Multigrid Hirsch-Fye quantum Monte Carlo algorithm for dynamical mean-field theory

Nils Blümer, Univ. Mainz

Outline

Introduction: quantum Monte Carlo simulations within dynamical mean-field theory

Unbiased Green functions and spectra from HF-QMC

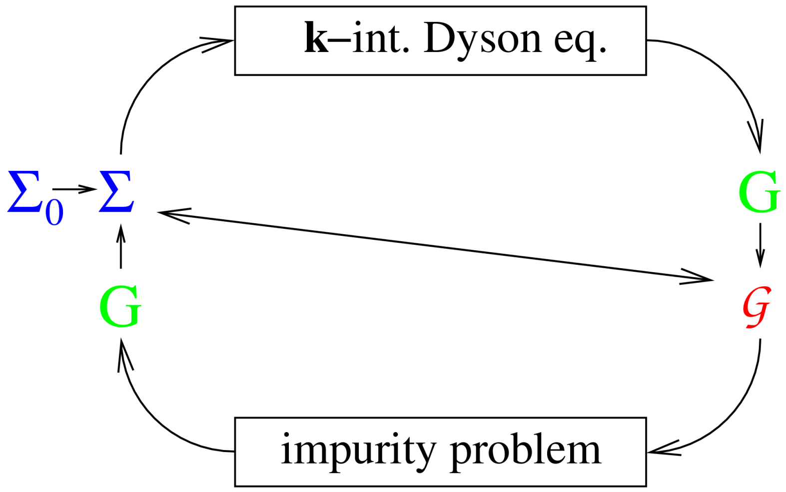
Multigrid Hirsch-Fye quantum Monte Carlo algorithm

Summary and outlook

Introduction: Dynamical mean-field theory

Iterative solution of DMFT equations

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



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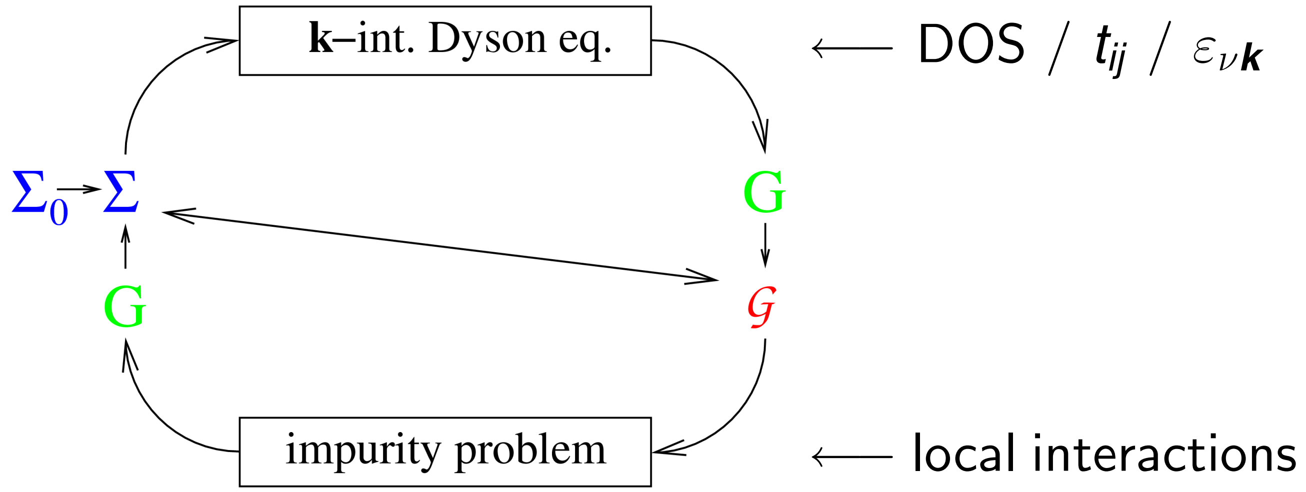

Impurity solver:

- Iterative perturbation theory (IPT; not controlled)
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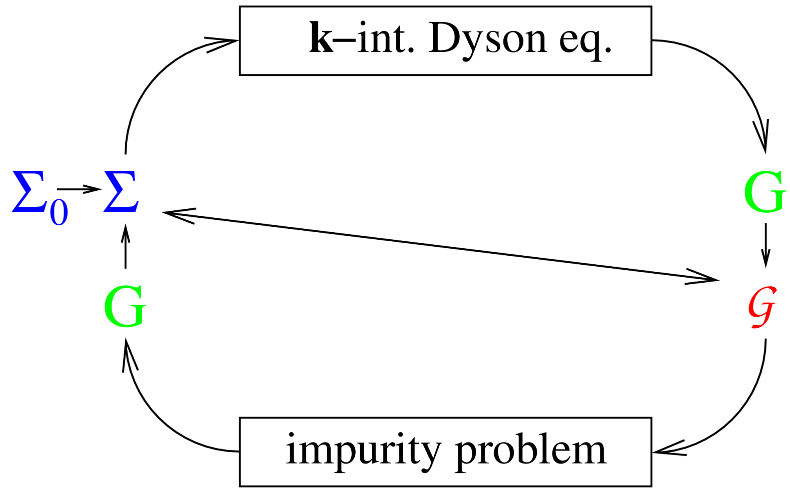

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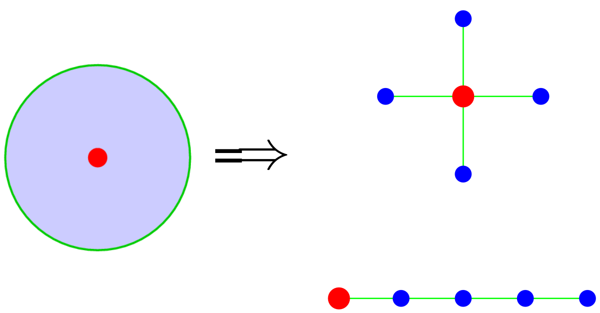
Impurity solver:

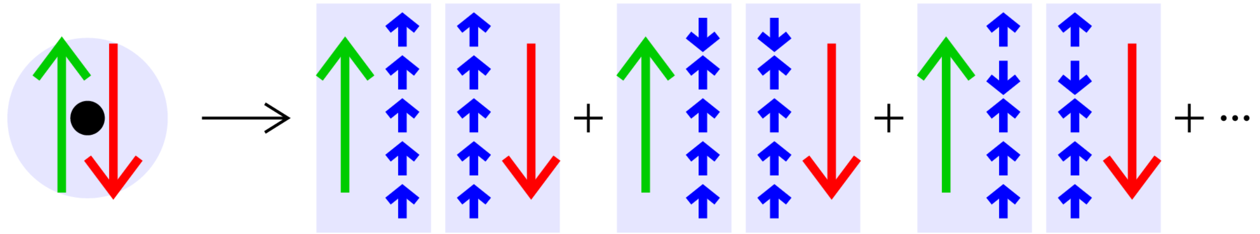
- Iterative perturbation theory (IPT; not controlled)
- Quantum Monte-Carlo (QMC)
- Exact diagonalization (ED; large finite-size errors)
- Numerical renormalization group (NRG; 1-2 bands)
- Density matrix renormalization group (DMRG)
- Self-energy functional theory (SFT) + ED



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

Wanted: Green function $G(\omega)$ Treatment in imaginary time $\tau \in [0, \beta]$

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



Wick theorem:

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

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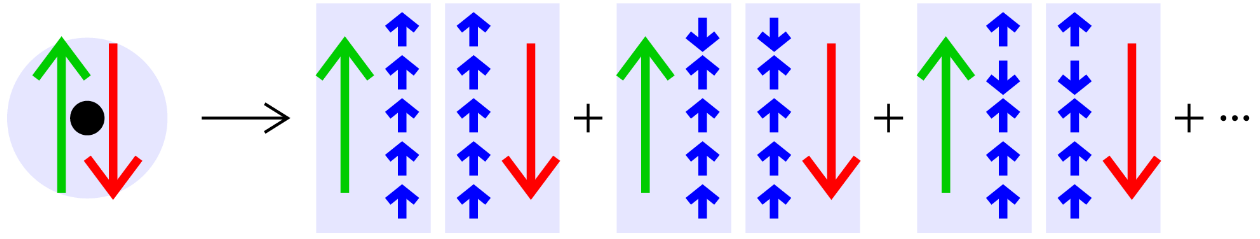

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MC importance sampling over auxiliary field, 2^Λ configurations ($50 \lesssim \Lambda \lesssim 400$)

+ + + nonperturbative, numerically exact

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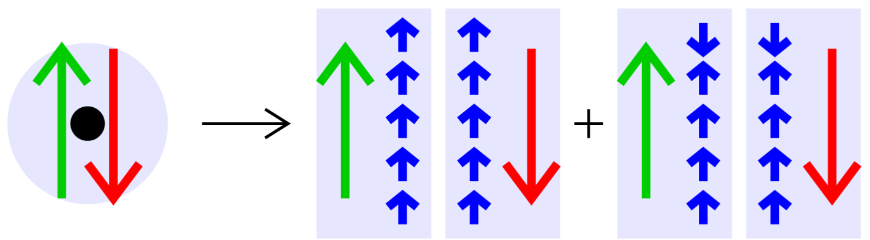

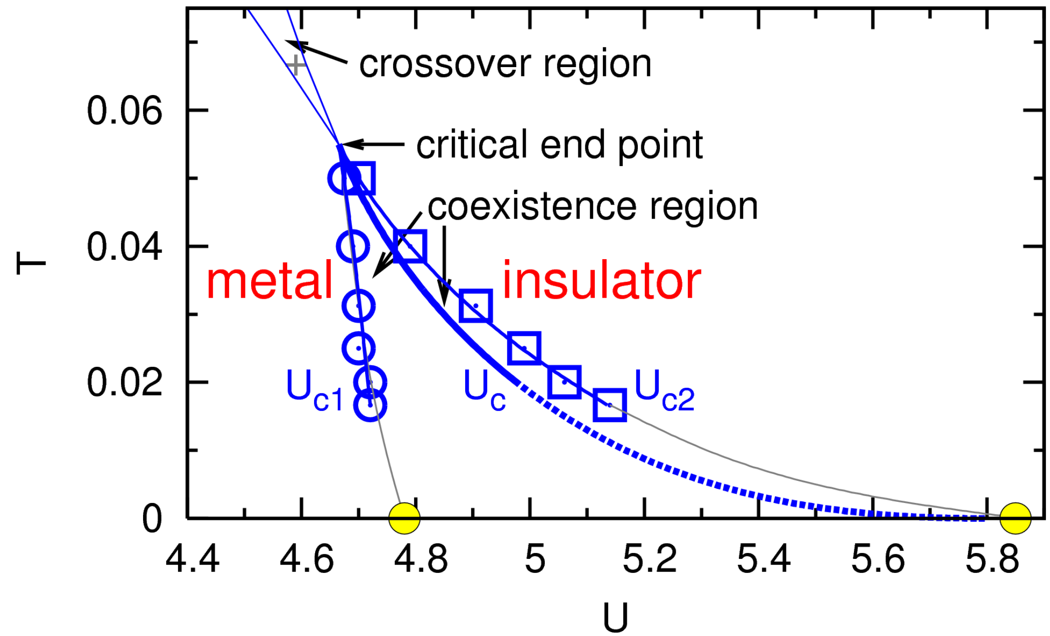

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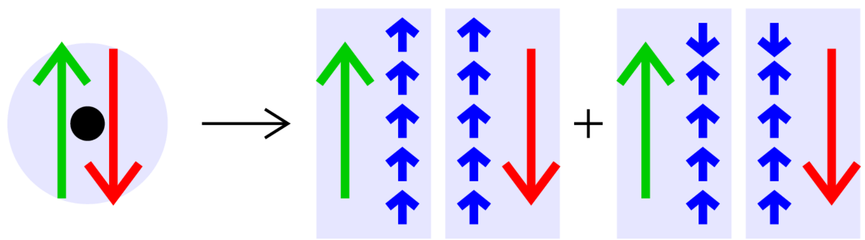

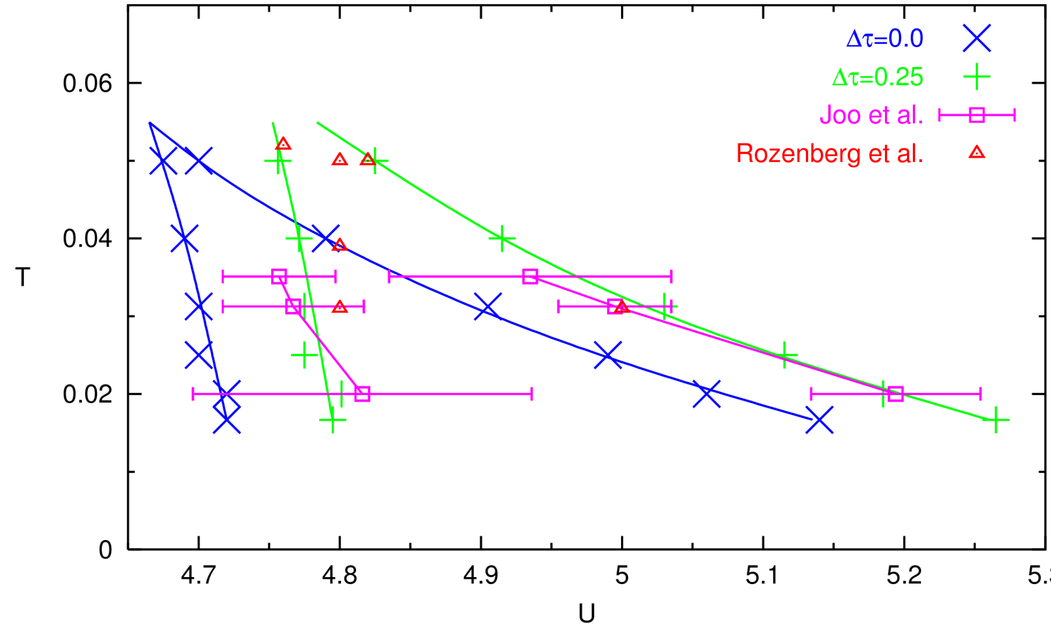

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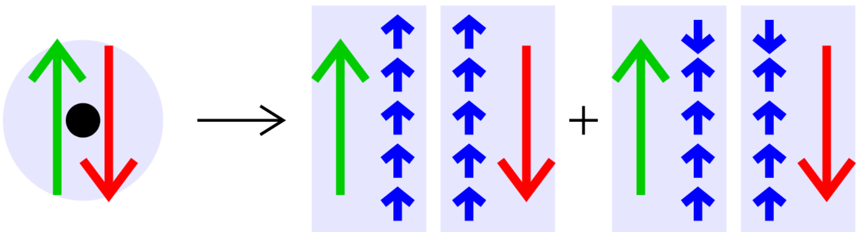

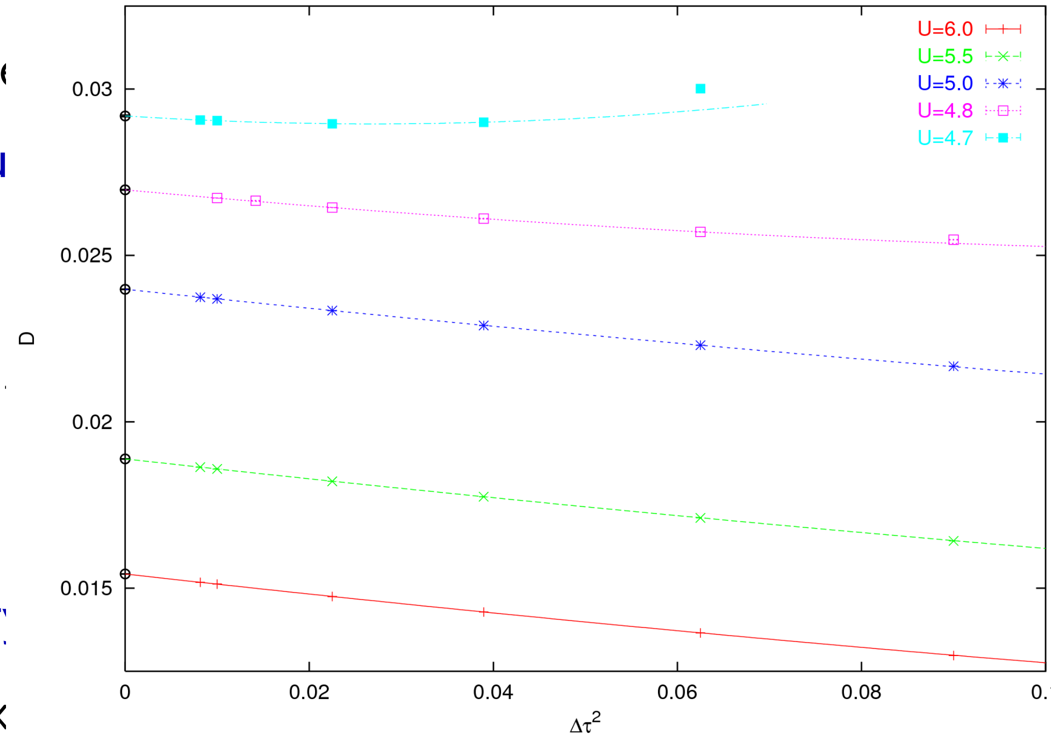

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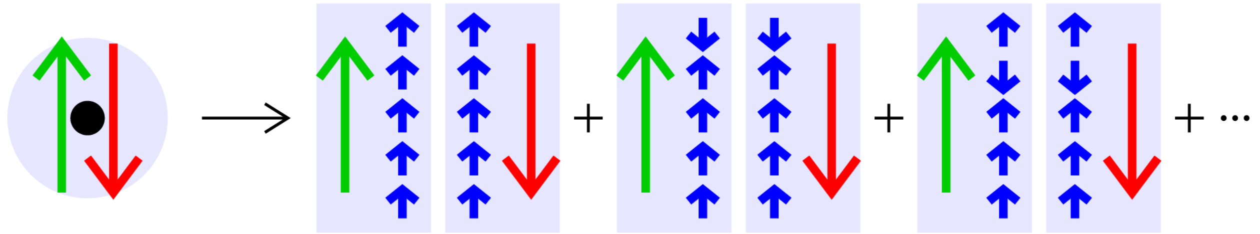

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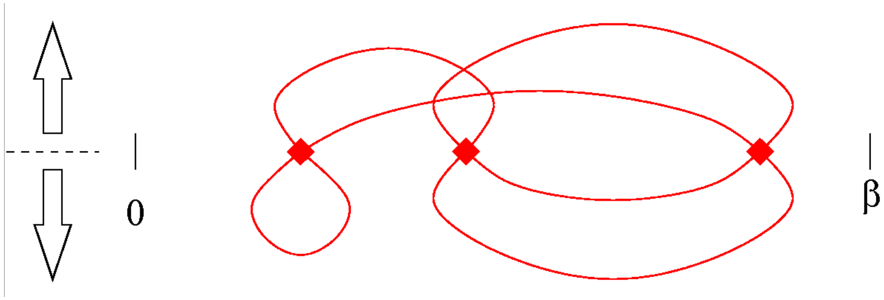
– – Green functions and spectra biased

Alternatives to Hirsch-Fye QMC as DMFT solver?

New development: continuous-time QMC algorithms

1. weak-coupling expansion

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



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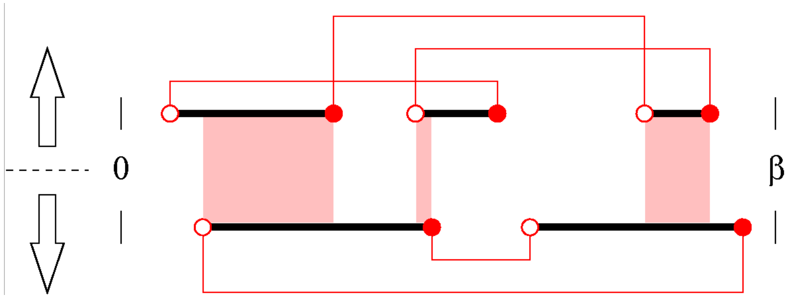

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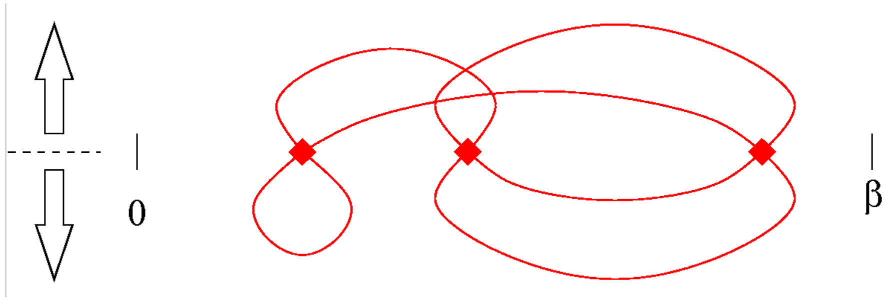

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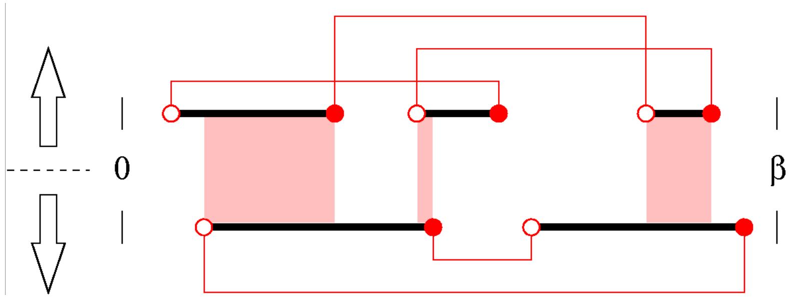
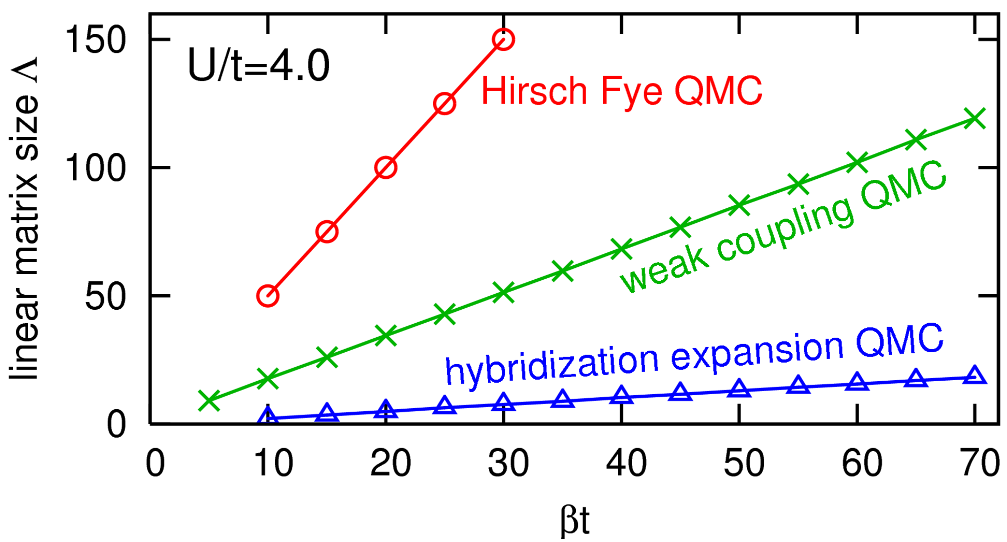


CT-QMC methods: smaller matrices

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



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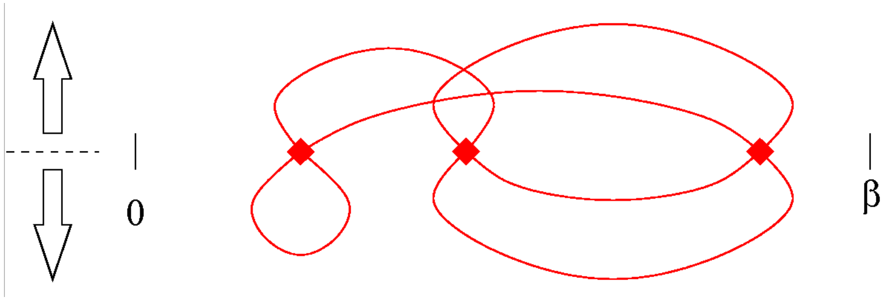

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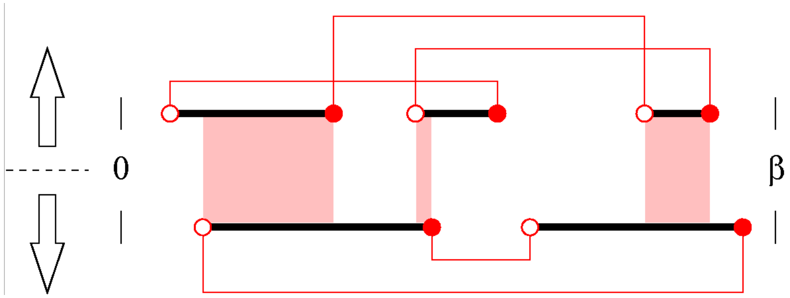

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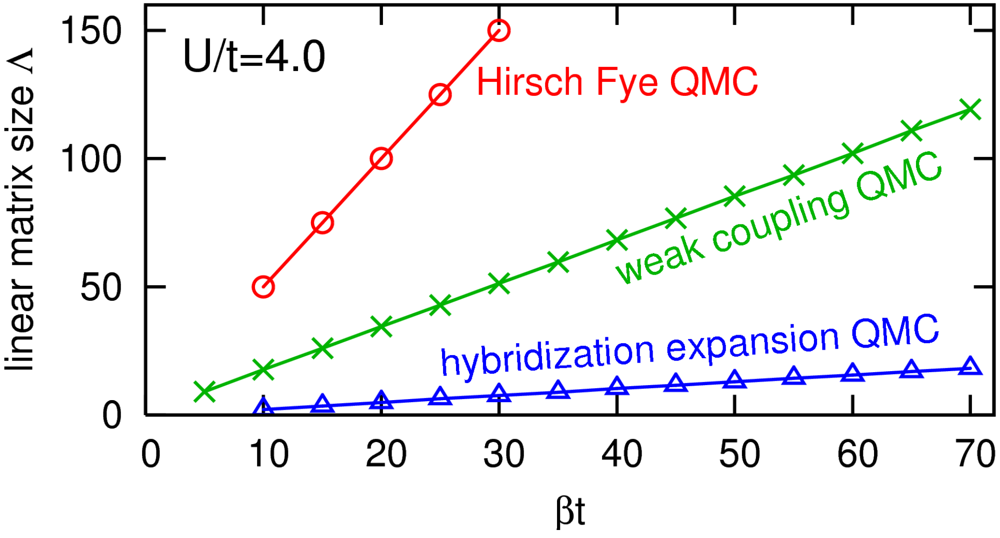
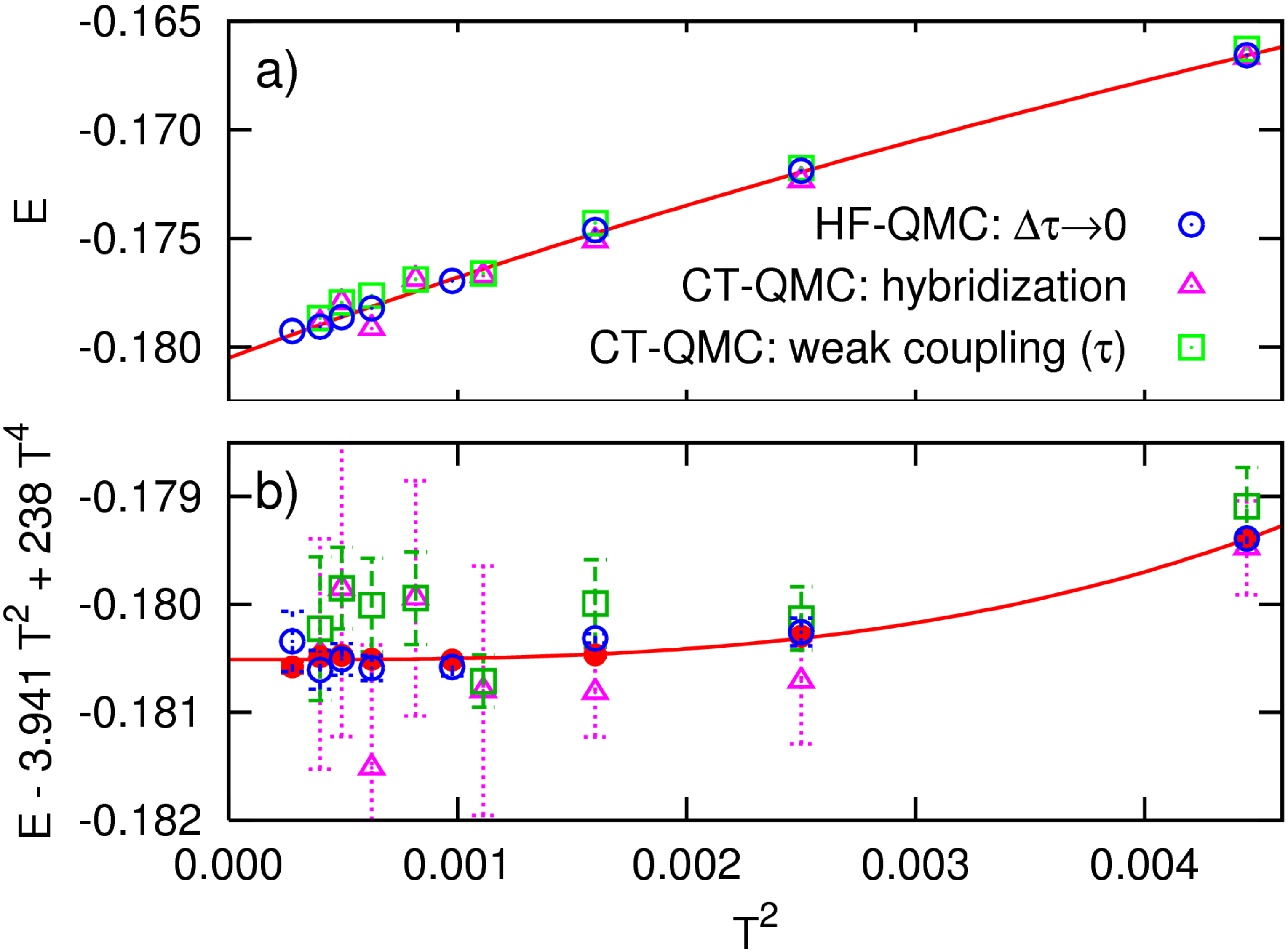
Claim [Troyer (2006)]:
CT-QMC more efficient than
HF-QMC by orders of magnitude



Comparison for total energy



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

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) $\Delta\tau$

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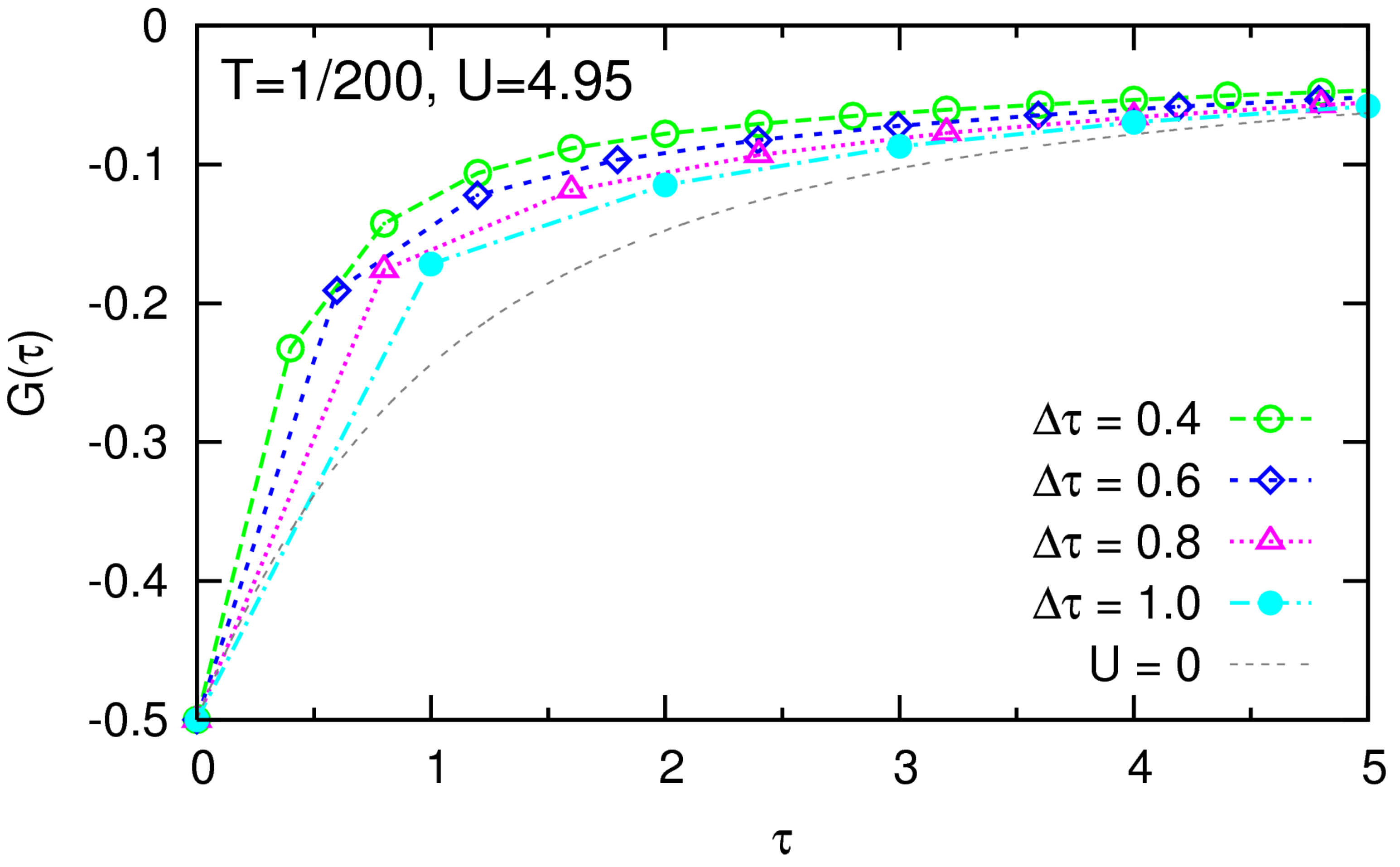
Reason: no obvious extrapolation scheme for $G(\tau)$



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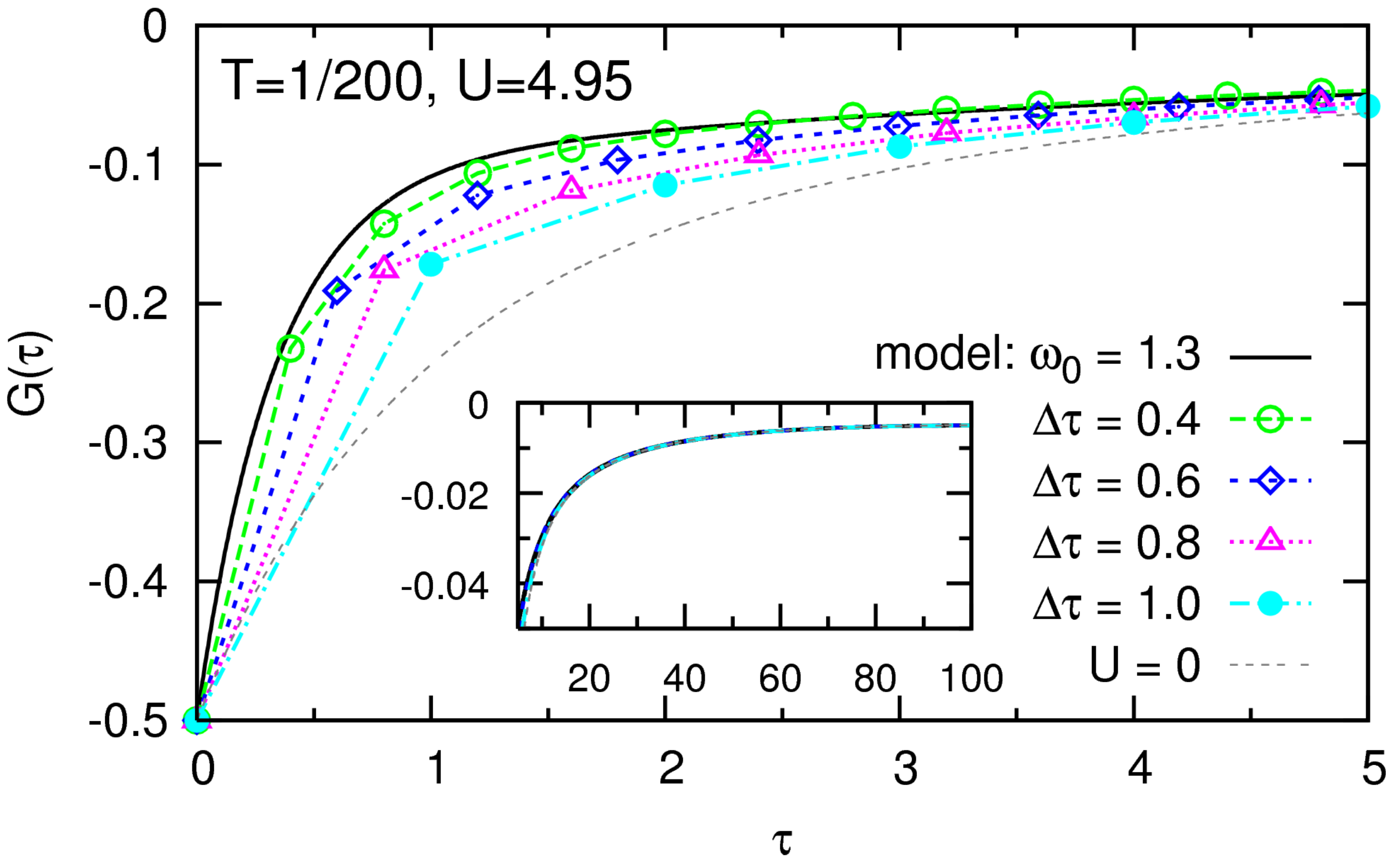

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Algorithm in more detail:

1. average $G(\tau)$ over parallel runs for same impurity model
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3. interpolate based on difference Green function $\{G(\tau)\} - G_{\text{model}}(\tau)$
4. extrapolate $\log[-G(\tau)]$ using cubic least-squares fits, overweighting low $\Delta\tau$

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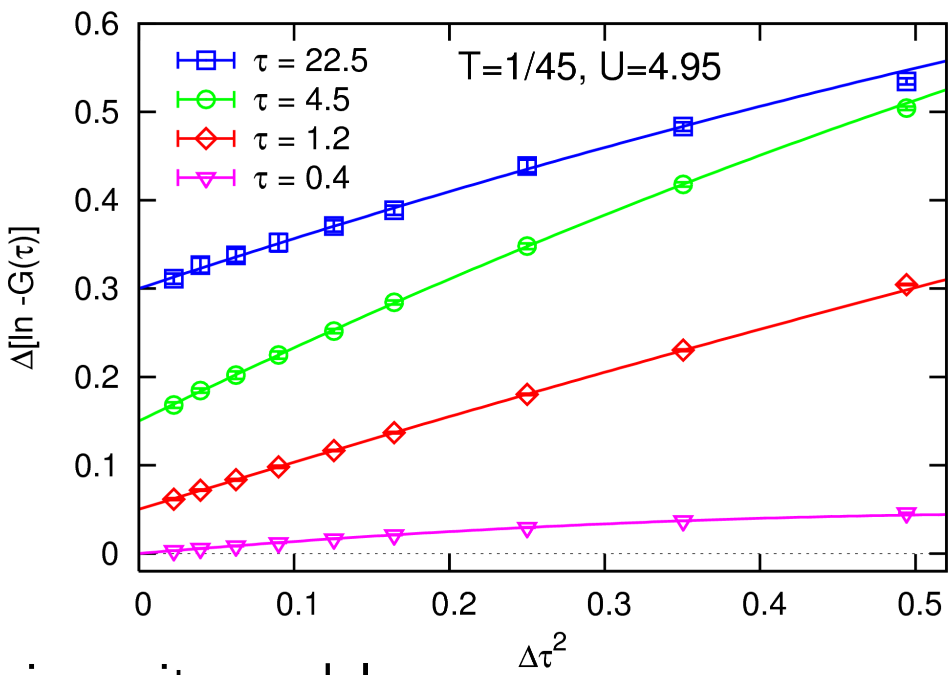

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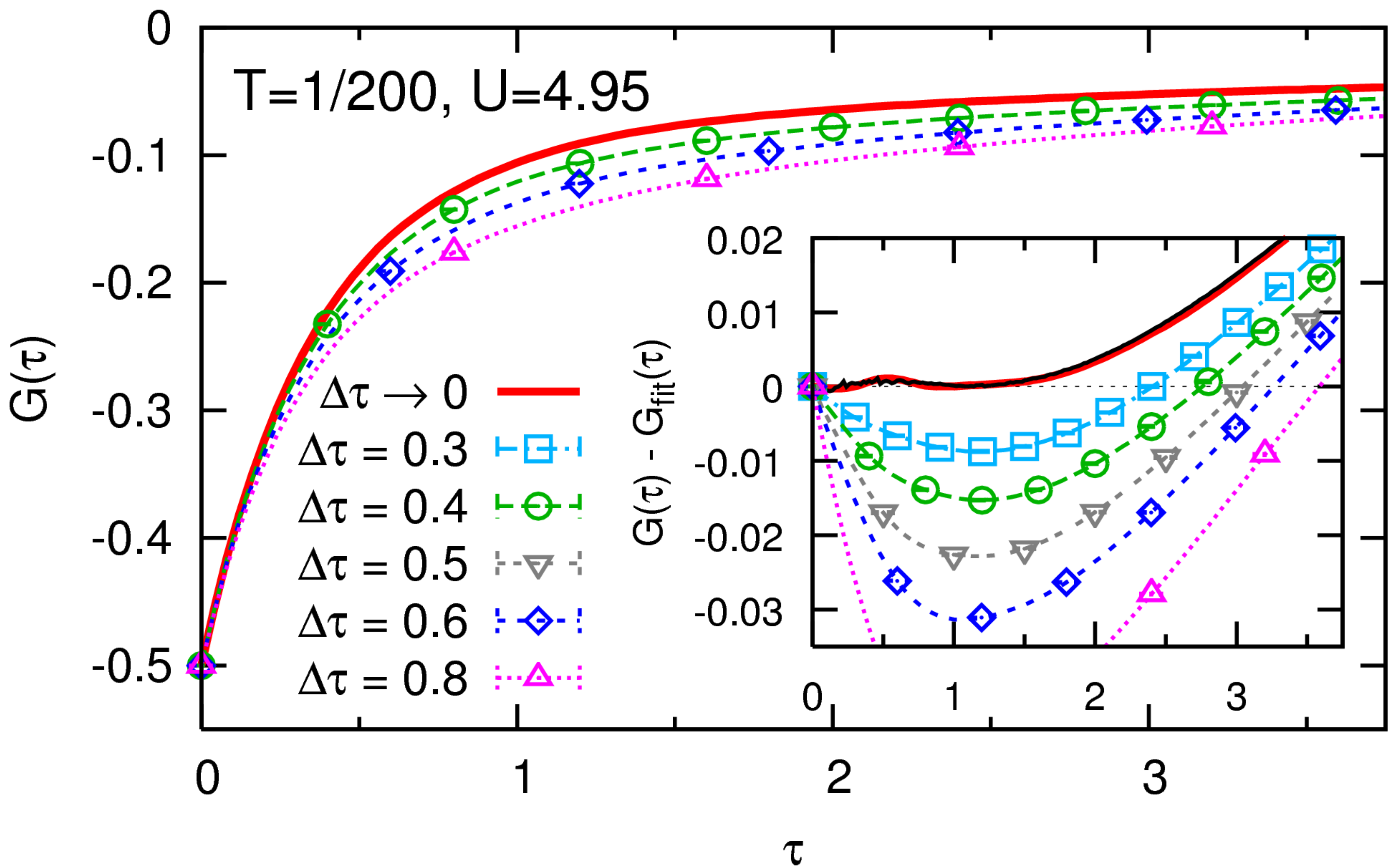
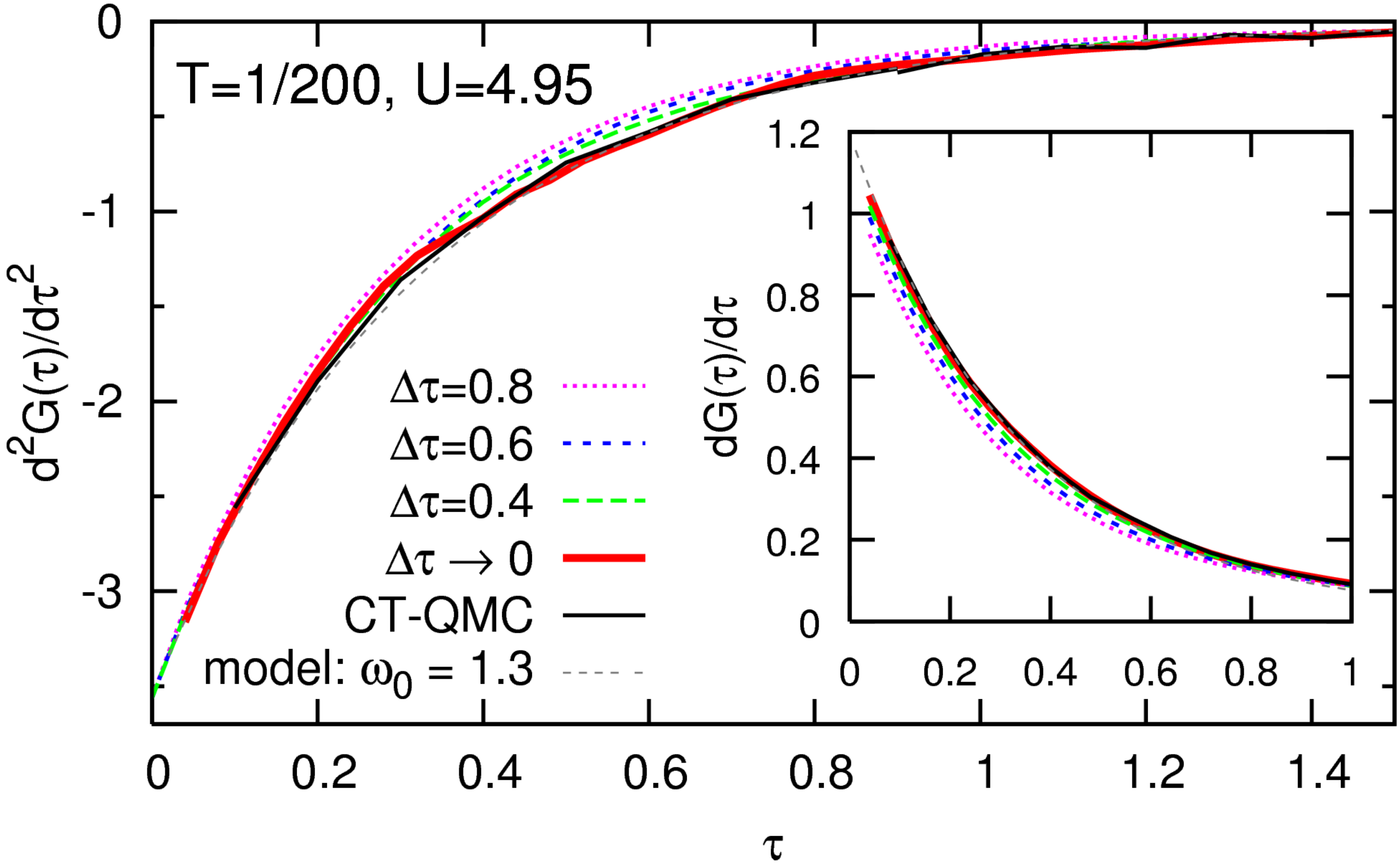
Result: unbiased, numerically exact Green function



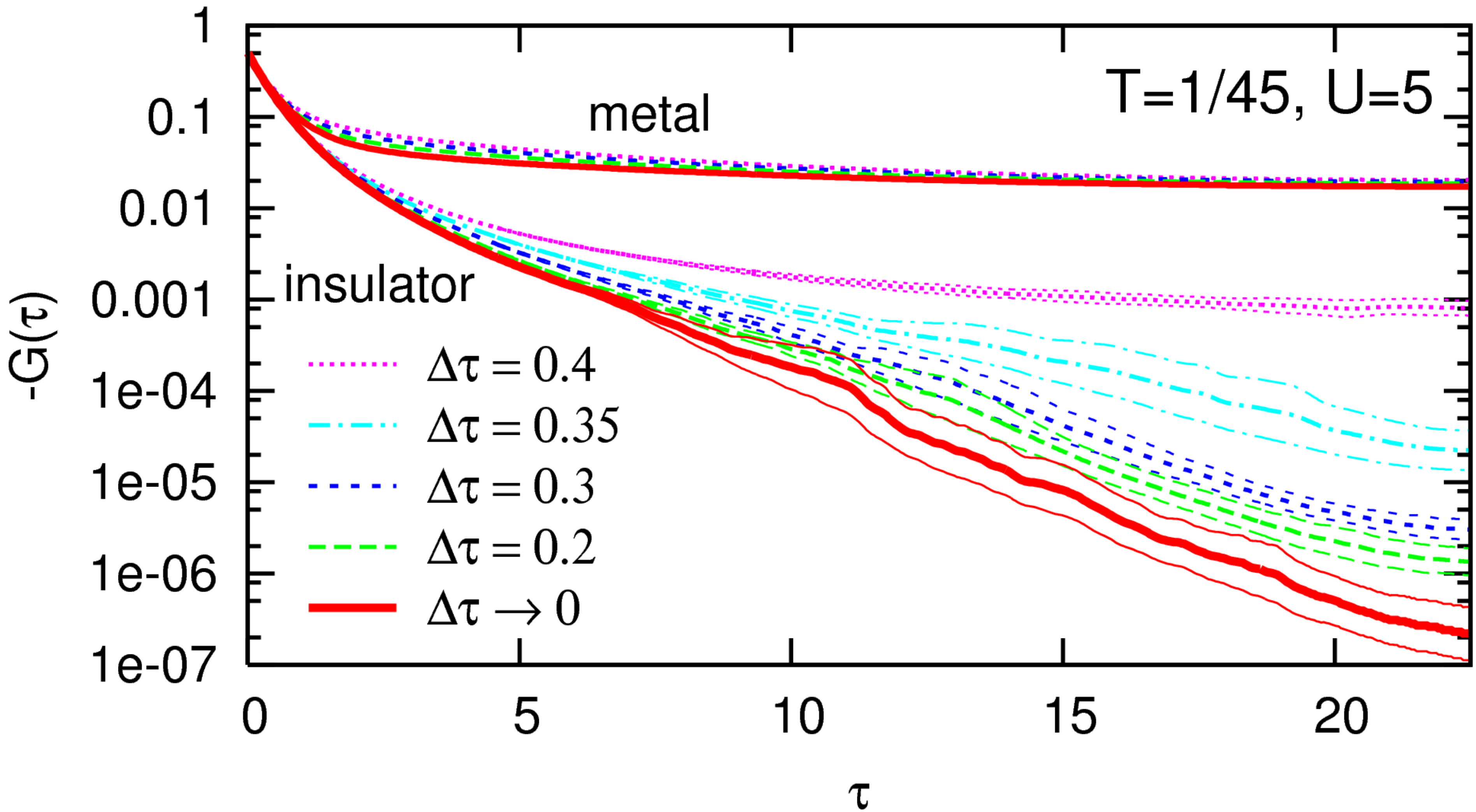
Excellent agreement with hybridization expansion CT-QMC [Werner et al., PRL (2006)]

2^{nd} and 1^{st} order derivatives of Green function



Exact asymptotics $d^2G(\tau)/d\tau^2|_{\tau=0+} = \frac{1}{2}(1 + U^2/4)$; $dG(\tau)/d\tau|_{\tau=0+}$ nonuniversal

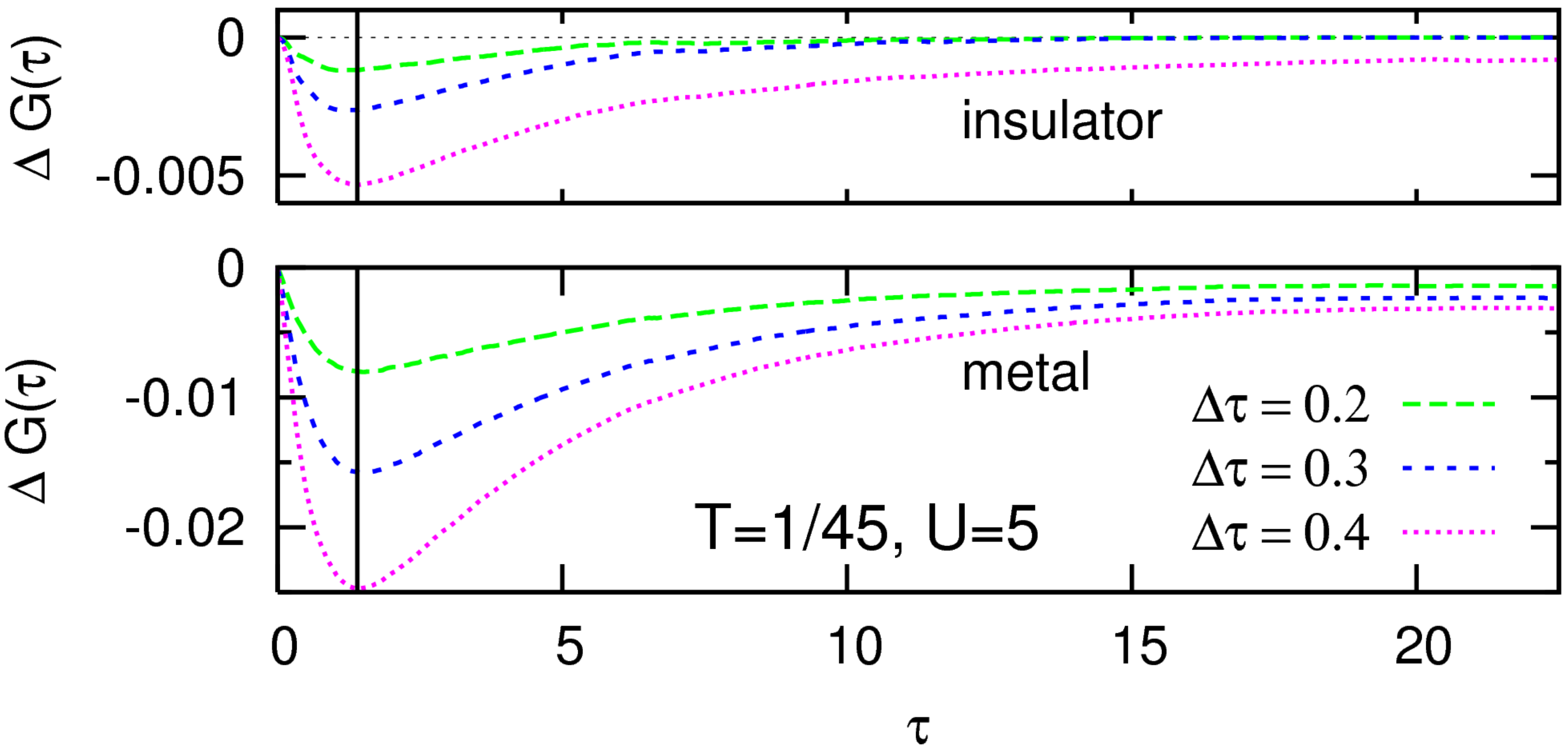
Why average and extrapolation on logarithmic scale?



Difference metal–insulator and $\Delta\tau$ dependence involves orders of magnitude!

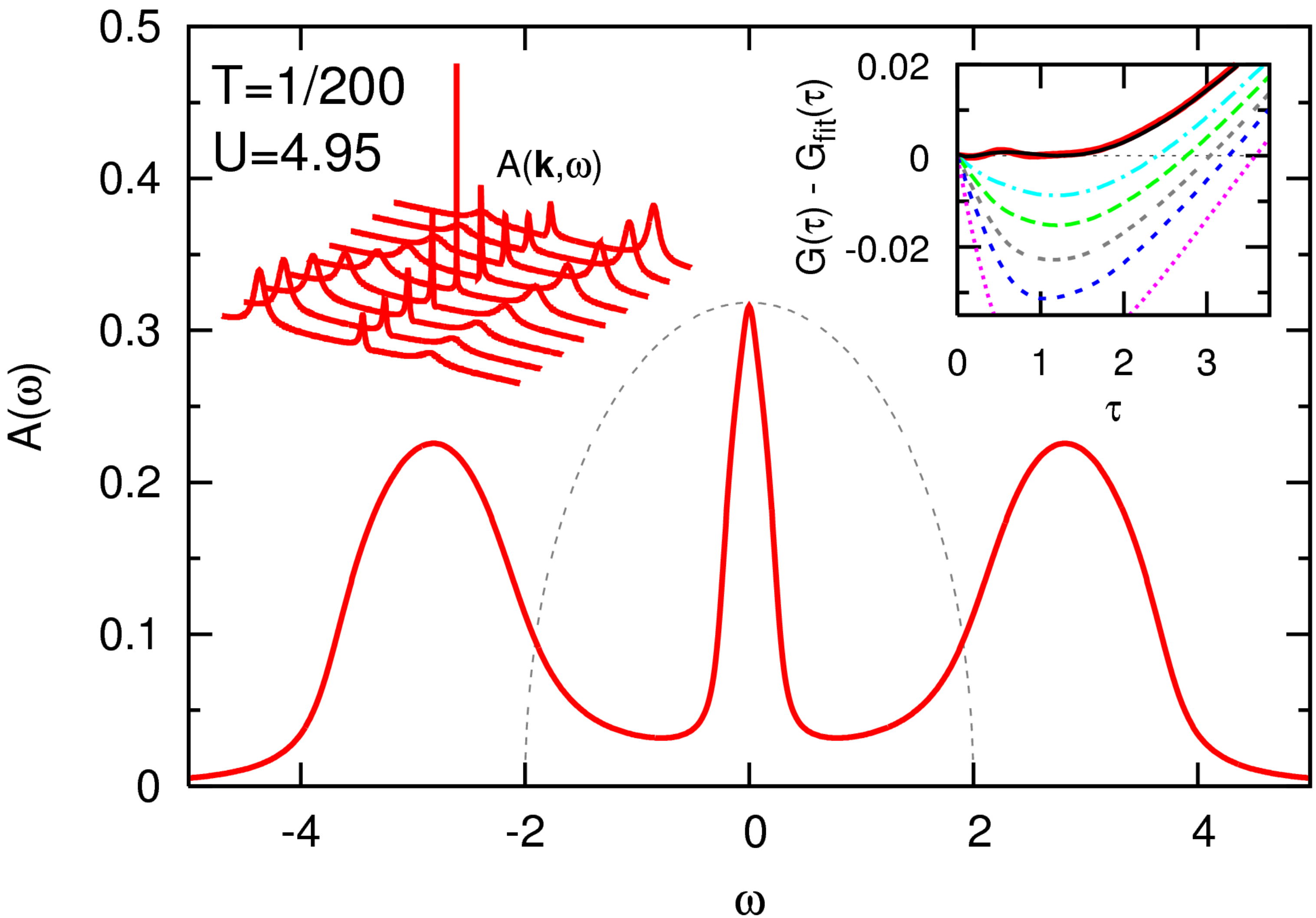
Even max statistical/iteration errors nearly order of magnitude

Low-τ resolution limited by $\Delta\tau$?



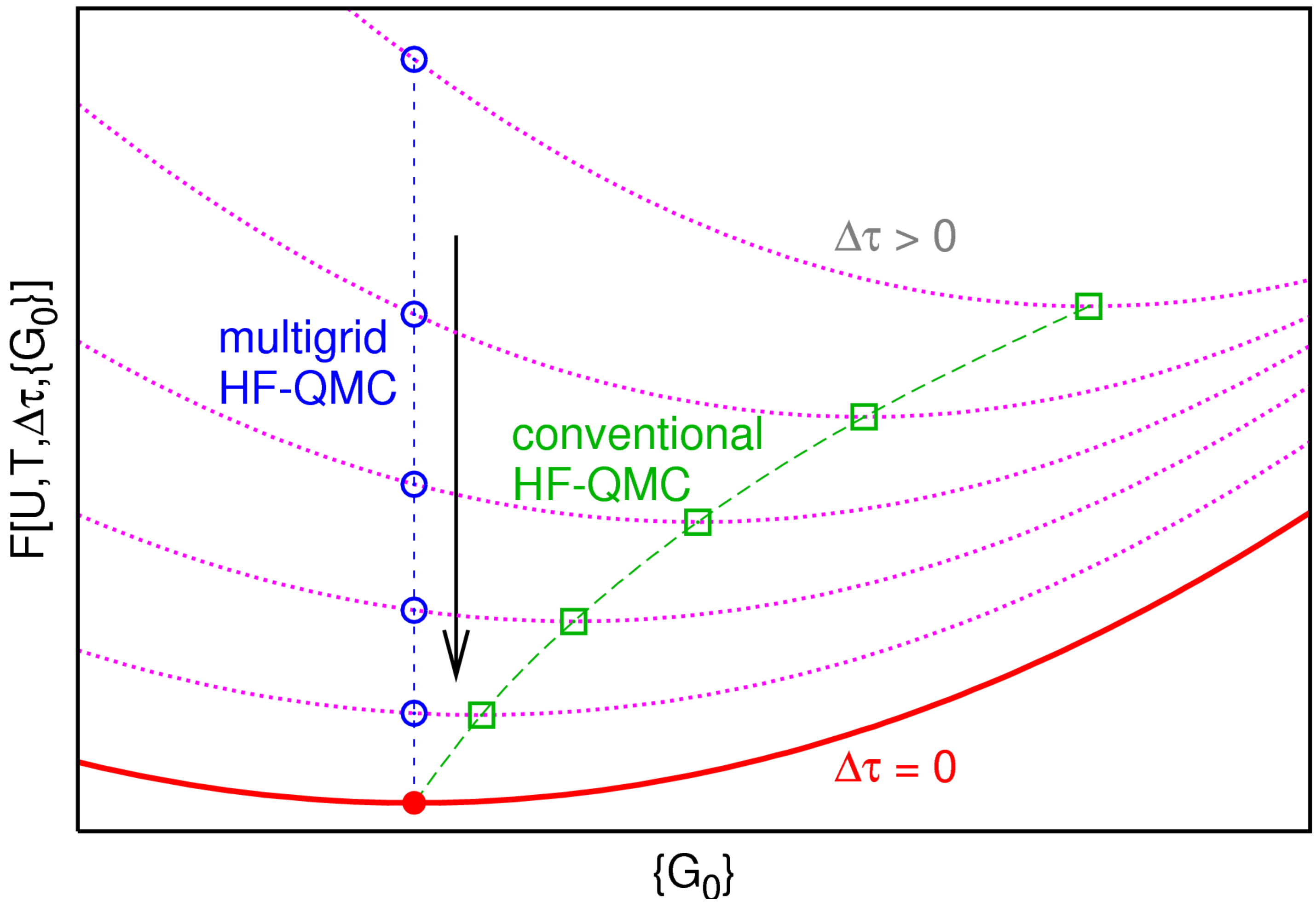
No, uniform $\Delta\tau$ dependence, position of max error independent of $\Delta\tau$ and phase!

Analytic continuation using Padé approximant for self-energy



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

Multigrid Hirsch-Fye quantum Monte Carlo algorithm

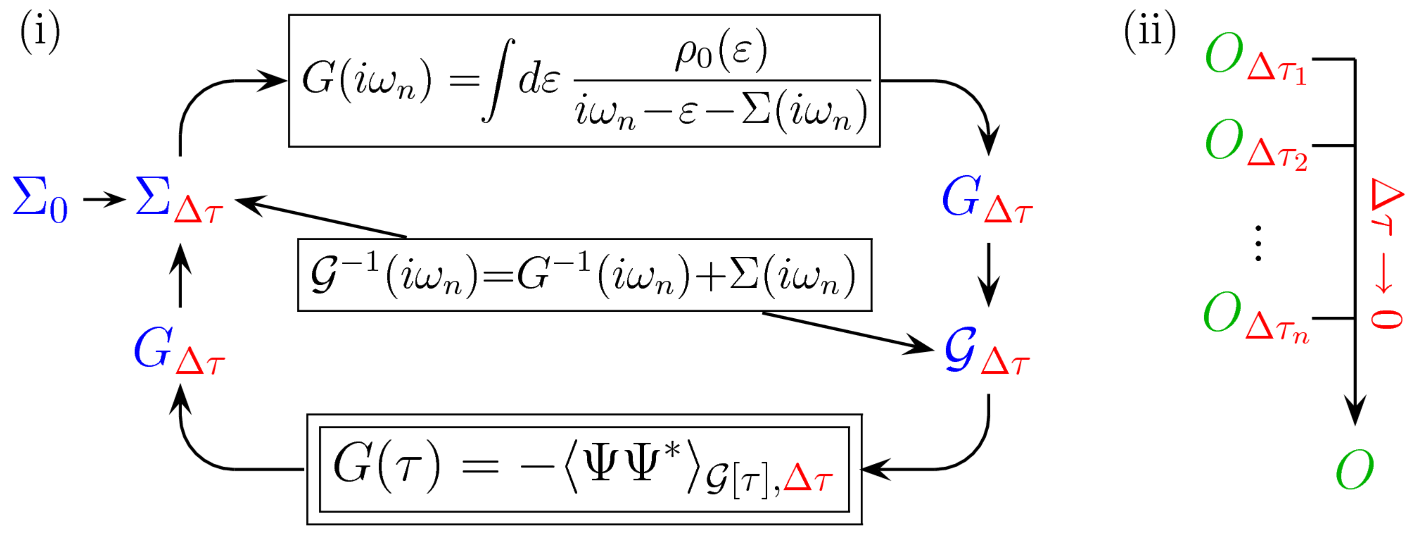


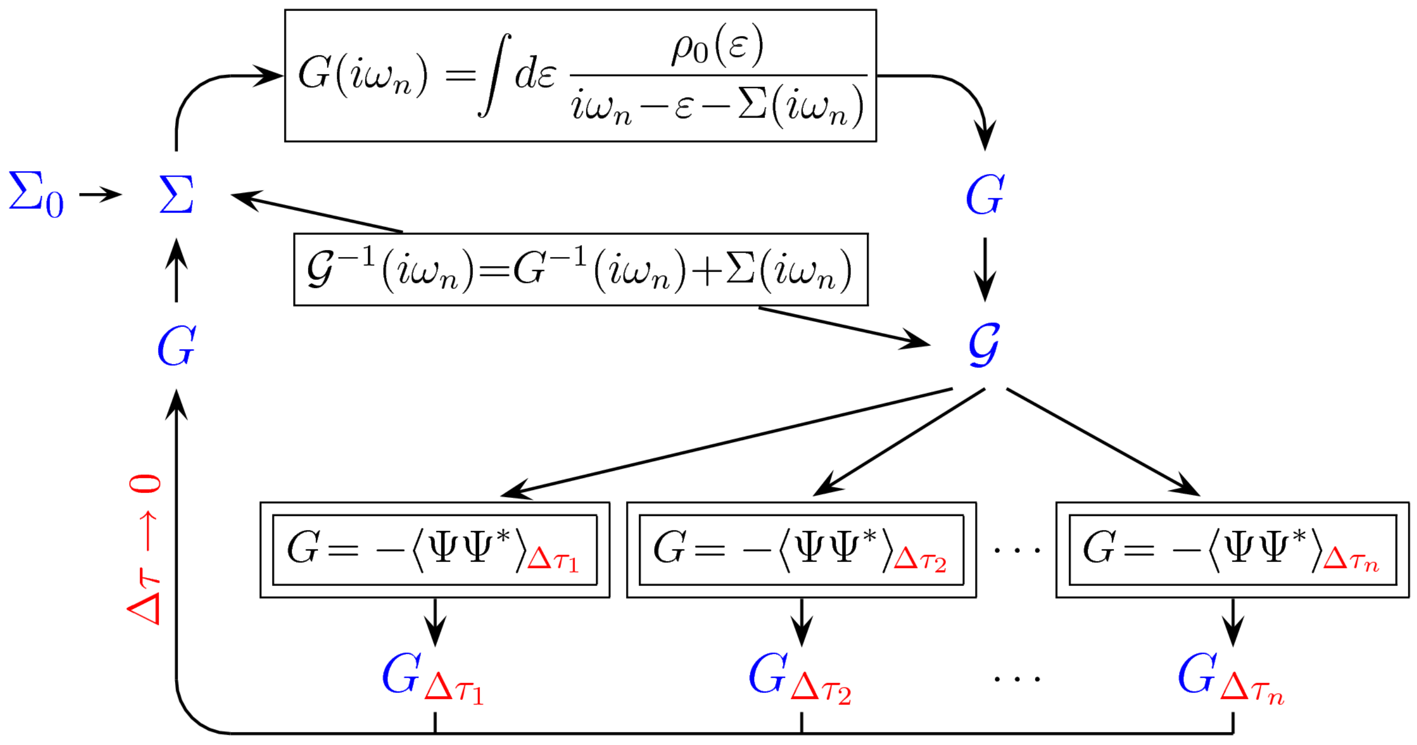
conventional Hirsch-Fye QMC: DMFT fixed point shifts with $\Delta\tau$

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

Comparison of schemes

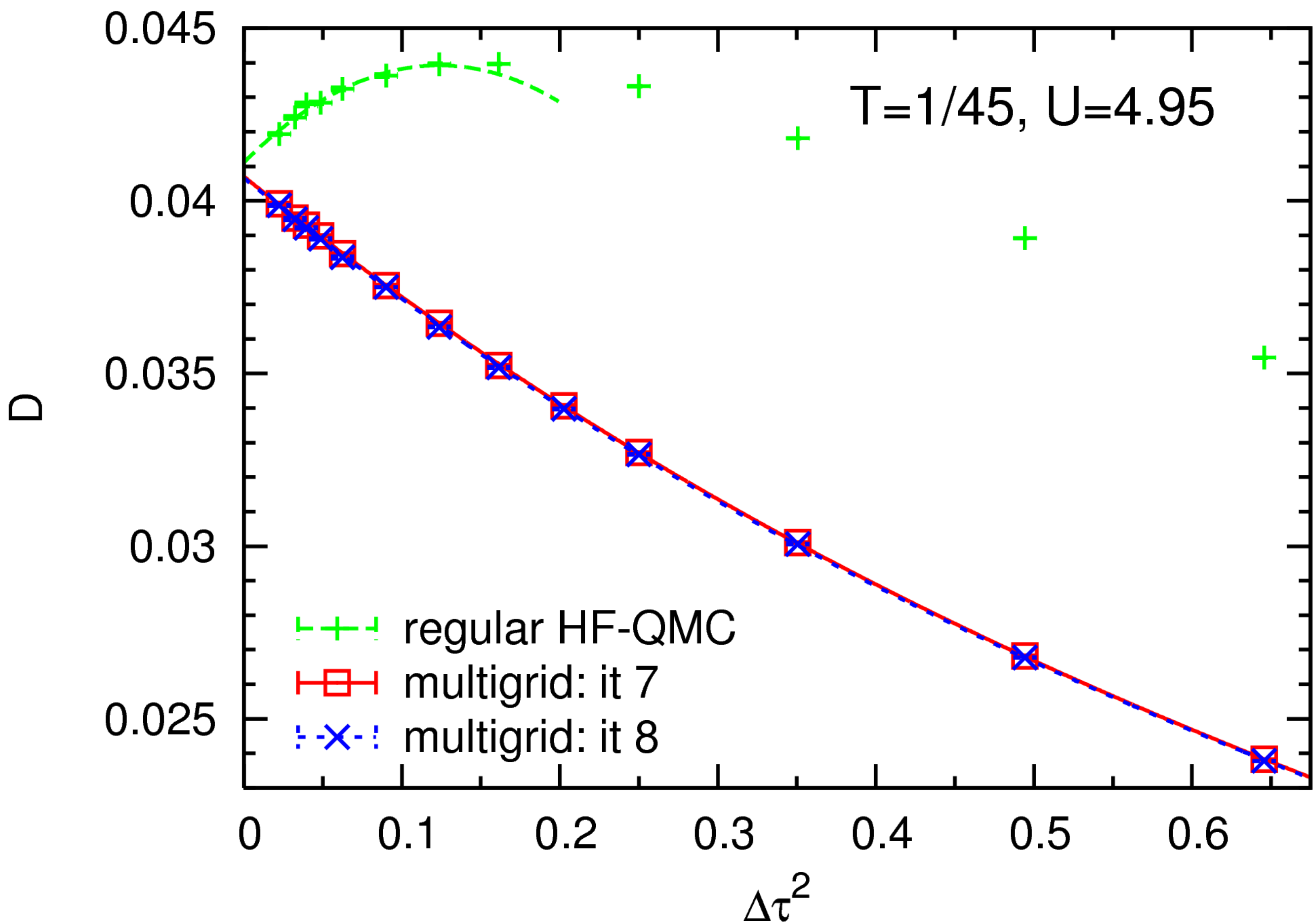
(a) conventional HF-QMC with extrapolation





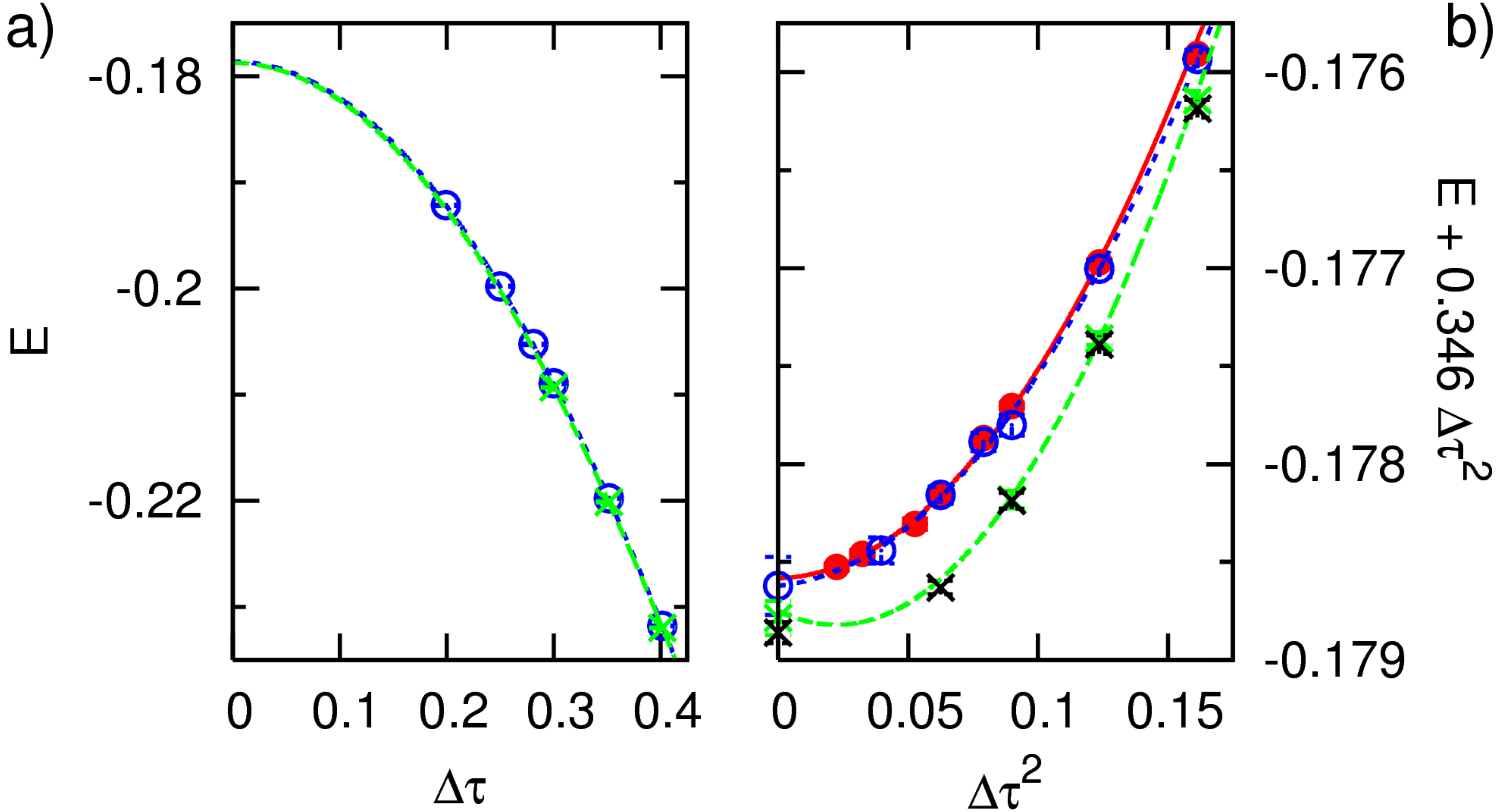
(b) multigrid HF-QMC

Preliminary study: double occupancy near Mott transition



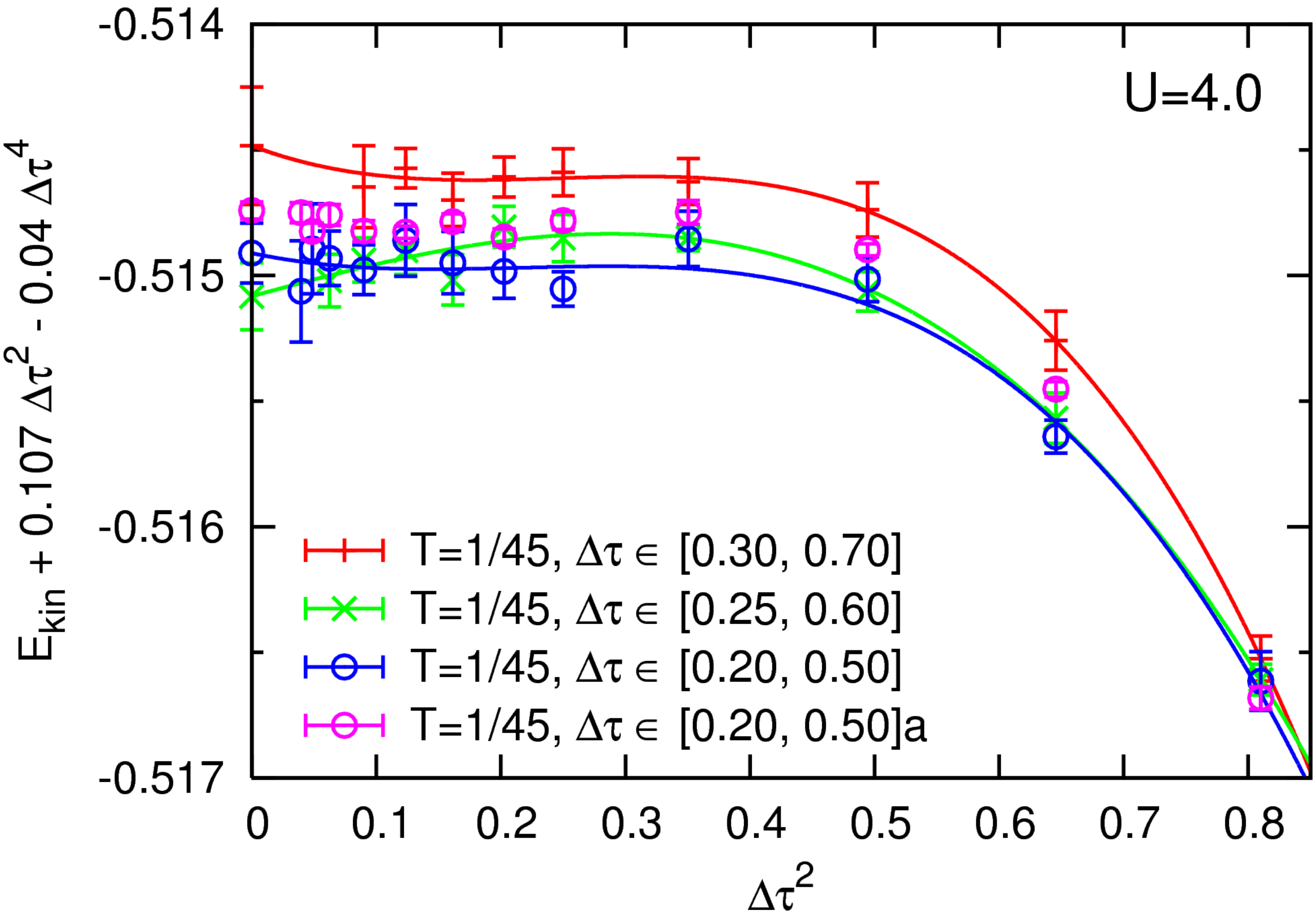
Useful $\Delta\tau$ range vastly larger for multigrid algorithm

Residual discretization errors?

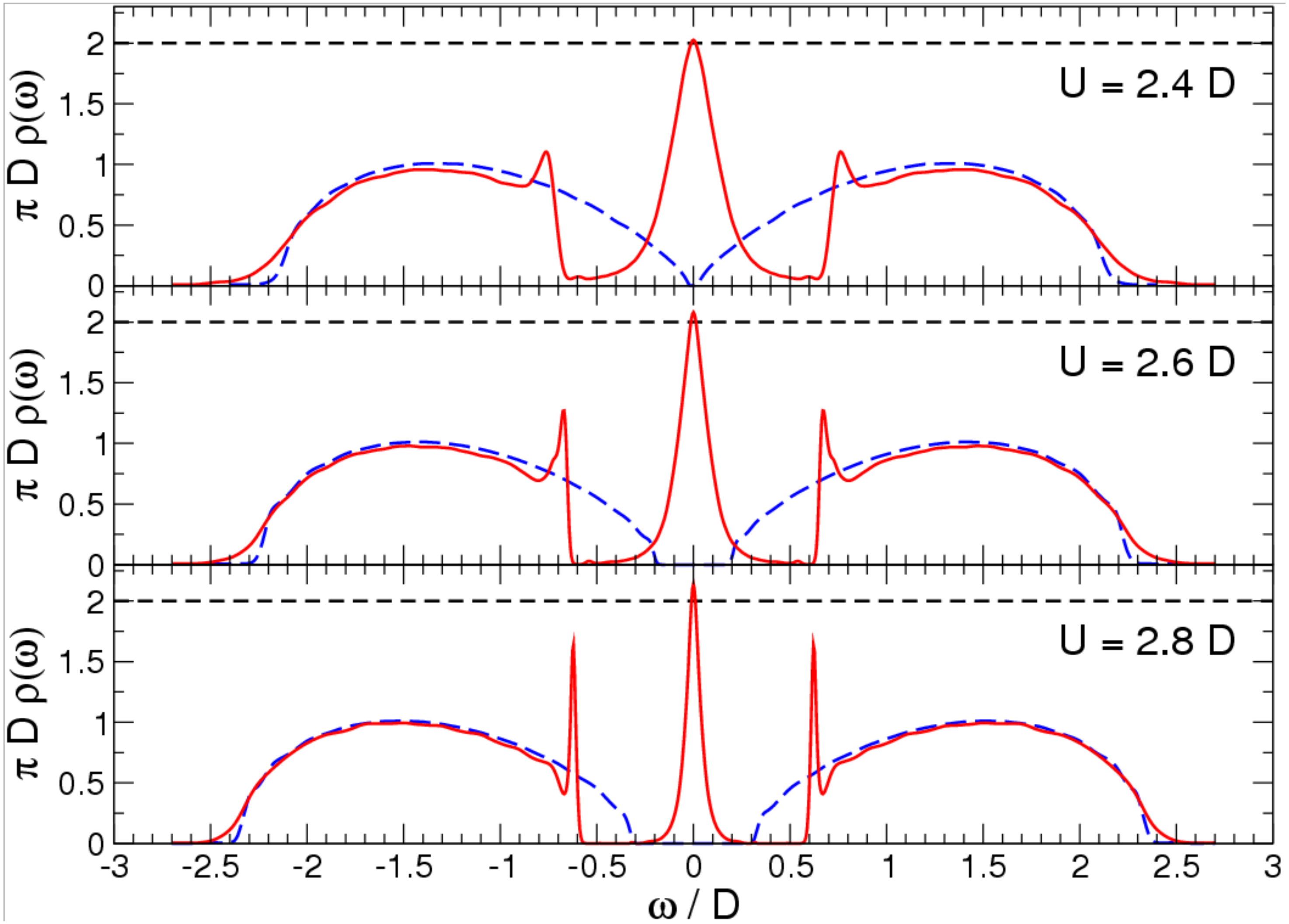


Extrapolated energy ($T = 1/45$, $U = 4$) slightly lower from multigrid algorithm

Systematic study of multigrid parameters

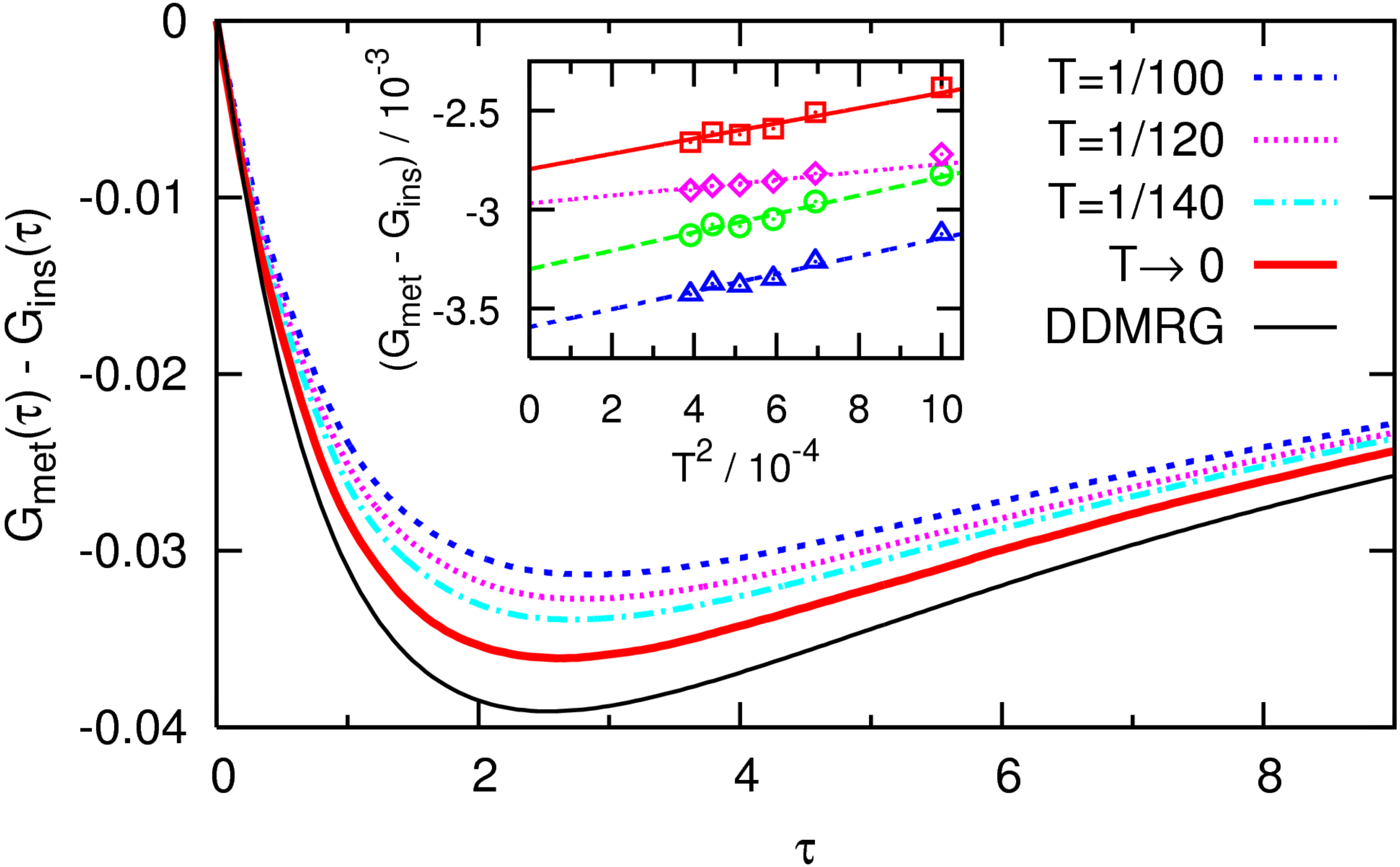


Application: spectral weight transfer at Mott transition



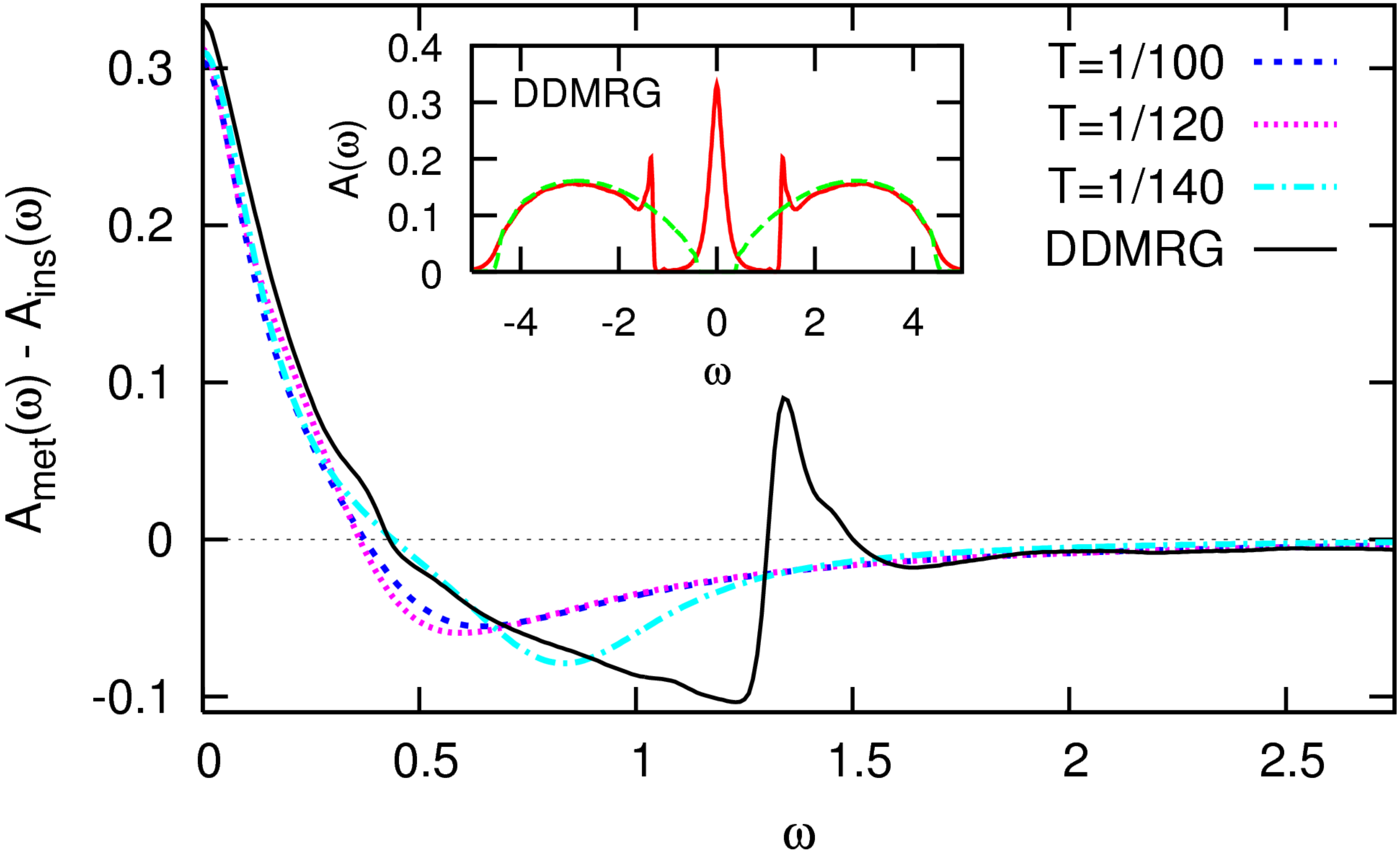
Substructures in Hubbard bands in metallic phase [Karski et al, PRB (2005)]?

Difference Green functions



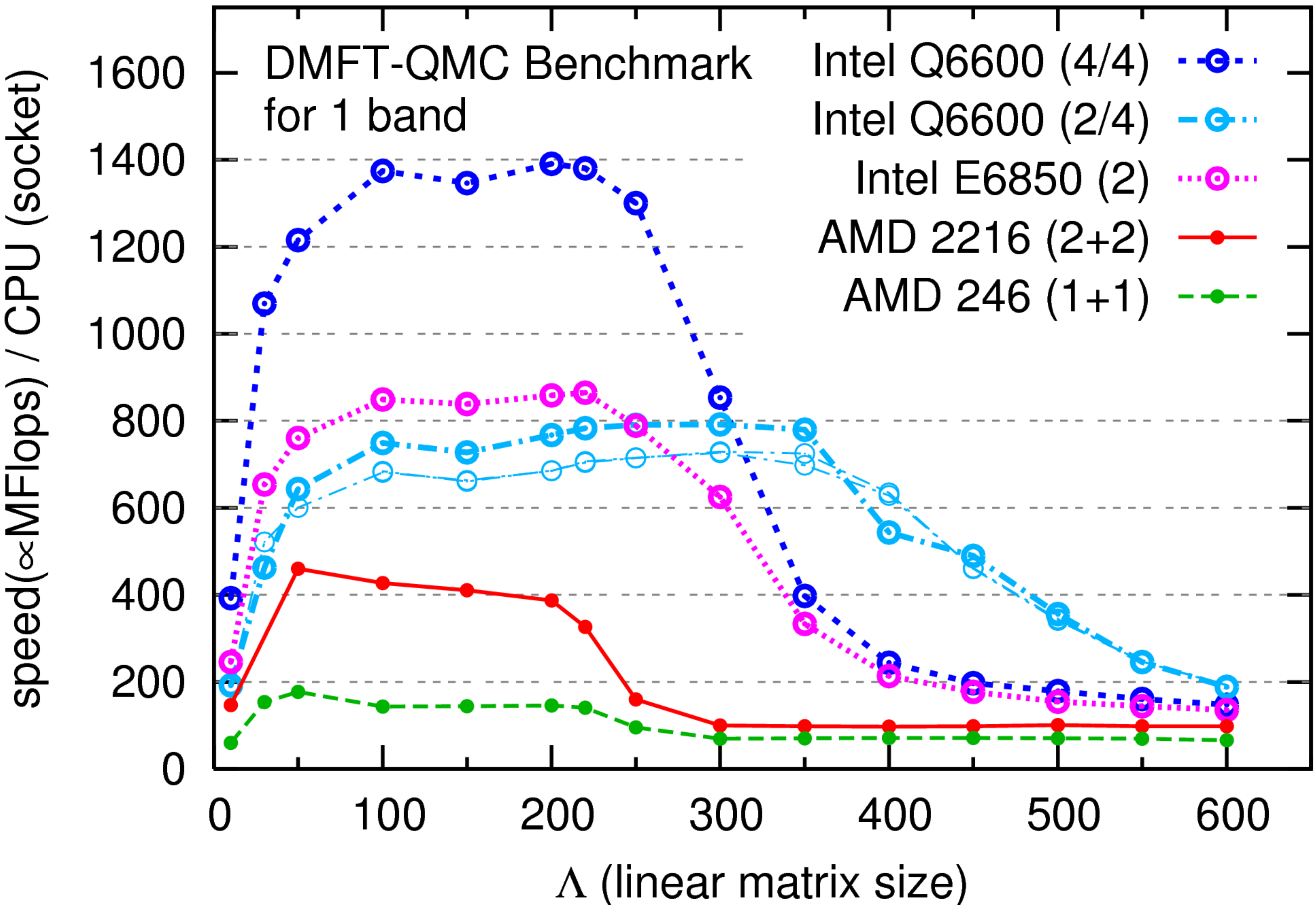
DDMRG spectra for $U = 5.2$ quantitatively incorrect!

Difference spectra



Similarities, but no indication for feature at $\omega = 1.3$ in QMC data

Summary


DMFT-QMC Benchmark
for 1 band
Intel Q6600 (4/4)
Intel Q6600 (2/4)
Intel E6850 (2)
AMD 2216 (2+2)
AMD 246 (1+1)
speed(∝MFlops) / CPU (socket)
0
200
400
600
800
1000
1200
1400
1600
0
100
200
300
400
500
600
Λ (linear matrix size)