Precise, efficient, and unbiased QMC simulations within DMFT

Nils Blümer, Univ. Mainz

Outline

Precise, efficient, and unbiased QMC simulations within DMFT

Nils Blümer, Univ. Mainz

Outline

Minimal background

What has been achieved? What is new?

Precise, efficient, and unbiased QMC simulations within DMFT

Nils Blümer, Univ. Mainz

Outline

Minimal background

What has been achieved? What is new?

Some more background

How does it work? Why?

Precise, efficient, and unbiased QMC simulations within DMFT

Nils Blümer, Univ. Mainz

Outline

Minimal background

What has been achieved? What is new?

Some more background

How does it work? Why?

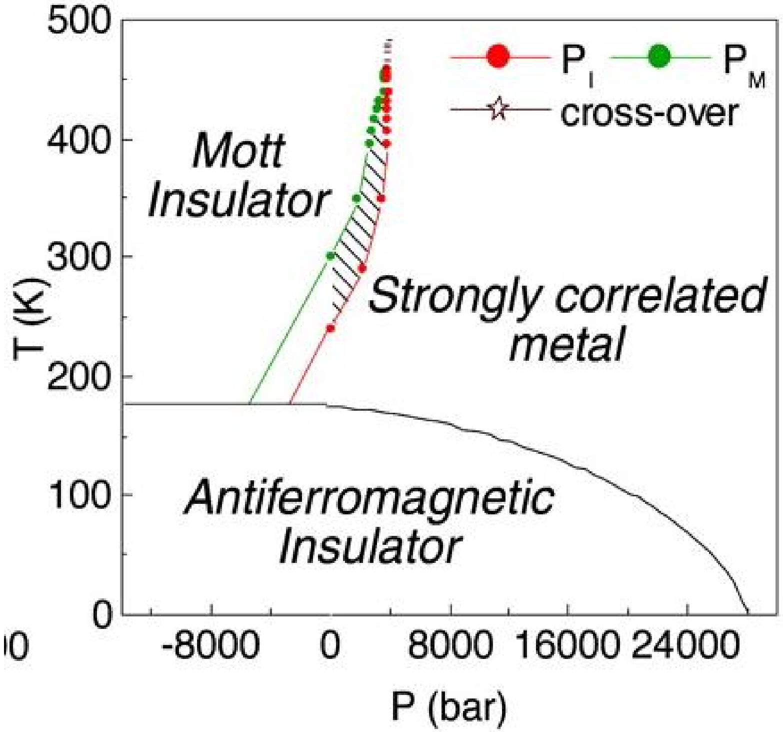
Application(s)

Minimal background

Mott metal-insulator transition

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

Phase diagram

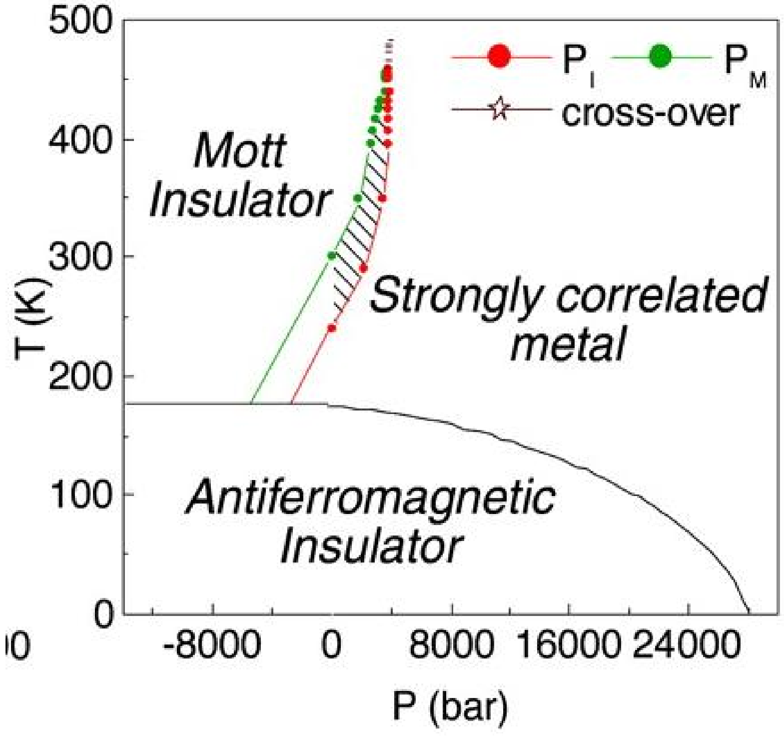


Minimal background

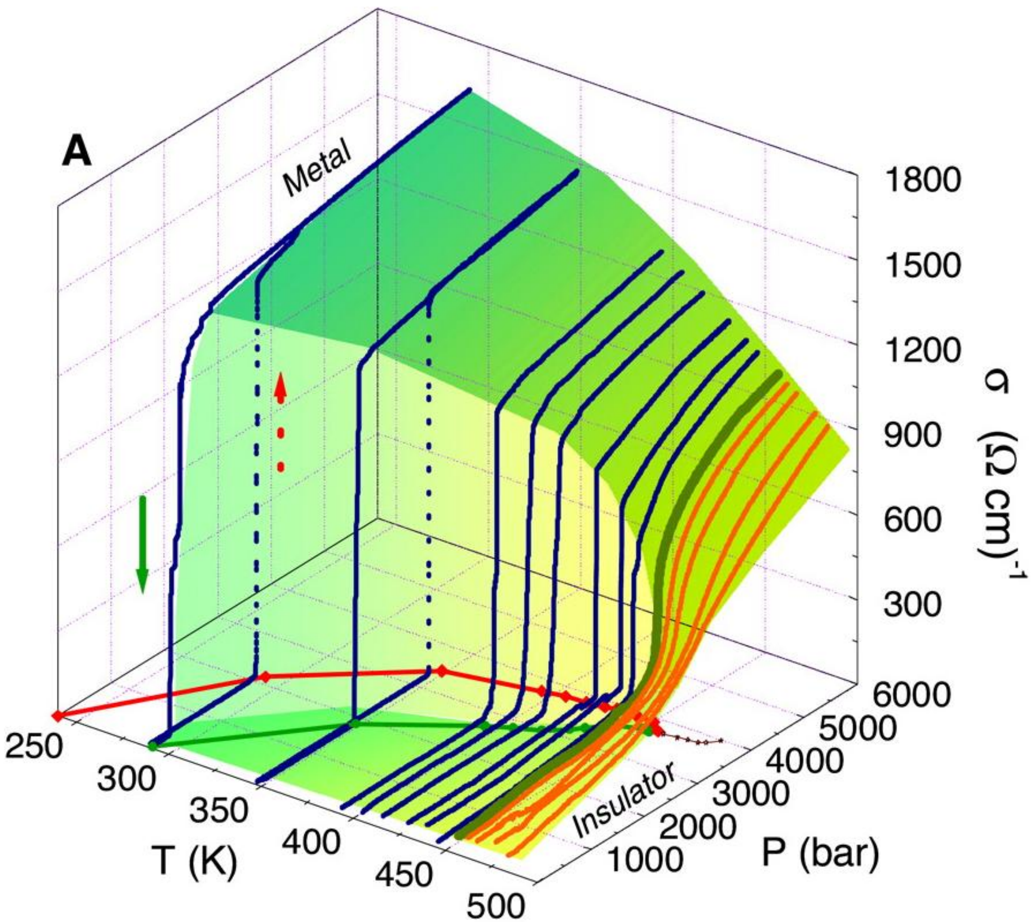
Mott metal-insulator transition

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

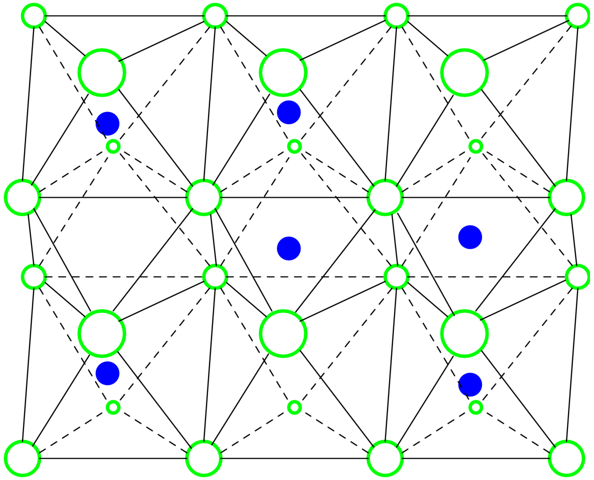
Phase diagram



Electrical conductivity



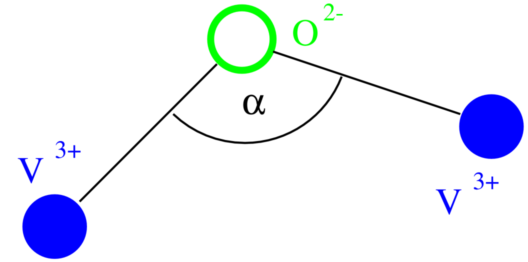
[Limelette et al., Science 302, 89 (2003)]



Corundum structure

Corundum structure:

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

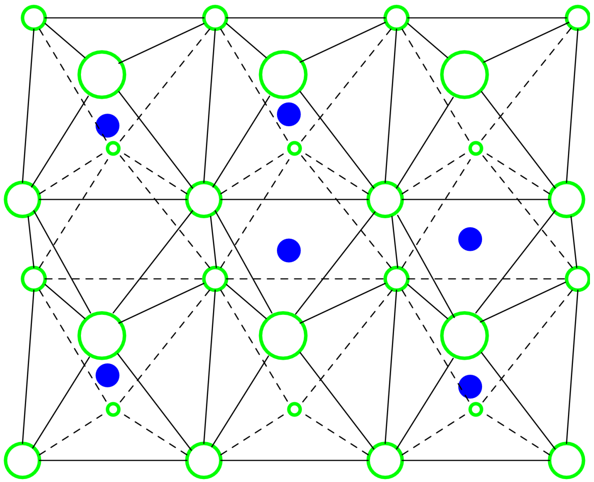


$\alpha_{Cr} < \alpha_V < \alpha_{Ti}$

parameters: pressure, isovalent doping with Ti, Cr

- larger lattice distortion ⇝ less overlap ⇝ MIT

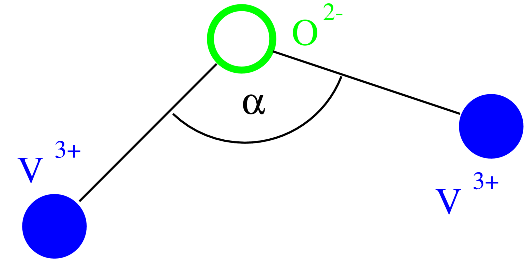
Paramagnetic, bandwidth-controlled metal-insulator transition in V_2O_3



Corundum structure

Corundum structure:

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



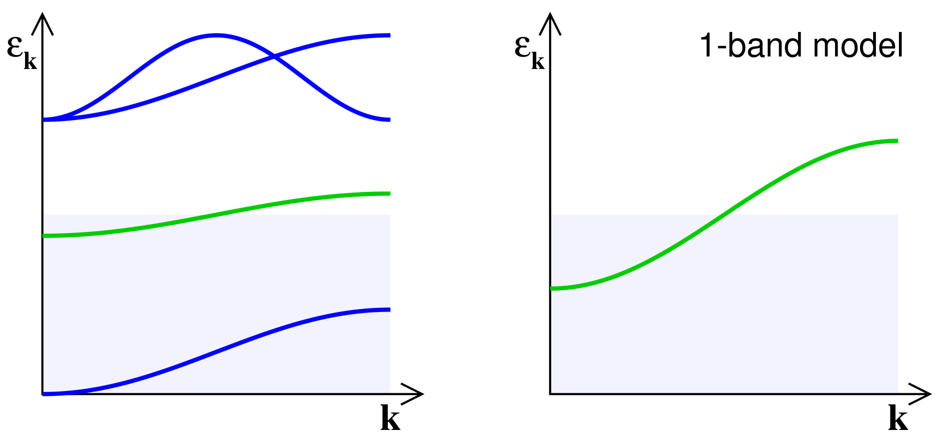
$\alpha_{Cr} < \alpha_{V} < \alpha_{Ti}$

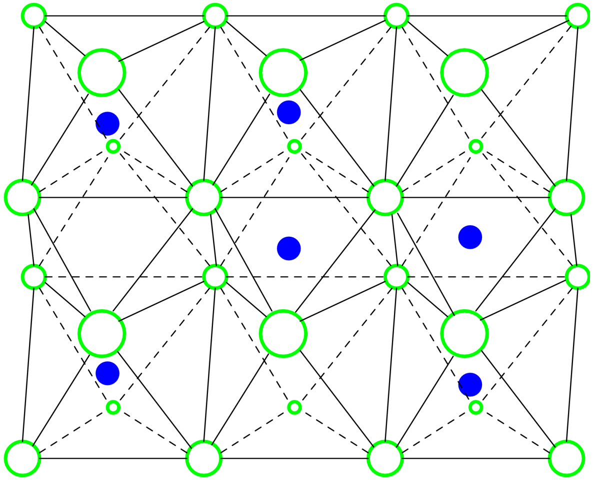
parameters: pressure, isovalent doping with Ti, Cr

- larger lattice distortion ⇝ less overlap ⇝ MIT

Paramagnetic, bandwidth-controlled metal-insulator transition in V_2O_3

Bloch states near Fermi energy,

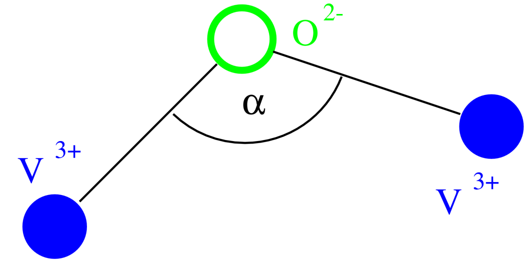




Corundum structure

Corundum structure:

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



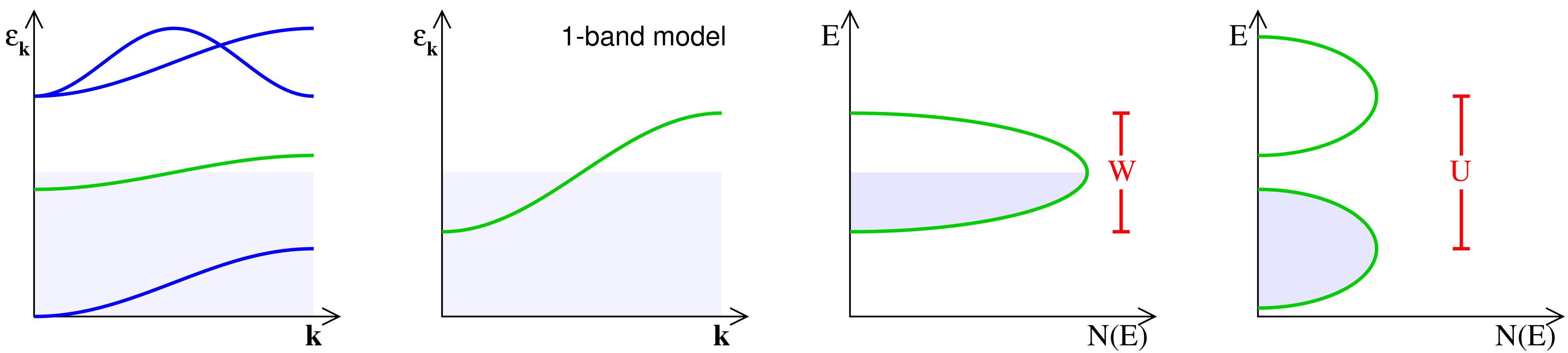
$\alpha_{Cr} < \alpha_{V} < \alpha_{Ti}$

parameters: pressure, isovalent doping with Ti, Cr

- larger lattice distortion ⇝ less overlap ⇝ MIT

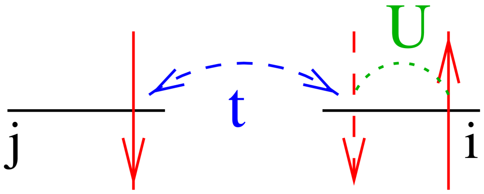
Paramagnetic, bandwidth-controlled metal-insulator transition in V_2O_3

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



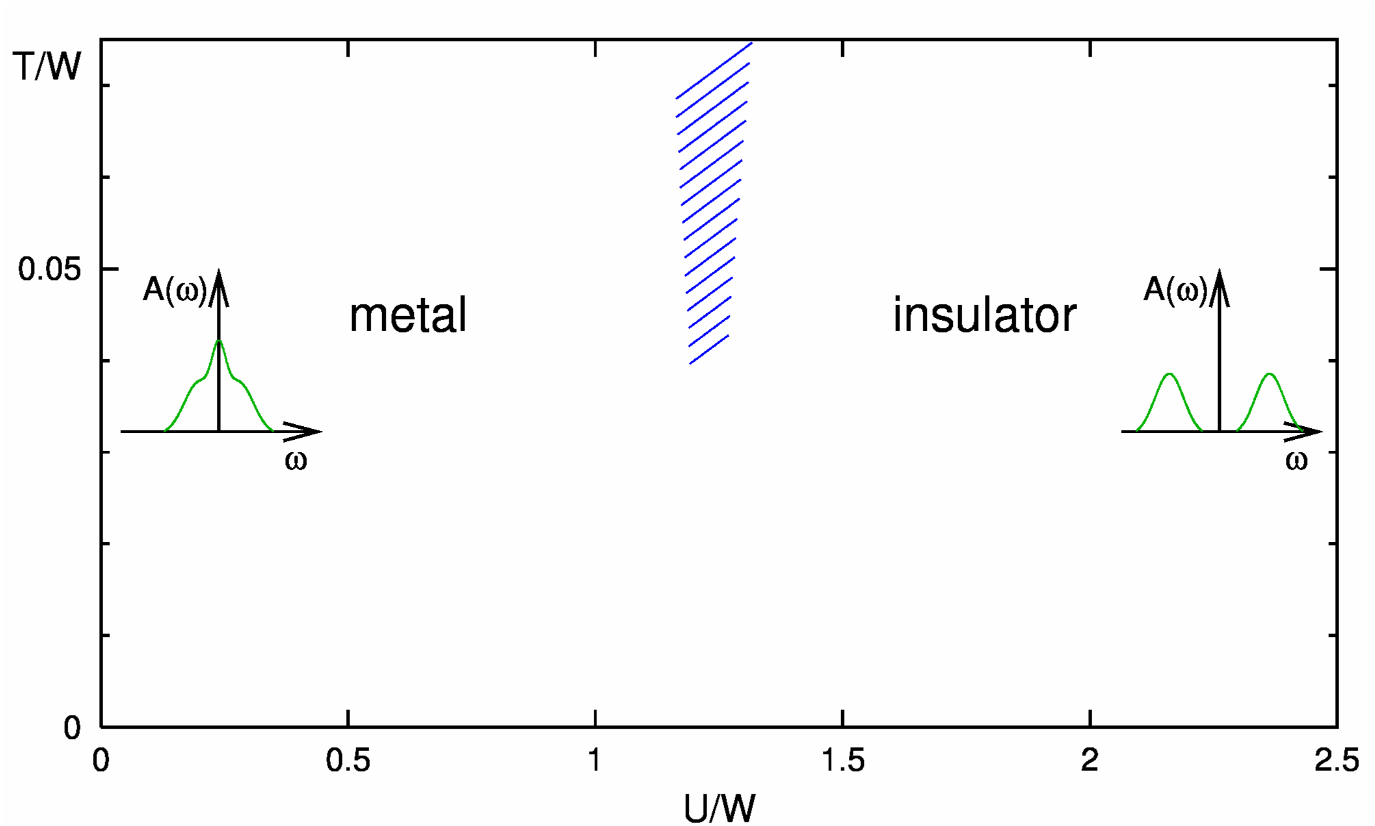
Paramagnetic MIT: no doubling of the unit cell ⇝ beyond single-particle theories!

Hubbard model $\hat{H} = -t \sum_{\langle i,j\rangle,\sigma} (\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$

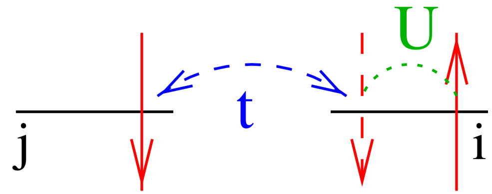


Minimal model for correlated electrons

MIT/crossover at $U/W \approx 1$ (and $n = 1$)



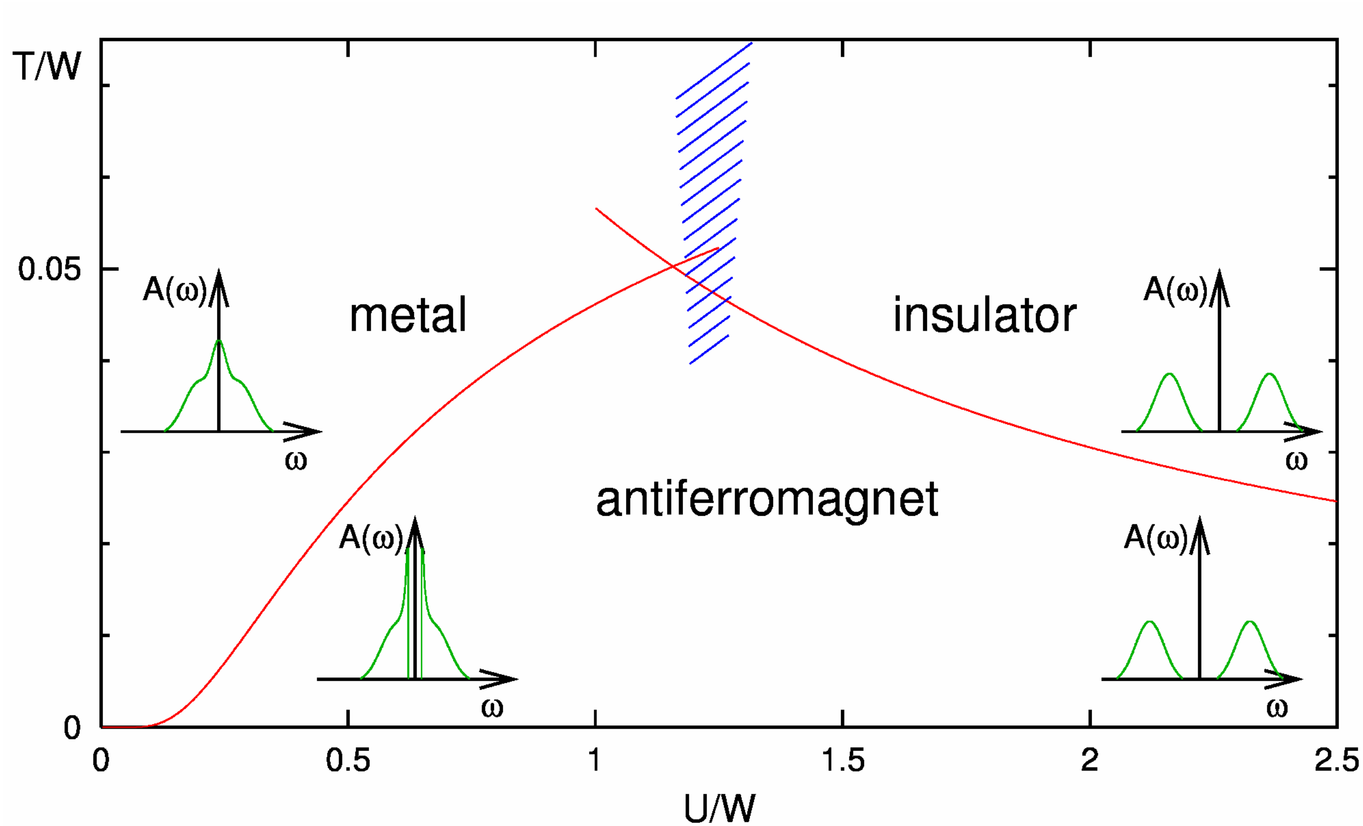
Hubbard model $\hat{H} = -t \sum_{\langle i,j\rangle,\sigma} (\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$



Minimal model for correlated electrons

MIT/crossover at $U/W \approx 1$ (and $n = 1$)

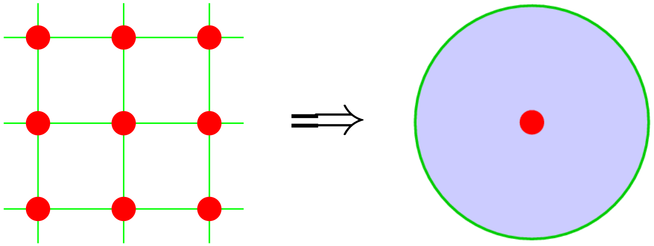
Generically antiferromagnetism at low T



Dynamical mean-field theory (DMFT)

- local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$
- mapping to impurity + self-consistency

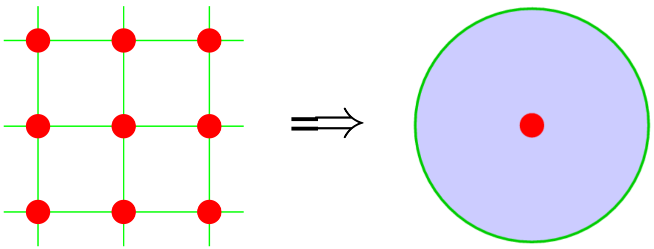
[Metzner, Vollhardt; Georges, Kotliar; Jarrell]

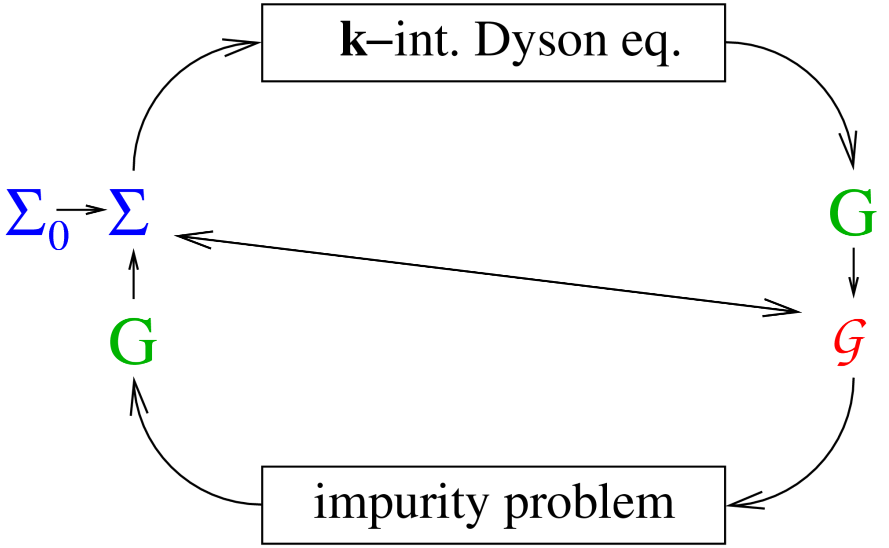


Dynamical mean-field theory (DMFT)

- local self-energy $\Sigma(\boldsymbol{k},\omega) \equiv \Sigma(\omega)$
- mapping to impurity + self-consistency

[Metzner, Vollhardt; Georges, Kotliar; Jarrell]

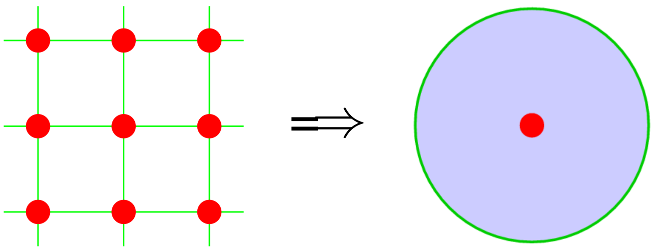


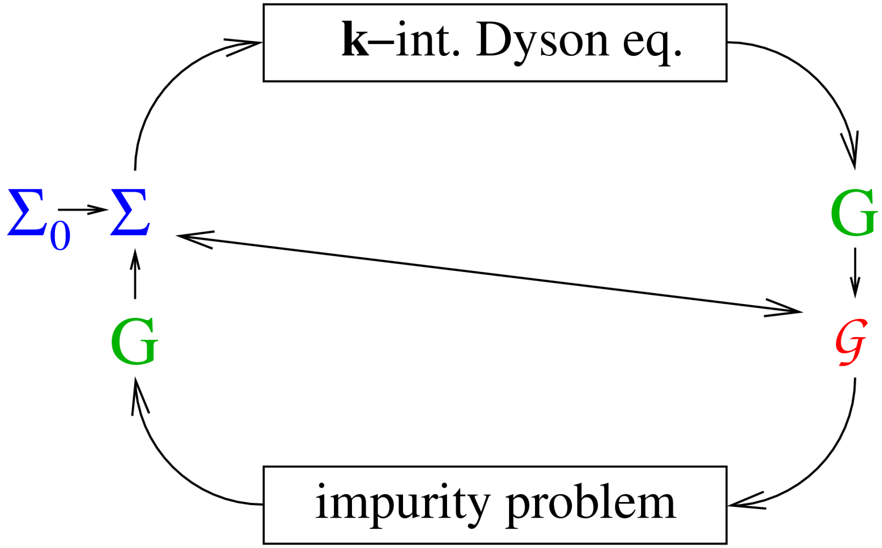


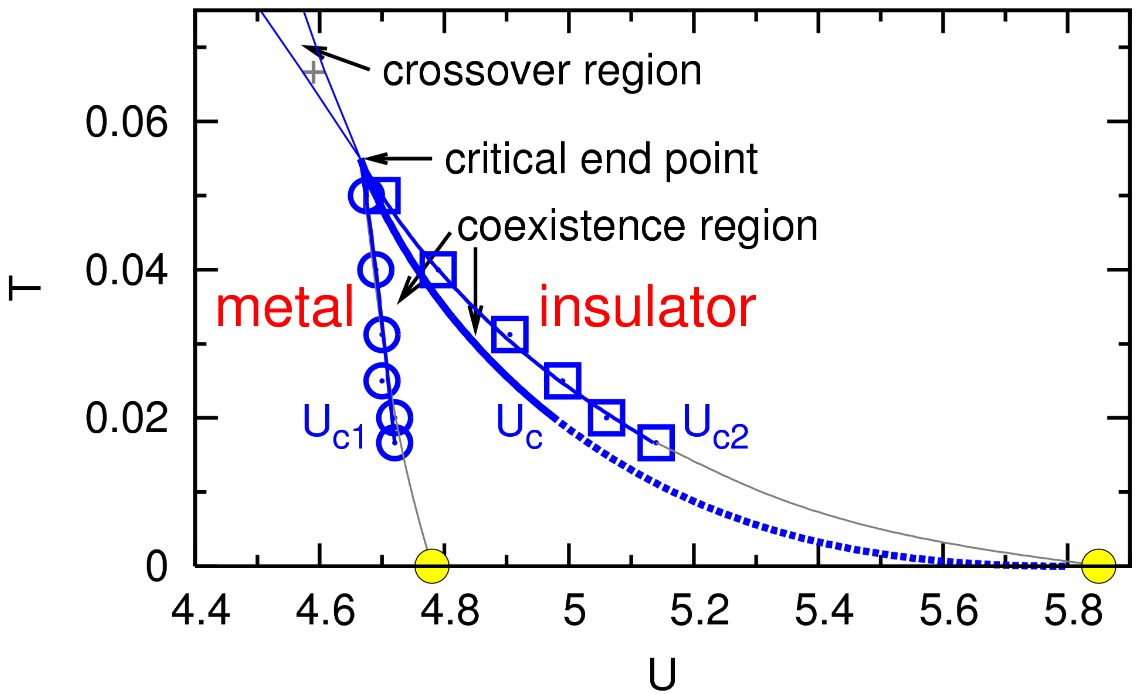
Dynamical mean-field theory (DMFT)

- local self-energy $\Sigma(\boldsymbol{k},\omega) \equiv \Sigma(\omega)$
- mapping to impurity + self-consistency

[Metzner, Vollhardt; Georges, Kotliar; Jarrell]







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)

Most results: HF-QMC

What has been achieved? What is new?

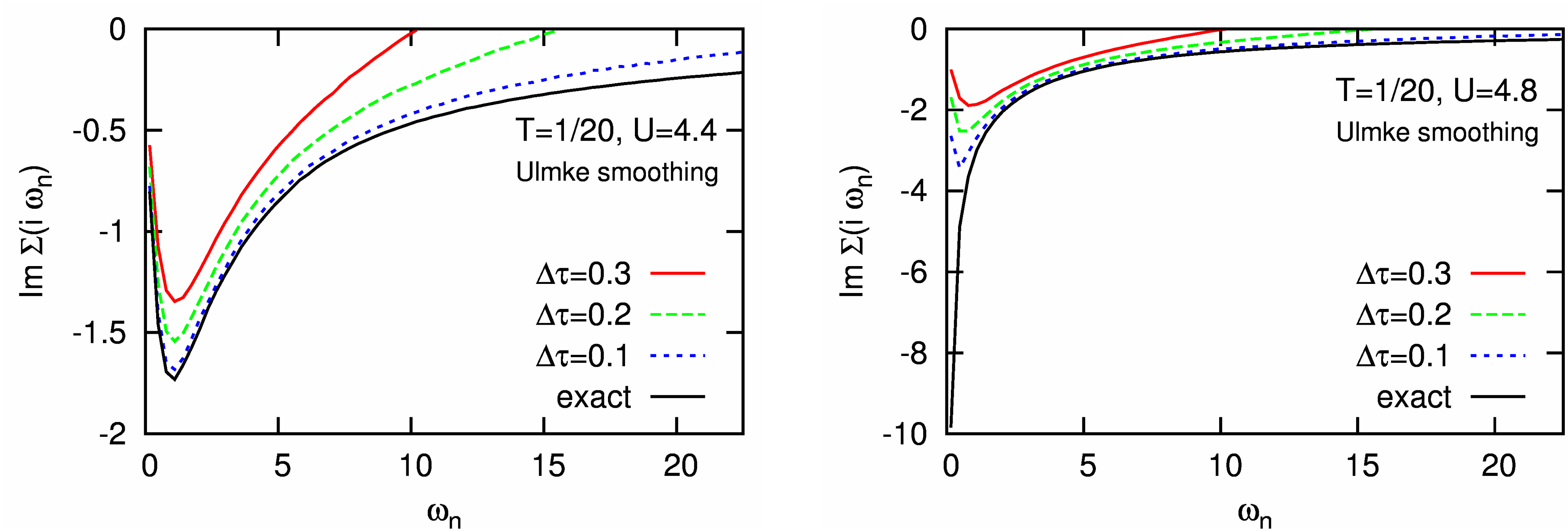
Promised: (i) precise, (ii) efficient, and (iii) unbiased QMC simulations within DMFT

What has been achieved? What is new?

Promised: (i) precise, (ii) efficient, and (iii) unbiased QMC simulations within DMFT

(0) Prehistory (1992-2000): "Ulmke smoothing"

- uncontrolled bias: insulator looks metallic-like at attainable $\Delta\tau$



What has been achieved? What is new?

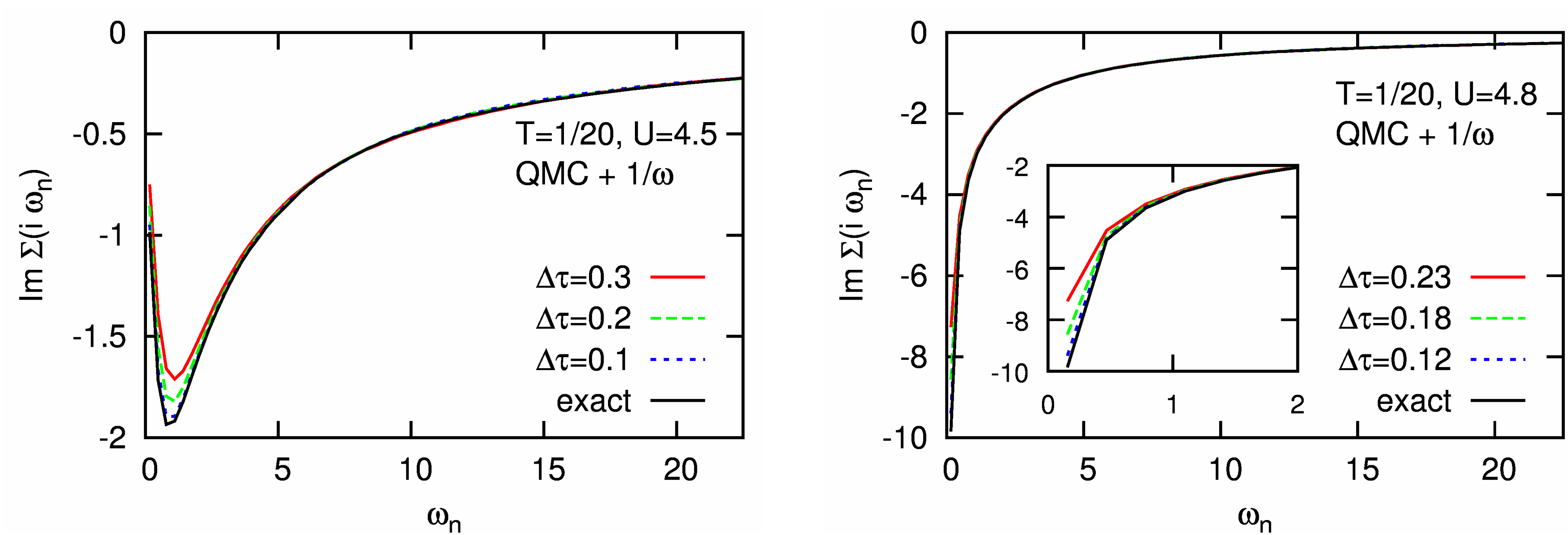
Promised: (i) precise, (ii) efficient, and (iii) unbiased QMC simulations within DMFT

(0) Prehistory (1992-2000): "Ulmke smoothing"

- uncontrolled bias: insulator looks metallic-like at attainable $\Delta\tau$

(i) Precise (2002-2007): HF-QMC supplemented with large-ω expansion

- minimal + controlled bias of raw results
- $\Delta\tau$-extrapolation $\rightsquigarrow$ unbiased high-precision results in favorable cases



(ii) Efficient: (Comparisons between HF-QMC and continuous-time QMC methods)

- Troyer group HF-QMC implementation apparently inferior
- HF-QMC needs $\Delta\tau$-extrapolation for high accuracy (and efficiency)
- HF-QMC is competitive with CT-QMC for all test cases, superior for energy

(ii) Efficient: (Comparisons between HF-QMC and continuous-time QMC methods)

- Troyer group HF-QMC implementation apparently inferior
- HF-QMC needs $\Delta\tau$-extrapolation for high accuracy (and efficiency)
- HF-QMC is competitive with CT-QMC for all test cases, superior for energy

(iii) Unbiased: (2007-) Multigrid Hirsch-Fye QMC algorithm

- Unbiased quasi-continuous-time solution of DMFT self-consistency equations
- High precision/efficiency for all observables, even close to phase transitions
- Unbiased: systematic errors smaller than statistical errors

(ii) Efficient: (Comparisons between HF-QMC and continuous-time QMC methods)

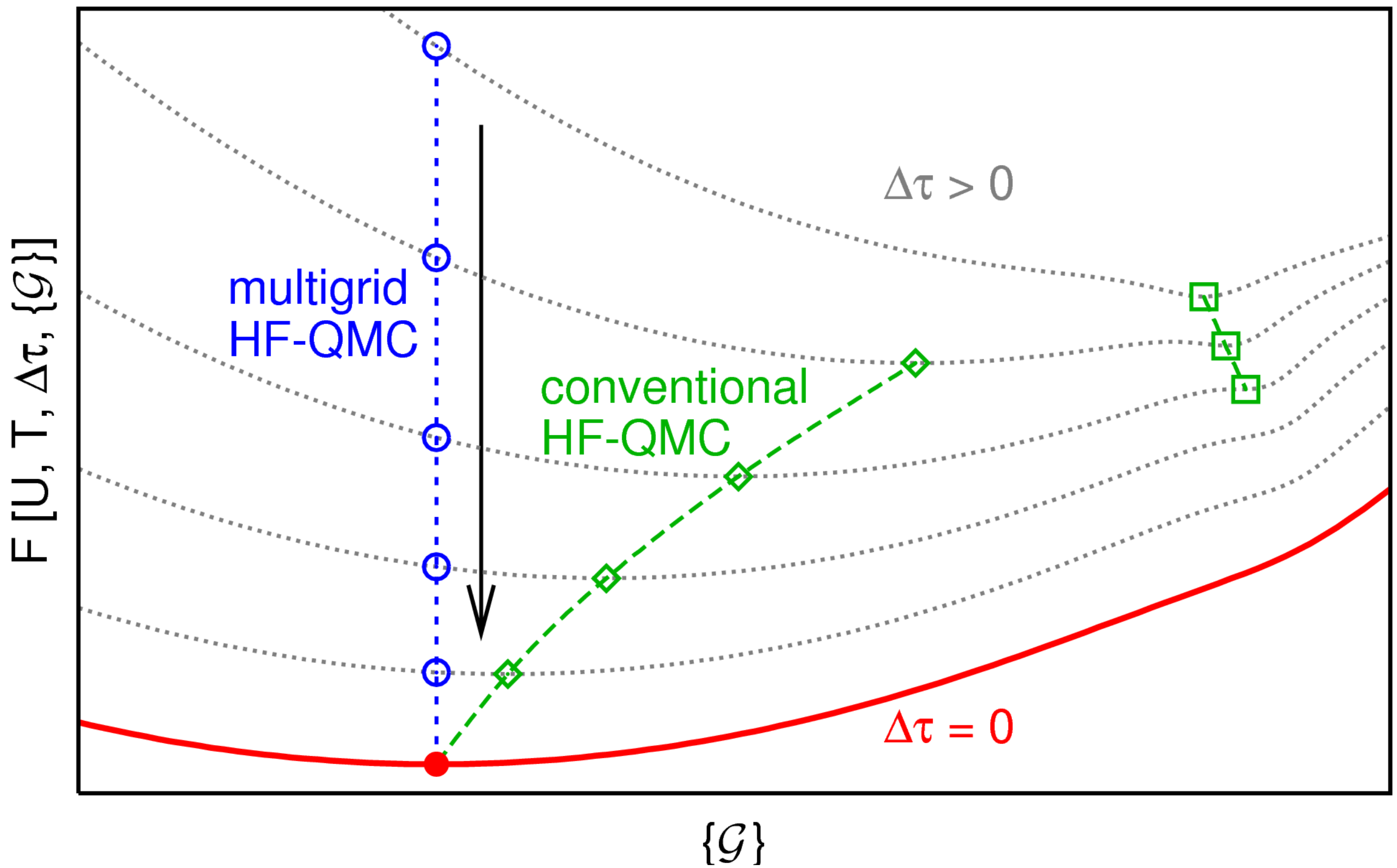
- Troyer group HF-QMC implementation apparently inferior
- HF-QMC needs $\Delta\tau$-extrapolation for high accuracy (and efficiency)
- HF-QMC is competitive with CT-QMC for all test cases, superior for energy

(iii) Unbiased: (2007-) Multigrid Hirsch-Fye QMC algorithm

- Unbiased quasi-continuous-time solution of DMFT self-consistency equations
- High precision/efficiency for all observables, even close to phase transitions
- Unbiased: systematic errors smaller than statistical errors
- Significant progress since last talk:

	2/2008	5/2008	9/2008	10/2008
Precise for $M = 1$, $n = 1$	V	V	V	V
Unbiased for $M = 1$, $n = 1$	(V)	?	V	V
Precise for $M > 1$			V	V
Precise at arbitrary filling				V
Unbiased for $M > 1$, $n \neq M$				(V)

Schematic comparison via generalized Ginzburg-Landau functionals



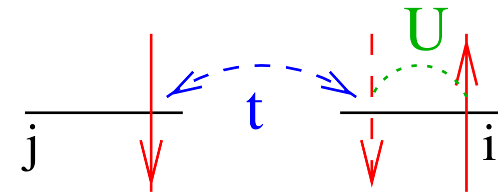
Conventional Hirsch-Fye QMC: DMFT fixed point shifts with $\Delta\tau$

Multigrid Hirsch-Fye QMC: DMFT iteration towards exact fixed point

Some more background

Hubbard model

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



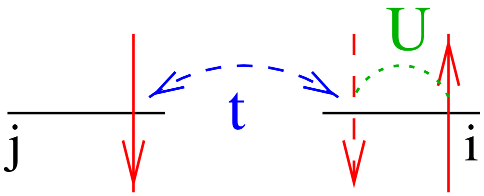
Captures important strong-correlation phenomena: Mott metal-insulator transition, (anti-) ferromagnetism, heavy fermions, high-T_c superconductivity (?), . . .

Few parameters: interaction U/W, temperature T/W, filling n, dispersion $\epsilon_{\boldsymbol{k}}$

Some more background

Hubbard model

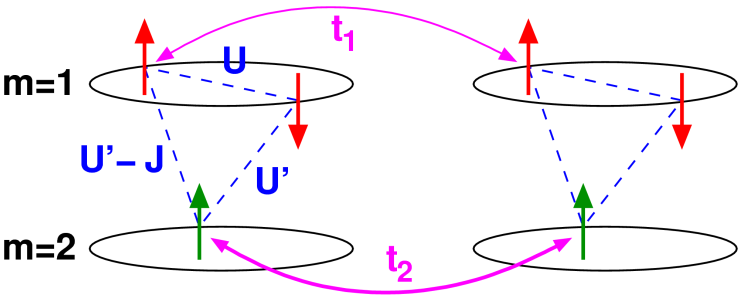
(i) Single band: $\hat{H} = \sum_{(i,j),\sigma} t_{ij} (\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$



Captures important strong-correlation phenomena: Mott metal-insulator transition, (anti-) ferromagnetism, heavy fermions, high-T_c superconductivity (?), . . .

Few parameters: interaction U/W, temperature T/W, filling n, dispersion $\epsilon_{\boldsymbol{k}}$

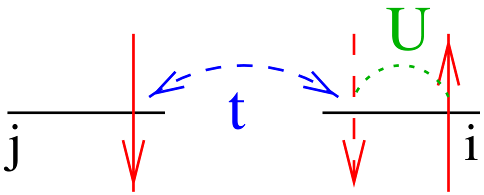
(ii) Multi-band model, e.g., 2-band model with inequivalent bands:



Some more background

Hubbard model

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

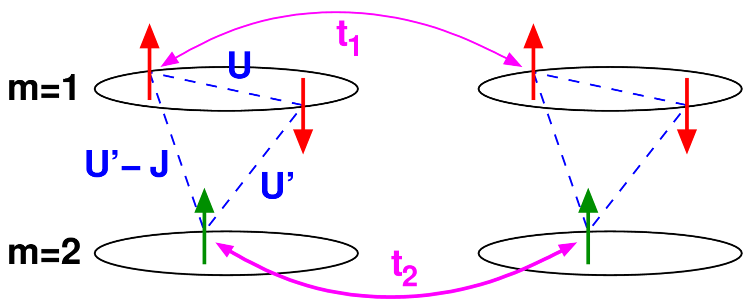


Captures important strong-correlation phenomena: Mott metal-insulator transition, (anti-) ferromagnetism, heavy fermions, high-T_c superconductivity (?), . . .

Few parameters: interaction U/W, temperature T/W, filling n, dispersion $\epsilon_{\boldsymbol{k}}$

(ii) Multi-band model, e.g., 2-band model with inequivalent bands:

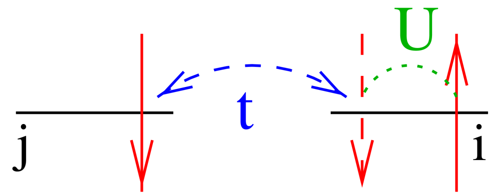
$$H = \sum_{m=1}^{2} \Big[-\sum_{\langle ij\rangle\sigma} t_m \, c^{\dagger}_{im\sigma} c_{jm\sigma} + U \sum_i n_{im\uparrow} n_{im\downarrow} \Big]$$
$$+ \sum_{i\sigma\sigma'} (U' - \delta_{\sigma\sigma'} J_z) \, n_{i1\sigma} \, n_{i2\sigma'}$$
$$+ \tfrac{1}{2} J_\perp \sum_{i\sigma} \Big[c^{\dagger}_{i1\sigma}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



Some more background

Hubbard model

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

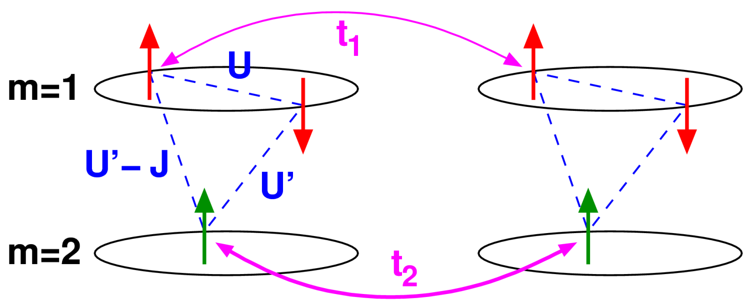


Captures important strong-correlation phenomena: Mott metal-insulator transition, (anti-) ferromagnetism, heavy fermions, high-T_c superconductivity (?), . . .

Few parameters: interaction U/W, temperature T/W, filling n, dispersion $\epsilon_{\boldsymbol{k}}$

(ii) Multi-band model, e.g., 2-band model with inequivalent bands:

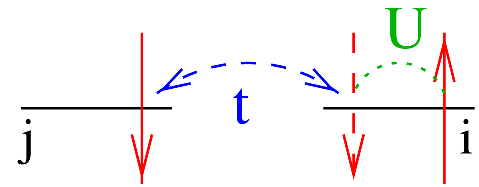
$$
\begin{aligned}
H \;=\; & \sum_{m=1}^{2} \Big[- \sum_{\langle ij \rangle \sigma} t_m \, c^\dagger_{im\sigma} c_{jm\sigma} + U \sum_i n_{im\uparrow} n_{im\downarrow} \Big] \\
& + \sum_{i\sigma\sigma'} (U' - \delta_{\sigma\sigma'} J_z) \, n_{i1\sigma} \, n_{i2\sigma'} \\
& + \tfrac{1}{2} J_\perp \sum_{i\sigma}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



More complexity, more realistic: OSMT, spin+orbital order, LDA+DMFT, . . .

Approaches for Hubbard-type models

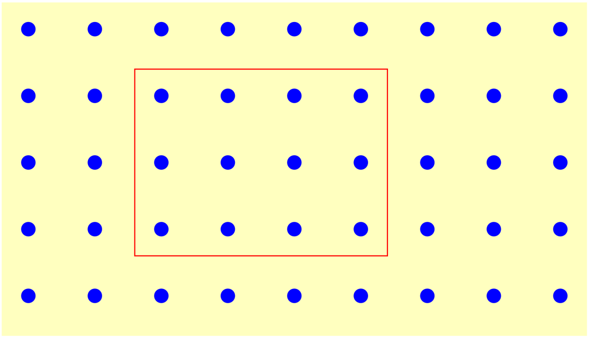
$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} \, (\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



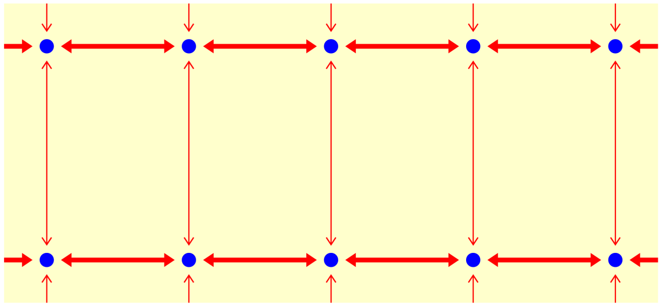
Perturbation theory

- $U \longrightarrow 0$: Hartree-Fock
  2$^{\text{nd}}$ order PT, . . .
- $t/U \longrightarrow 0$ (for $n = 1$)
  $\rightsquigarrow$ Heisenberg model

finite clusters: ED, QMC

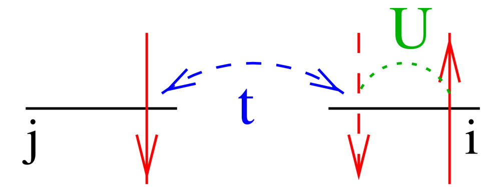


$d \rightarrow 1$: Bethe ansatz, DMRG



Approaches for Hubbard-type models

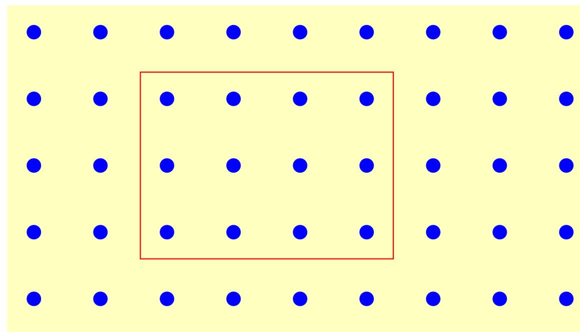
$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}\right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



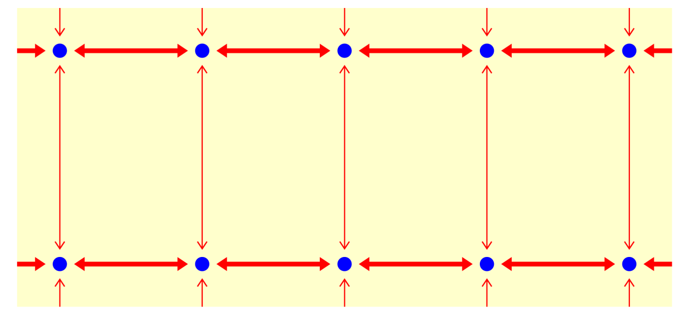
Perturbation theory

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

finite clusters: ED, QMC



$d \rightarrow 1$: Bethe ansatz, DMRG

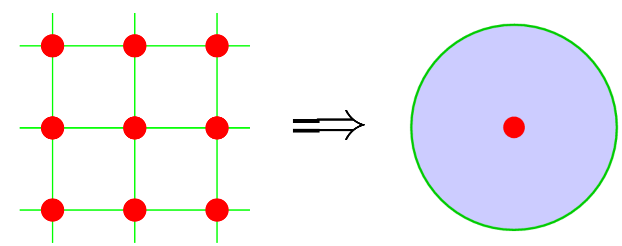


Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$

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

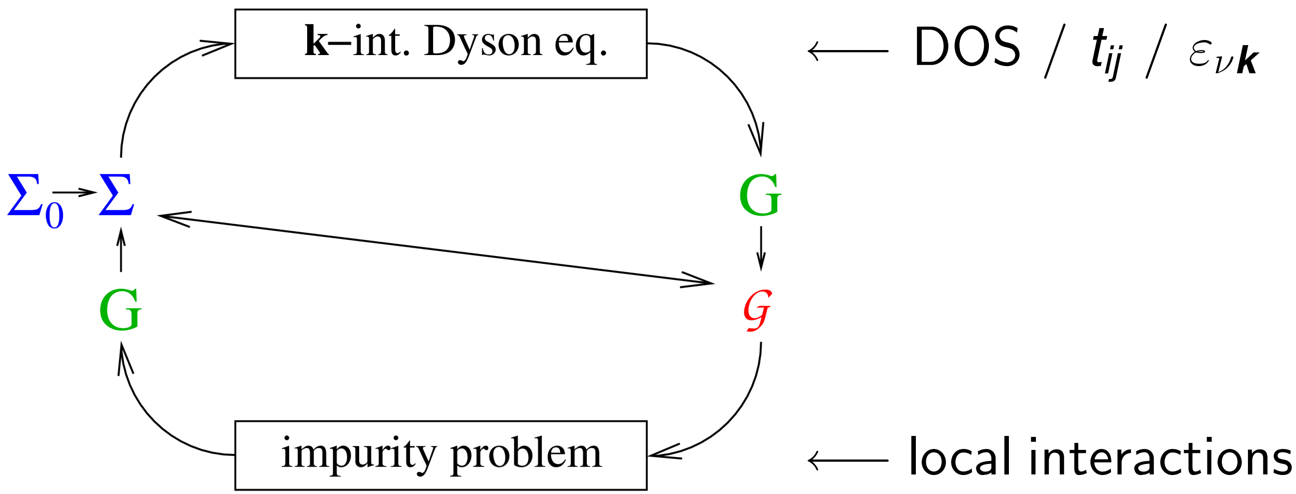
+ non-perturbative $\rightsquigarrow$ valid at MIT
+ dynamical on-site correlations preserved
+ in thermodynamic limit $\rightsquigarrow$ resolves MIT

+/− exact for coordination $Z \rightarrow \infty$



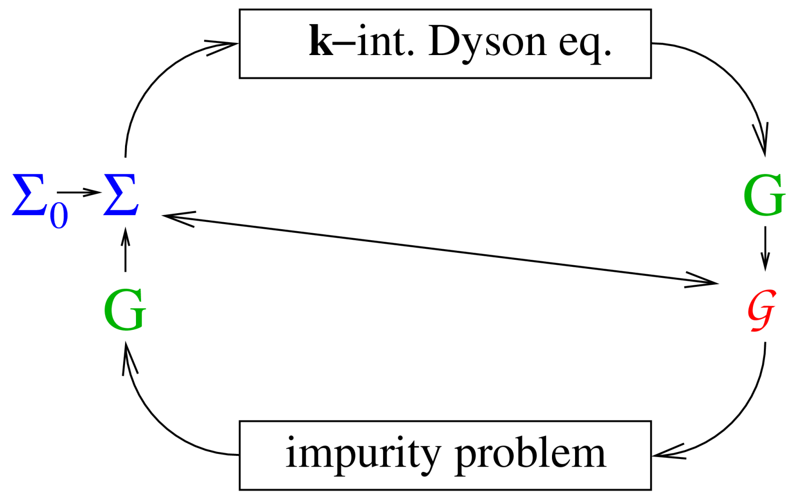
Iterative solution of DMFT equations

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



Iterative solution of DMFT equations

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



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

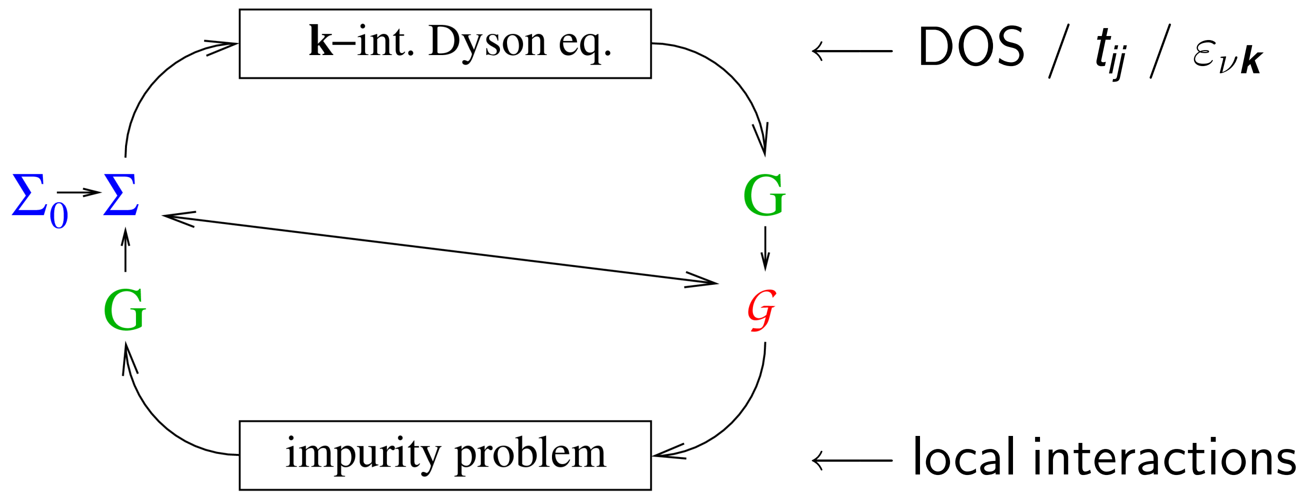
$\longleftarrow$ local interactions

Impurity solver:

- Iterative perturbation theory (IPT; not controlled)
- Quantum Monte Carlo (QMC)

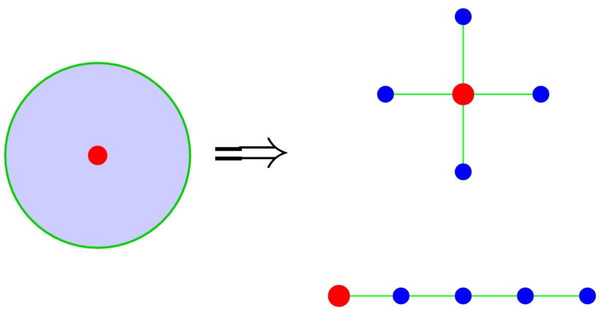
Iterative solution of DMFT equations

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 function G in imaginary time (fermionic Grassmann variables ψ, ψ^*):

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

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

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

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

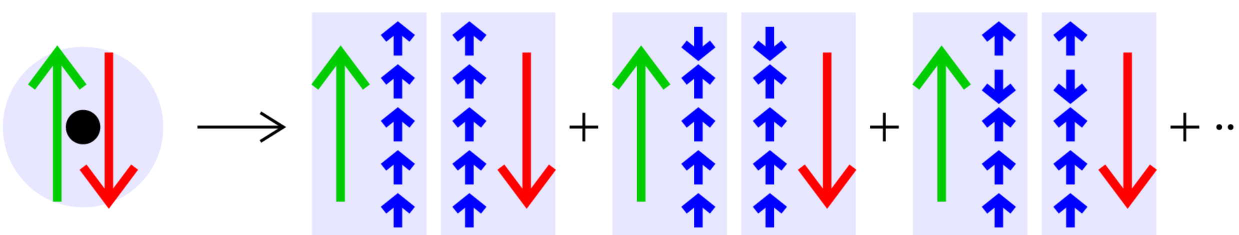
- Discretization $\beta = \Lambda\,\Delta\tau$,
- Trotter decoupling $\quad e^{-\beta(\hat{T}+\hat{V})} = \lim_{\Lambda\to\infty} \left[e^{-\Delta\tau\,\hat{T}} e^{-\Delta\tau\,\hat{V}}\right]^\Lambda$

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

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

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

- Discretization $\beta = \Lambda\,\Delta\tau$,
- Trotter decoupling $e^{-\beta(\hat{T}+\hat{V})} = \lim_{\Lambda\to\infty}\left[e^{-\Delta\tau\hat{T}}e^{-\Delta\tau\hat{V}}\right]^\Lambda$
- Discrete Hubbard-Stratonovich transformation $e^{\Delta\tau U(\hat{n}_\uparrow-\hat{n}_\downarrow)^2/2} = \frac{1}{2}\sum_{s=\pm1} e^{\lambda s(\hat{n}_\uparrow-\hat{n}_\downarrow)}$



Wick theorem:

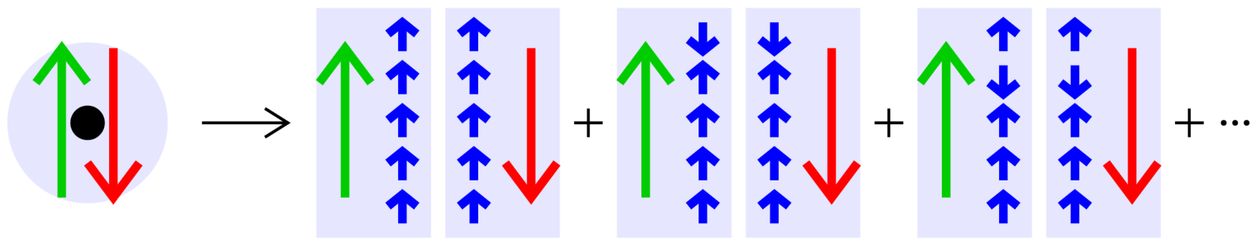
$$G = \frac{\sum M \det\{M\}}{\sum \det\{M\}}$$

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

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

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

- Discretization $\beta = \Lambda\,\Delta\tau$,
- Trotter decoupling $e^{-\beta(\hat{T}+\hat{V})} = \lim_{\Lambda\to\infty}\left[e^{-\Delta\tau\hat{T}}e^{-\Delta\tau\hat{V}}\right]^\Lambda$
- Discrete Hubbard-Stratonovich transformation $e^{\Delta\tau U(\hat{n}_\uparrow-\hat{n}_\downarrow)^2/2} = \frac{1}{2}\sum_{s=\pm1} e^{\lambda s\,(\hat{n}_\uparrow-\hat{n}_\downarrow)}$



Wick theorem:

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

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

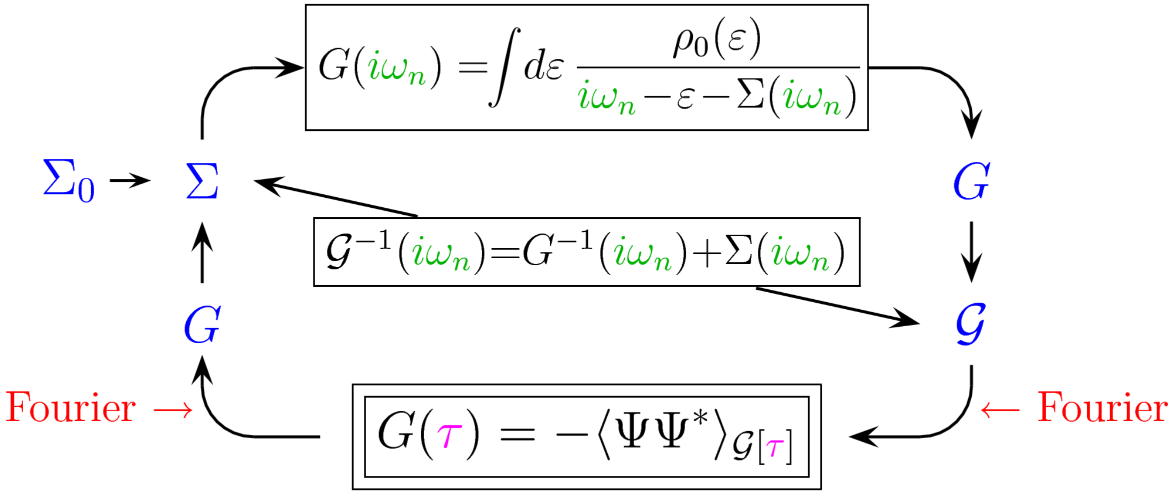
+ numerically exact, + no sign problem (density-type int.), − effort scales as T^{-3}

How does it work? Why?

How does it work? Why?

(i) Fourier trafos in DMFT-QMC cycle

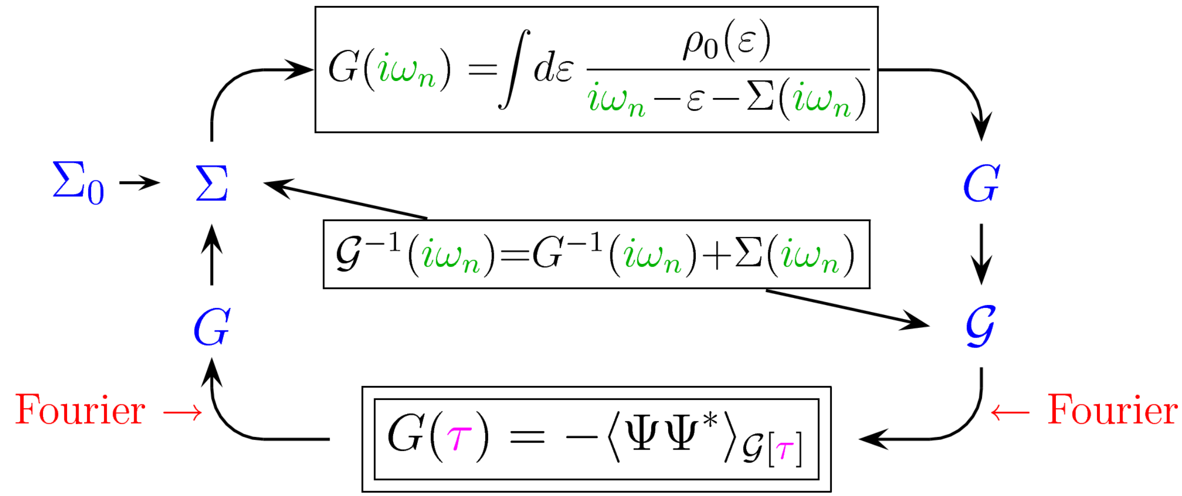
Iterative solution of DMFT equations (for imaginary-time impurity solver)



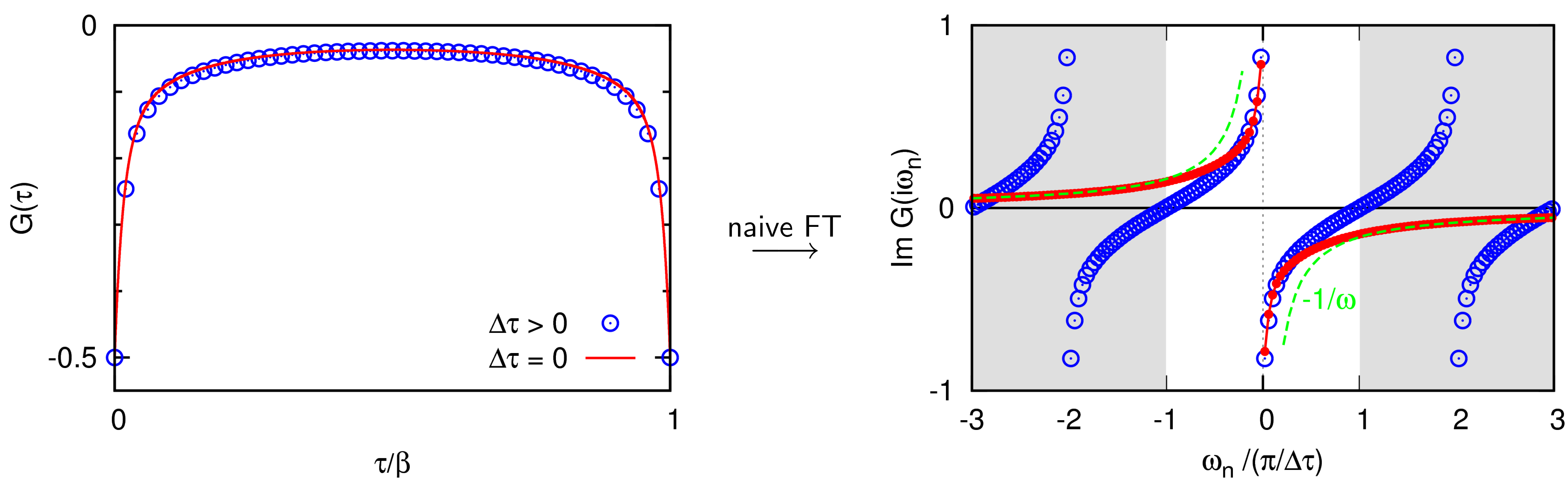
How does it work? Why?

(i) Fourier trafos in DMFT-QMC cycle

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



Naive discrete Fourier transformation $\rightsquigarrow$ oscillations (instead of $G(\omega) \overset{\omega\to\infty}{\longrightarrow} 1/\omega$)



Possible solution: interpolate $G_{\text{QMC}}(\tau)$, e.g., by cubic splines [Jarrell, Krauth, Gull, ...]

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

Possible solution: interpolate $G_{\text{QMC}}(\tau)$, e.g., by cubic splines [Jarrell, Krauth, Gull, . . .]

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

- adjust boundary cond.
  [Oudovenko]

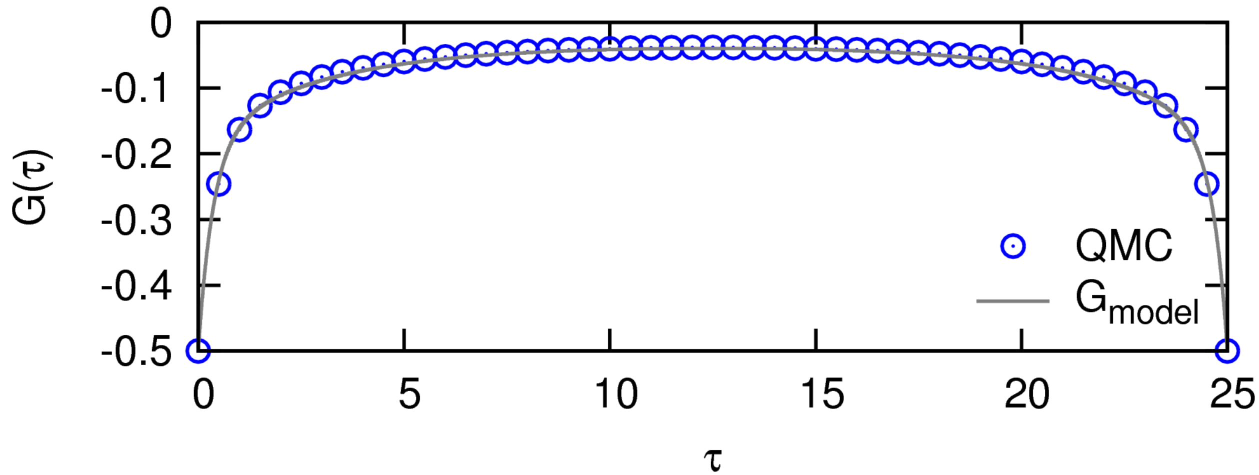
- spline-fit only
  difference w.r.t.
  reference problem:

  - IPT [Jarrell]

Possible solution: interpolate $G_{\text{QMC}}(\tau)$, e.g., by cubic splines [Jarrell, Krauth, Gull, ...]

But: $\dfrac{d^2G(\tau)}{d\tau^2}$ maximal for $\tau \to 0, \beta$ $\rightsquigarrow$ 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]

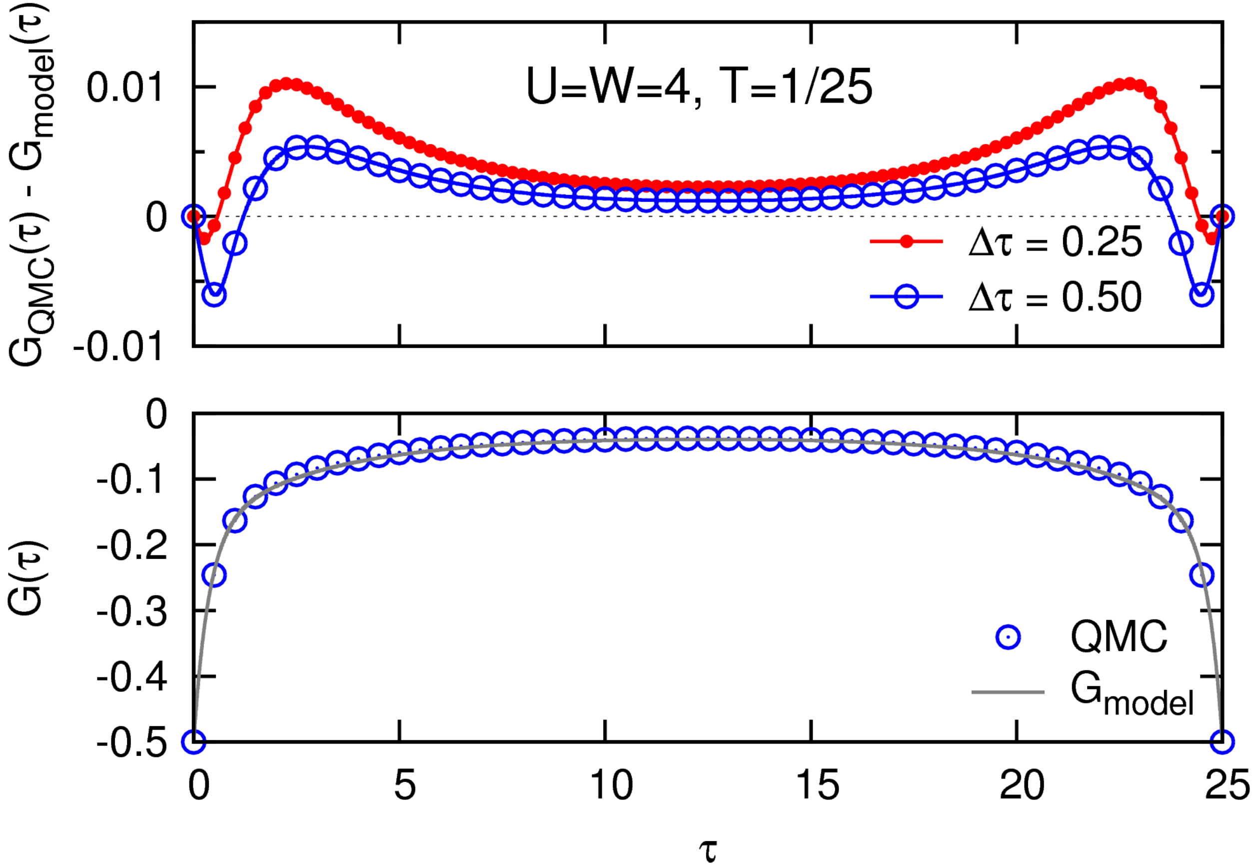


$$\Sigma_\sigma(\omega) = U\left(\langle \hat{n}_{-\sigma}\rangle - \tfrac{1}{2}\right)\omega^{0} + U^2\langle \hat{n}_{-\sigma}\rangle\left(1 - \langle \hat{n}_{-\sigma}\rangle\right)\omega^{-1} + \mathcal{O}(\omega^{-2})$$

Possible solution: interpolate $G_{\text{QMC}}(\tau)$, e.g., by cubic splines [Jarrell, Krauth, Gull, ...]

But: $\dfrac{d^2G(\tau)}{d\tau^2}$ maximal for $\tau \to 0, \beta$ $\rightsquigarrow$ 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]



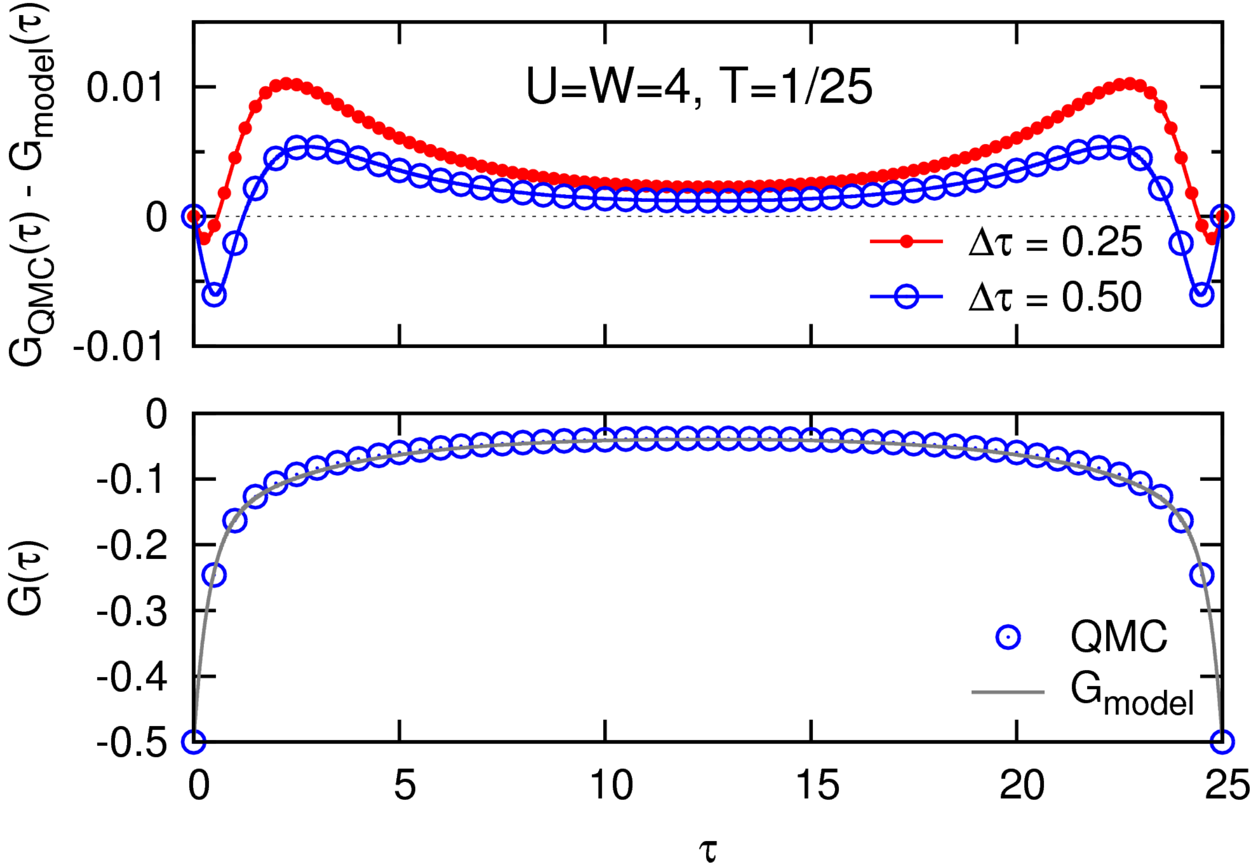
$$\Sigma_\sigma(\omega) = U\left(\langle \hat{n}_{-\sigma}\rangle - \tfrac{1}{2}\right)\omega^0 + U^2\langle \hat{n}_{-\sigma}\rangle\left(1 - \langle \hat{n}_{-\sigma}\rangle\right)\omega^{-1} + \mathcal{O}(\omega^{-2})$$

multi-band case: additional terms

Possible solution: interpolate $G_{\text{QMC}}(\tau)$, e.g., by cubic splines [Jarrell, Krauth, Gull, . . .]

But: $\dfrac{d^2G(\tau)}{d\tau^2}$ maximal for $\tau \to 0, \beta$ $\rightsquigarrow$ 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]



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

multi-band case: additional terms

Current project: replace spline interpolation by smooth fit!

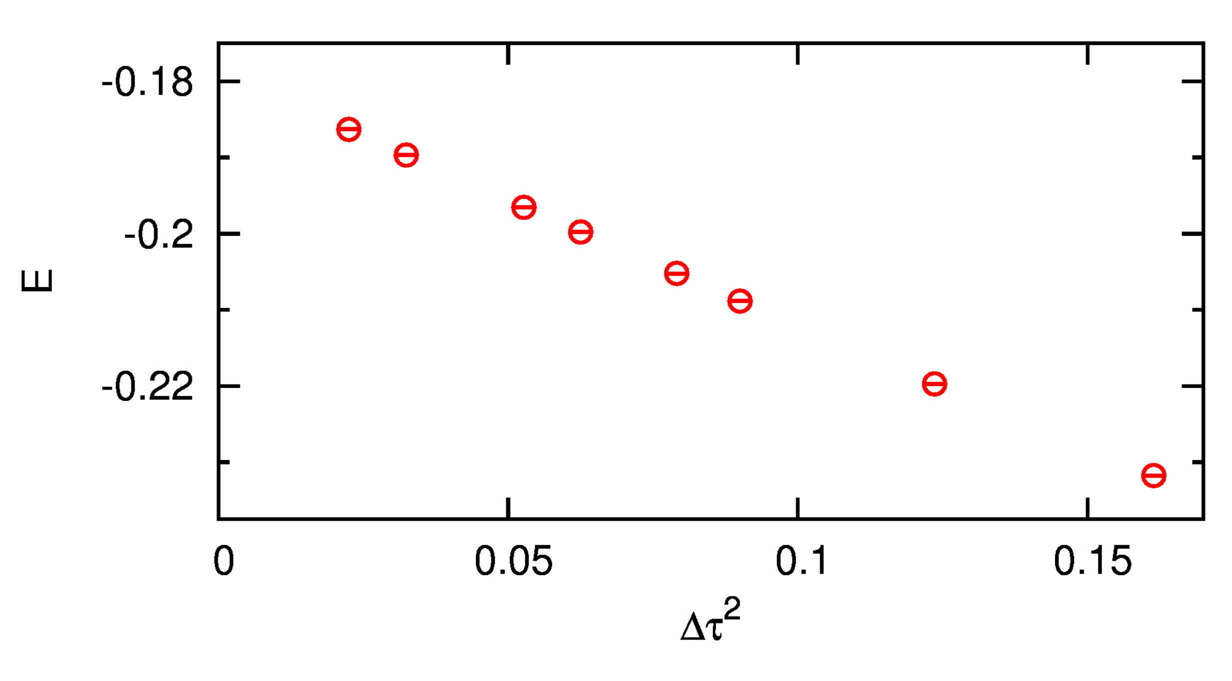
Extrapolation $\Delta\tau \to 0$

can improve accuracy of observable estimates by several orders of magnitude ($\sim$same cost)

Extrapolation $\Delta\tau \to 0$

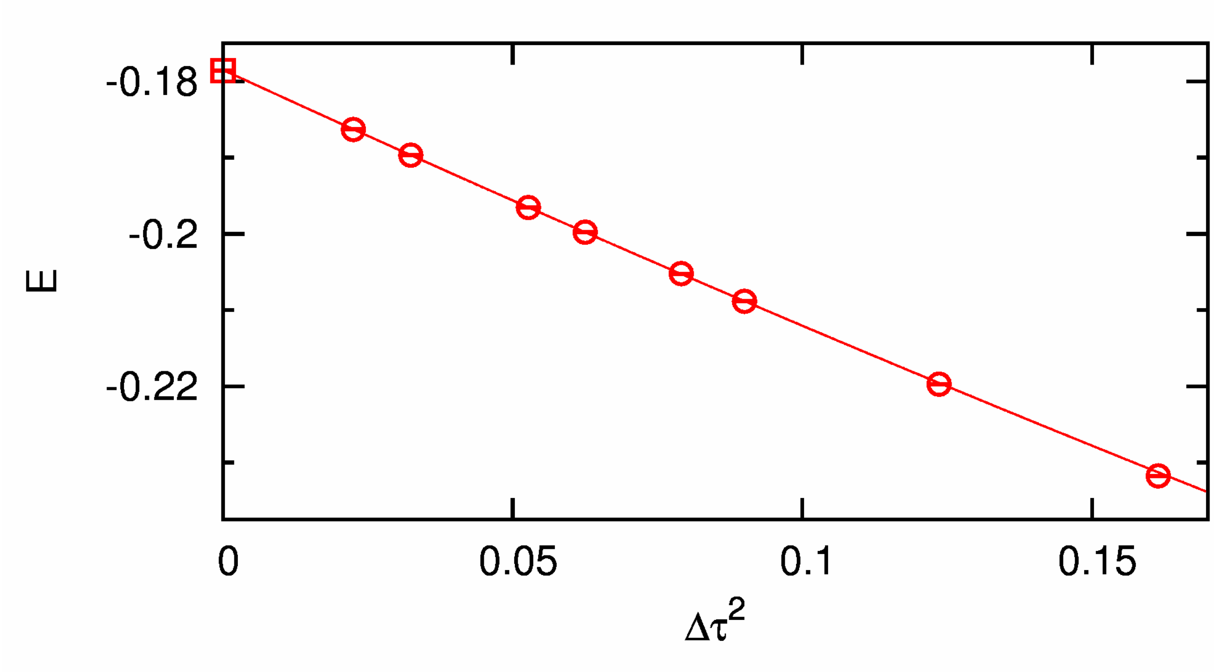
can improve accuracy of observable estimates by several orders of magnitude (∼same cost)

Example: energy E for $U = W = 4$ (Bethe DOS), $T = 1/45$
[NB, PRB (2007)]

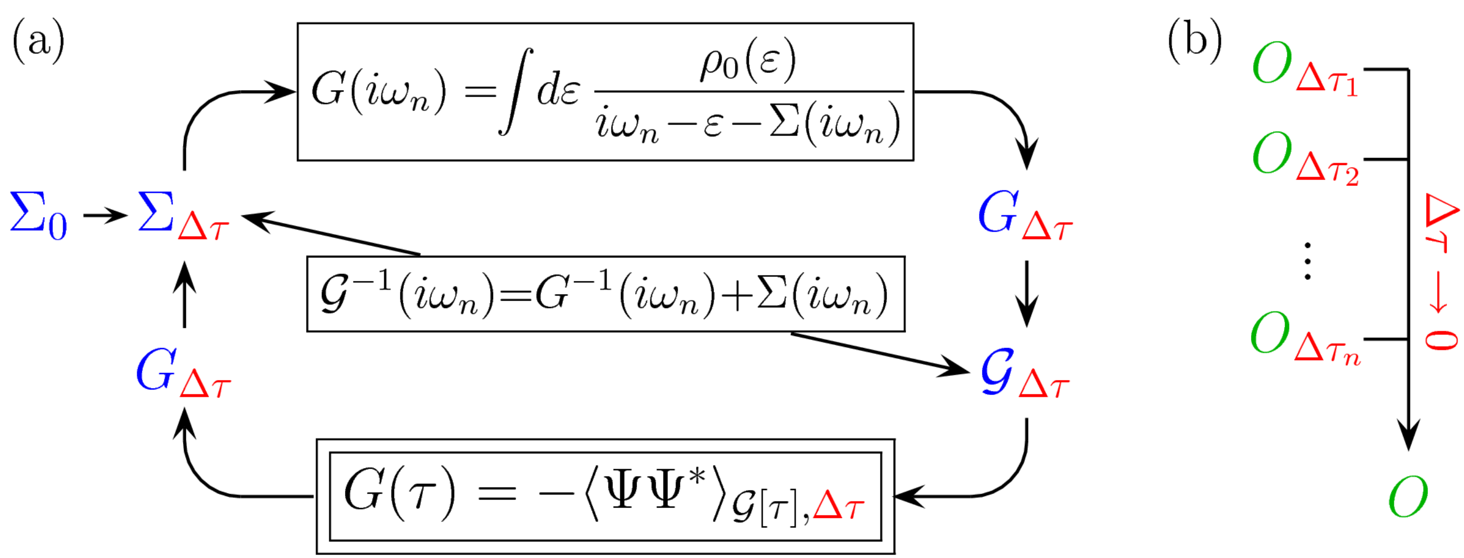


Extrapolation $\Delta\tau \to 0$ can improve accuracy of observable estimates by several orders of magnitude (∼same cost)

Example: energy E for $U = W = 4$ (Bethe DOS), $T = 1/45$ [NB, PRB (2007)]



Self-consistency cycle using conventional HF-QMC



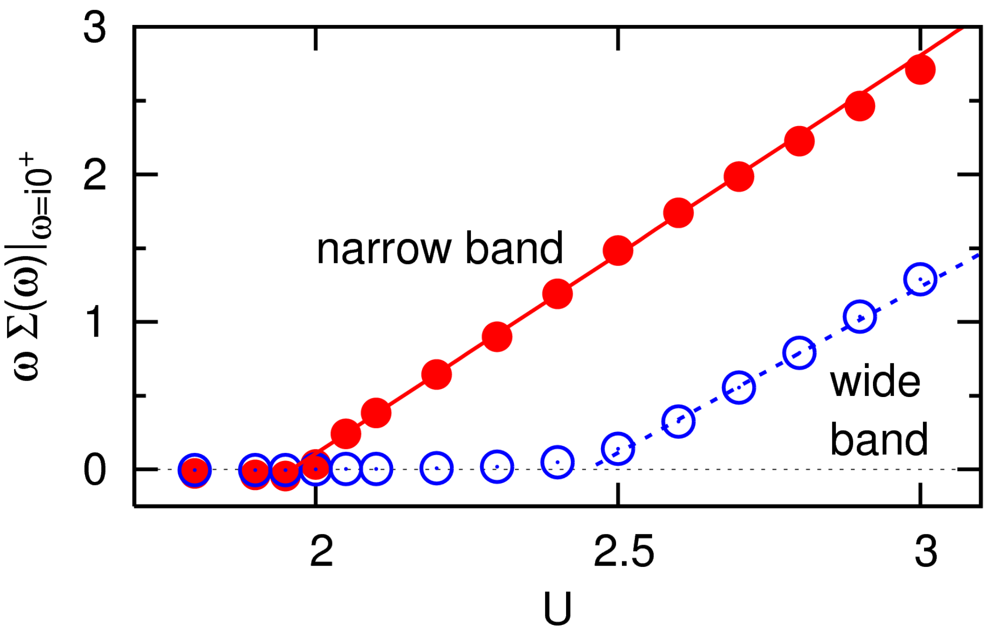
Selected applications

High-precision calculations for 1-band model, extrapolation $T \to 0$:

benchmark results (E, D, Z) unmatched by ED, DMRG, PQMC, NRG

revealed errors in weak-coupling expansions

Orbital-selective Mott transitions in 2-band model



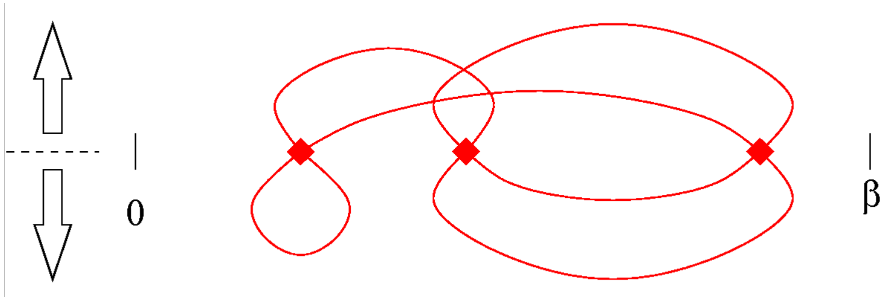
[C. Knecht, NB, and P.G.J. van Dongen, PRB 72, 081103(R) (2005)]

Efficiency of QMC DMFT solvers

New development: continuous-time QMC algorithms

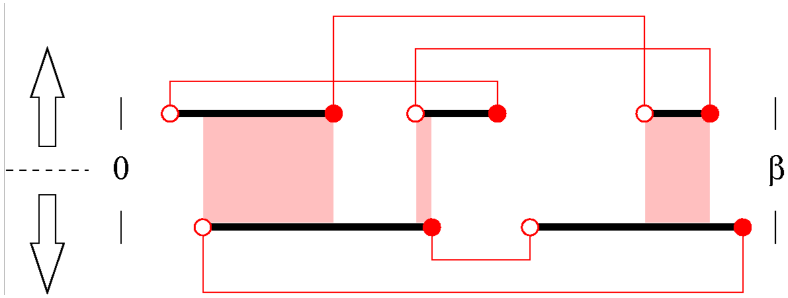
1. weak-coupling expansion

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



2. hybridization expansion

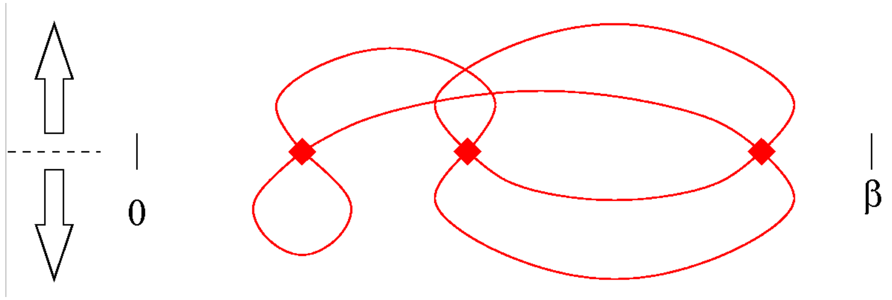
[Werner et al., PRL (2006)]



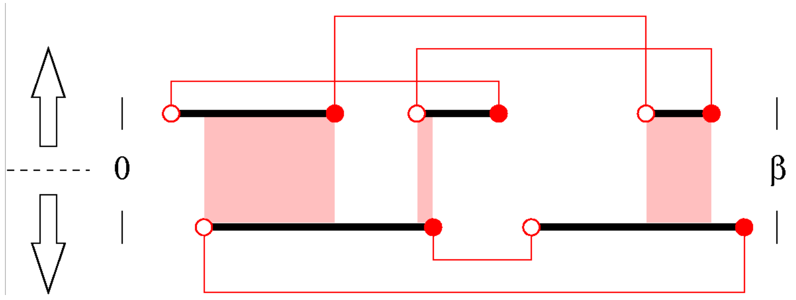
Efficiency of QMC DMFT solvers

New development: continuous-time QMC algorithms

1. weak-coupling expansion
[Rubtsov, Savkin, Lichtenstein, PRB (2005)]

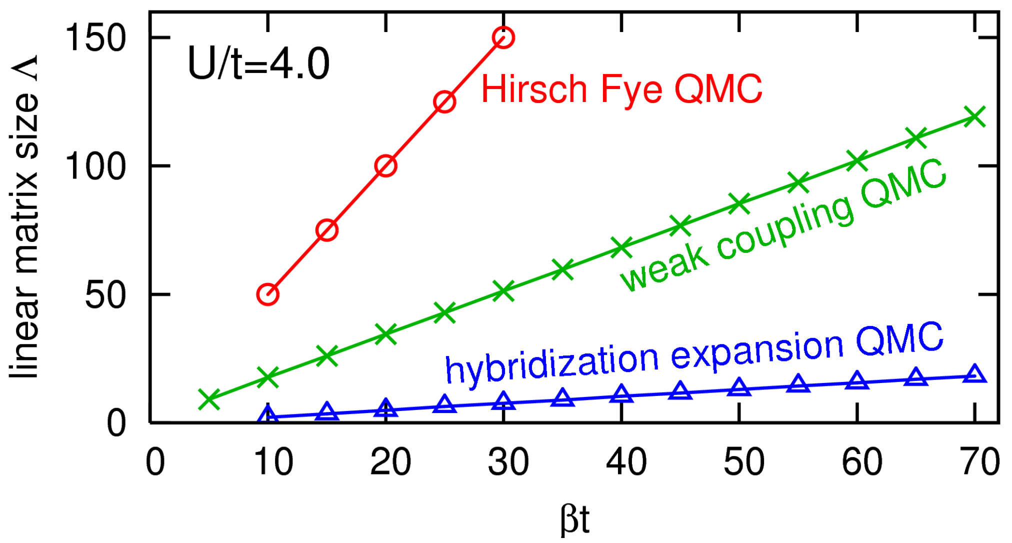


2. hybridization expansion
[Werner et al., PRL (2006)]



CT-QMC methods: smaller matrices

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

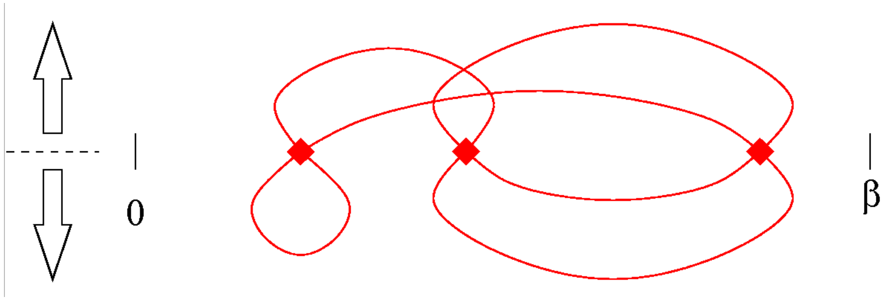


Efficiency of QMC DMFT solvers

New development: continuous-time QMC algorithms

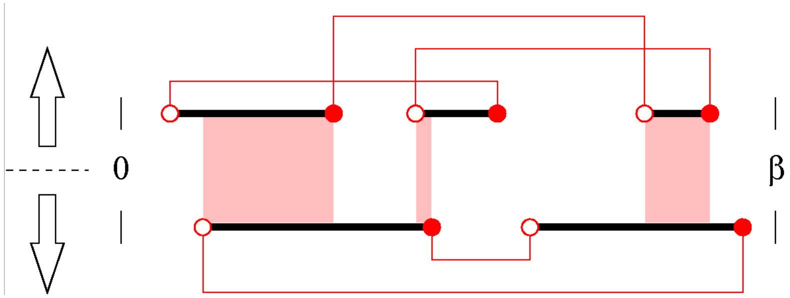
1. weak-coupling expansion

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



2. hybridization expansion

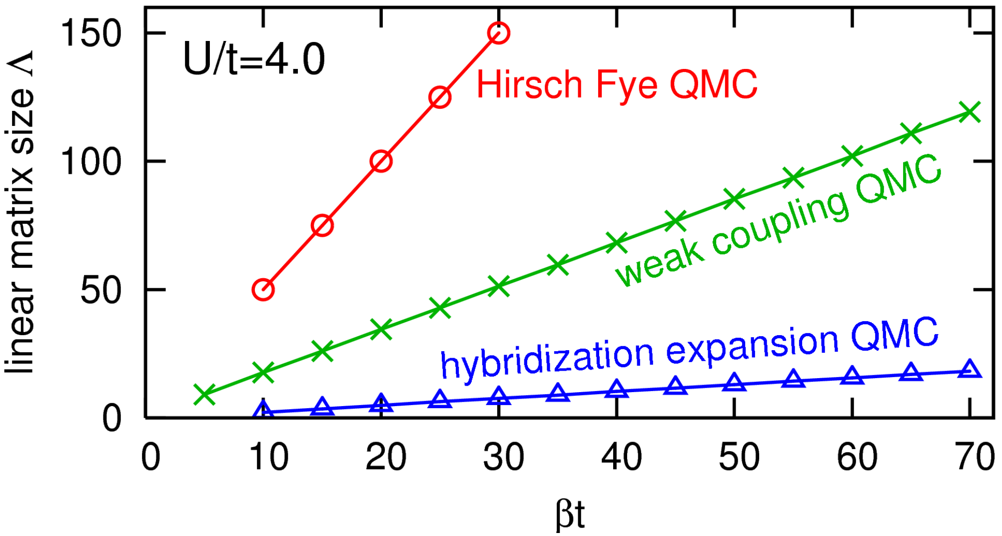
[Werner et al., PRL (2006)]



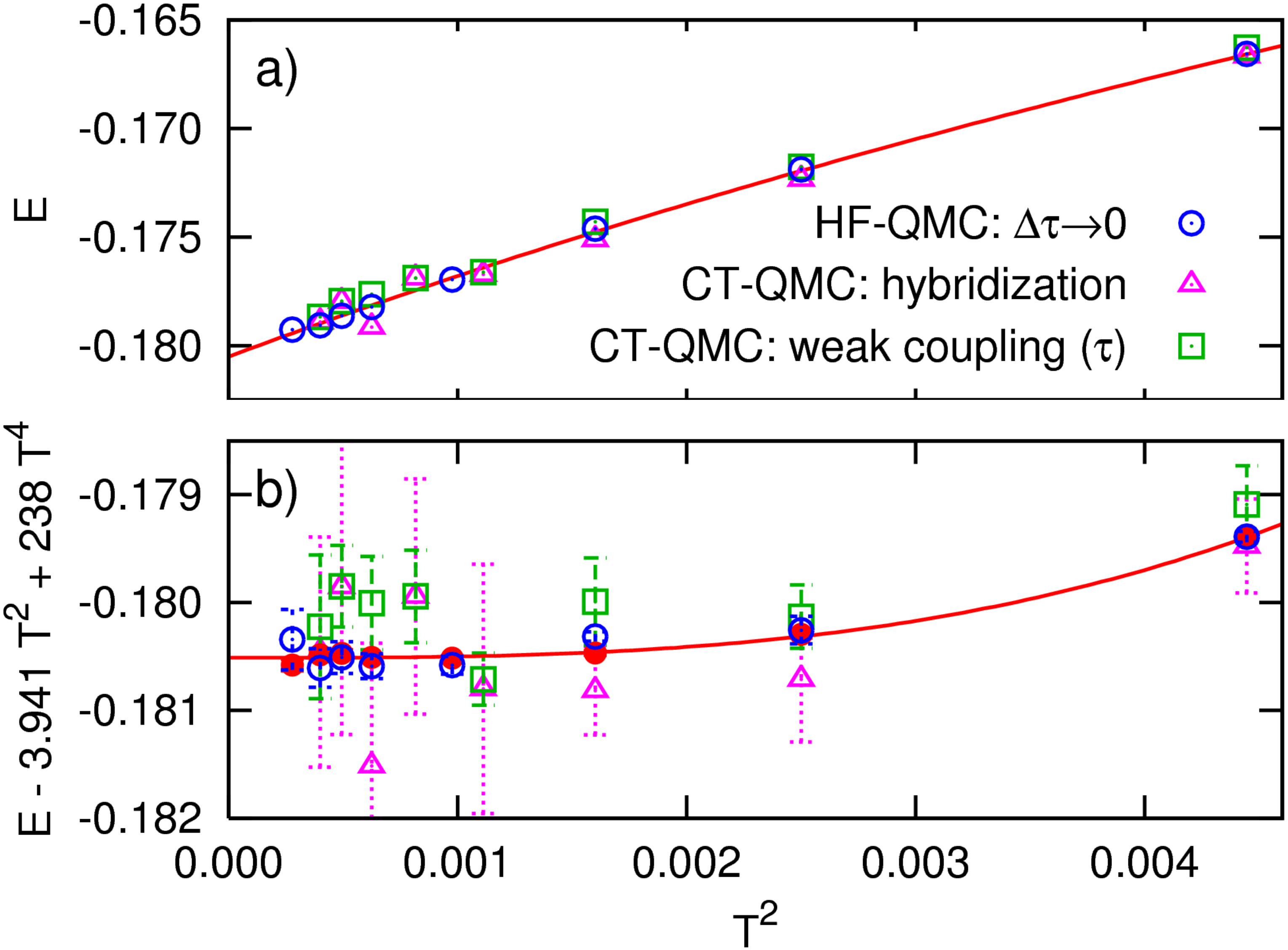
CT-QMC methods: smaller matrices

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

Claim [Troyer (2006)]:
"CT-QMC more efficient than HF-QMC by orders of magnitude"

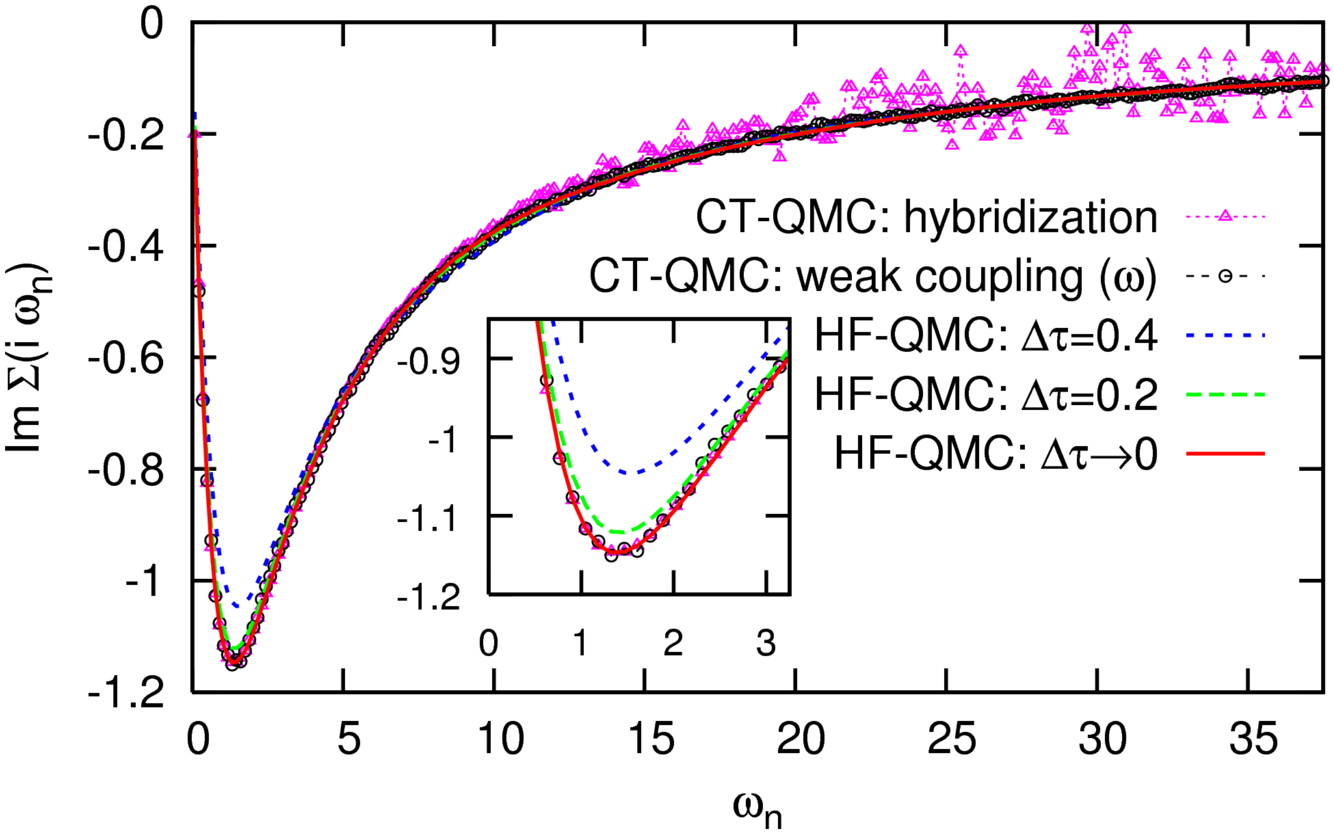


Comparisons at constant CPU time: total energy (at $U = W = 4$)



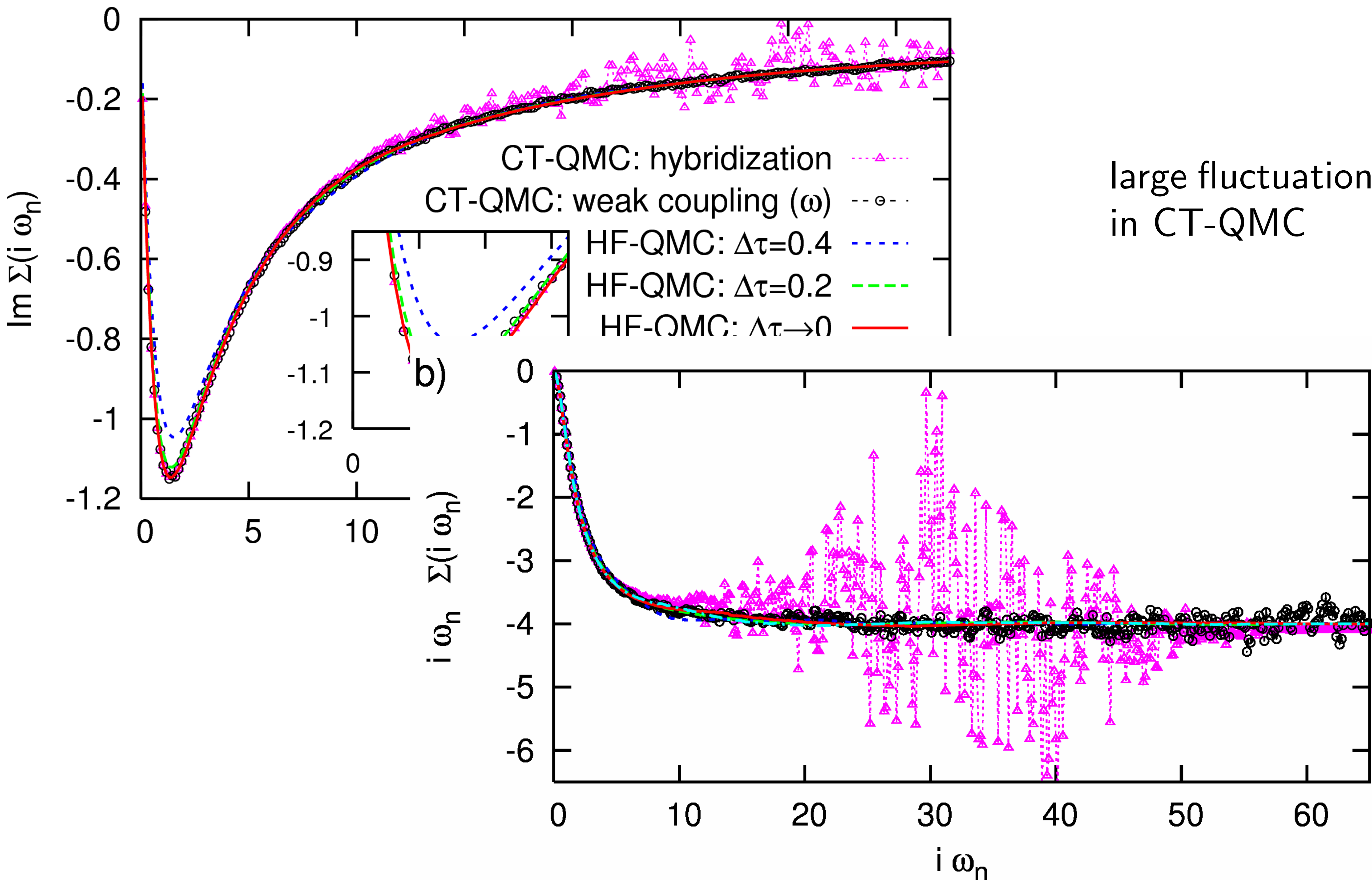
HF-QMC more efficient (higher precision at same cost) [NB, PRB **76**, 205120 (2007)]

Comparison of self energies (at $U = W = 4$)



large fluctuations in CT-QMC

Comparison of self energies (at $U = W = 4$)



large fluctuations in CT-QMC

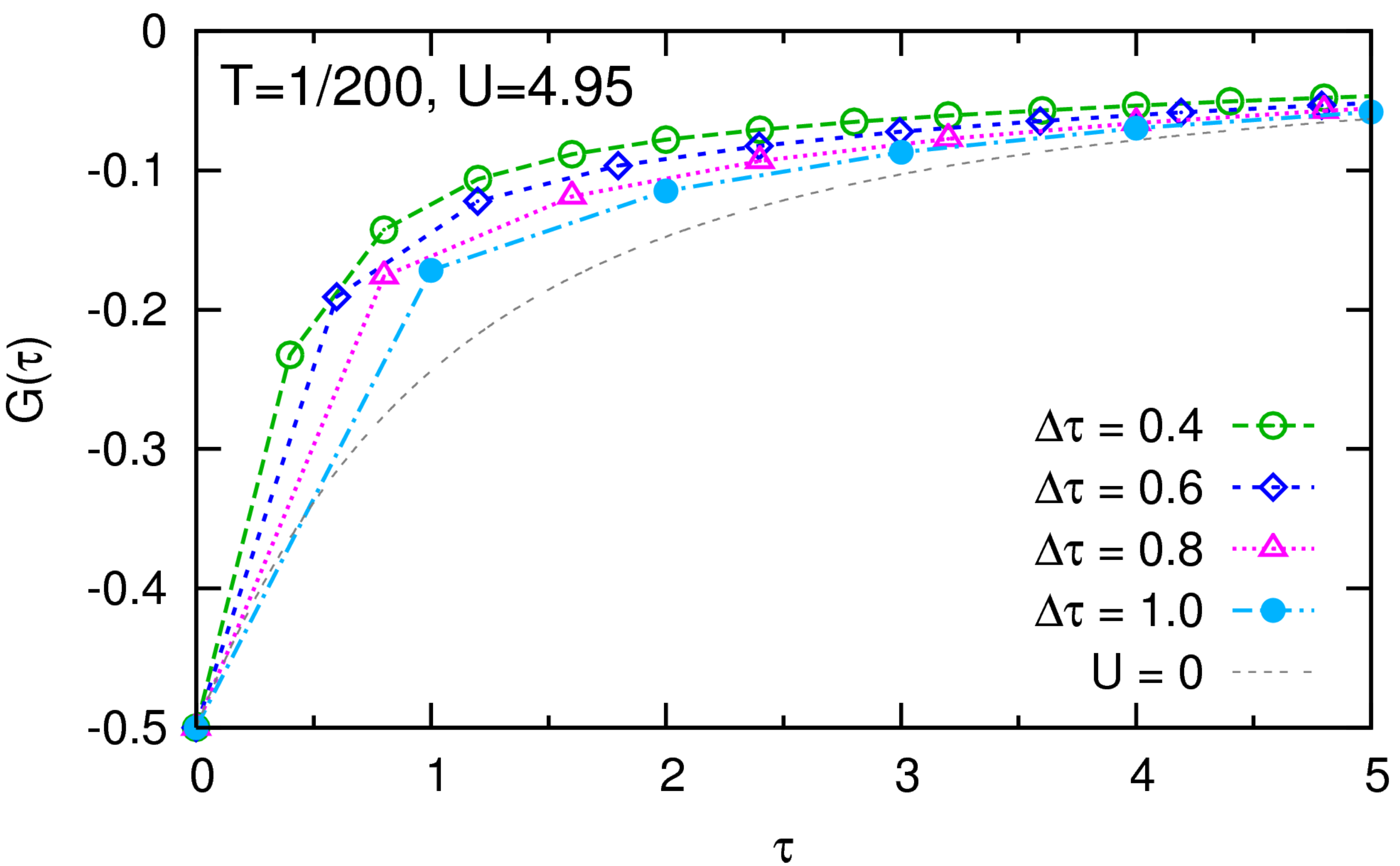
Unbiased Green functions and spectra from HF-QMC

State of the art: analytic continuation (using MEM) of imaginary-time Green function at fixed finite (often large) $\Delta\tau$ $\rightsquigarrow$ bias

Unbiased Green functions and spectra from HF-QMC

State of the art: analytic continuation (using MEM) of imaginary-time Green function at fixed finite (often large) $\Delta\tau$ $\rightsquigarrow$ bias

Reason: no obvious extrapolation scheme for $G(\tau)$

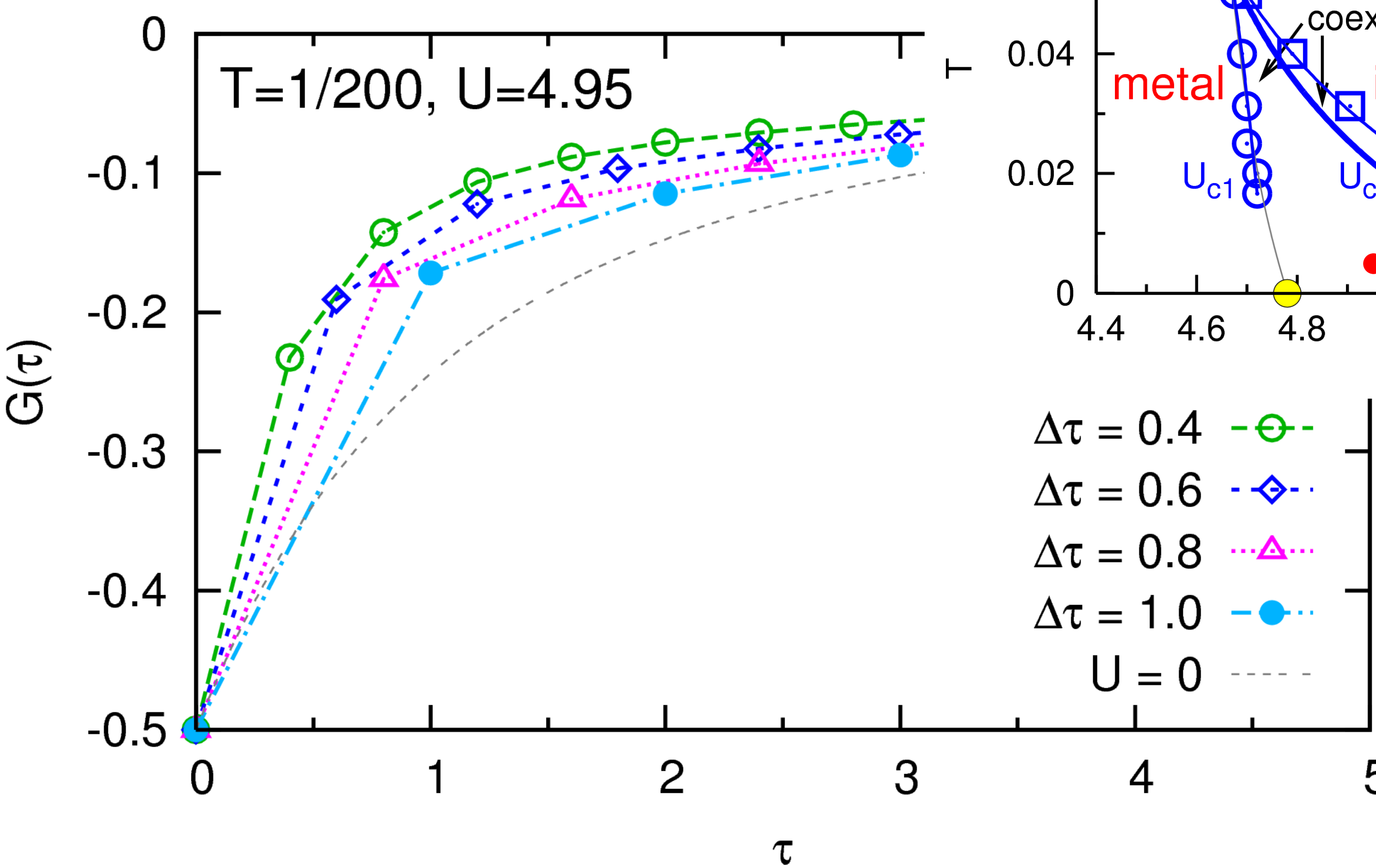


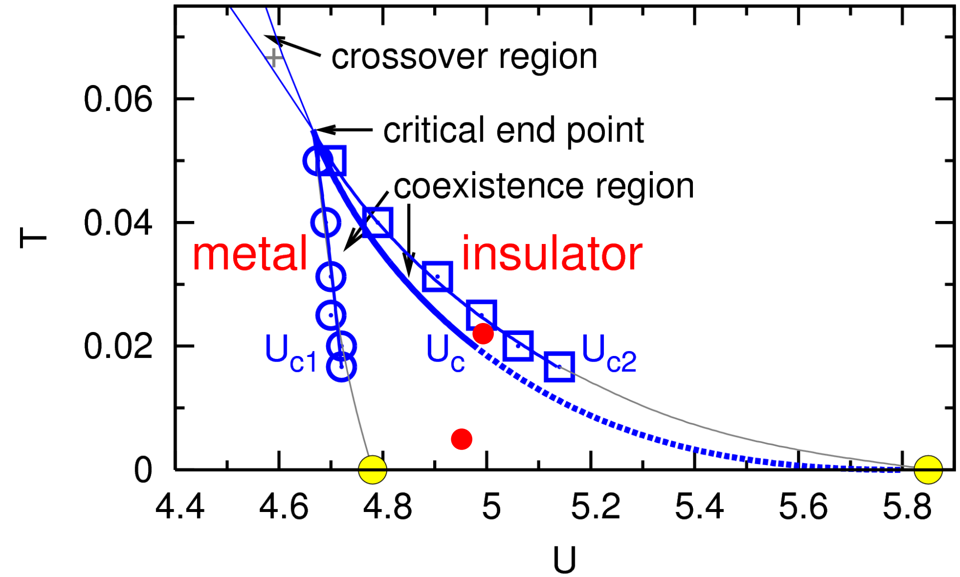
Low temperature ("beyond HF-QMC"): large $\Delta\tau$ $\rightsquigarrow$ large biases [NB, arXiv:0712.1290]

Unbiased Green functions and spectra from HF-QMC

State of the art: analytic continuation (using MEM) of imaginary-time Green function at fixed

Reason: no obvious extrapolatic



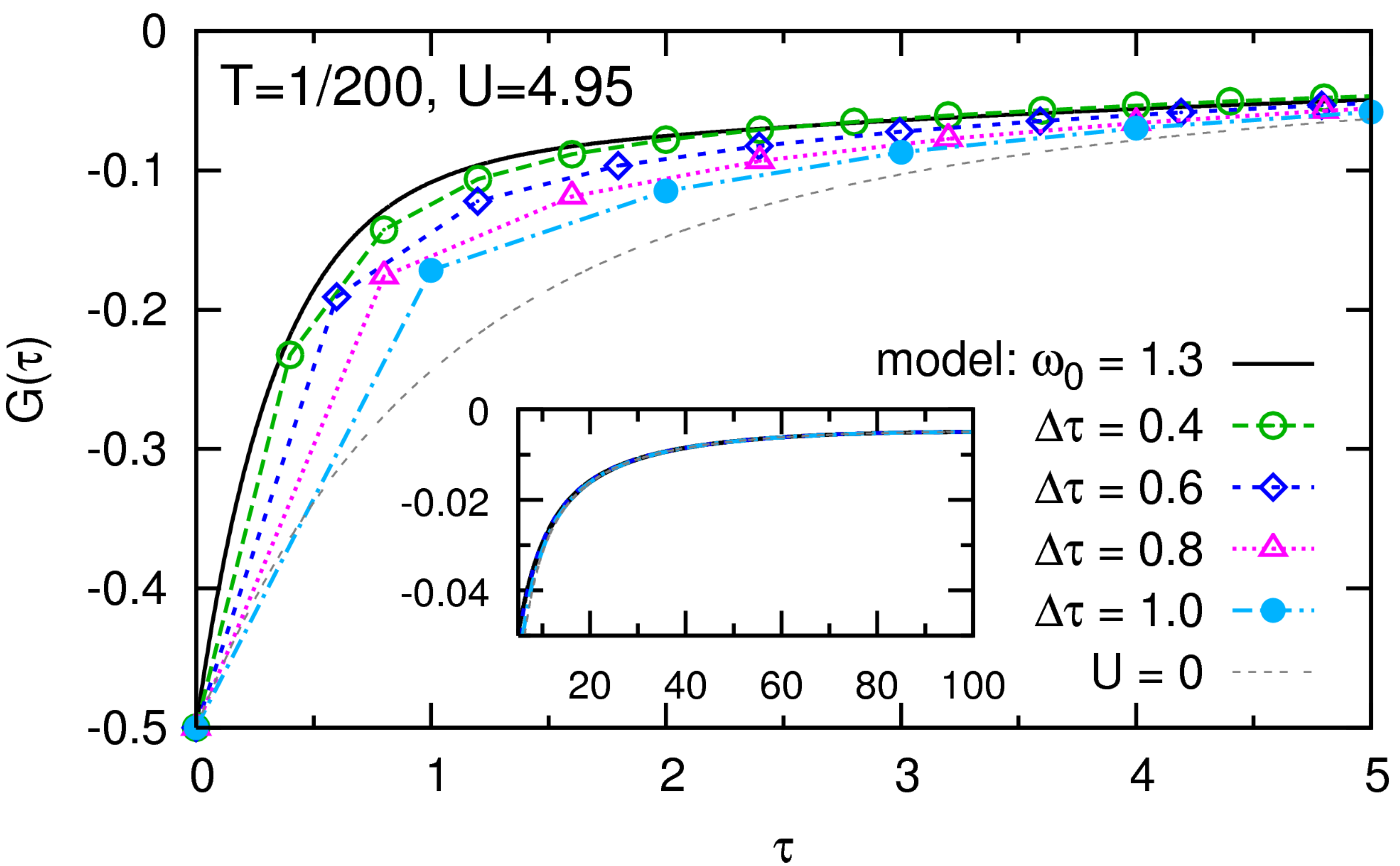


Low temperature ("beyond HF-QMC"): large $\Delta\tau \rightsquigarrow$ large biases [NB, arXiv:0712.1290]

Unbiased Green functions and spectra from HF-QMC

State of the art: analytic continuation (using MEM) of imaginary-time Green function at fixed finite (often large) $\Delta\tau$ $\rightsquigarrow$ bias

Reason: no obvious extrapolation scheme for $G(\tau)$



Low temperature ("beyond HF-QMC"): large $\Delta\tau$ $\rightsquigarrow$ large biases [NB, arXiv:0712.1290]

New Green function extrapolation scheme

For each $\Delta\tau$:
- average $G_{\Delta\tau}(\tau)$ over parallel runs for same impurity model
- average $\log[-G_{\Delta\tau}(\tau)]$ over iterations ($\sim$ geometric av. for $G_{\Delta\tau}(\tau)$)
- interpolate via difference Green function $G_{\Delta\tau}(\tau) - G_{\text{model}}(\tau)$

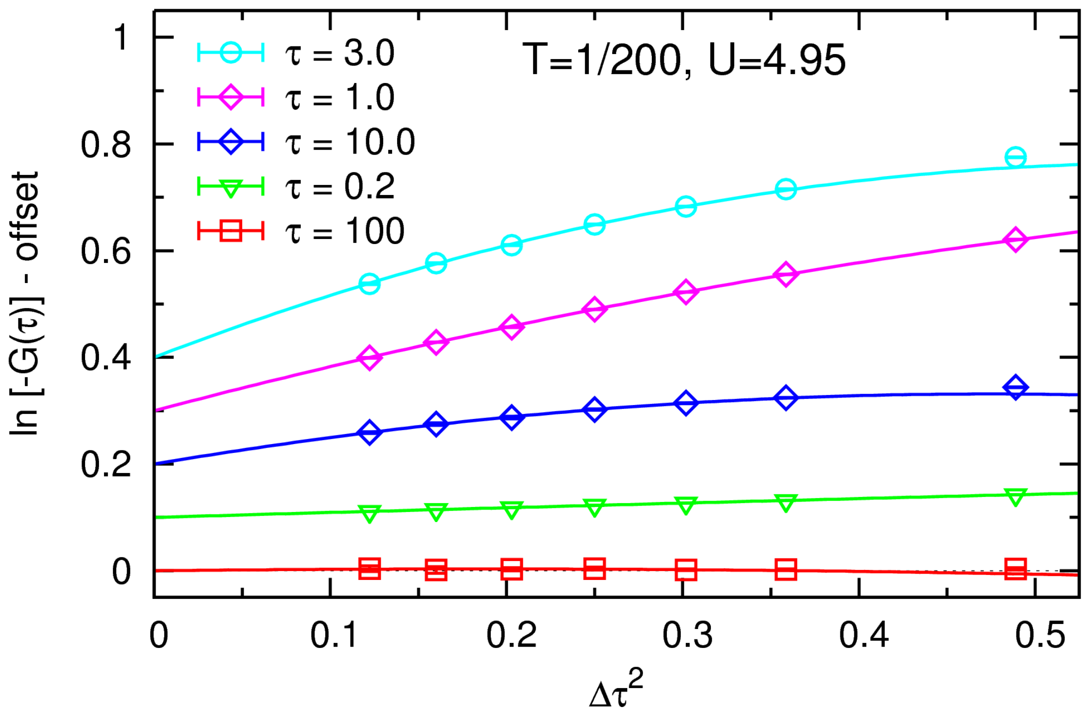
$\rightsquigarrow$ $G_{\Delta\tau_1}$, $G_{\Delta\tau_2}$, ... $G_{\Delta\tau_n}$ (with error bars) on common fine τ grid

New Green function extrapolation scheme

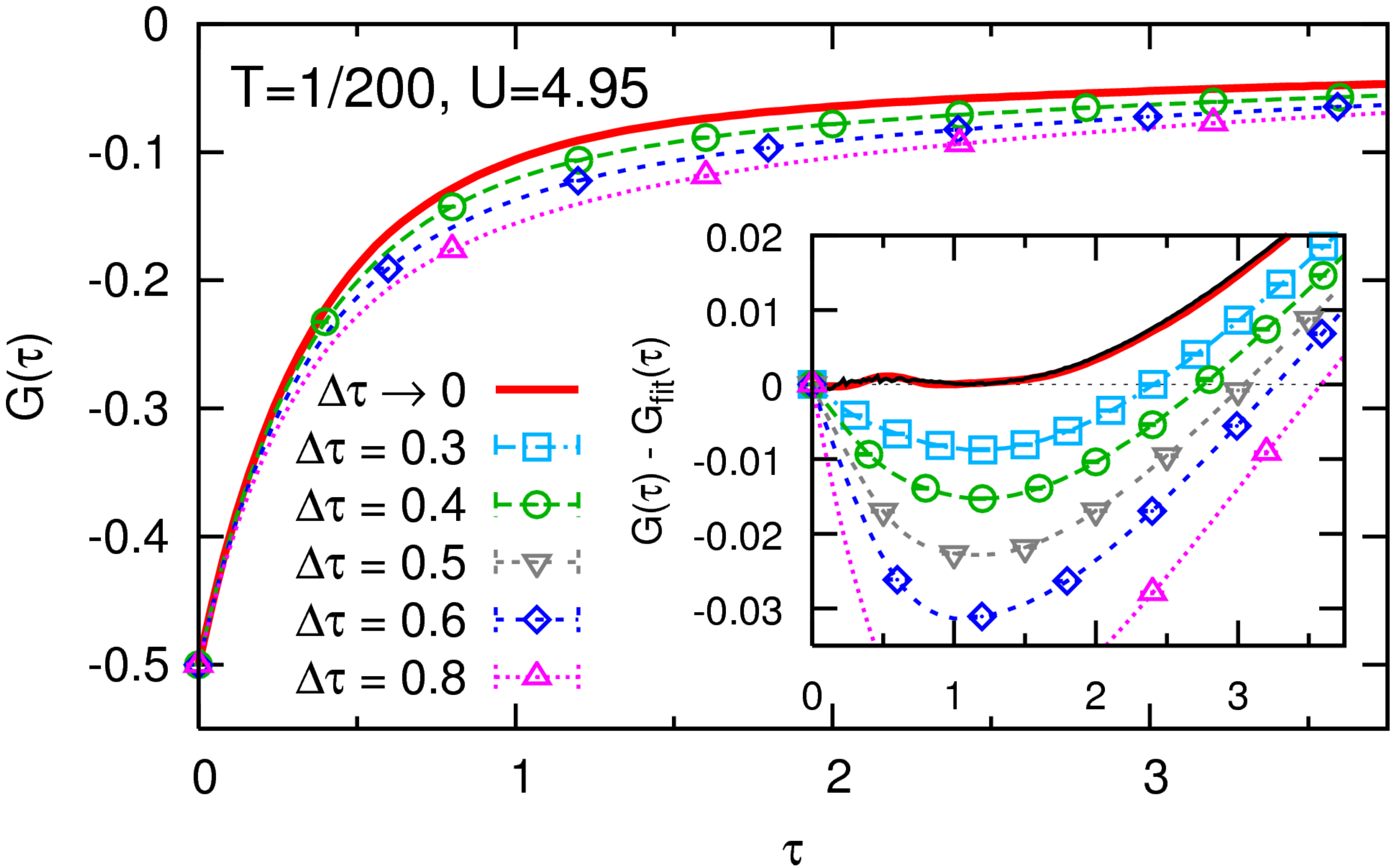
For each $\Delta\tau$:
- average $G_{\Delta\tau}(\tau)$ over parallel runs for same impurity model
- average $\log[-G_{\Delta\tau}(\tau)]$ over iterations ($\sim$ geometric av. for $G_{\Delta\tau}(\tau)$)
- interpolate via difference Green function $G_{\Delta\tau}(\tau) - G_{\text{model}}(\tau)$

$\rightsquigarrow$ $G_{\Delta\tau_1}$, $G_{\Delta\tau_2}$, . . . $G_{\Delta\tau_n}$ (with error bars) on common fine τ grid

- Extrapolate $\log[-G(\tau)]$ using cubic least-squares fits, overweighting low $\Delta\tau$



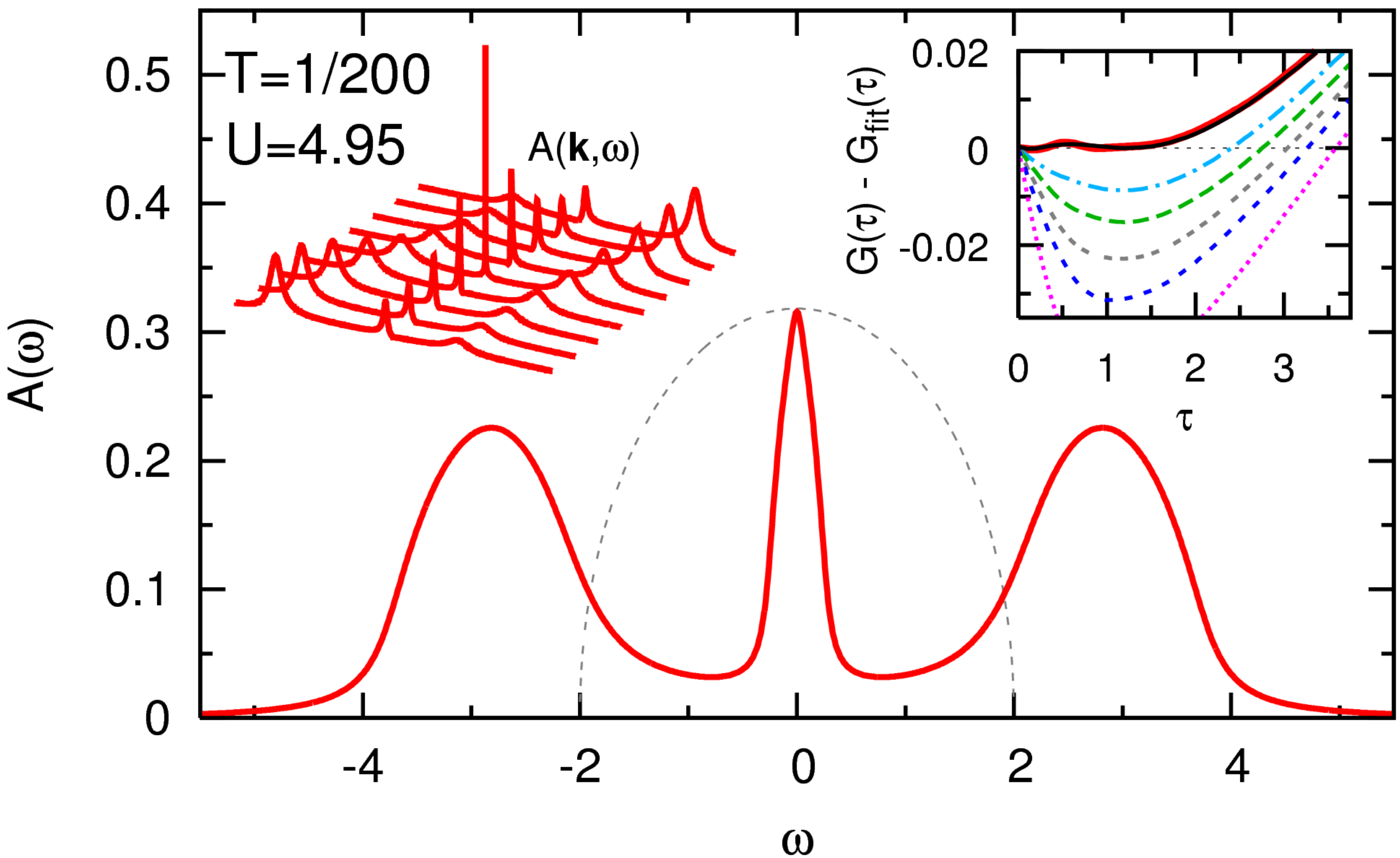
Result: unbiased, numerically exact Green function



[NB, arXiv:0712.1290]

Excellent agreement with hybridization expansion CT-QMC [Werner et al., PRL (2006)]

Analytic continuation using Padé approximant for self-energy



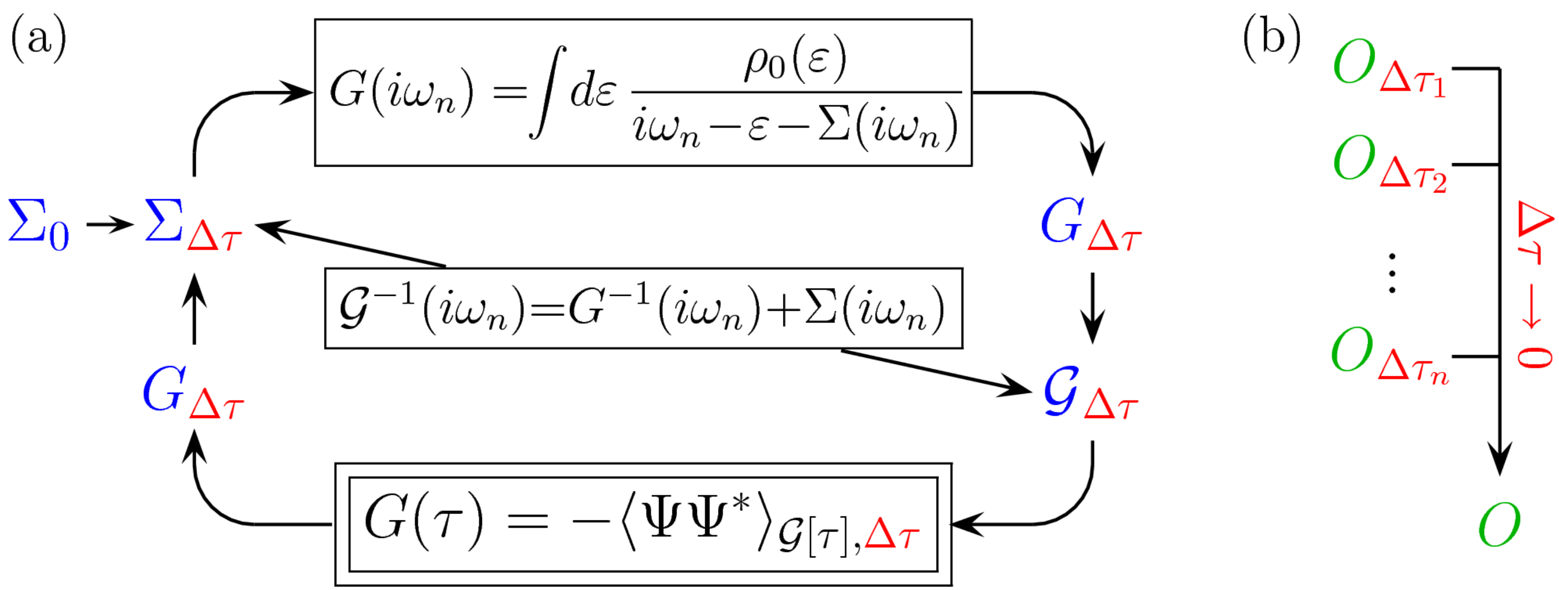
First spectra without discretization error from HF-QMC, at ultra-low T

Method directly applicable, e.g., to LDA+DMFT calculations [NB, arXiv:0712.1290]

Multigrid Hirsch-Fye quantum Monte Carlo algorithm

State of the art: (a) conventional HF-QMC

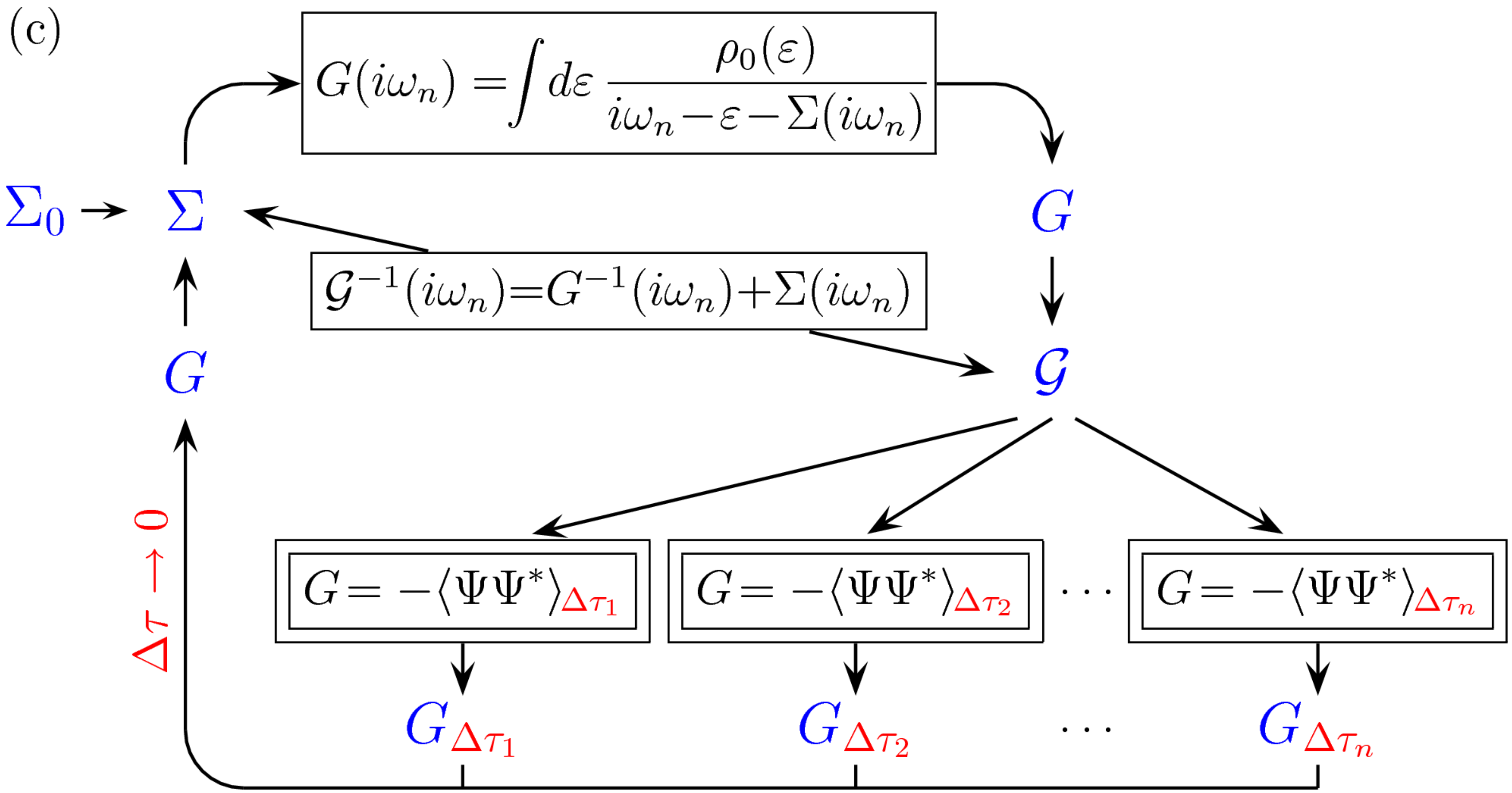
(b) *a posteriori* extrapolation of selected observables



Multigrid Hirsch-Fye quantum Monte Carlo algorithm

State of the art: (a) conventional HF-QMC

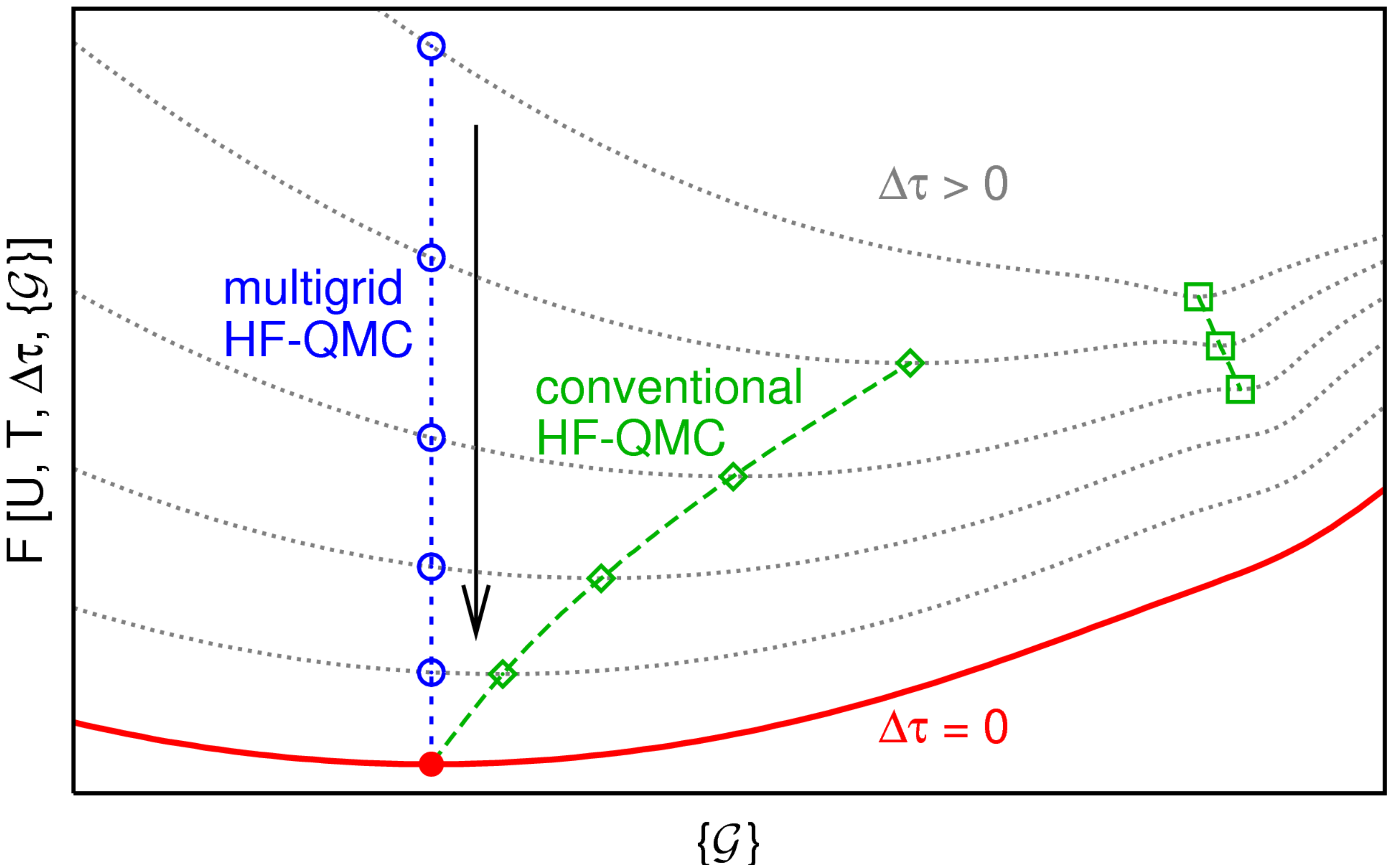
(b) *a posteriori* extrapolation of selected observables



(c) Multigrid HF-QMC: internal elimination of Trotter error

$\rightsquigarrow$ quasi continuous time algorithm [NB, arXiv:0801.1222]

Schematic comparison via generalized Ginzburg-Landau functionals

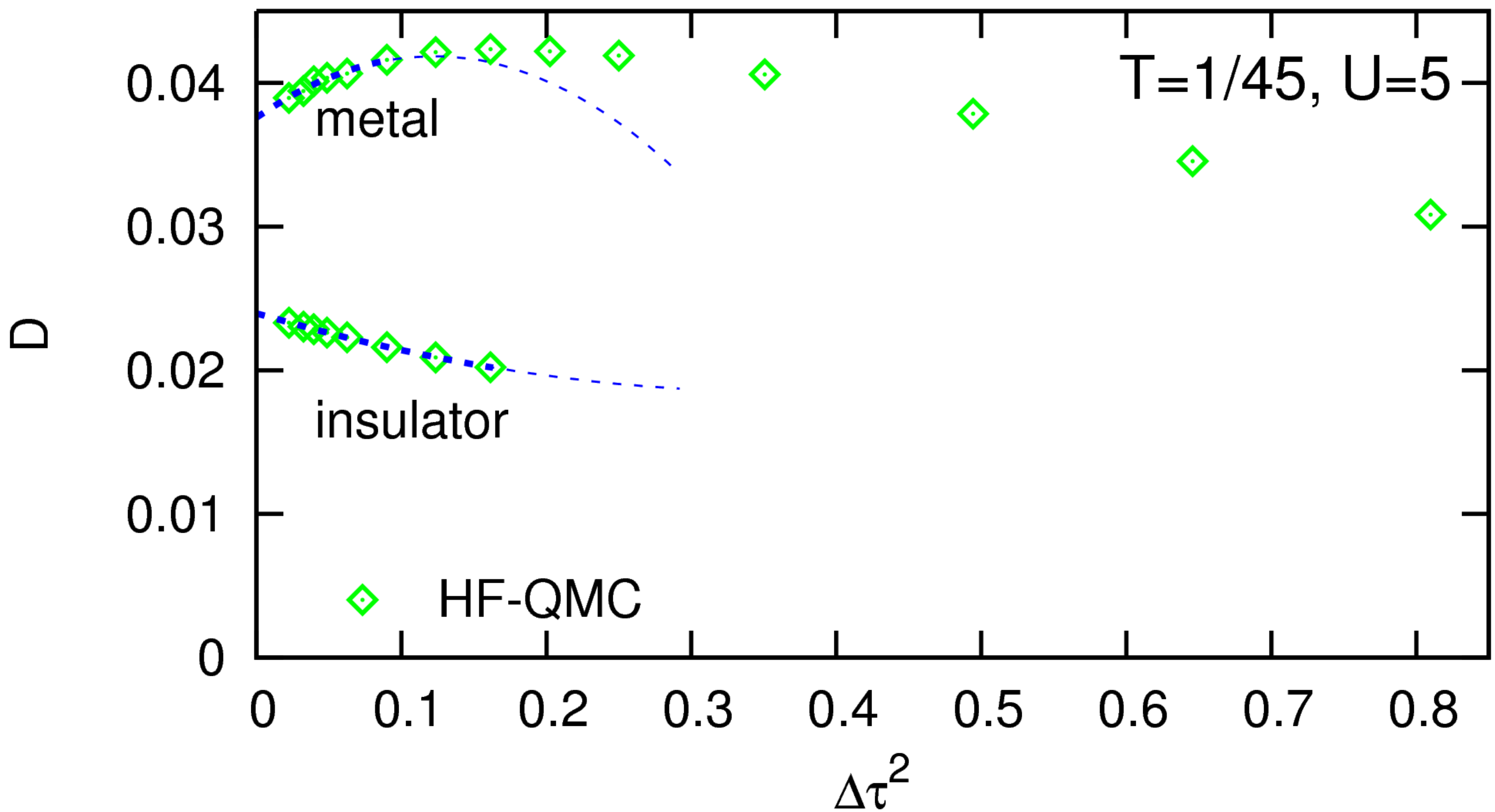


Conventional Hirsch-Fye QMC: DMFT fixed point shifts with $\Delta\tau$

Multigrid Hirsch-Fye QMC: DMFT iteration towards exact fixed point

Implementation: Green function extrapolation, hierarchy of frequency scales

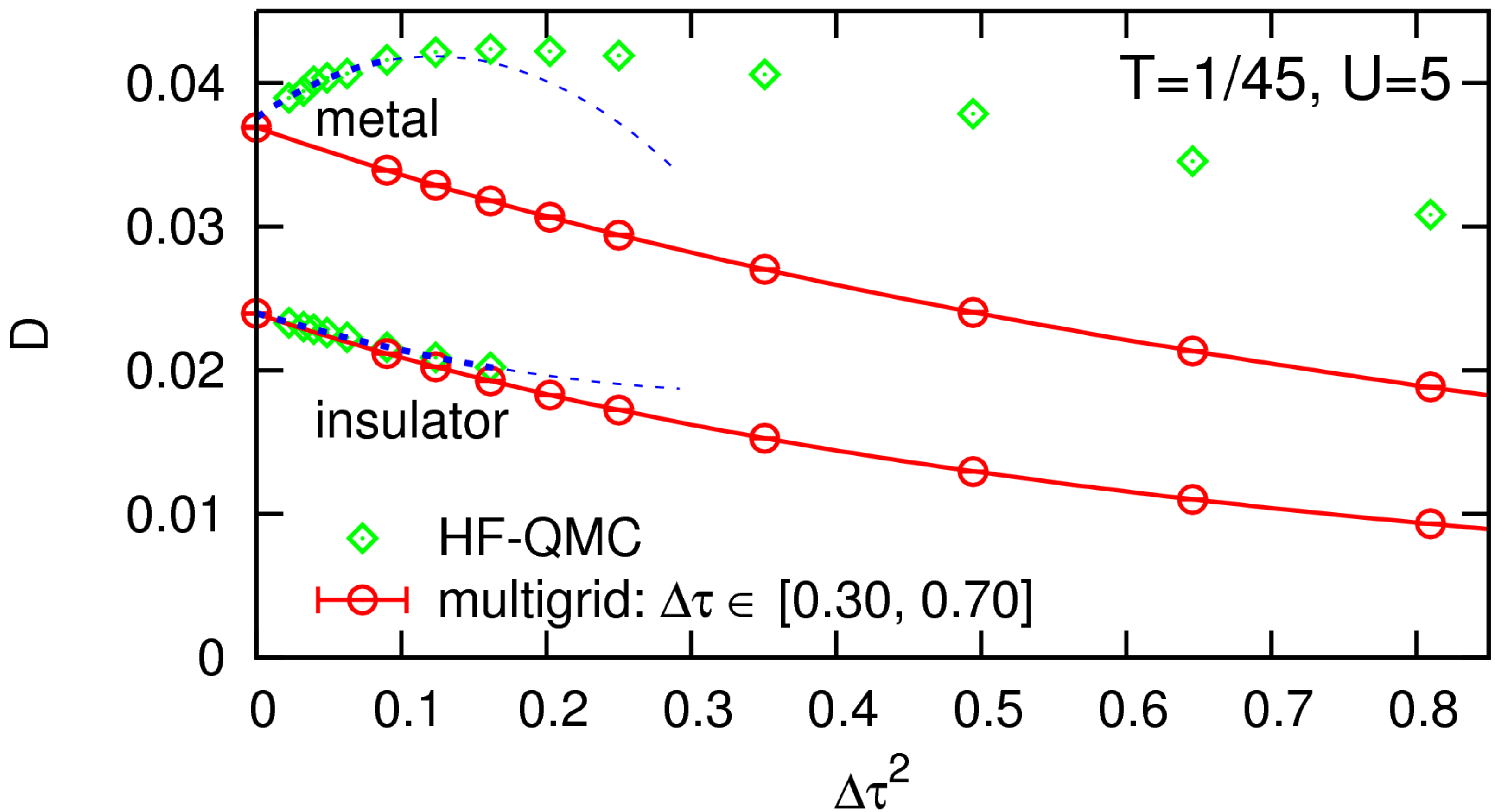
Comparison: double occupancy $D = \langle n_{i\uparrow} n_{i\downarrow} \rangle$ near Mott transition



Conventional HF-QMC: no insulating solution for $\Delta\tau \gtrsim 0.4$

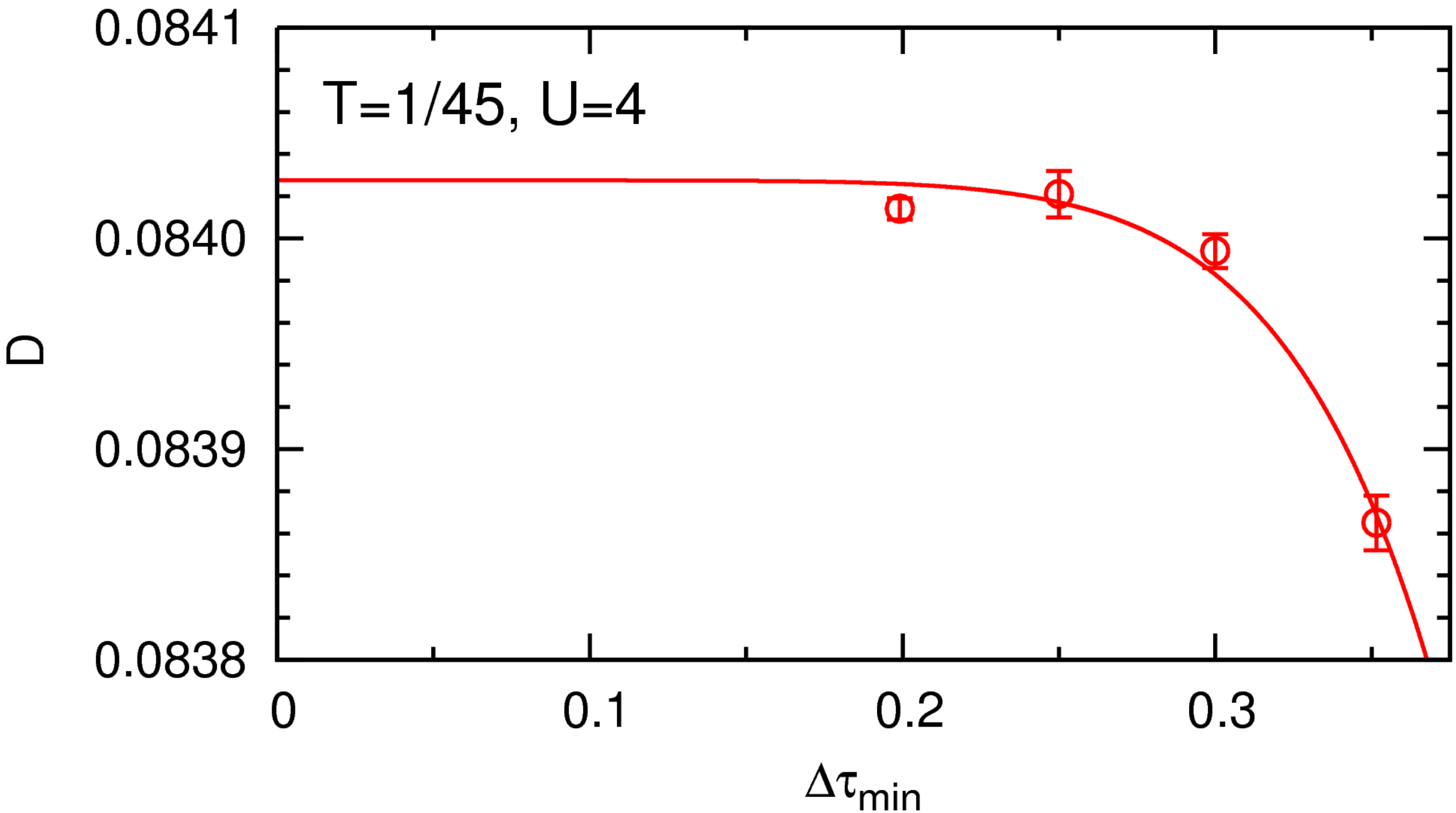
very irregular $\Delta\tau$ dependence beyond $\Delta\tau \approx 0.3$

Comparison: double occupancy $D = \langle n_{i\uparrow} n_{i\downarrow} \rangle$ near Mott transition



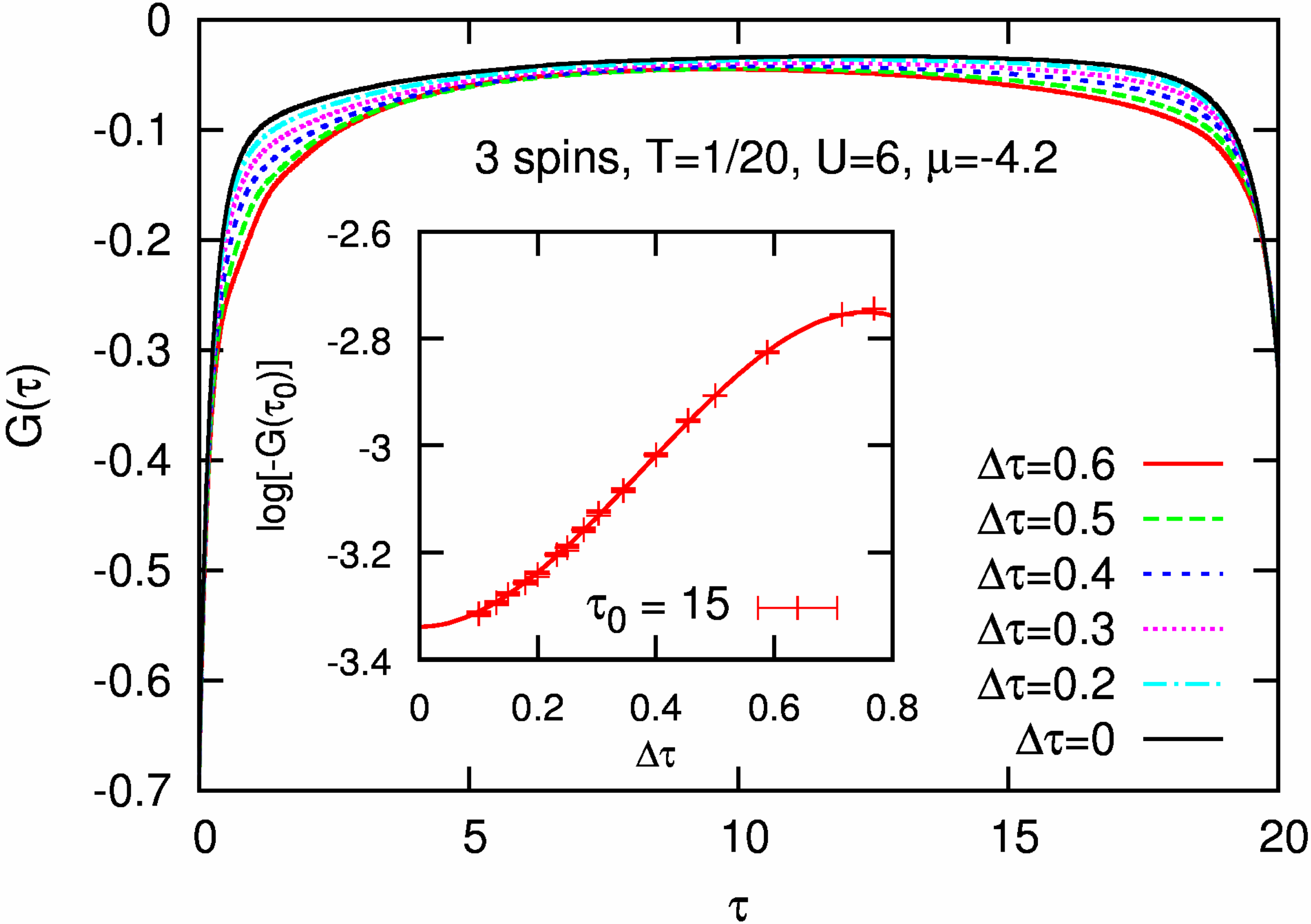
Conventional HF-QMC:	no insulating solution for $\Delta\tau \gtrsim 0.4$
	very irregular $\Delta\tau$ dependence beyond $\Delta\tau \approx 0.3$
Multigrid HF-QMC:	vastly larger useful range of $\Delta\tau$

Systematic study: impact of grid range (on double occupancy)



Multigrid HF-QMC usually "numerically exact" for $\tau_{\text{min}} \lesssim 0.3$

General (metallic) test case for $\Delta\tau$ extrapolation of $G(\tau)$



Summary

Auxiliary-field Hirsch-Fye QMC + high-frequency corrections

Efficiency of QMC DMFT solvers: HF-QMC competitive (for not too low T)

Unbiased Green functions and spectra from HF-QMC

Multigrid Hirsch-Fye quantum Monte Carlo algorithm

Applications (Gorelik): Mott transitions at large degeneracy / in 3-spin system

Summary

Auxiliary-field Hirsch-Fye QMC + high-frequency corrections

Efficiency of QMC DMFT solvers: HF-QMC competitive (for not too low T)

Unbiased Green functions and spectra from HF-QMC

Multigrid Hirsch-Fye quantum Monte Carlo algorithm

Applications (Gorelik): Mott transitions at large degeneracy / in 3-spin system

On request: Spectral weight transfer at Mott transition, high-precision specific heat, superlinear MPI + OpenMP scaling

New project: real-space DMFT+QMC for ultracold atom clouds on optical lattices

Not yet considered: spin-flip terms, superconductivity, . . .

Acknowledgements:

Carsten Knecht, **Elena Gorelik**, Eberhard Jakobi, Peter van Dongen;
Funding by state RLP (Forschungsfonds 2007) and DFG (FG 559, SFB/TR 49)