

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

Nils Blümer, Univ. Mainz

Outline

Introduction: DMFT, HF-QMC

Unbiased Green functions and spectra from HF-QMC

Multigrid Hirsch-Fye quantum Monte Carlo algorithm

Spectral weight transfer at the Mott transition

Summary

Introduction

Target: Hubbard-type models

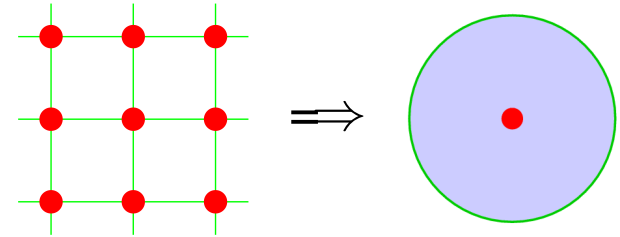
$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

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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 $Z \rightarrow \infty$

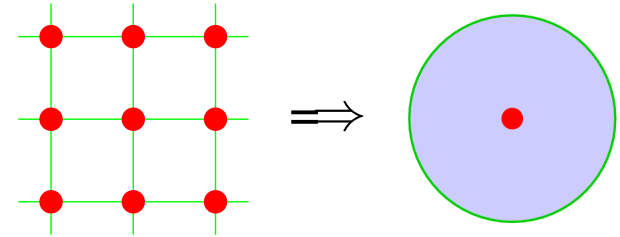


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Numerically exact impurity solvers:

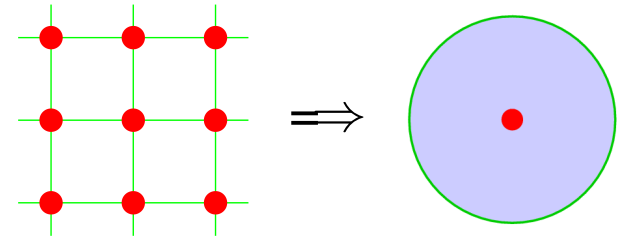
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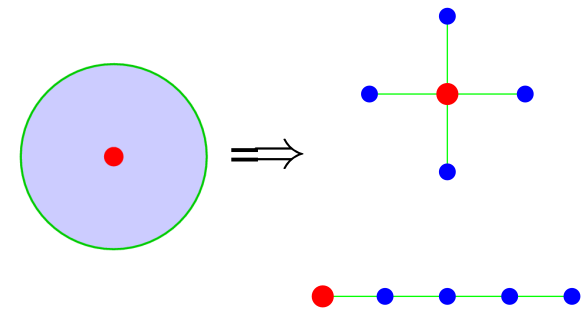
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Numerically exact impurity solvers:

- Quantum Monte Carlo (QMC)
- Exact diagonalization (ED; large finite-size errors)
- Numerical renormalization group (NRG; 1-2 bands)
- Density matrix renormalization group (DMRG)



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

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

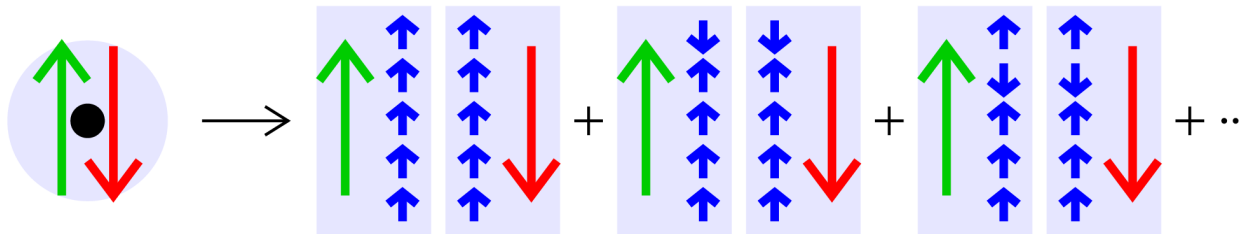
$$G_{\sigma}(\tau_2 - \tau_1) = \frac{1}{Z} \int \mathcal{D}[\psi] \mathcal{D}[\psi^*] \psi_{\sigma}(\tau_1) \psi_{\sigma}^*(\tau_2) \exp \left[\mathcal{A}_0 - U \sum_{\sigma\sigma'} \int_0^{\beta} d\tau \psi_{\sigma}^* \psi_{\sigma} \psi_{\sigma'}^* \psi_{\sigma'} \right]$$

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



Wick theorem:

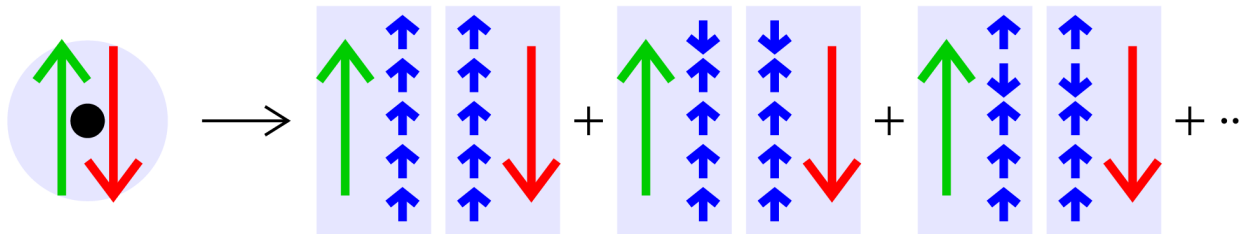
$$G = \frac{\sum M \det\{M\}}{\sum \det\{M\}}$$

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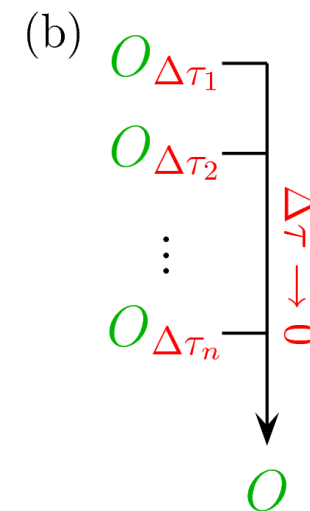
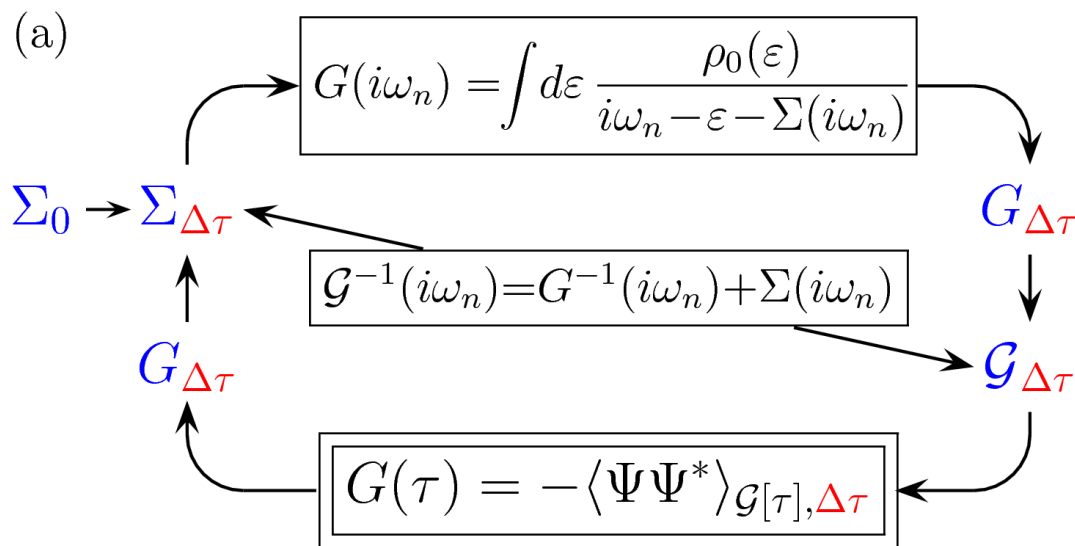
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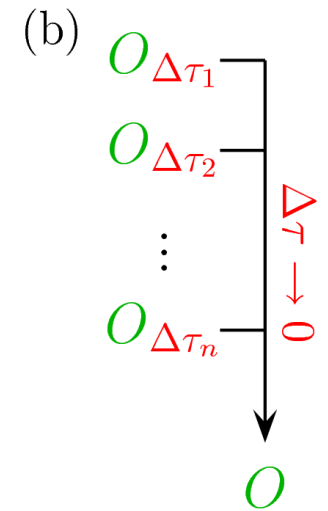
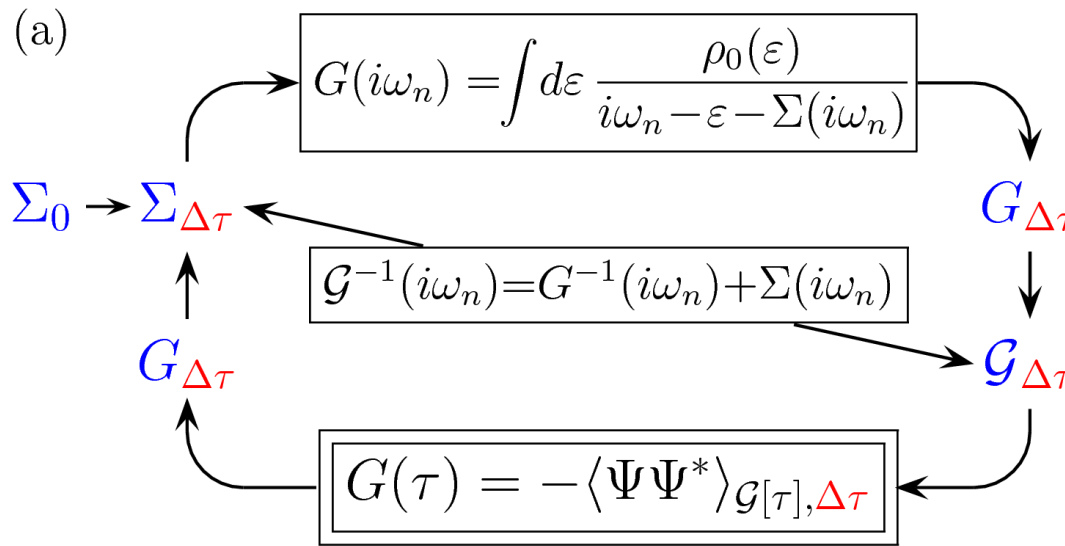
Metropolis MC importance sampling over auxiliary Ising field $\{s\}$: 2^{Λ} configurations

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

Self-consistency cycle using conventional HF-QMC

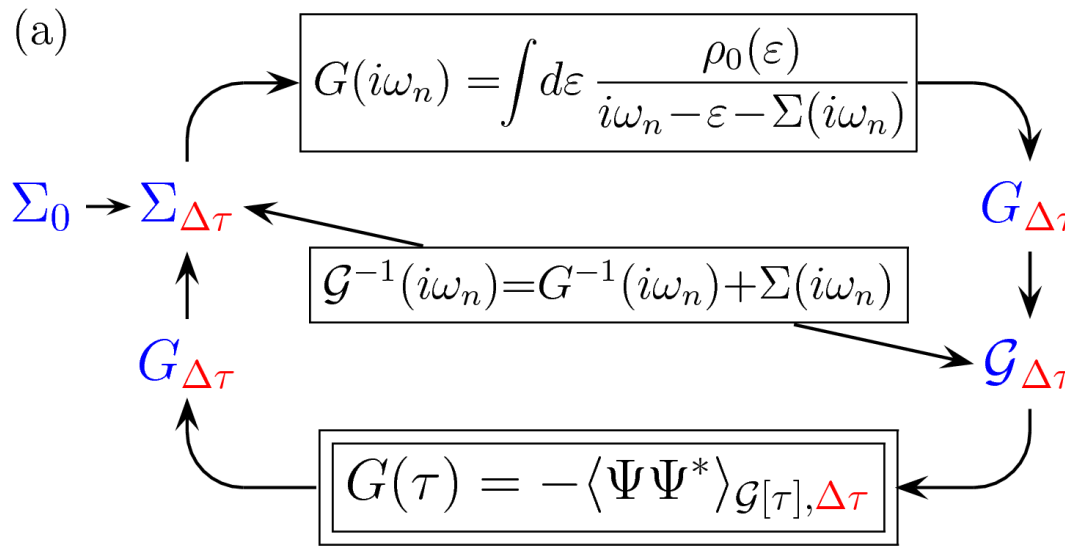


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Extrapolation $\Delta\tau \rightarrow 0$ can improve accuracy of observable estimates by several orders of magnitude!

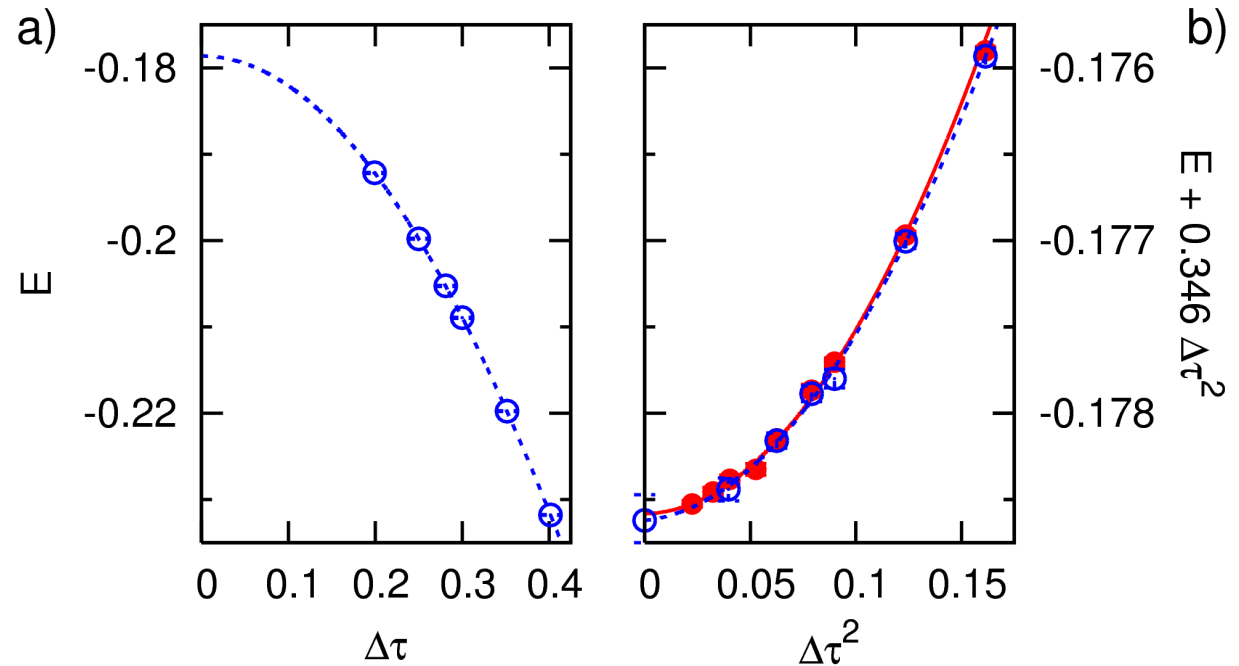
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Example: energy for $U = W = 4$ (Bethe DOS), $T = 1/45$

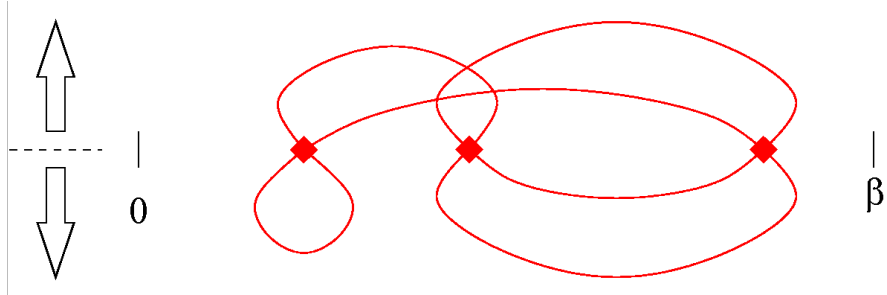
[NB, PRB (2007)]



New development: continuous-time QMC algorithms

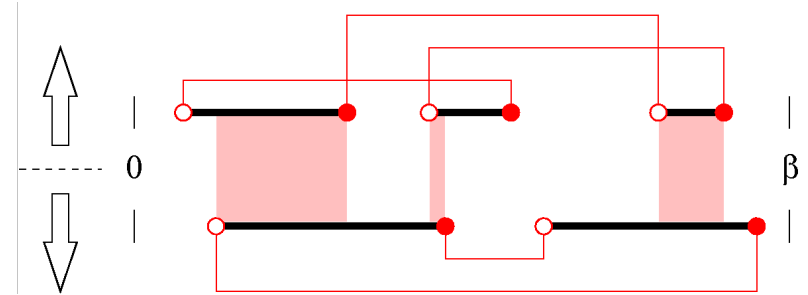
1. weak-coupling expansion

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



2. hybridization expansion

[Werner et al., PRL (2006)]

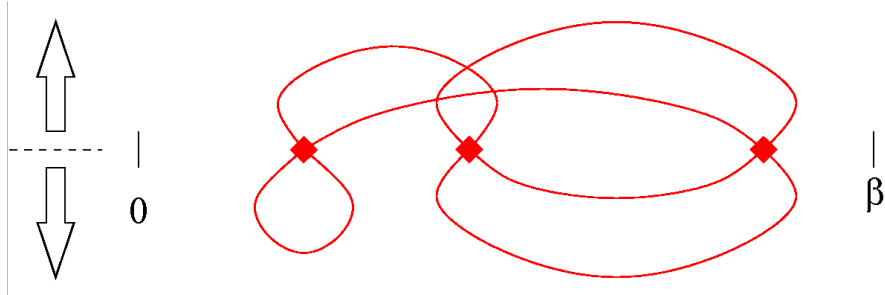


No systematic errors (in principle). Also more efficient than HF-QMC?

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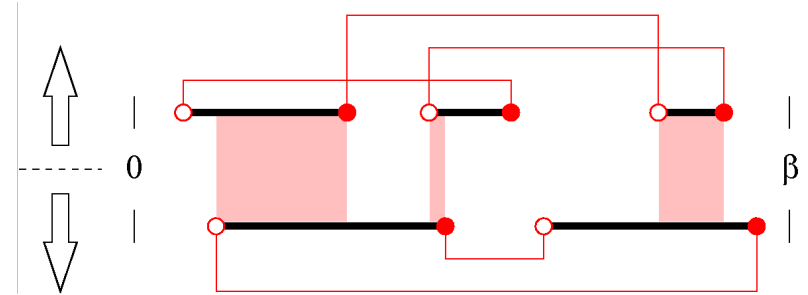
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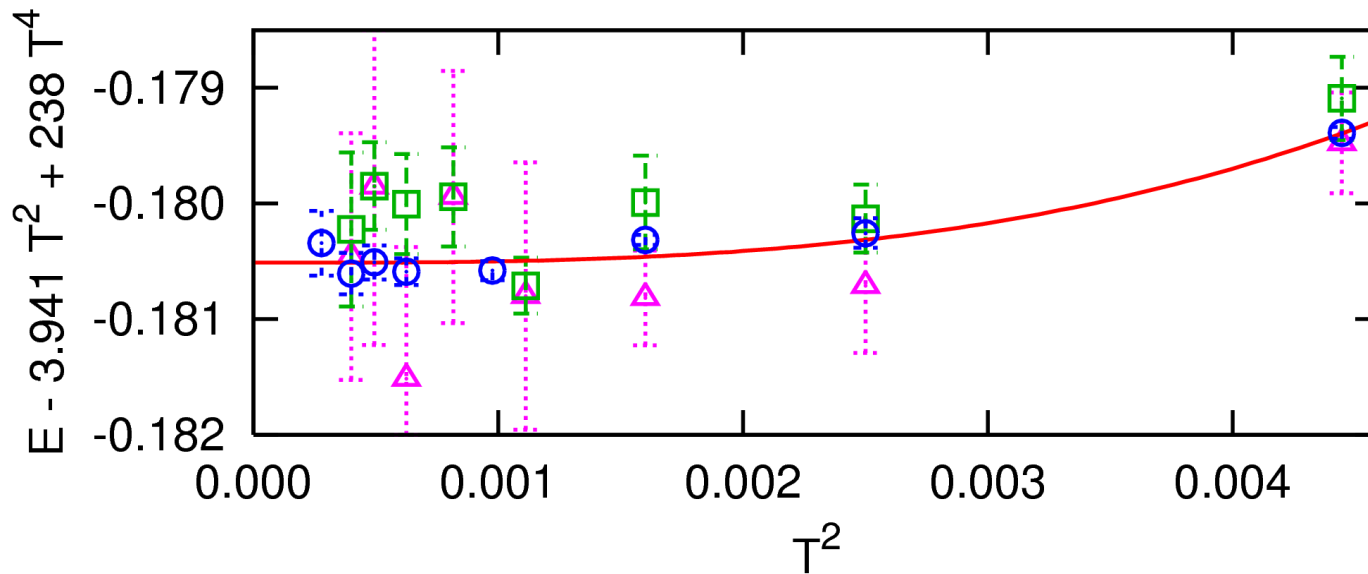


2. hybridization expansion

[Werner et al., PRL (2006)]



No systematic errors (in principle). Also more efficient than HF-QMC? **No!**



- HF-QMC ($\Delta\tau \rightarrow 0$)
- weak-coupling CT-QMC
- △ hybridization CT-QMC

HF-QMC + extrapolation $\Delta\tau \rightarrow 0$ can be more efficient [NB, PRB 76, 205120 (2007)]

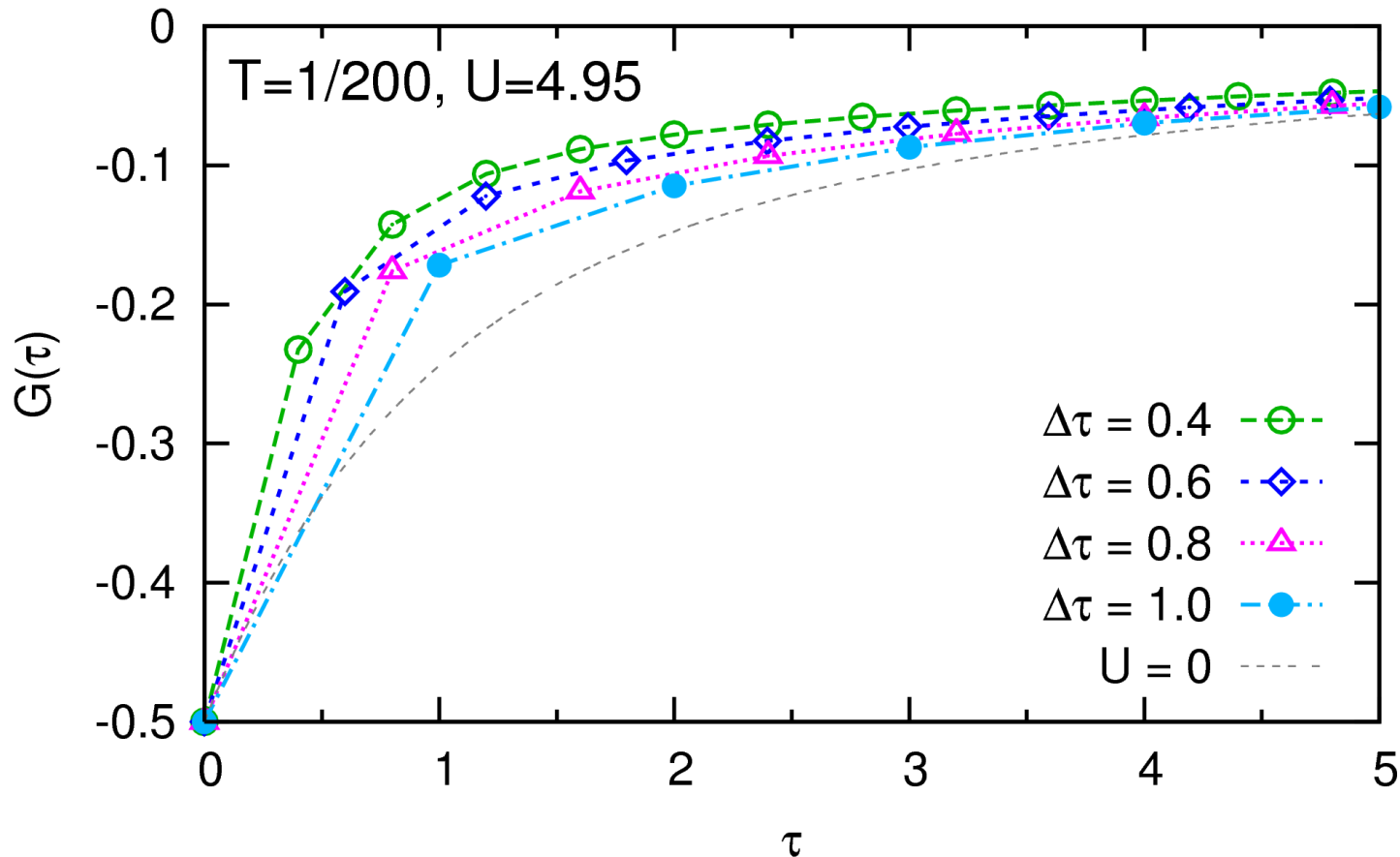
Unbiased Green functions and spectra from HF-QMC

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

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

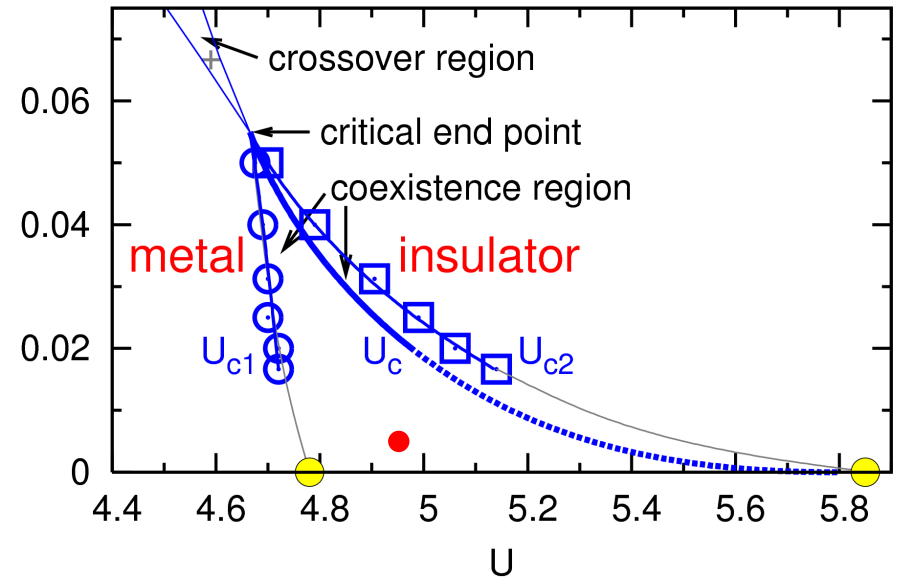
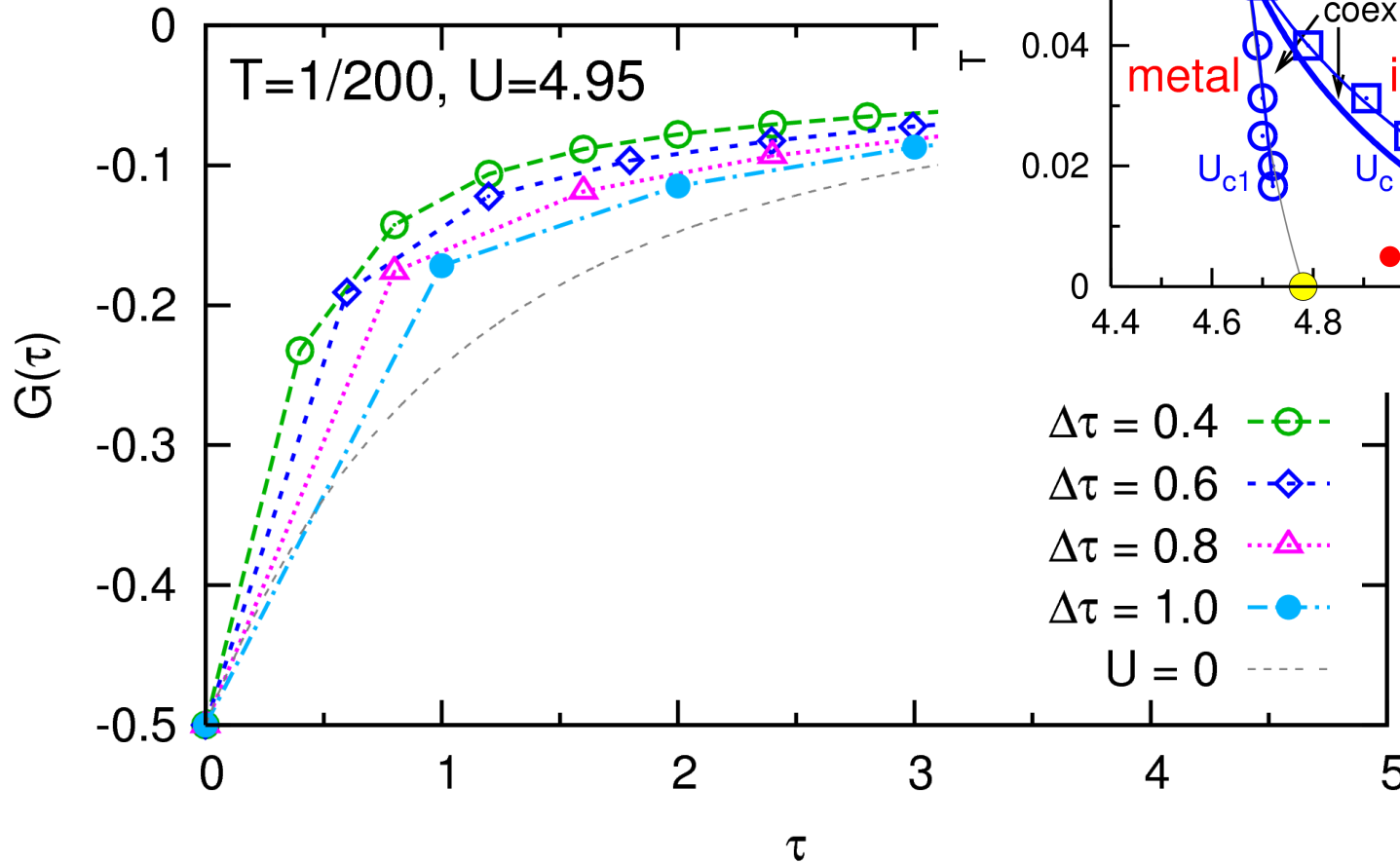


Low temperature (“beyond HF-QMC”): large $\Delta\tau \rightsquigarrow$ large biases [NB, arXiv:0712.1290]

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New Green function extrapolation scheme

For each $\Delta\tau$: • average Green functions $\rightsquigarrow G_{\Delta\tau}(\tau_i), \Delta G_{\Delta\tau}(\tau_i)$
• interpolate via difference Green function $G_{\Delta\tau}(\tau) - G_{\text{model}}(\tau)$
 $\rightsquigarrow G_{\Delta\tau_1}, G_{\Delta\tau_2}, \dots, G_{\Delta\tau_n}$ (with error bars) on common fine τ grid

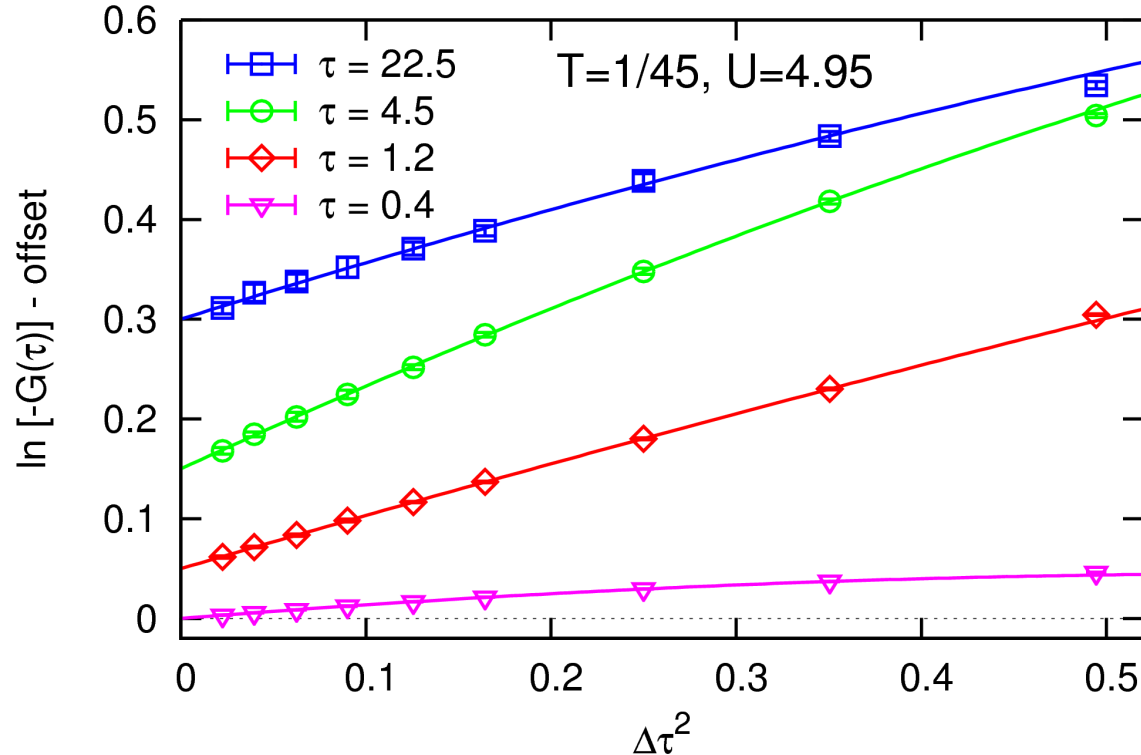
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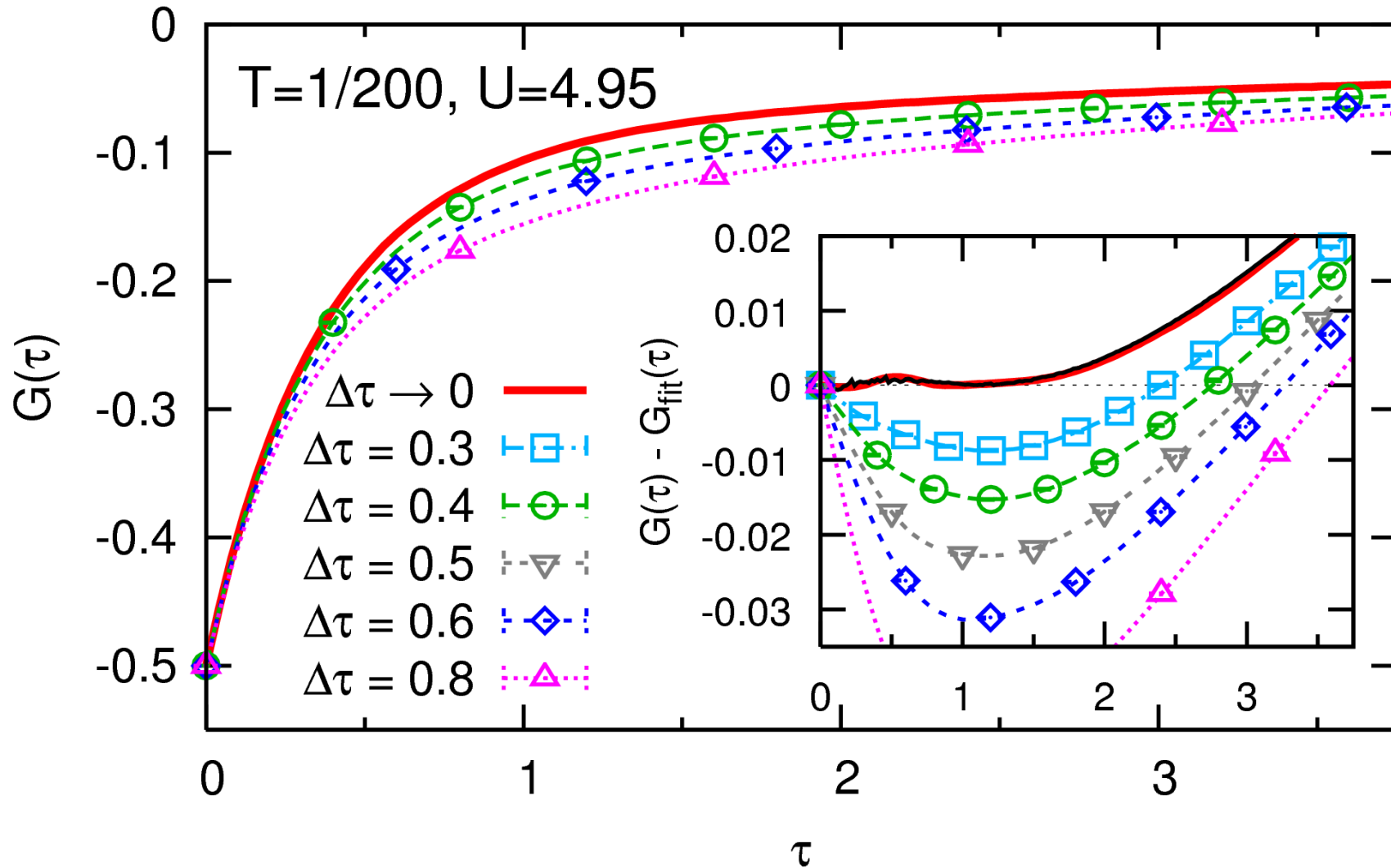
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• Extrapolate $\log[-G(\tau)]$ using cubic least-squares fits, overweighting low $\Delta\tau$



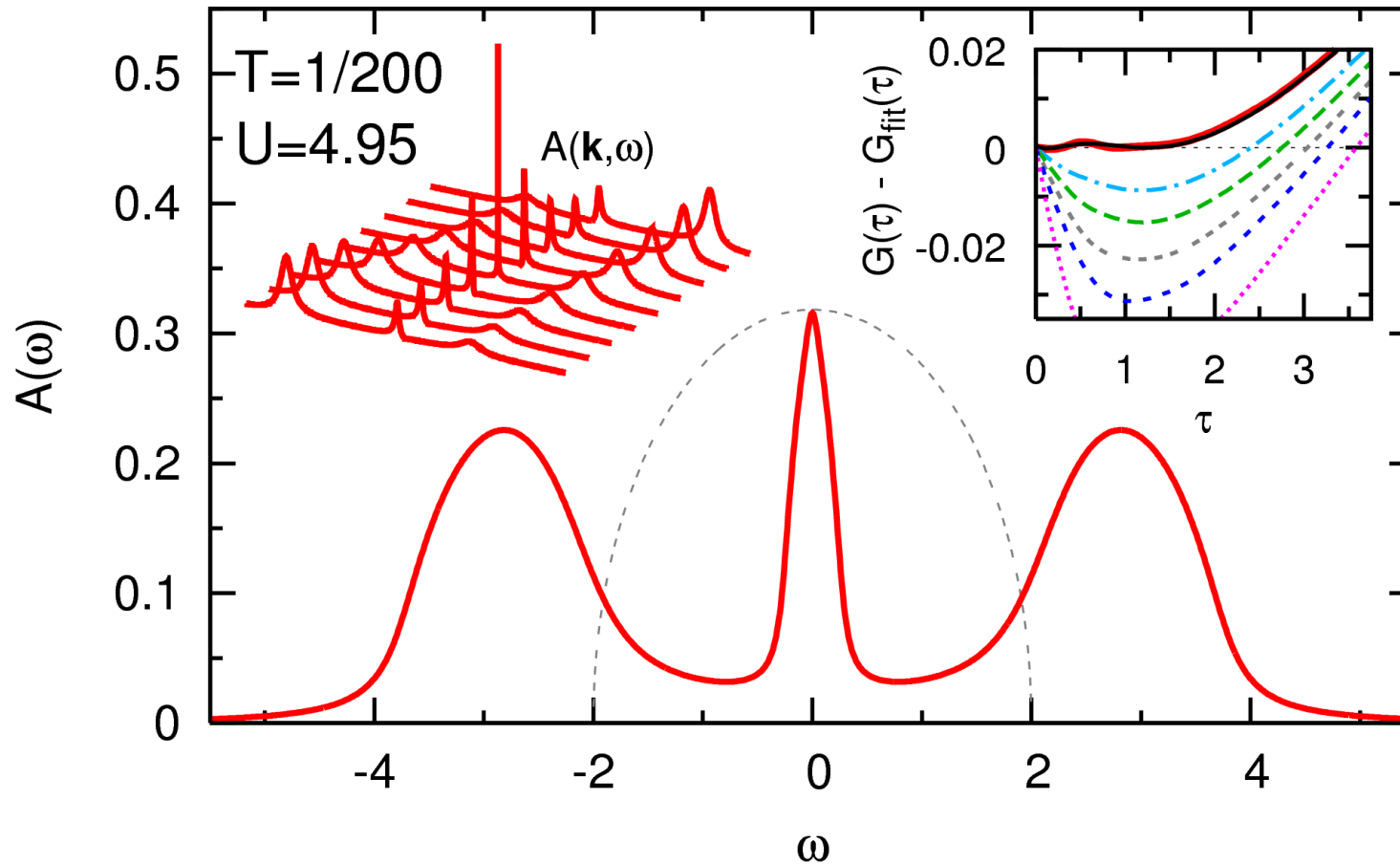
Result: unbiased, numerically exact Green function



[NB, arXiv:0712.1290]

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

Analytic continuation using Padé approximant for self-energy



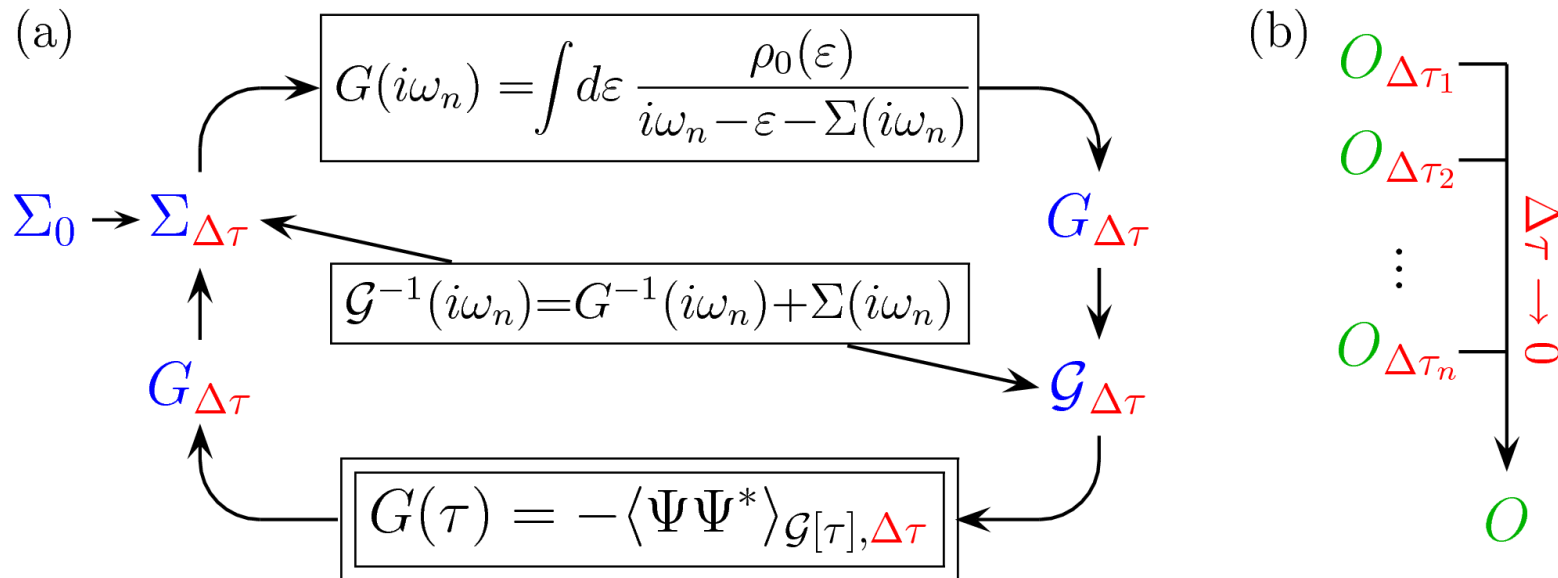
First spectra without discretization error from HF-QMC, at ultra-low T

Method directly applicable, e.g., to LDA+DMFT calculations [NB, [arXiv:0712.1290](https://arxiv.org/abs/0712.1290)]

Multigrid Hirsch-Fye quantum Monte Carlo algorithm

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

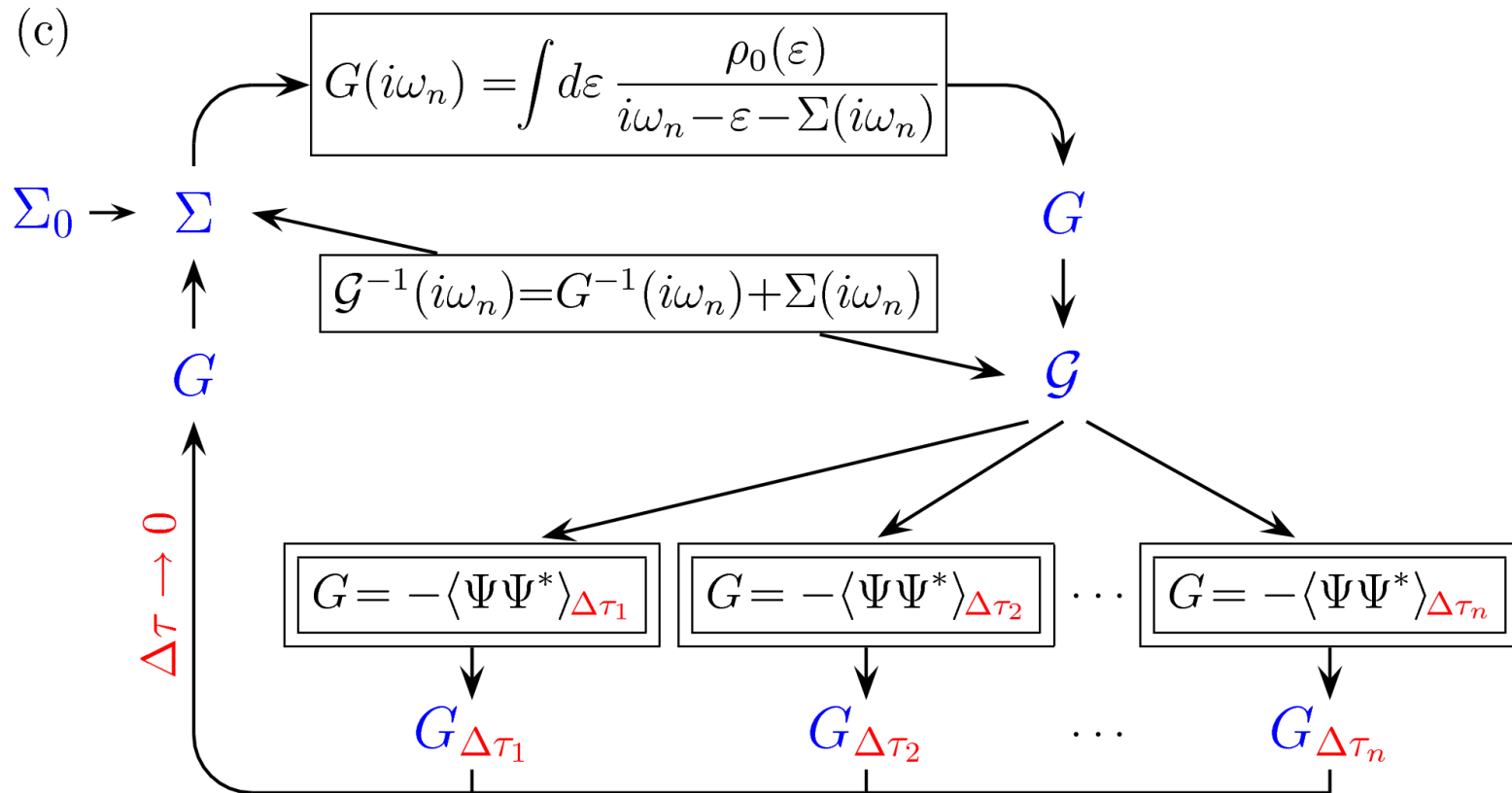
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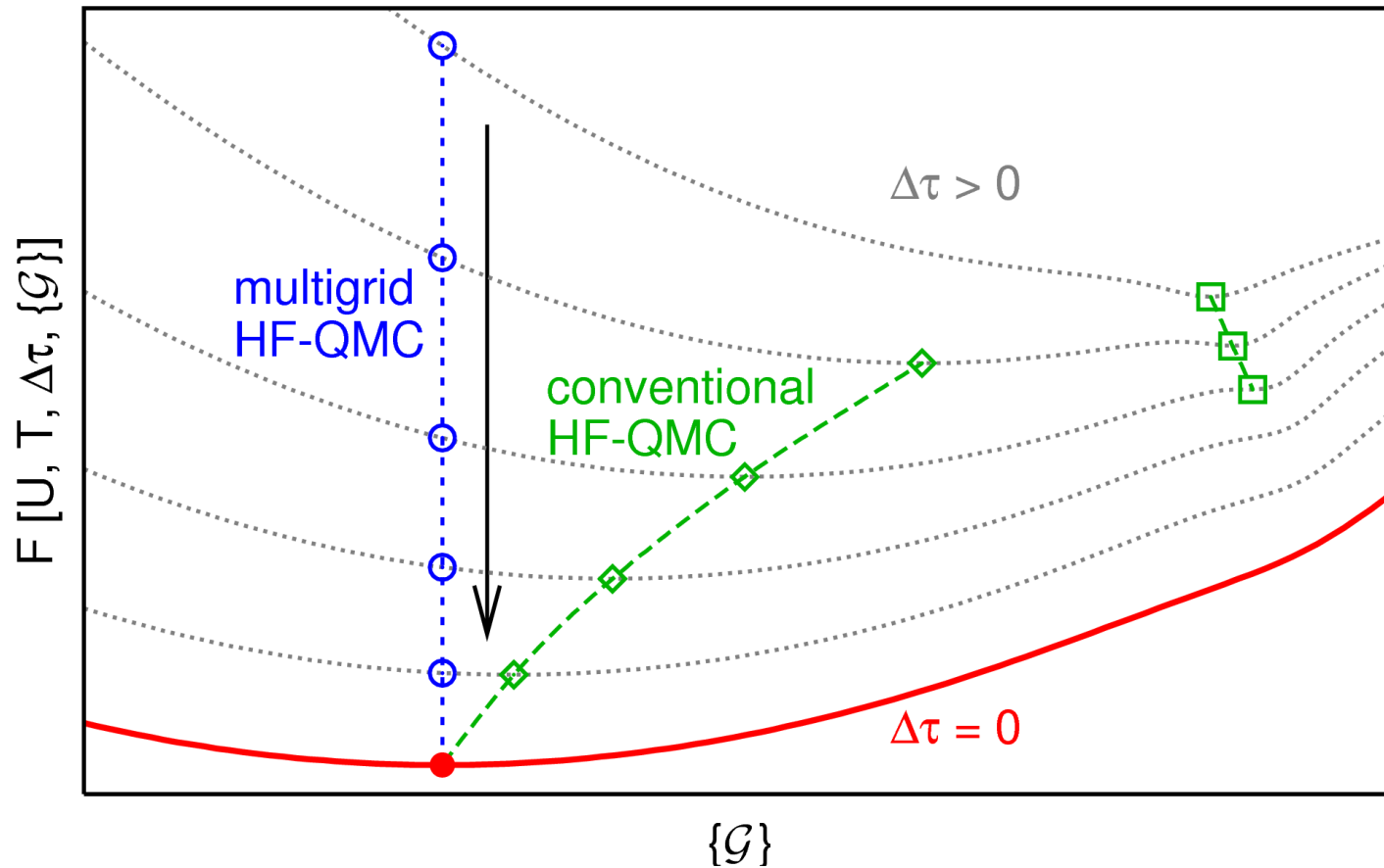
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(c) Multigrid HF-QMC: internal elimination of Trotter error

\rightsquigarrow quasi continuous time algorithm [NB, [arXiv:0801.1222](https://arxiv.org/abs/0801.1222)]

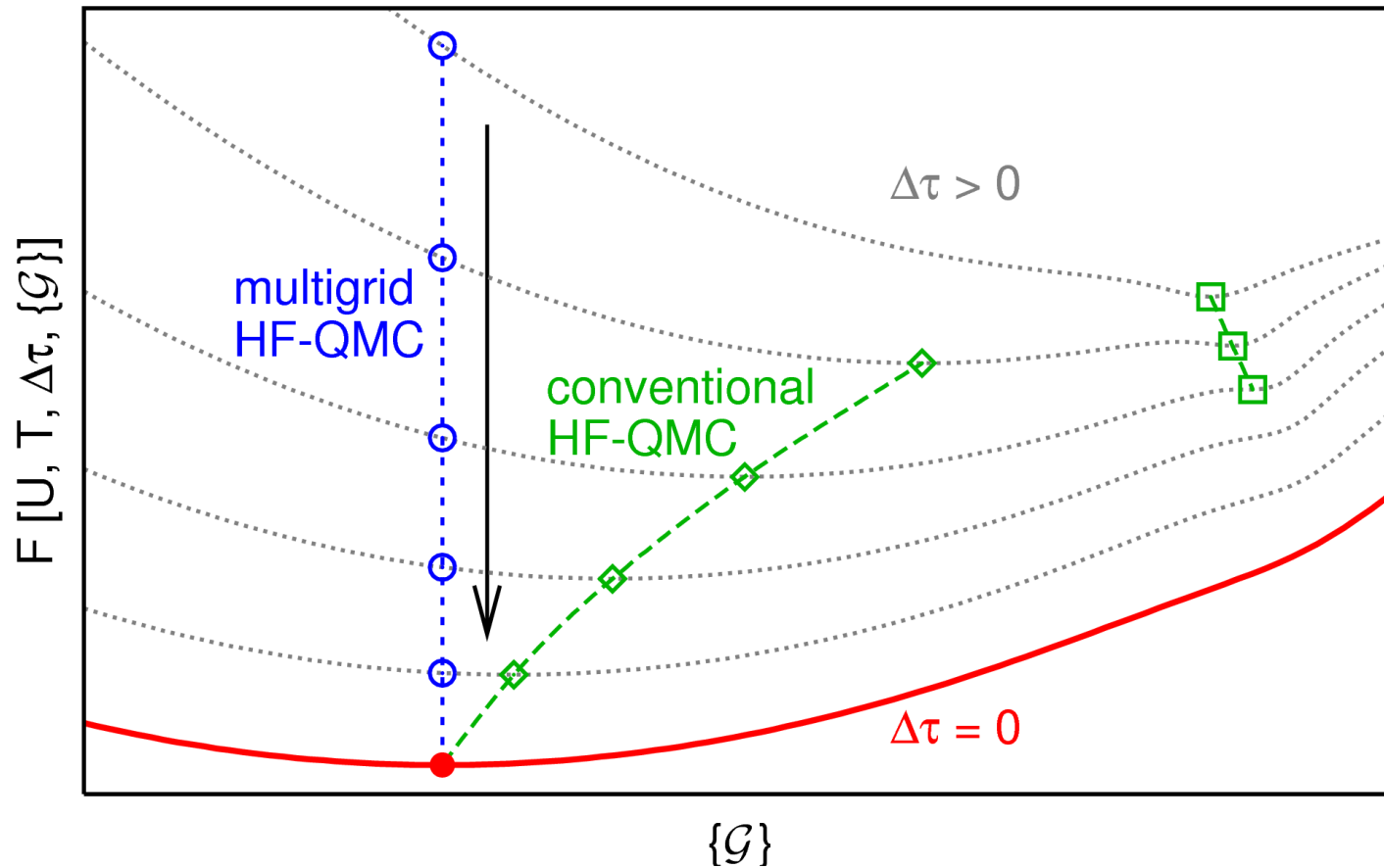
Schematic comparison via generalized Ginzburg-Landau functionals



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

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

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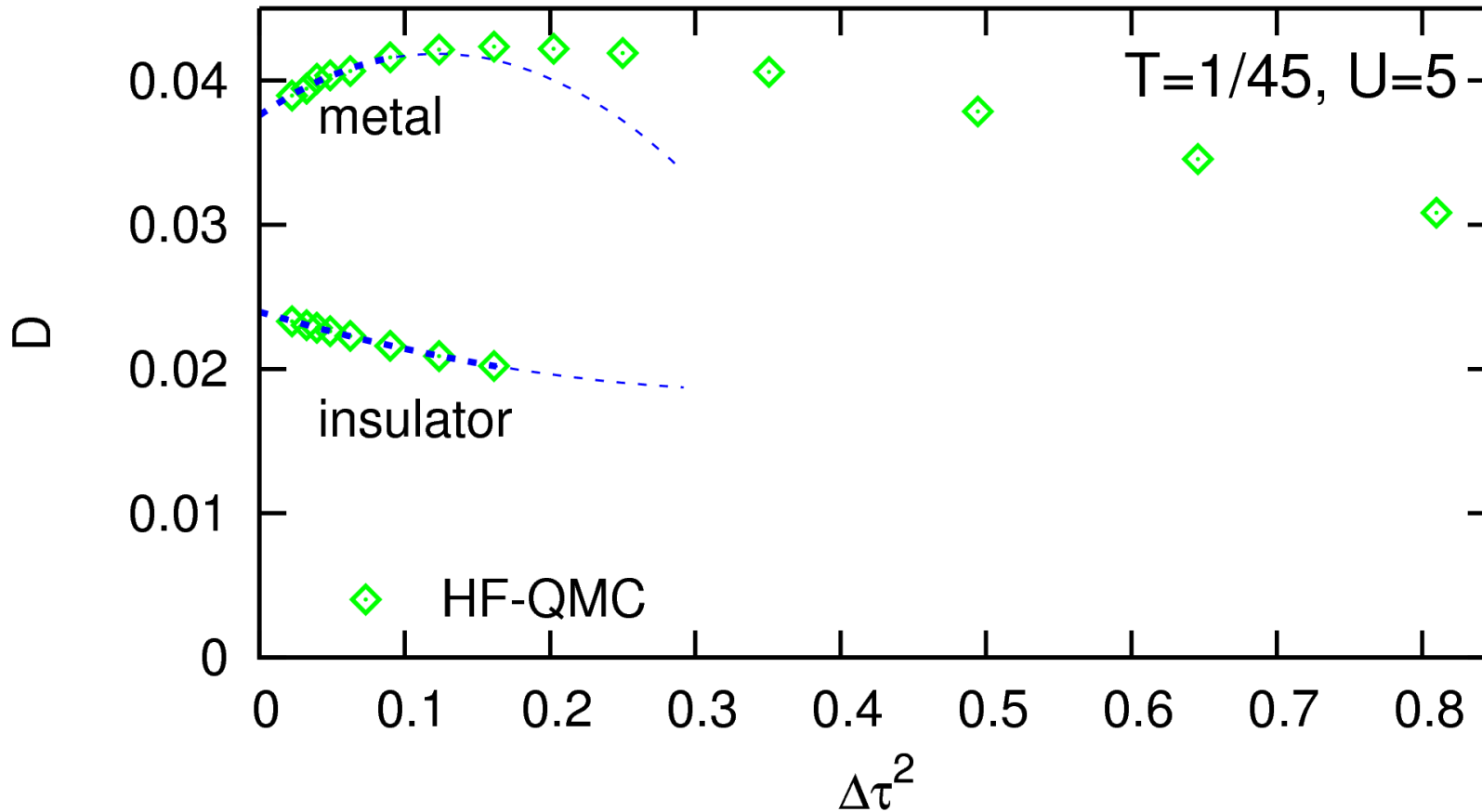


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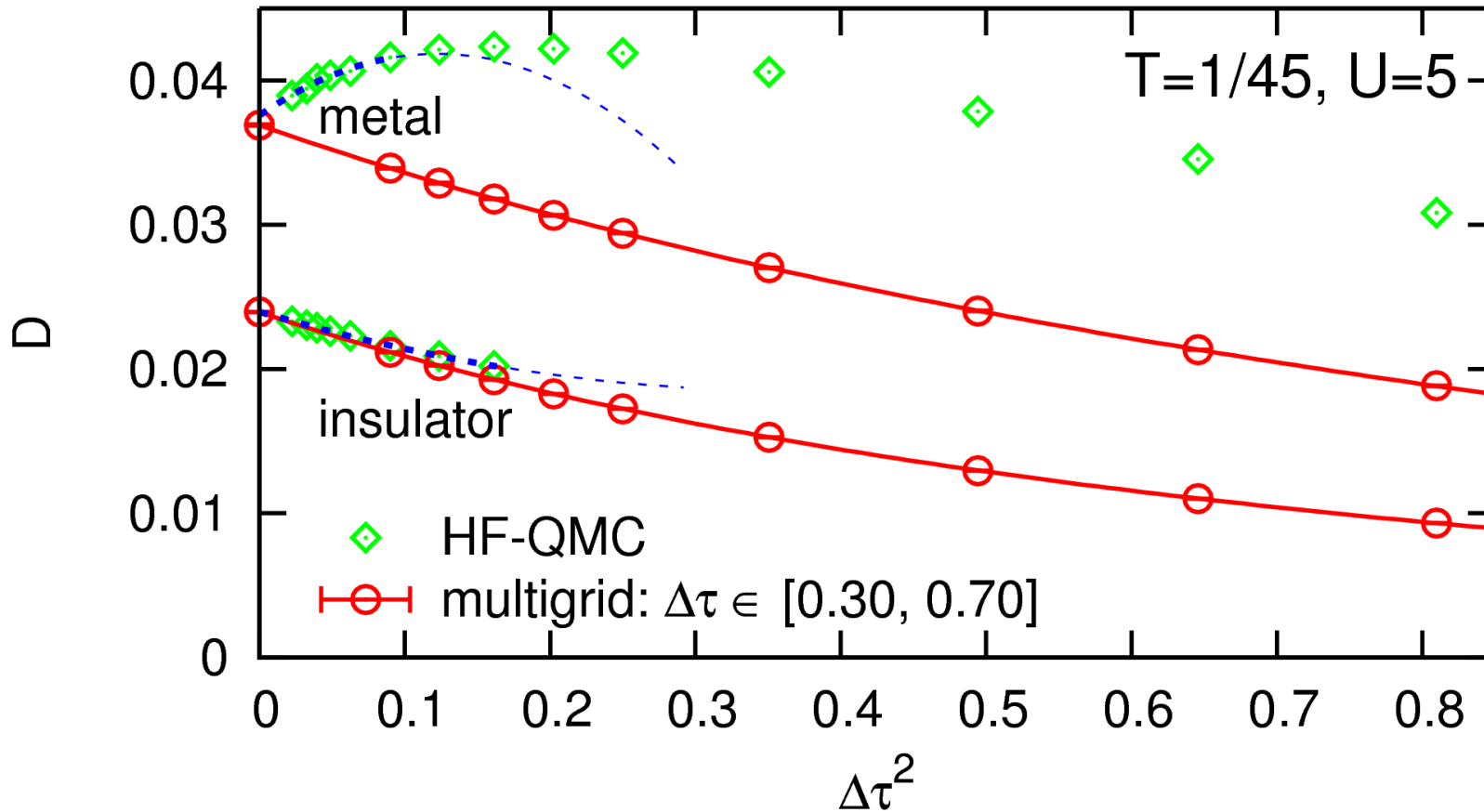
Implementation: Green function extrapolation, hierarchy of frequency scales, . . .

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 $\Delta\tau \approx 0.3$

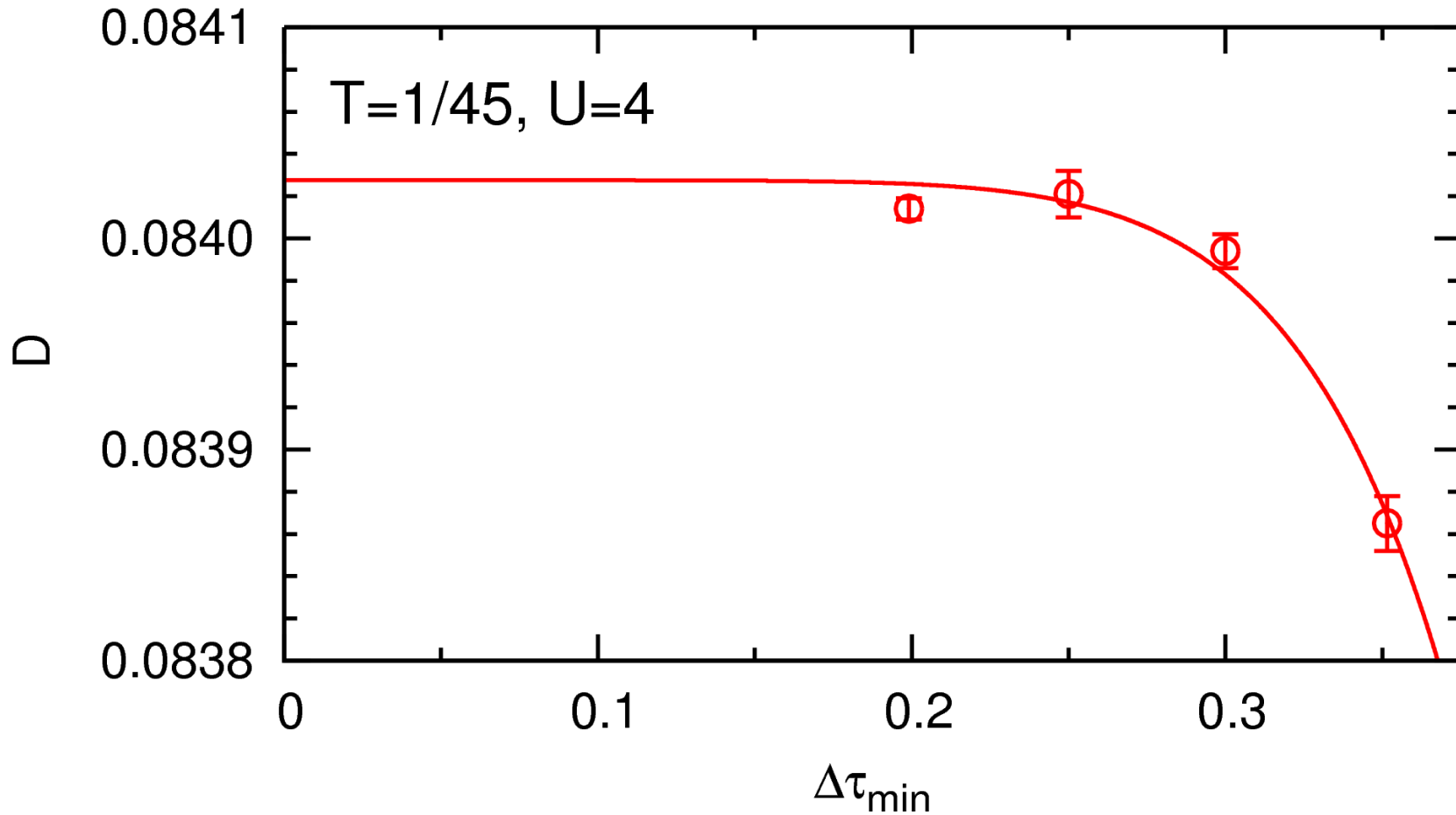
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Multigrid HF-QMC: vastly larger useful range of $\Delta\tau$

Systematic study: impact of grid range $[\Delta\tau_{\min}, \Delta\tau_{\max}]$



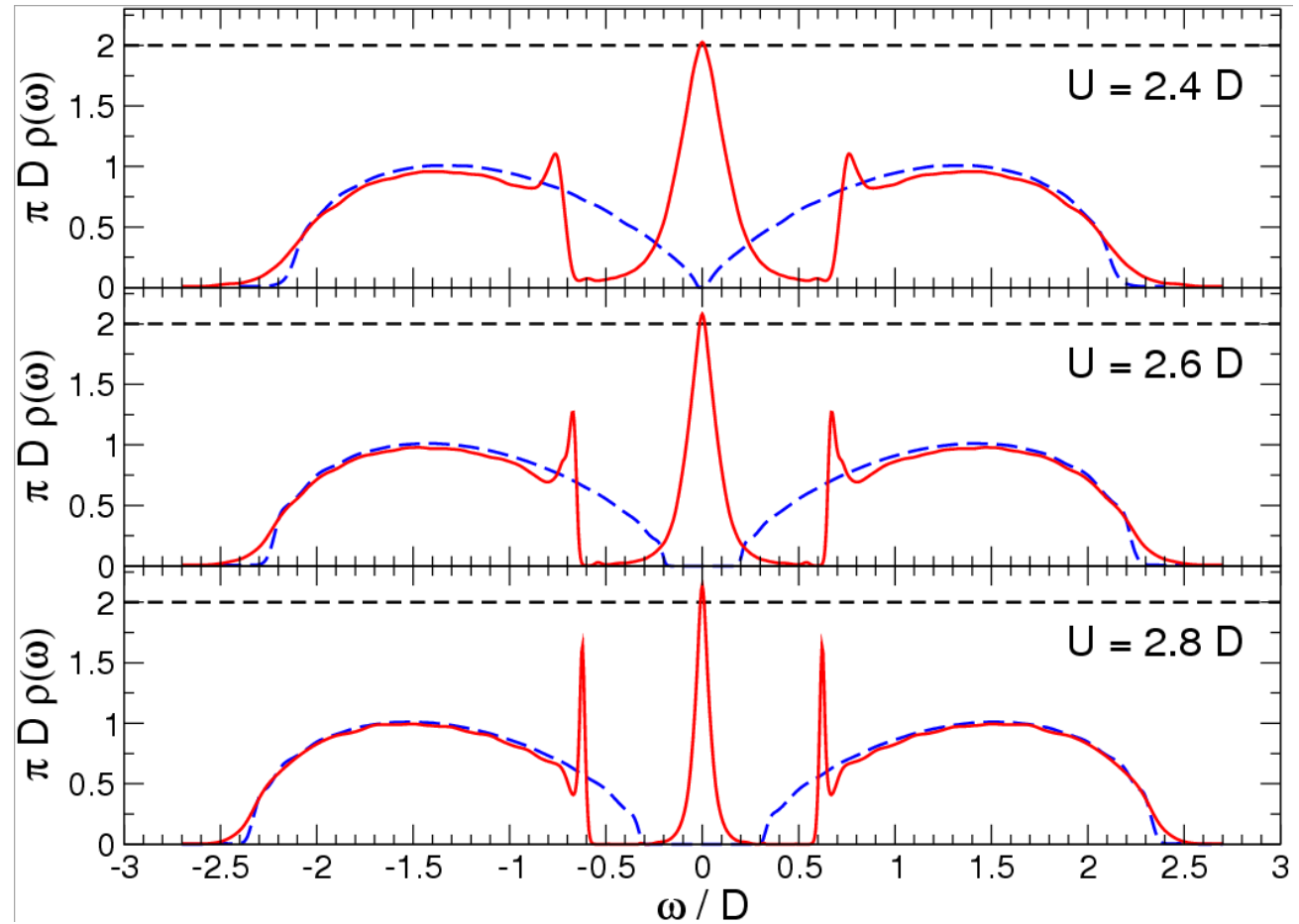
Multigrid HF-QMC usually “numerically exact” for $\tau_{\min} \lesssim 0.3$

Spectral weight transfer at the Mott transition

Question: how does the Mott metal-insulator transition take place, precisely?

Spectral weight transfer at the Mott transition

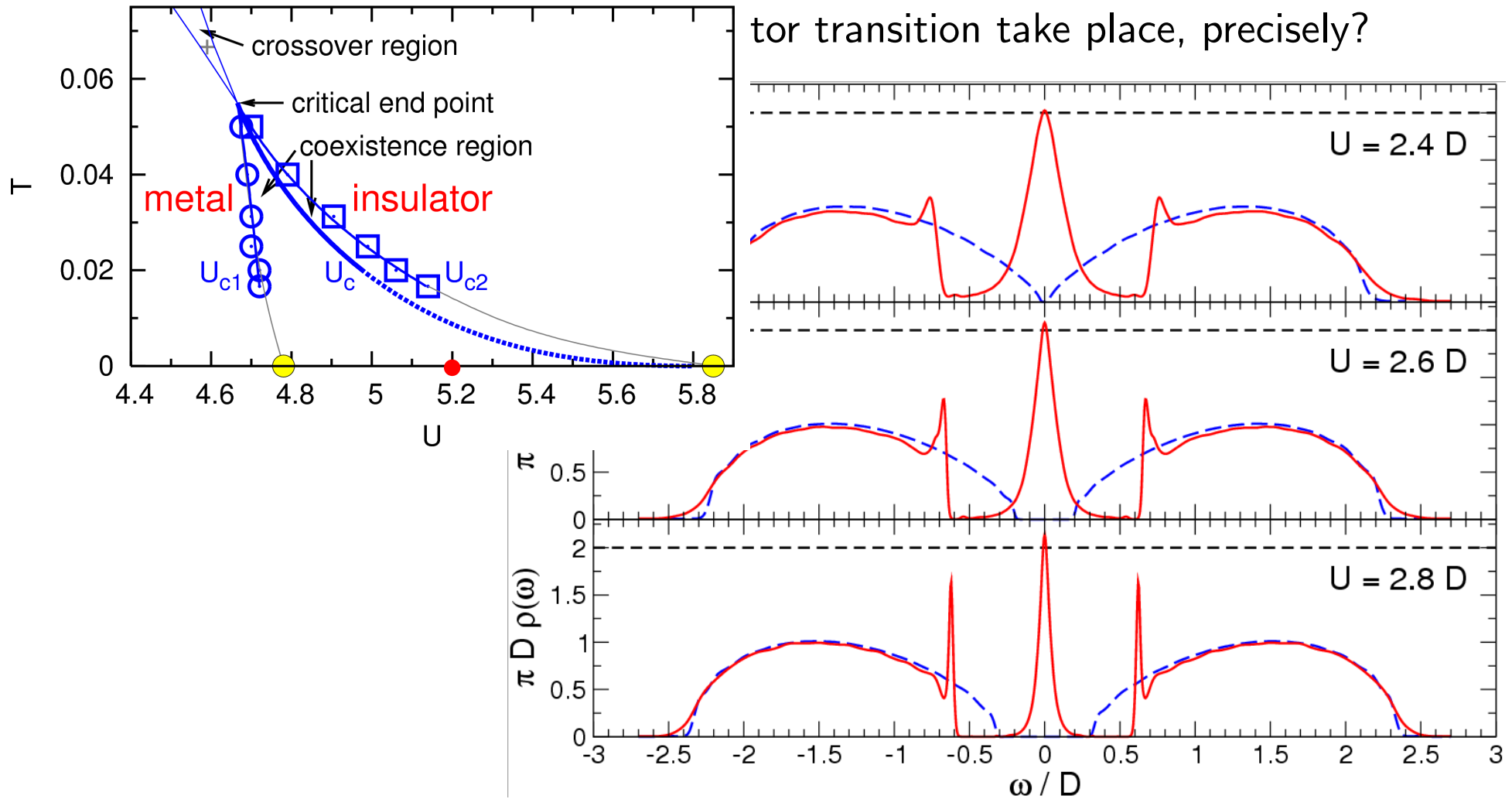
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Dynamical DMRG \rightsquigarrow Hubbard band subpeaks in metallic phase (at $T = 0$)

[Karski, Raas, Uhrig, PRB (2005)]

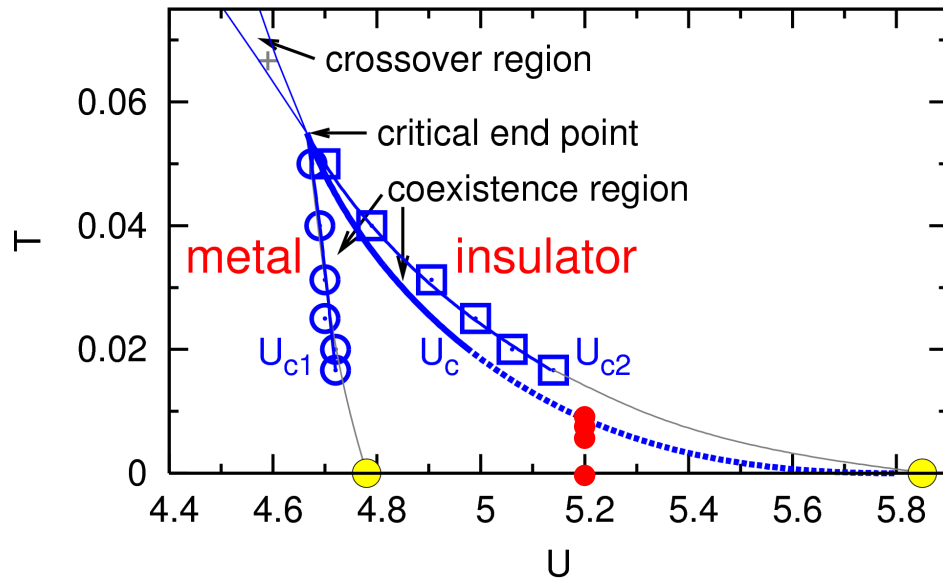
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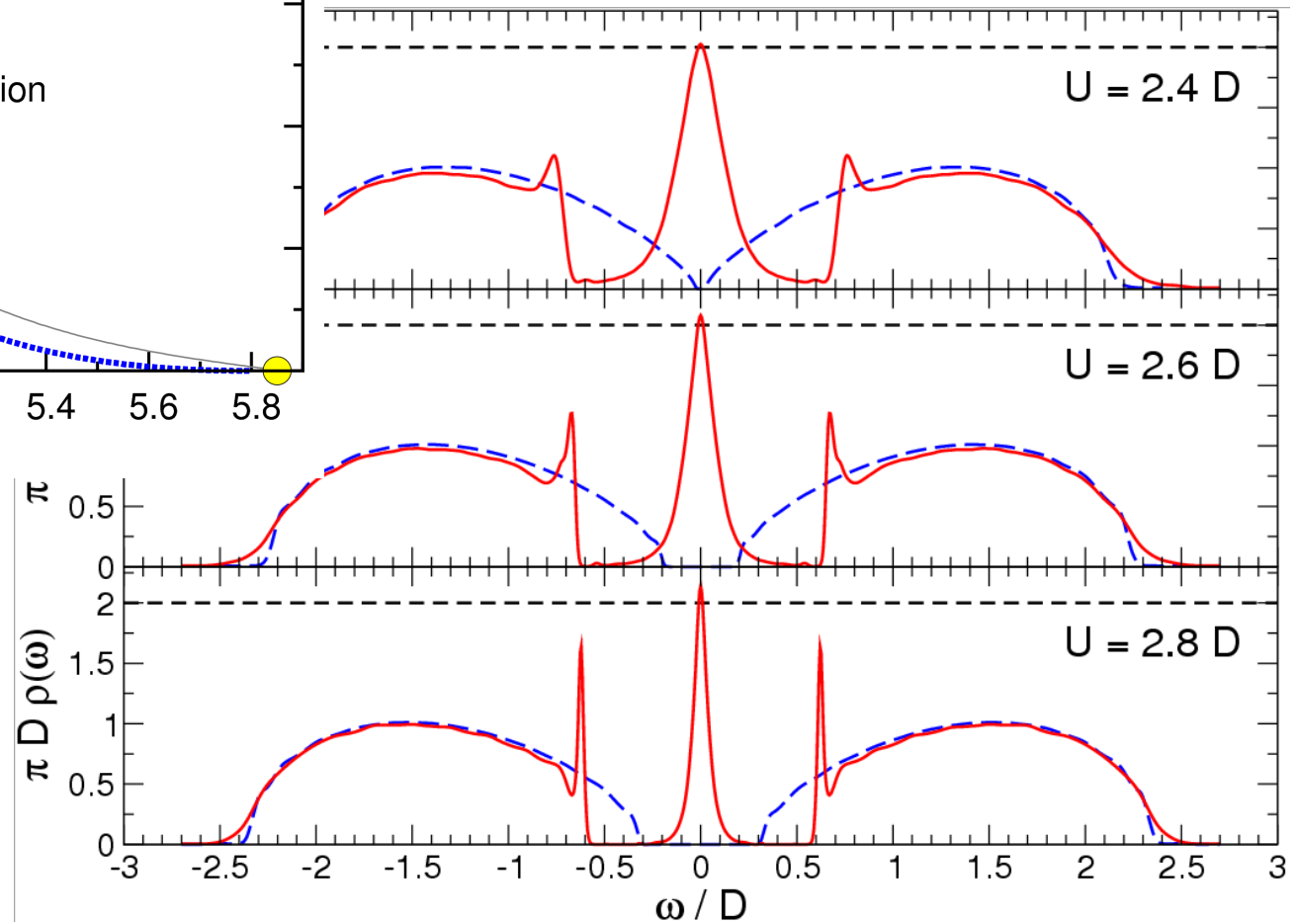
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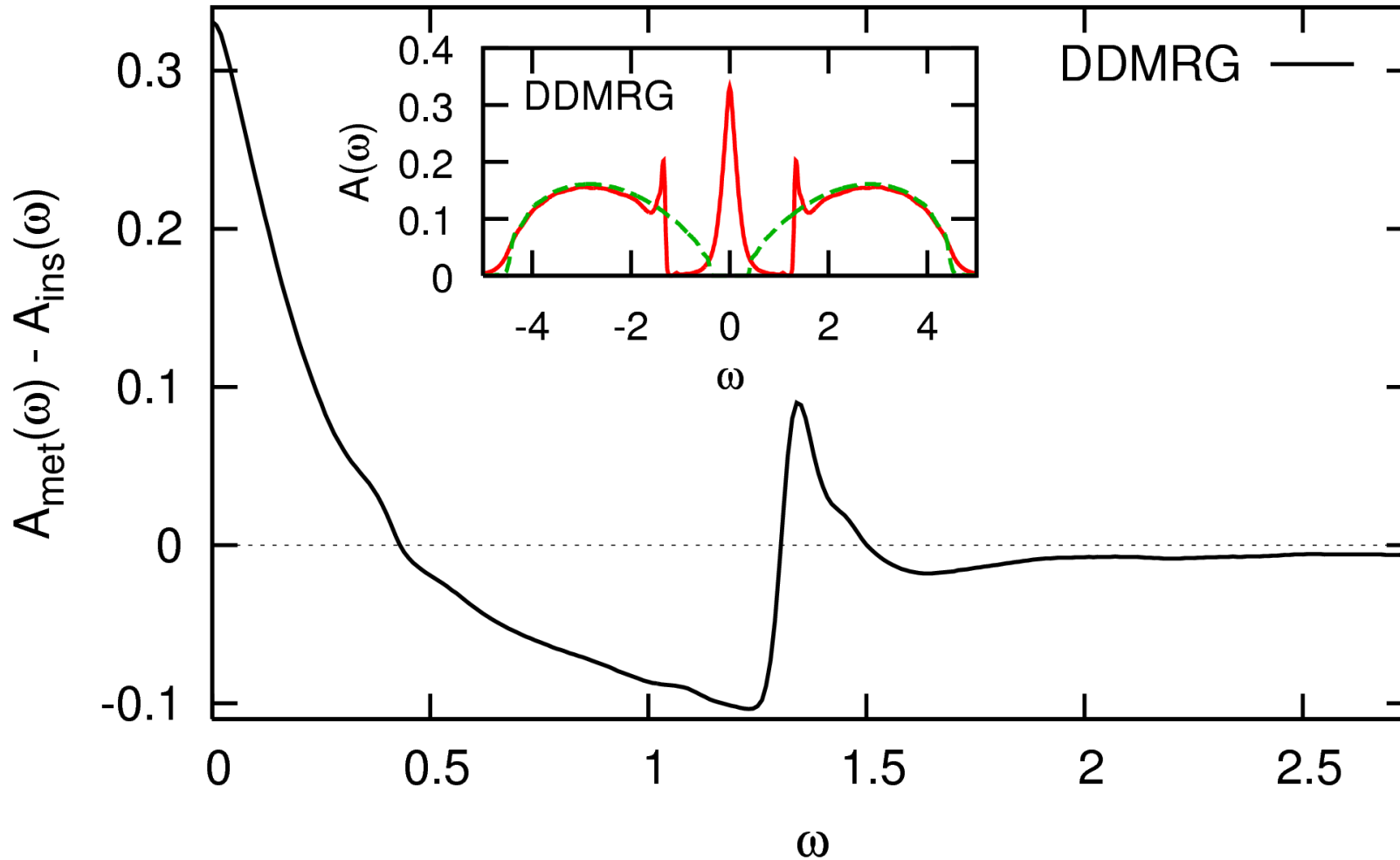


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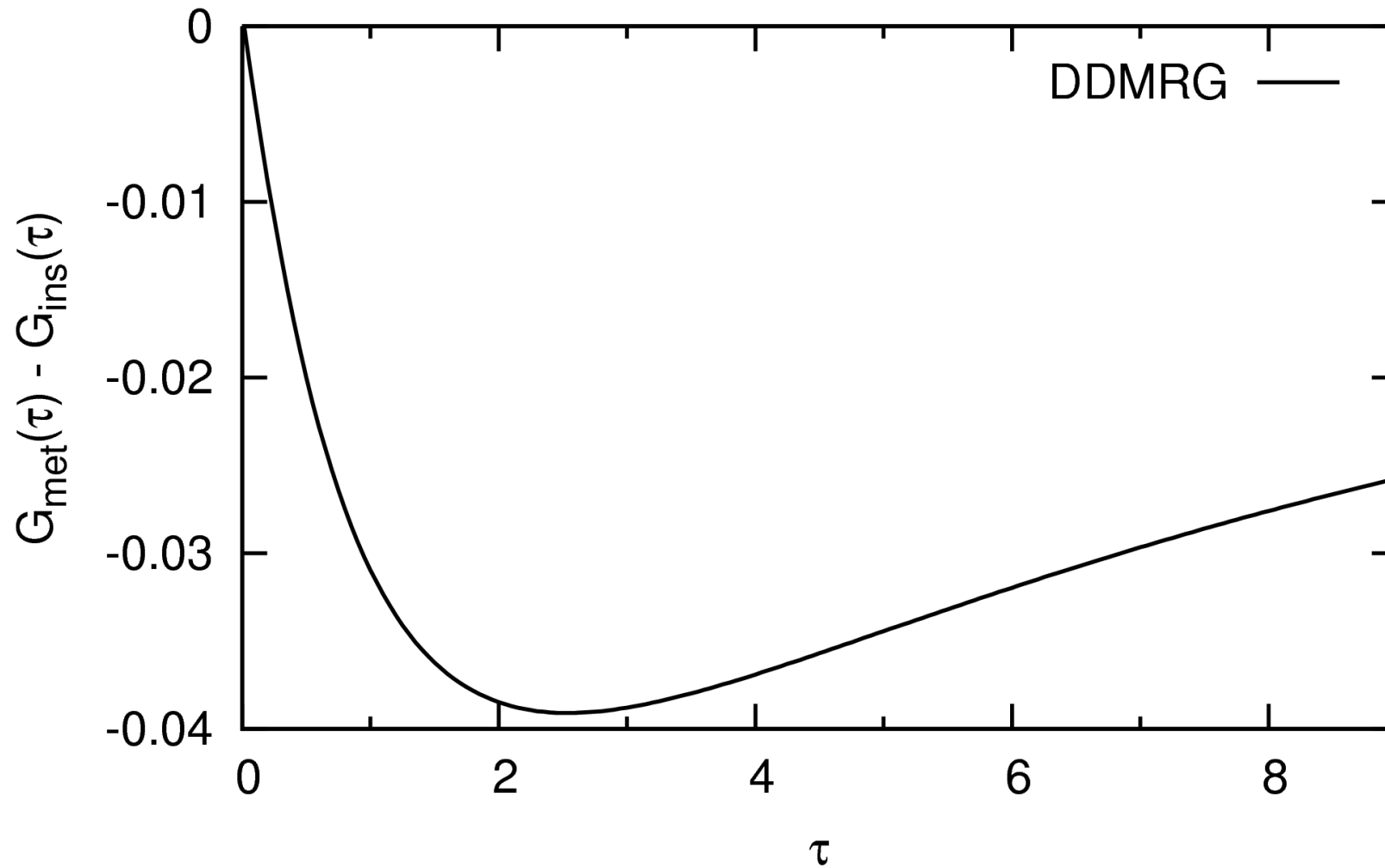
Verify using multigrid HF-QMC...

Analysis via difference of spectral functions (symmetric in ω) at $U = 5.2$

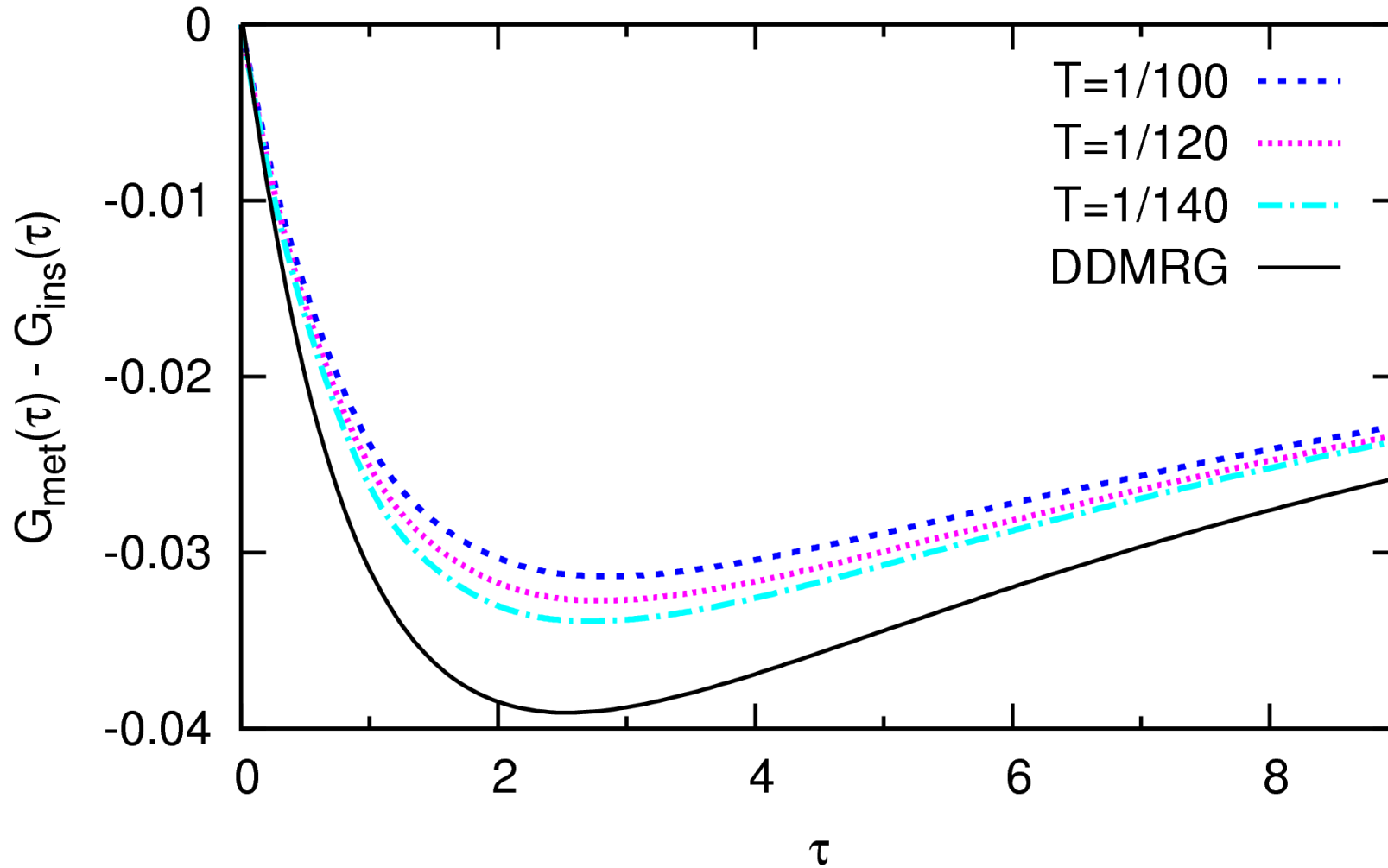


- Problems for QMC:
- (i) analytic continuation of QMC data ill-conditioned
 - (ii) no $T \rightarrow 0$ extrapolation of spectra

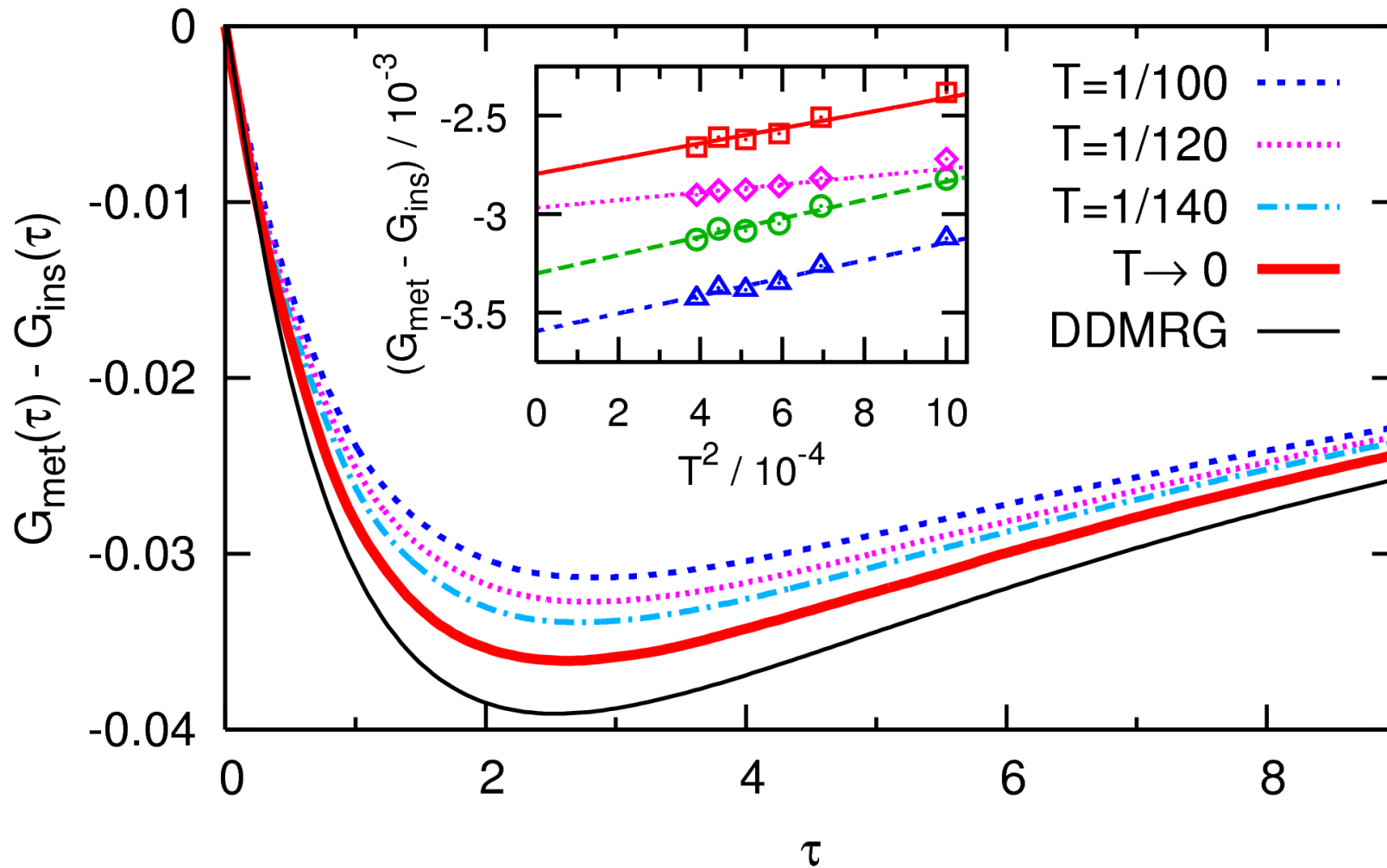
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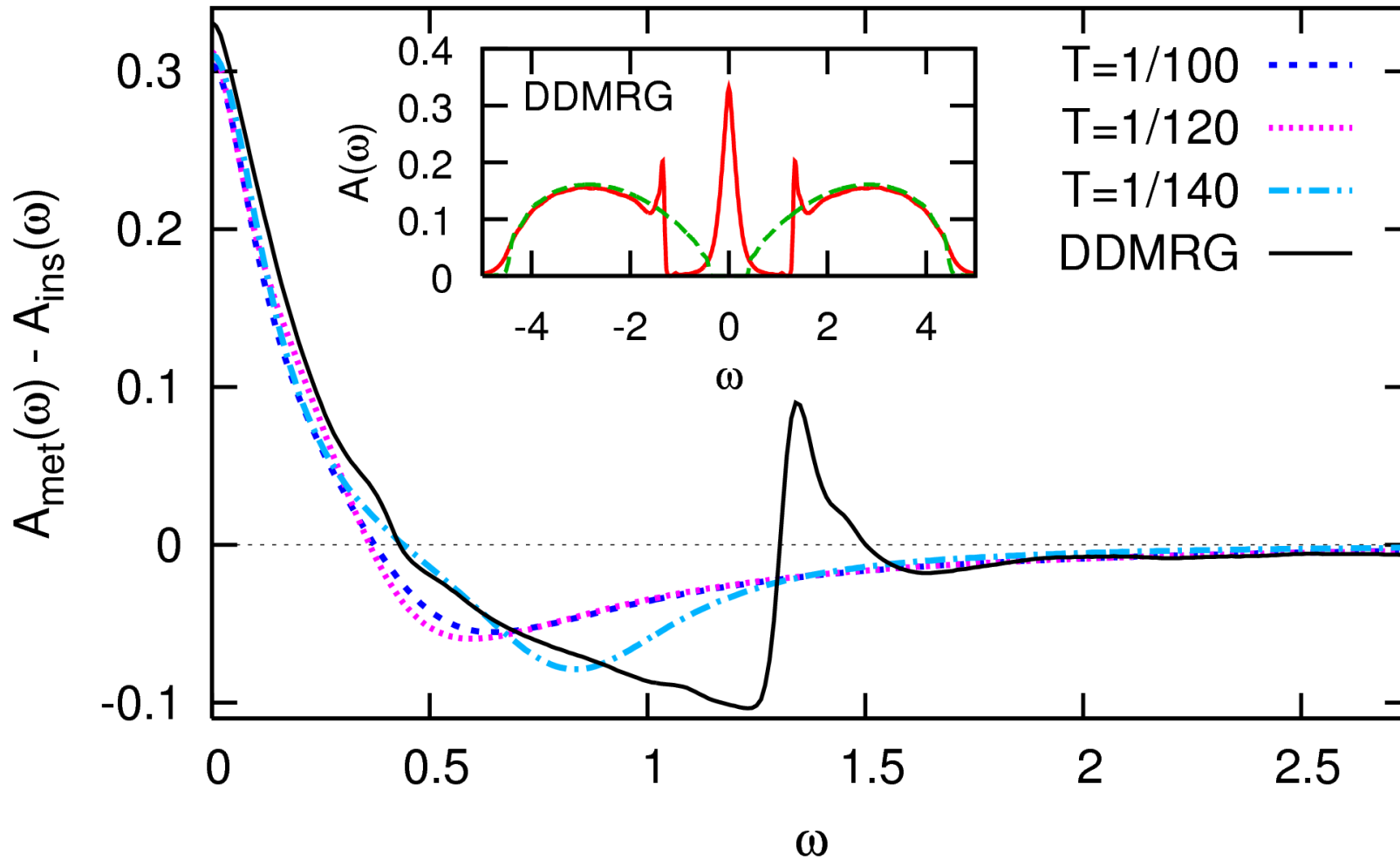
Difference Green functions in imaginary time



Multigrid HF-QMC data precise within linewidths [NB, arXiv:0801.1222]

DDMRG overestimates spectral weight transfer at $U = 5.2$ by about 10%!

Difference spectra



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

QMC spectral data via Padé interpolation, may be overly smooth [NB, [arXiv:0801.1222](https://arxiv.org/abs/0801.1222)]

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

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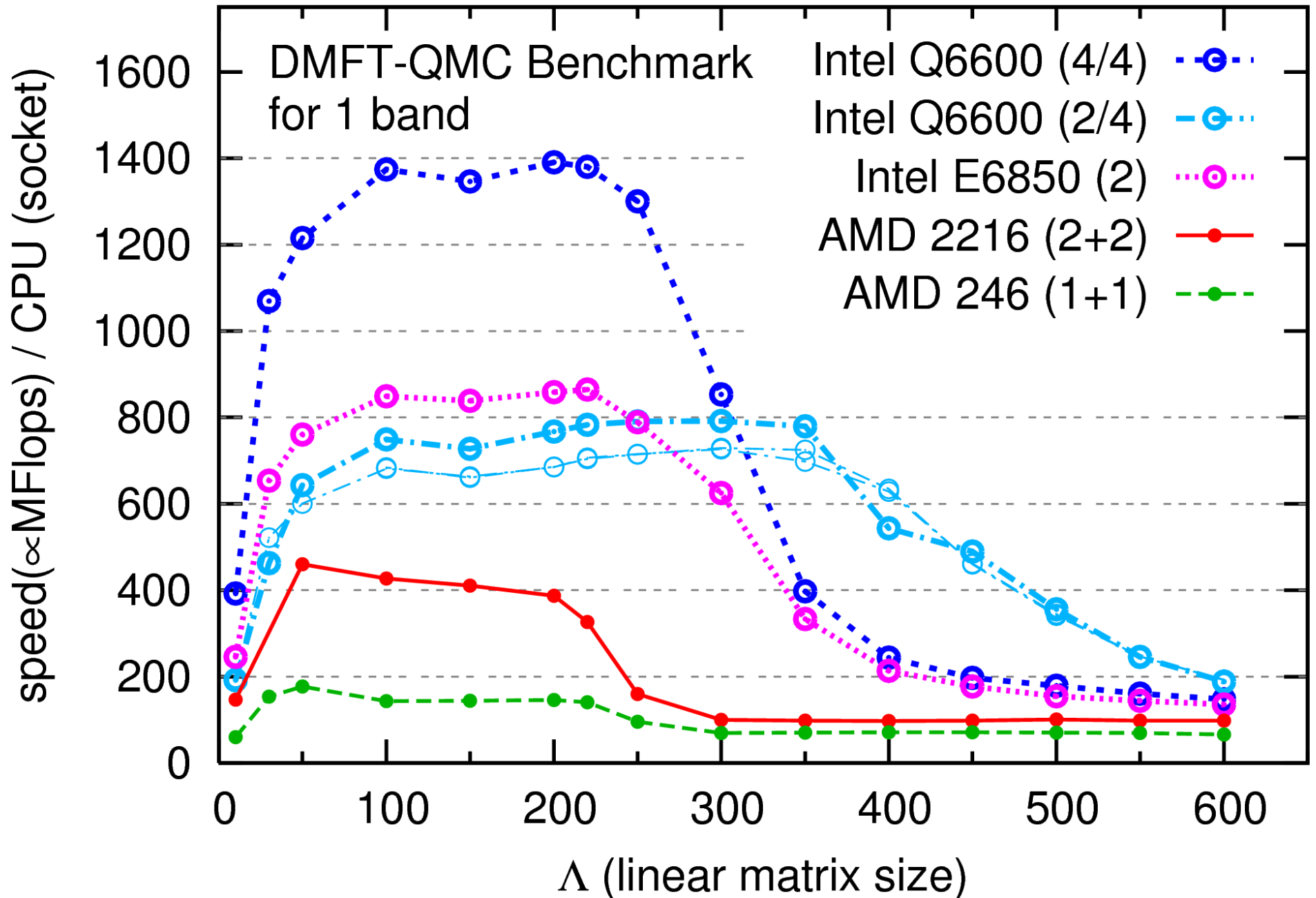
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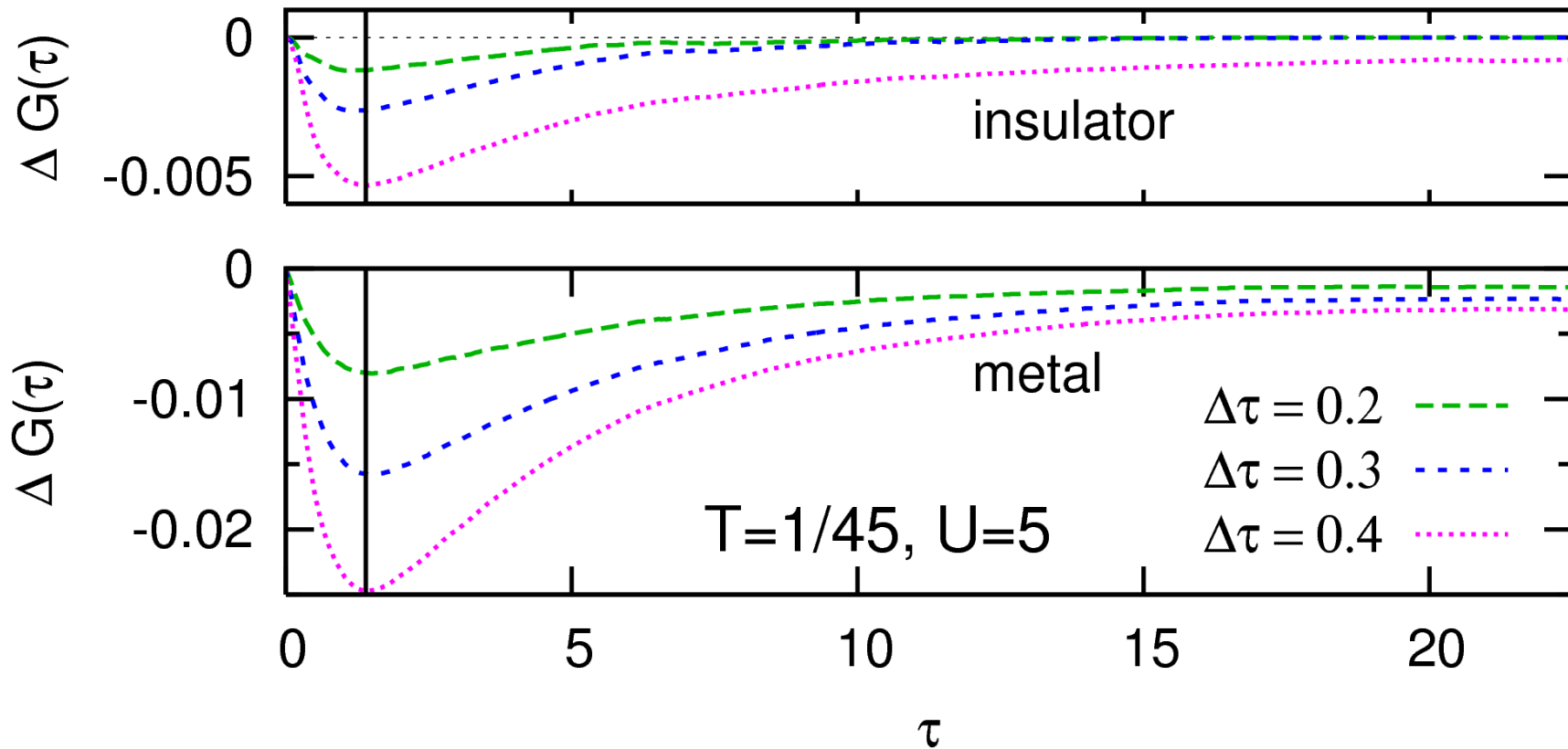
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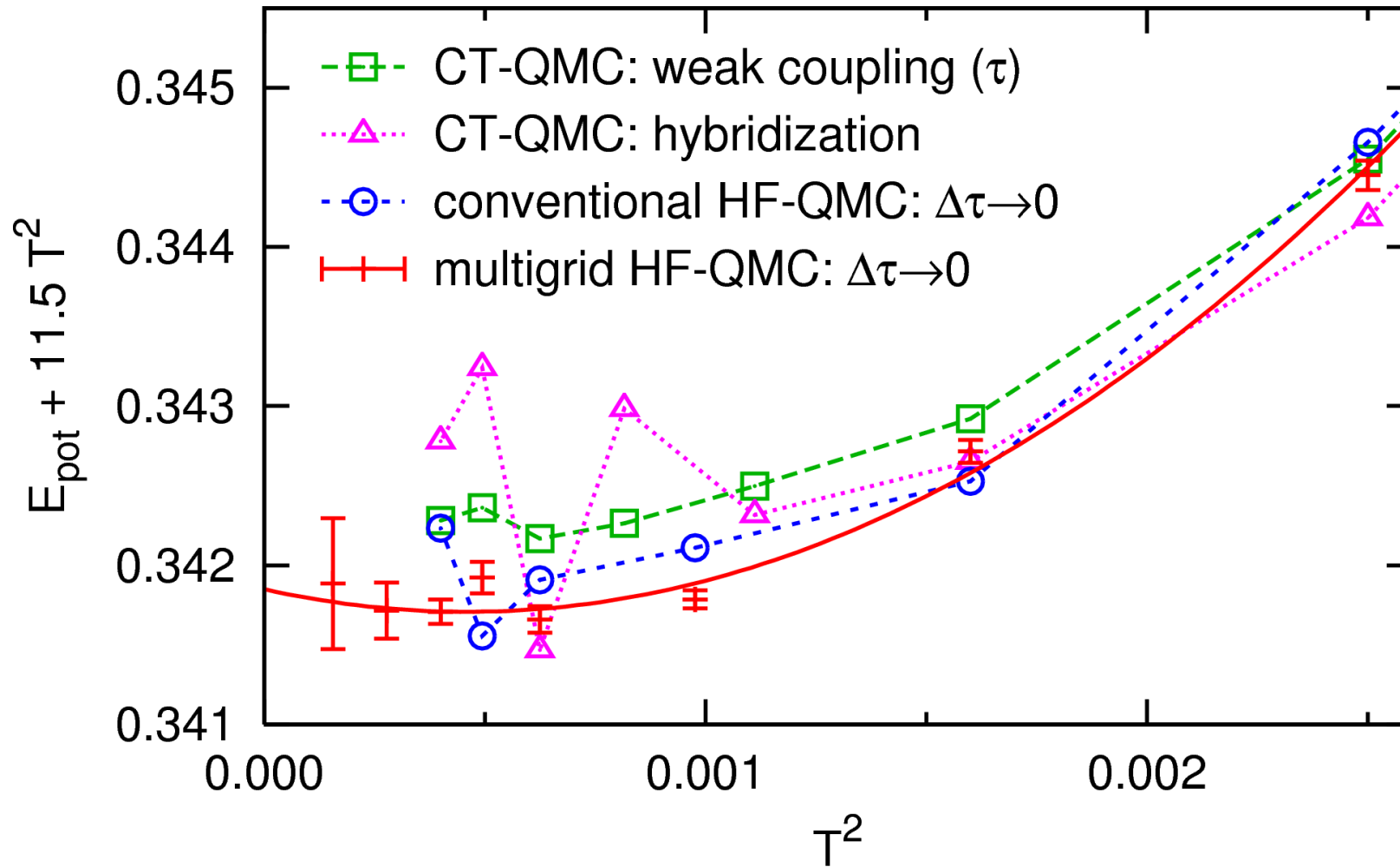


Low- τ resolution limited by $\Delta\tau$? **No!**



Uniform $\Delta\tau$ dependence, position of max. error independent of $\Delta\tau$ and phase!

Efficiency: potential energy $E_{\text{pot}} = UD$ (at $U = W = 4$)



No more “difficult observables” for multigrid HF-QMC
Higher precision than CT-QMC methods at same effort