

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

Nils Blümer, Univ. Mainz

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Outline

A brief reminder

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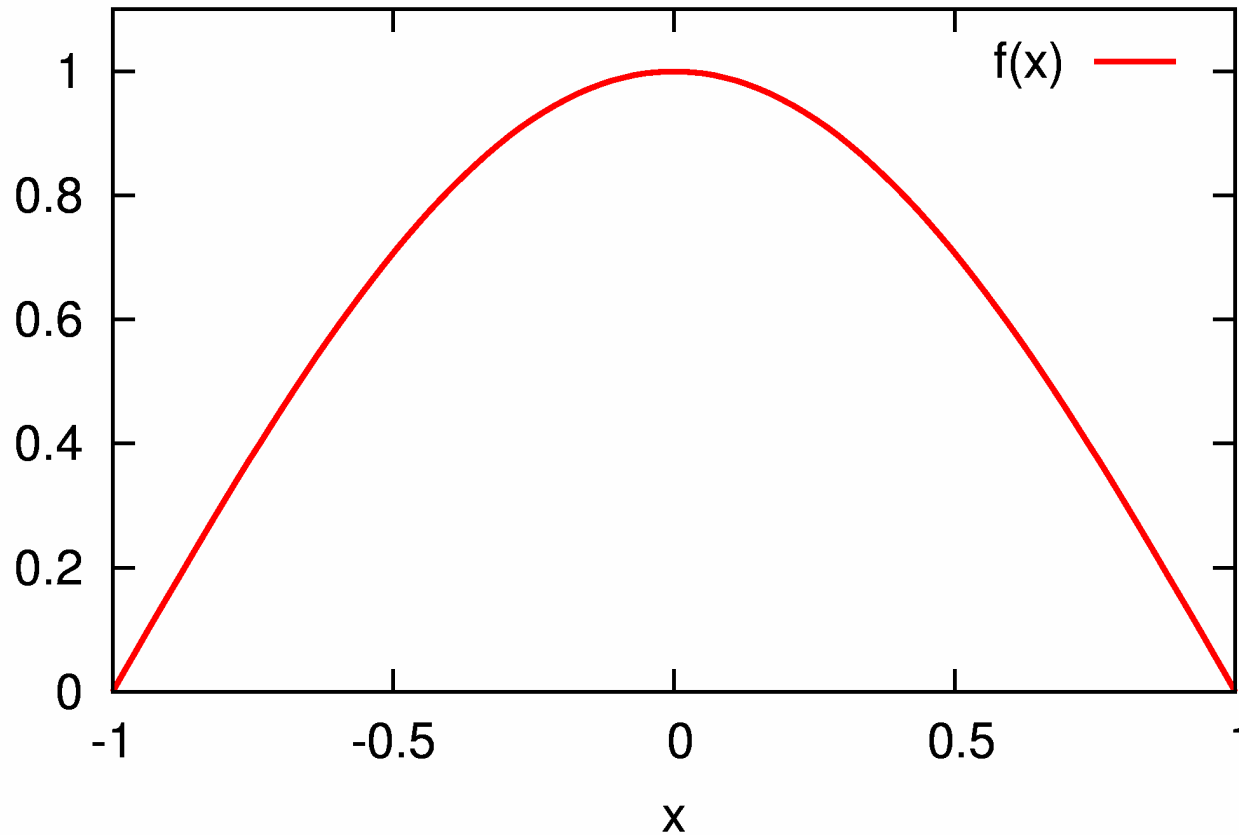
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The (brief?) remainder

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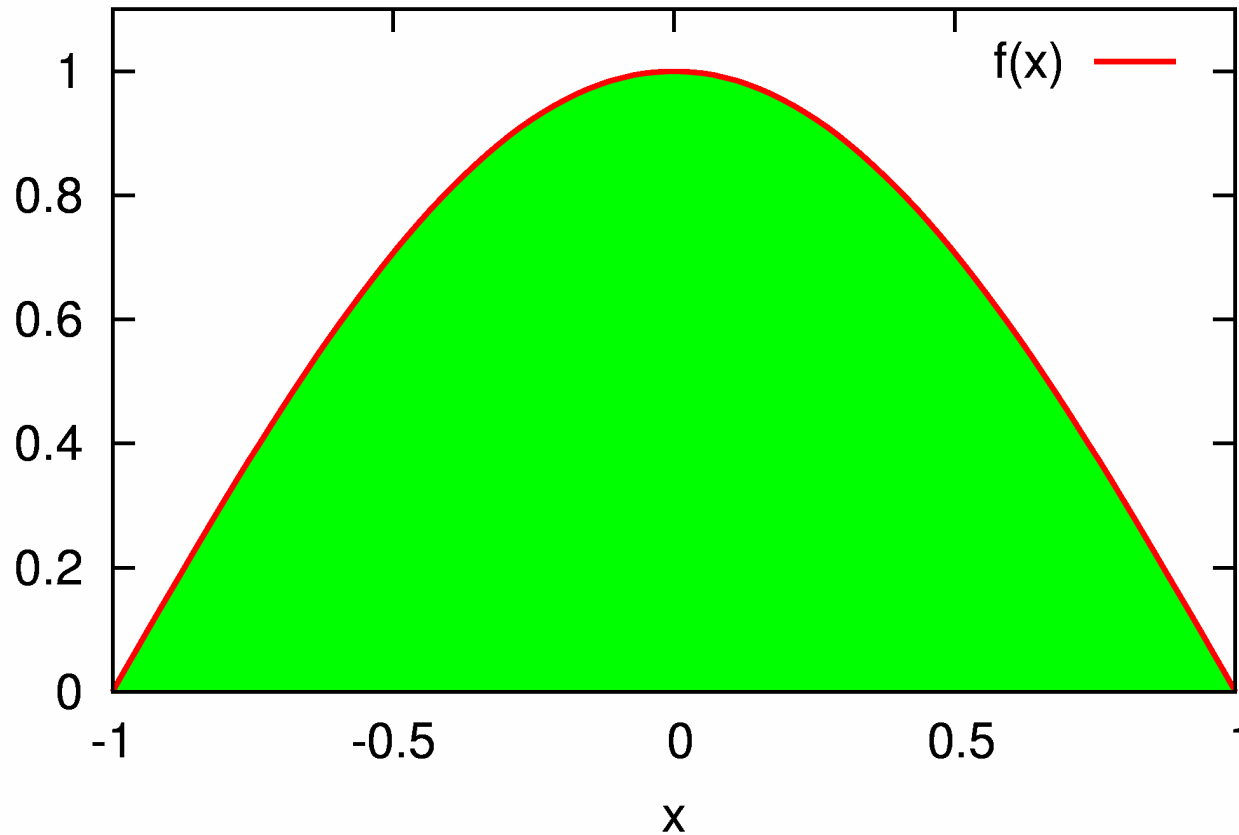
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$$I = \int_a^b f(x) dx = ?$$

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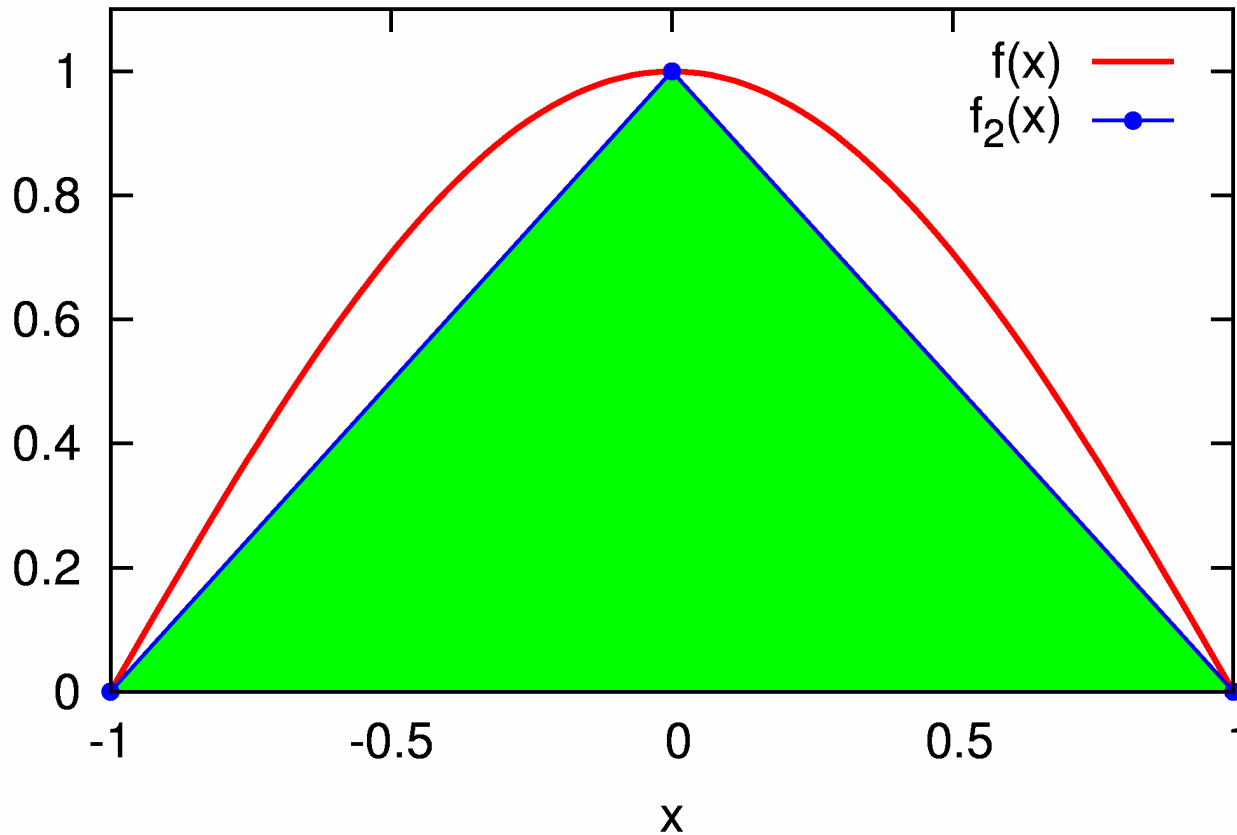
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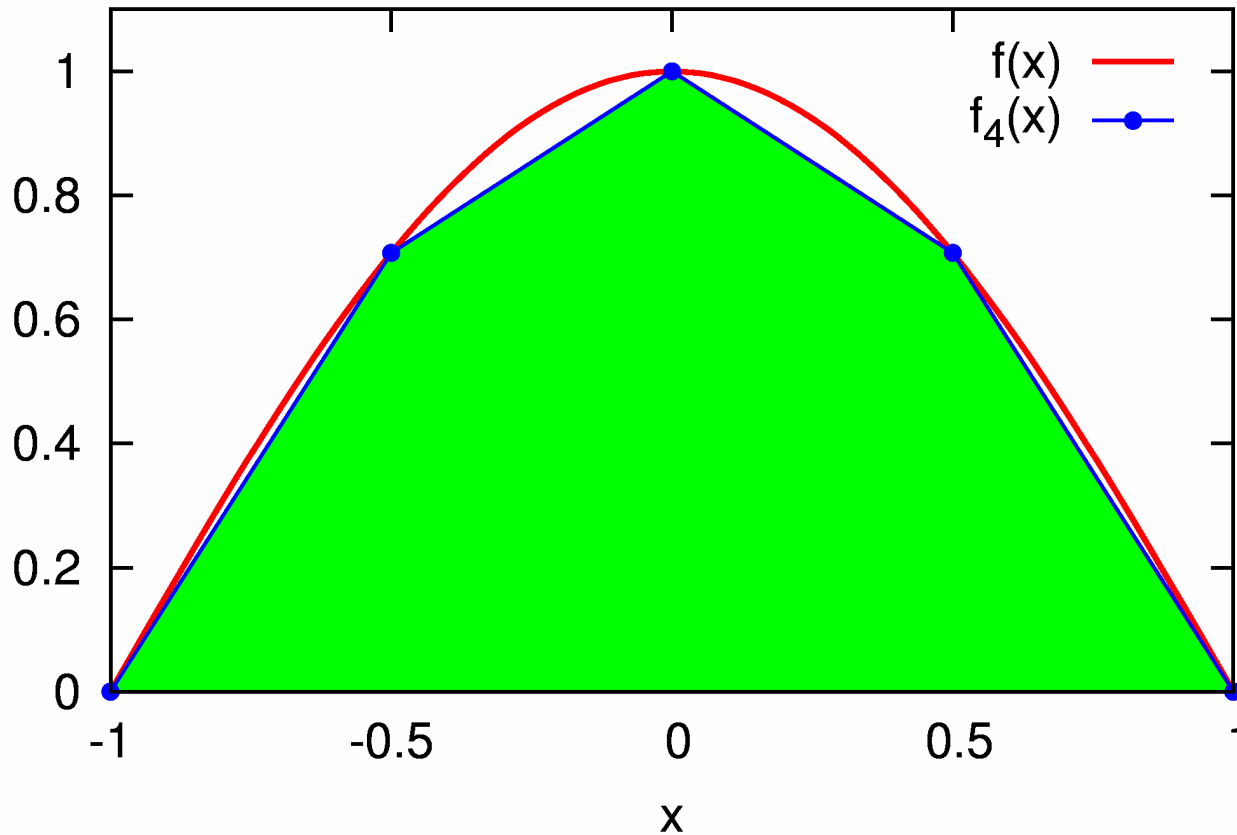
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Numerical methods:

- discretization

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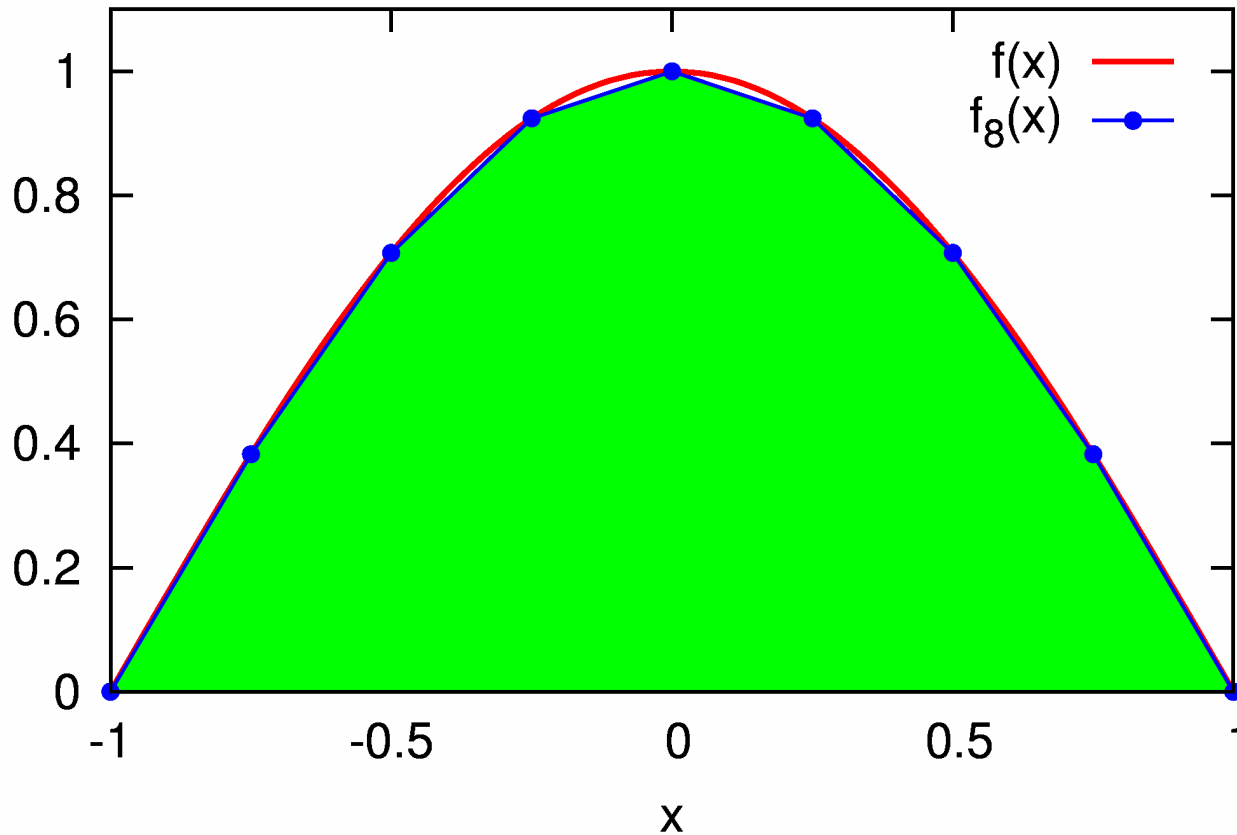
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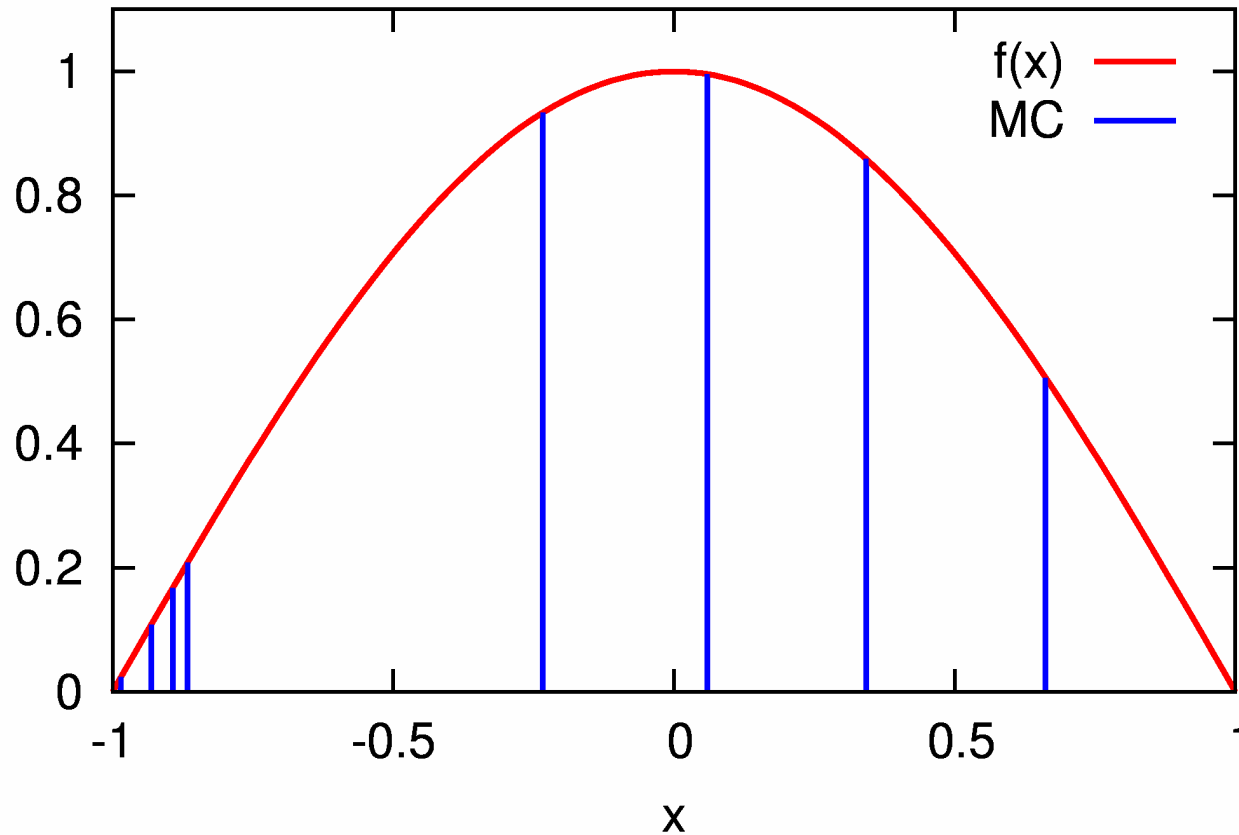
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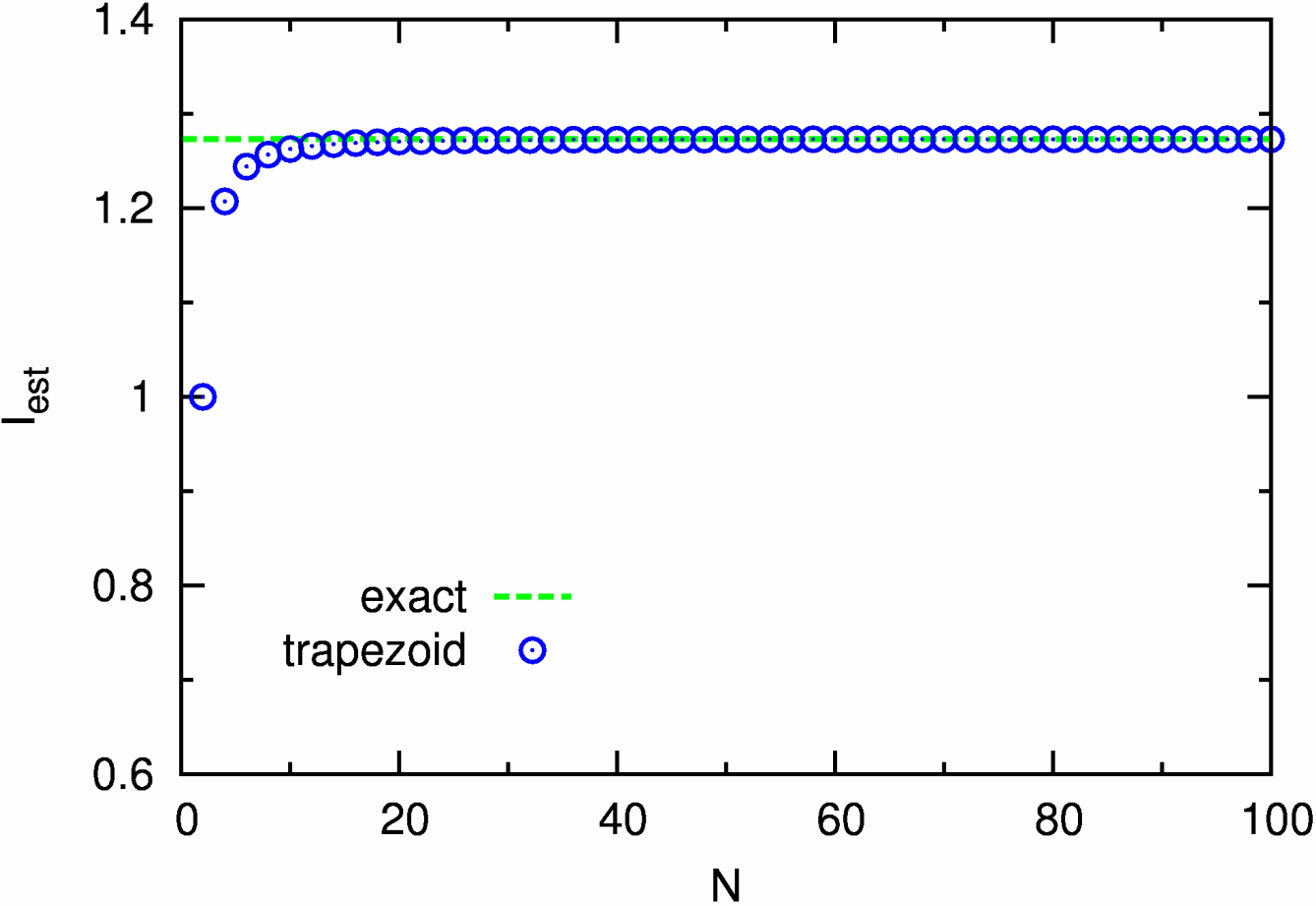


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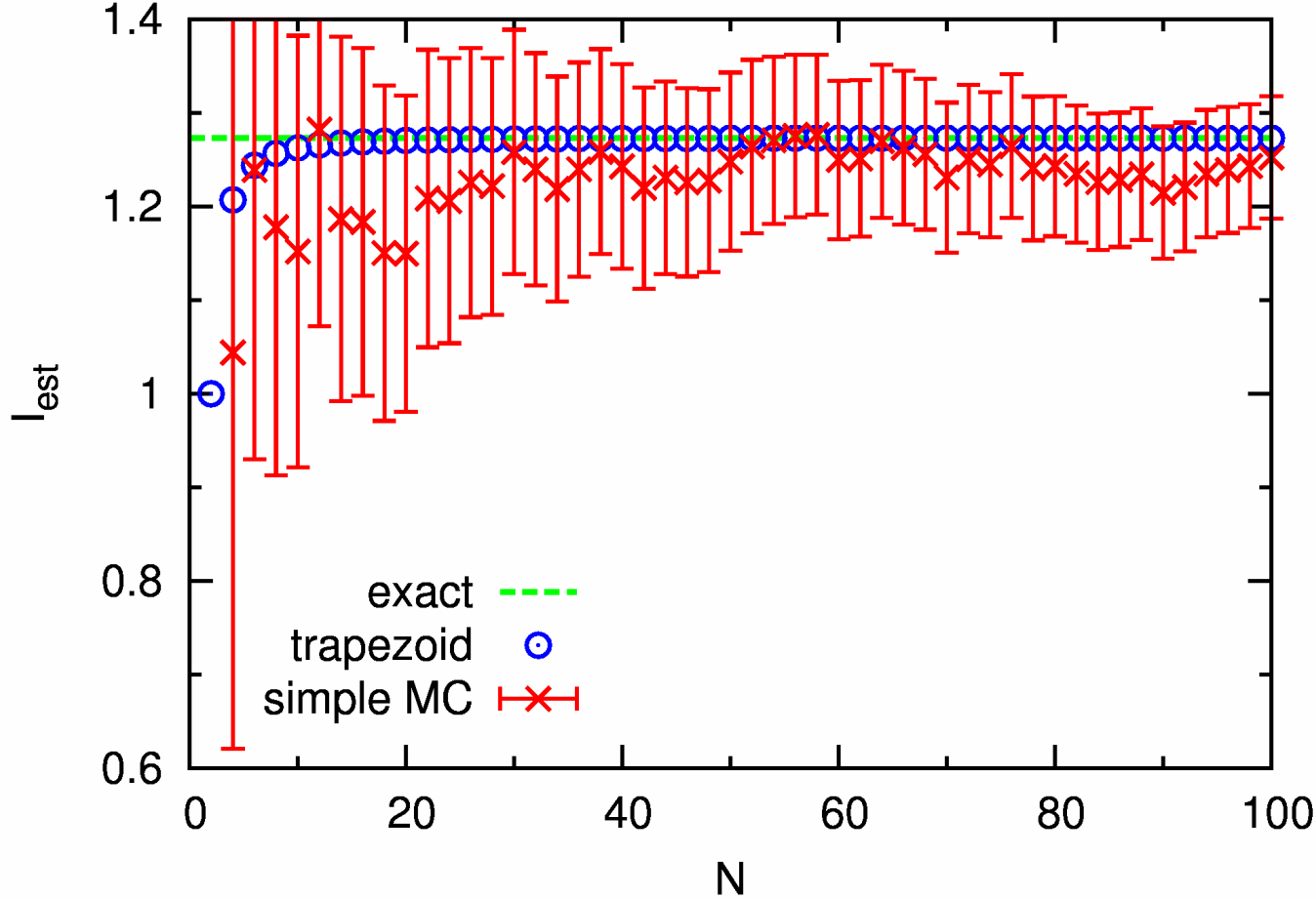
Numerical methods:

- discretization
- Monte Carlo

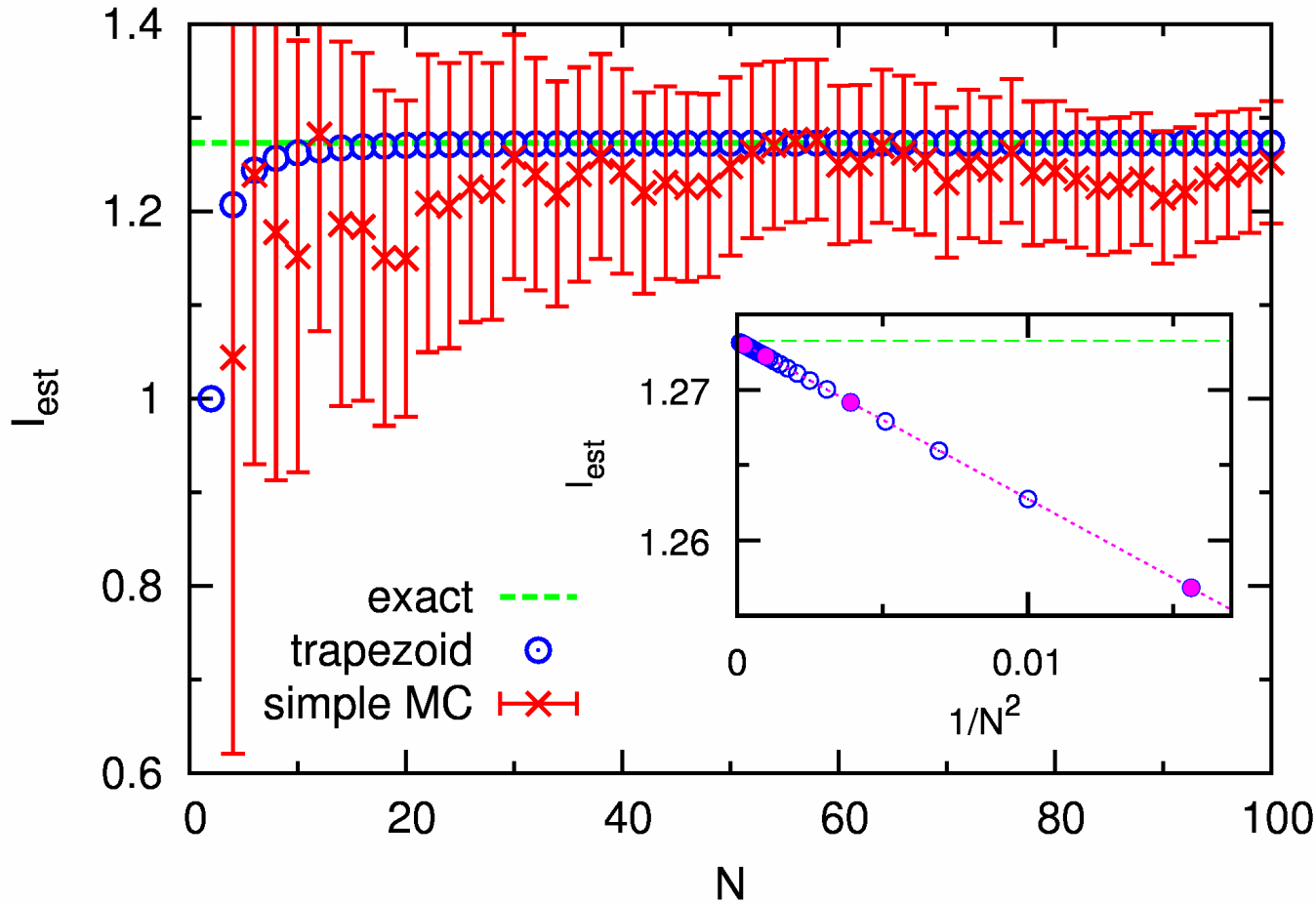
Convergence of results?



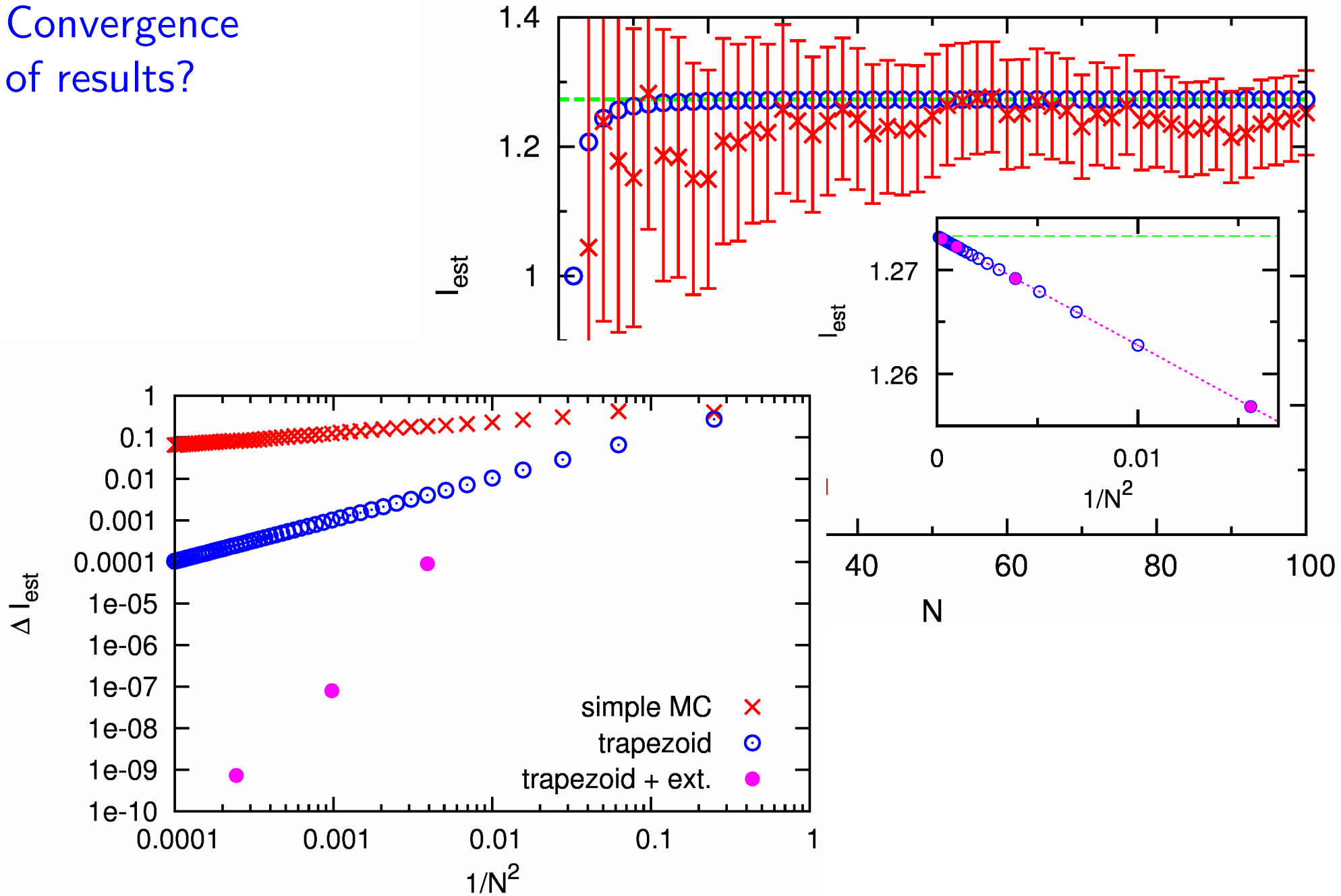
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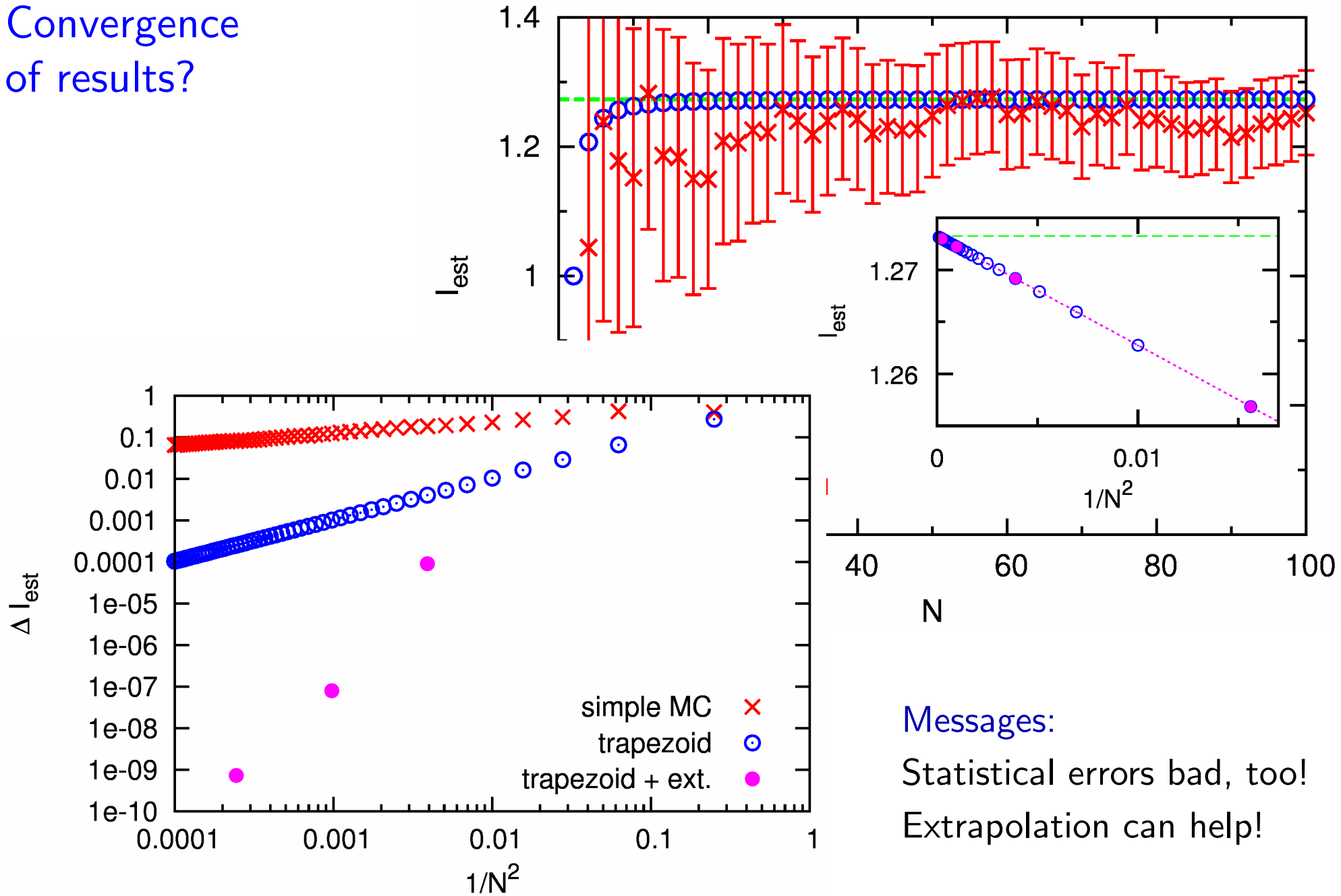
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Convergence of results?



Messages:

Statistical errors bad, too!
Extrapolation can help!

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Introduction: DMFT, HF-QMC

Unbiased Green functions and spectra from HF-QMC

Multigrid Hirsch-Fye quantum Monte Carlo algorithm

Applications: spectral-weight transfer, specific heat

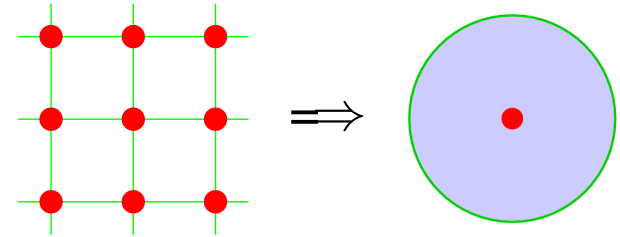
Summary

Introduction

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

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 $Z \rightarrow \infty$

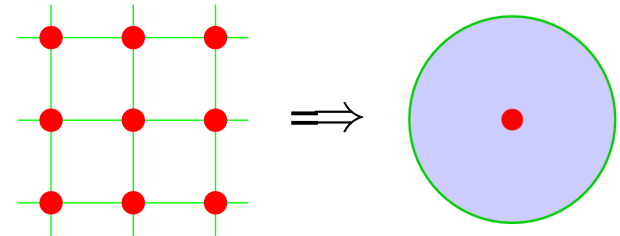


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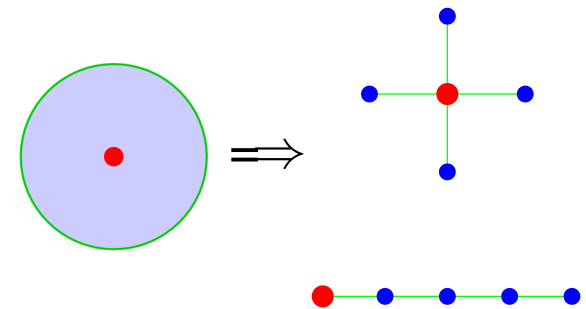
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Numerically exact impurity solvers:

- 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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(i) Imaginary-time discretization $\beta = \Lambda \Delta\tau$

(ii) Trotter decoupling $e^{-\beta(\hat{T}+\hat{V})} \approx [e^{-\Delta\tau\hat{T}} e^{-\Delta\tau\hat{V}}]^{\Lambda}$

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

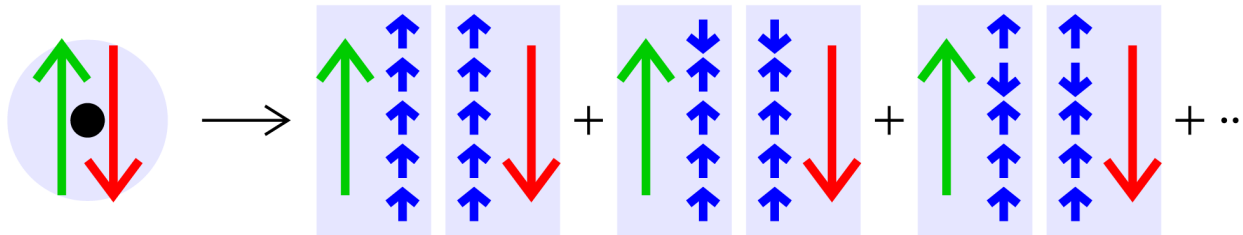
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(iii) Hubbard-Stratonovich transformation



Wick theorem:

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

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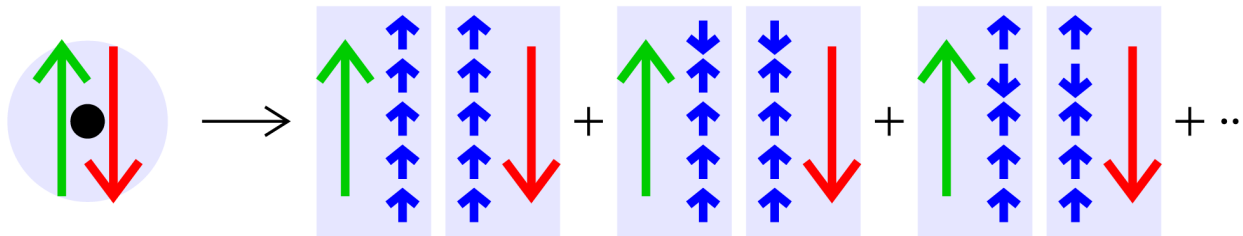
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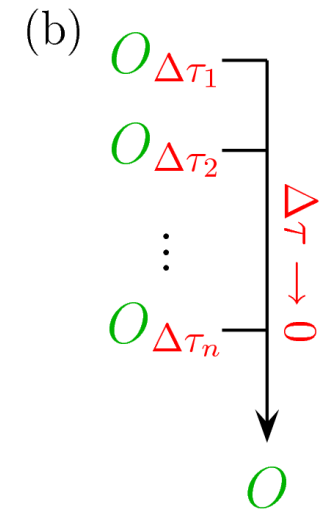
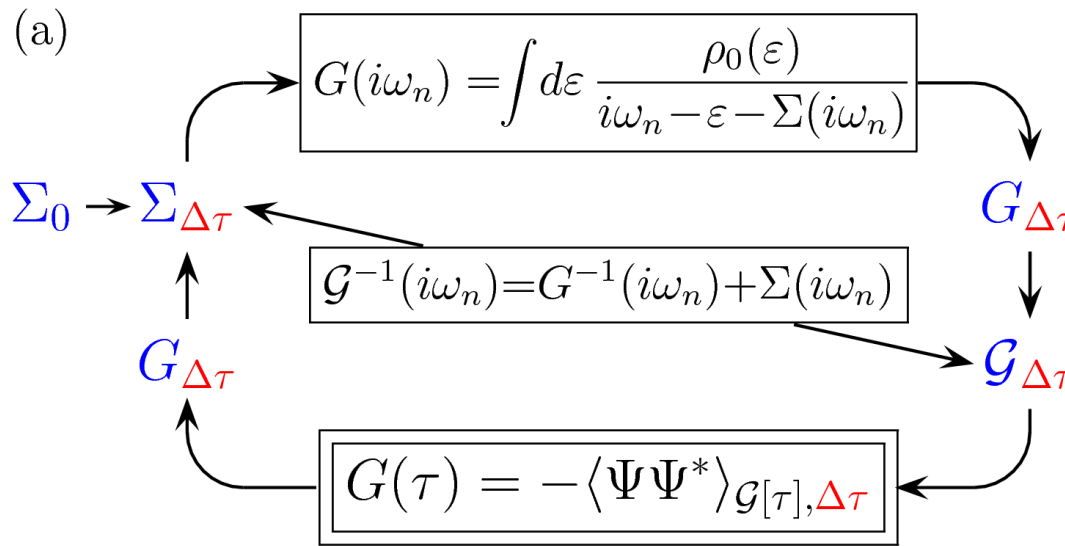
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(iv) MC importance sampling over auxiliary Ising field $\{s\}$: 2^{Λ} configurations

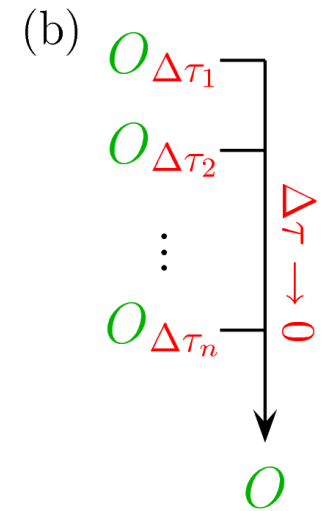
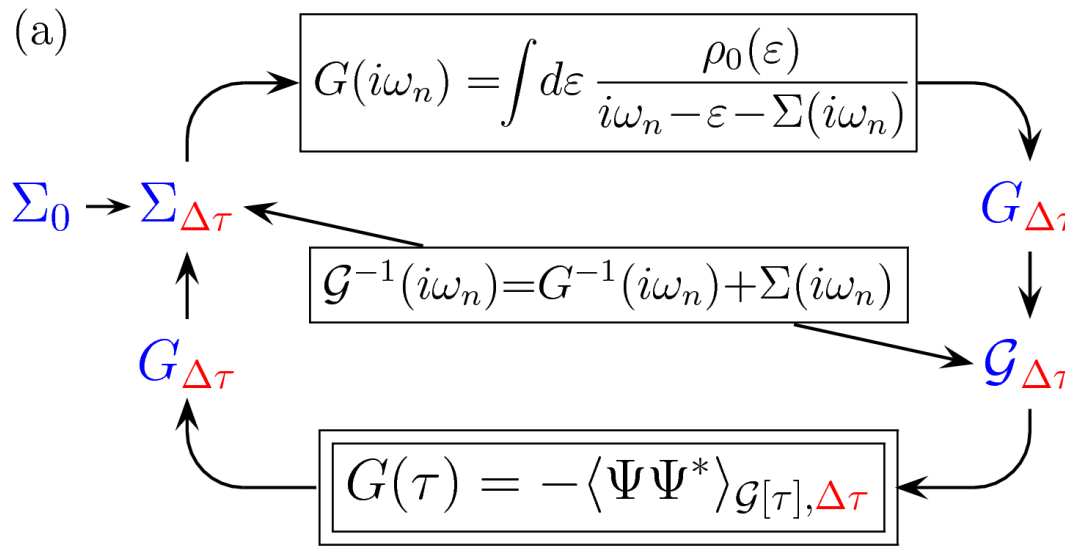
+ numerically exact, + no sign problem, – effort scales as T^{-3}
(density-type interactions)

Self-consistency cycle using conventional HF-QMC



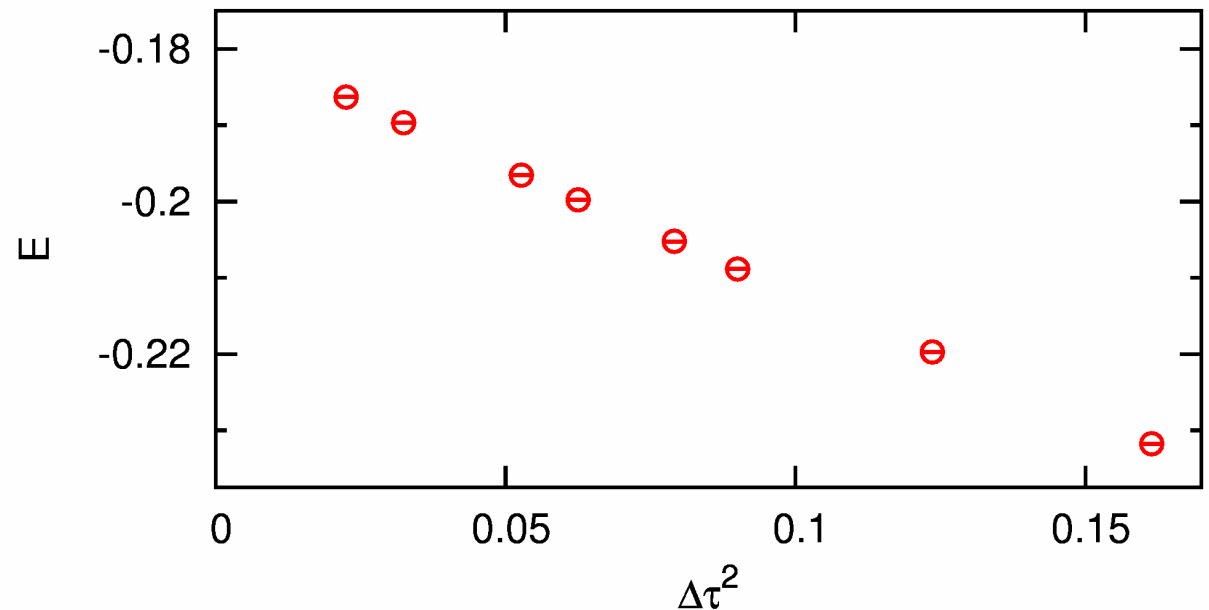
Extrapolation $\Delta\tau \rightarrow 0$ can improve accuracy of observable estimates by several orders of magnitude (\sim same cost)

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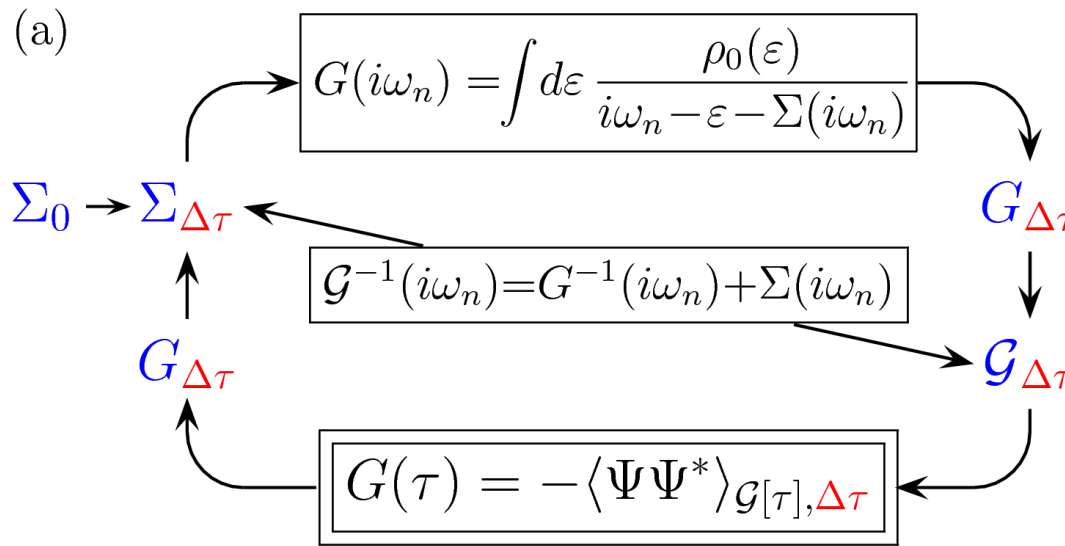


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Example: energy E for $U = W = 4$ (Bethe DOS), $T = 1/45$
 [NB, PRB (2007)]

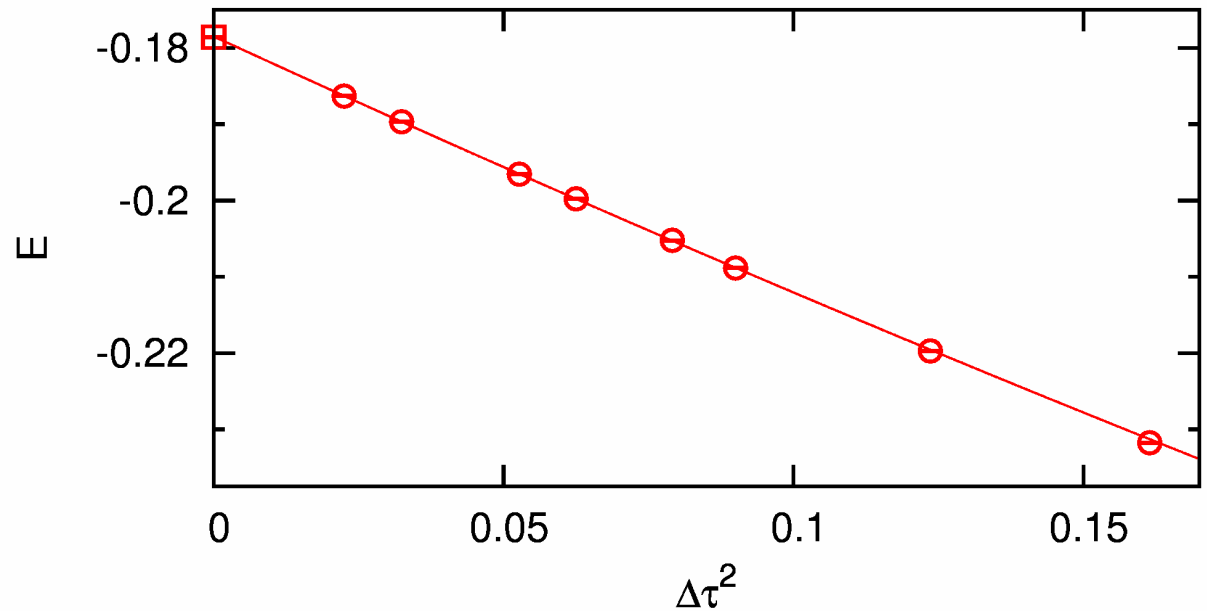


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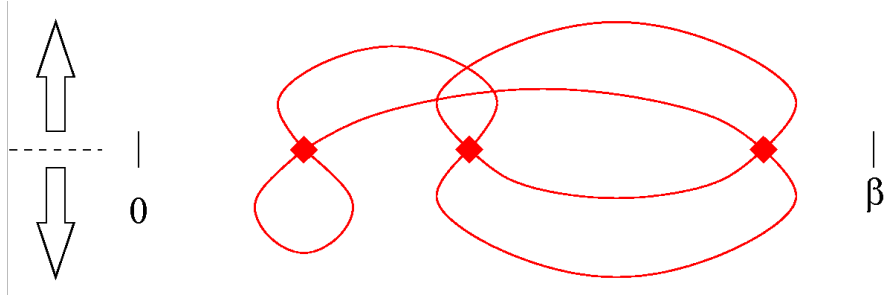
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New development: continuous-time QMC algorithms

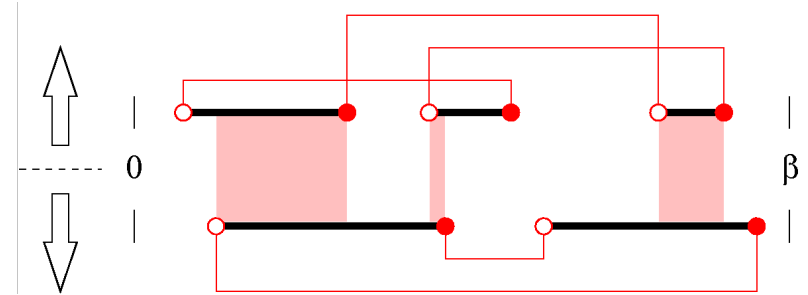
1. weak-coupling expansion

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



2. hybridization expansion

[Werner et al., PRL (2006)]

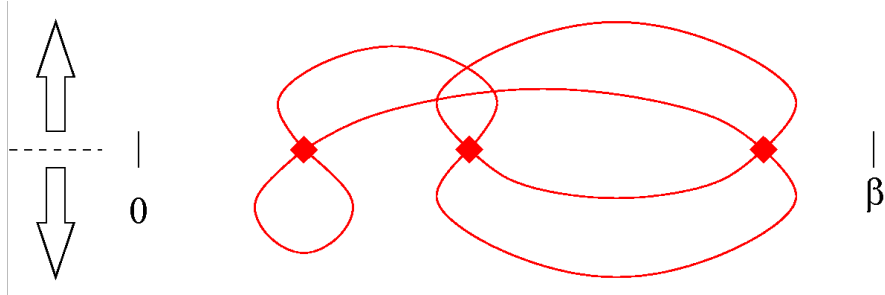


No systematic errors (in principle). Also more efficient than HF-QMC?

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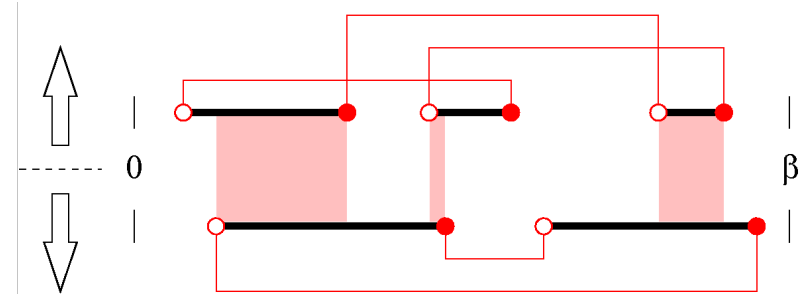
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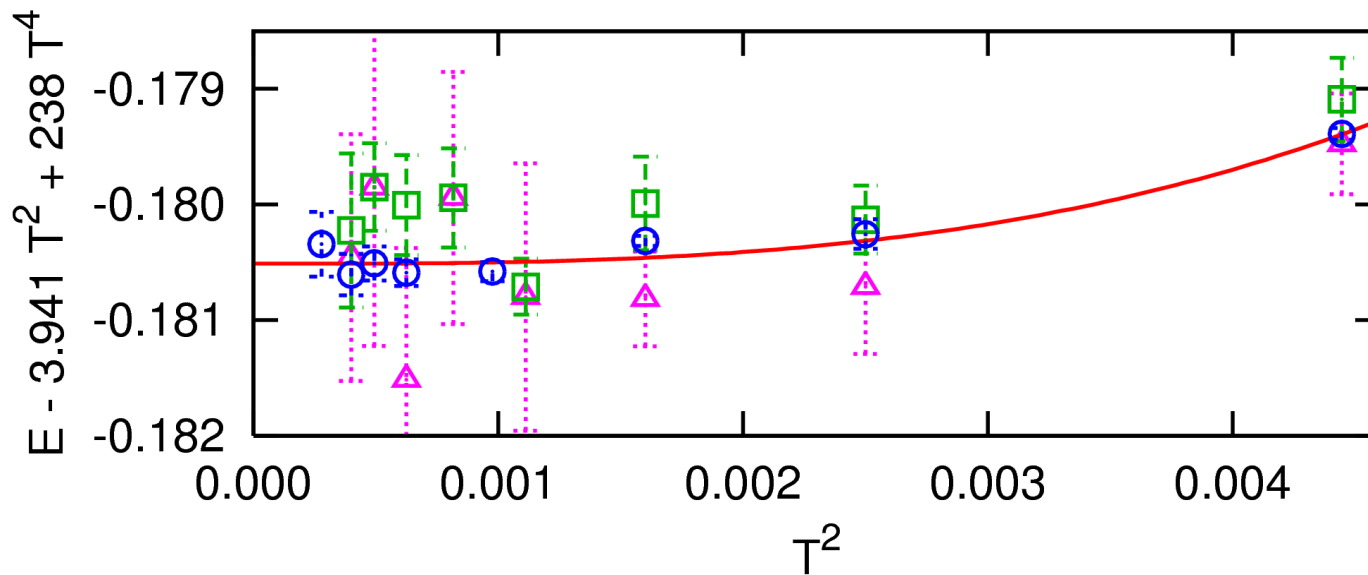


2. hybridization expansion

[Werner et al., PRL (2006)]



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



- 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)]

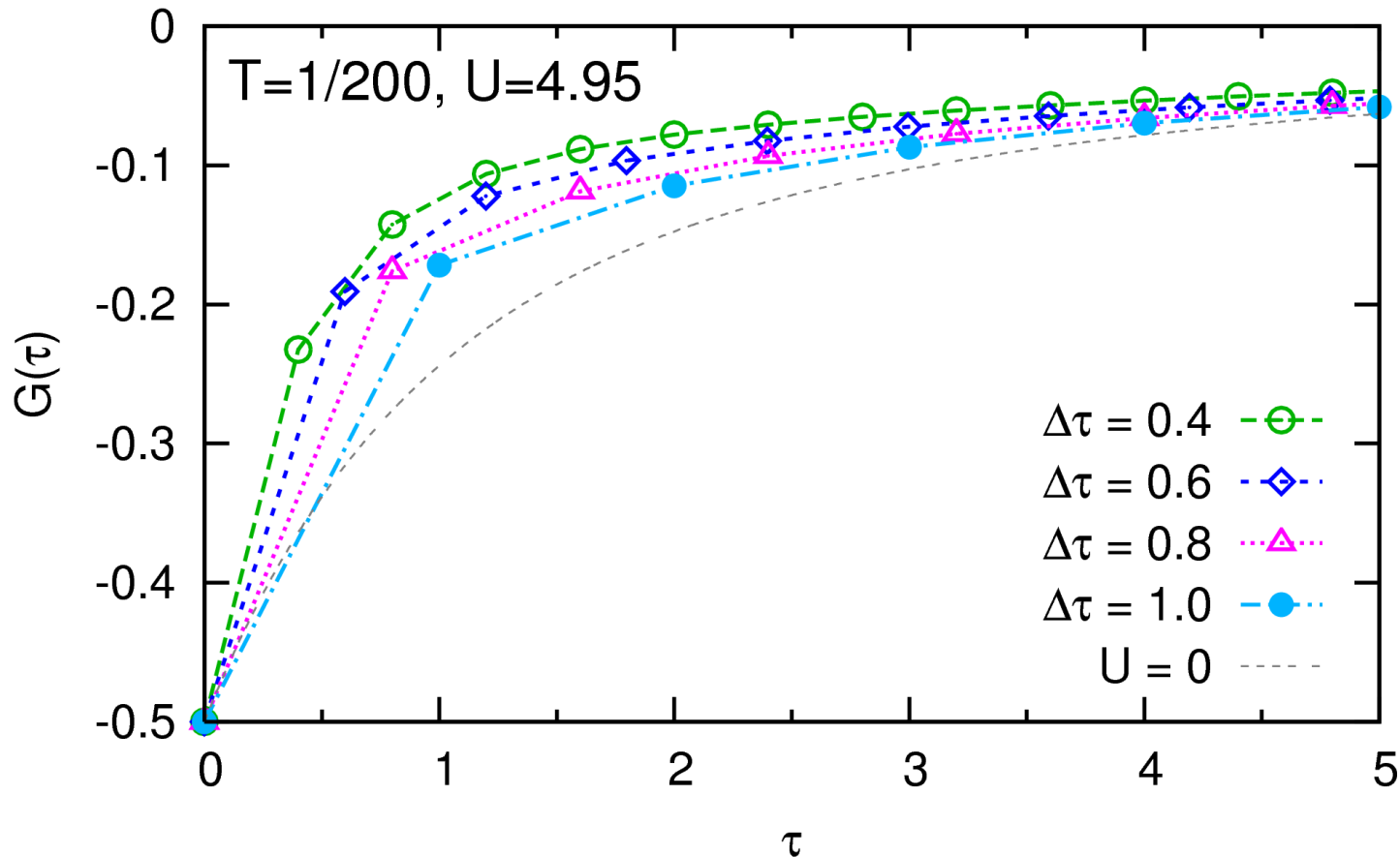
Unbiased Green functions and spectra from HF-QMC

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 $G(\tau)$

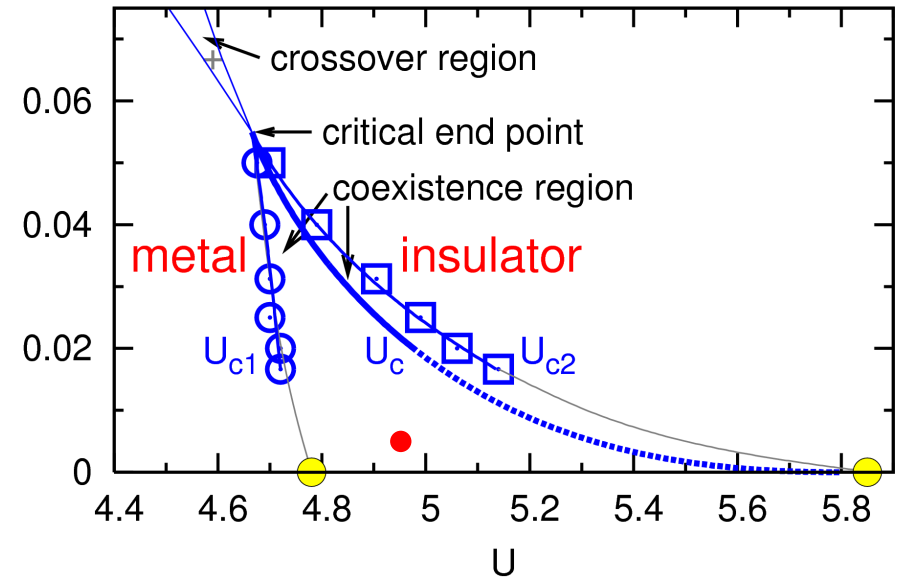
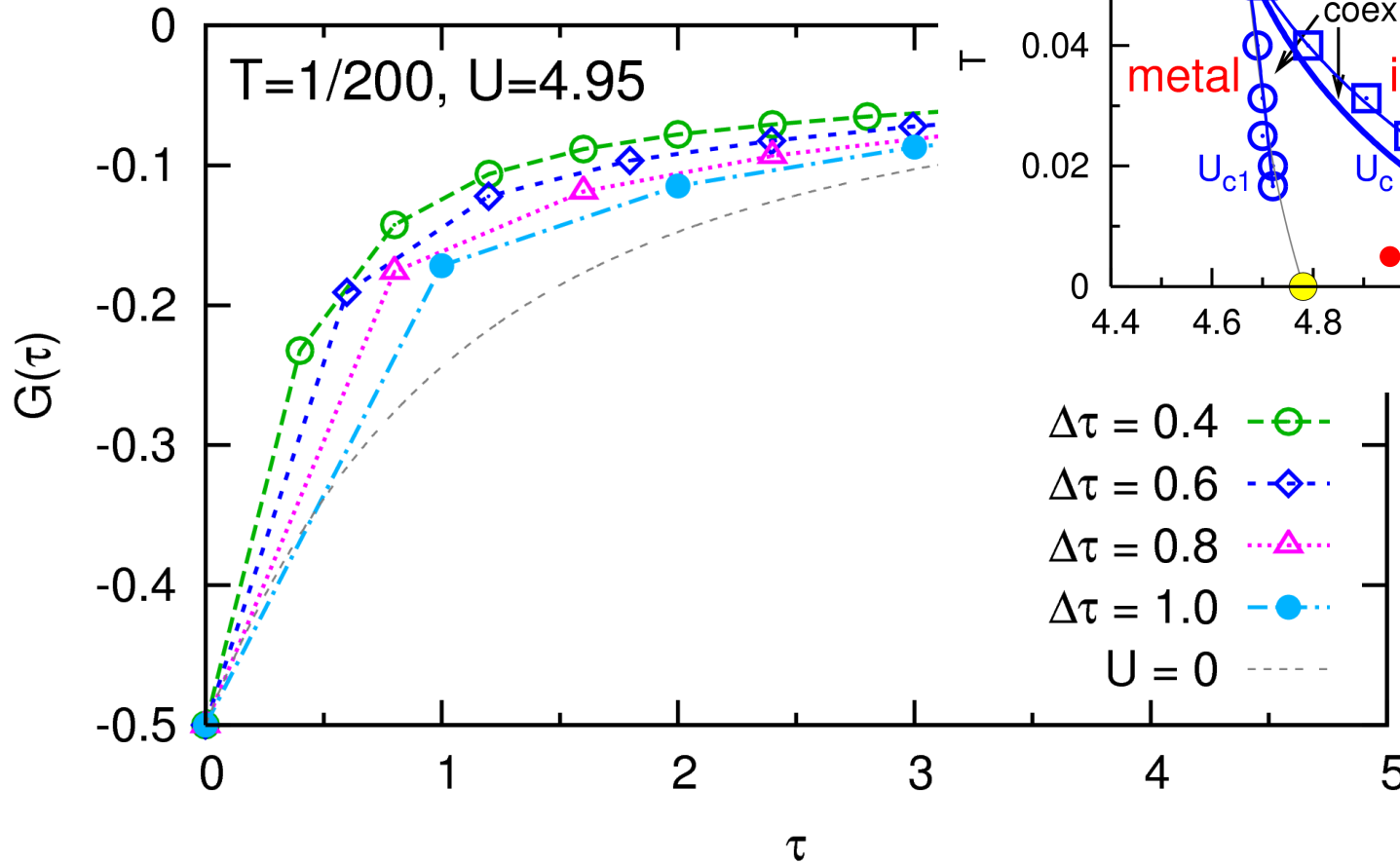


Low temperature (“beyond HF-QMC”): large $\Delta\tau \rightsquigarrow$ large biases [NB, arXiv:0712.1290]

Unbiased Green functions and spectra from HF-QMC

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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

\uparrow
weak-coupling expansion

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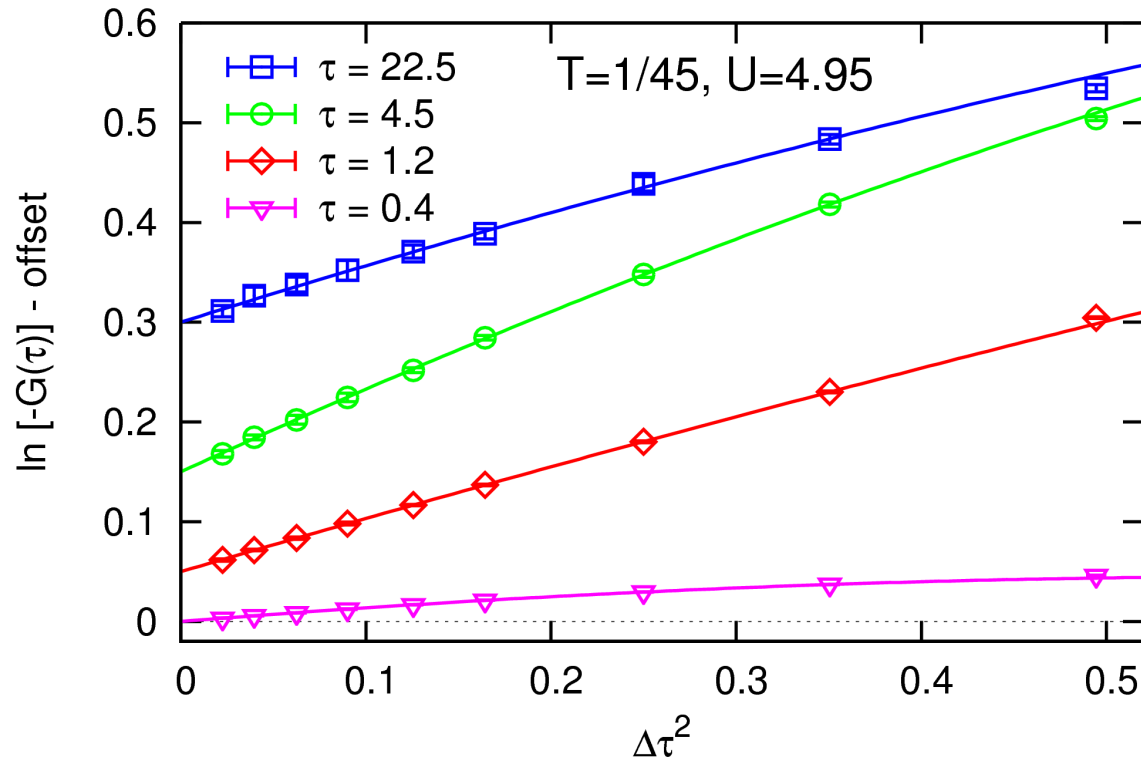
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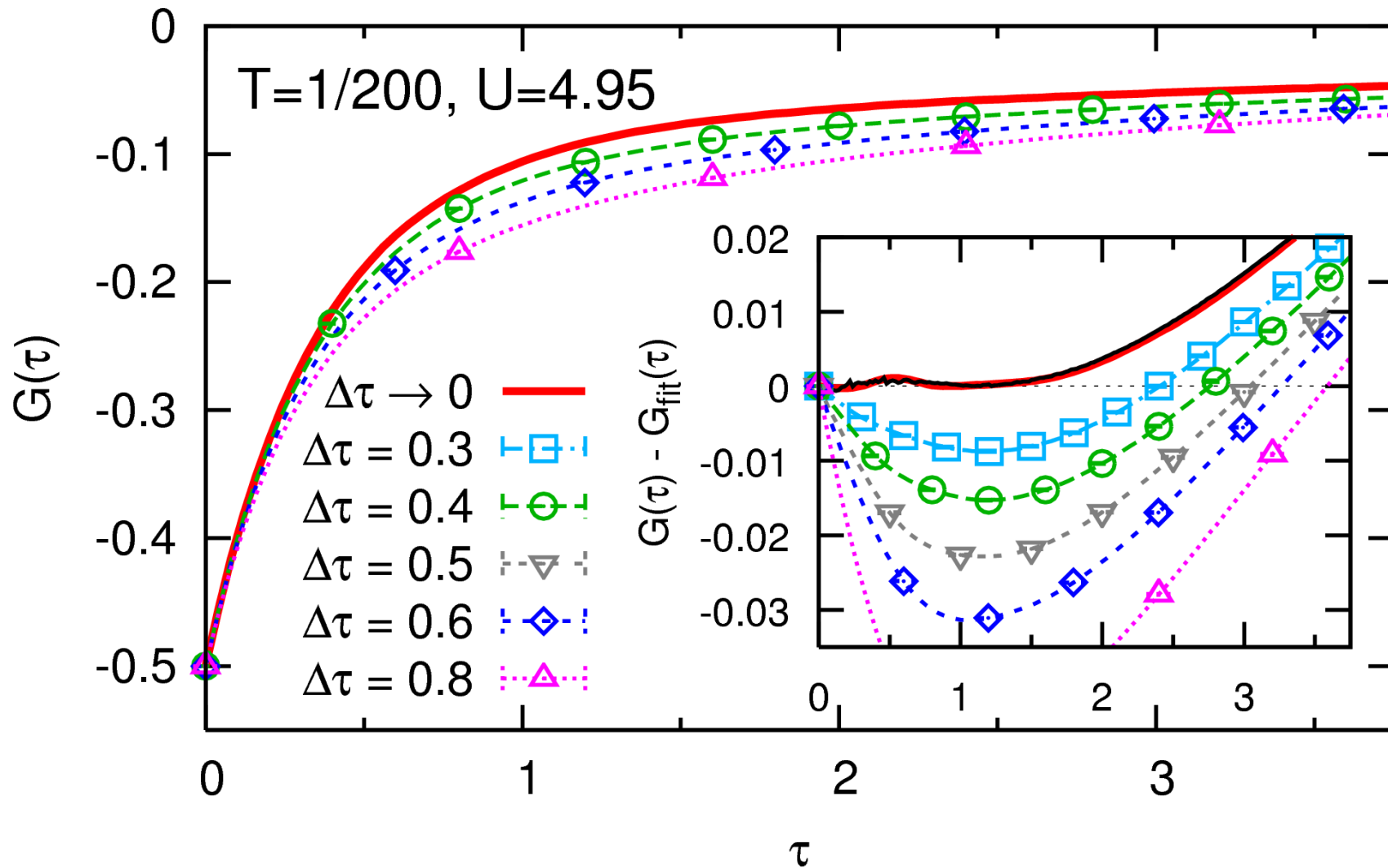
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• Extrapolate $\log[-G(\tau)]$ using cubic least-squares fits



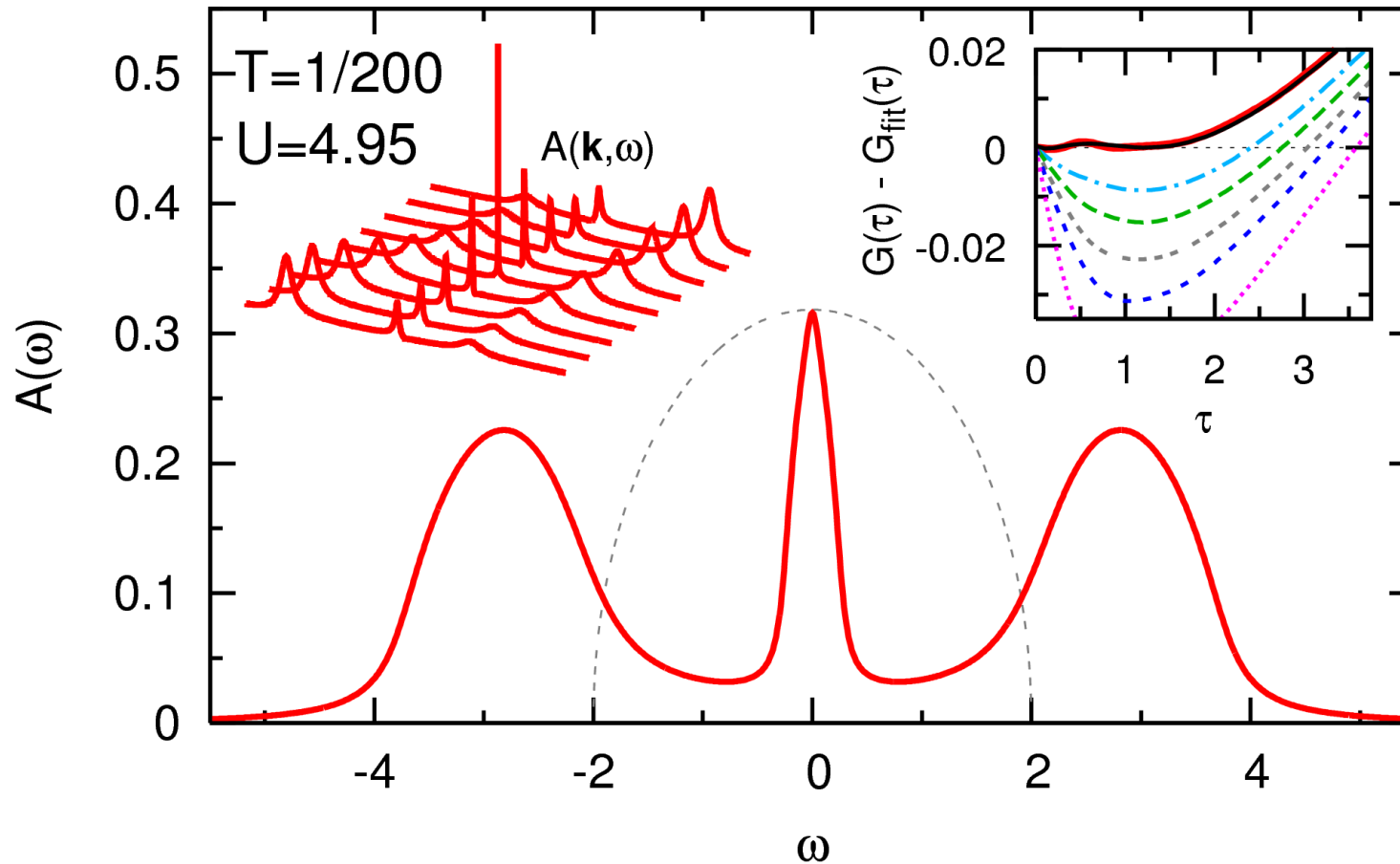
Result: unbiased, numerically exact Green function



[NB, arXiv:0712.1290]

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

Analytic continuation using Padé approximant for self-energy



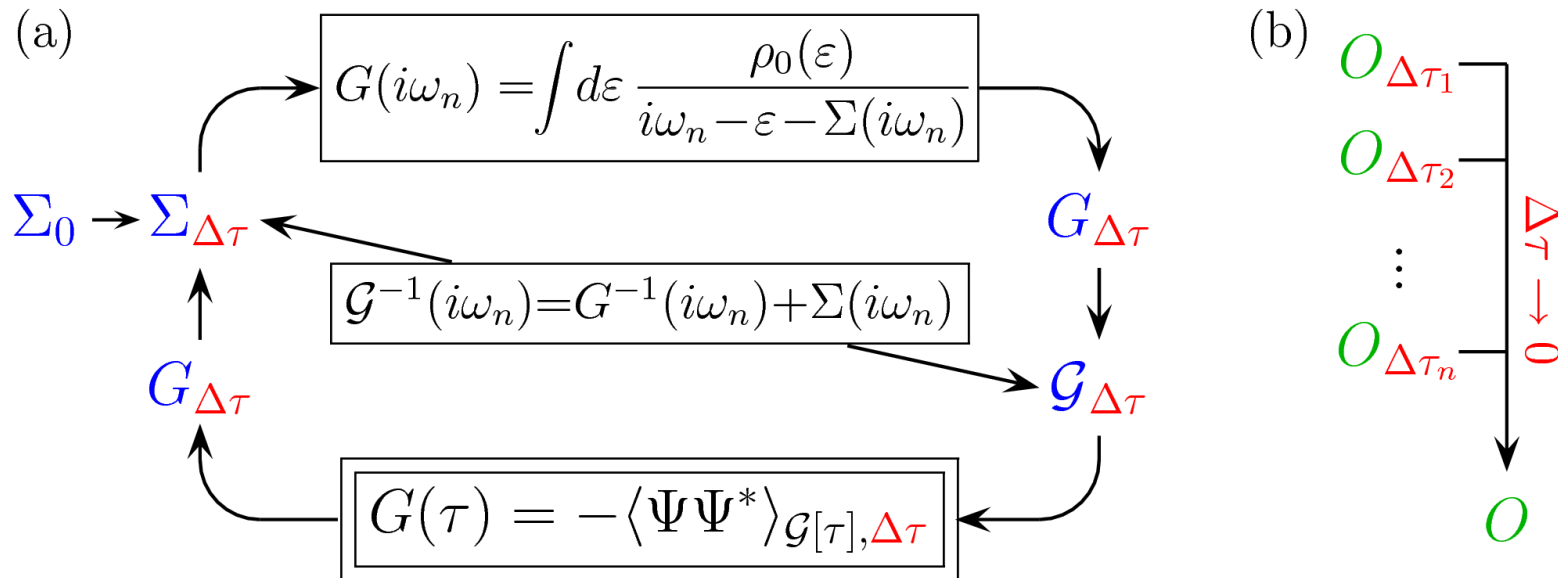
First spectra without discretization error from HF-QMC, at ultra-low T

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

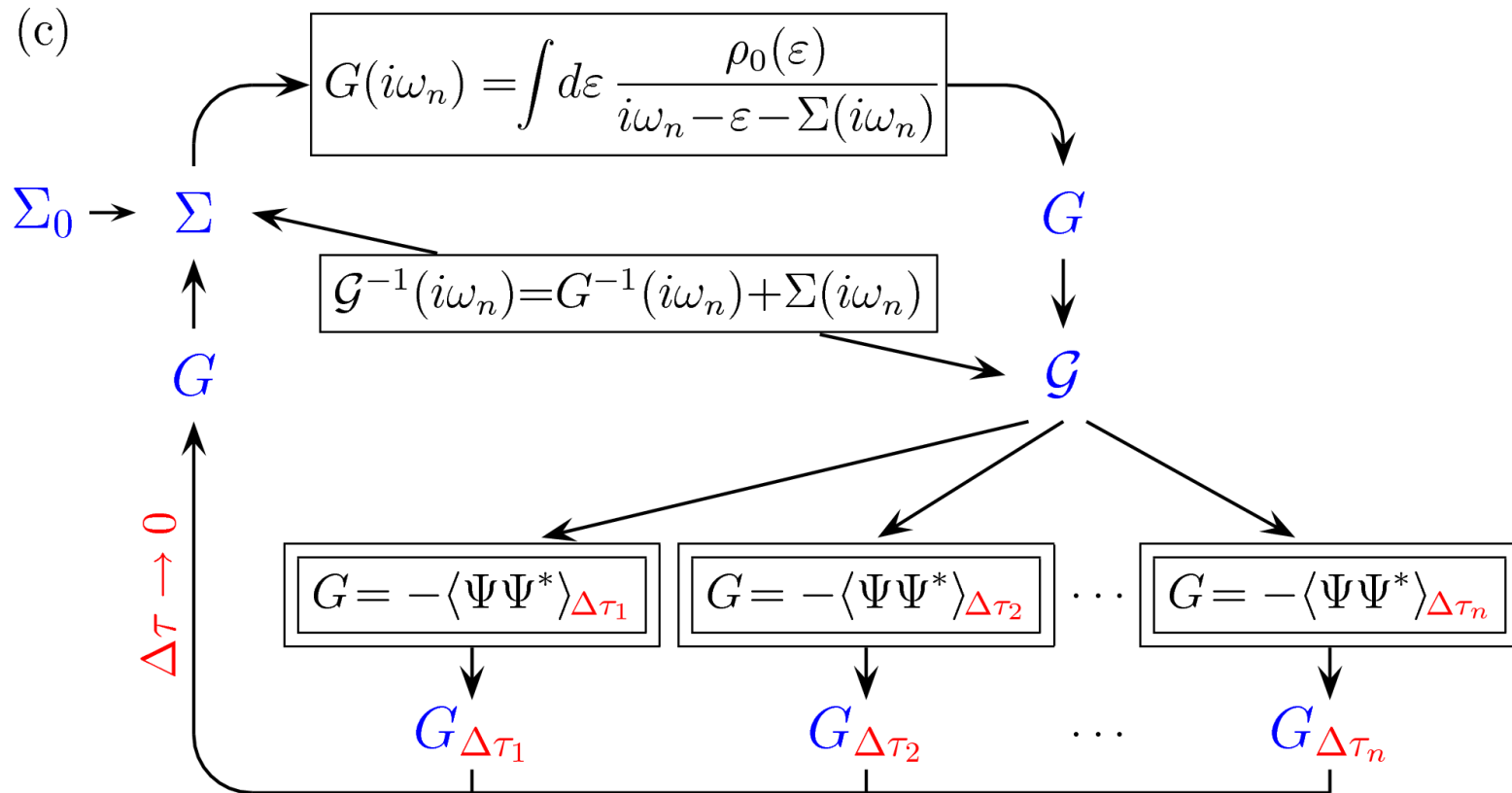
(b) *a posteriori* extrapolation of selected observables



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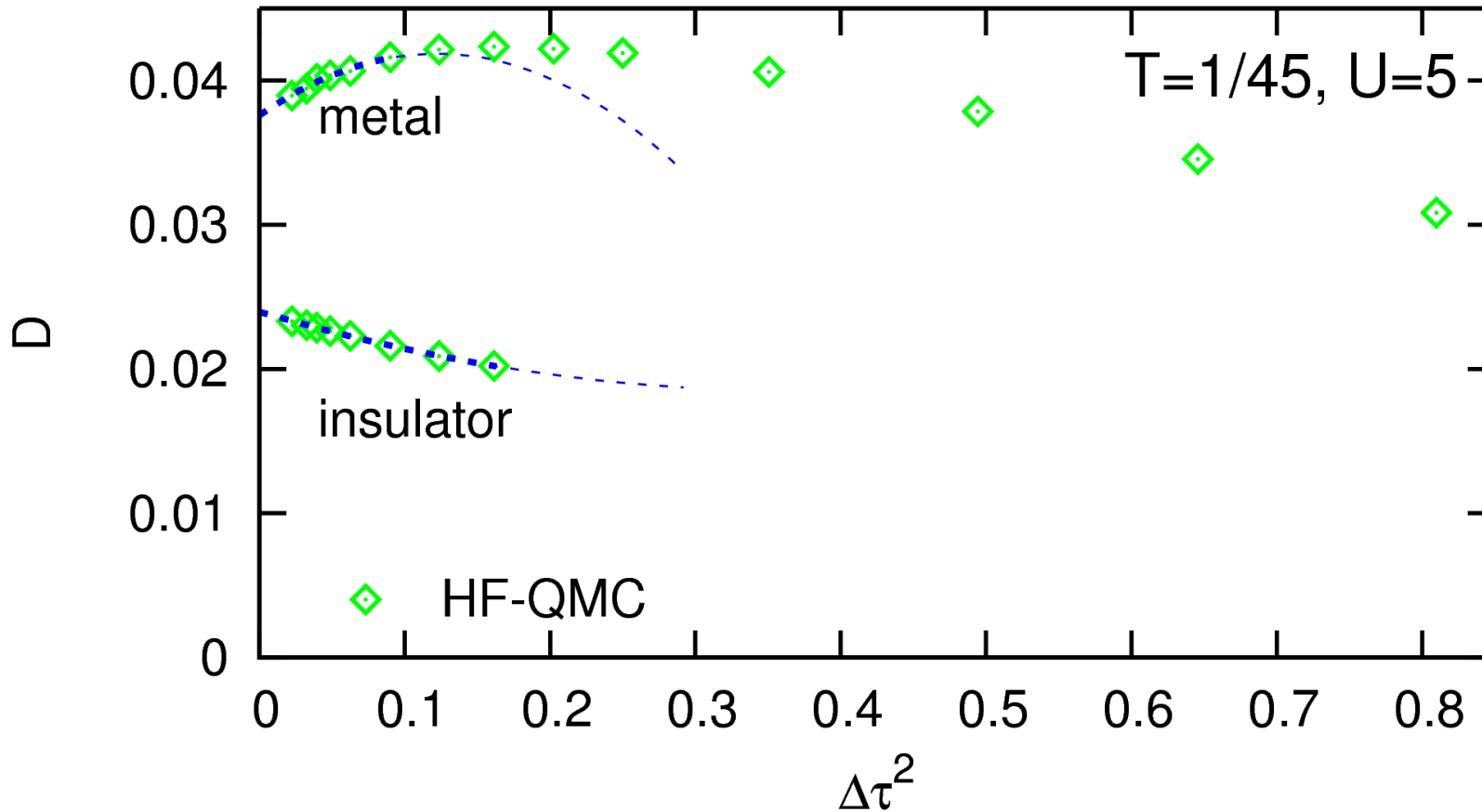
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(c) Multigrid HF-QMC: internal elimination of Trotter error

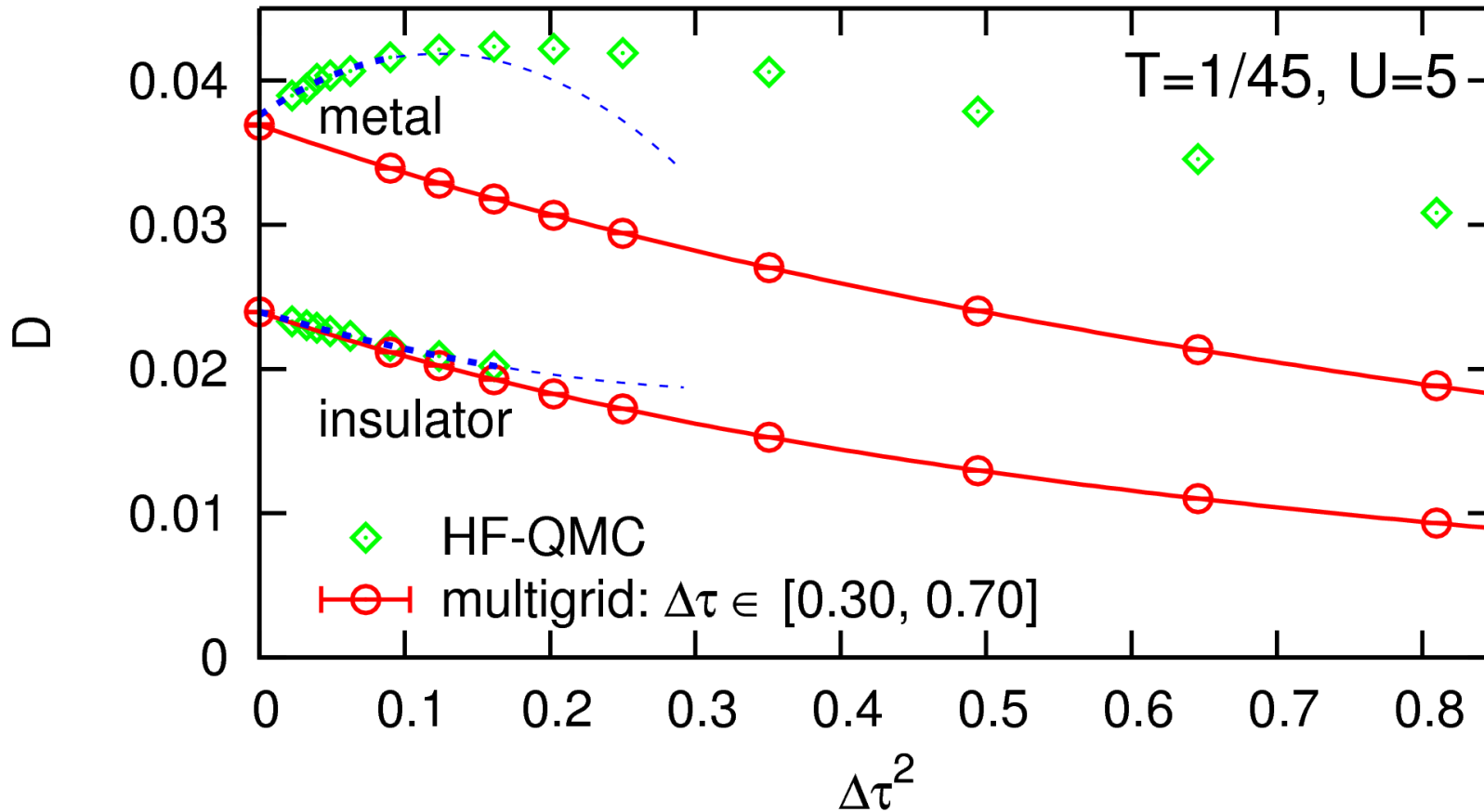
\rightsquigarrow quasi continuous time algorithm [NB, [arXiv:0801.1222](https://arxiv.org/abs/0801.1222)]

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



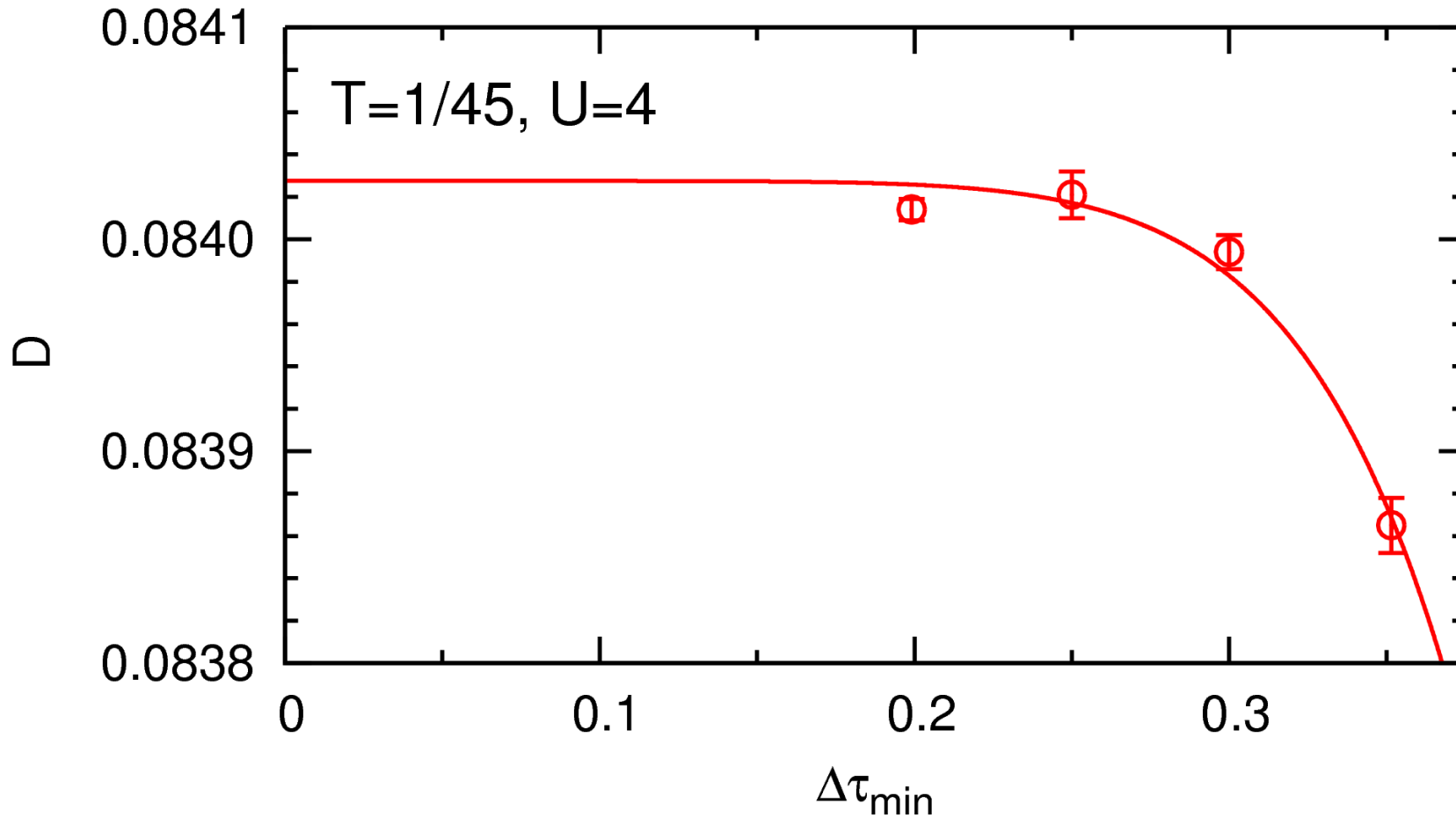
Conventional HF-QMC: no insulating solution for $\Delta\tau \gtrsim 0.4$
very irregular $\Delta\tau$ dependence beyond $\Delta\tau \approx 0.3$

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- 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 $\Delta\tau$

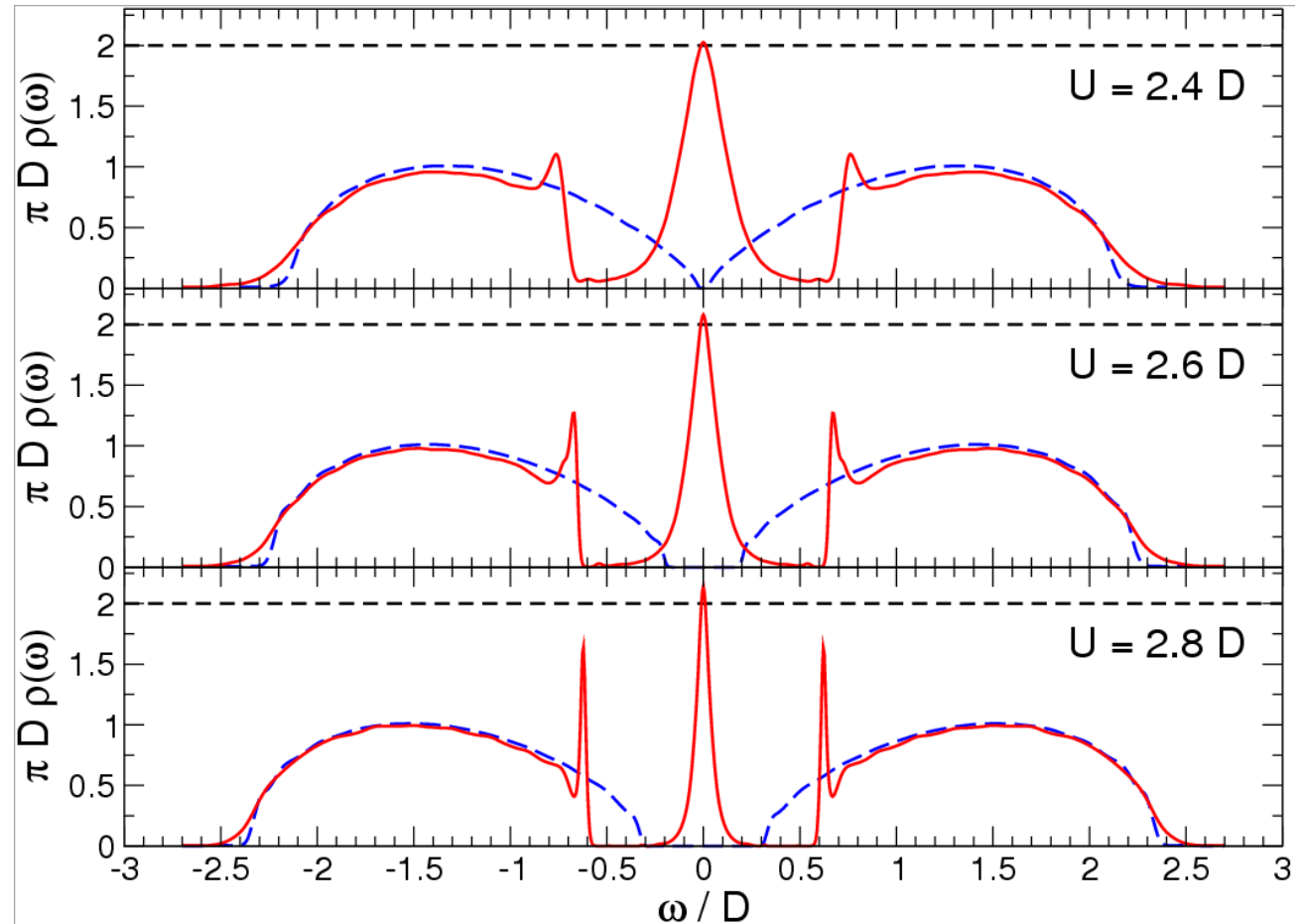
Systematic study: impact of grid range $[\Delta\tau_{\min}, \Delta\tau_{\max}]$



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

Spectral weight transfer at the Mott transition

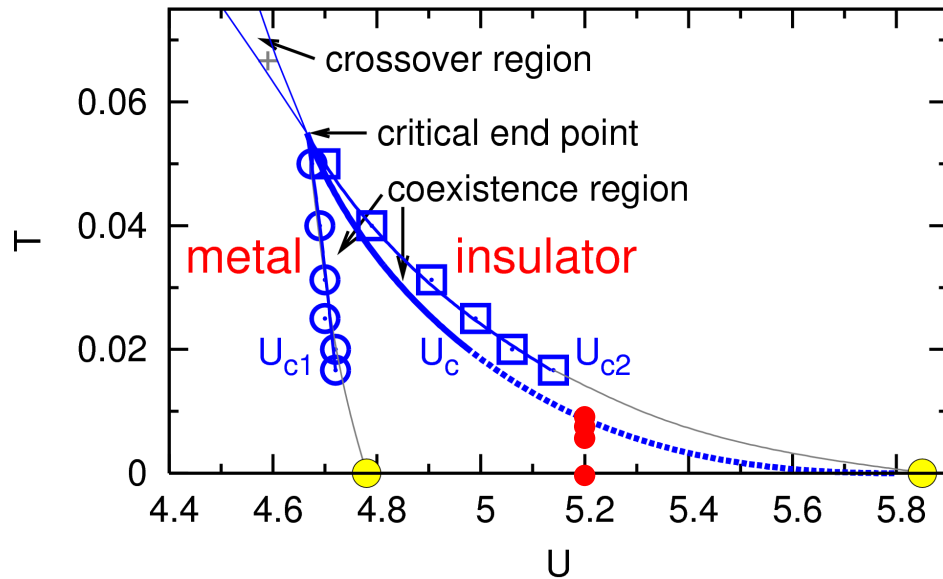
Question: how does the Mott metal-insulator transition take place, precisely?



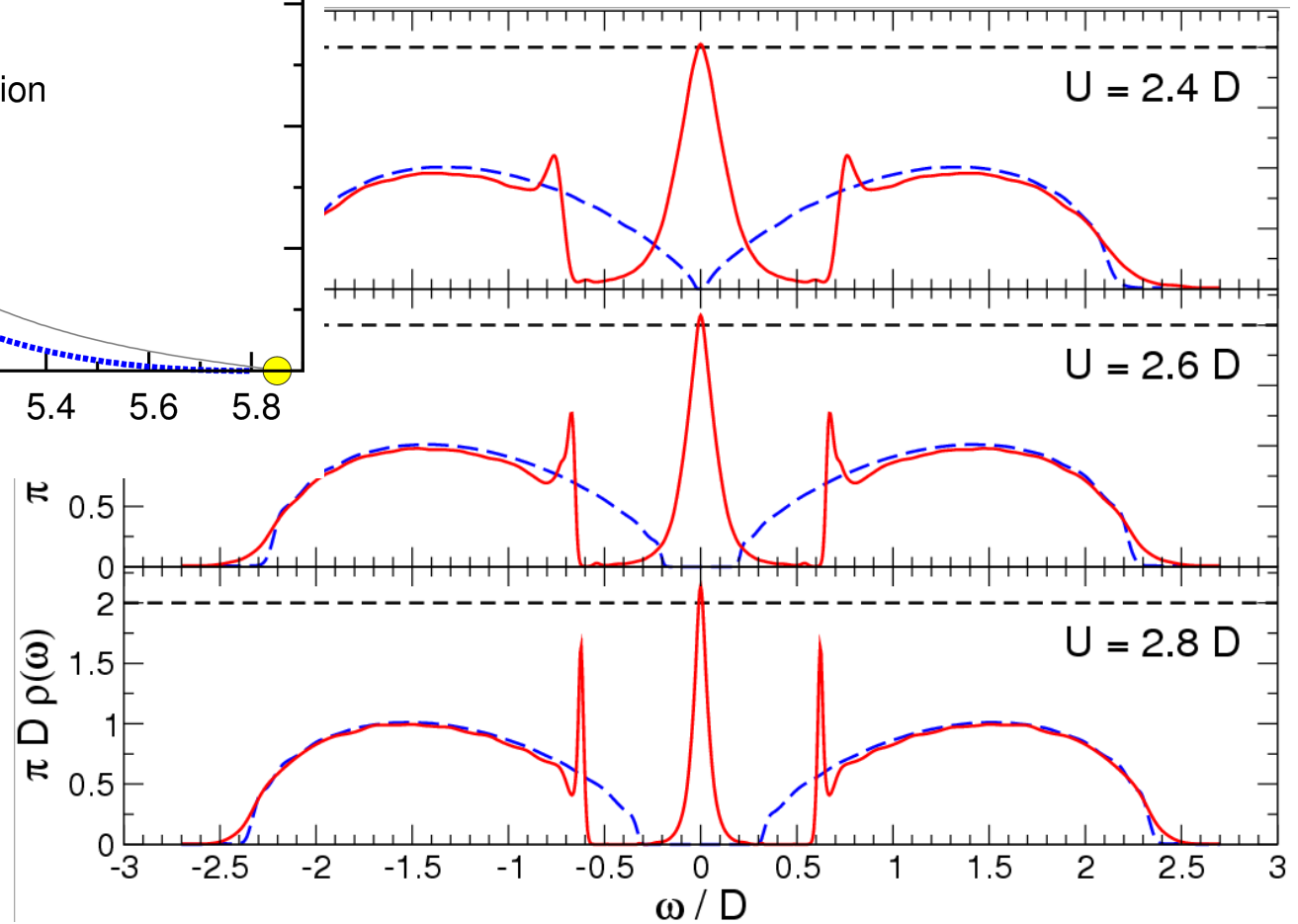
Dynamical DMRG \rightsquigarrow Hubbard band subpeaks in metallic phase (at $T = 0$)

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

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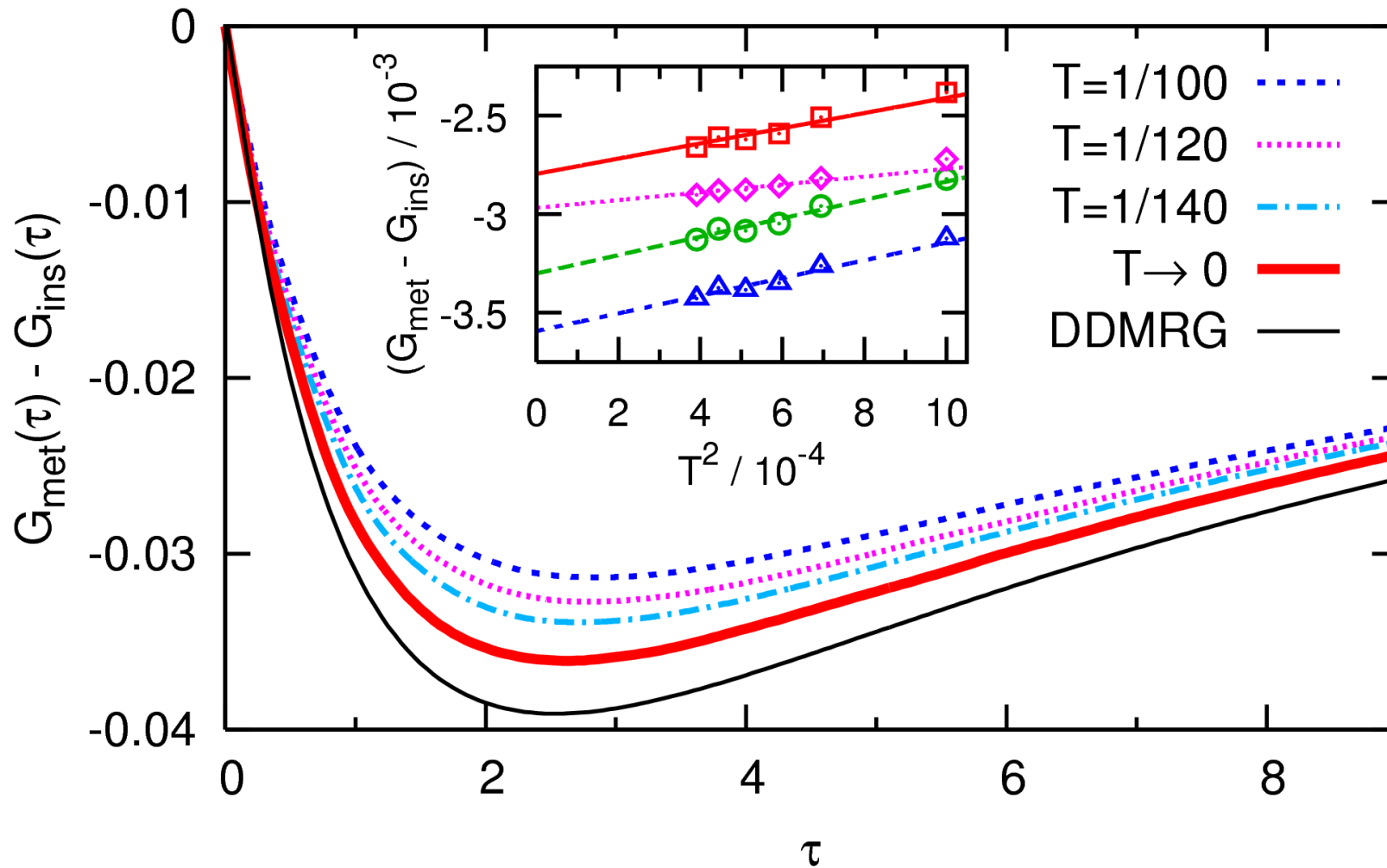


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Check using multigrid HF-QMC...

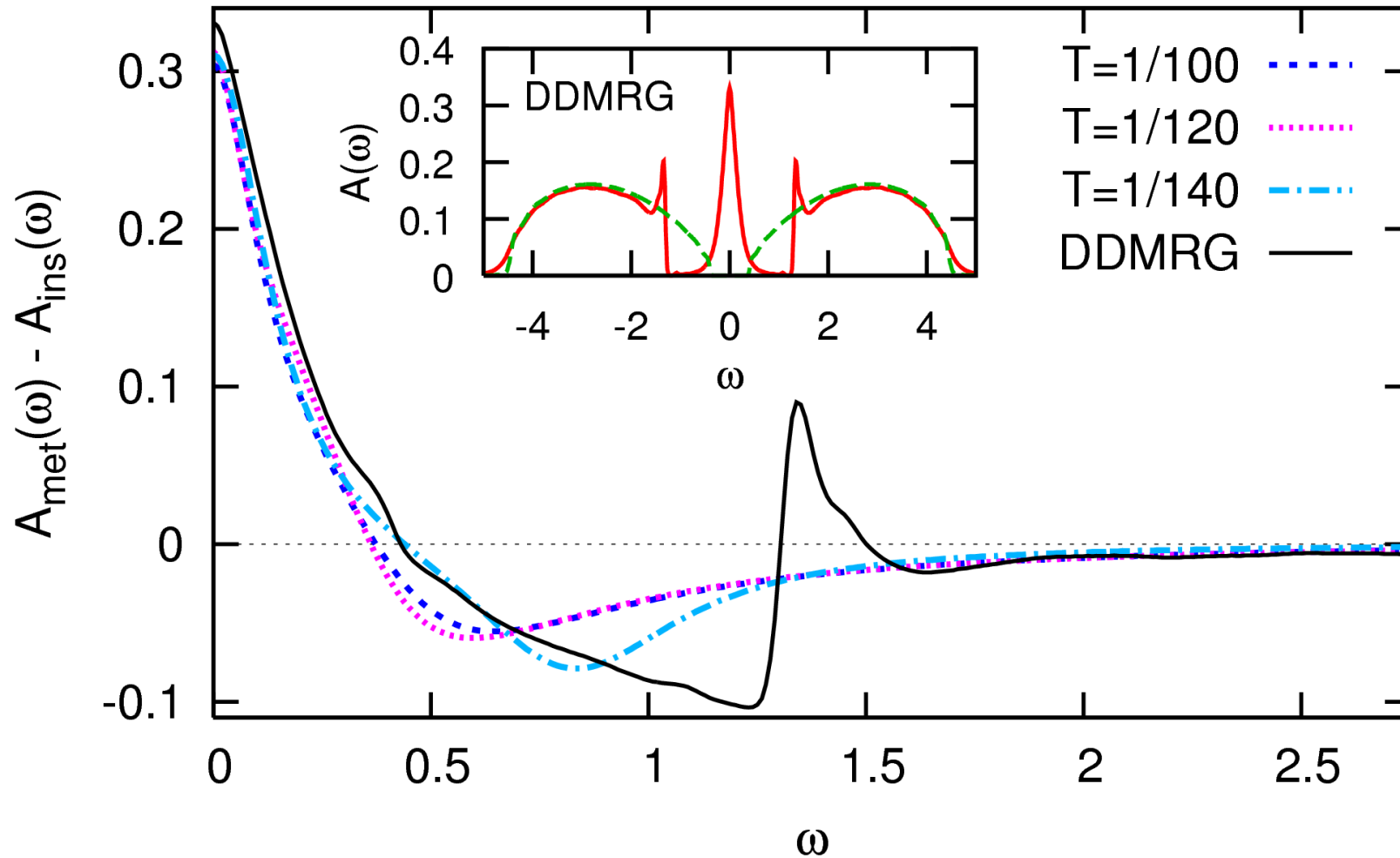
Difference Green functions in imaginary time



Multigrad 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 [NB, arXiv:0801.1222]

Thermal breakdown of a Fermi liquid

Fermi liquid theory: linear specific heat $c_V = \gamma T$
linear entropy $S = \gamma T$
quadratic resistivity $\rho \propto T^2$ for “low enough” T

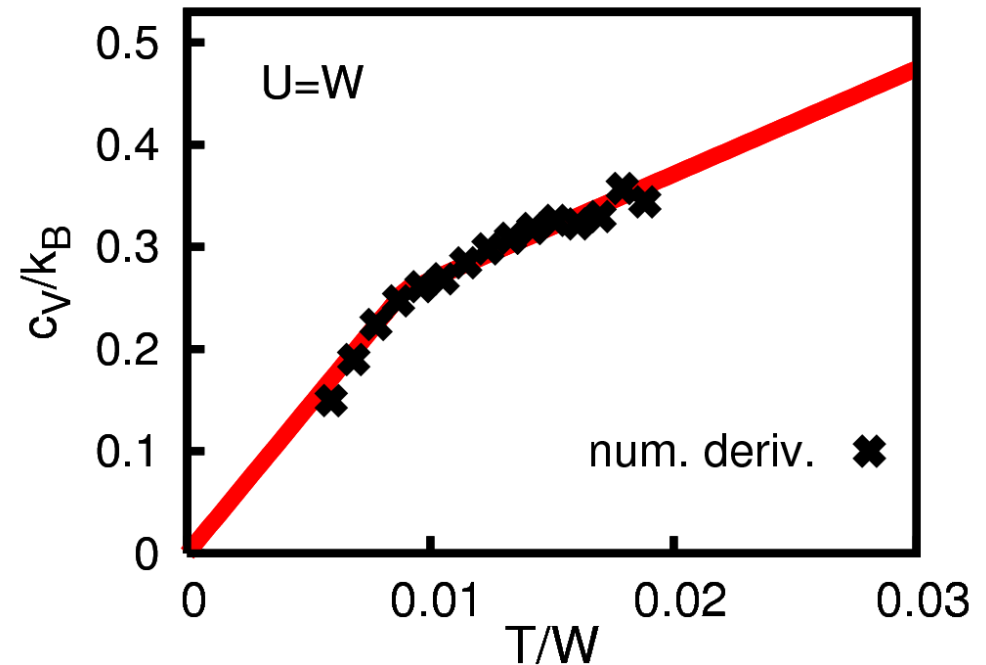
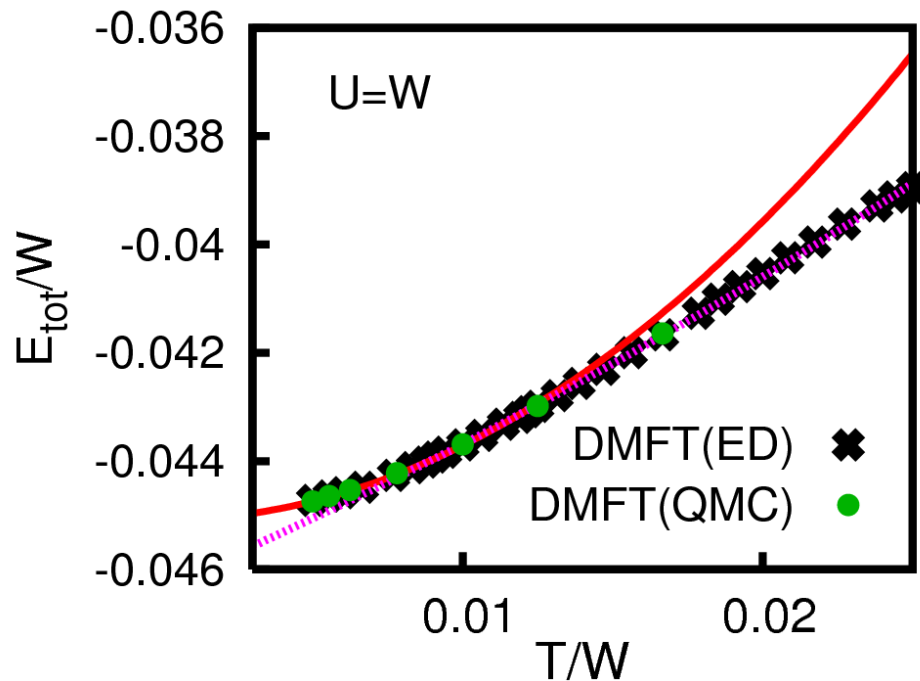
When/how do these laws break down?

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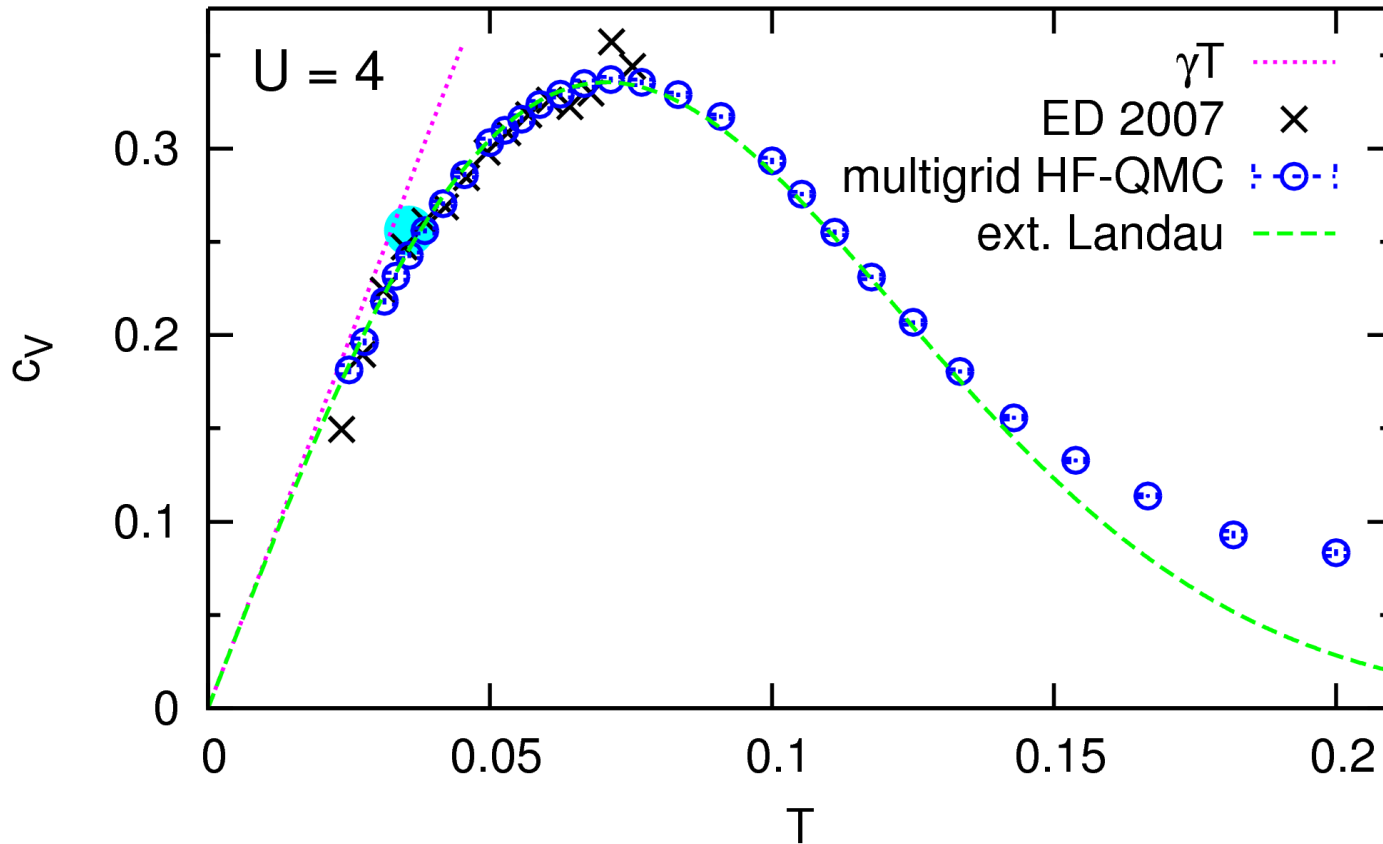
When/how do these laws break down?

Exact diagonalization study (8 sites) for 1-band Hubbard model



Distinct kink in c_V !

[A. Toschi, M. Capone, C. Castellani, K. Held, [arXiv:0712.3723](https://arxiv.org/abs/0712.3723)]



High-precision results \rightsquigarrow no kink!

Full agreement of (multigrid) HF-QMC with **extended Landau** theory (parameter: Z)

$$c_V(T) = \frac{2\pi}{3Z} T \exp \left[- (T/T_0)^2 \right]; \quad T_0 = \frac{3 \log(2)}{\pi^{3/2}} Z \quad (\text{Bethe DOS})$$

Summary

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

Quasi continuous time \rightsquigarrow strictly “numerically exact”

Stable and precise even at phase boundaries

More efficient, reaches lower T

Spectral weight transfer at the Mott transition

Thermal breakdown of a Fermi liquid

Not shown: arbitrary filling, multiple bands . . .

Outlook: flavor-selective Mott transitions in ultracold quantum gases

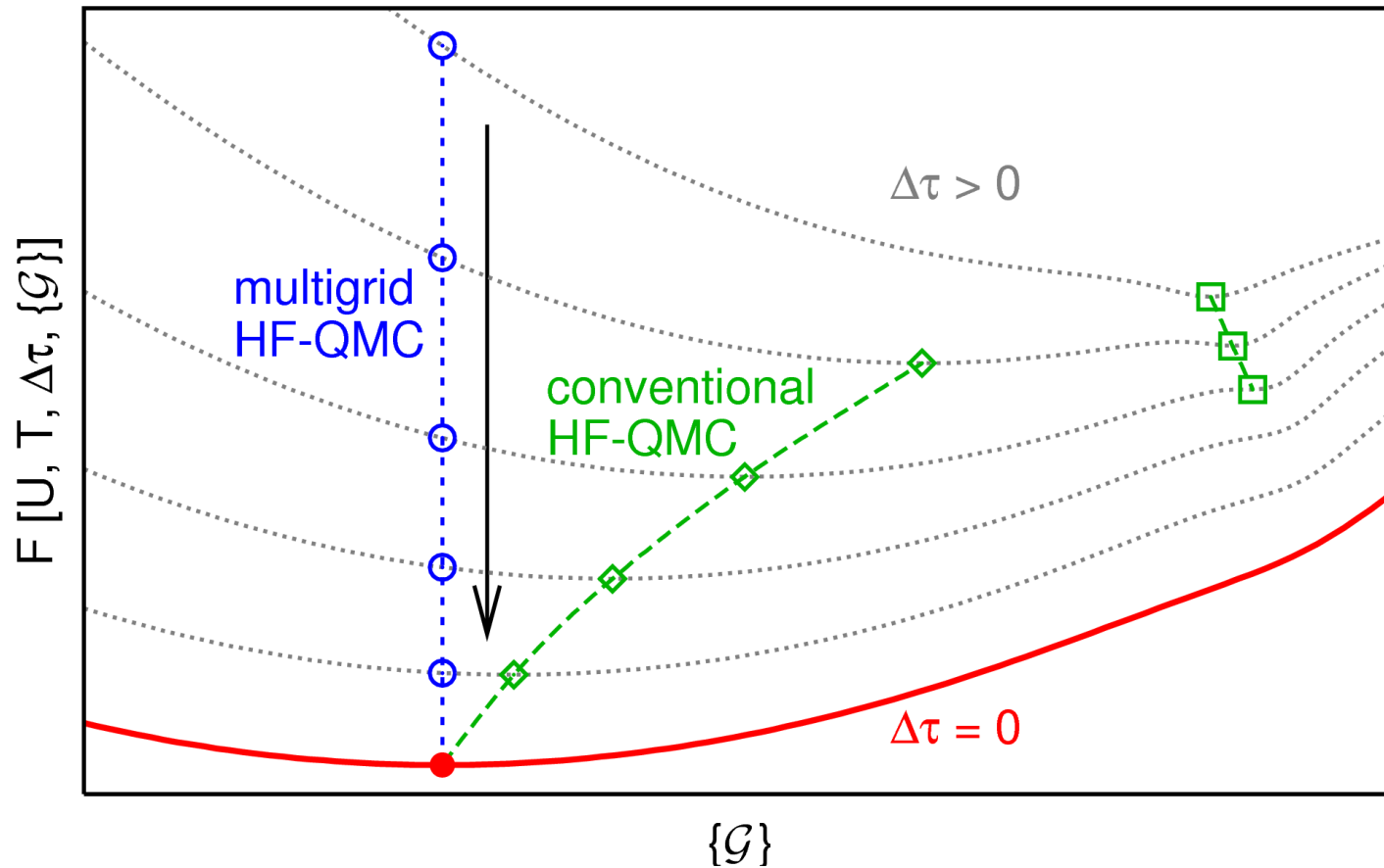
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Schematic comparison via generalized Ginzburg-Landau functionals

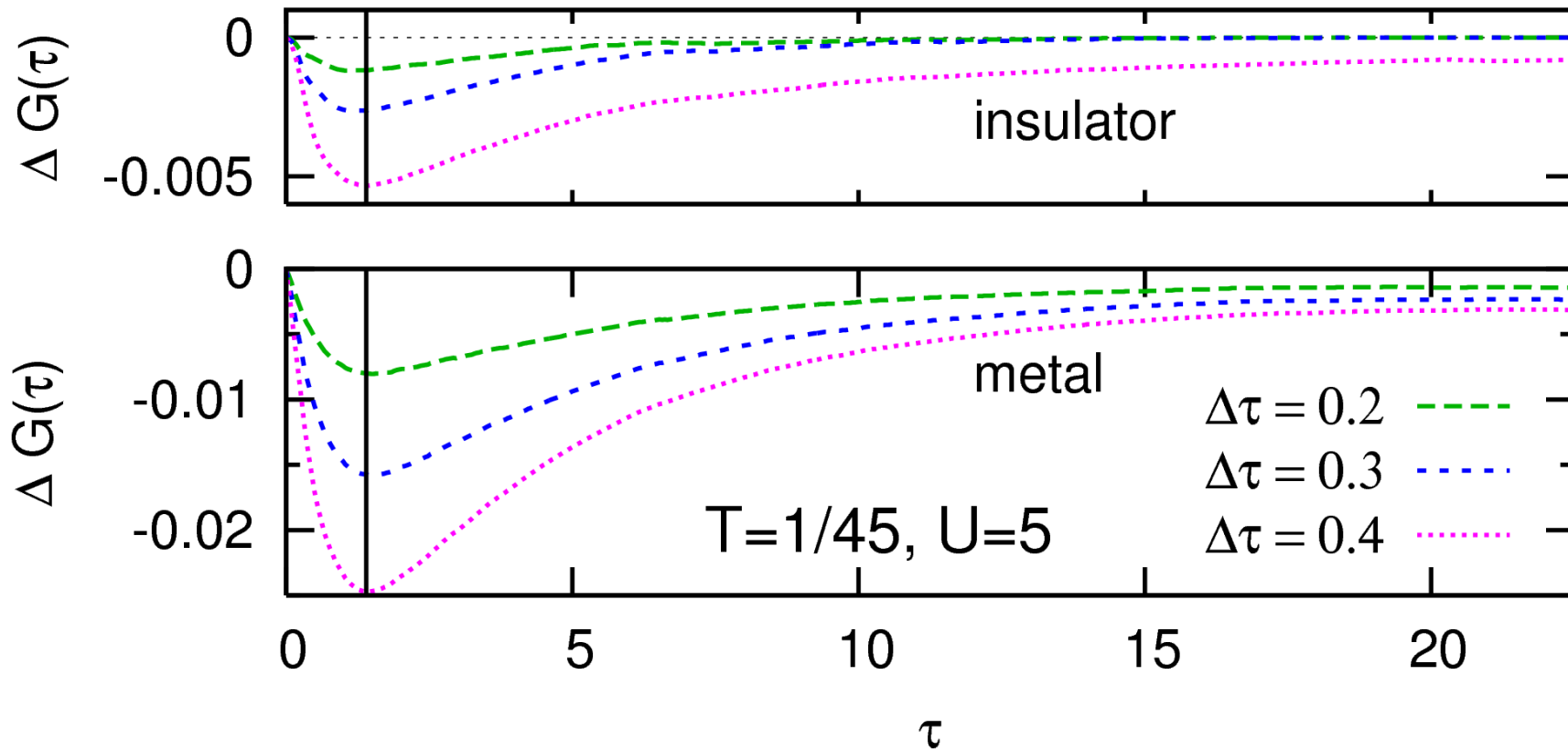


Conventional Hirsch-Fye QMC: DMFT fixed point shifts with $\Delta\tau$

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

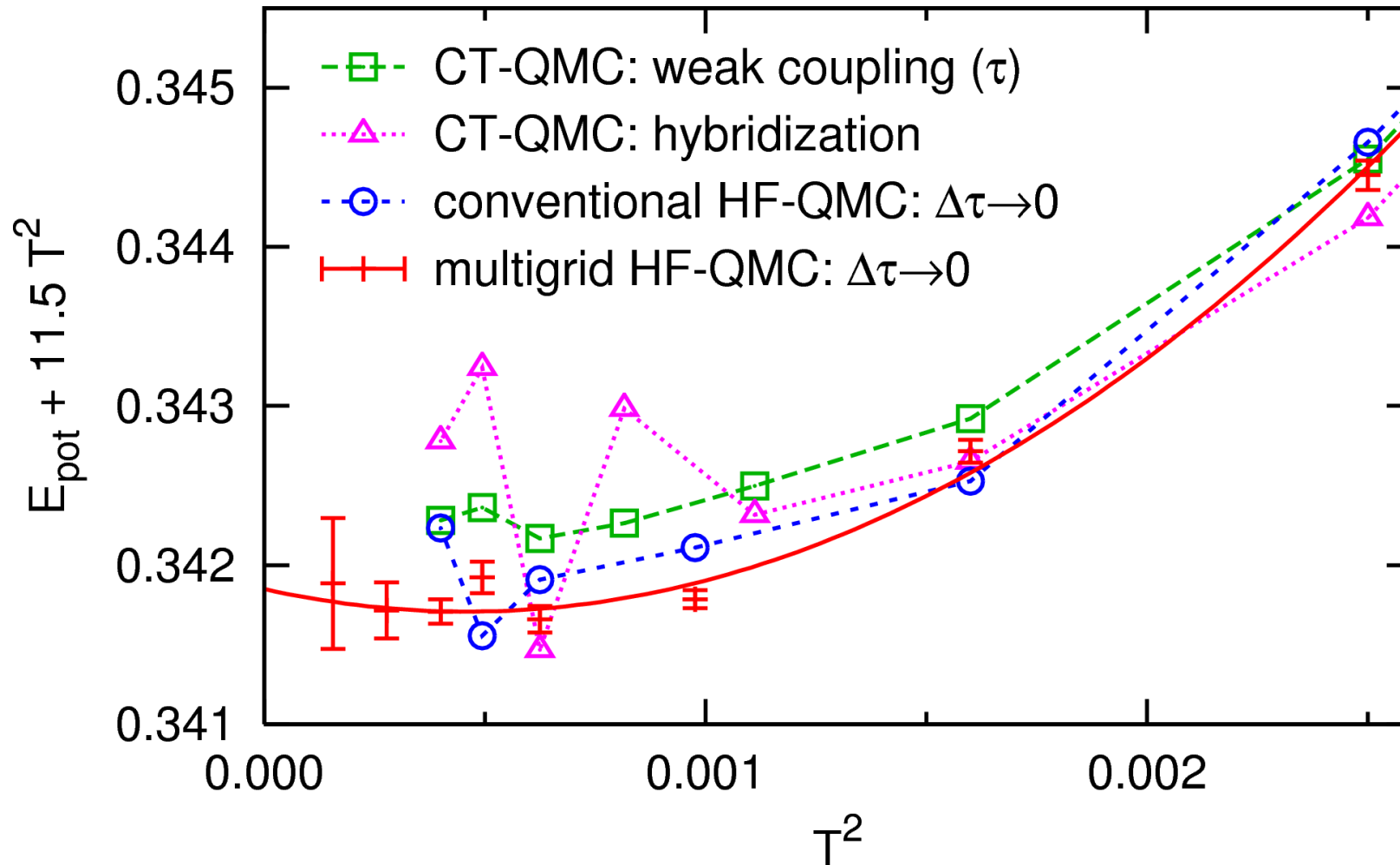
Implementation: Green function extrapolation, hierarchy of frequency scales, . . .

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