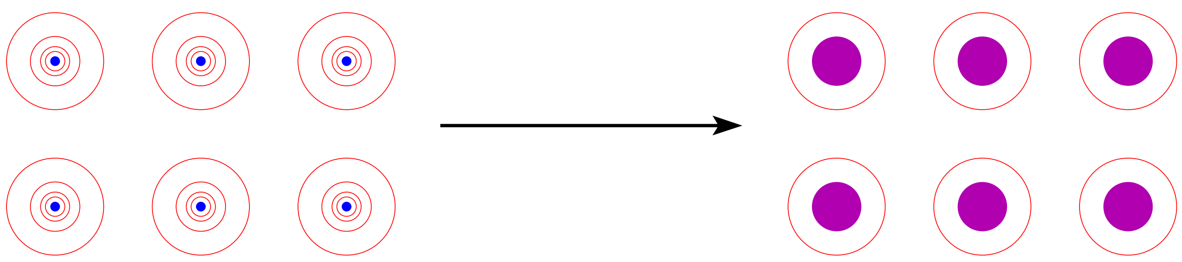

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occupation number formalism, Wannier orbitals ↓

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

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← **density functional theory (DFT)**

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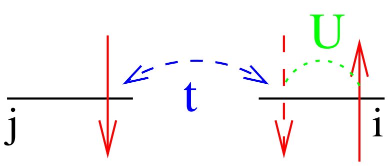
Hubbard model

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



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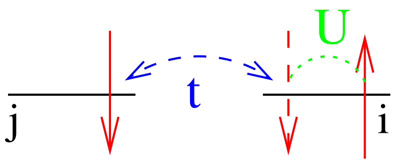

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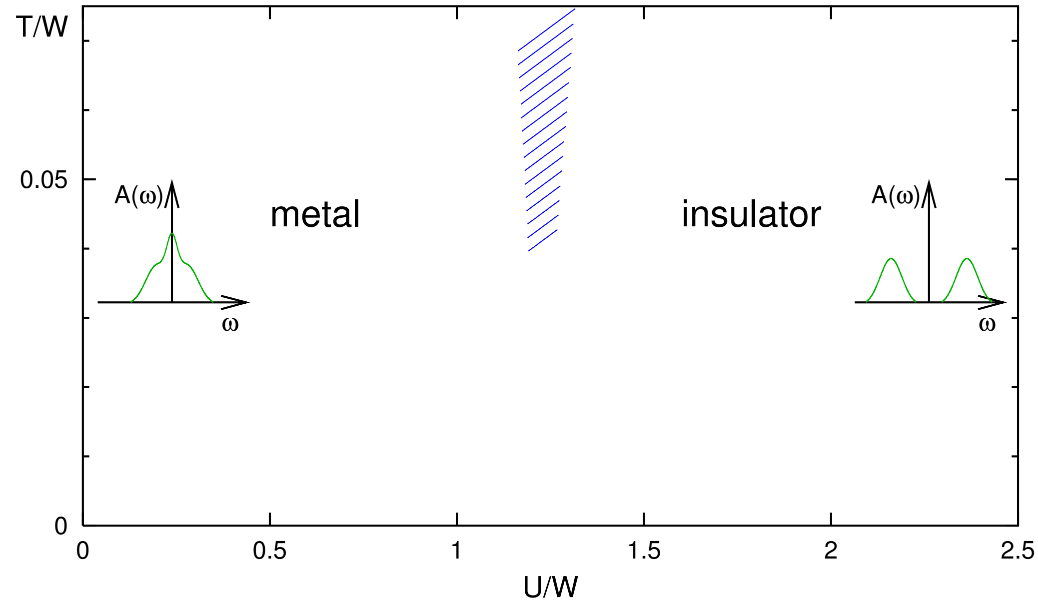
Minimal model for correlated electrons

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



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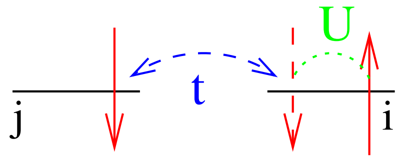

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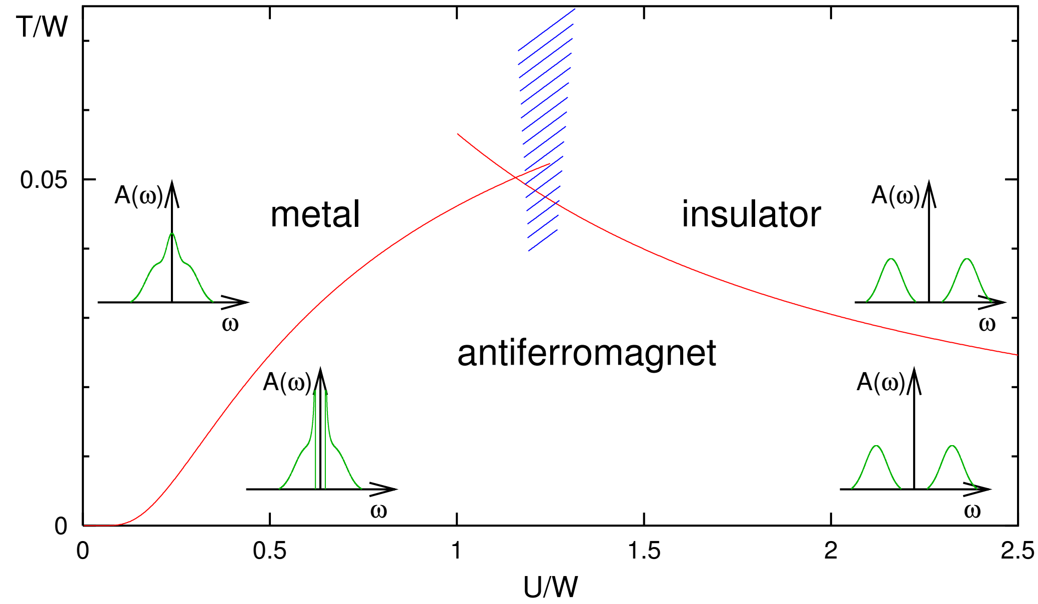
But: generically antiferromagnetism at low T



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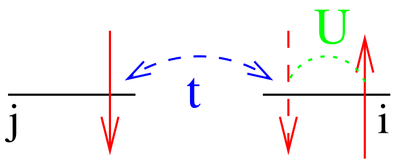

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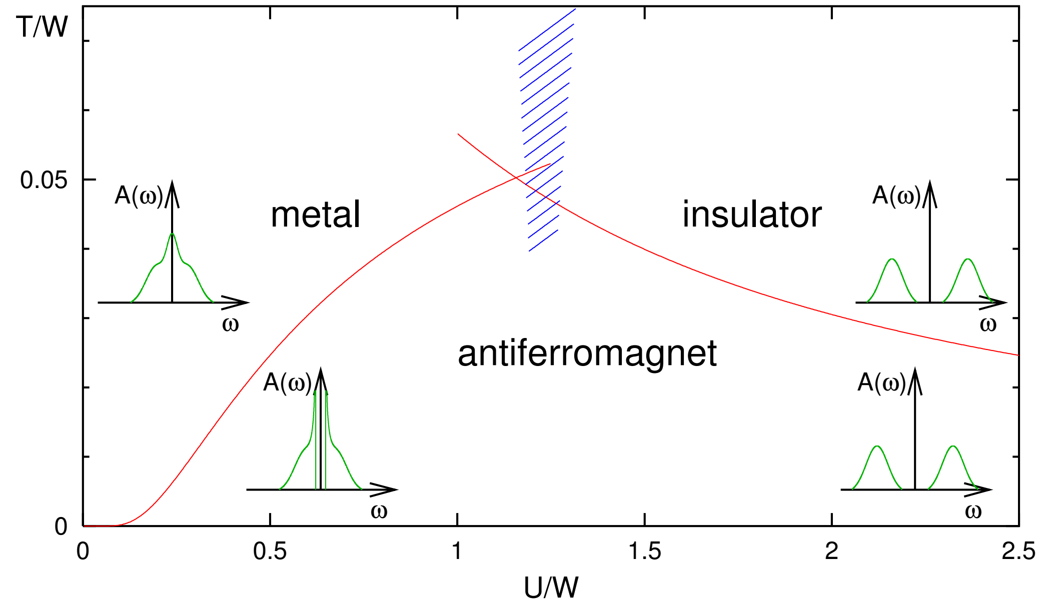

How to solve (frustrated) Hubbard model in regime of $W \sim U$?

Approaches for Hubbard-type models

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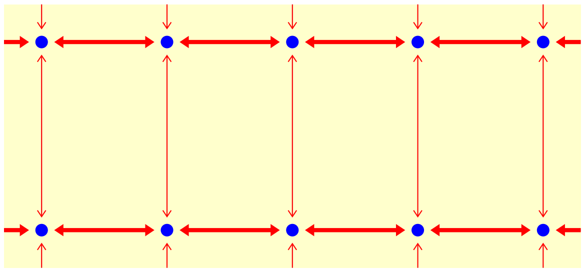
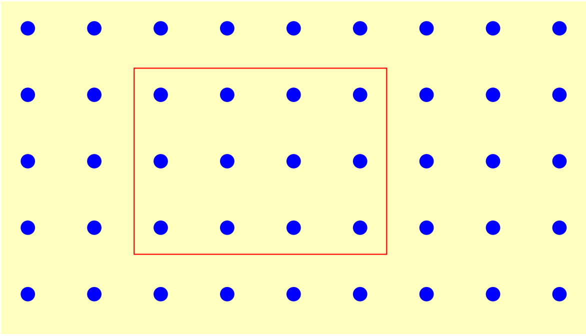
Perturbation theory, e.g.

- $U \longrightarrow 0$: 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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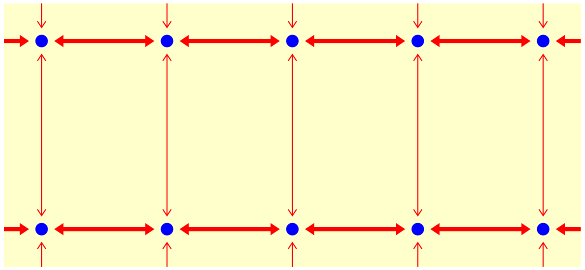

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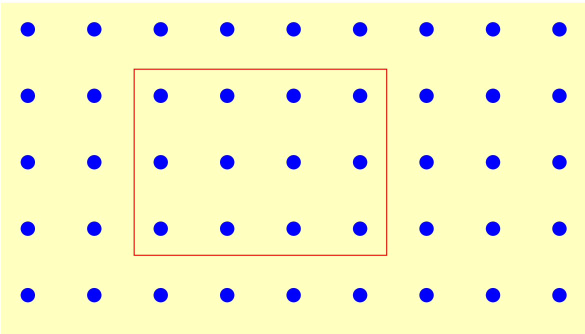

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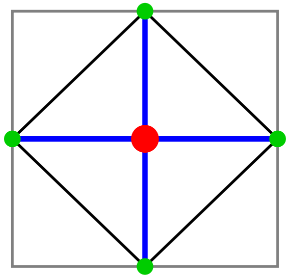
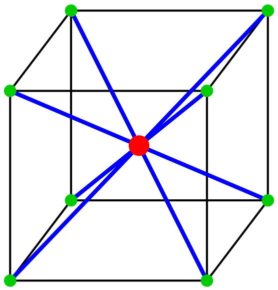
Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$

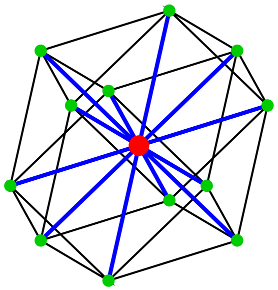
+ non-perturbative $\rightsquigarrow$ valid at MIT
+ dynamical on-site correlations preserved
+ in thermodynamic limit
+ exact for $Z \rightarrow \infty$



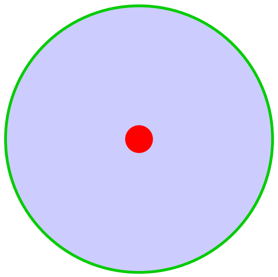
d=2: $Z = 4$



bcc: $Z = 8$



fcc: $Z = 12$



DMFT: $Z = \infty$

Iterative solution of DMFT equations

$$G(\tau) = -\langle \Psi \Psi^* \rangle_{\mathcal{G}[\tau]}$$

single-impurity problem

$\mathcal{G}$ $\uparrow$ G

$$\mathcal{G}^{-1}(i\omega_n) = G^{-1}(i\omega_n) + \Sigma(i\omega_n)$$

G $\downarrow$ impurity Dyson equation

$\Sigma \leftarrow \Sigma_0$

$$G(i\omega_n) = \int d\epsilon \, \frac{\rho(\epsilon)}{i\omega_n - \epsilon - \Sigma(i\omega_n)}$$

lattice Dyson equation

Impurity solver:

- Quanten-Monte-Carlo (QMC)
- Iterative perturbation theory (IPT; not controlled)
- Non-crossing approximation (NCA; not controlled)
- Numerical renormalization group (NRG; 1-2 bands)

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- Iterative perturbation theory (IPT; not controlled)
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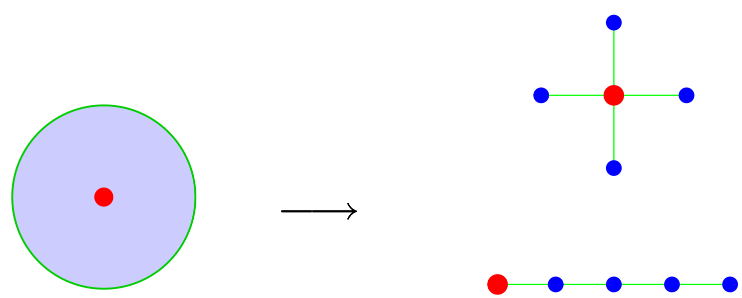
- Numerical renormalization group (NRG; 1-2 bands)
- Exact diagonalization (ED; large finite-size errors)
- Density matrix renormalization group (DMRG)
- Self-energy functional theory (SFT) + ED



Direct $d = \infty$ solution: PT, ePT

Hirsch-Fye QMC algorithm for DMFT impurity problem

Green-Funktion G in imaginary time (fermionic Grassmann variables ψ, ψ^*):

$$\begin{aligned} G_\sigma(\tau_2 - \tau_1) \equiv G_\sigma(\tau_1, \tau_2) &= \frac{1}{\mathcal{Z}} \int \mathcal{D}[\psi]\,\mathcal{D}[\psi^*]\ \psi_\sigma(\tau_1)\psi^*_\sigma(\tau_2)\ e^{\mathcal{A}}\,, \\ \mathcal{A} &= \mathcal{A}_0 - \frac{U}{2}\sum_{\sigma\sigma'}\int_0^\beta d\tau\,\psi^*_\sigma(\tau)\psi_\sigma(\tau)\psi^*_{\sigma'}(\tau)\psi_{\sigma'}(\tau) \end{aligned}$$

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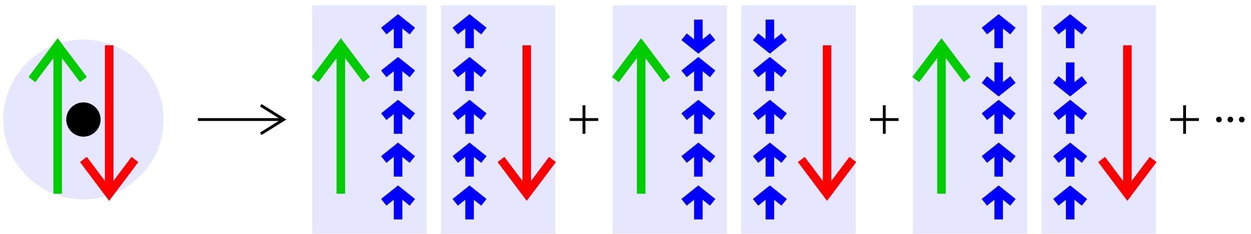
discretization $\beta = \Lambda\,\Delta\tau$, Trotter decoupling, discrete Hubbard-Stratonovich transformation



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}

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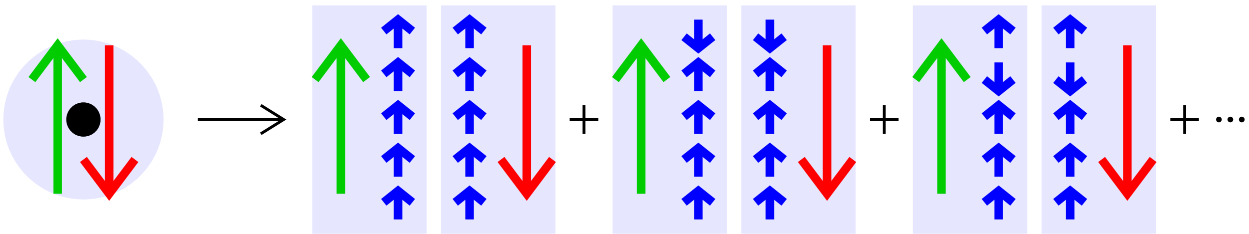

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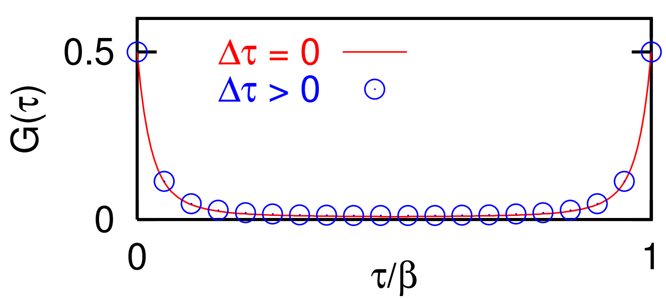
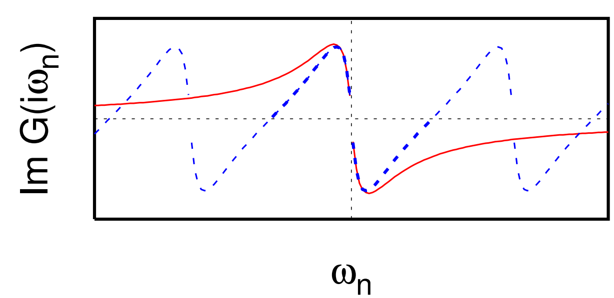
− effort scales as T^{-3}
− no info for $\omega \gtrsim \omega_{\text{Nyquist}}$





Mott transition in frustrated 1-band Hubbard model

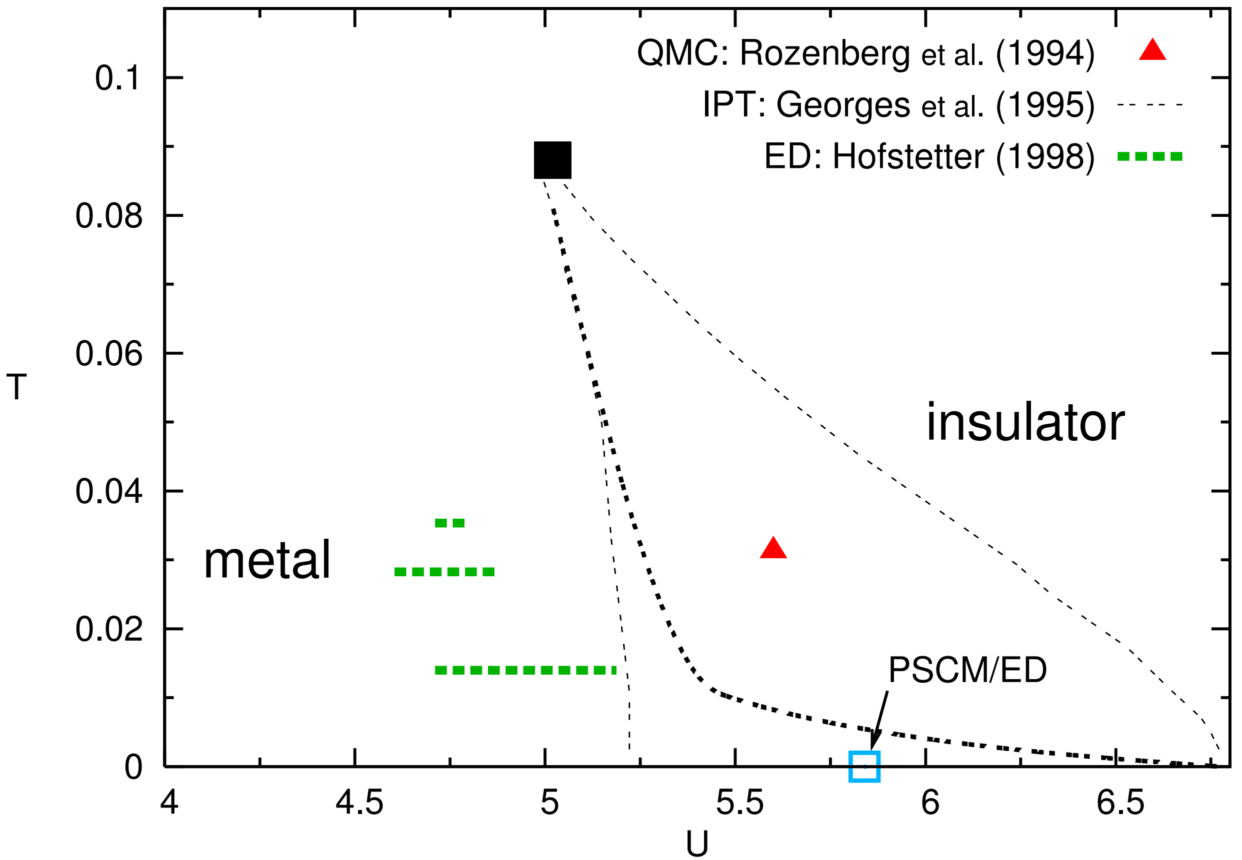
Controversy in 1999:

1st order MIT ("Bethe" DOS)?

Hysteresis in DMFT cycle?

Coexistence of metal + insulator?

- IPT, ED: yes!



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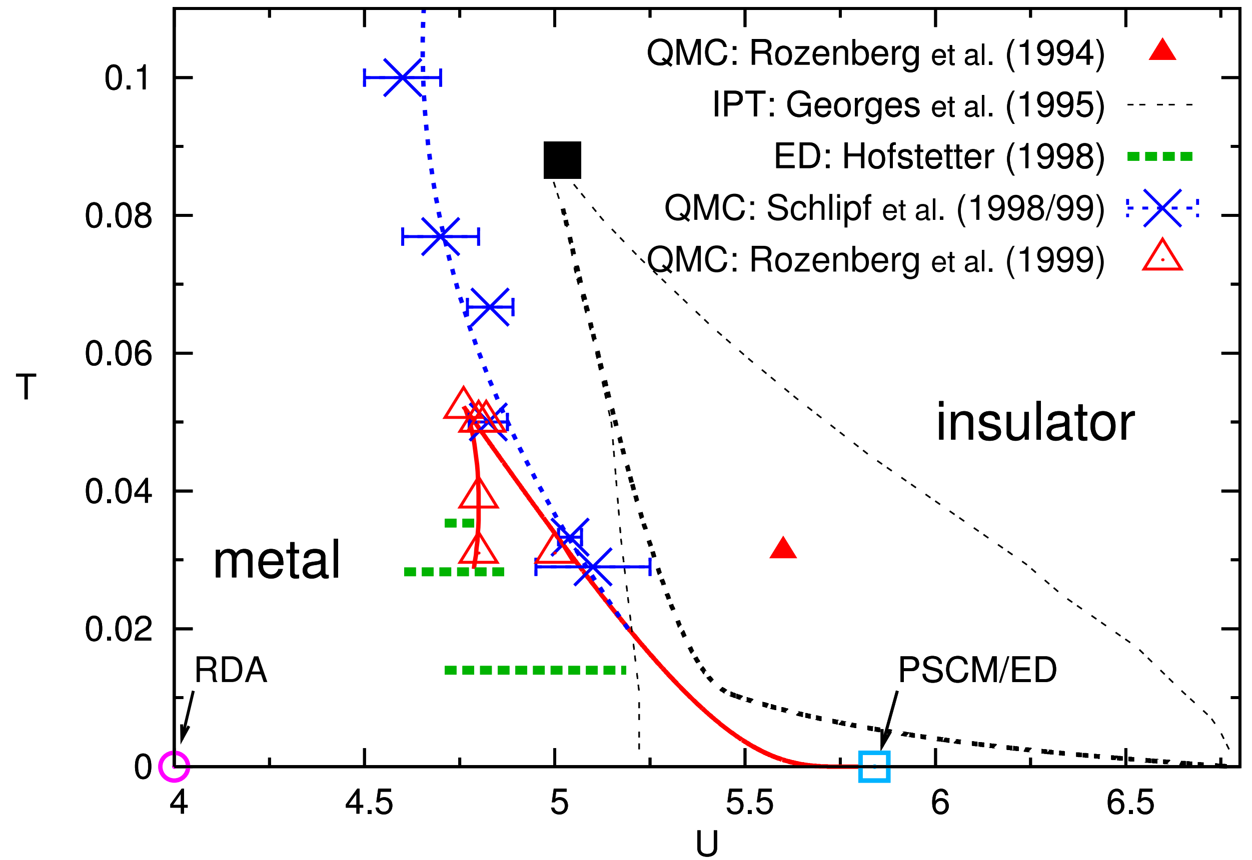
Controversy in 1999:

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?

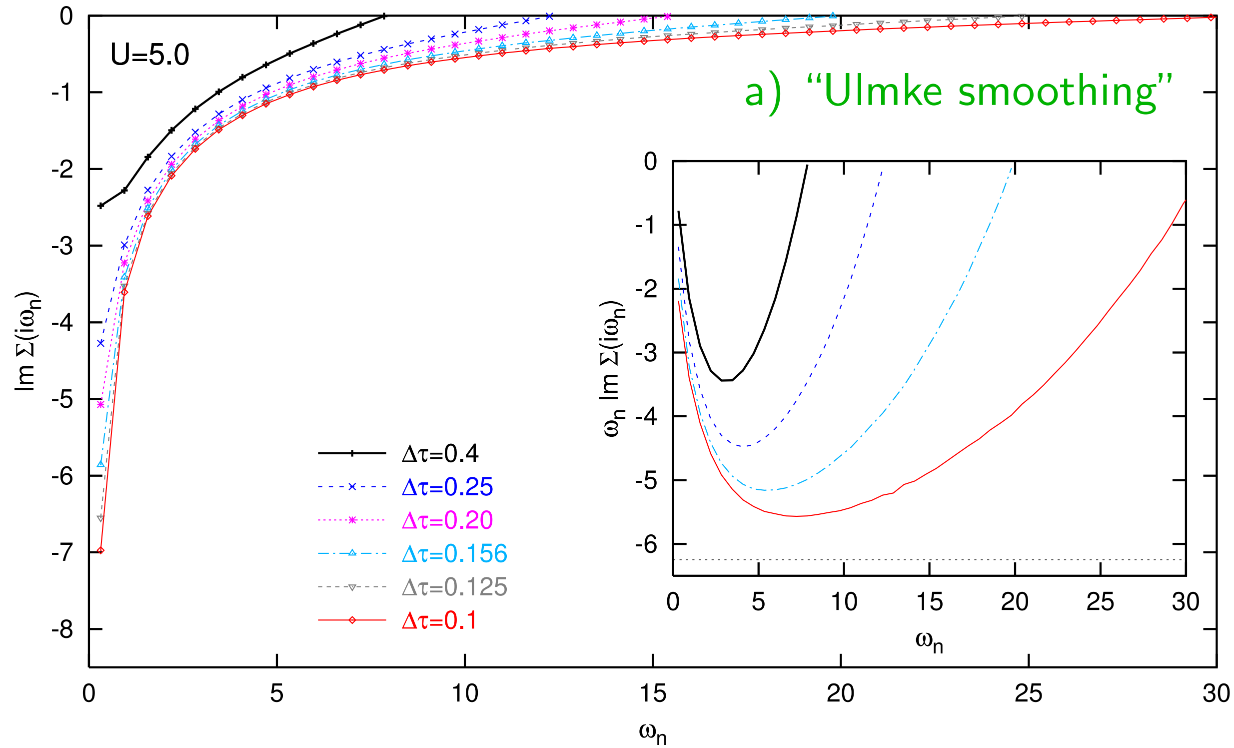
Impact of Fourier transformation schemes in DMFT-QMC:

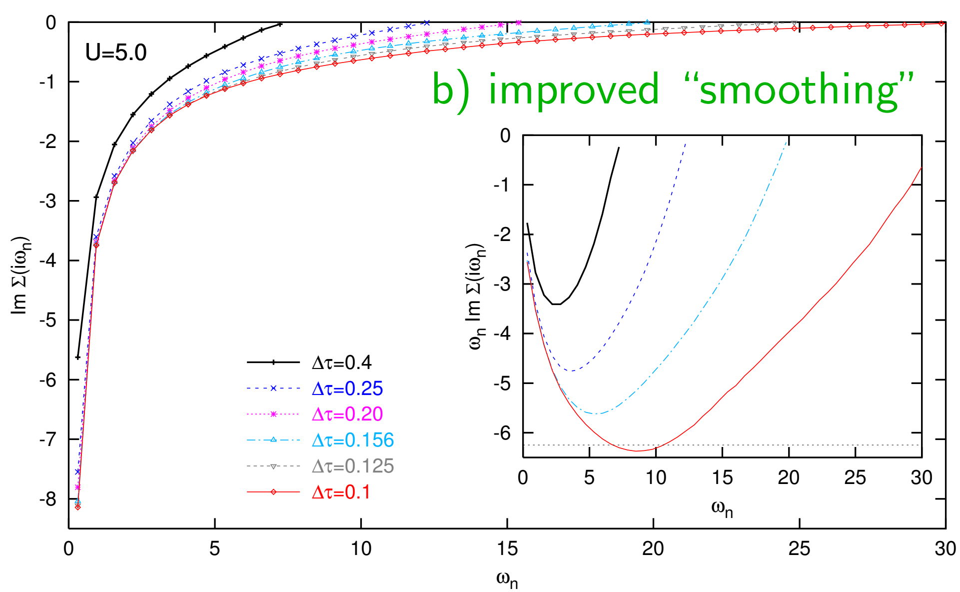
self-energy Σ $(T = 0.1, U = 5.0)$

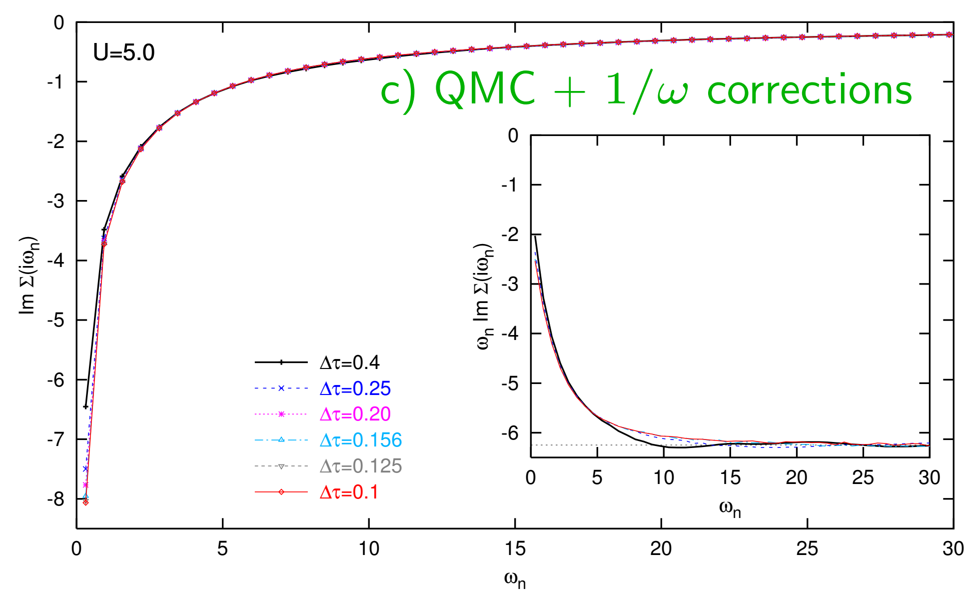
large errors even for $\omega \longrightarrow 0$ in a)

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

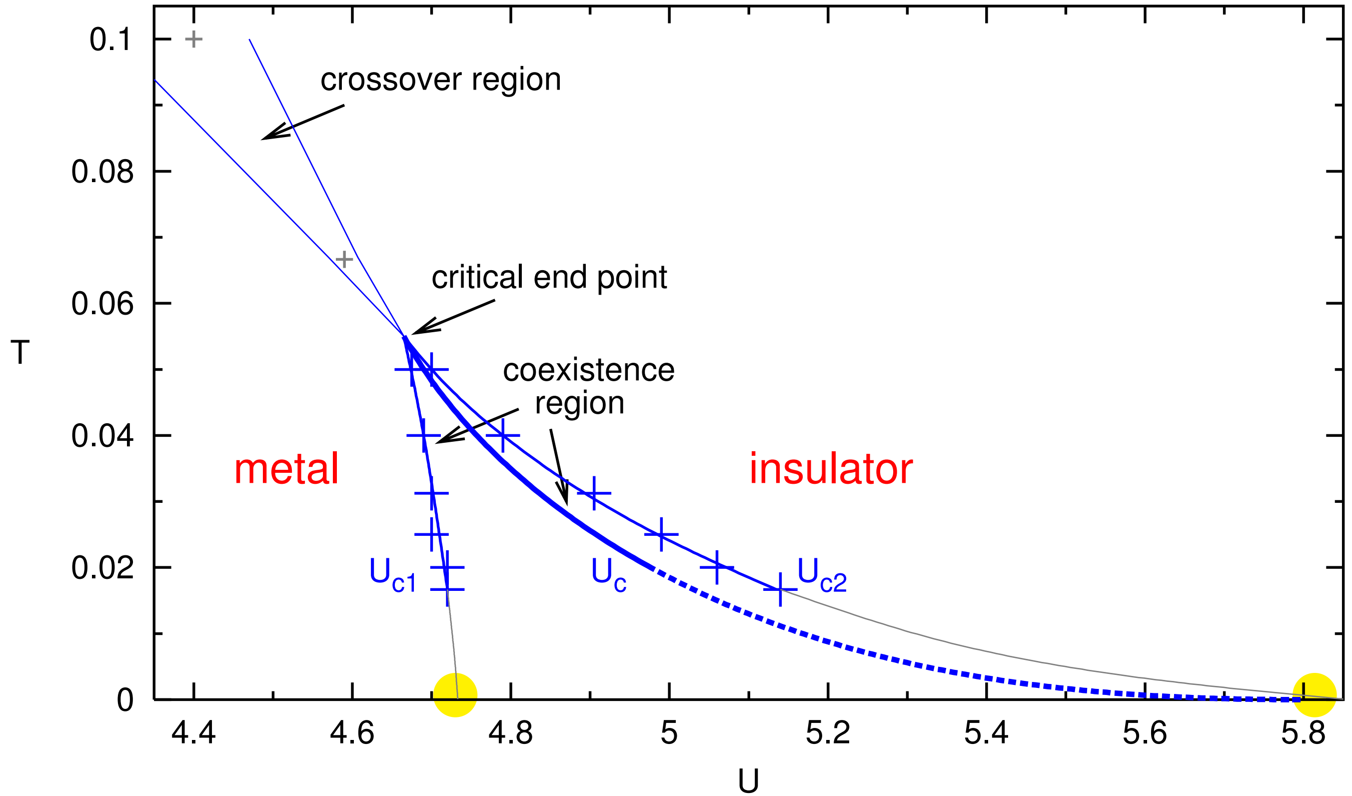
correct $\omega \longrightarrow \infty$ asymptotics in c)







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)

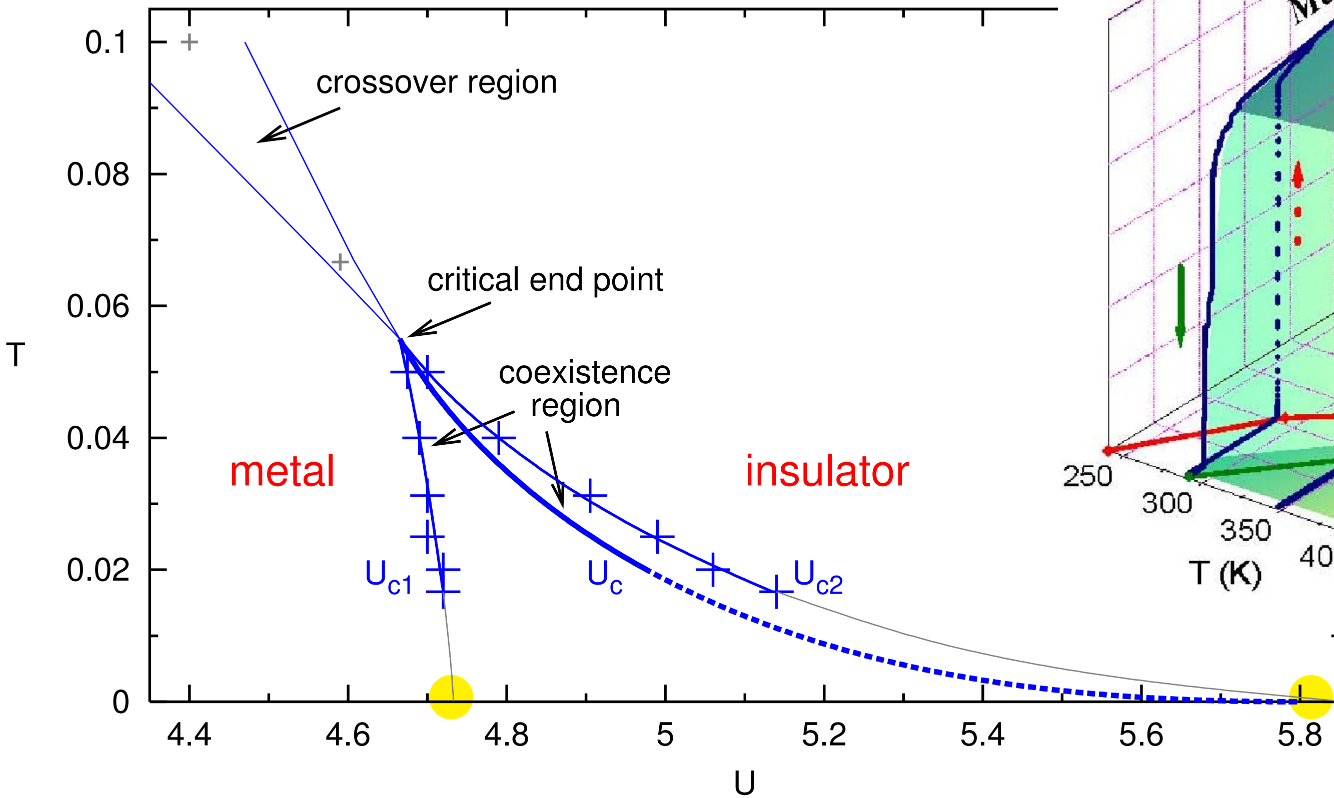
Blümer (2000, 2002)

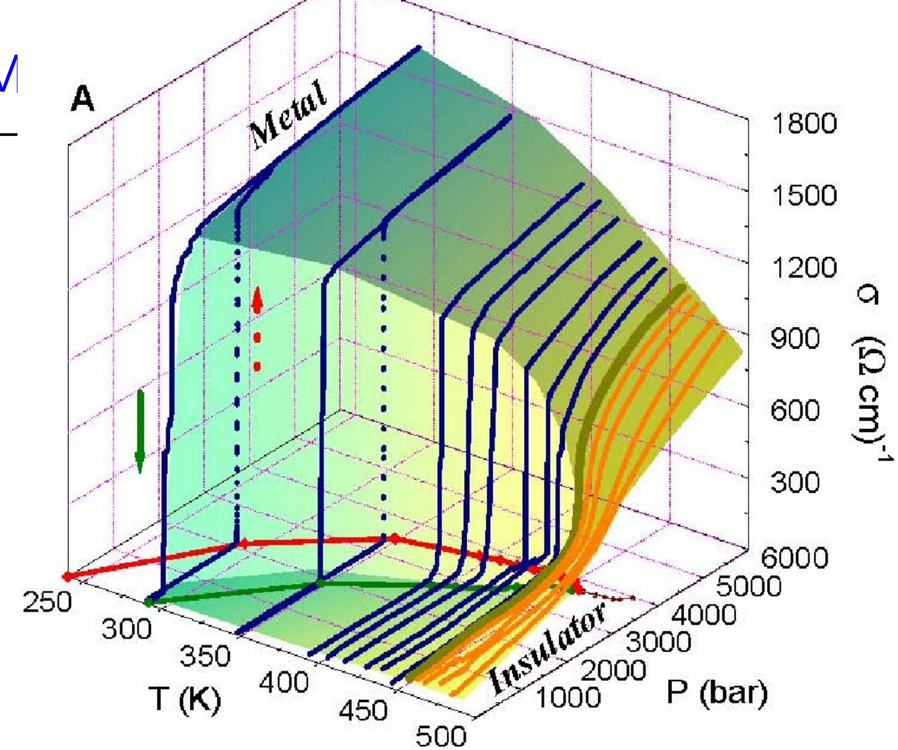
1^{st} order line from $$\frac{\mathrm{d}U_c(T)}{\mathrm{d}T} = f(T, U_c(T)); \quad f(T,U) := \frac{\Delta E(T,U)}{T\,\Delta D(T,U)}$$

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

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

Frustrated 1-band Hubbard model: 1^{st} order M





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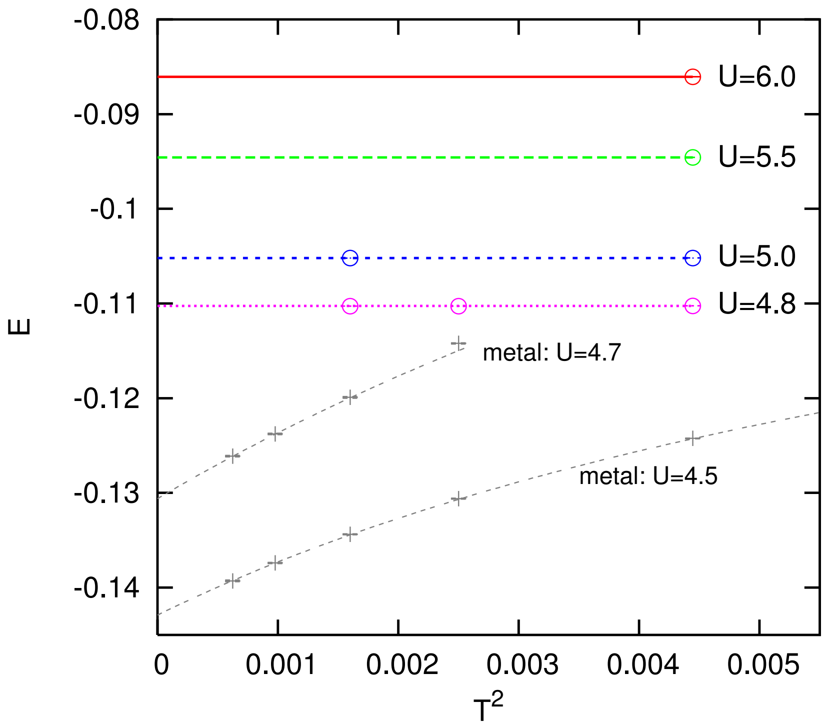
High-precision ground state estimates from QMC and ePT

Energy E and double occupancy D
for Mott insulator

High-precision quantum Monte Carlo

$$\left.\begin{array}{l}\Sigma(\omega) = \frac{U^2}{4\omega} + \mathcal{O}(\omega^{-2}) \\ 40 \times 10^7 \text{ sweeps} \\ \text{careful } \Delta\tau \text{ extrapolation}\end{array}\right\} \quad \begin{array}{l}\Delta E \approx 10^{-5} \\ \Delta D \approx 10^{-5}\end{array}$$

nearly negligible T-dependence for Mott insulator



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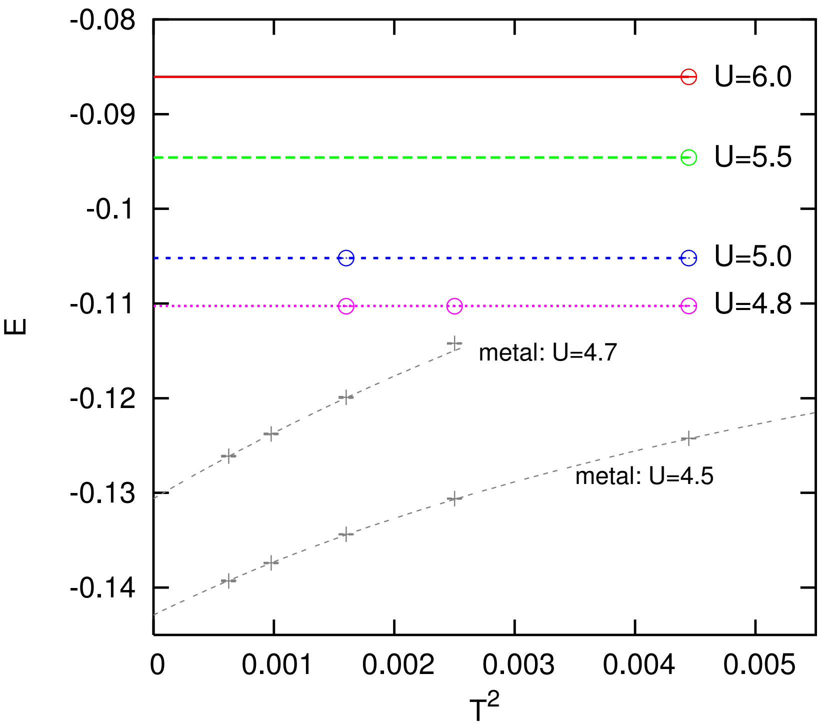

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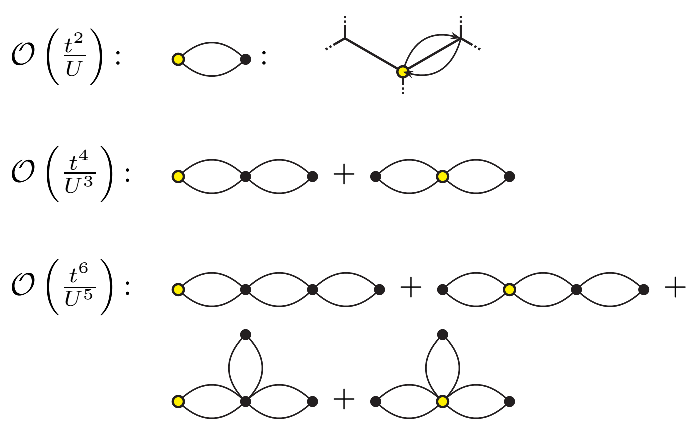
10^{th} order Kato-Takahashi perturbation theory at $T = 0$:

$$E_{\text{PT}}(U) = -\frac{1}{2\,U} - \frac{1}{2\,U^3} - \frac{19}{8\,U^5} - \frac{593}{32\,U^7} - \frac{23877}{128\,U^9}$$

accurate at $U \gtrsim 6$: $\Delta E_{\text{PT}} \leq 10^{-5}$, $\Delta D_{\text{PT}} \leq 10^{-5}$



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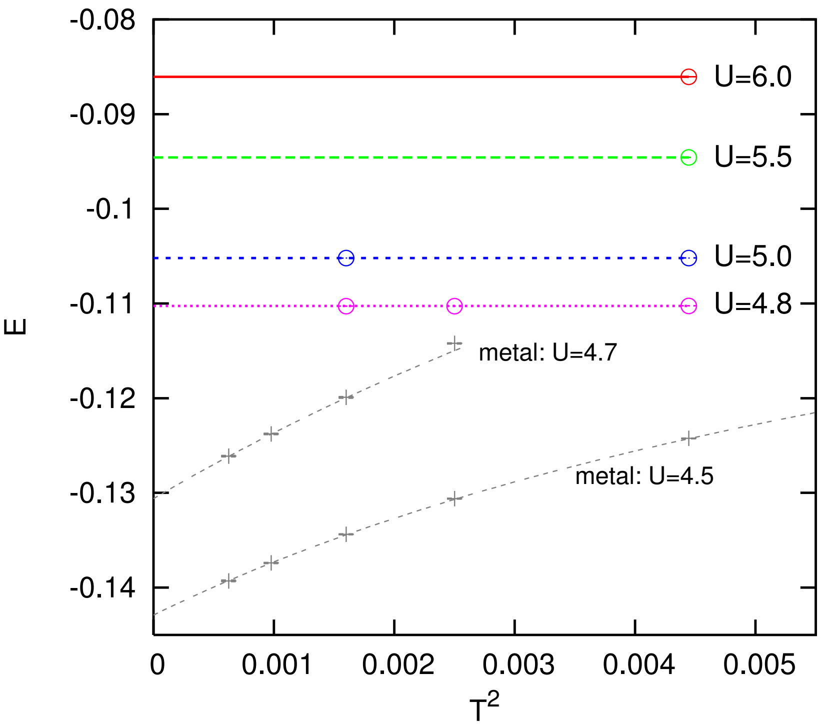

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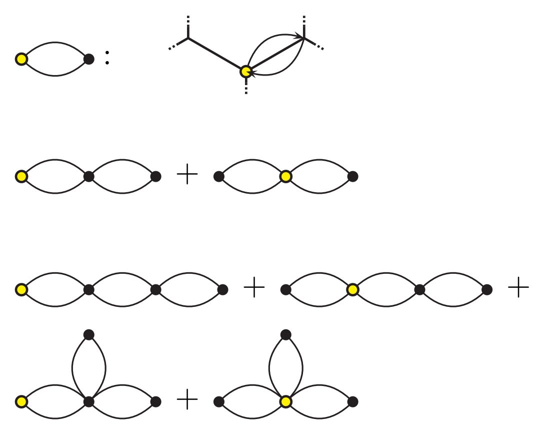
ratios of coefficients: 1 4.8 7.8 10.1

accurate at $U \gtrsim 6$: $\Delta E_{\text{PT}} \leq 10^{-5}$, $\Delta D_{\text{PT}} \leq 10^{-5}$

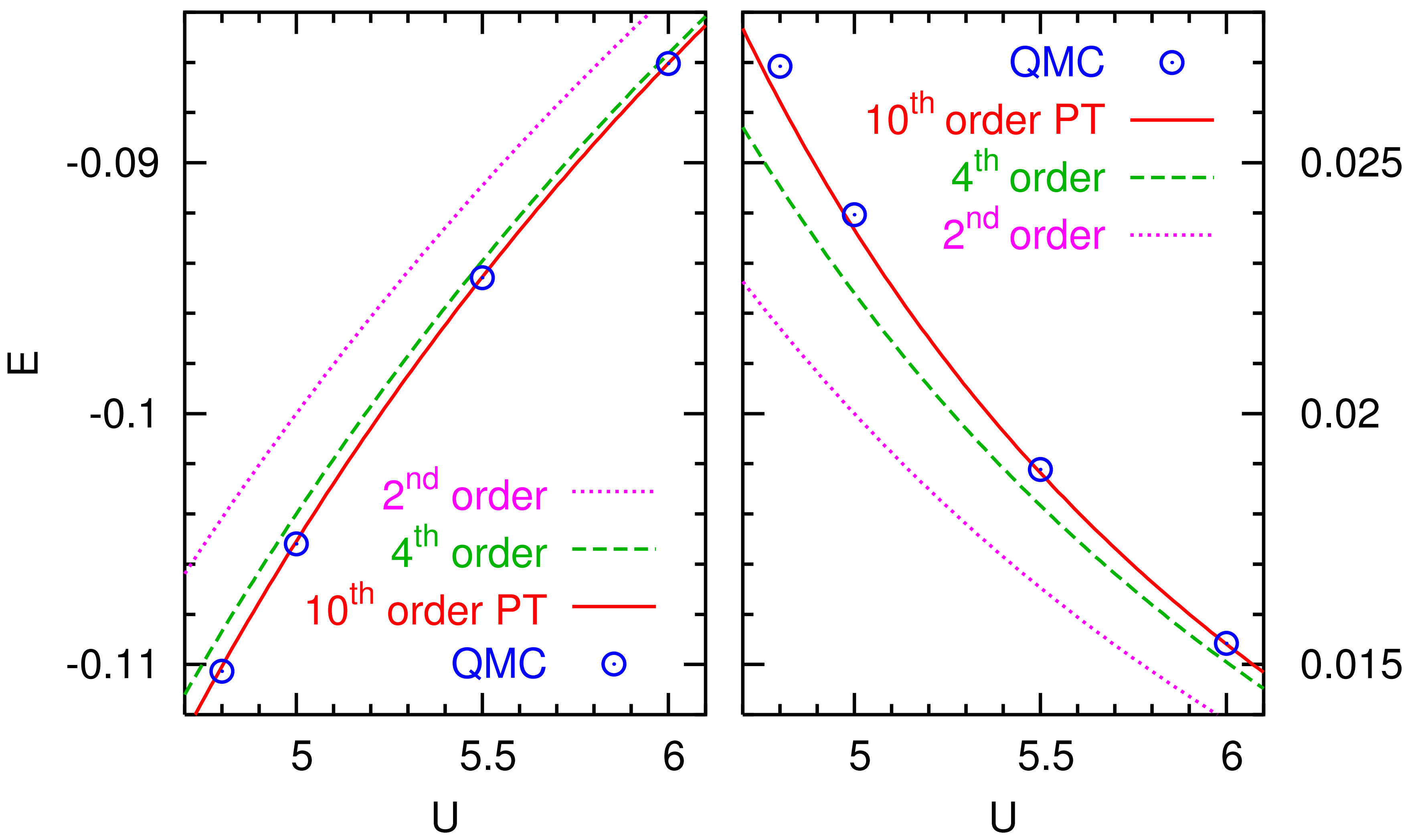
$\mathcal{O}\left(\frac{t^2}{U}\right)$:

$\mathcal{O}\left(\frac{t^4}{U^3}\right)$:

$\mathcal{O}\left(\frac{t^6}{U^5}\right)$:



Mott insulator: energy + double occupancy (QMC+$1/\omega$ vs. PT)



Excellent agreement at $U = 6.0$, deviations below. **continuous fit + critical behavior?**

Extended perturbation theory: ePT

Extrapolate coefficients in PT series

$$E_{\mathsf{PT}} = \sum_{i=1}^{\infty} a_{2i}\, U^{1-2i}$$

by fitting ratios $U_{c1}[2i] \equiv \sqrt{a_{2i+2}/a_{2i}}$.

to $U_{c1}[n] \approx U_{c1} + u_1\, n^{-1} + u_2\, n^{-2}$

General consequences:

$$U_{c1} \;=\; \lim_{i\to\infty} U_{c1}[2i]$$

$$a_n \;\propto\; n^{\tau}\, U_{c1}^{n}; \qquad \tau = -\tfrac{u_1}{U_{c1}}$$

$$E(U) \;\propto\; (U - U_{c1})^{\tau - 1}$$

$$D(U) \;\propto\; (U - U_{c1})^{\tau - 2}$$

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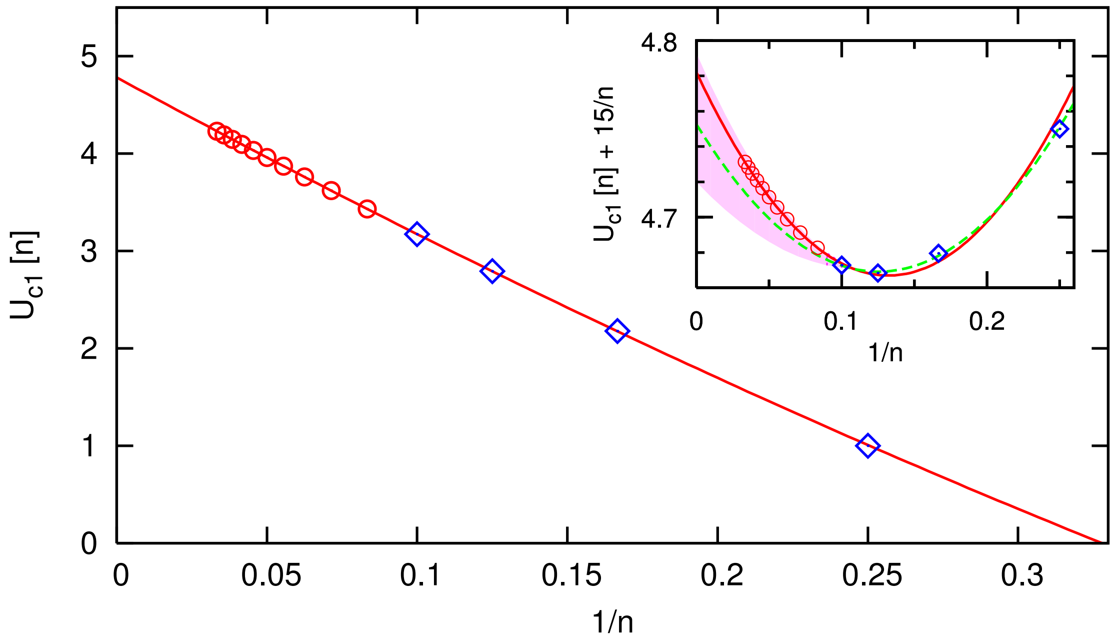

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$$E(U) \;\propto\; (U - U_{c1})^{\tau-1}$$

$$D(U) \;\propto\; (U - U_{c1})^{\tau-2}$$

Specifics / numerical results of extrapolation:

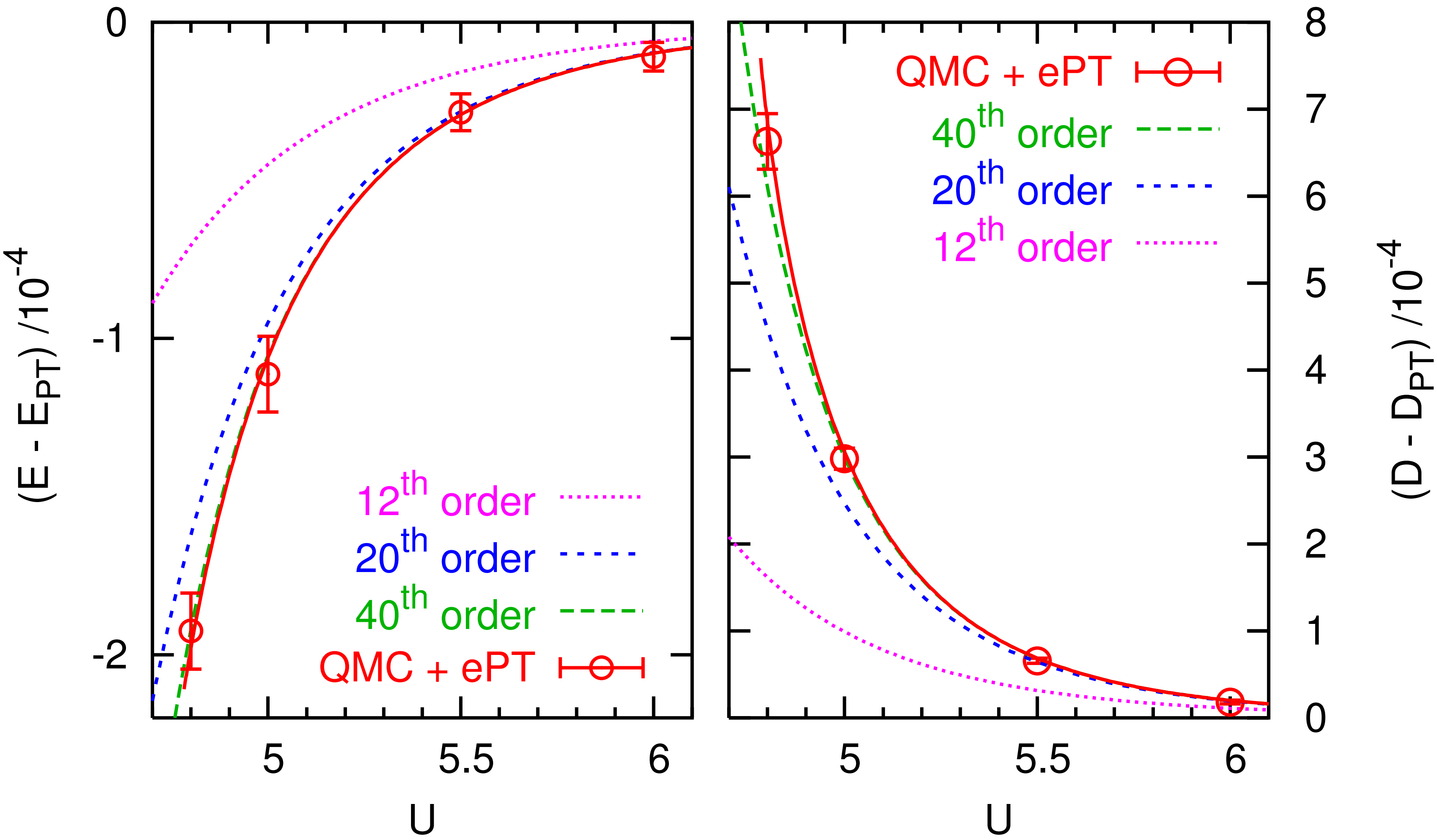
Unrestricted quadratic fit (dashed) $\rightsquigarrow$ $\tau \approx 3.44$, $U_{c1} \approx 4.75$

Comparison of $E(U)$, $D(U)$ with QMC $\rightsquigarrow$ $3.36 \leq \tau \leq 3.53$

Half-integer exponents likely for (dynamical) mean-field theory

Assume $\tau = 3.5$ $\rightsquigarrow$ $U_{c1} = 4.782$, $E_{\text{ePT}}(U)$, $D_{\text{ePT}}(U)$

Mott insulator: energy + double occupancy II (QMC+$1/\omega$ vs. ePT)

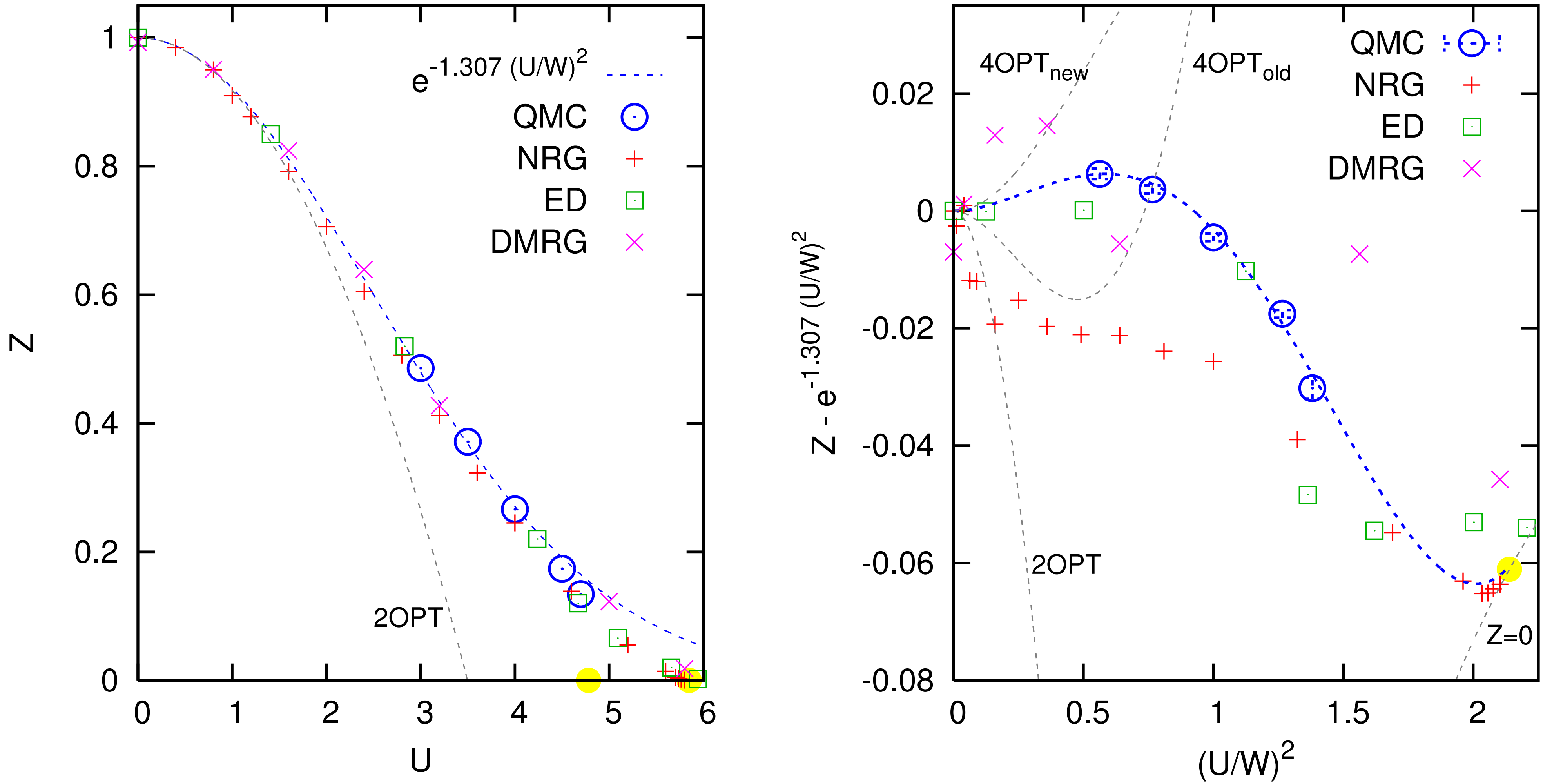


Mott insulator: U_{c1}, critical exponents, low-T parameter for $U_c(T)$

high-precision results for E, D at all U (parametrizations available) $\rightsquigarrow$ benchmark

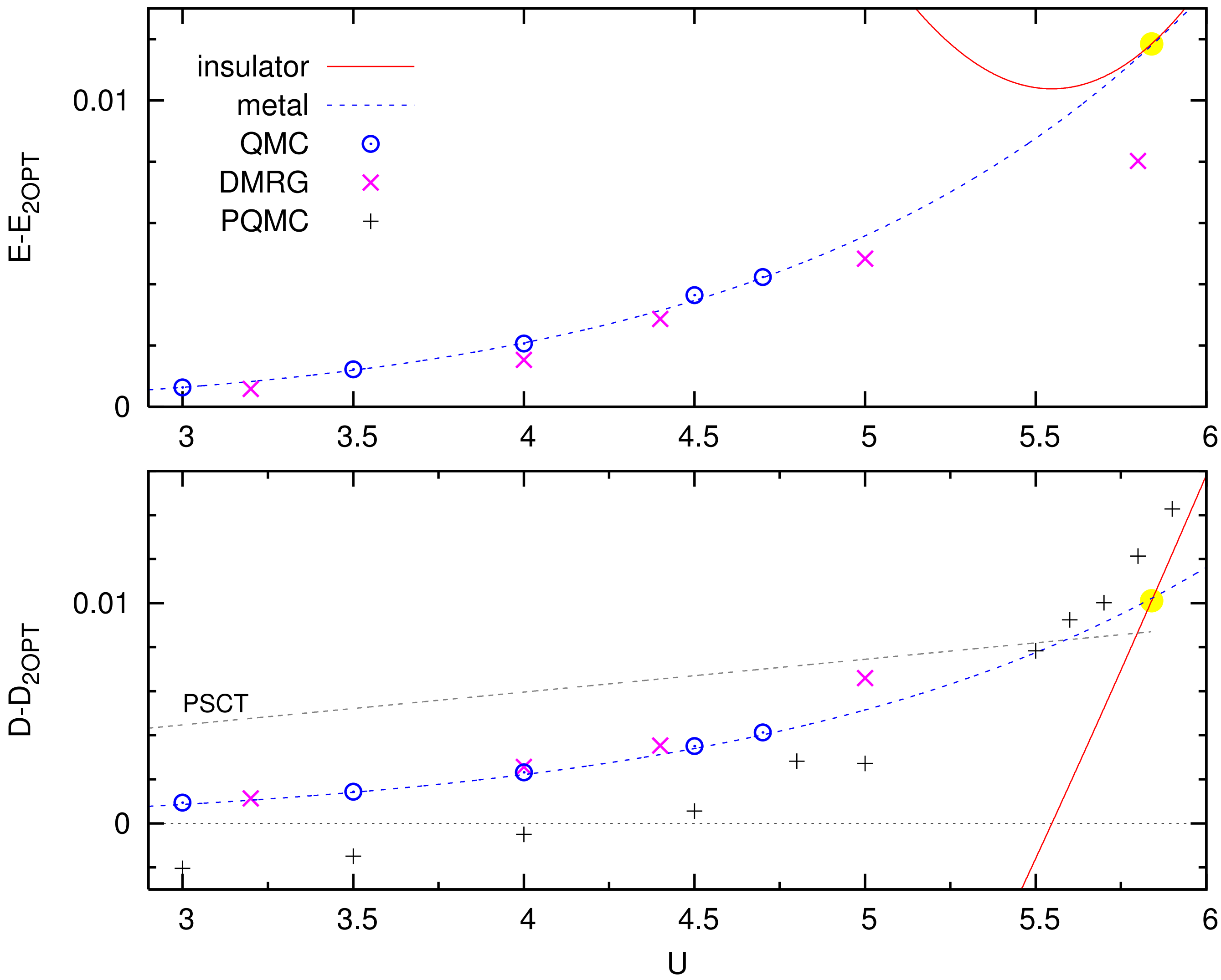
[Blümer, Kalinowski, Phys. Rev. B **71**, 195102 (2005)]

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



T-extrapolated QMC even beats ground state methods!

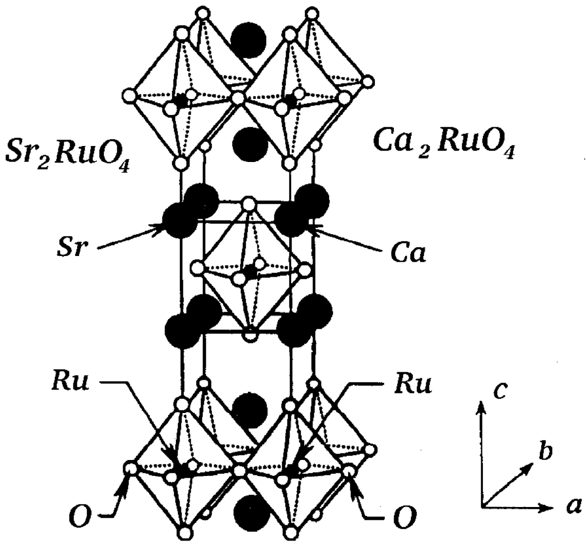
Energetics: differences w.r.t. 2^{nd} order weak-coupling PT for E and D



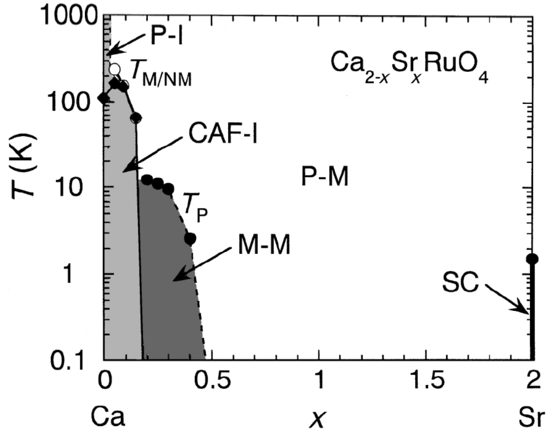
QMC-fit consistent with ePT for insulator; large deviations of PQMC, PSCT.

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)]

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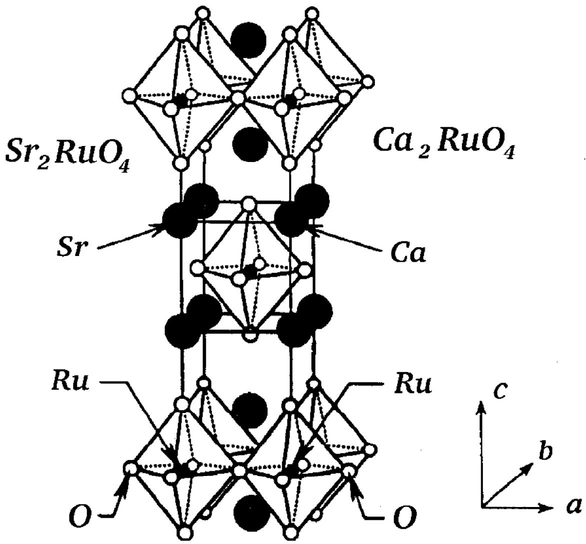

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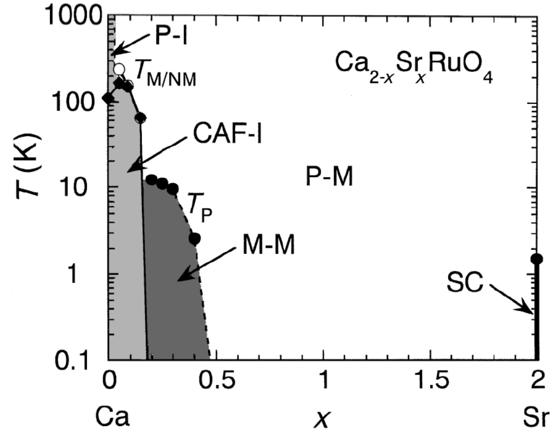

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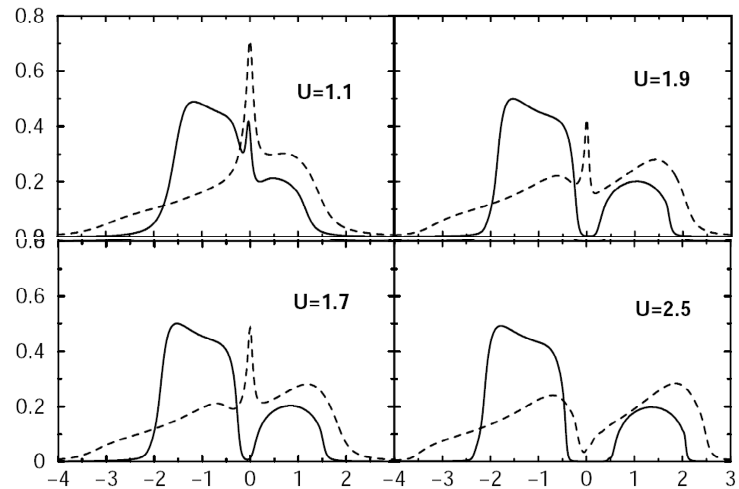
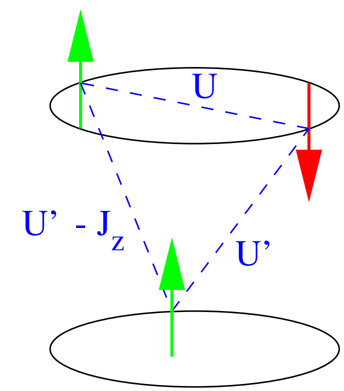


[Anisimov et al. (2002)]

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

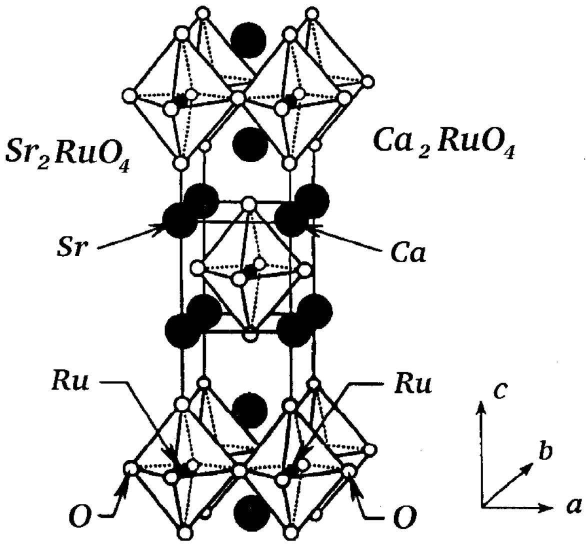
$$+ \sum_{i\sigma\sigma'} (U' - \delta_{\sigma\sigma'} J_z)\, n_{i1\sigma}\, n_{i2\sigma'}$$

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



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

Orbital-selective Mott transition in 2-band Hubbard model



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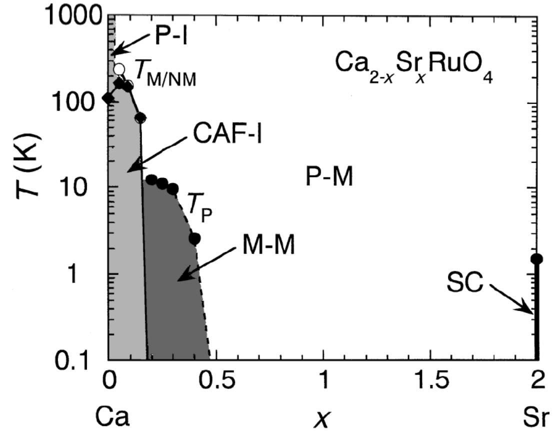

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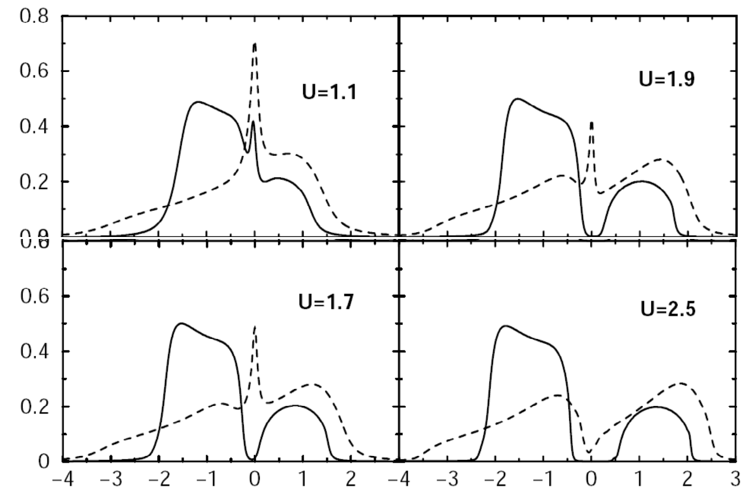

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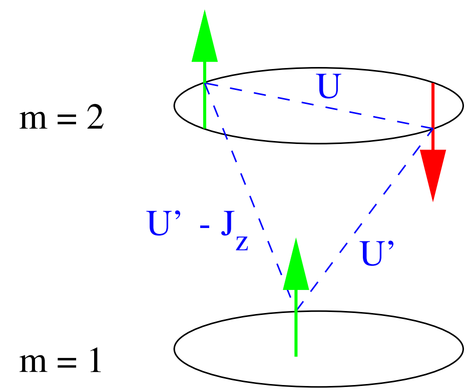
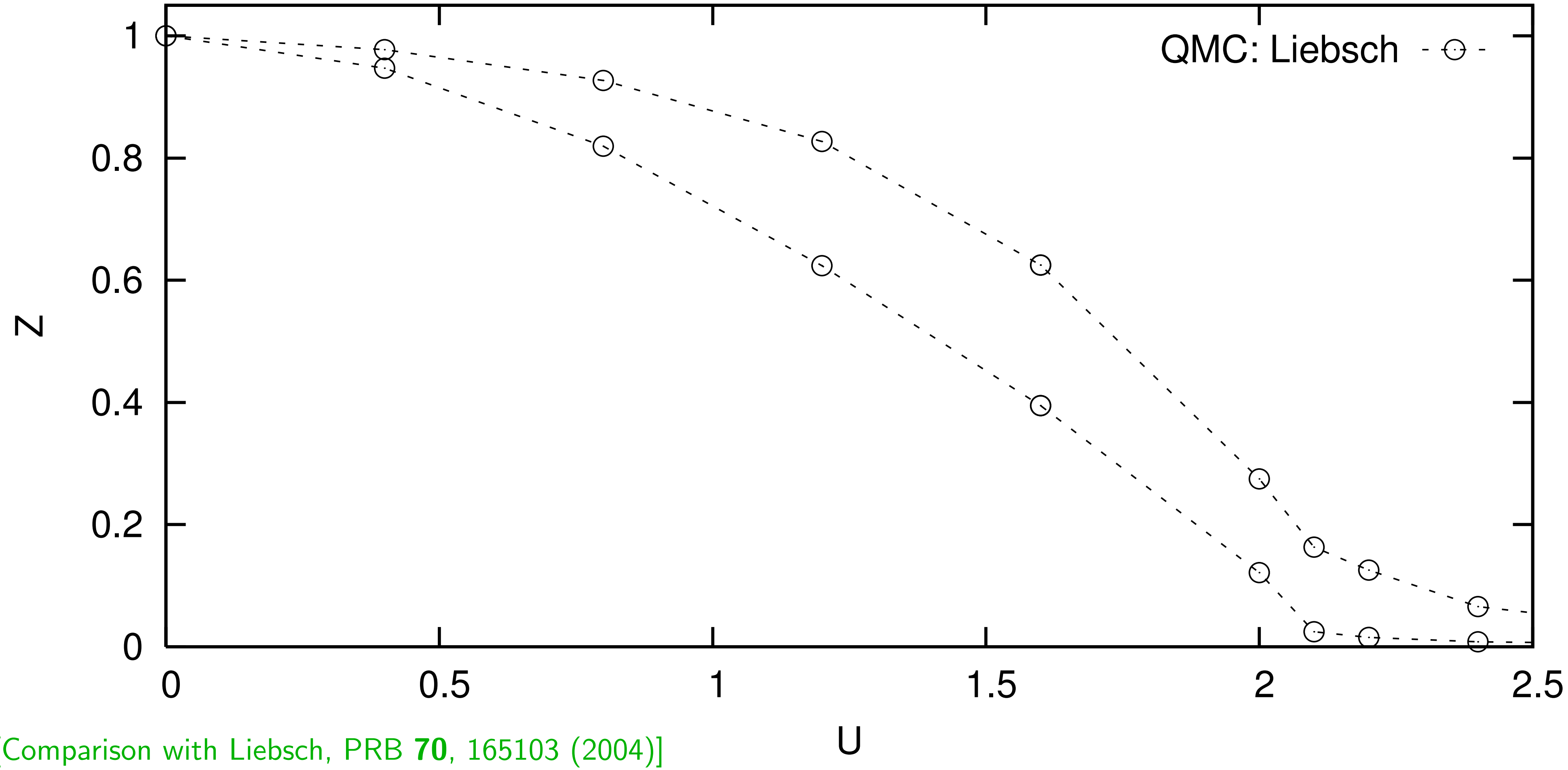


For Bethe DOS, $t_2 = 2\, t_1$: two 1^{st} order MITs for $U' = J_z = J_\perp = 0$

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)]

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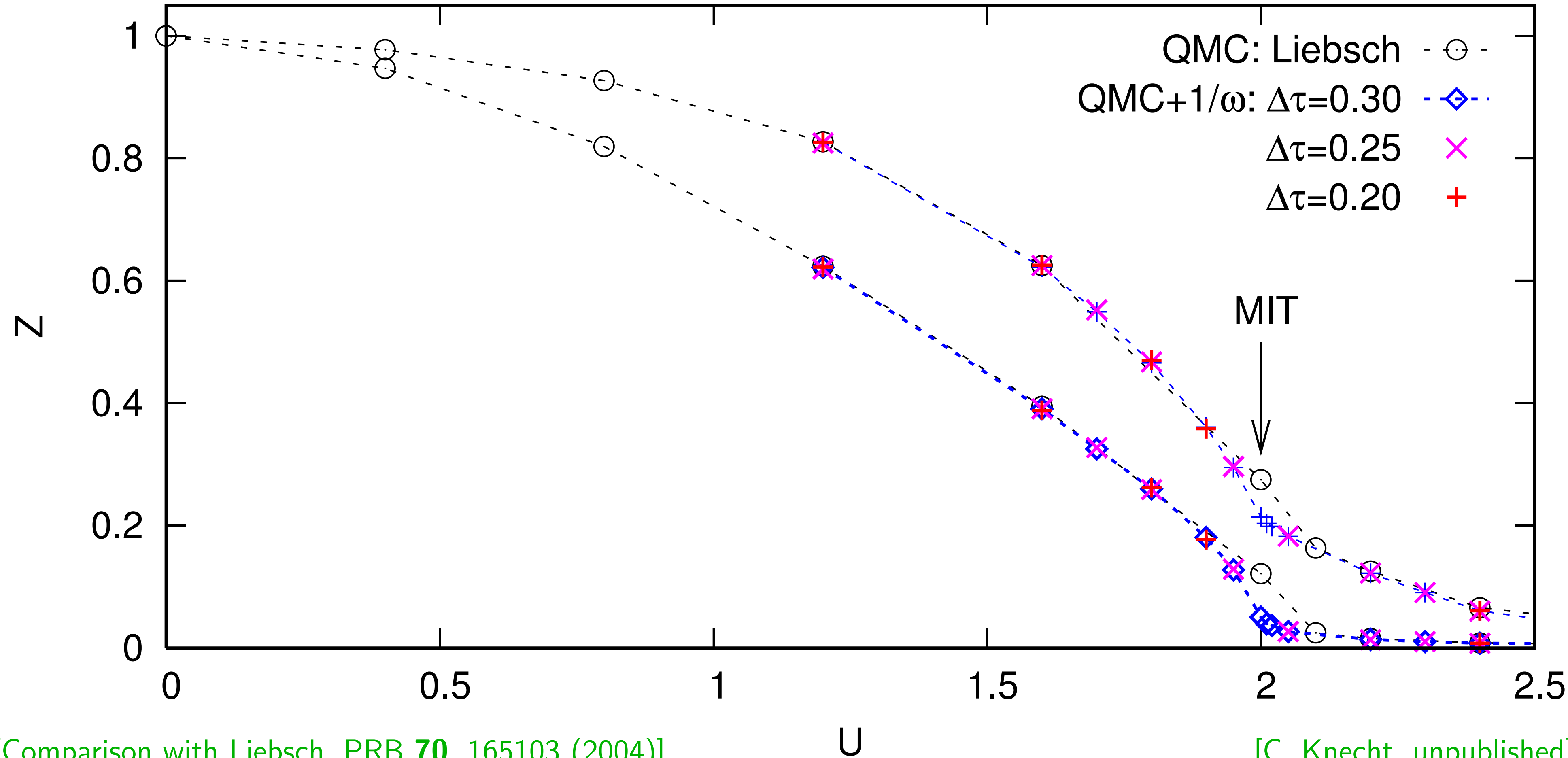


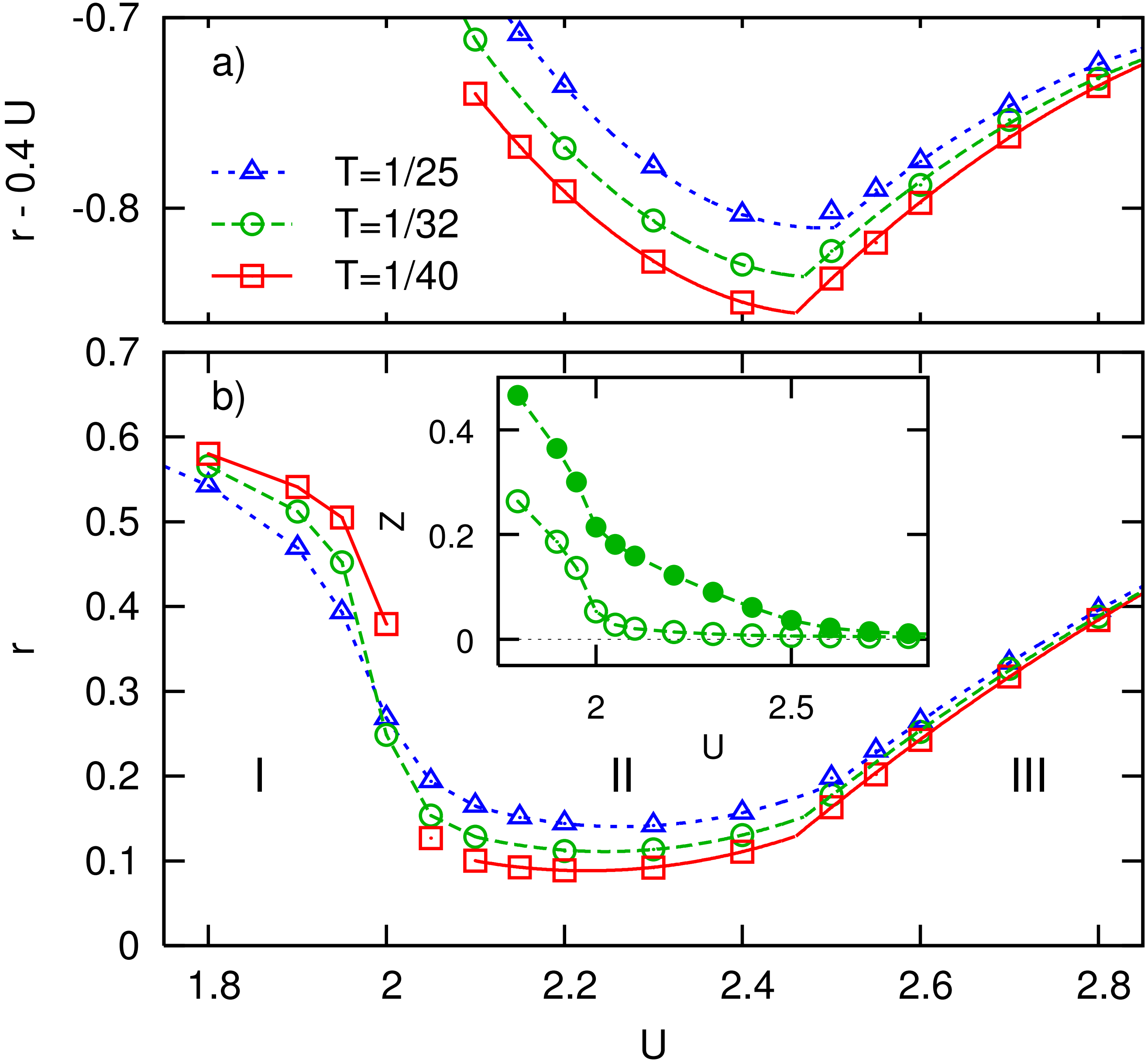
[Comparison with Liebsch, PRB **70**, 165103 (2004)] [C. Knecht, unpublished]

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 $U > 2.0$ – $2^{\rm nd}$ transition?

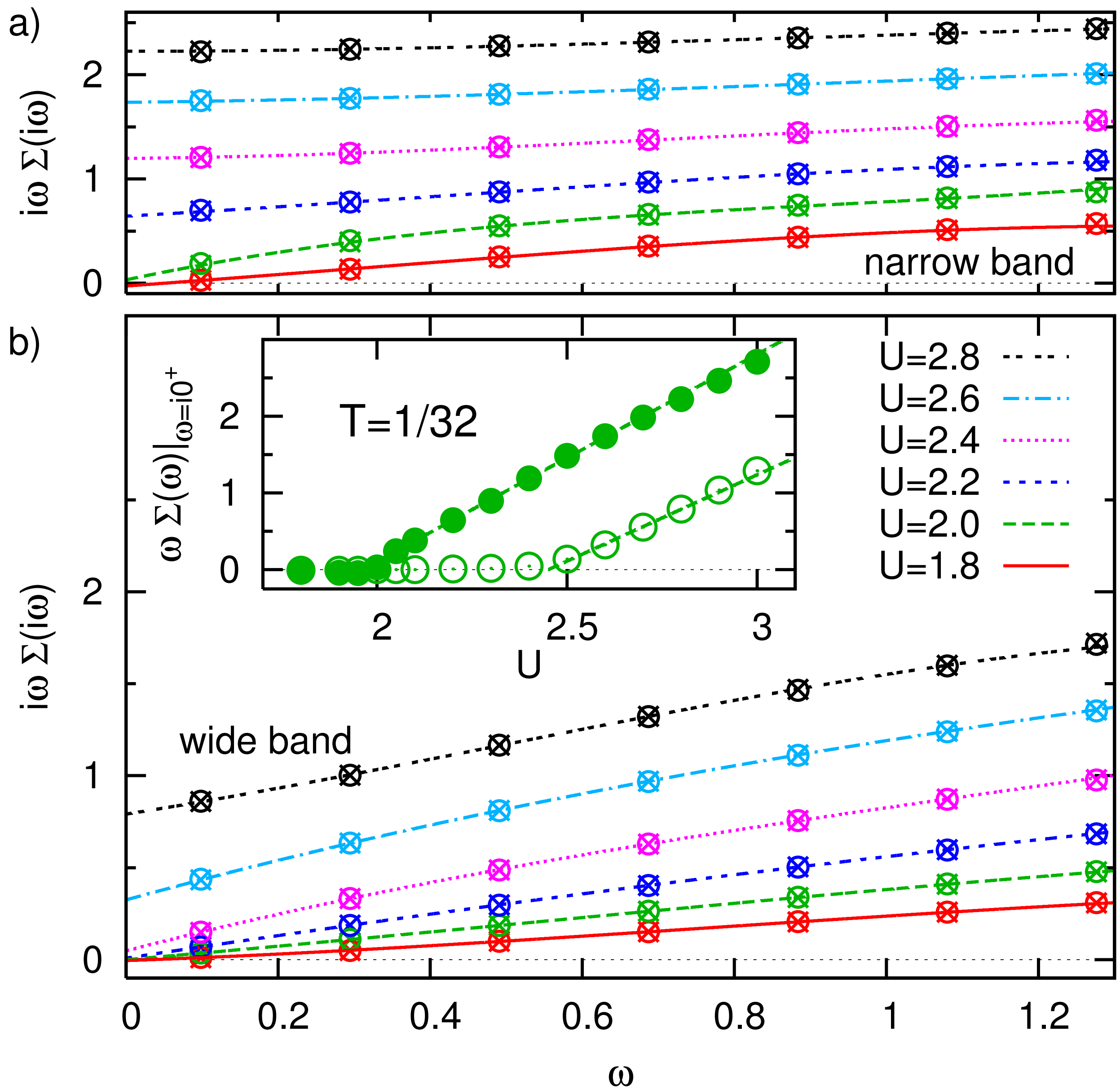
Ratio of quasiparticle weights $r = Z_{\text{narrow}}/Z_{\text{wide}}$



3 regions of different character

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

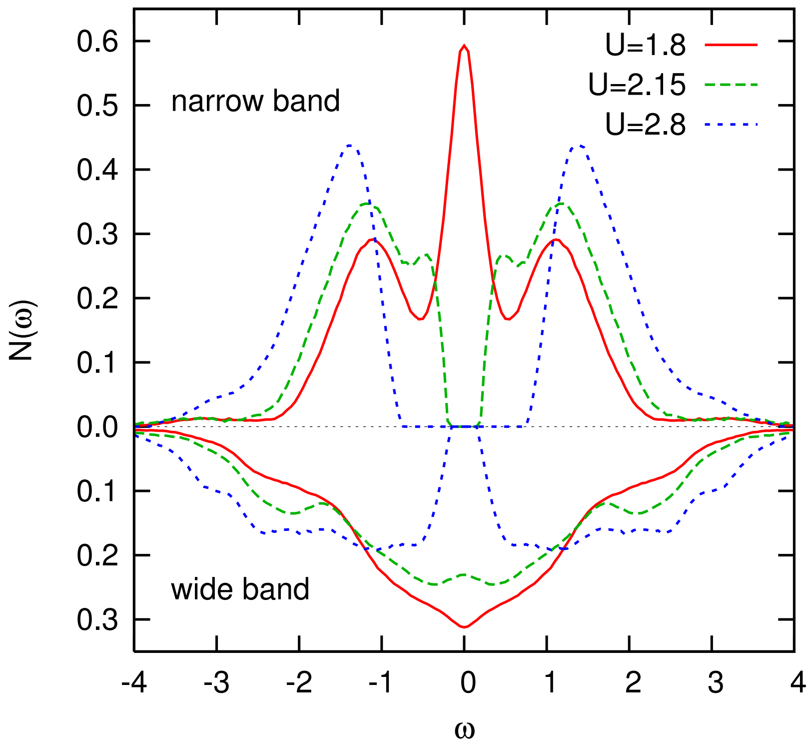
Low-frequency analysis of self-energy

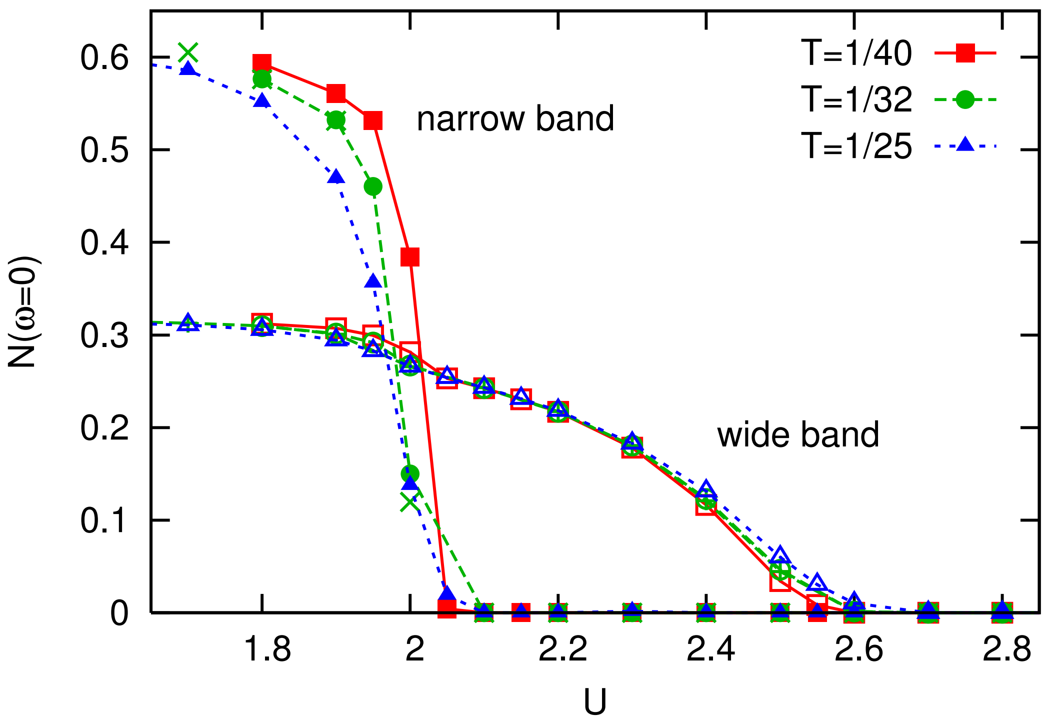


for regular self-energy:
$\omega\Sigma(\omega) \xrightarrow{\omega\to 0} 0$

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

Spectral function (interacting DOS)





Clear indications for second singularity

Wide band remains metallic at $U \approx 2.0$

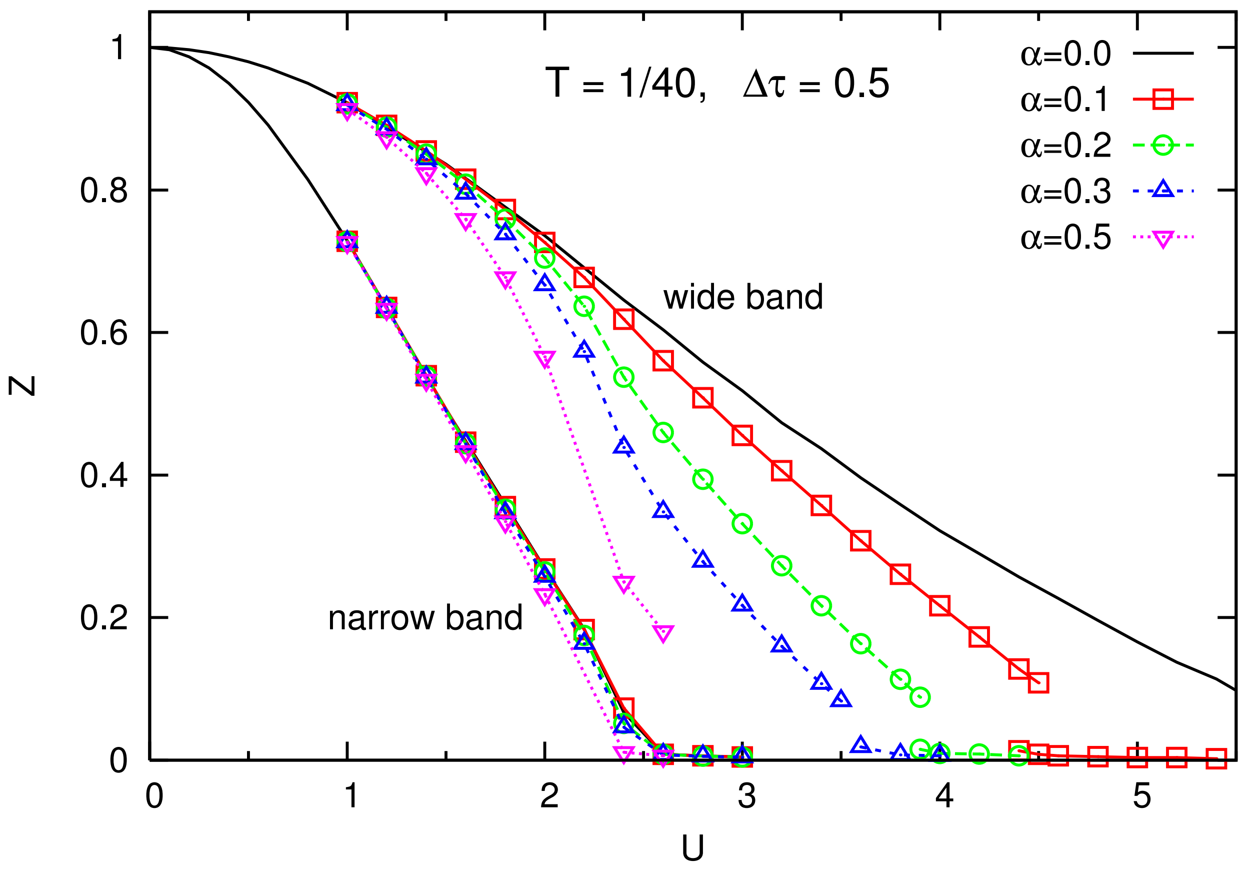
$\rightsquigarrow$ **two orbital-selective Mott transitions**

[Knecht, NB, van Dongen, cond-mat/0505106]

Comment: [Liebsch, cond-mat/0506138], Reply: [Knecht, NB, van Dongen, cond-mat/0506450]

Systematic study on 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 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

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Critical exponents from (infinite-order) ePT

Orbital-selective Mott transition in 2-band Hubbard model

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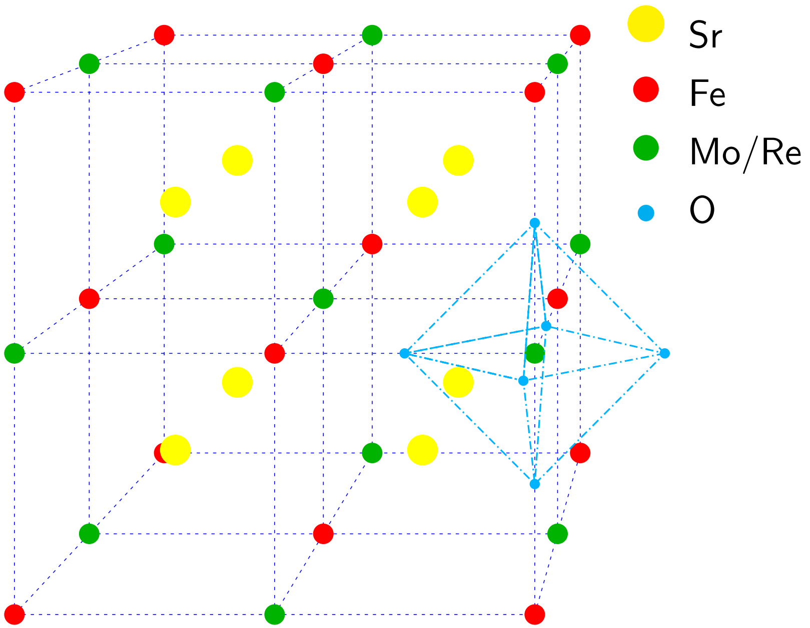
Outlook: realistic material-specific calculations with LDA+DMFT . . .

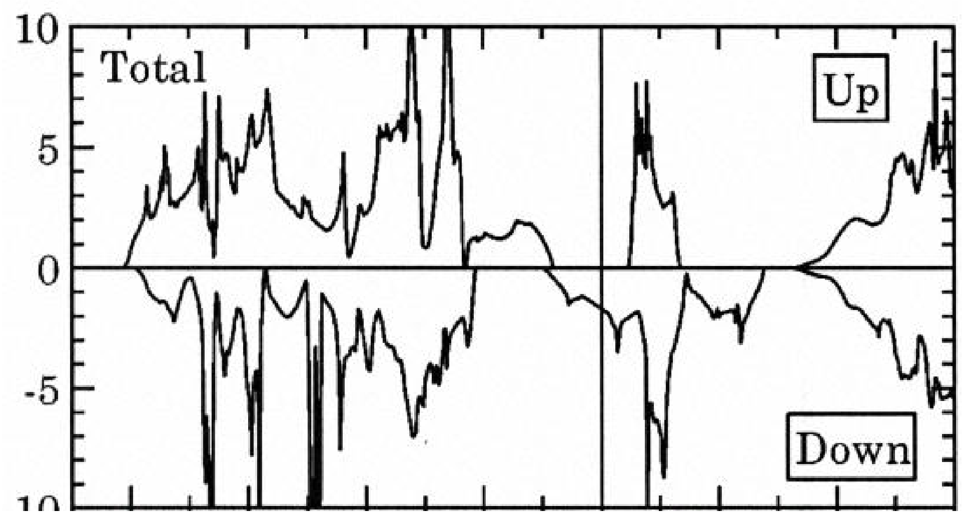
Thanks to: NIC Jülich, DFG (Bl775/1)

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)]

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

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

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

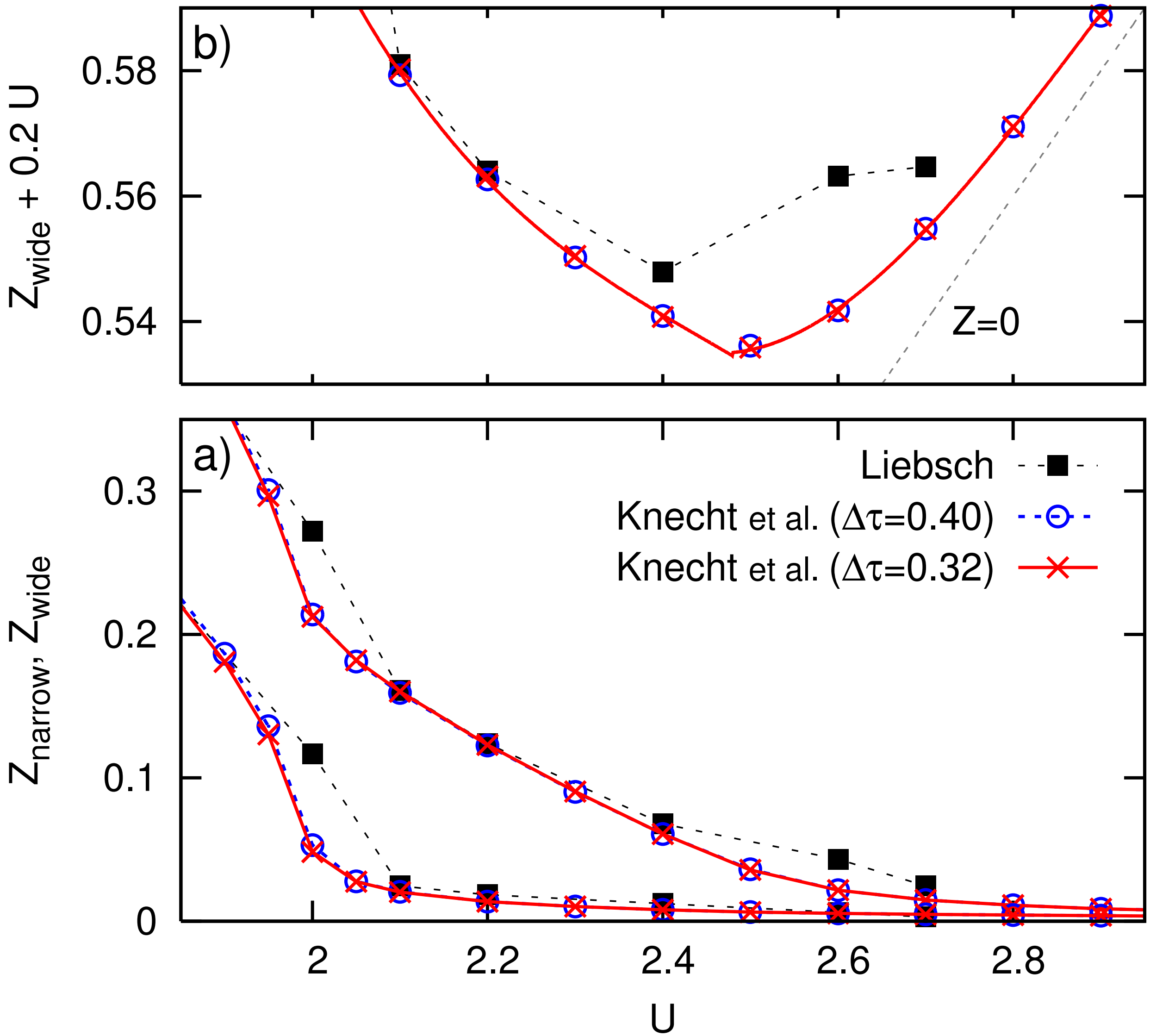
Speakers: Felser (Mainz), Hillebrands (Kaiserslautern)

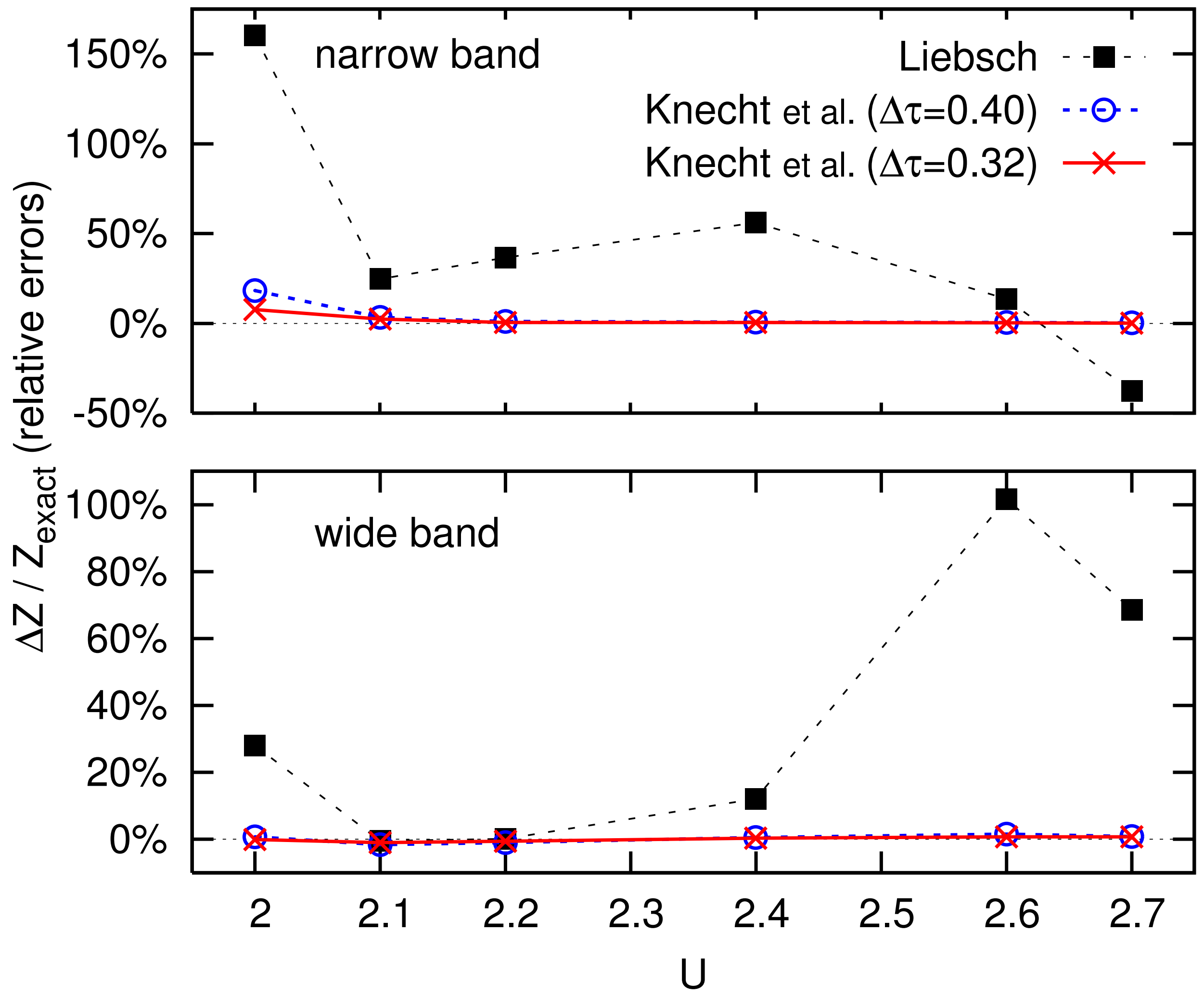
List of projects

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)





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