

# Quantum Monte Carlo simulations within dynamical mean-field theory

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## Outline

Motivation: cooperative phenomena in solids

Approaches for correlated electron systems  $\rightsquigarrow$  DMFT

Auxiliary-field quantum Monte Carlo algorithm

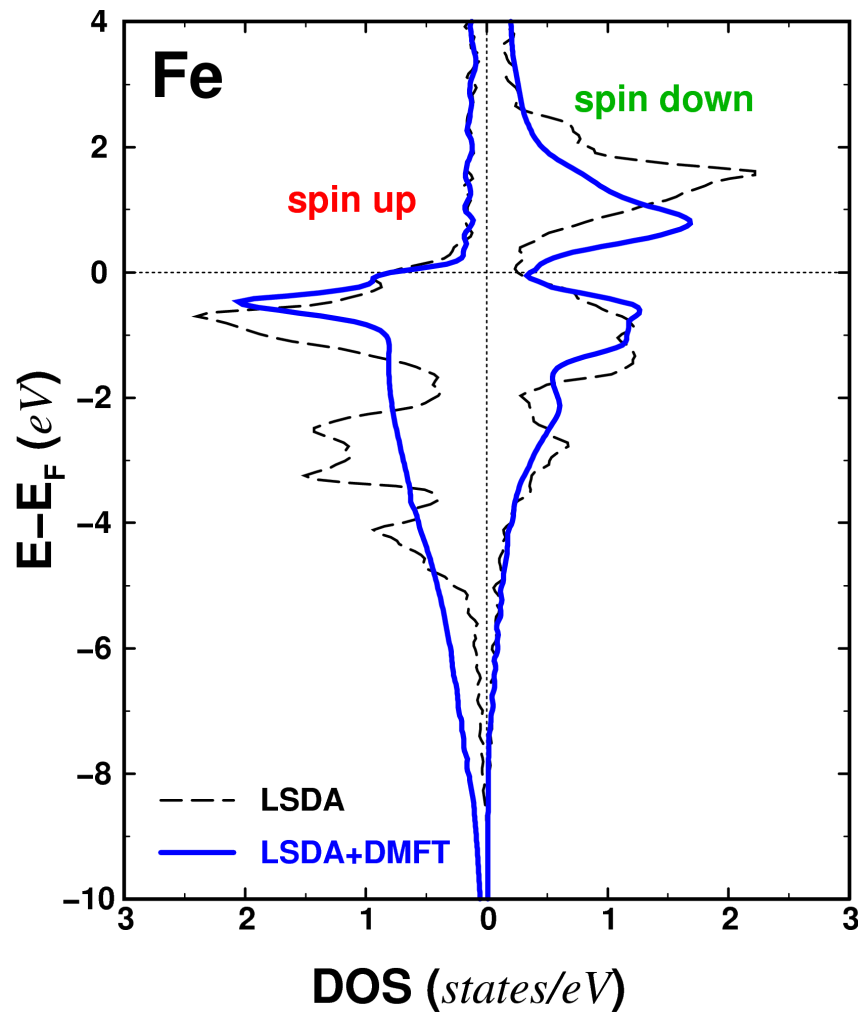
Update: orbital-selective Mott transitions

Efficiency of QMC DMFT solvers

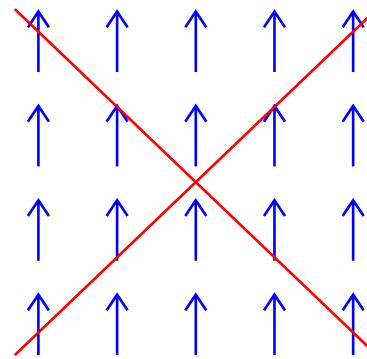
Summary and outlook

# Motivation: cooperative phenomena in solids

## Itinerant ferromagnetism and half-metallicity

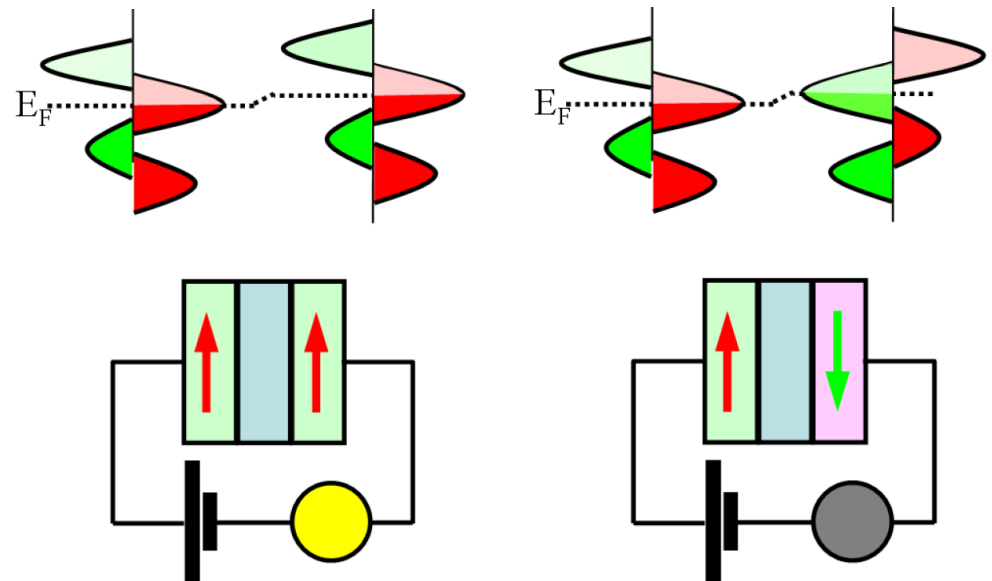


[Chioncel et. al, PRB (2003)]



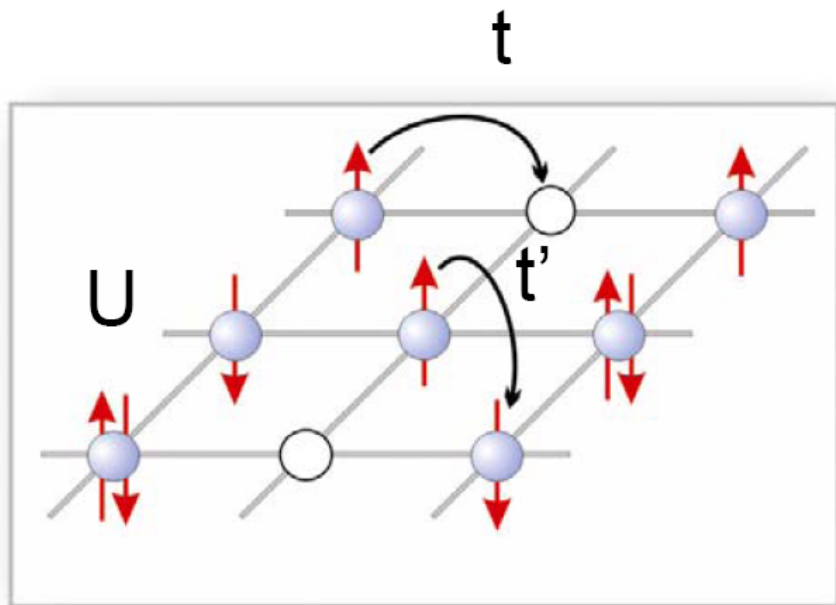
Spin models  
insufficient

Technological goal: TMR with half metals

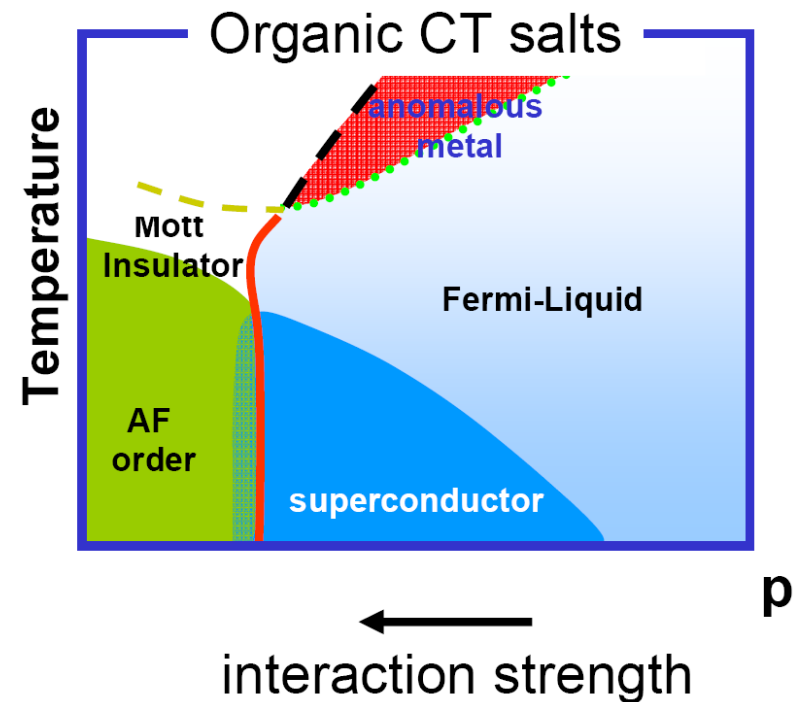
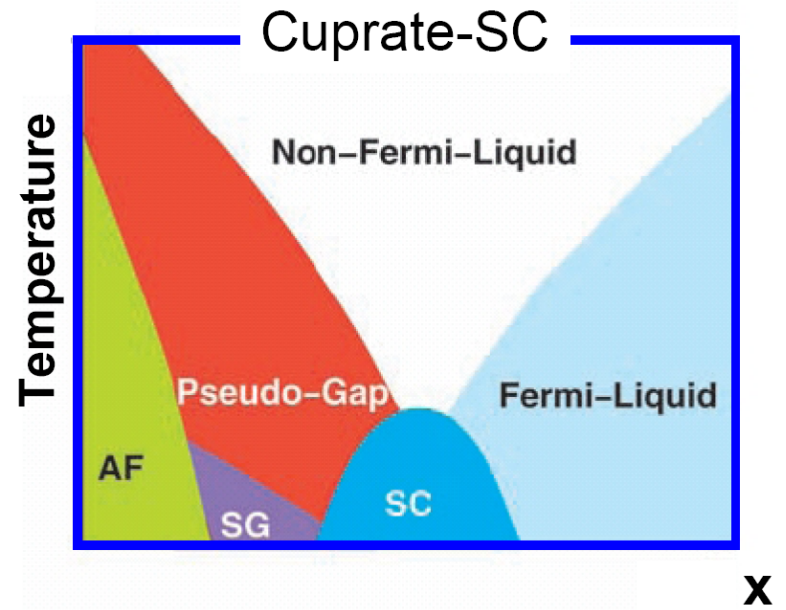


# Complex phases of cuprate and organic superconductors

High- $T_c$  physics contained in 2D Hubbard model?



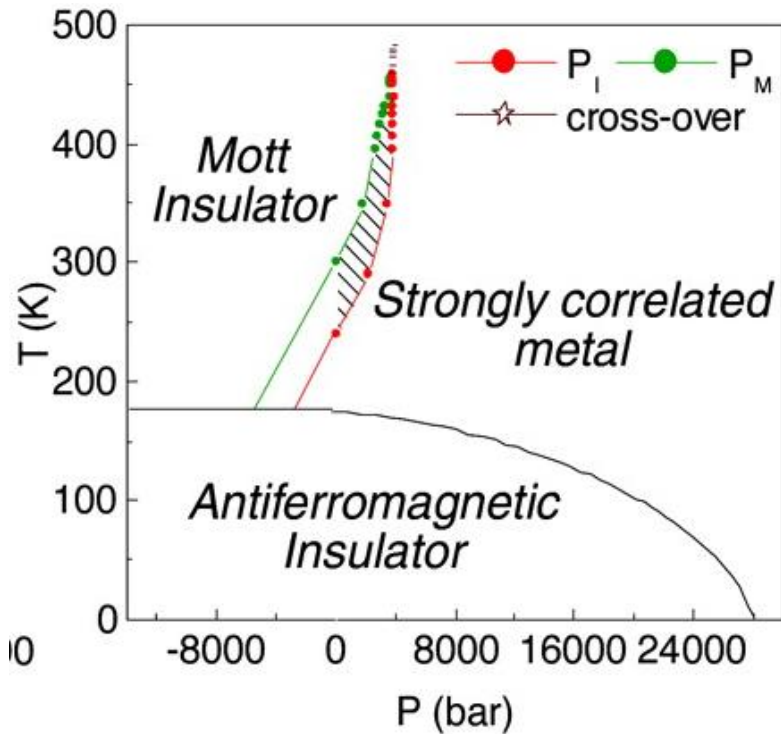
Are antiferromagnetic (AF) and Mott insulating phases essential for superconductivity?



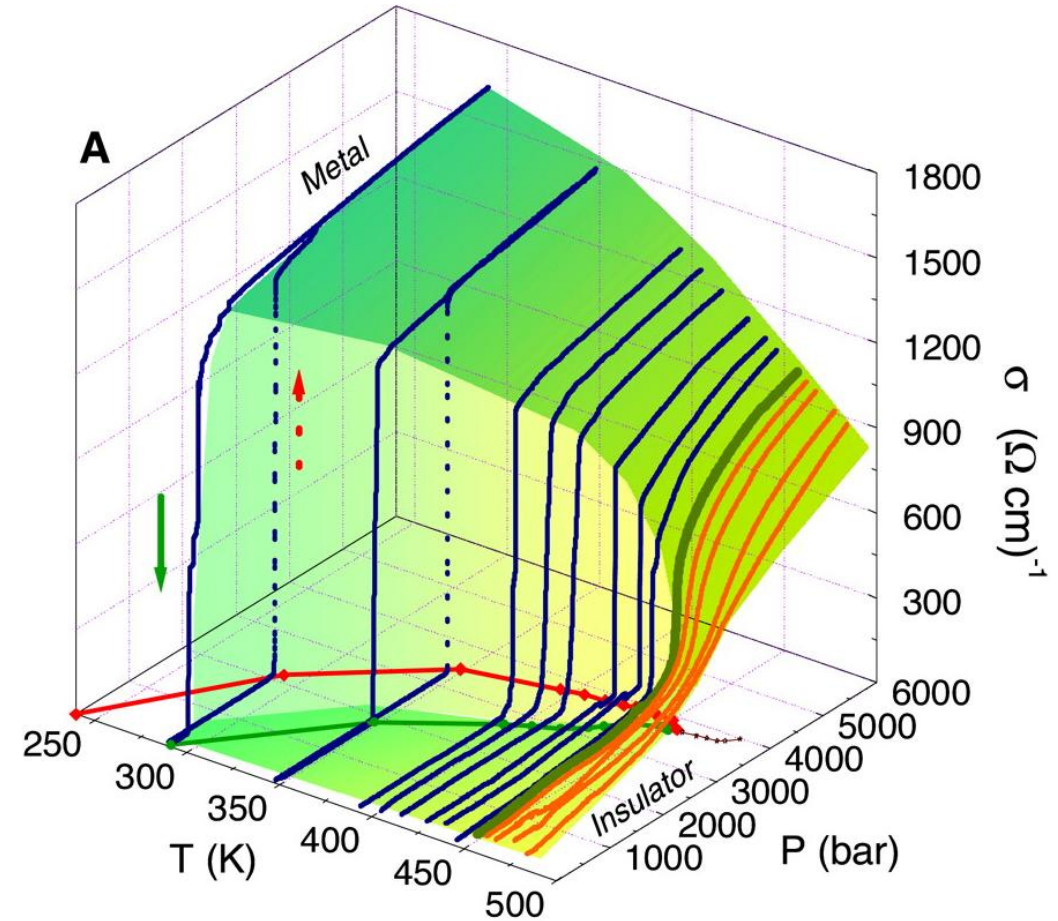
# Mott metal-insulator transition

Prototype example:  $V_2O_3$  doped with Cr/Ti and/or under pressure

## Phase diagram

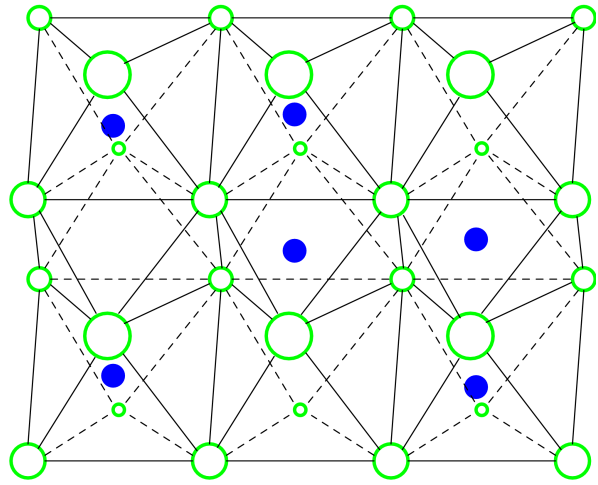


## Electrical conductivity



[Limelette et al., Science 302, 89 (2003)]

# Bandwidth control of metal-insulator transitions



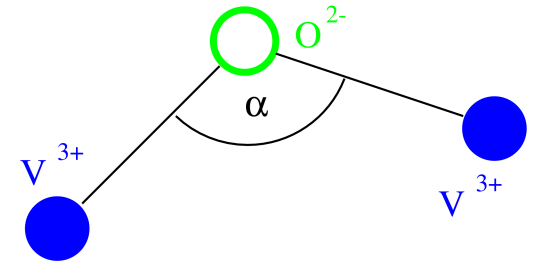
Corundum structure

Hydrostatic pressure or isovalent doping change

● lattice spacings

● bond angles

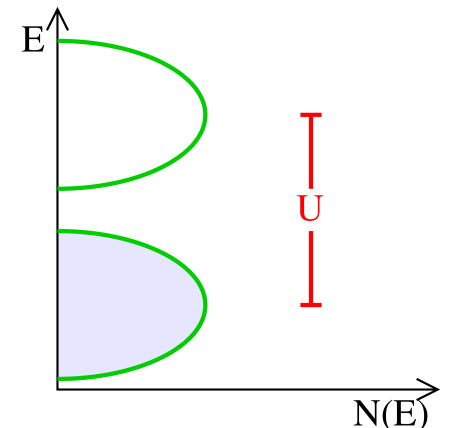
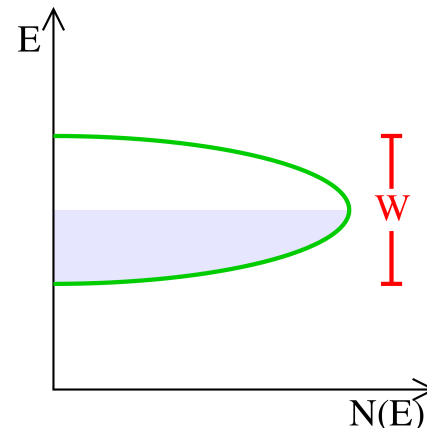
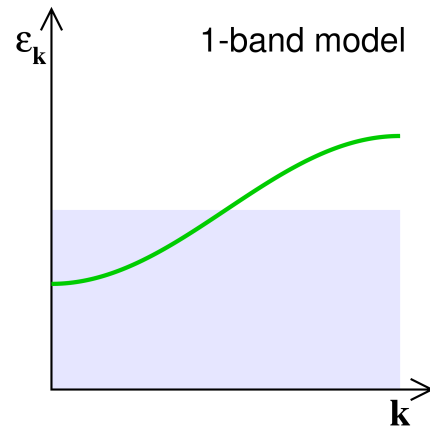
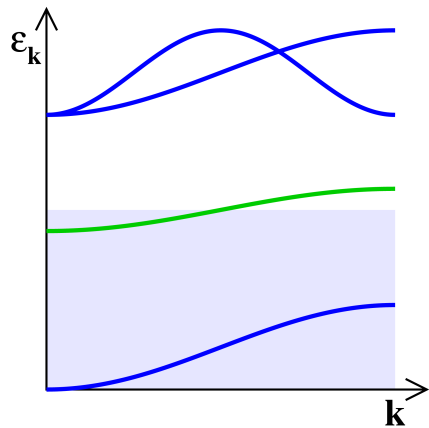
↪ hopping amplitudes



$$\alpha_{Cr} < \alpha_V < \alpha_{Ti}$$

Bond angles for  $V_2O_3$  doped with Cr or Ti

# Breakdown of Bloch band description at paramagnetic Mott transition



Bloch states near Fermi energy,

band-splitting by Coulomb correlations

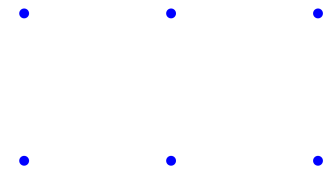
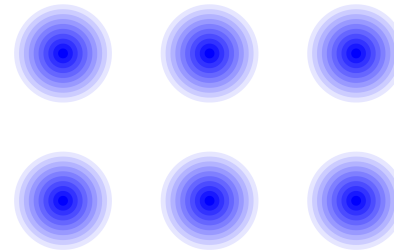
# Approaches for correlated electron systems

## Microscopic modeling I

### General Hamiltonian for nuclei and electrons

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

Born-Oppenheimer approximation (0<sup>th</sup> order)



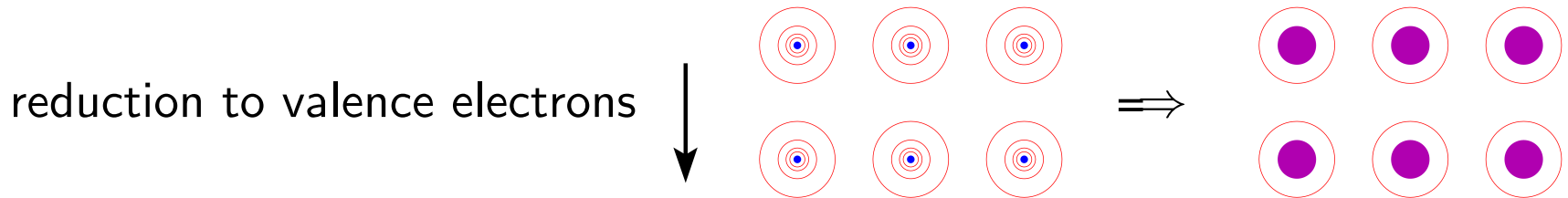
$$H = \sum_{i=1}^{N_e} \frac{\mathbf{p}_i^2}{2m} + \sum_i V(\mathbf{r}_i) + \sum_{i<j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

### Classes of theoretical approaches for electronic problem

- continuum methods: density functional theory (DFT), variational+diffusion QMC, . . .
- methods for lattice electrons

# Microscopic modeling II

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



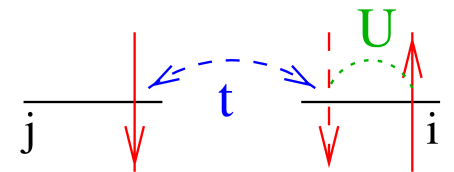
$$H = \sum_{i=1}^{N_v} \frac{\mathbf{p}_i^2}{2m} + \sum_{i=1}^{N_v} V^{\text{ion}}(\mathbf{r}_i) + \sum_{i=1}^{N_v-1} \sum_{j=i+1}^{N_v} V^{ee}(\mathbf{r}_i, \mathbf{r}_j)$$



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

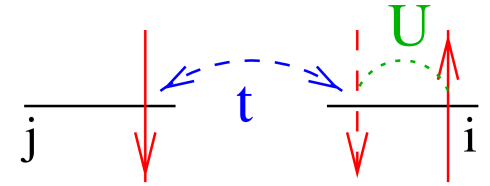
## Hubbard model

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



# Approaches for Hubbard-type models

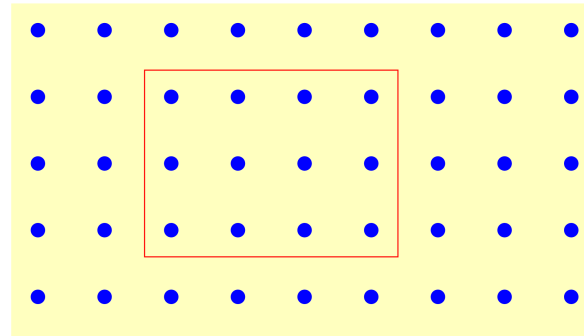
$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



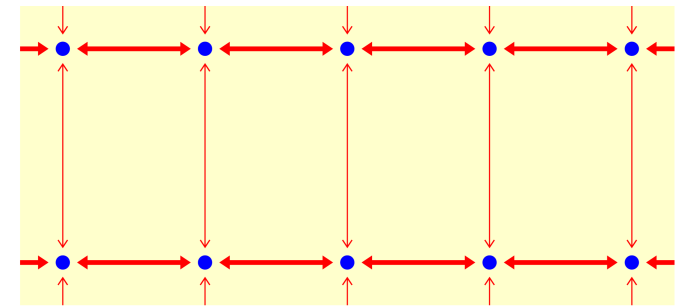
## Perturbation theory

- $U \rightarrow 0$ : Hartree-Fock  
2<sup>nd</sup> order PT, . . . .
- $t/U \rightarrow 0$  (for  $n = 1$ )  
 $\rightsquigarrow$  Heisenberg model

## finite clusters: ED, QMC



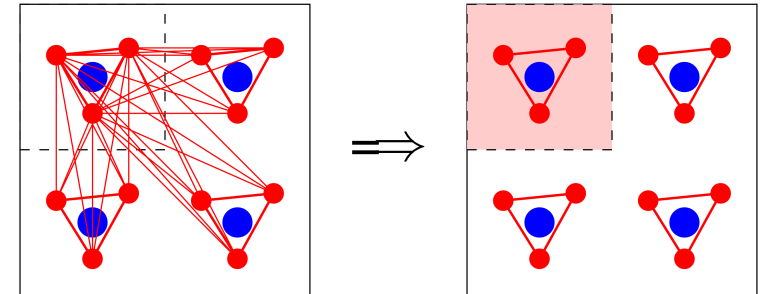
## $d \rightarrow 1$ : Bethe ansatz, DMRG



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

[Metzner, Vollhardt, PRL (1989), Georges, Kotliar, PRL (1992), Jarrell, PRL (1992)]

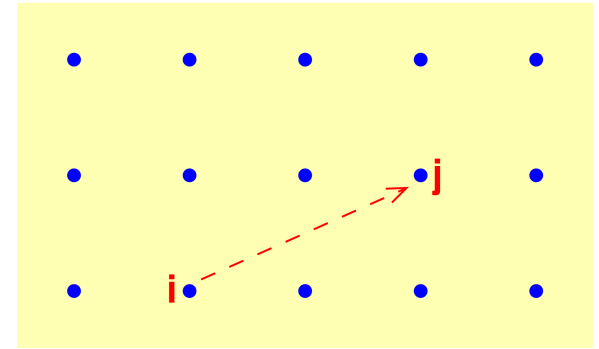
- + non-perturbative  $\rightsquigarrow$  valid at MIT
- + dynamical on-site correlations preserved
- + in thermodynamic limit
- +/- exact for coordination  $Z \rightarrow \infty$



# Excursus: Green function and self-energy

Single-particle Green function (lattice sites  $i, j$ ):

$$G_{ij}(t_1, t_2) = -\langle c_j(t_2) c_i^\dagger(t_1) \rangle$$

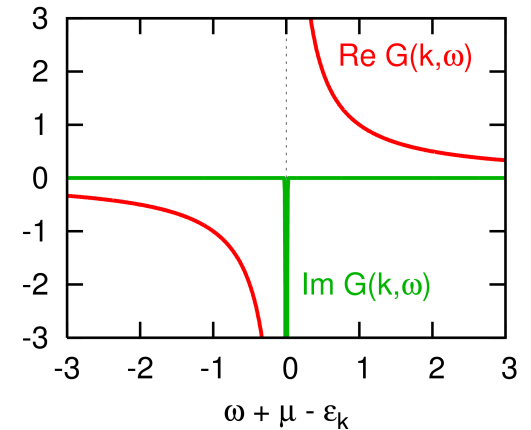


Translation invariance in space and time:  $G_{ij}(t_1, t_2) \equiv G_{j-i}(t_2 - t_1) \xrightarrow{\text{Fourier}} G(\mathbf{k}, \omega)$

Noninteracting limit (dispersion  $\epsilon_{\mathbf{k}}$ ):  $G_0(\mathbf{k}, \omega) = \frac{1}{\omega + \mu - \epsilon_{\mathbf{k}}}$

Self-energy  $\Sigma$  quantifies impact of interactions:

$$G(\mathbf{k}, \omega) = \frac{1}{\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, \omega)}$$



Locality of self-energy  $\Sigma(\mathbf{k}, \omega) \equiv \Sigma(\omega)$  within DMFT simplifies local Green function:

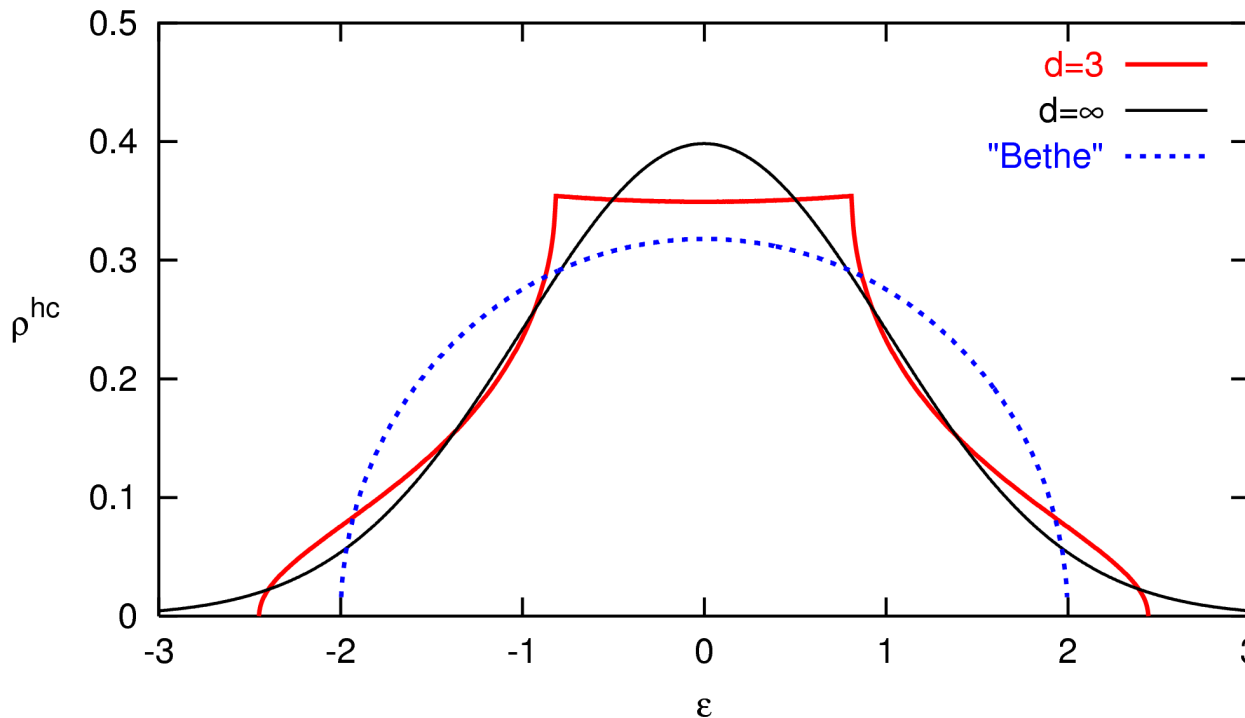
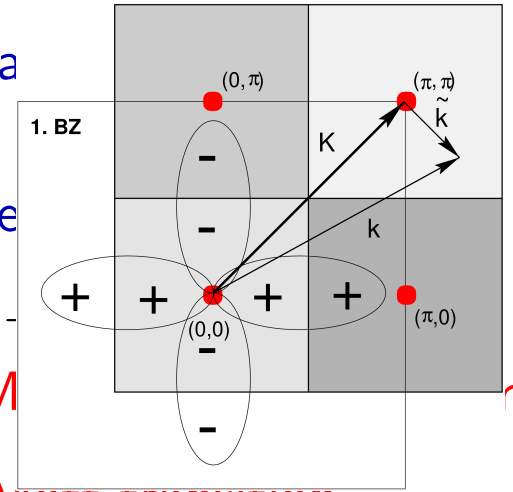
$$G(\omega) \equiv G_{ii}(\omega) = \int d\epsilon \frac{\rho(\epsilon)}{\omega + \mu - \epsilon - \Sigma(\omega)} ; \quad \rho(\epsilon) = \frac{1}{N} \sum_{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}})$$

$\mathbf{k}$  integrated Dyson equation

noninteracting DOS

# Brief History of DMFT

- 1989 Metzner, Vollhardt: **limit**  $d \rightarrow \infty$ : Gutzwiller approximation  
 Müller-Hartmann: **local self-energy**:  $\Sigma(\mathbf{q}, \omega) \rightarrow \Sigma(\omega)$   
 Brandt, Mielsch: exact solution of Falicov-Kimball model
- 1992 Georges, Kotliar: mapping to Anderson impurity model  
 Jarrell: **quantum Monte Carlo**  $\rightsquigarrow$  antiferromagnetism, Mott transition
- 1993 Georges et al., Kotliar et al.: **frustrated Bethe lattice**  $\rightsquigarrow$  Mott transition



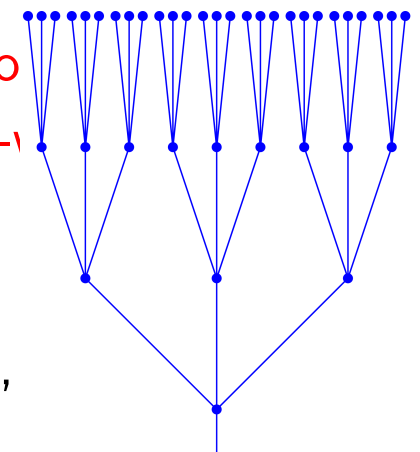
d. Phys. article

emission spectra (PES)

$\hookrightarrow$   $\rightsquigarrow$  PES for

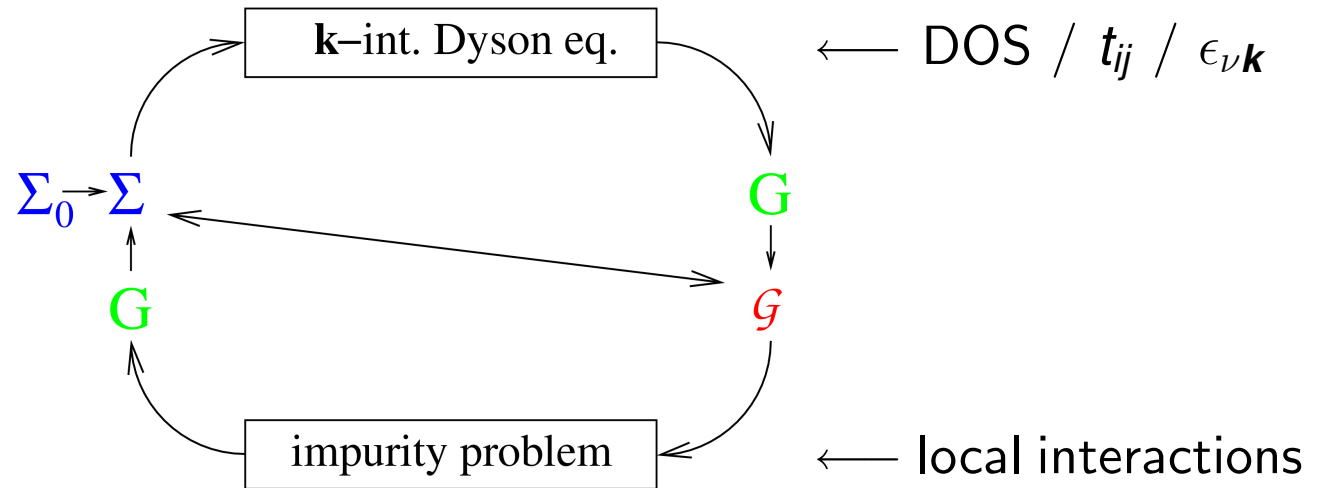
DCA)  $\rightsquigarrow$   $d \rightarrow \infty$

Methods (DCA,



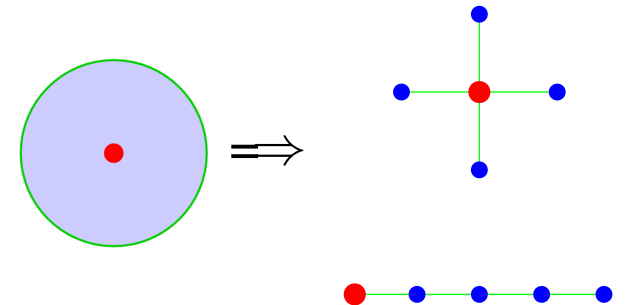
# Iterative solution of DMFT equations

0. Initialize self-energy
1. Solve Dyson equation
2. Solve **single impurity Anderson model (SIAM)**



## Impurity solver:

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



# Auxiliary-field QMC algorithm [Hirsch, Fye (1986)]

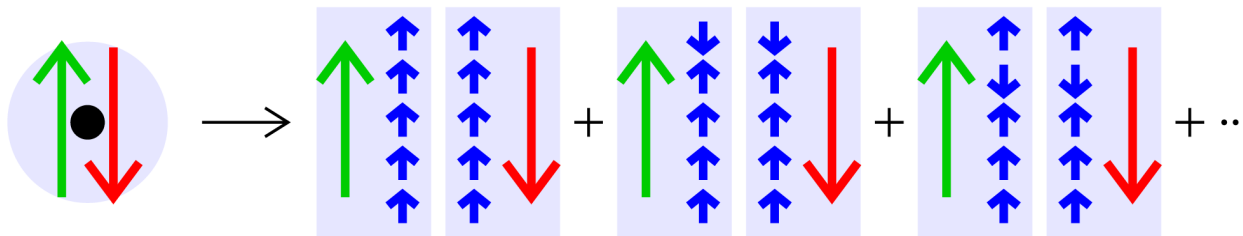
Green-Funktion  $G$  in imaginary time (fermionic Grassmann variables  $\psi, \psi^*$ ):

$$G_{\sigma}(\tau_2 - \tau_1) = \frac{1}{Z} \int \mathcal{D}[\psi] \mathcal{D}[\psi^*] \psi_{\sigma}(\tau_1) \psi_{\sigma}^*(\tau_2) \exp \left[ \mathcal{A}_0 - U \sum_{\sigma\sigma'} \int_0^{\beta} d\tau \psi_{\sigma}^* \psi_{\sigma} \psi_{\sigma'}^* \psi_{\sigma'} \right]$$

Discretization  $\beta = \Lambda \Delta\tau$ , Trotter decoupling  $e^{-\beta(\hat{T}+\hat{V})} = \lim_{\Lambda \rightarrow \infty} [e^{-\Delta\tau \hat{T}} e^{-\Delta\tau \hat{V}}]^{\Lambda}$

Use  $\hat{n}_{\uparrow} \hat{n}_{\downarrow} = \frac{1}{2} [\hat{n}_{\uparrow} + \hat{n}_{\downarrow} - (\hat{n}_{\uparrow} - \hat{n}_{\downarrow})^2]$ ; discrete Hubbard-Stratonovich transformation

$$\exp[\Delta\tau U (\hat{n}_{\uparrow} - \hat{n}_{\downarrow})^2 / 2] = \frac{1}{2} \sum_{s=\pm 1} \exp[\lambda s (\hat{n}_{\uparrow} - \hat{n}_{\downarrow})]; \quad \cosh(\lambda) = \exp(\Delta\tau U / 2)$$



Wick theorem:

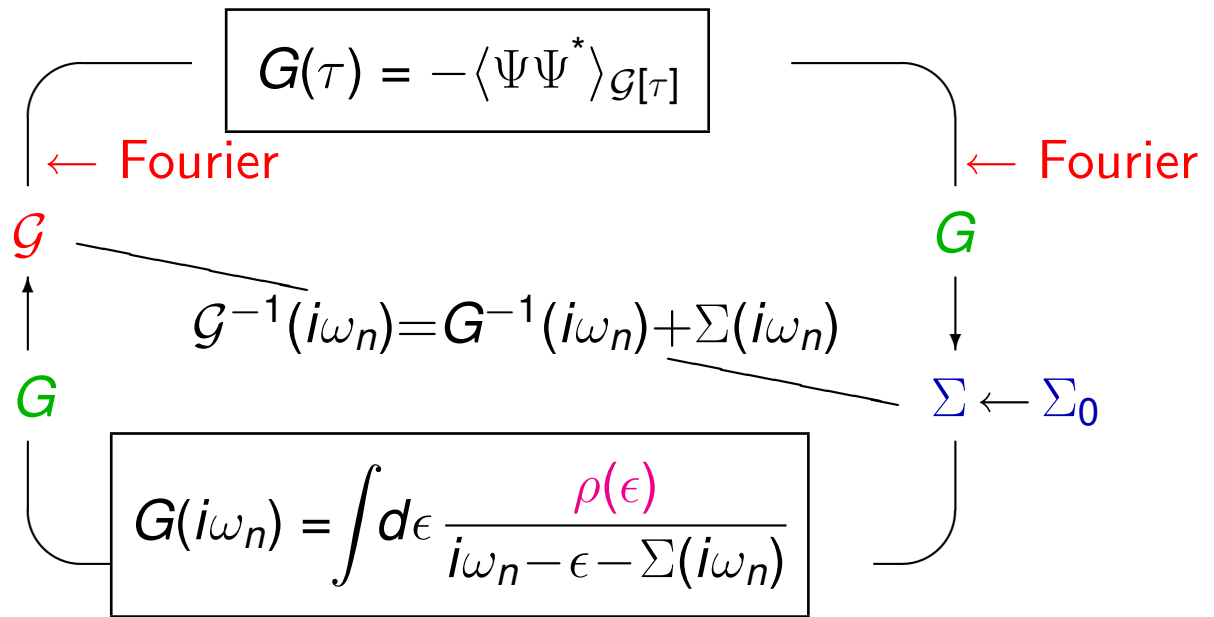
$$G = \frac{\sum M \det\{M\}}{\sum \det\{M\}}$$

Metropolis MC importance sampling over auxiliary Ising field  $\{s\}$ :  $2^{\Lambda}$  configurations

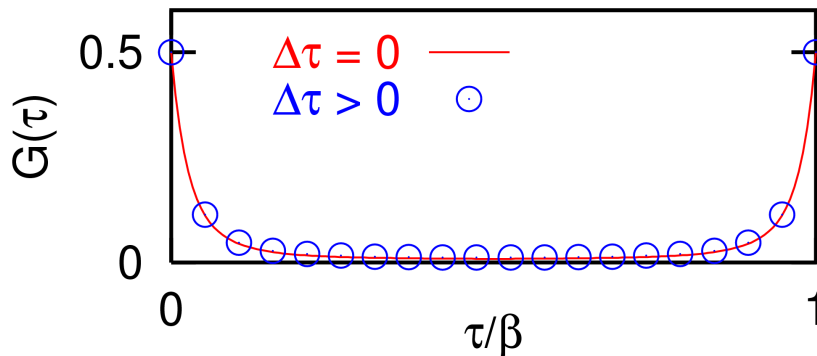
+ numerically exact, + no sign problem, – effort scales as  $T^{-3}$ ,

# Problems with Fourier transformations in DMFT-QMC cycle

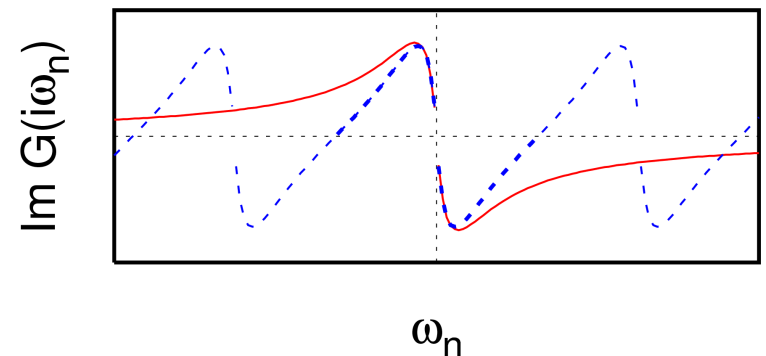
Iterative solution of DMFT equations (for imaginary-time impurity solver)



Naive discrete Fourier transformation  $\rightsquigarrow$  oscillations (instead of  $G(\omega) \xrightarrow{\omega \rightarrow \infty} 1/\omega$ )



naive FT  $\rightarrow$

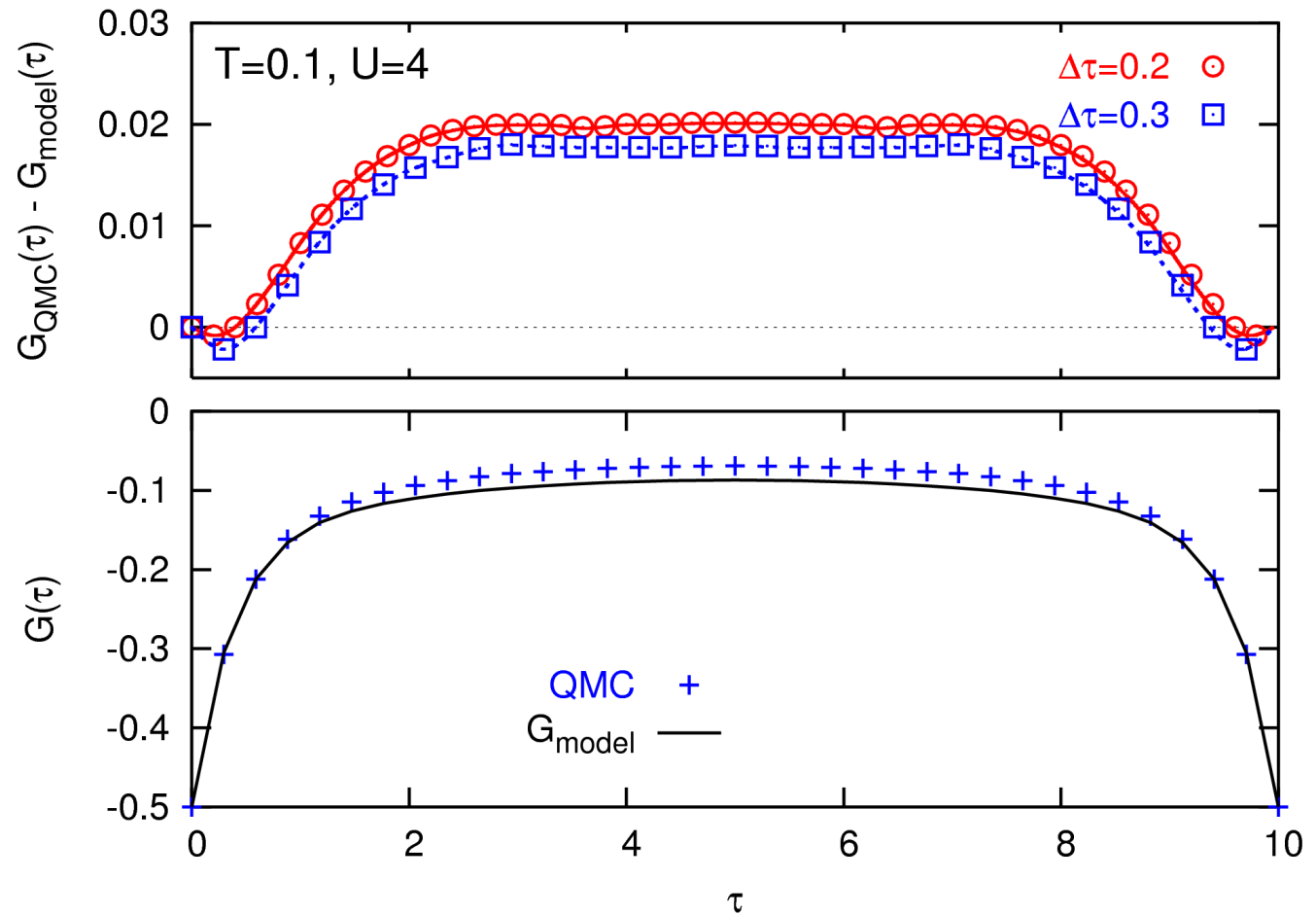


1<sup>st</sup> solution: correct unphysical behavior for  $|\omega| \lesssim \omega_{\text{Nyquist}}$  by transformation [Ulmke]

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

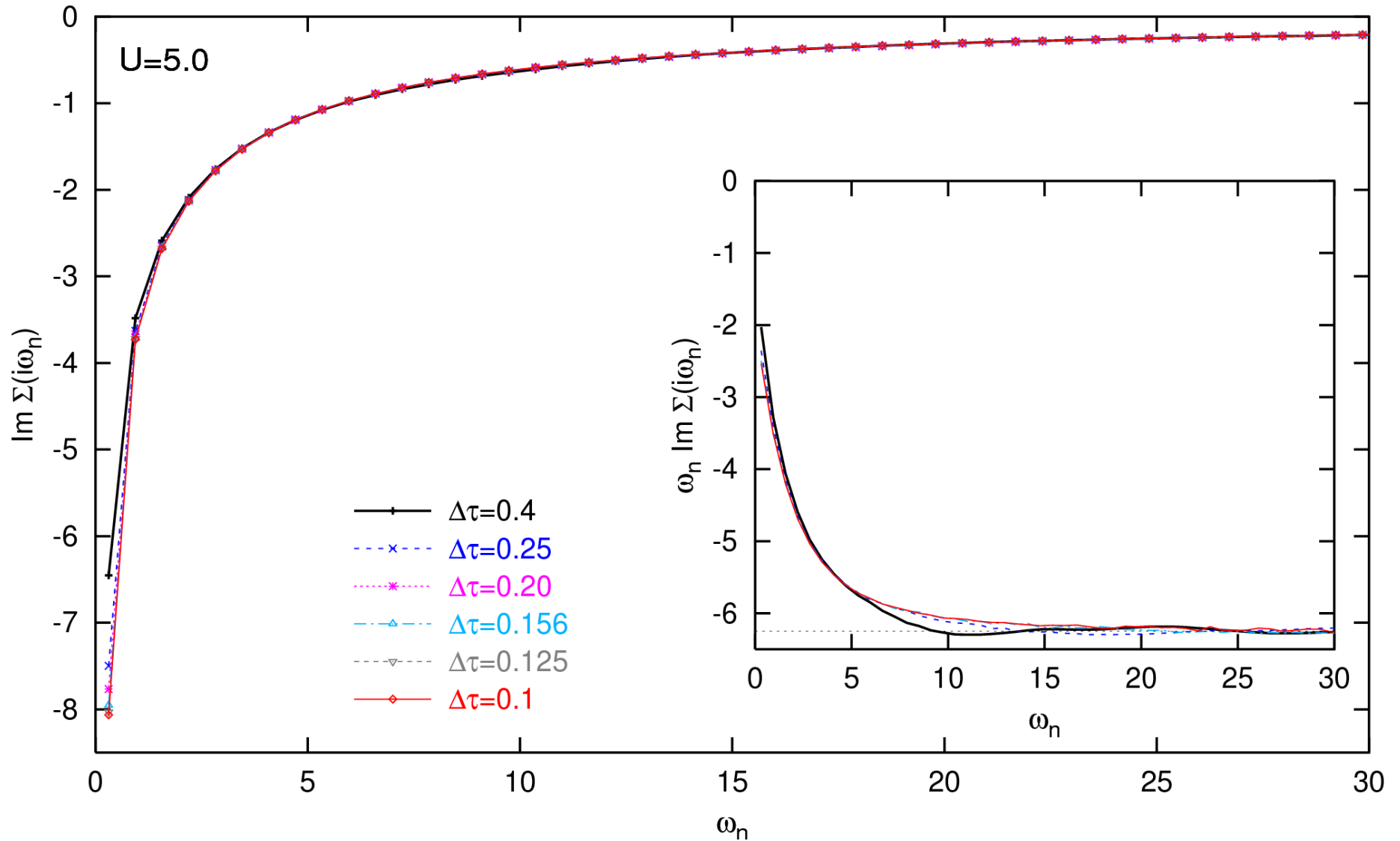
But:  $\frac{d^2 G(\tau)}{d\tau^2}$  maximal for  $\tau \rightarrow 0, \beta \rightsquigarrow$  natural boundary conditions inappropriate

- adjust boundary cond. [Oudovenko]
- spline-fit only difference w.r.t. reference problem:
  - IPT [Jarrell]
  - high-frequency expansion for  $\Sigma(\omega)$  + param. [Knecht, NB]



$$\Sigma_{\sigma}(\omega) = U \left( \langle \hat{n}_{-\sigma} \rangle - \frac{1}{2} \right) \omega^0 + U^2 \langle \hat{n}_{-\sigma} \rangle (1 - \langle \hat{n}_{-\sigma} \rangle) \omega^{-1} + \mathcal{O}(\omega^{-2})$$

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

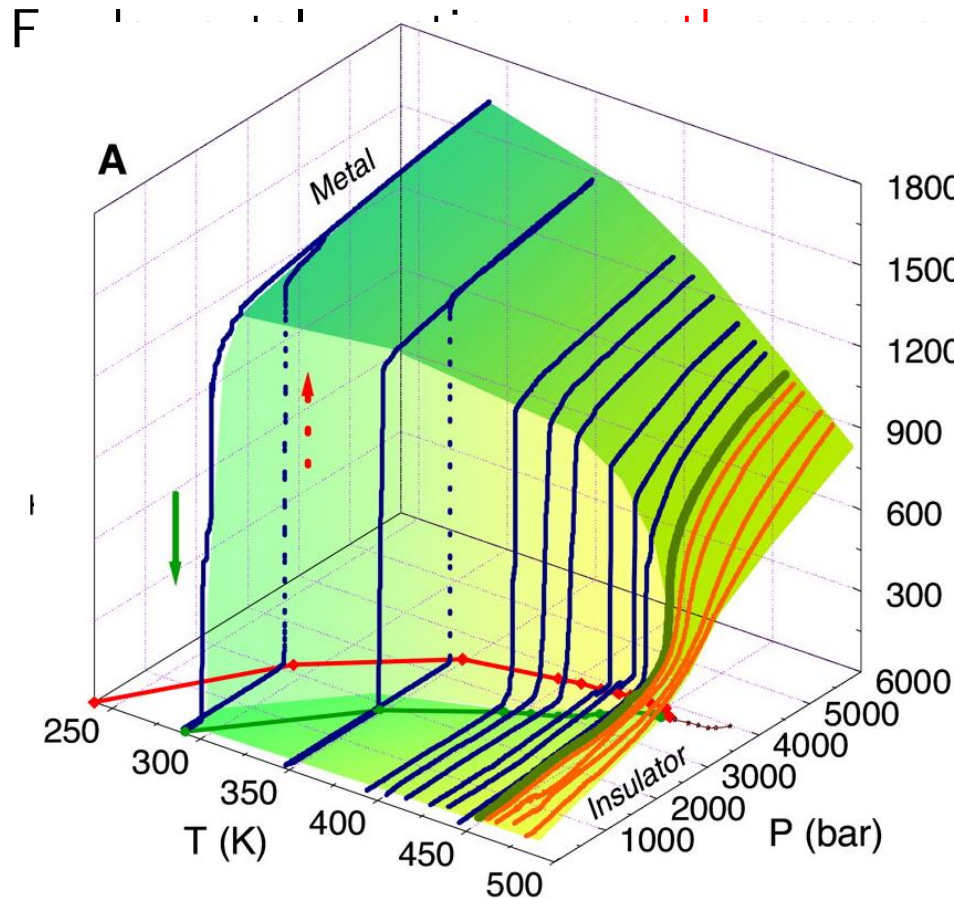
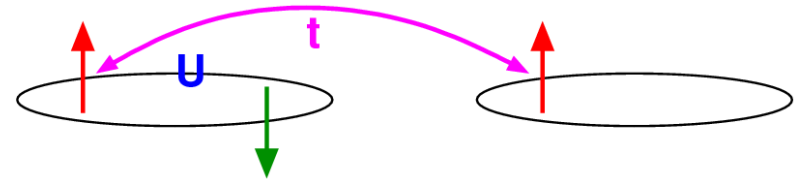


Rapid convergence at all frequencies for “QMC +  $1/\omega$ ” DMFT solver

# Update: Orbital-selective Mott transitions

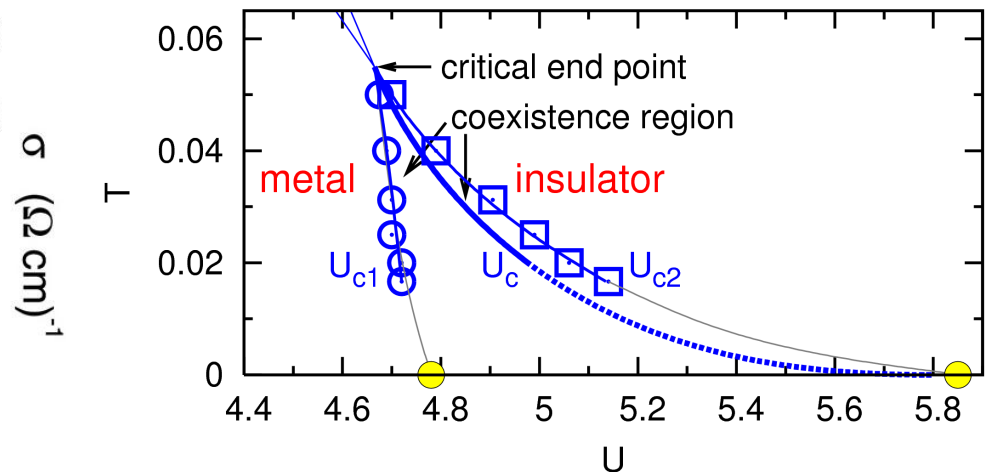
Step back: Mott transition in frustrated 1-band Hubbard model

$$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



From metal to insulator or (within DMFT)?

No conclusive answer up to 1999

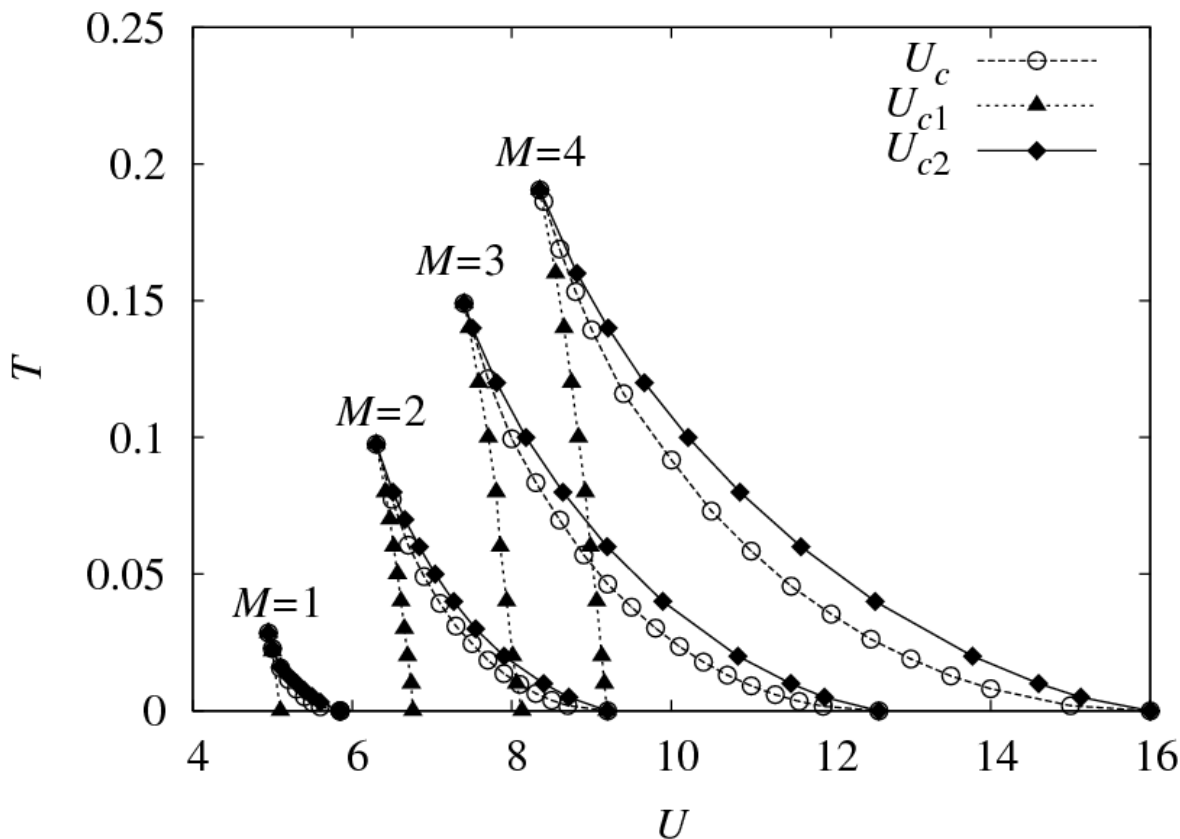


Now accepted: 1<sup>st</sup> order transition for  $0 < T < T^*$  (QMC + ePT, 2000-2005)

# Multiorbital case ( $M > 1$ orbitals, half filling $n = M$ )?

Extension without additional parameters: SU(2M) symmetric case:

$$H = -t \sum_{\langle i,j \rangle, m, \sigma} c_{im\sigma}^\dagger c_{jm\sigma} + \frac{U}{2} \sum_i \sum_{(m,\sigma) \neq (m'\sigma')} n_{im\sigma} n_{im\sigma'}$$



$$U_c(M) \propto \sqrt{M}$$

[Koch et al., PRB(1999)]

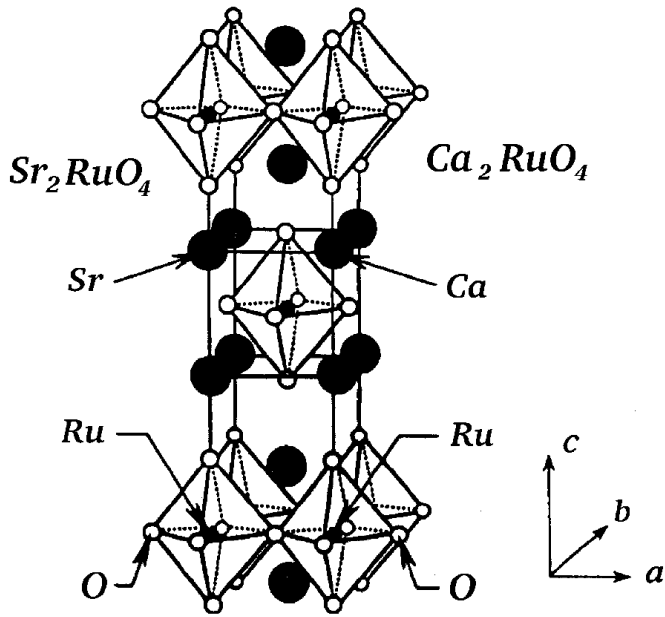
$$U_{c1} \propto \sqrt{M}, \quad U_{c2}(M) \sim 2M E_{\text{kin}}^0$$

[Florens et al., PRB (2002)]

but still **single Mott transition**

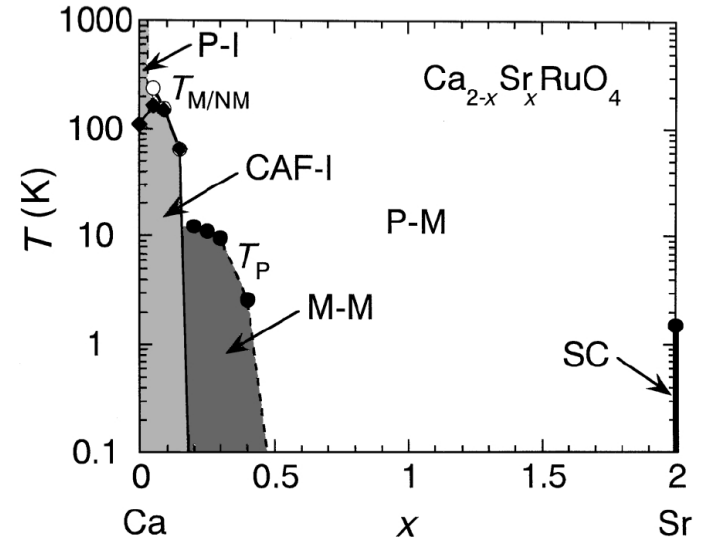
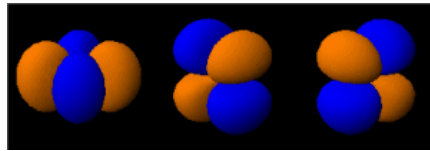
[Inaba, Koga, Suga, Kawakami, PRB **72**, 085112 (2005)]

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



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

4 valence electrons  
in 3 Ru  $t_{2g}$  orbitals



[Nakatsuji, Maeno, PRL (2000)]

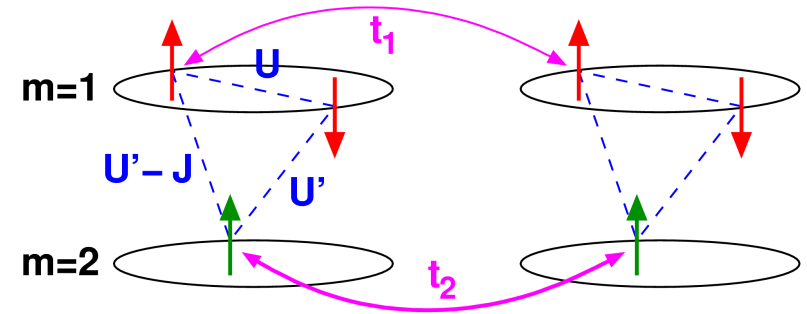
susceptibility, MR  $\rightsquigarrow$   $S = 1/2$  system (+ easy axis) for  $0.2 < x \lesssim 0.5$  (not  $S = 1$ )

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

Possible mechanism: different effective hopping amplitudes for in-plane and out-of-plane orbitals [Anisimov et al., EPJB (2002)]

# 2-band model with orbital-dependent hopping

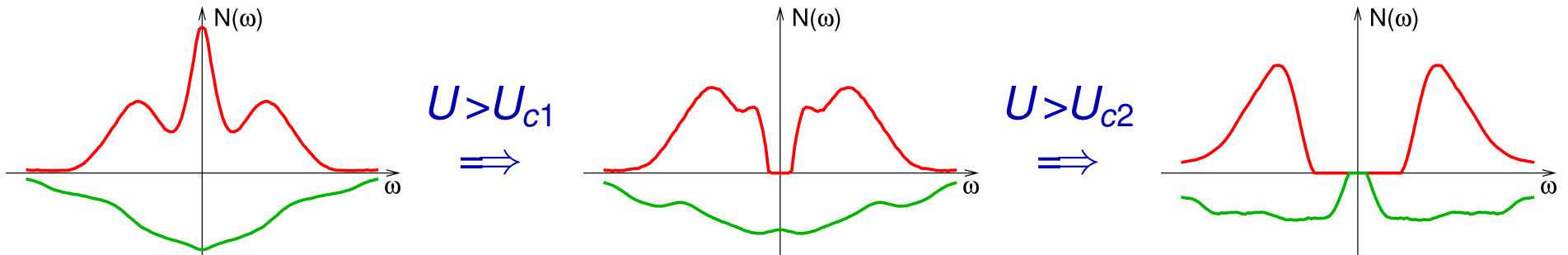
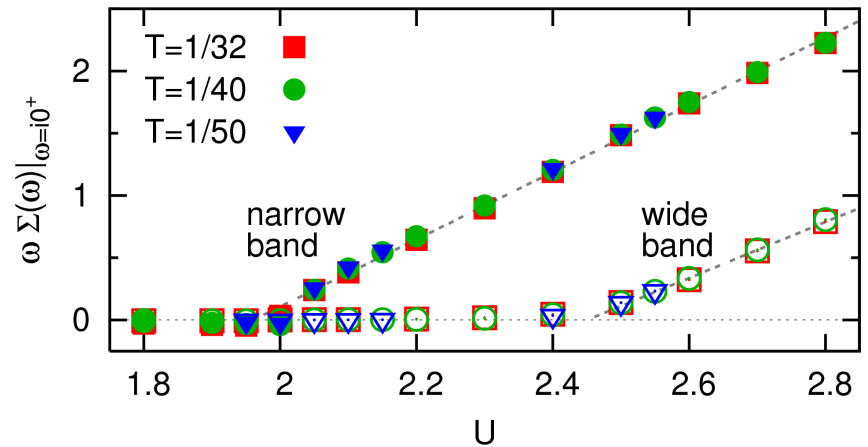
$$H = \sum_{m=1}^2 \left[ - \sum_{\langle ij \rangle \sigma} t_m c_{im\sigma}^\dagger c_{jm\sigma} + U \sum_i n_{im\uparrow} n_{im\downarrow} \right] + \sum_{i\sigma\sigma'} (U' - \delta_{\sigma\sigma'} J_Z) n_{i1\sigma} n_{i2\sigma'}$$



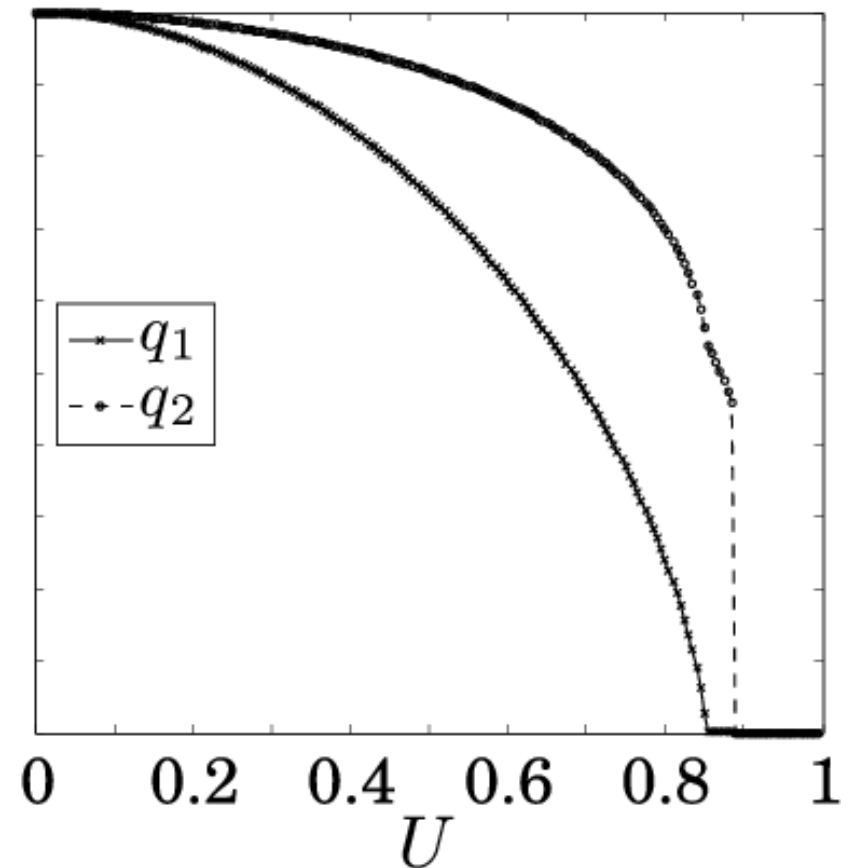
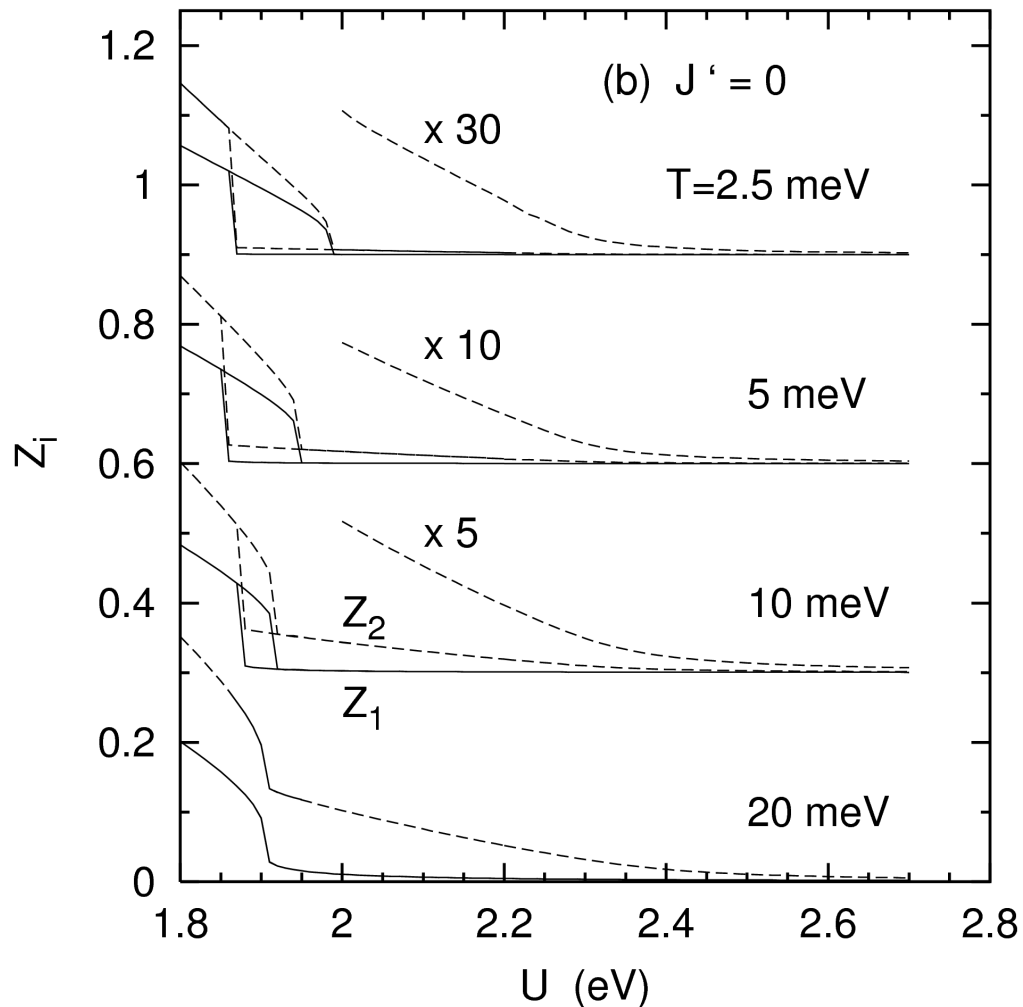
Ising-type Hund couplings with  $t_2/t_1 = 2$  and  $U' = U/2$ ,  $J_Z = U/4$  [Liebsch, PRB (2004)]

## 2 well-defined phase transitions

[Knecht et al. (PRB 2005), de' Medici et al. (PRB 2005), Rüegg et al. (EPJB 2005)]



# Order of wide-band transition in anisotropic model

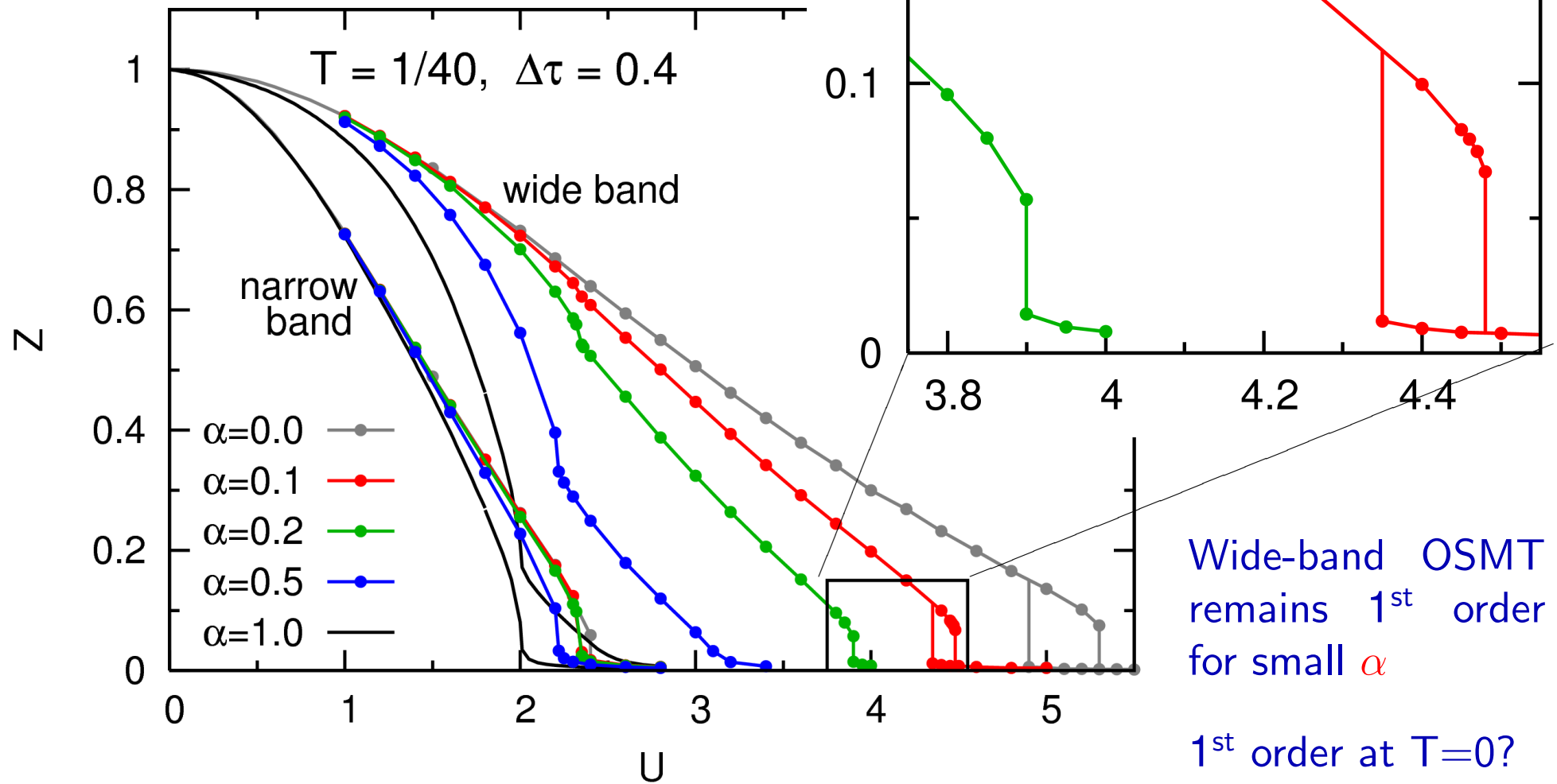


Slave-boson MF  $\rightsquigarrow$  1<sup>st</sup> order wide-band transition (at  $T = 0$ ) [Rüegg, Indergand, Pilgram, Sigrist, EPJB (2005)]

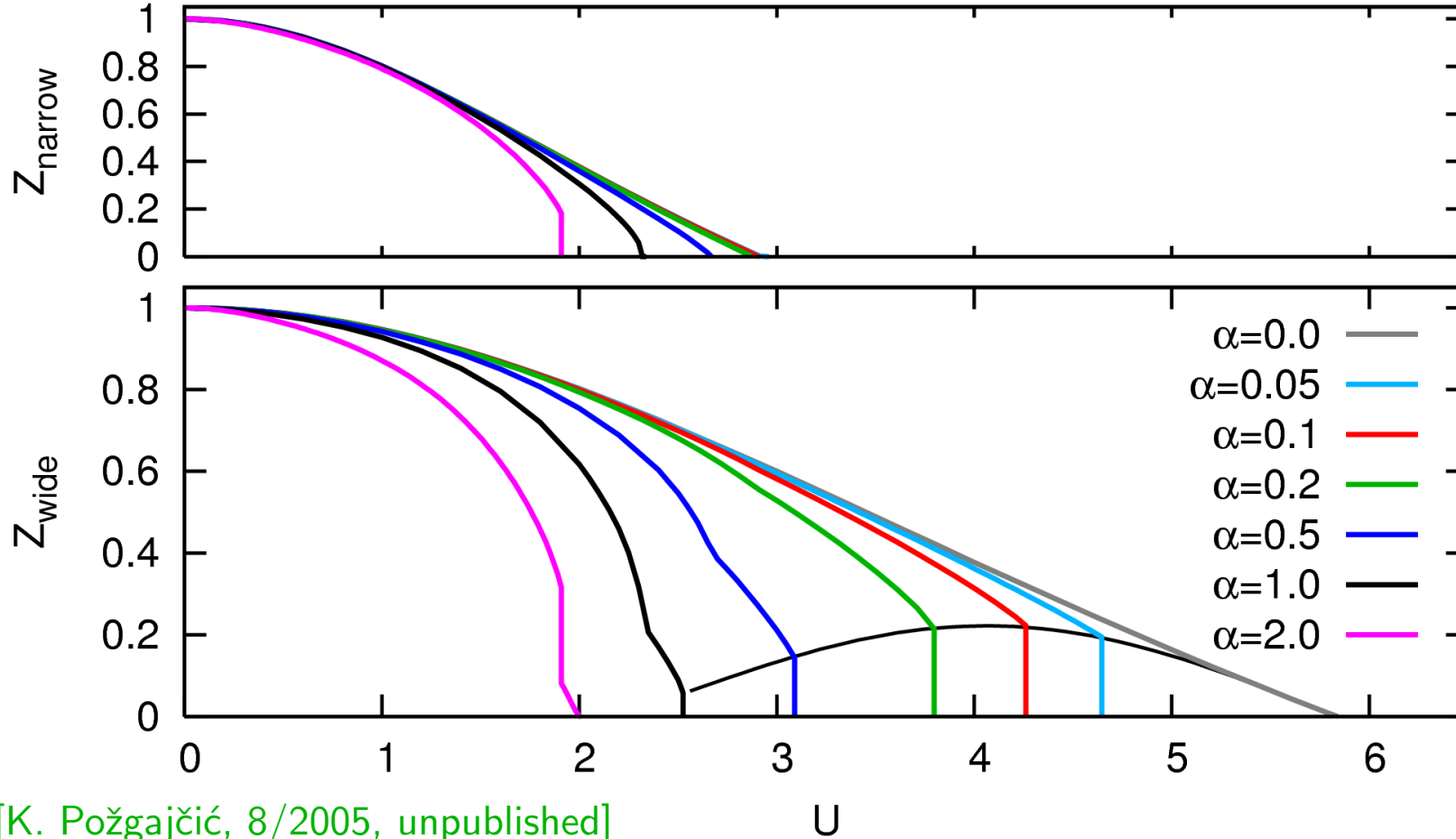
ED  $\rightsquigarrow$  no hysteresis at low  $T$  for wide-band transition [Liebsch, PRL (2005)]

# Systematic study: effect of inter-orbital coupling

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



# Self-energy functional theory (SFT+ED) with 1 bath site per orbital



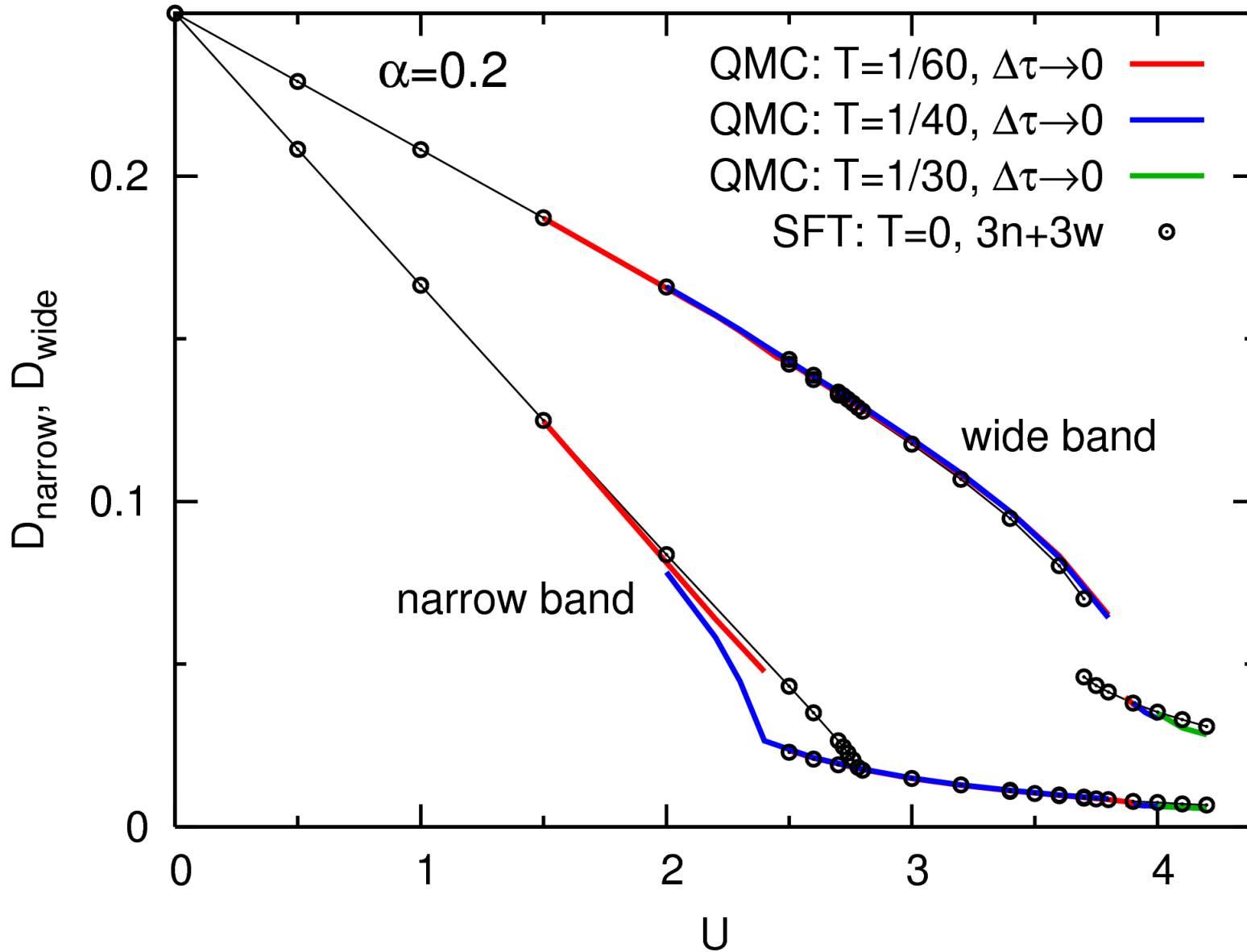
[K. Požgajčić, 8/2005, unpublished]

- 1<sup>st</sup> order wide-band transition for  $0 < \alpha \lesssim 1.5$
- larger  $\alpha$ : 2<sup>nd</sup> order  $\leftrightarrow$  1<sup>st</sup> order

**Problems:**

- Low-frequency part of  $\Sigma(\omega)$  inconsistent with QMC
- $Z$  ill-defined in OSM phase
- strong finite-size effects

# Double occupancy (1<sup>st</sup> order derivative of $\Omega$ )



Excellent agreement between SFT and QMC

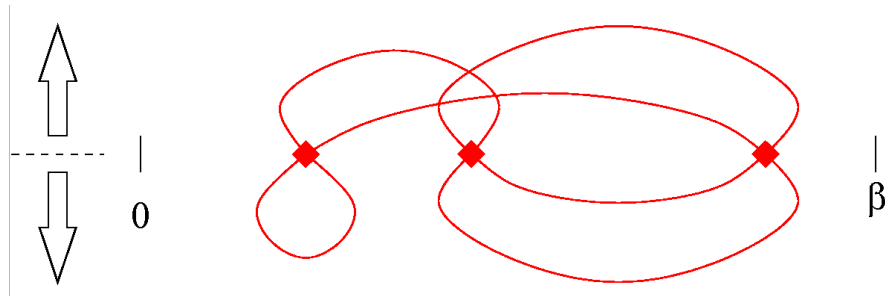
1<sup>st</sup> order at  $T=0$  (at least) for  $0 < \alpha \leq 0.2$

# Efficiency of Quantum Monte Carlo DMFT solvers

New development: continuous-time QMC algorithms

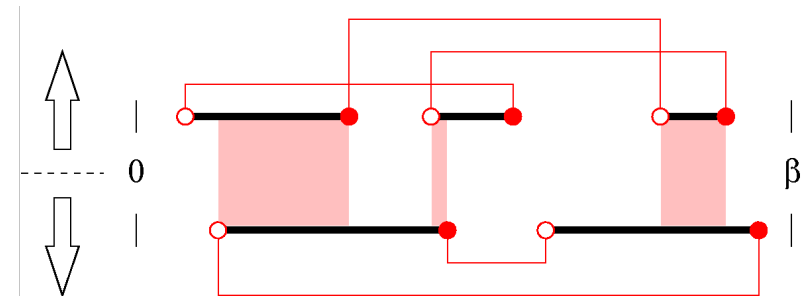
1. weak-coupling expansion

[Rubtsov, Savkin, Lichtenstein, PRB (2005)]



2. hybridization expansion

[Werner et al., PRL (2006)]

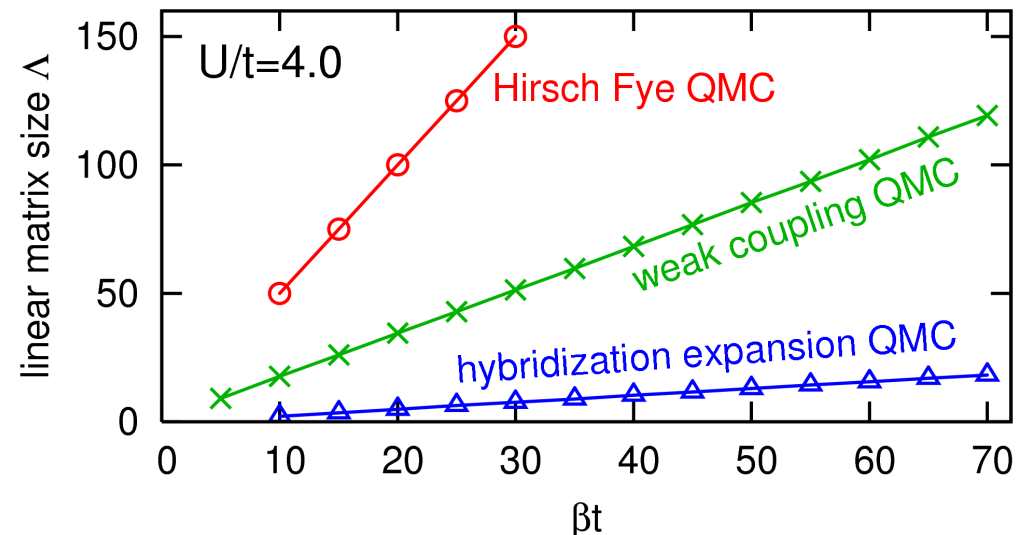


CT-QMC methods: smaller matrices

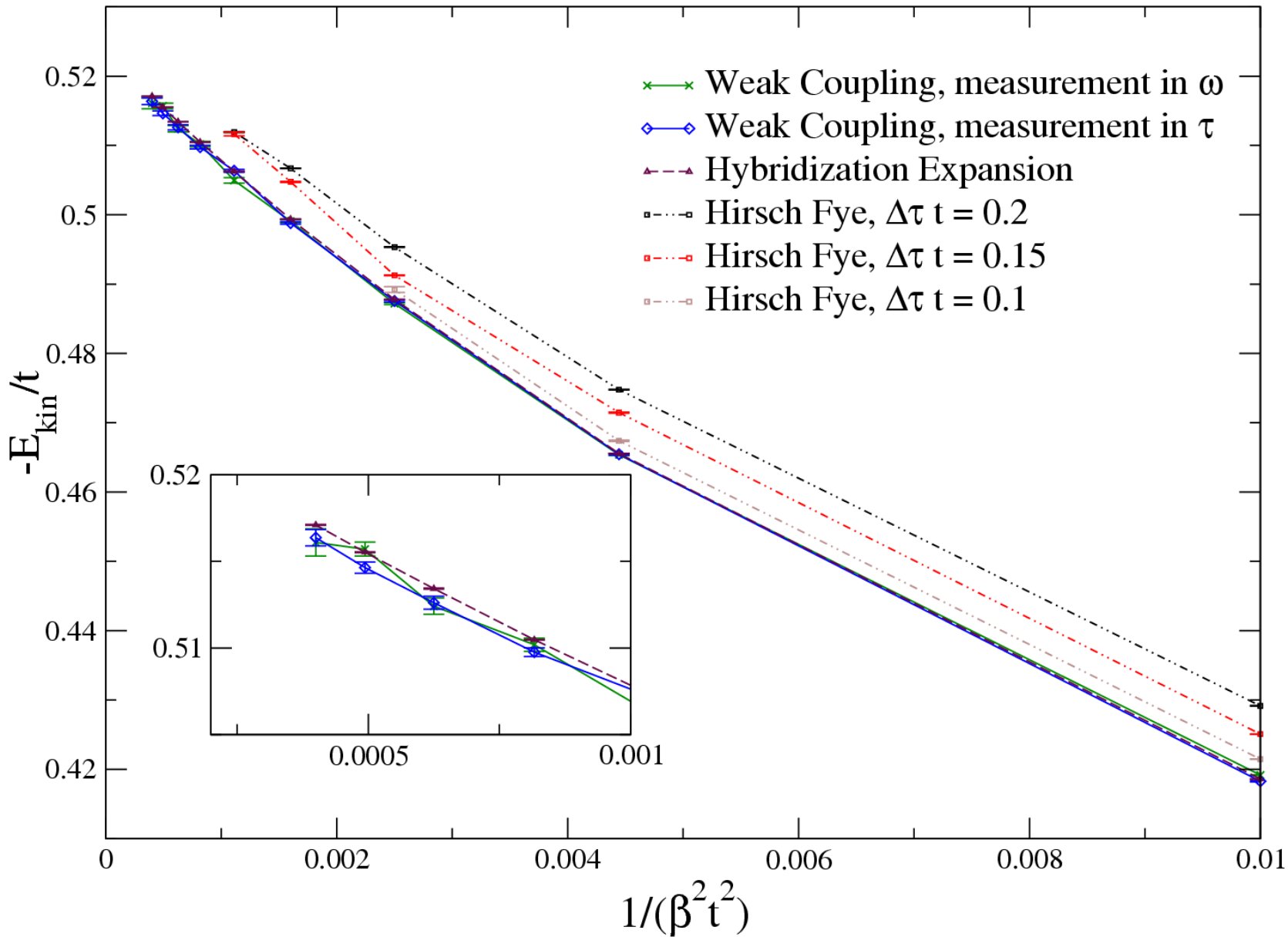
All QMC methods: effort  $\propto \Lambda^3$

Claim [Troyer (2006)]:

CT-QMC more efficient than HF-QMC by orders of magnitude



# Kinetic energy vs. squared temperature ( $U/t = 4.0$ )



[Gull et al., cond-mat/0609438]

HF-QMC useless at small T!?

# Performance analysis: CT-QMC methods versus HF-QMC

## Performance analysis of continuous-time solvers for quantum impurity models

Emanuel Gull,<sup>1</sup> Philipp Werner,<sup>2</sup> Andrew Millis,<sup>2</sup> and Matthias Troyer<sup>1</sup>

<sup>1</sup>*Institut für theoretische Physik, ETH Zürich, CH-8093 Zürich, Switzerland*

<sup>2</sup>*Columbia University, 538 West, 120th Street, New York, NY 10027, USA*

Impurity solvers play an essential role in the numerical investigation of strongly correlated electrons systems within the “dynamical mean field” approximation. Recently, a new class of **continuous-time solvers** has been developed, based on a diagrammatic expansion of the partition function in either the interactions or the impurity-bath hybridization. We **investigate the performance** of these two complimentary approaches and **compare them to the well-established Hirsch-Fye method**. The results show that the continuous-time methods, and in particular the version which expands in the hybridization, provide **substantial gains in computational efficiency**.

PACS numbers: 71.10.-w, 71.10.Fd, 71.28.+d, 71.30.+h

[\[cond-mat/0609438\]](#)

- Test case: 1-band Hubbard model (semi-elliptic DOS,  $n = 1$ ,  $W = 4$ ) for  $U = 4$
- Focus on low temperatures:  $T = 1/45$
- Additional results for doped model (also different  $U$ )

Good Hirsch-Fye implementation?

Fair comparison?

Precision of results?

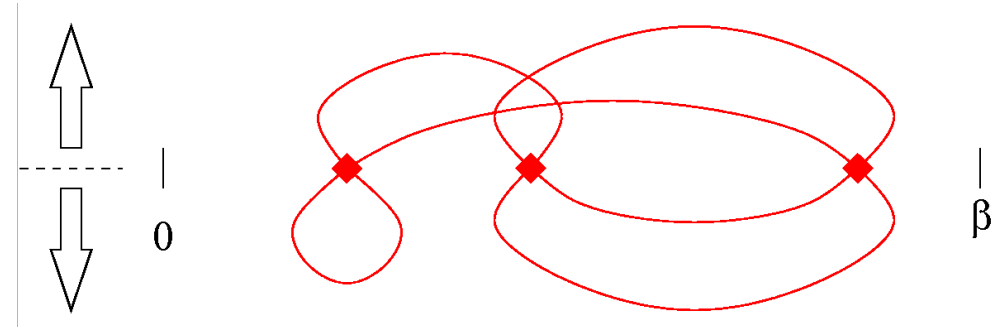
# Principles of weak-coupling CT-QMC

Decouple action into quadratic part

$$S_0 = - \int_0^\beta d\tau d\tau' \sum_\sigma c_\sigma(\tau) F_\sigma(\tau - \tau') c_\sigma^\dagger(\tau') - \mu \int_0^\beta d\tau (n_\uparrow + n_\downarrow)$$

and an interaction part

$$S_U = U \int_0^\beta d\tau n_\uparrow n_\downarrow,$$



where  $\mathcal{G}_{0,\sigma}^{-1}(i\omega) = i\omega + \mu - F_\sigma(-i\omega)$ .

[Gull et al. cond-mat/0609438]

$$Z = \sum_k \frac{(-U)^k}{k!} \int d\tau_1 \dots d\tau_k \text{Tr} T_\tau e^{-S_0} n_\uparrow(\tau_1) n_\downarrow(\tau_1) \dots n_\uparrow(\tau_k) n_\downarrow(\tau_k)$$

is sampled by random insertions/removals of vertices. Trick: avoid sign problem

[Rubtsov, Savkin, Lichtenstein, PRB **72**, 035122 (2005)]

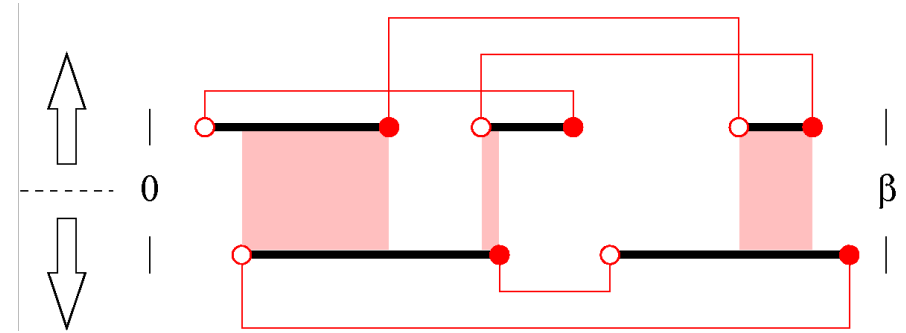
# Principles of hybridization expansion CT-QMC

Decompose action into local part

$$S_L = -\mu \int_0^\beta d\tau (n_\uparrow + n_\downarrow) + U \int_0^\beta d\tau n_\uparrow n_\downarrow$$

and hybridization part

$$S_F = - \int_0^\beta d\tau d\tau' \sum_\sigma c_\sigma(\tau) F_\sigma(\tau - \tau') c_\sigma^\dagger(\tau');$$



[Gull et al. cond-mat/0609438]

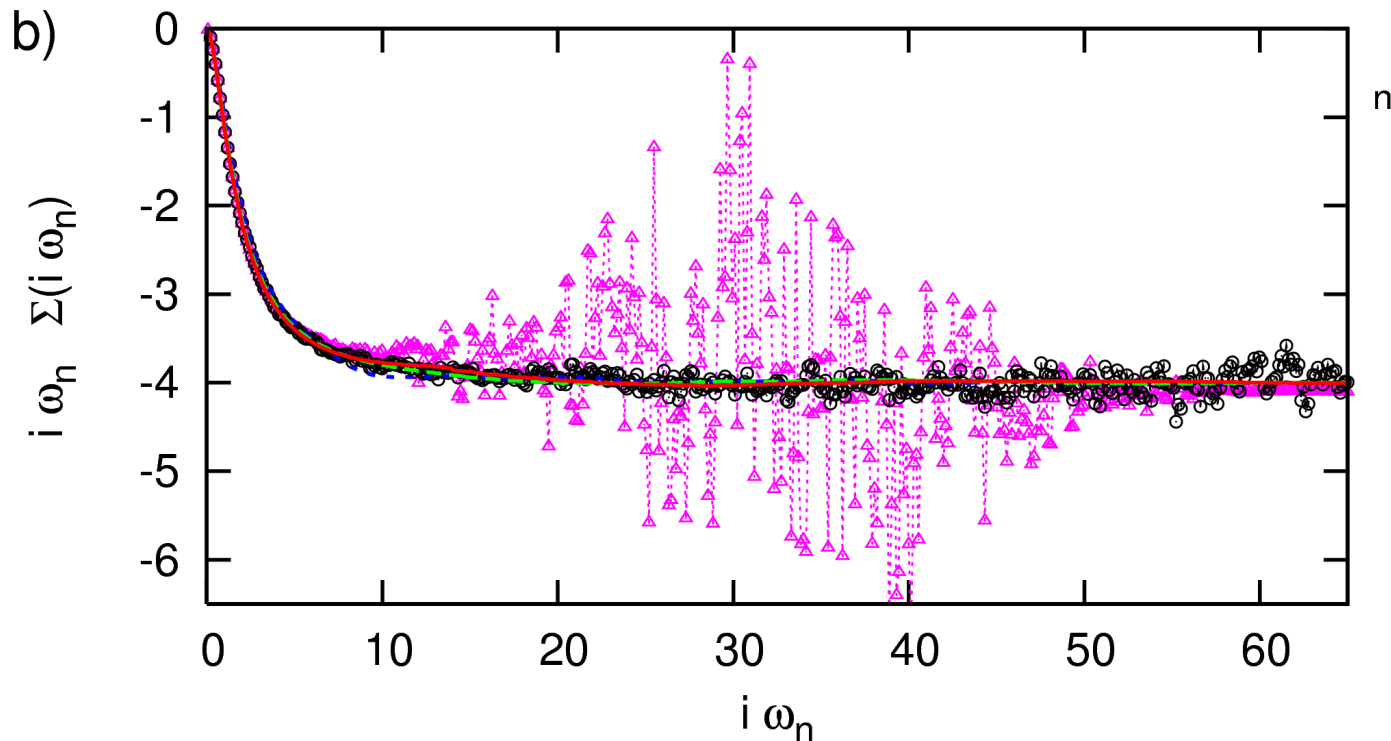
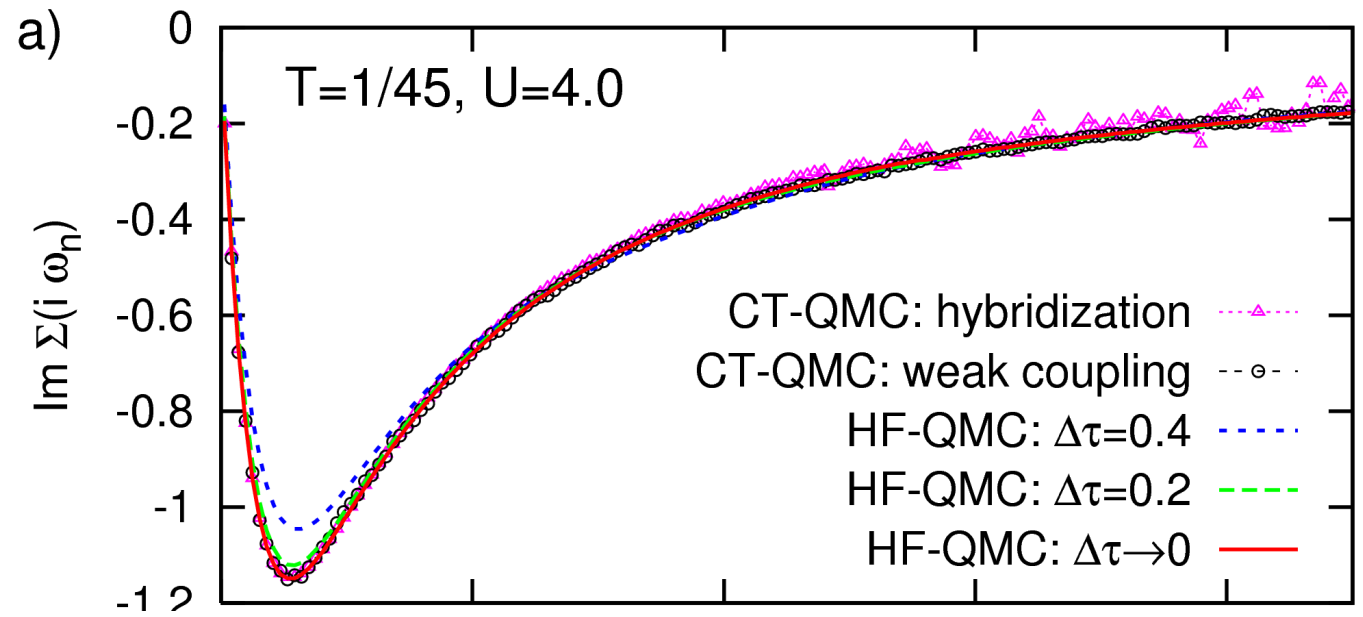
expanding the partition function in powers of  $F_\sigma$  leads to:

$$Z = \text{Tr} T_\tau e^{-S_L} \prod_\sigma \sum_{k_\sigma} \frac{1}{k_\sigma!} \int_0^\beta d\tau_1^\sigma \dots d\tau_{k_\sigma}^\sigma \int_0^\beta d\tilde{\tau}_1^\sigma \dots d\tilde{\tau}_{k_\sigma}^\sigma$$

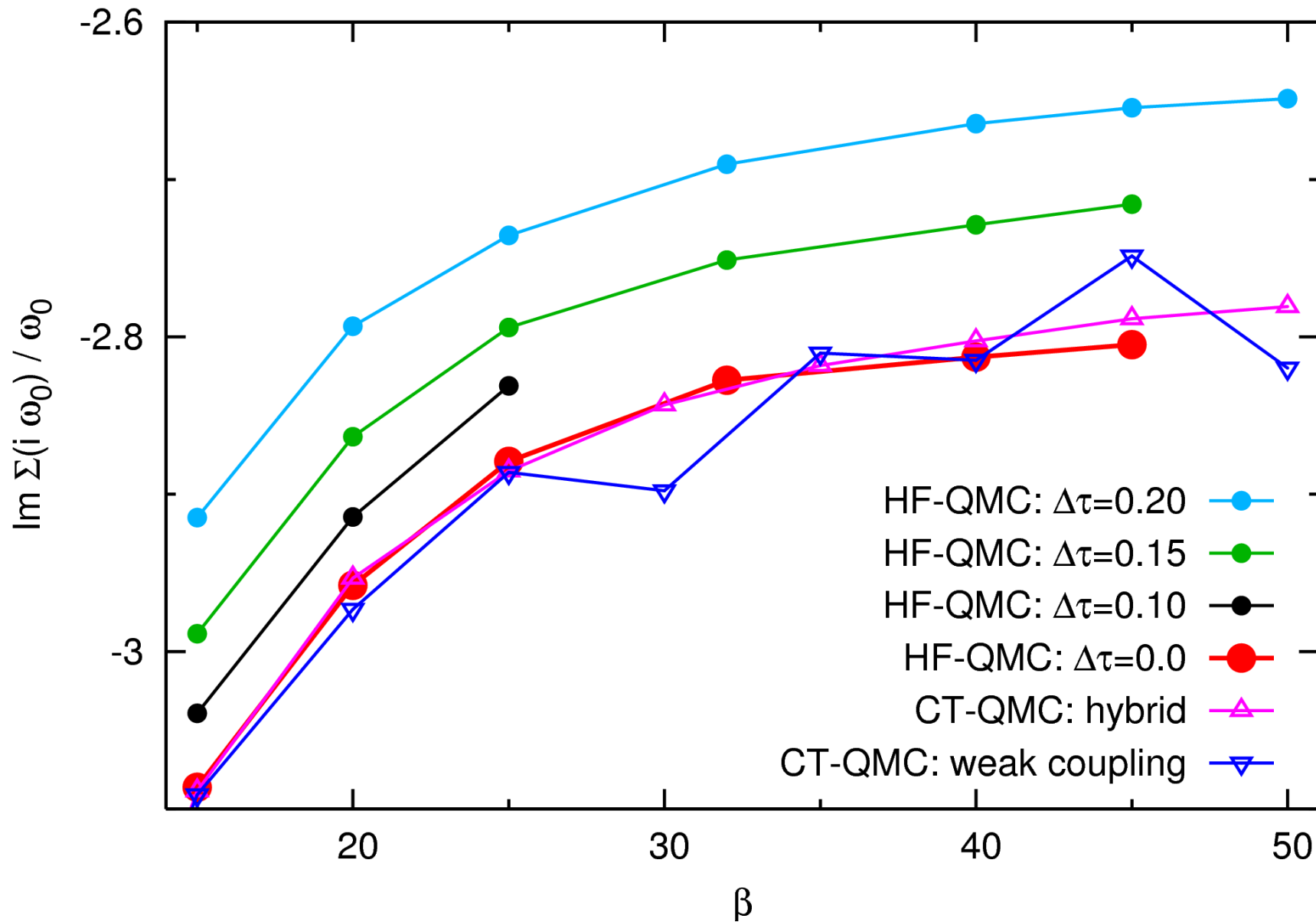
$$\times \left[ c_\sigma(\tau_1) F_\sigma(\tau_1 - \tilde{\tau}_1) c_\sigma^\dagger(\tilde{\tau}_1) \dots c_\sigma(\tau_{k_\sigma}) F_\sigma(\tau_{k_\sigma} - \tilde{\tau}_{k_\sigma}) c_\sigma^\dagger(\tilde{\tau}_{k_\sigma}) \right].$$

Express combined weight corresponding to given collection  $\{c_\sigma^\dagger(\tilde{\tau}_i), c_\sigma(\tau_i)\}_{i=1, \dots, k_\sigma}$  of creation and annihilation operators as the determinant of a matrix  $D_{F, \sigma}$ ,  
sample . . . [Werner et al., PRL **97**, 076405 (2006); Werner and Millis, PRB **76**, 1 (2006)]

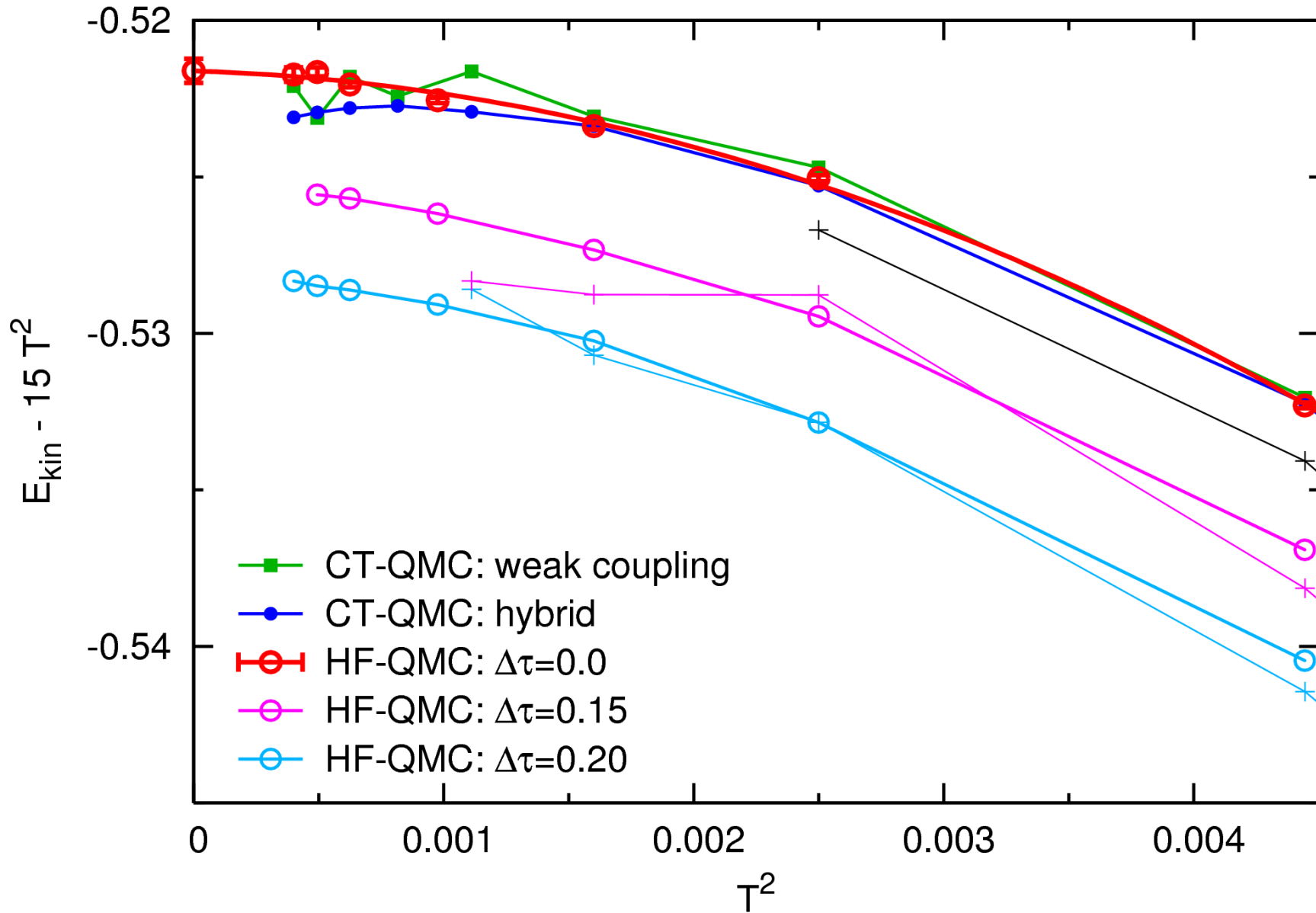
# Self-energy



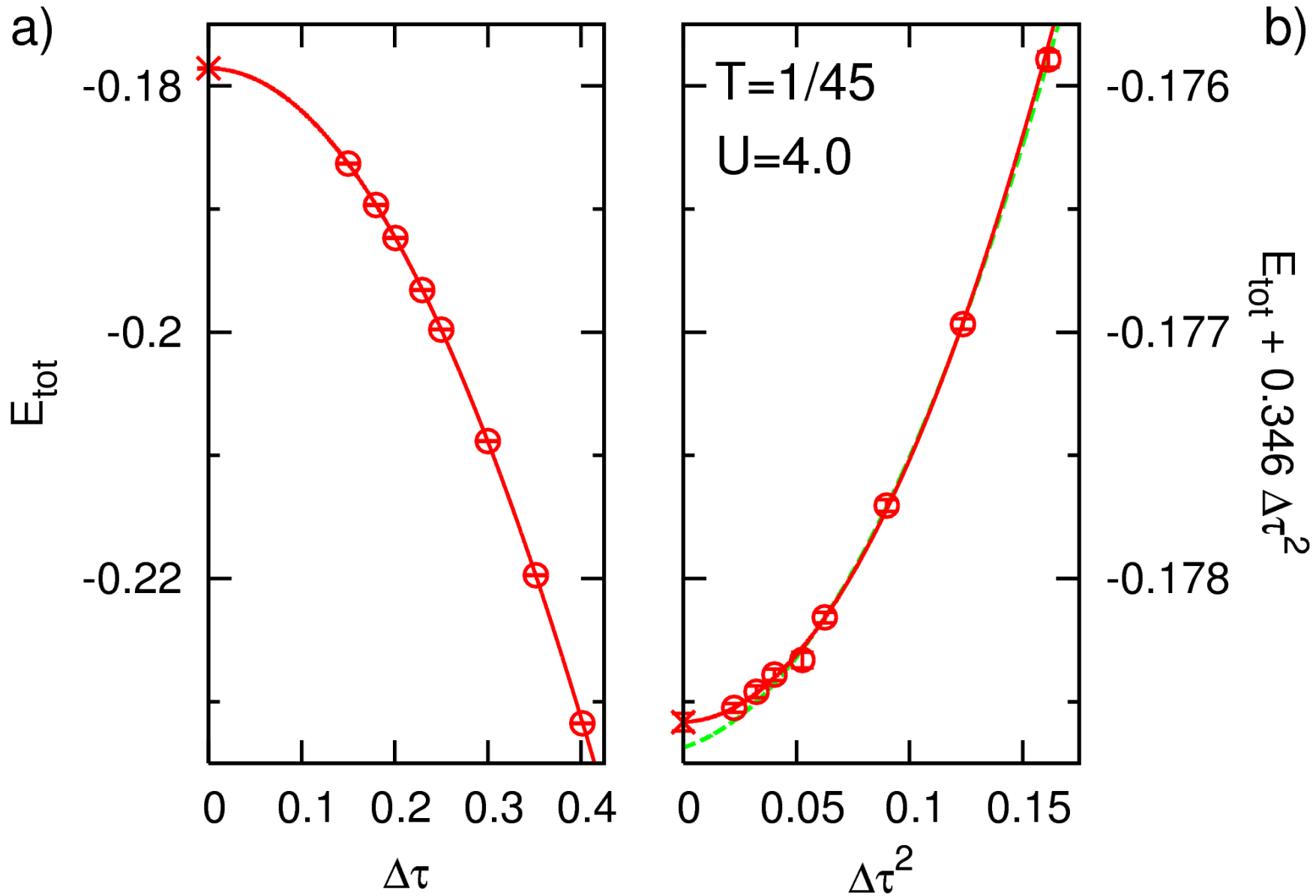
Self-energy:  $\text{Im}\Sigma(i\omega_0)/\omega_0 = 1 - 1/Z$  for  $U = 4$



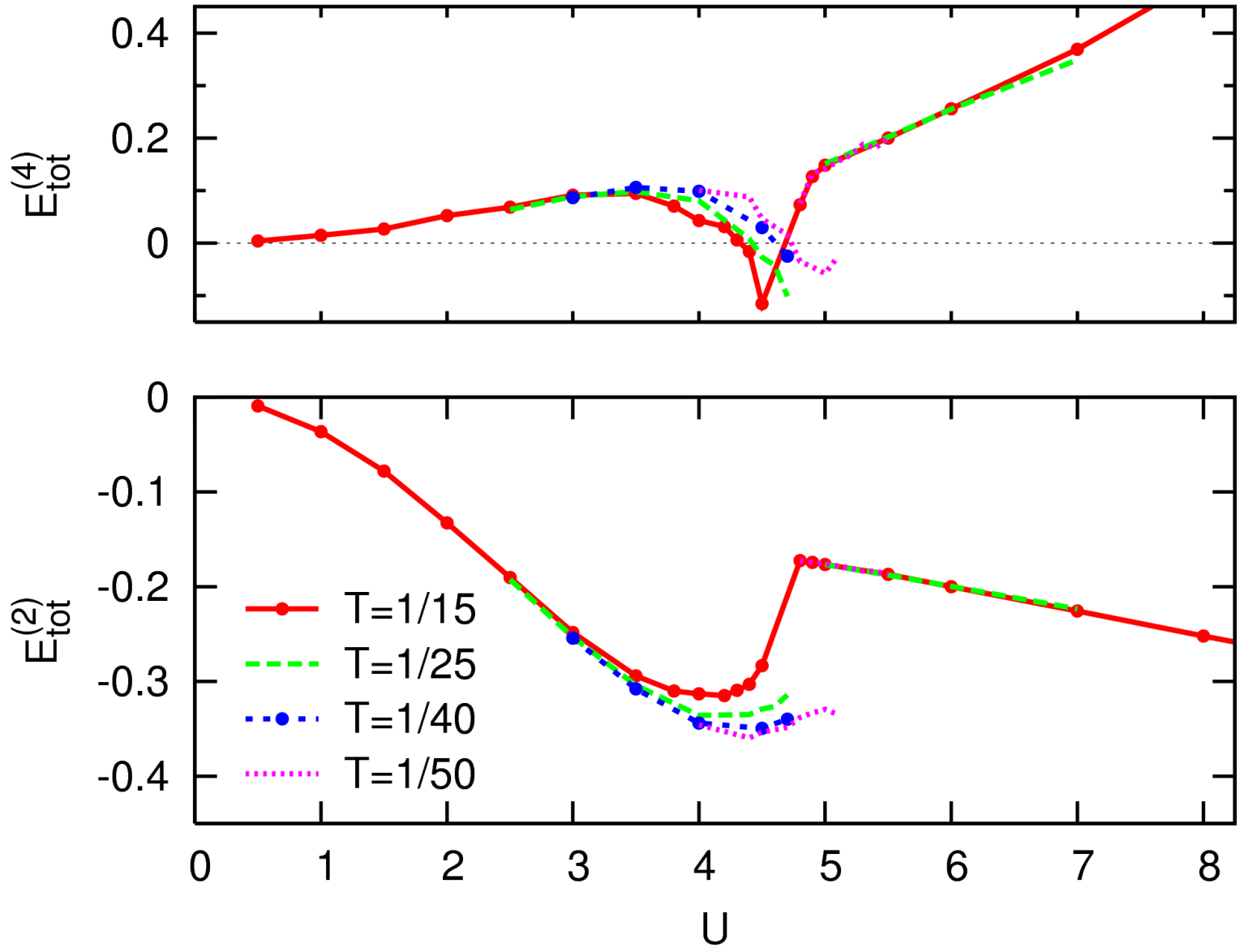
# Energetics: kinetic energy for $U = 4$



# Essential step in HF-QMC: extrapolation $\Delta\tau \rightarrow 0$

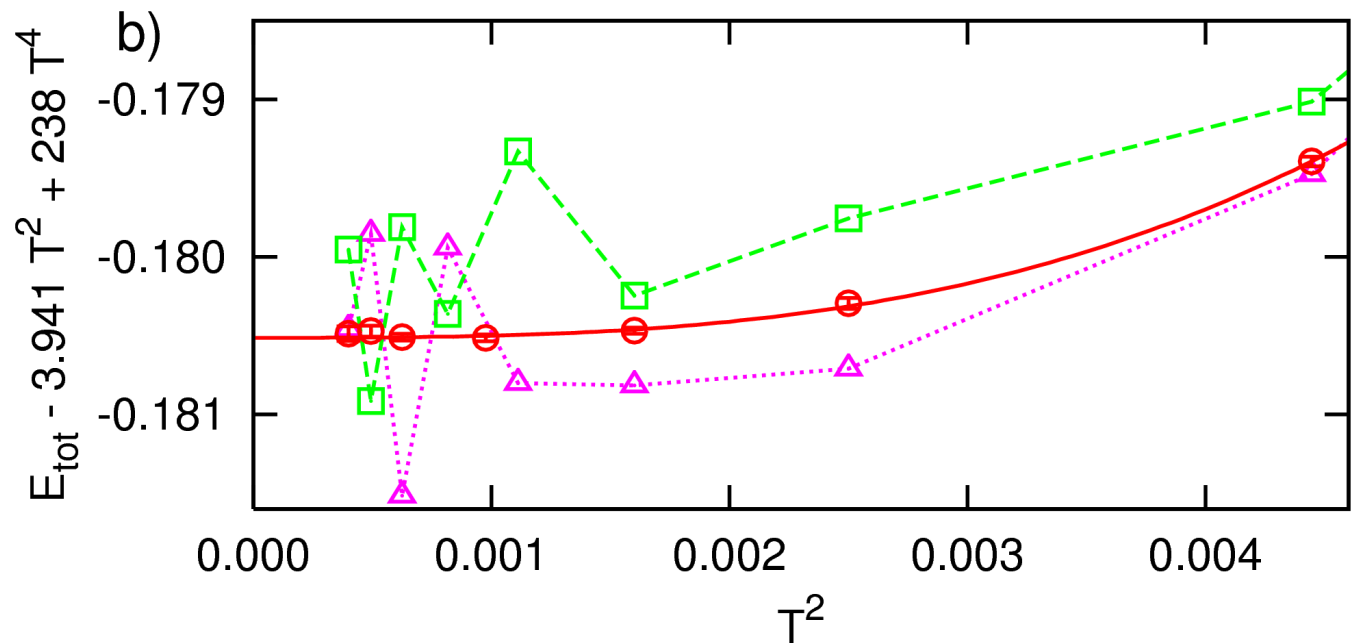
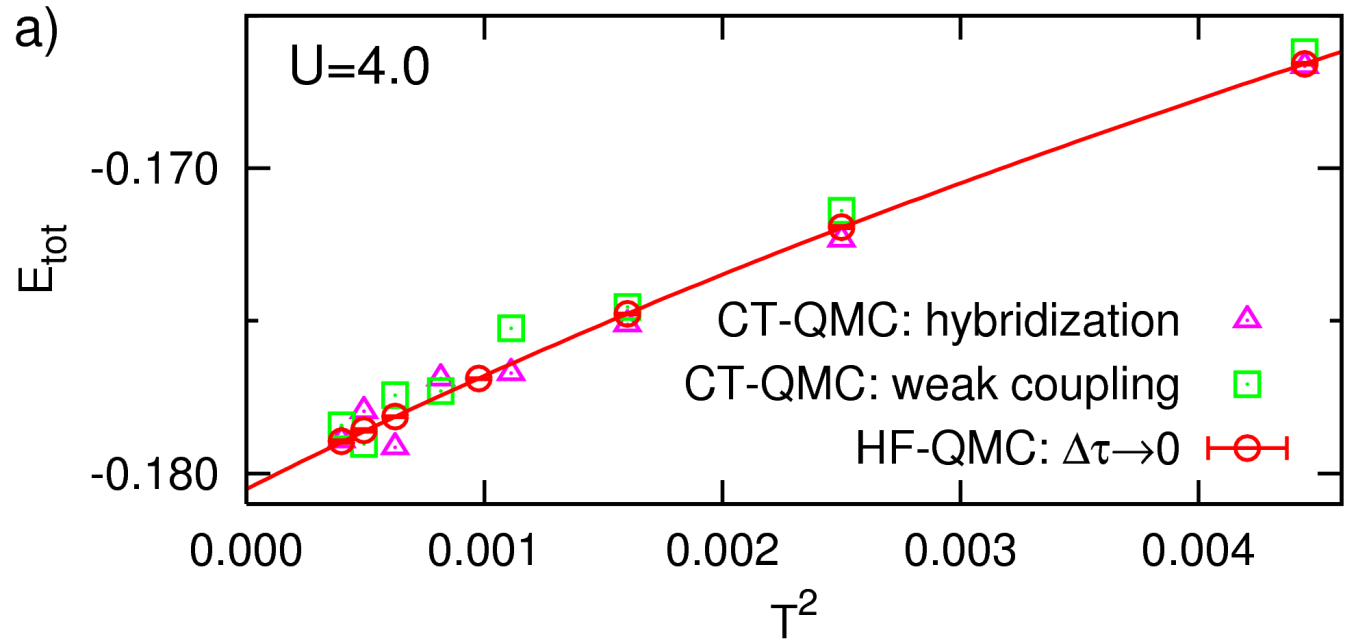


$\Delta\tau$  dependence very regular (except at phase transition)

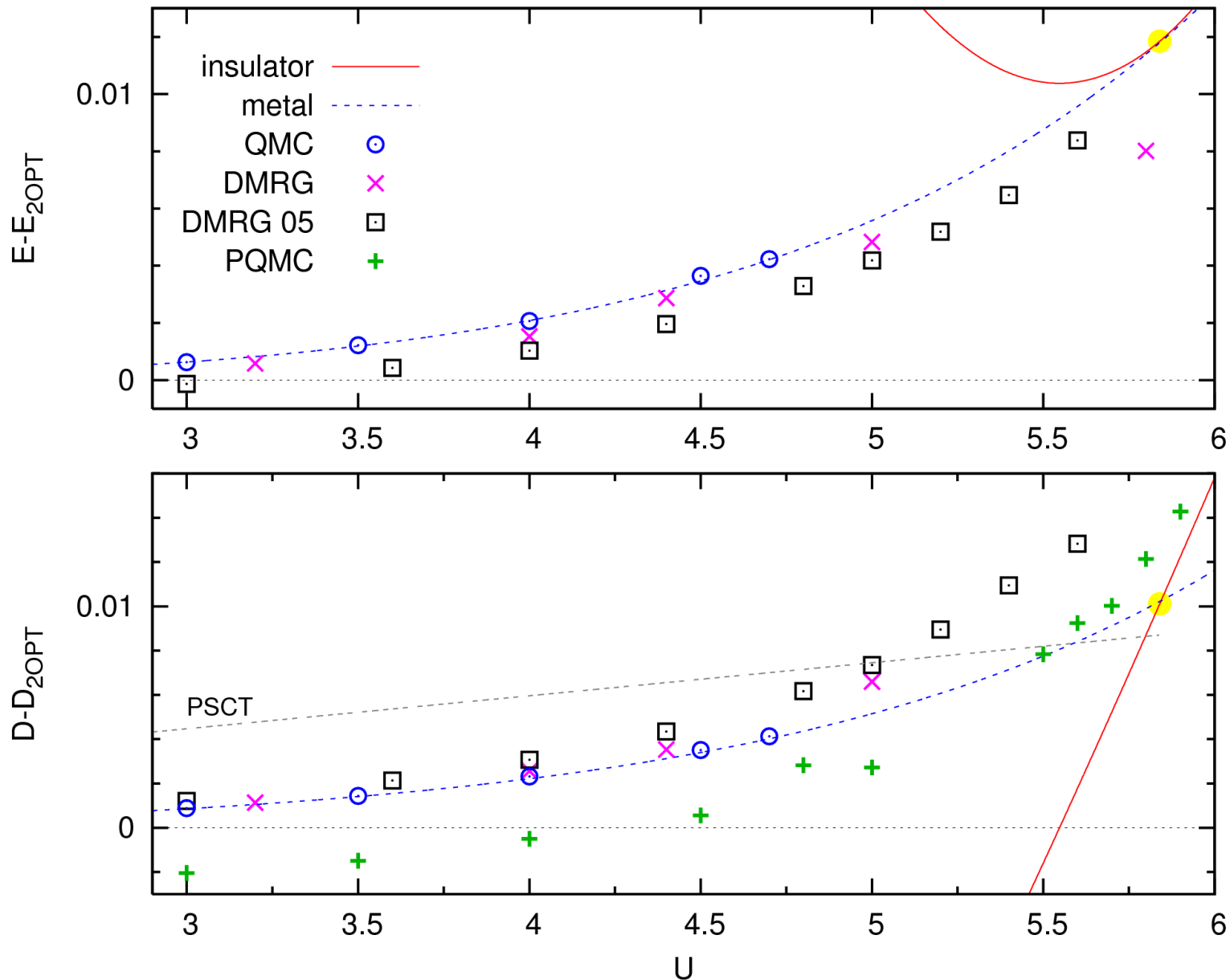


# Comparison for total energy

HF-QMC is more efficient (much higher precision at slightly higher cost)



# Precision: HF-QMC vs. ground state methods



# Summary

Cooperative phenomena in correlated electron systems

Theoretical approaches: (multi-band) Hubbard models, DMFT

High-precision Hirsch-Fye quantum Monte-Carlo algorithm

Orbital-selective Mott transitions: 1<sup>st</sup> order for wide band

Efficiency: HF-QMC competitive with continuous-time QMC

Not covered: Critical exponents from QMC and strong-coupling PT

[Theory of half-metallic double perovskites](#)

Realistic material-specific calculations with LDA+DMFT

# Outlook

Band structure calculations for correlated systems

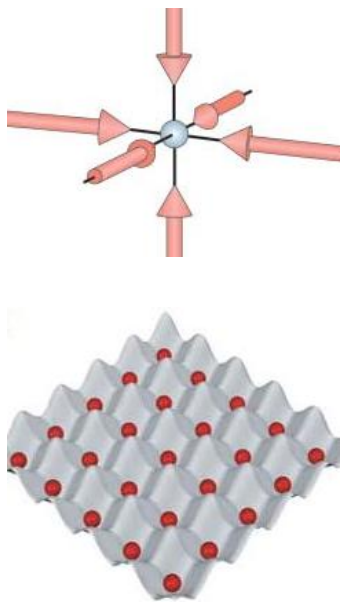
Cluster extensions of DMFT

[Ultracold quantum gases on optical lattices](#)

# Starting in 7/2007: SFB/TRR 49 (Frankfurt - Kaiserslautern - Mainz)

## Condensed matter systems with variable many-body interactions

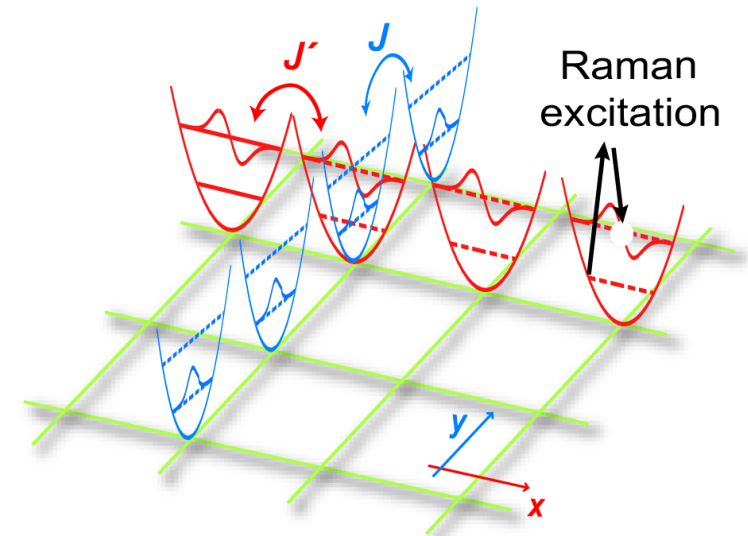
- A1 [Bloch] – Ultracold Fermi mixtures in optical lattices
  - A2 [Kuhr/Bloch] – Spatially addressable quantum gases in optical lattices
  - A3 [Hofstetter] – Inhomogeneous quantum phases in ultracold gases with strong correlations
  - A5 [Fleischhauer/Eggert] – Advanced numerical methods for correlated quantum gases
  - A6 [Blümer] – Flavour-selective Mott transitions of ultracold quantum gases on optical lattices
  - A7 [Hillebrands/Serha] – Collective effects and instabilities of a magnon gas
  - A8 [Kopietz] – Interacting magnons and critical behaviour of bosons
- project area B: real materials



A1 + A6: flavor selectivity in Fermi mixtures of different

- atomic species:  ${}^6\text{Li}$  and  ${}^{40}\text{K}$
  - hyperfine states
  - vibrational levels
- on optical lattices

Hopping amplitudes tunable and flavor-dependent!



[Müller, Fölling, Widera, Bloch (2007)]