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

Applications: spectral-weight transfer, specific heat

Summary

Introduction

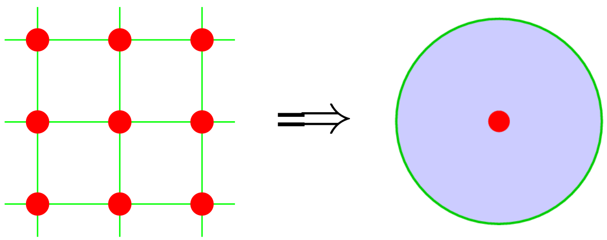
Target: Hubbard-type models $\hat{H} = \sum_{(i,j),\sigma} t_{ij} \, (\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$

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

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



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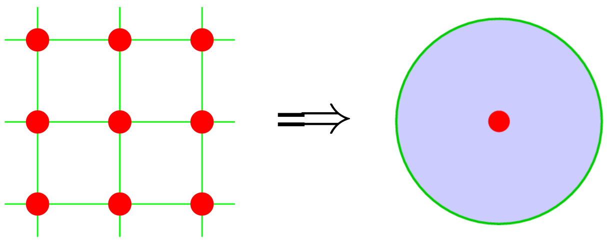

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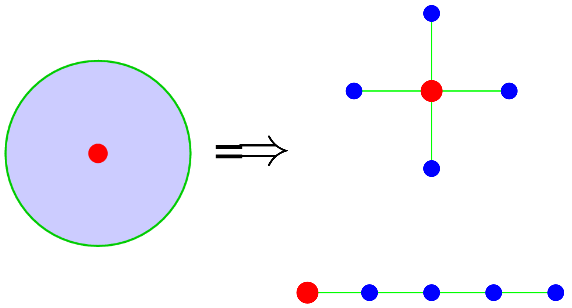
Numerically exact impurity solvers:

- 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^*):

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

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

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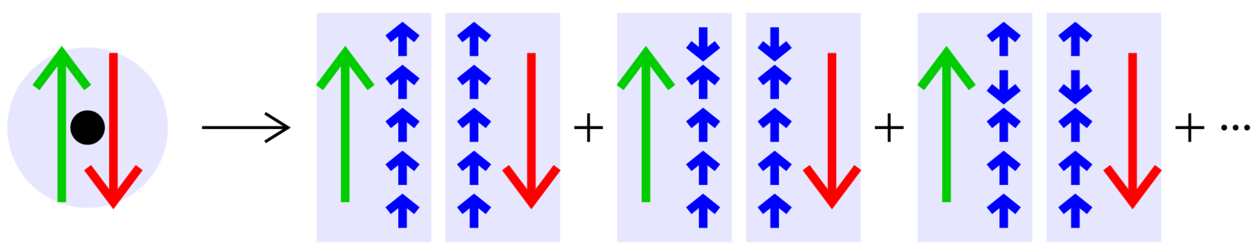
(iii) Hubbard-Stratonovich transformation



Wick theorem:

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

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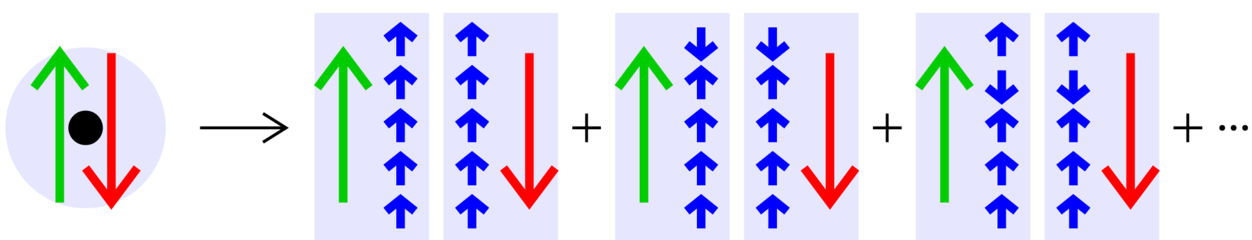

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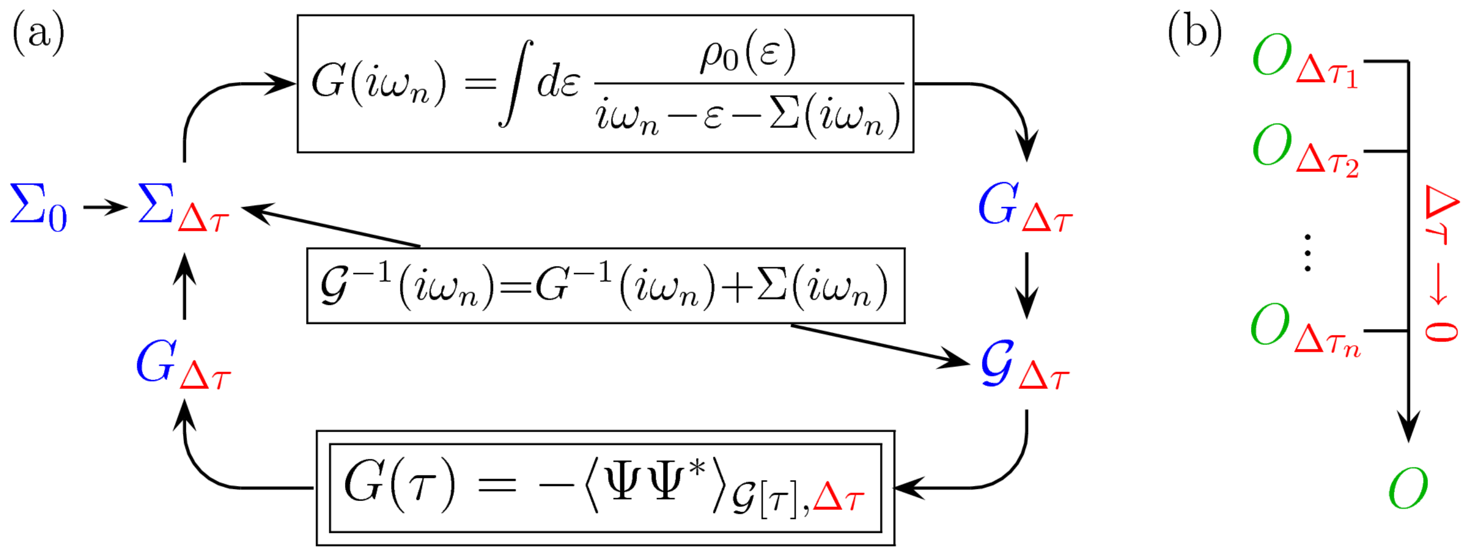
(iv) MC importance sampling over auxiliary Ising field $\{s\}$: 2^Λ configurations

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

(density-type interactions)

Self-consistency cycle using conventional HF-QMC



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

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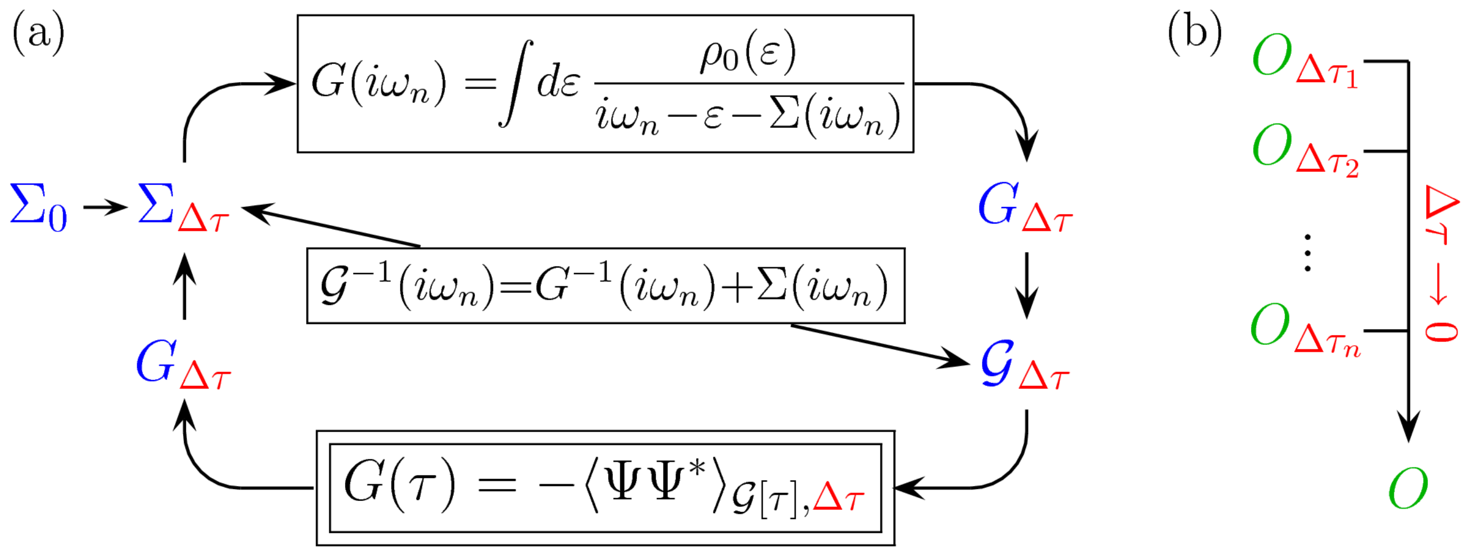

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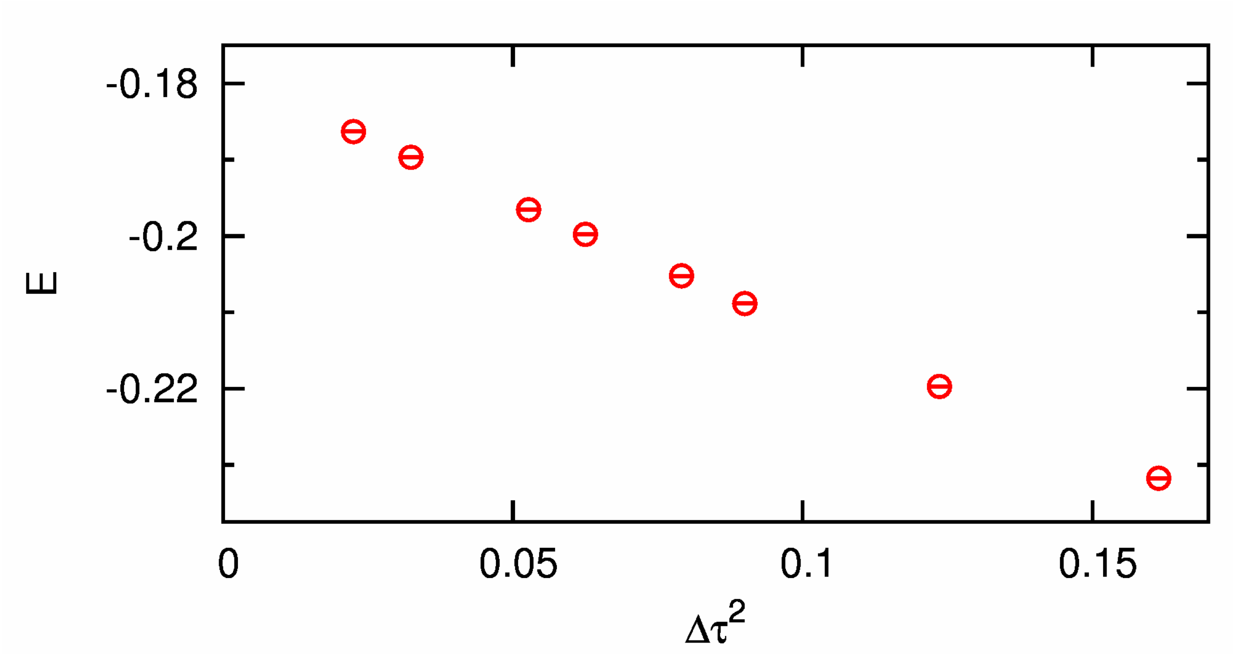
Example: energy E for $U = W = 4$ (Bethe DOS), $T = 1/45$ [NB, PRB (2007)]



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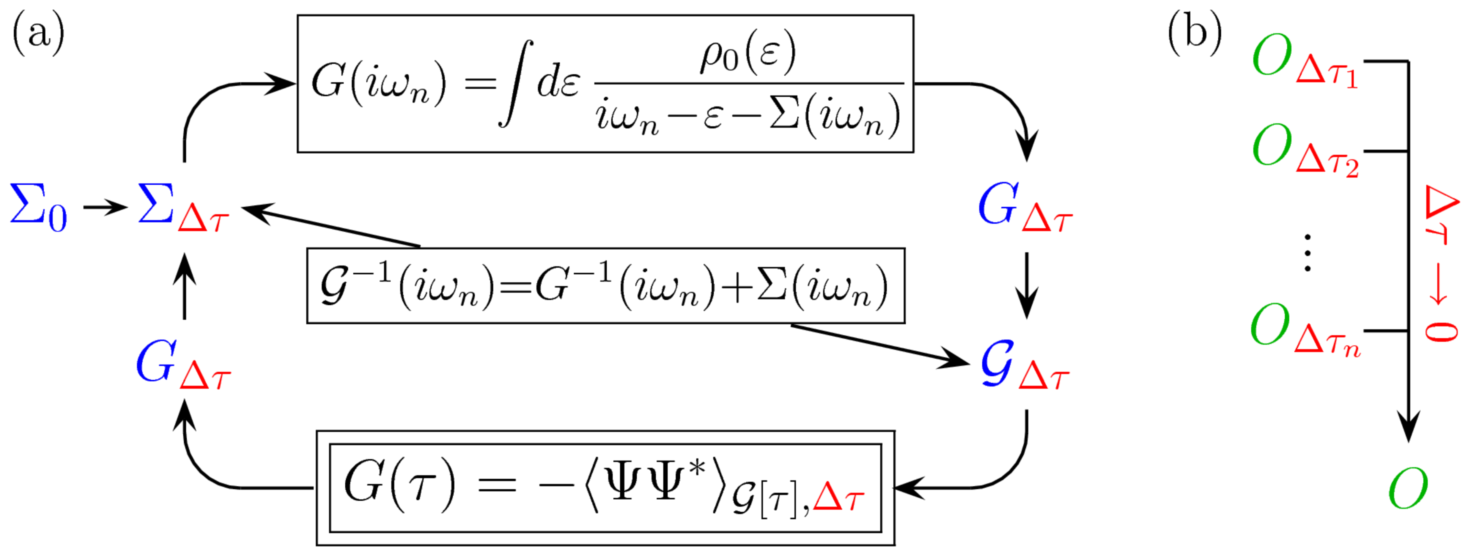

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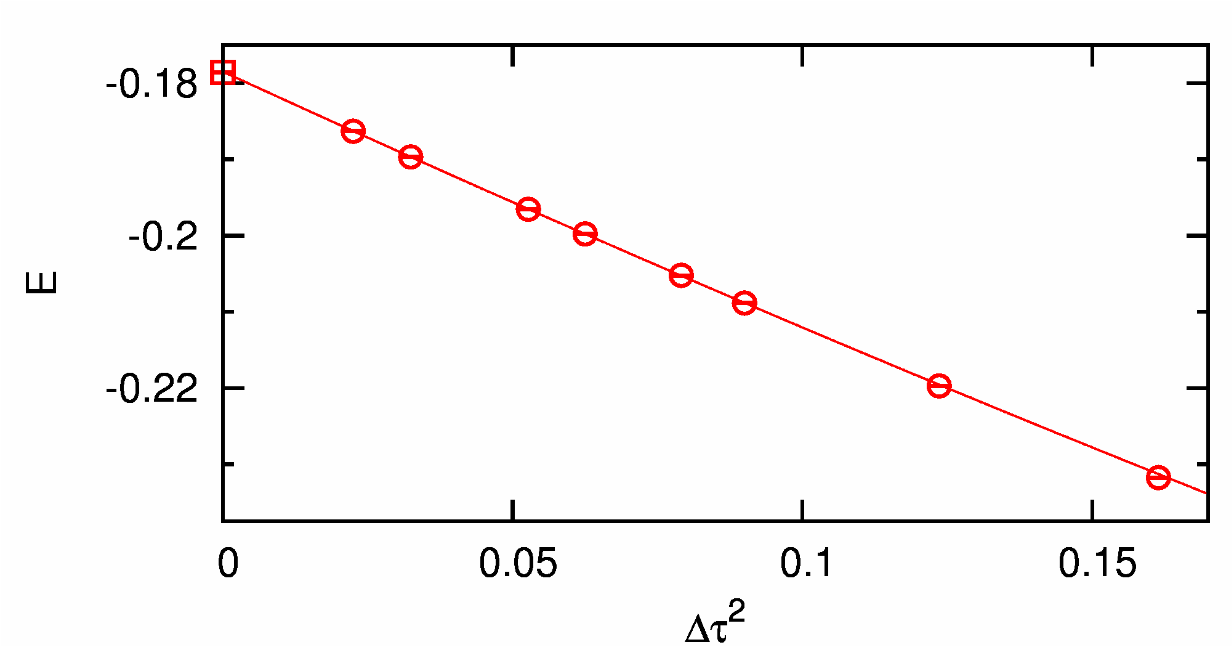
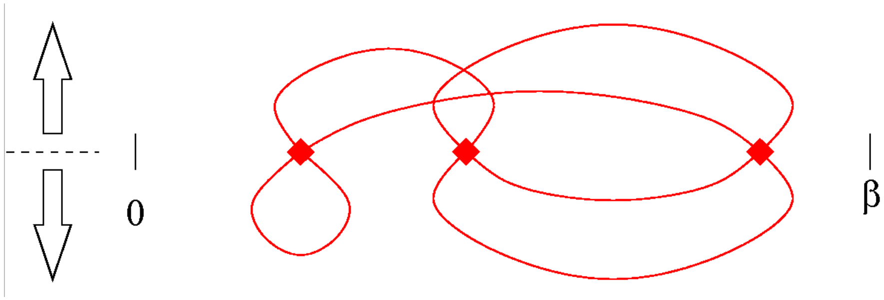


New development: continuous-time QMC algorithms

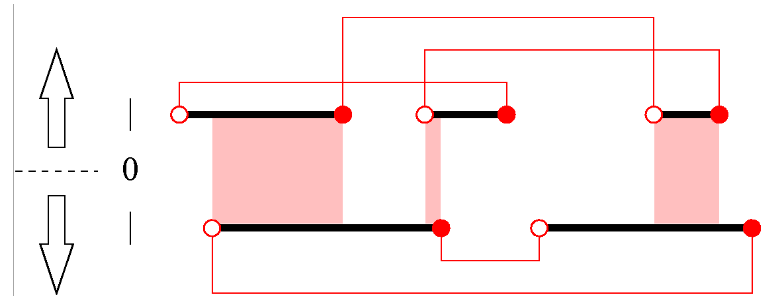
1. weak-coupling expansion

[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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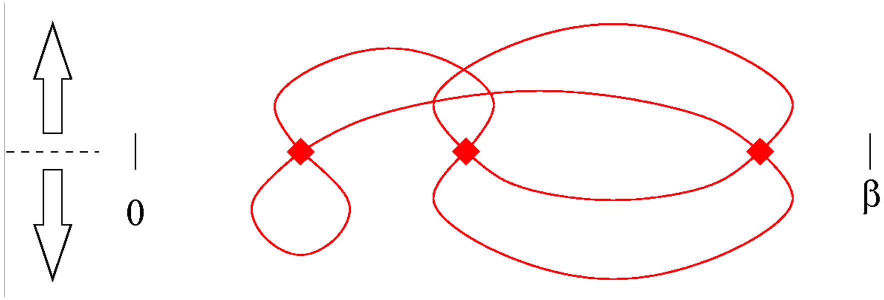

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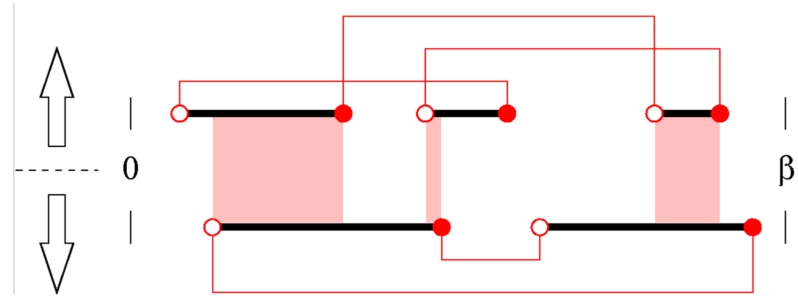
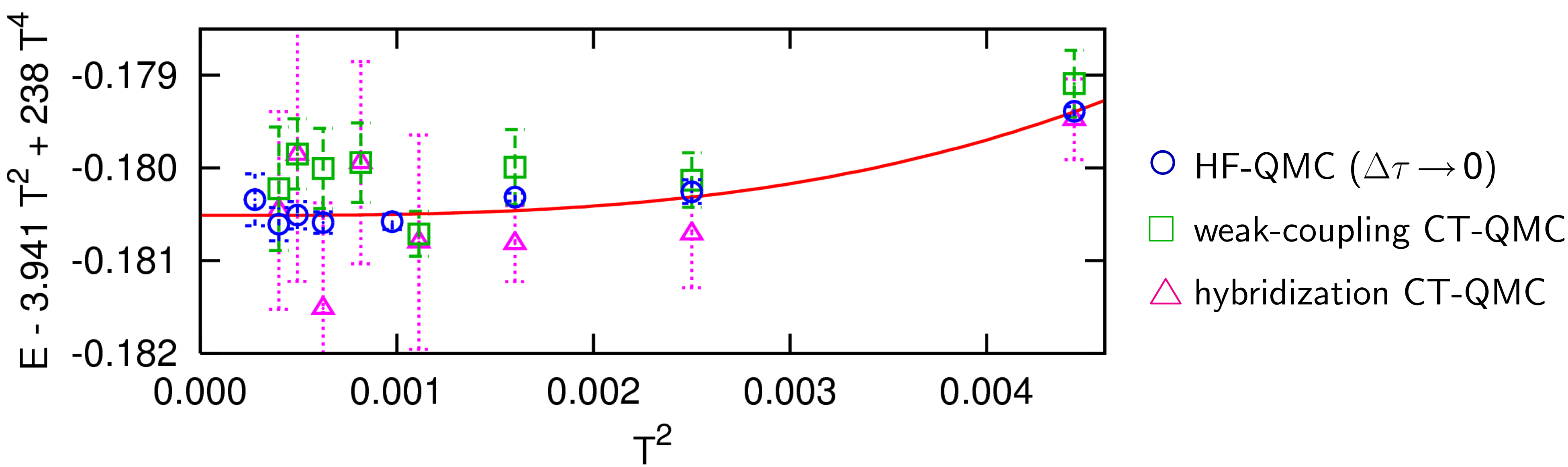


No systematic errors (in principle). Also more efficient than HF-QMC? Depends!



HF-QMC + extrapolation $\Delta\tau \to 0$ 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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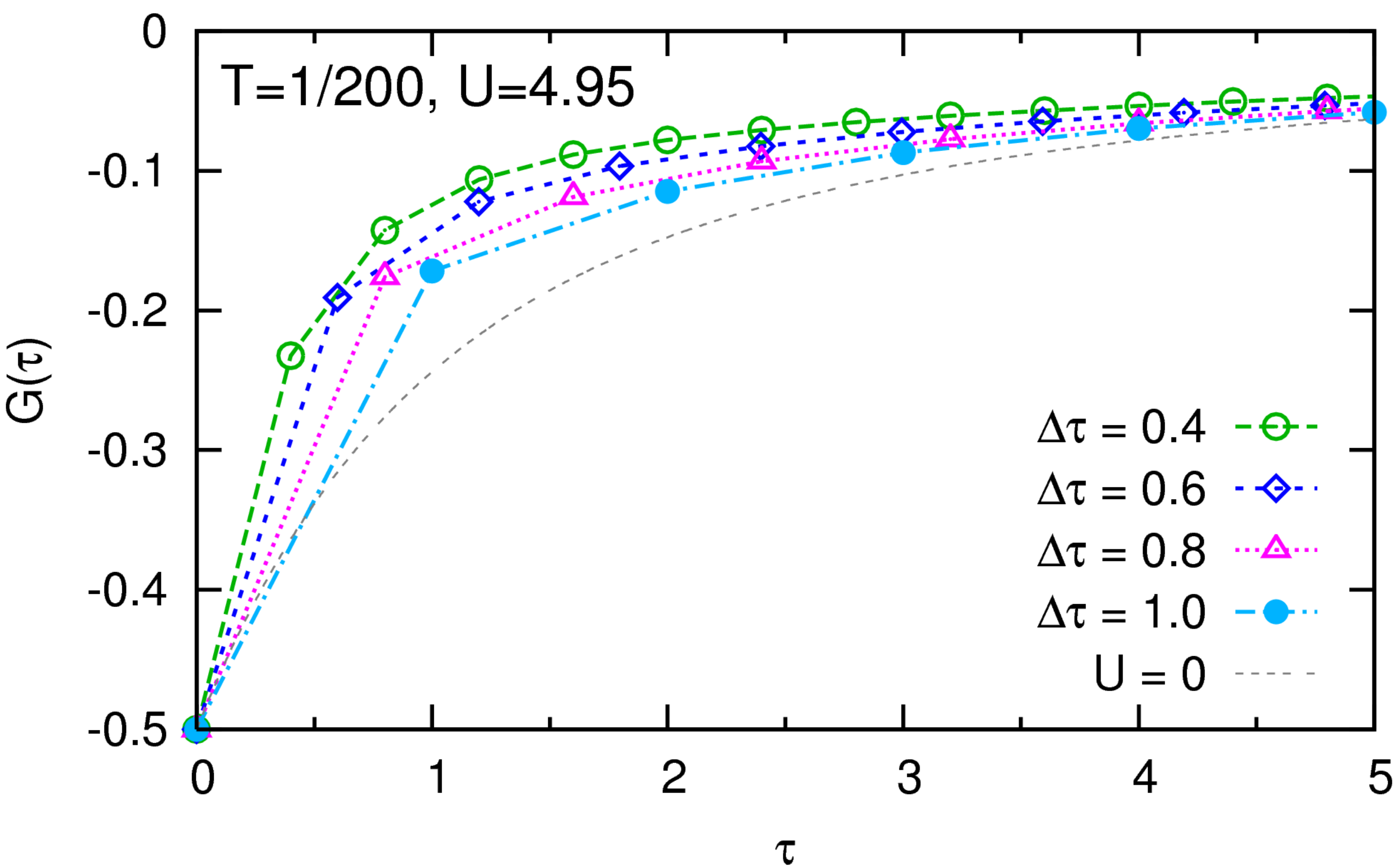
Reason: no obvious extrapolation scheme for $G(\tau)$



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

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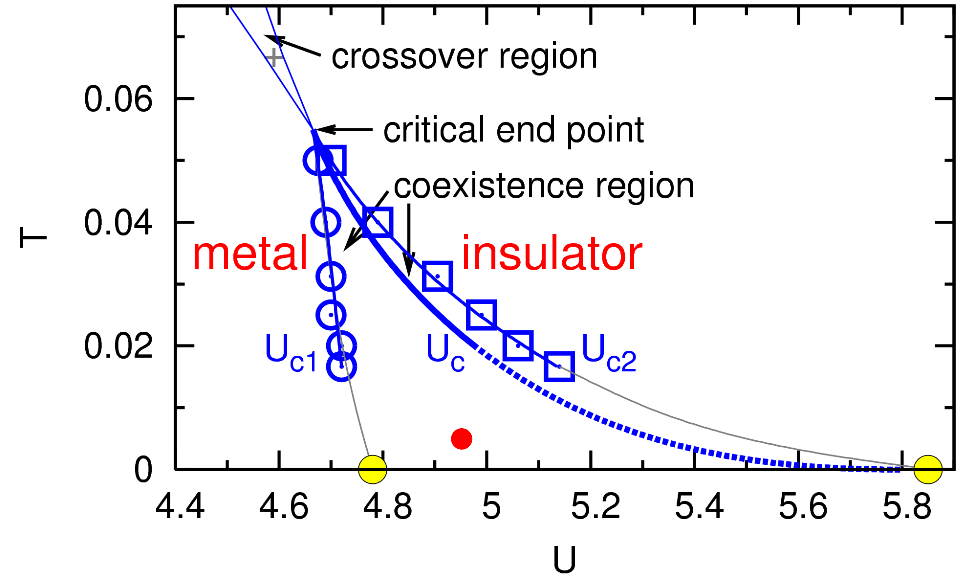

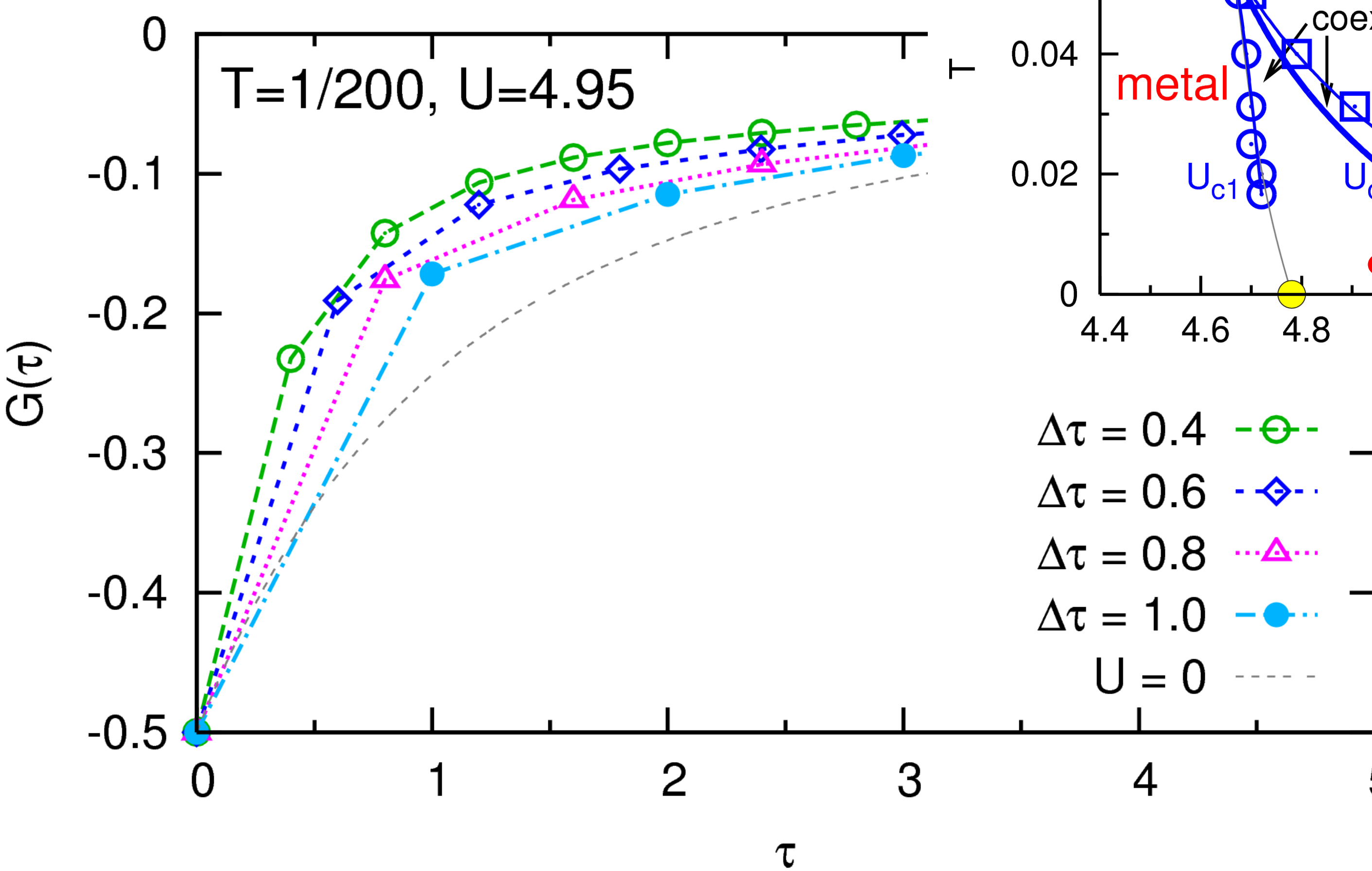

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New Green function extrapolation scheme

For each $\Delta\tau$: • average Green functions $\rightsquigarrow G_{\Delta\tau}(\tau_i)$, $\Delta G_{\Delta\tau}(\tau_i)$

• interpolate via difference Green function $G_{\Delta\tau}(\tau) - G_{\text{model}}(\tau)$

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

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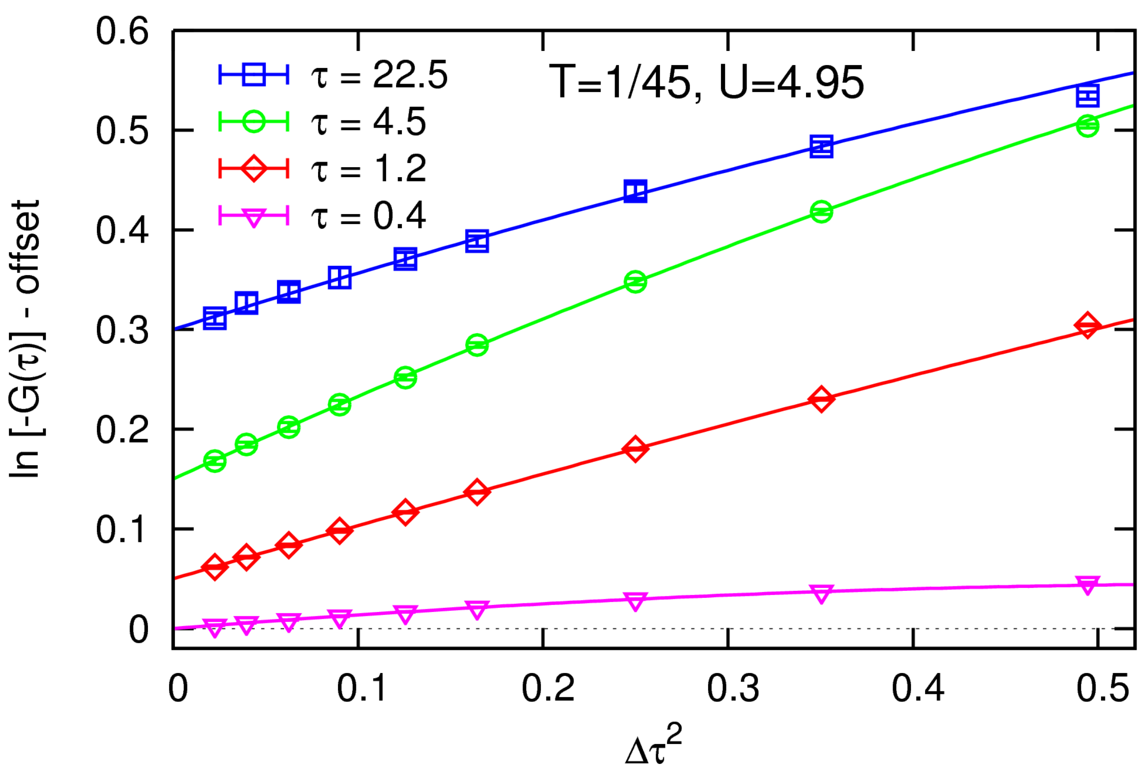
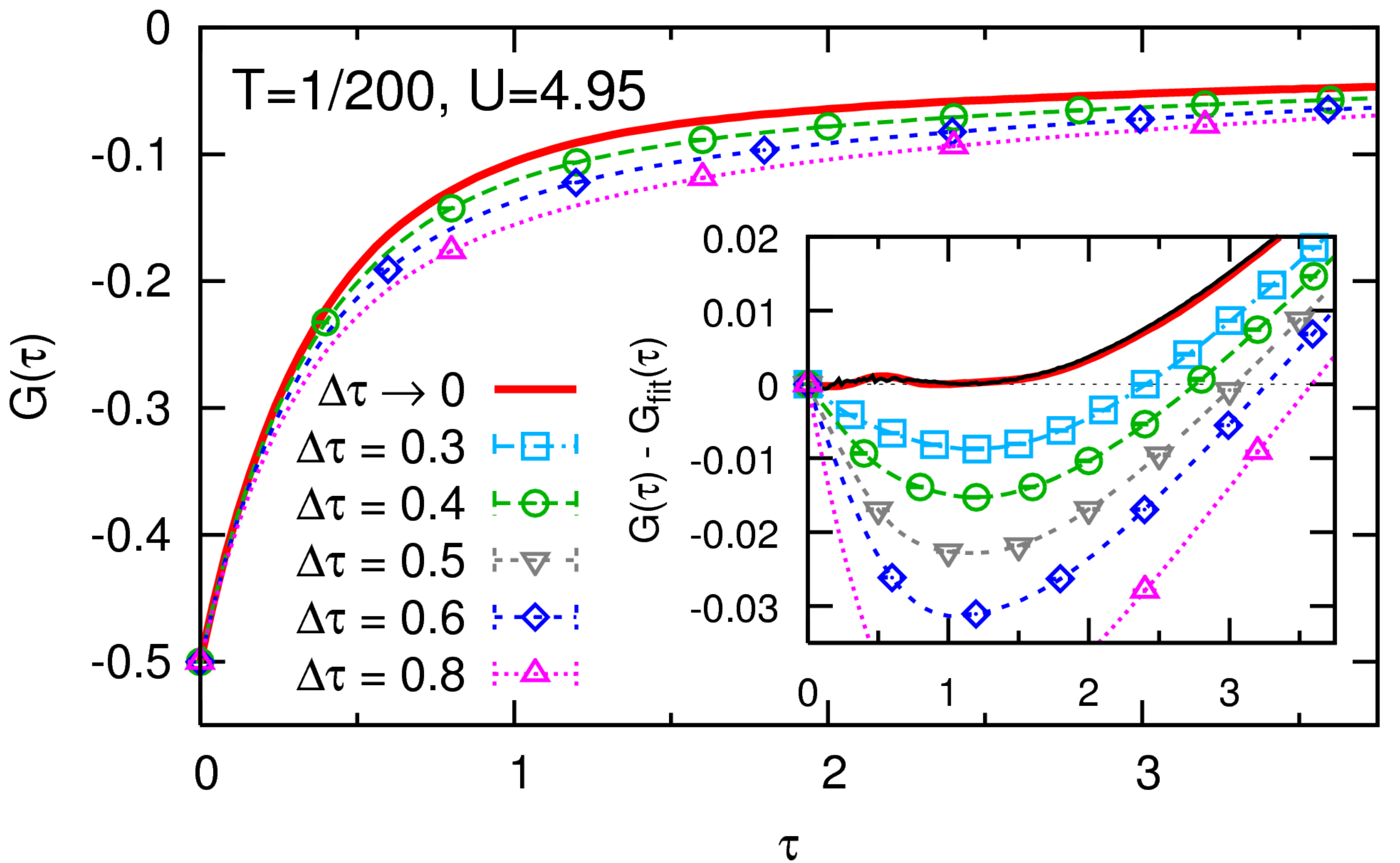
↑ weak-coupling expansion

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



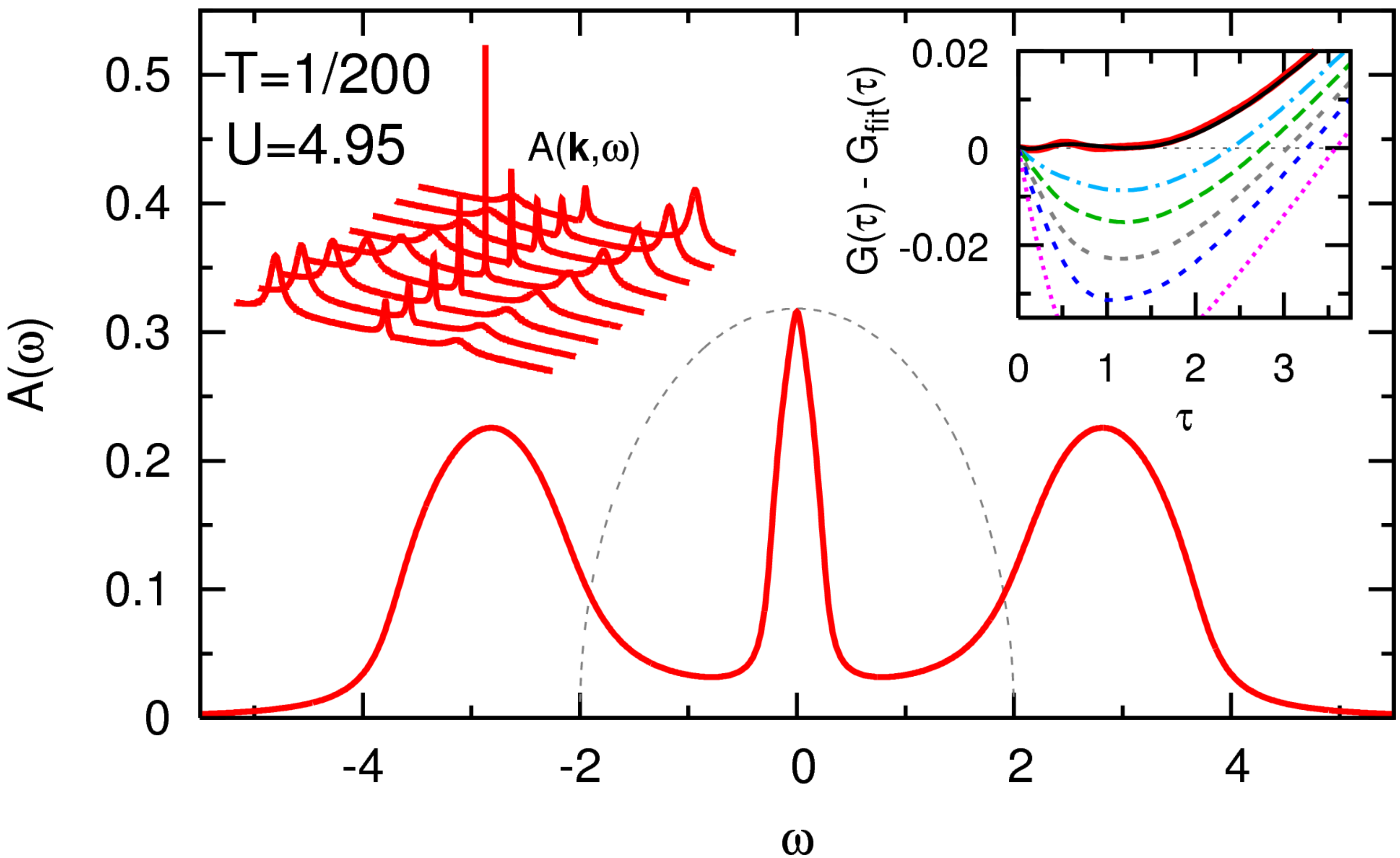
Result: unbiased, numerically exact Green function



[NB, arXiv:0712.1290]

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

Analytic continuation using Padé approximant for self-energy



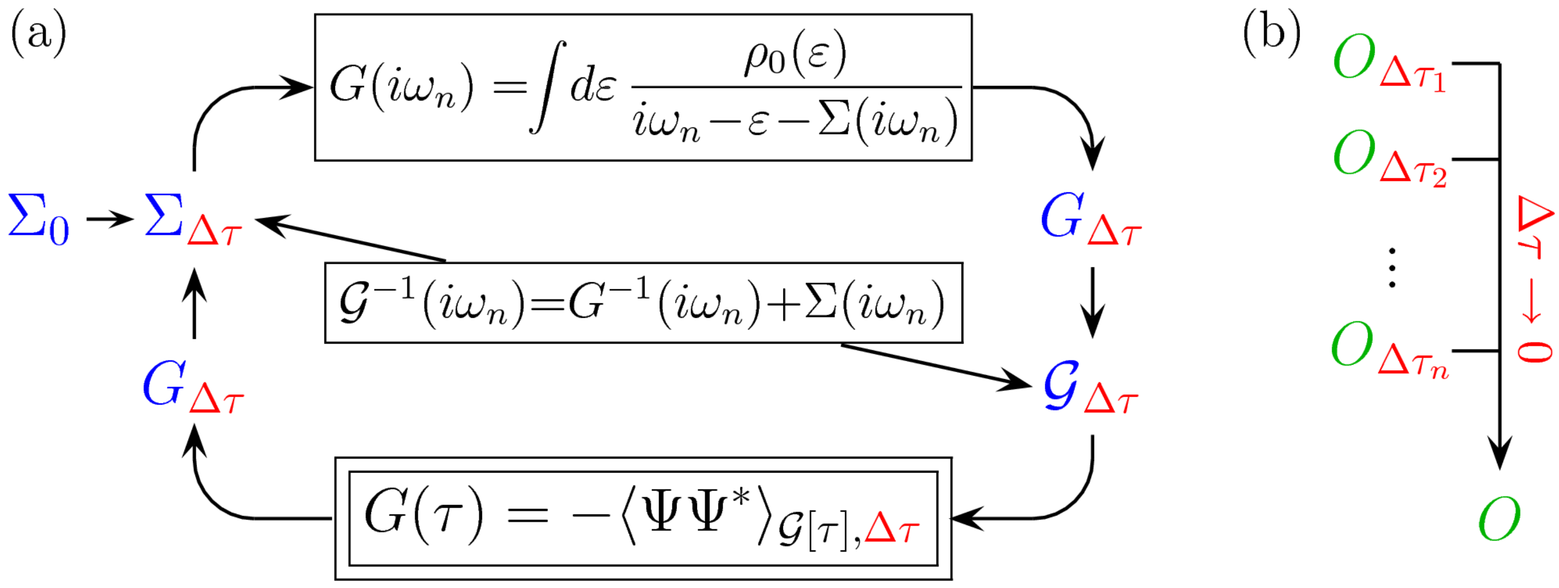
First spectra without discretization error from HF-QMC, at ultra-low *T*

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

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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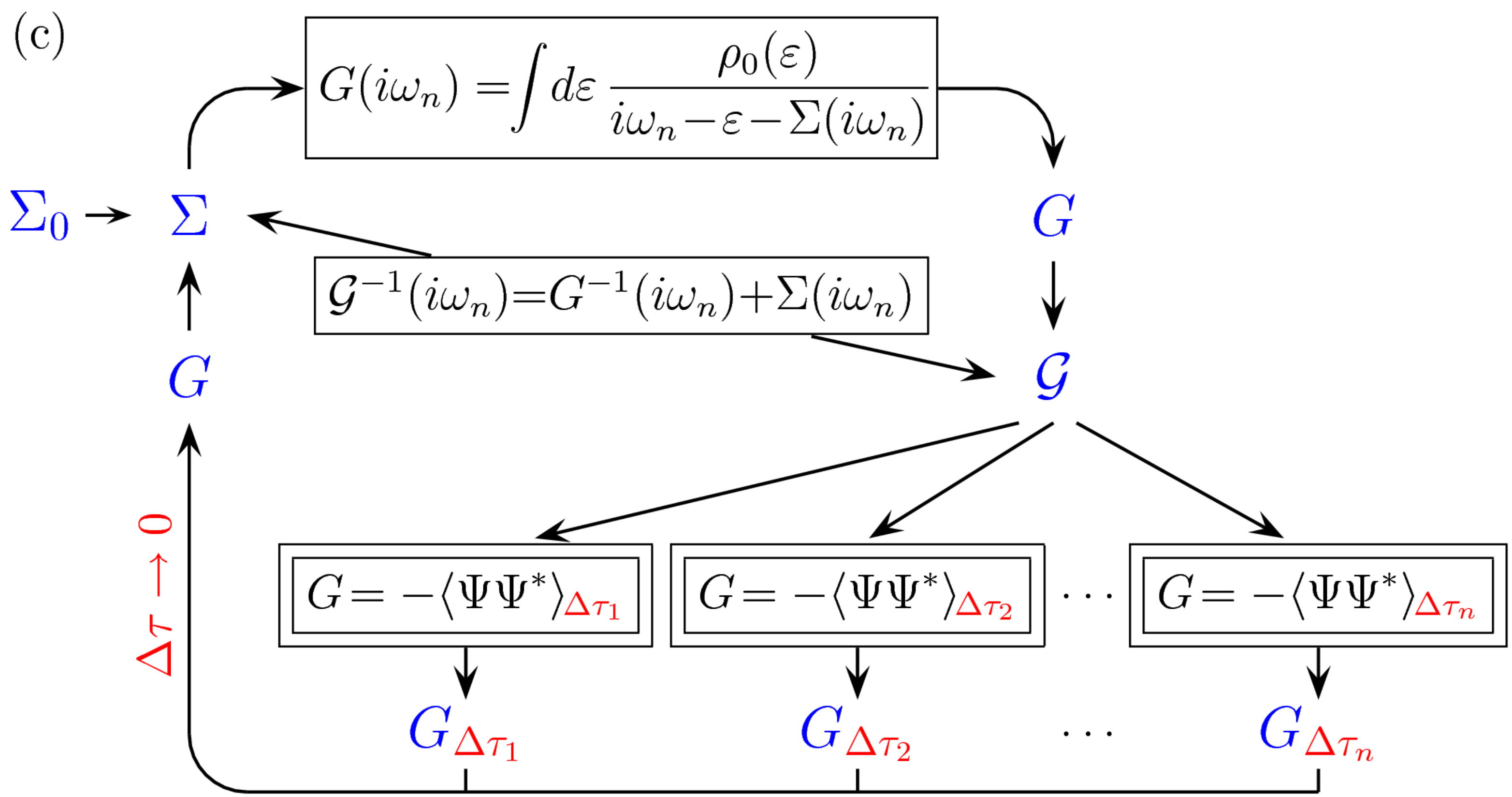
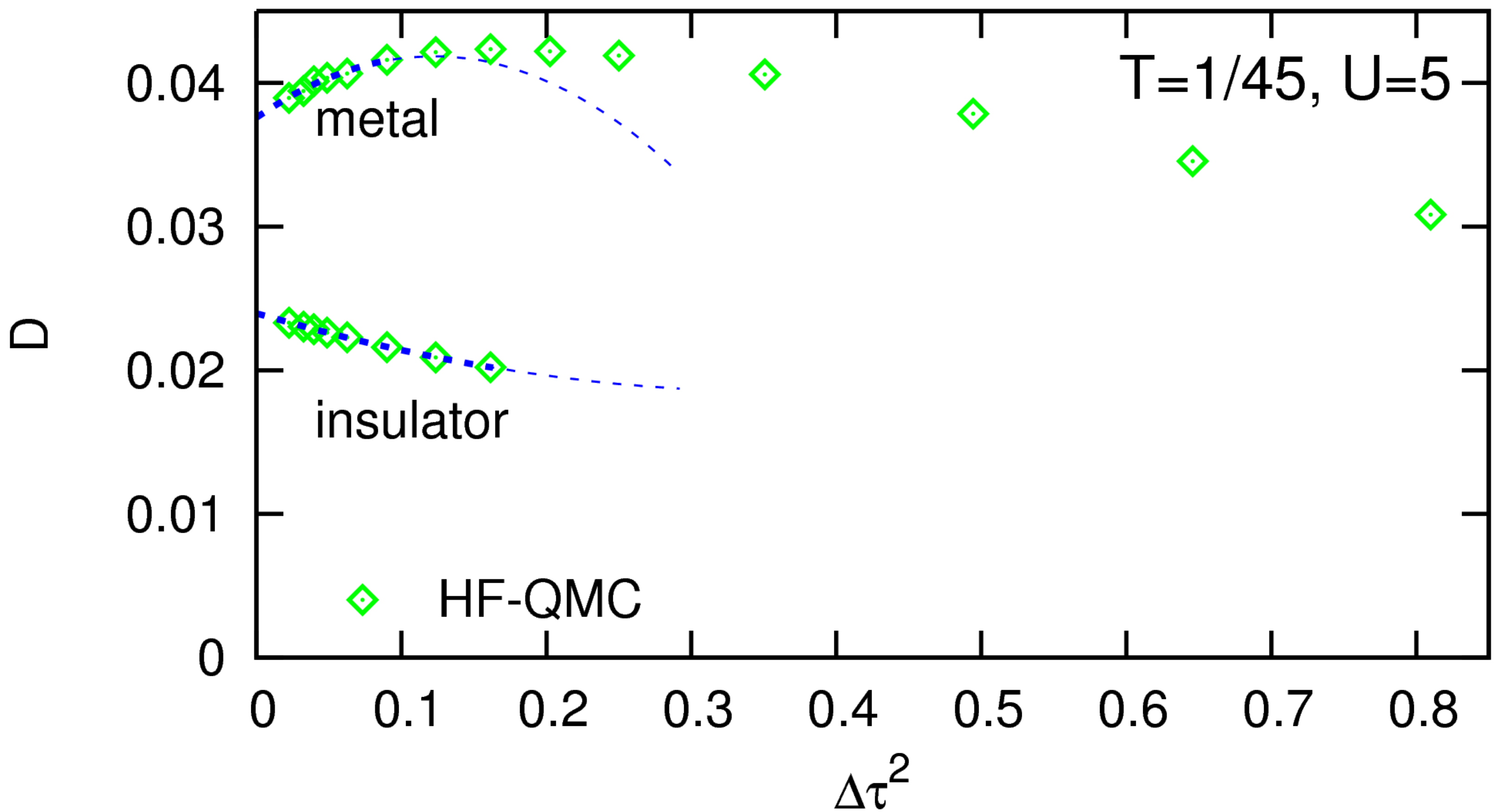


(c) Multigrid HF-QMC: internal elimination of Trotter error

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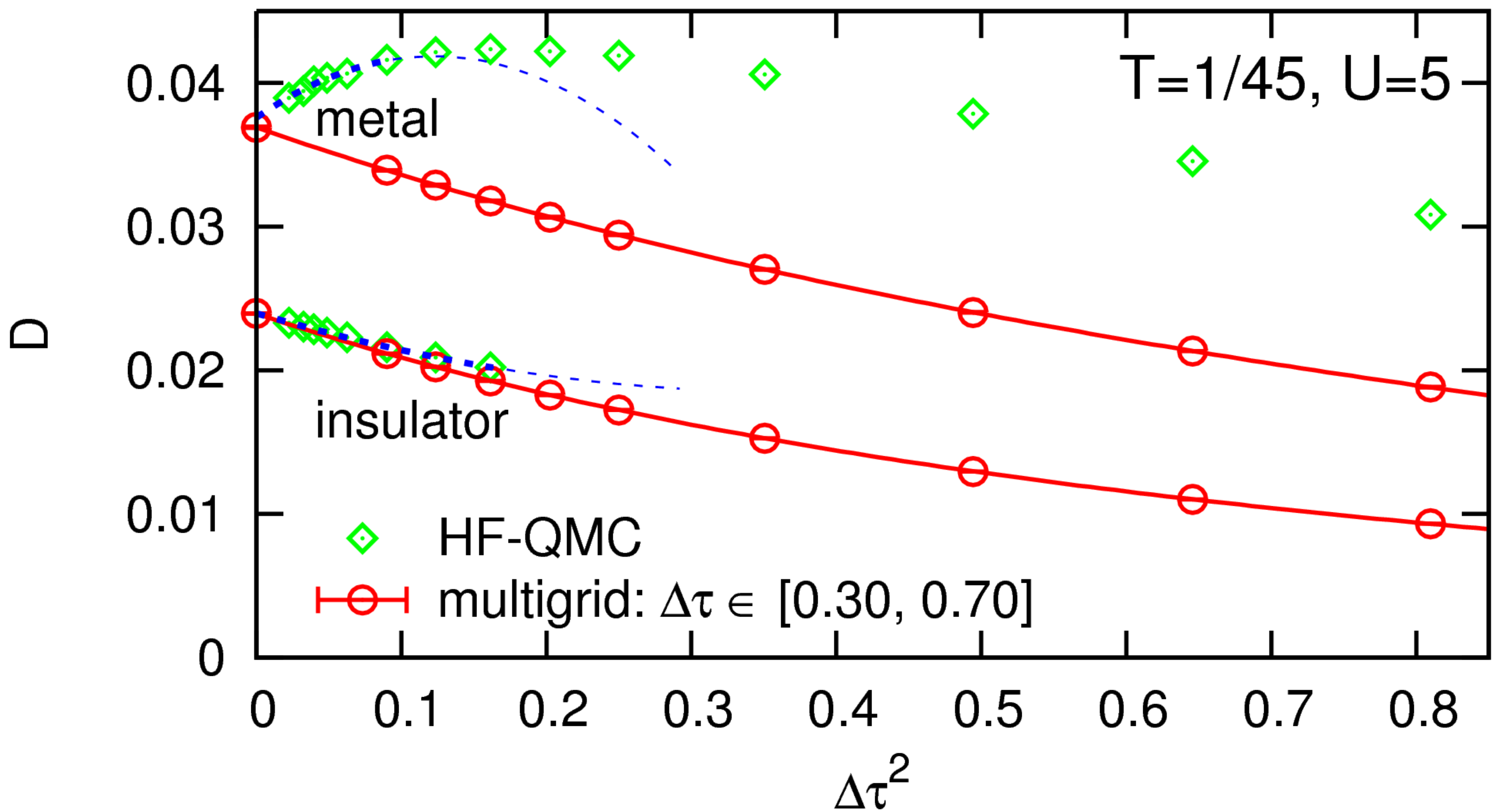
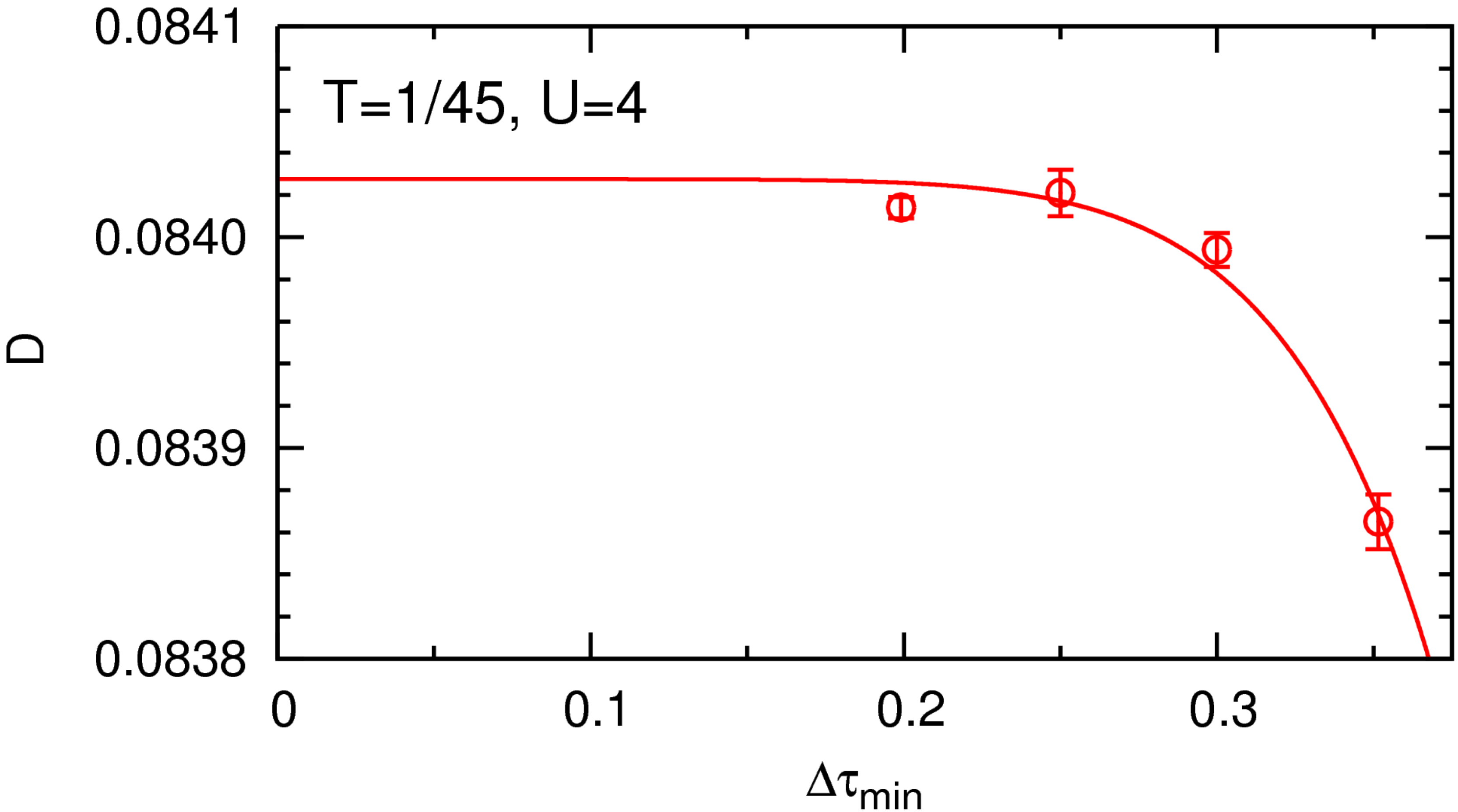


Conventional HF-QMC:	no insulating solution for $\Delta\tau \gtrsim 0.4$
	very irregular $\Delta\tau$ dependence beyond $\Delta\tau \approx 0.3$
Multigrid HF-QMC:	vastly larger useful range of $\Delta\tau$

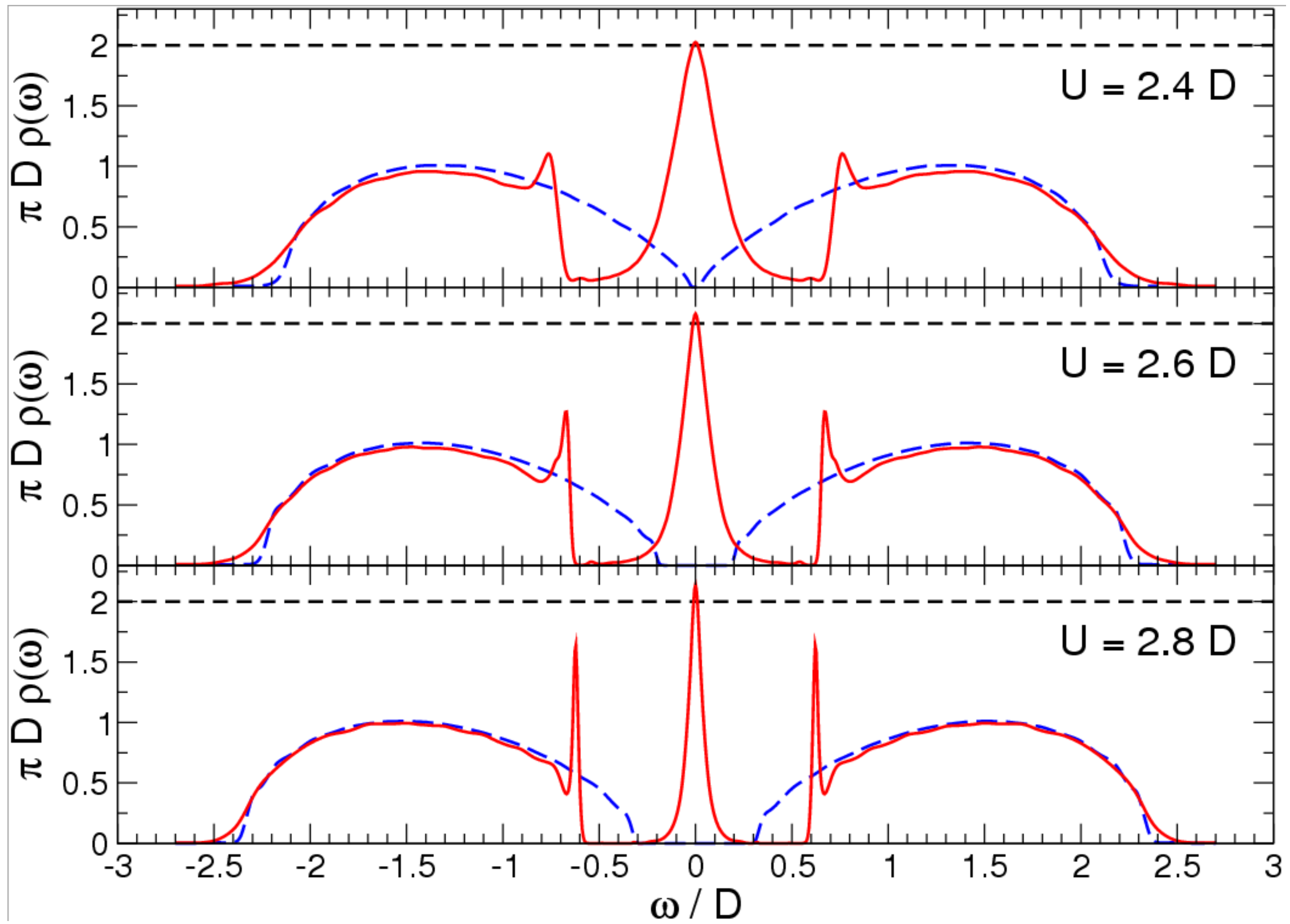
Systematic study: impact of grid range $[\Delta\tau_{\text{min}}, \Delta\tau_{\text{max}}]$



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

Spectral weight transfer at the Mott transition

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



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

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

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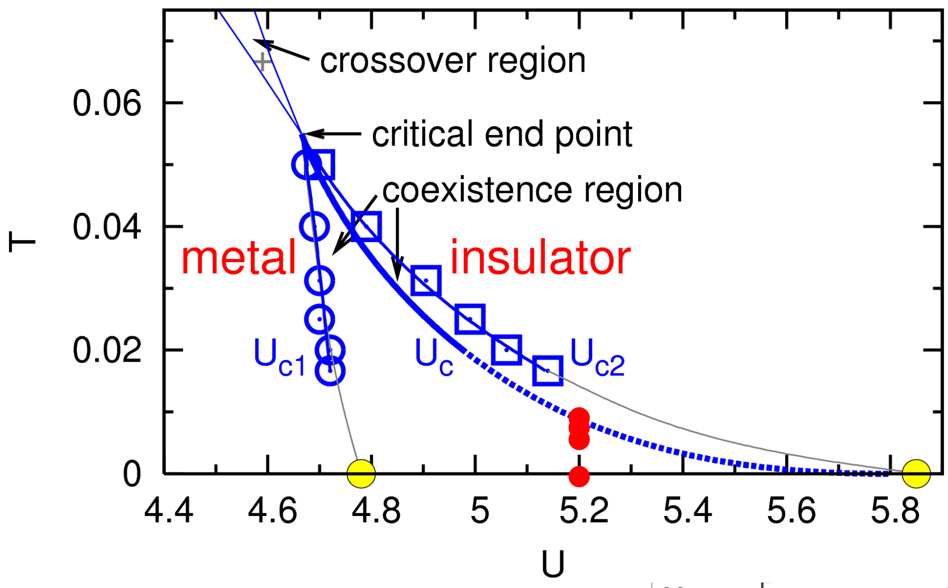
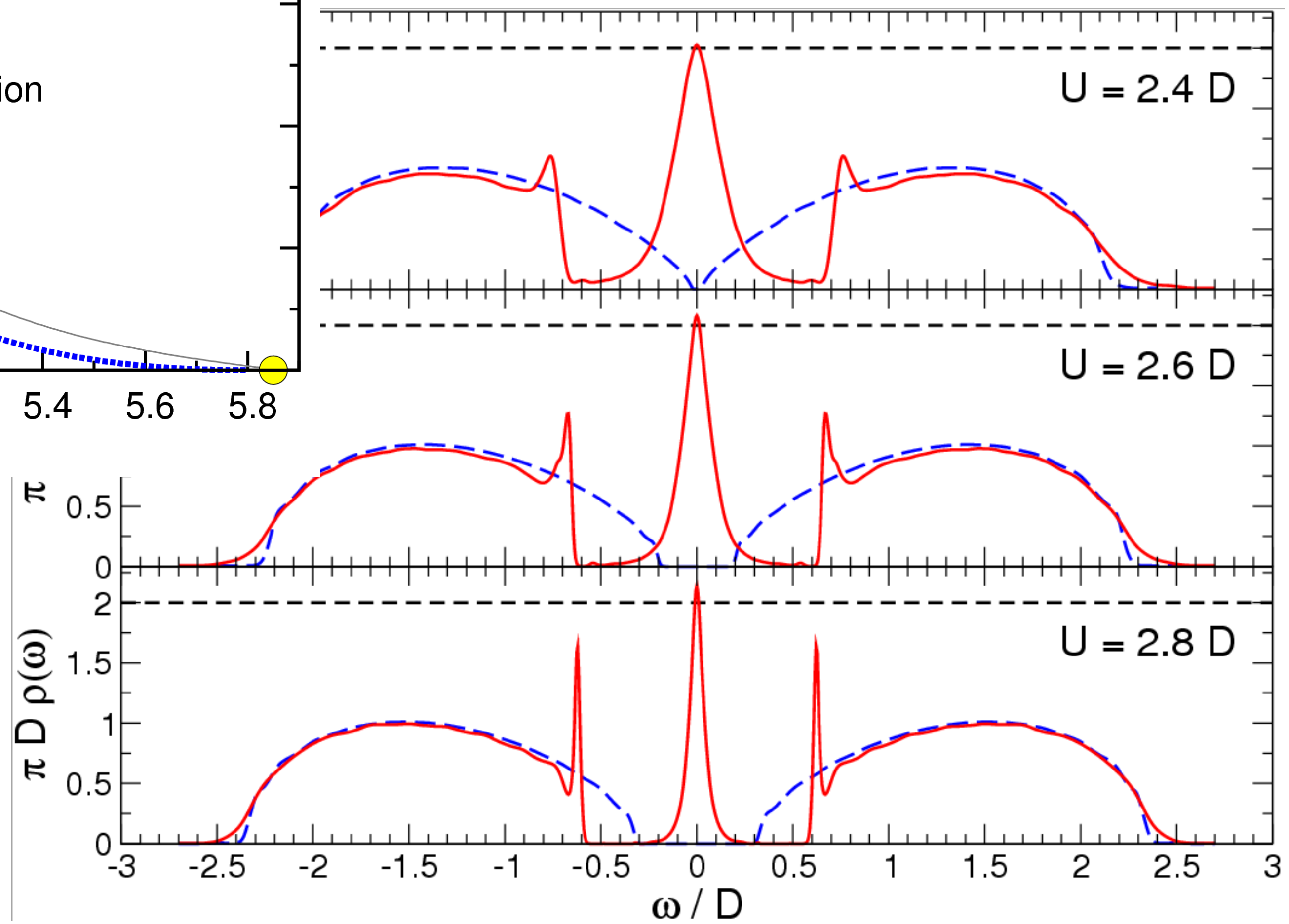


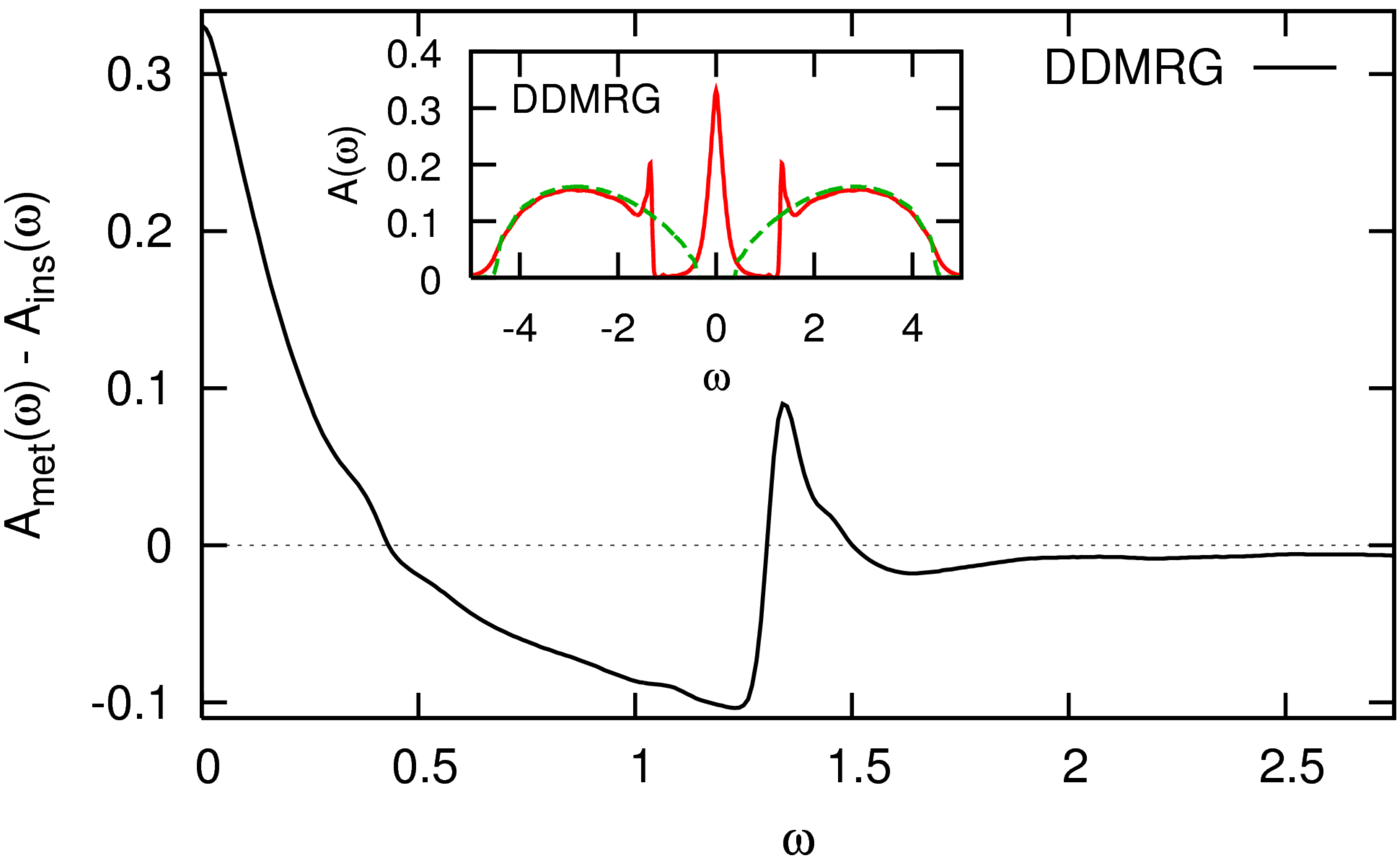


Dynamical DMRG $\rightsquigarrow$ Hubbard band subpeaks in metallic phase (at $T = 0$)

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

Check using multigrid HF-QMC. . .

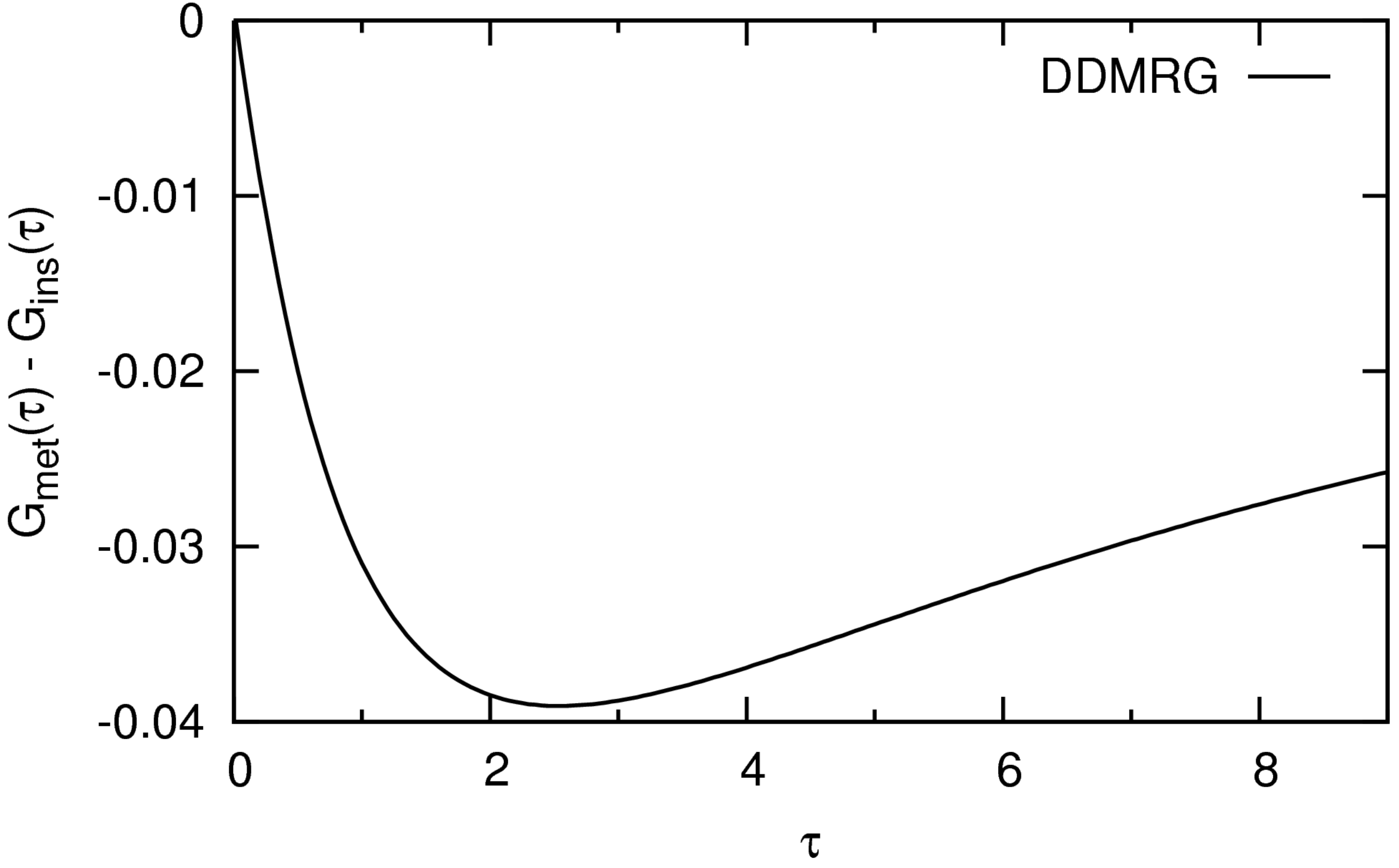
Analysis via difference of spectral functions (symmetric in ω) at $U = 5.2$



Problems for QMC: (i) analytic continuation of QMC data ill-conditioned

(ii) no $T \to 0$ extrapolation of spectra

Difference Green functions in imaginary time



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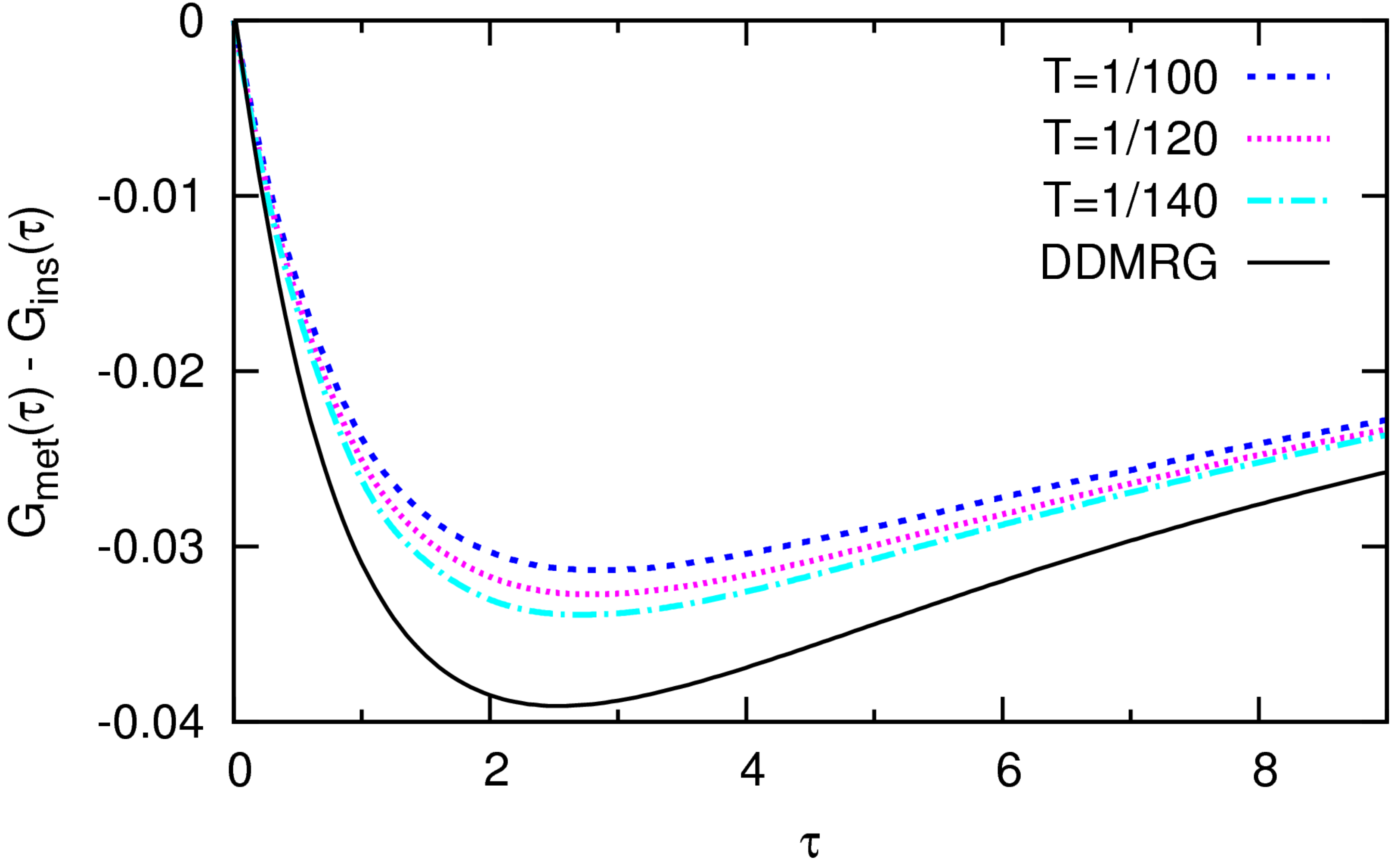

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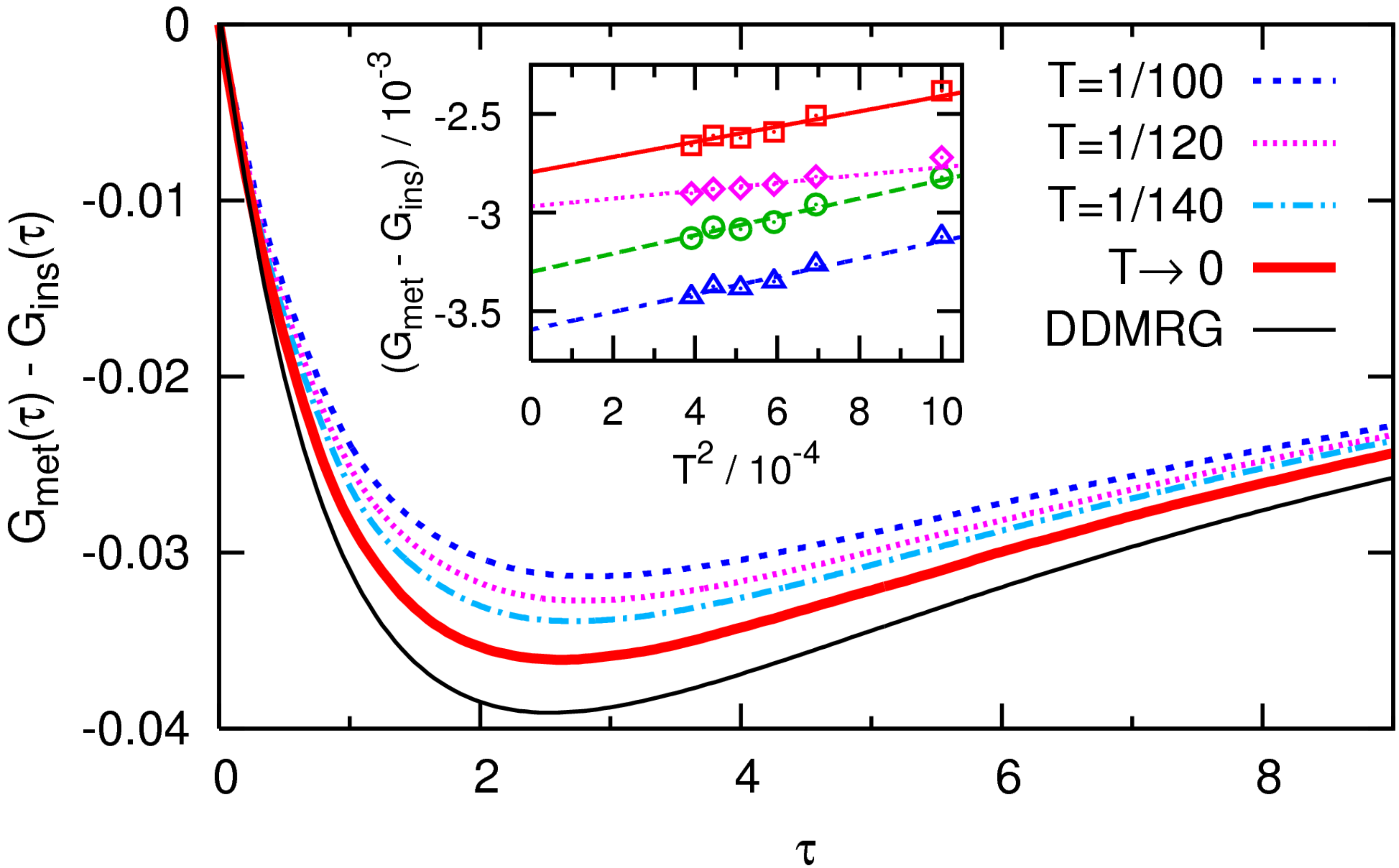
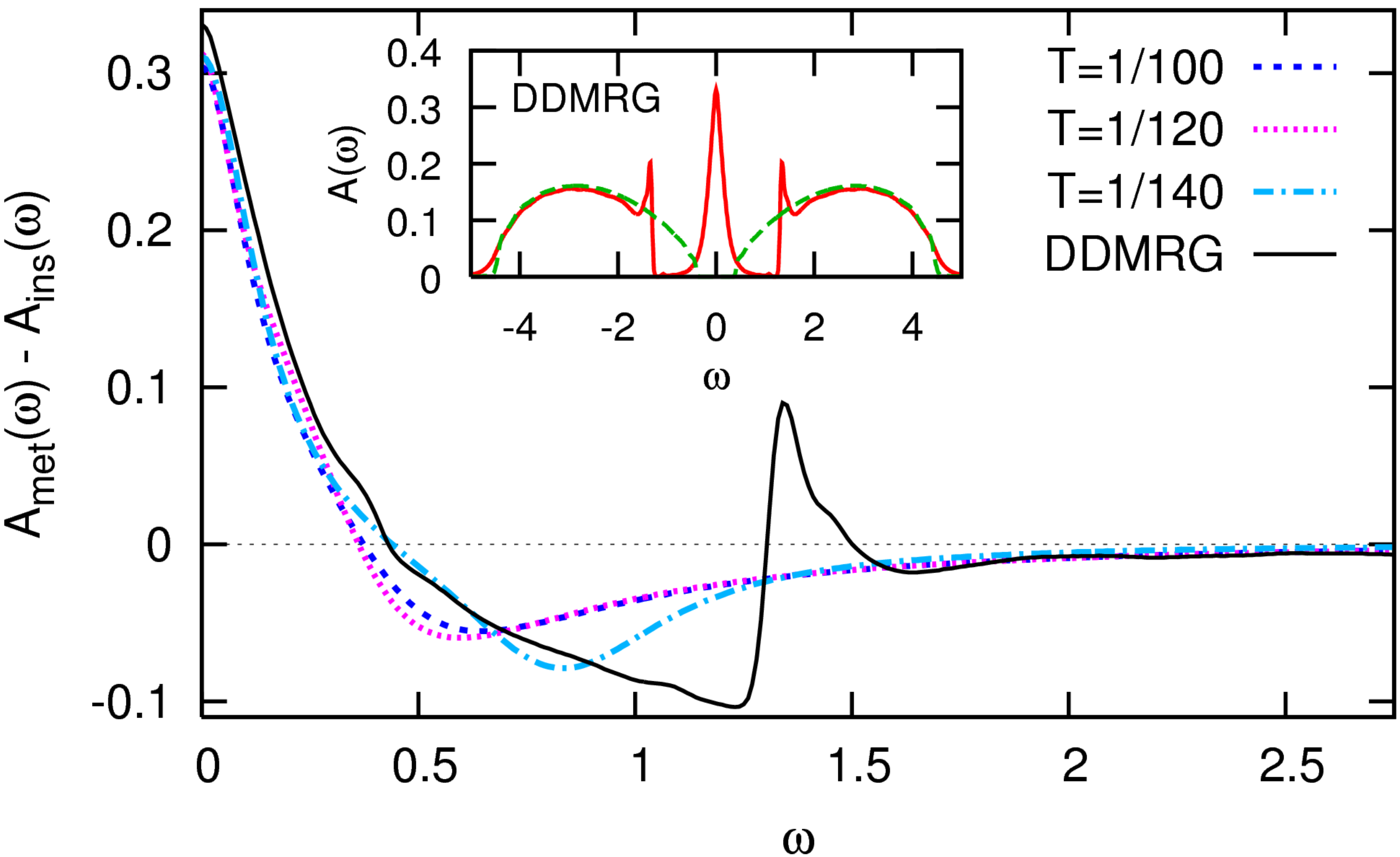


Multigrid HF-QMC data precise within linewidths [NB, arXiv:0801.1222]

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 [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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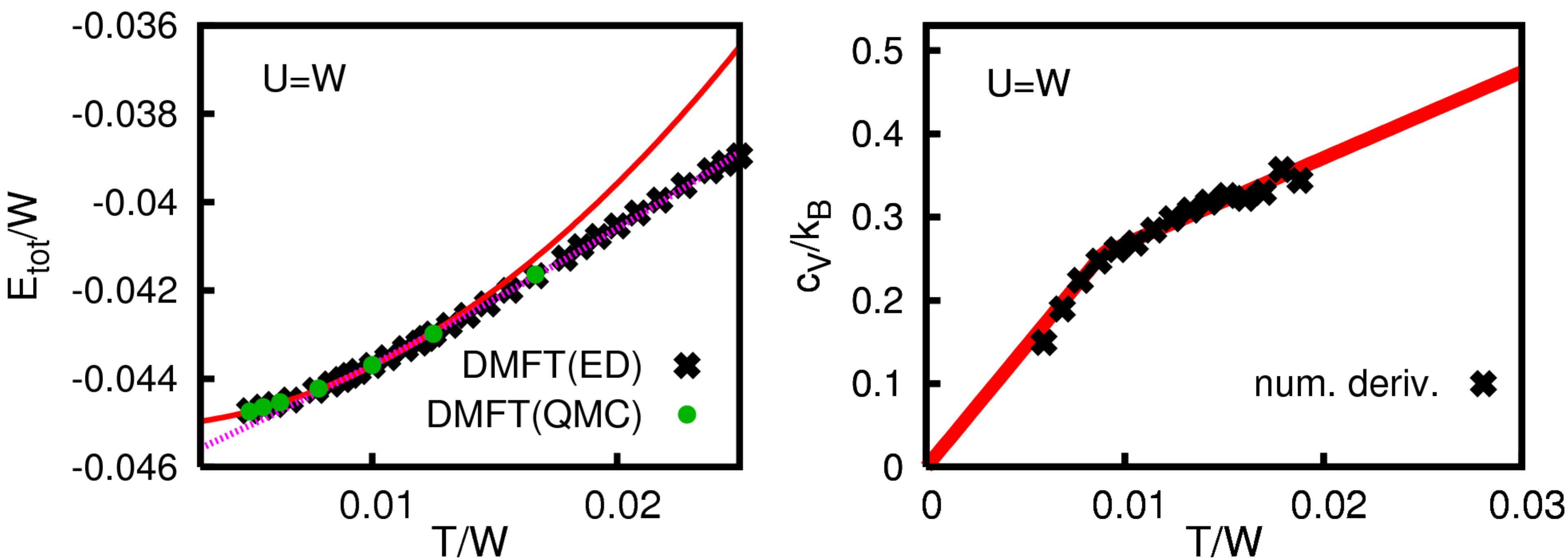
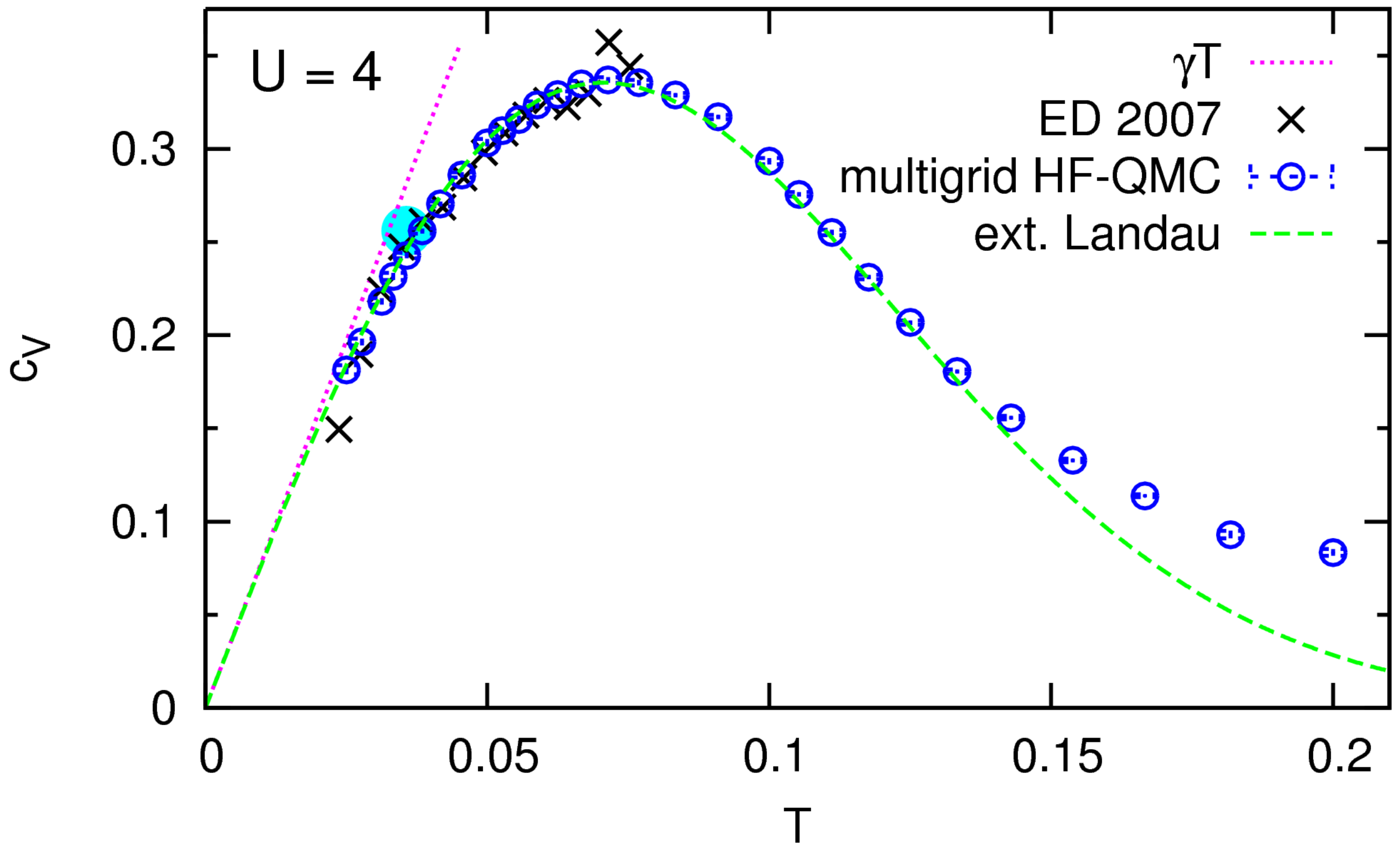
When/how do these laws break down?

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]

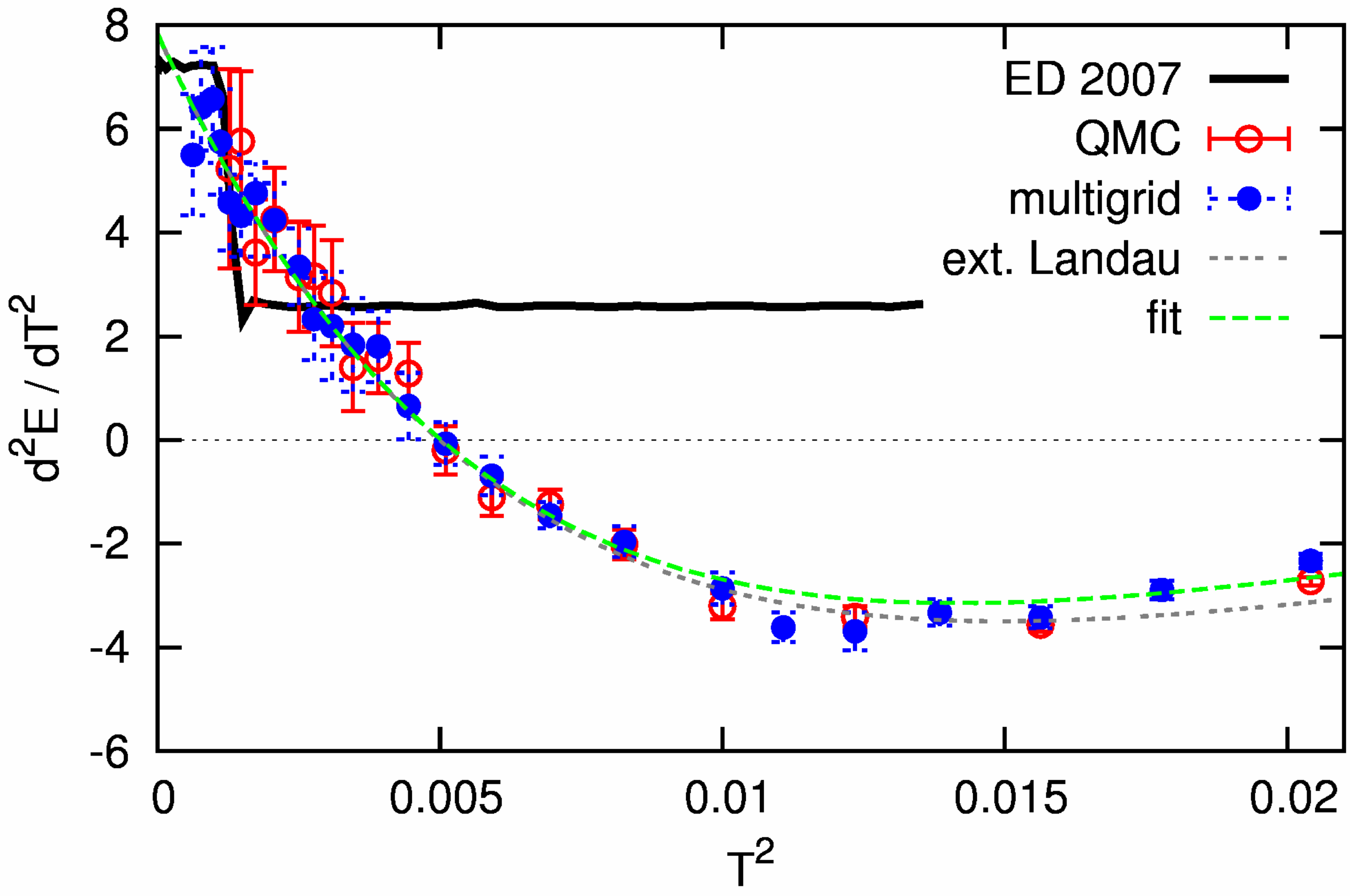


High-precision results $\rightsquigarrow$ no kink!

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

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

Direct measure of "kinkiness": energy curvature



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

Initial slope: contributions from Sommerfeld expansion + T-dependence of $\Sigma(\omega)$

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, multi-band [e.g. SU(2M) symmetric for M=1,2,4,8] . . .

Outlook: flavor-selective Mott transitions in ultracold quantum gases

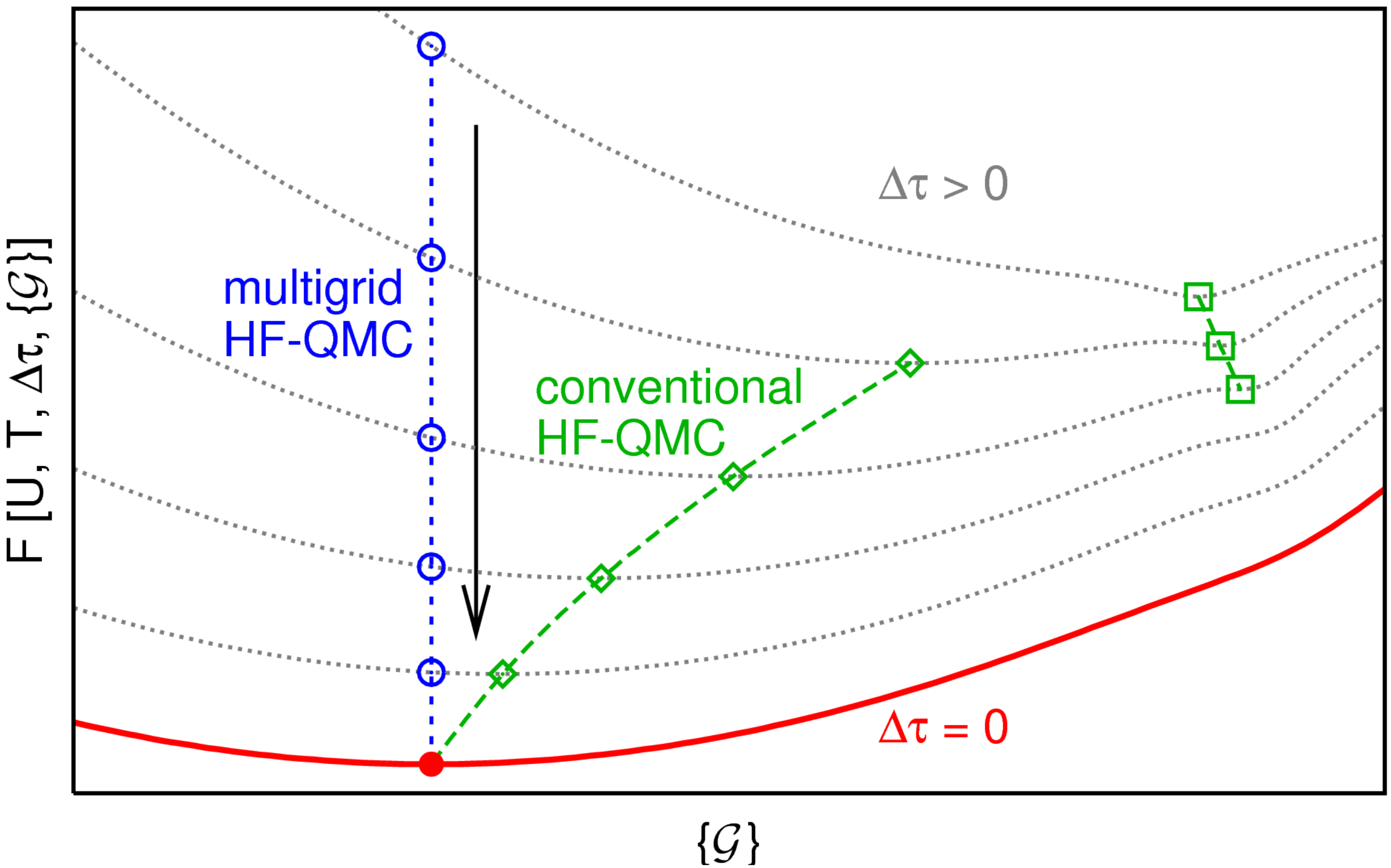
Acknowledgements

Carsten Knecht, Elena Gorelik

Eberhard Jacobi, Peter van Dongen

Funding by state RLP (Forschungsfonds 2007) and DFG (in SFB/TR 49)

Schematic comparison via generalized Ginzburg-Landau functionals

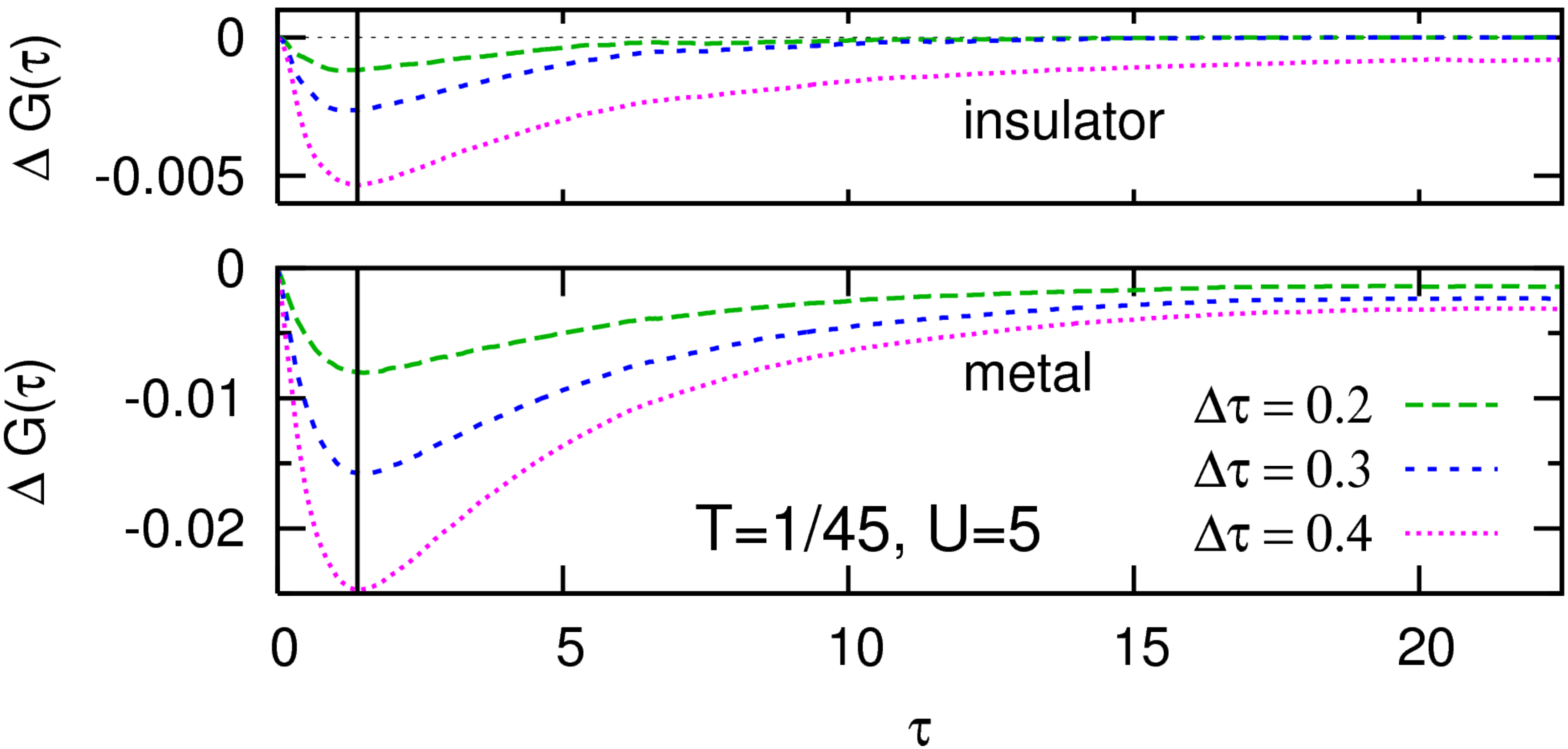


Conventional Hirsch-Fye QMC: DMFT fixed point shifts with $\Delta\tau$

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

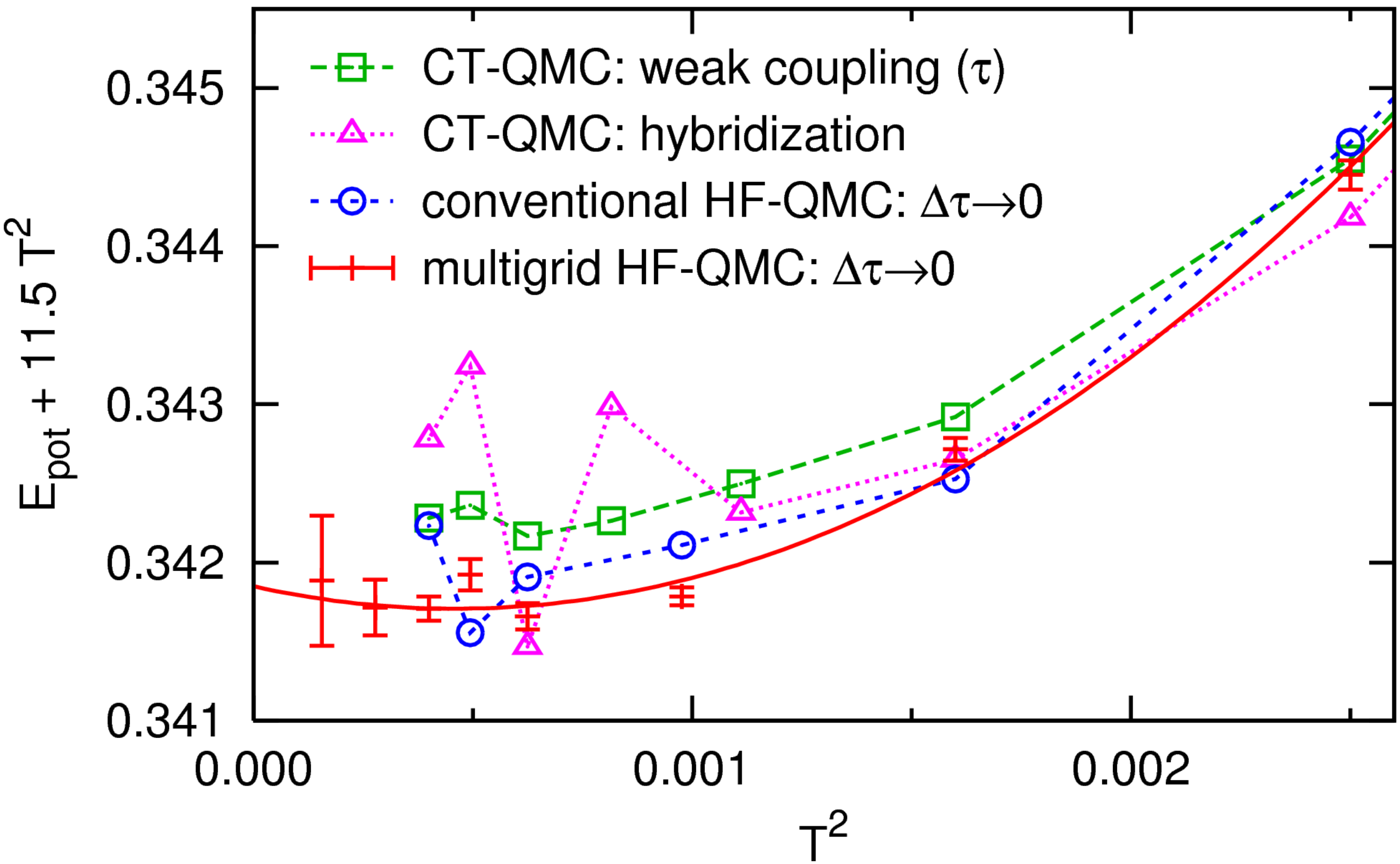
Implementation: Green function extrapolation, hierarchy of frequency scales, . . .

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



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

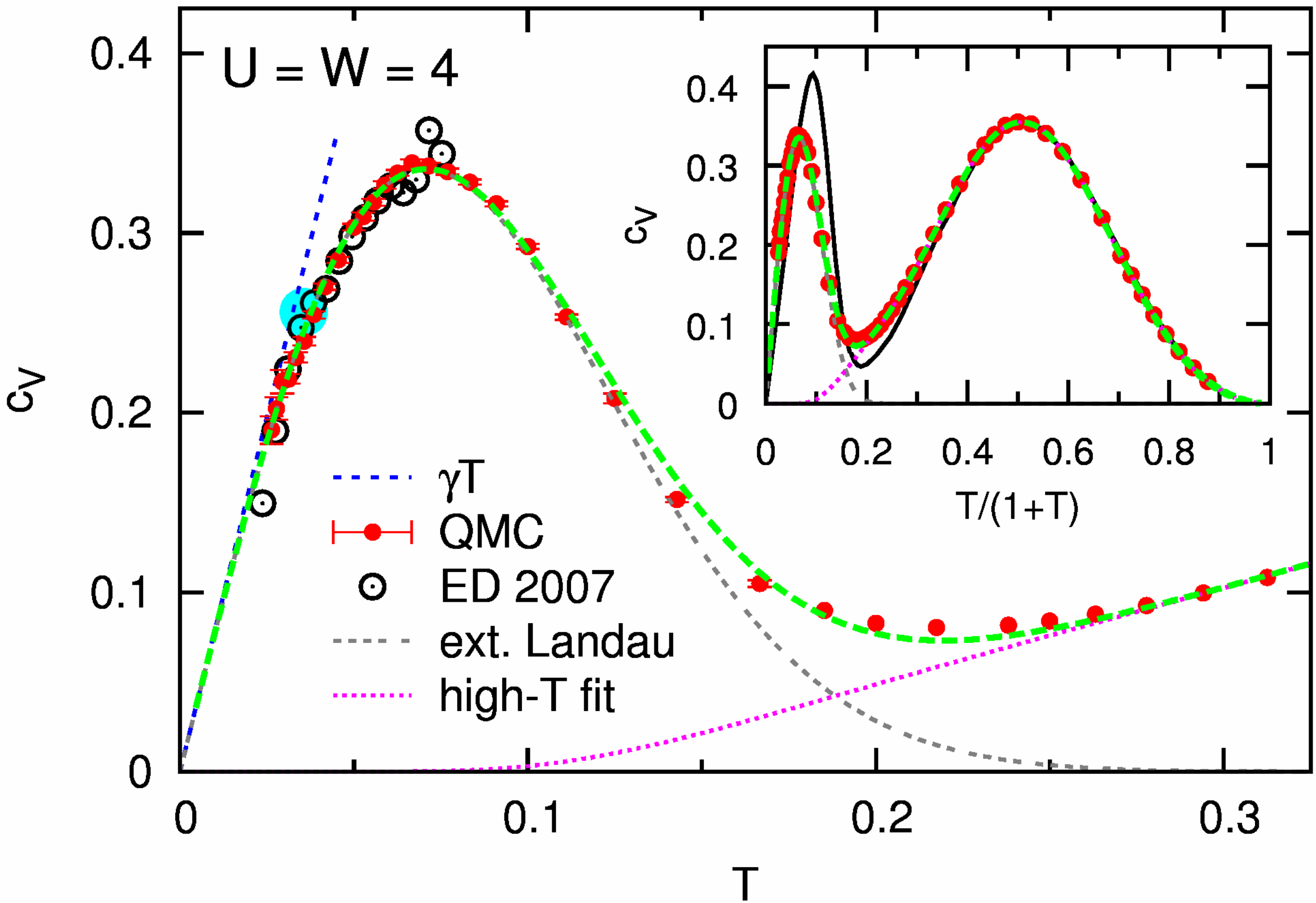
Efficiency: potential energy $E_{\rm pot} = UD$ (at $U = W = 4$)



No more "difficult observables" for multigrid HF-QMC

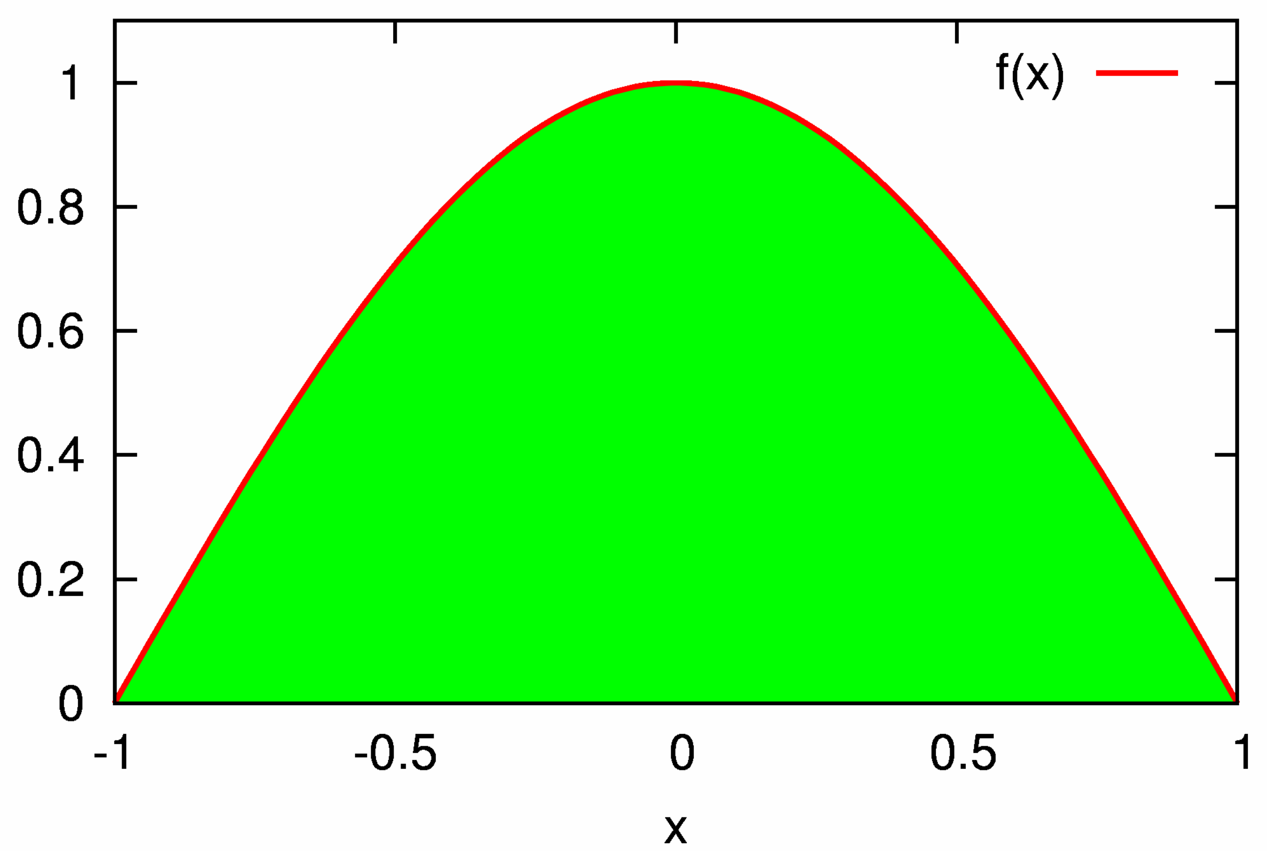
Higher precision than CT-QMC methods at same effort

Specific heat over full temperature range



A brief reminder

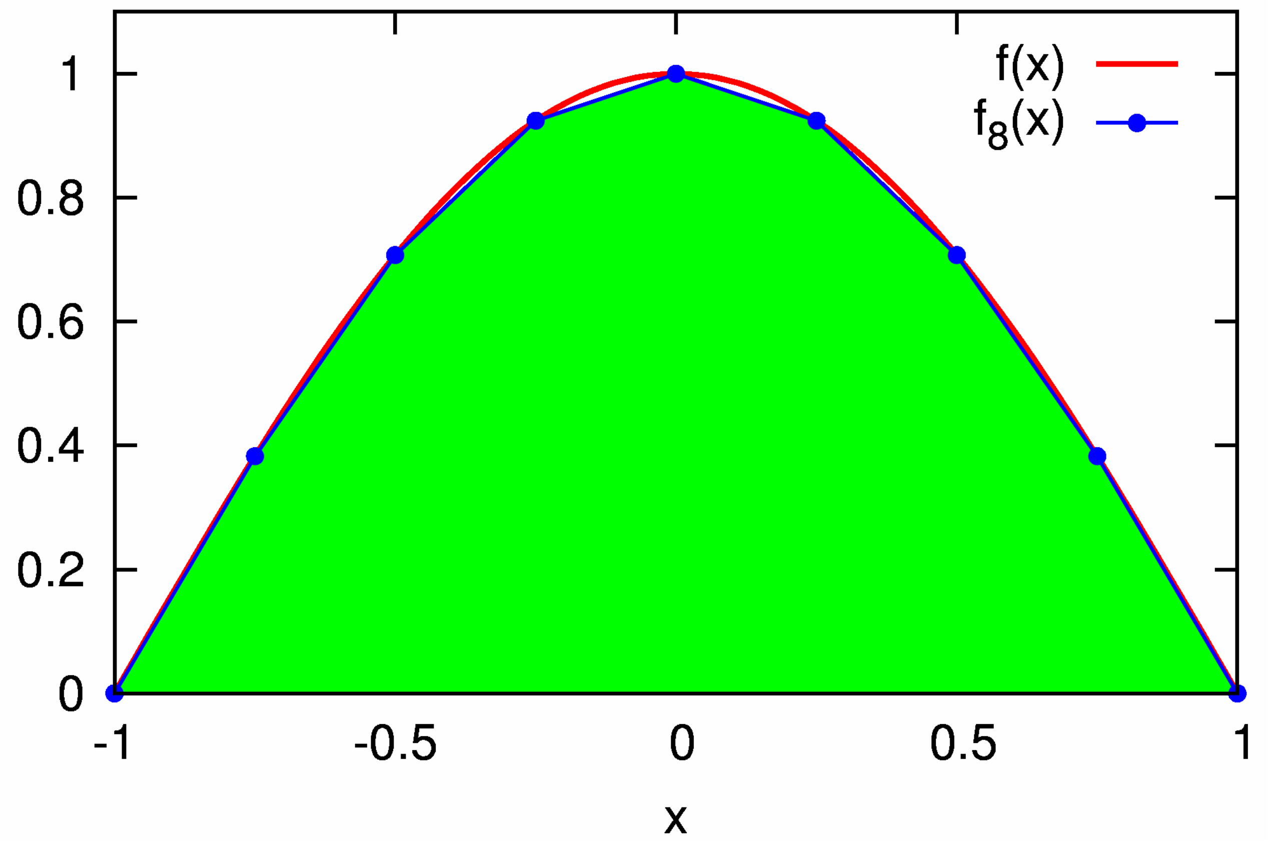
Simple example: quadrature of a convex function (in $d = 1$)



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

A brief reminder

Simple example: quadrature of a convex function (in $d = 1$)



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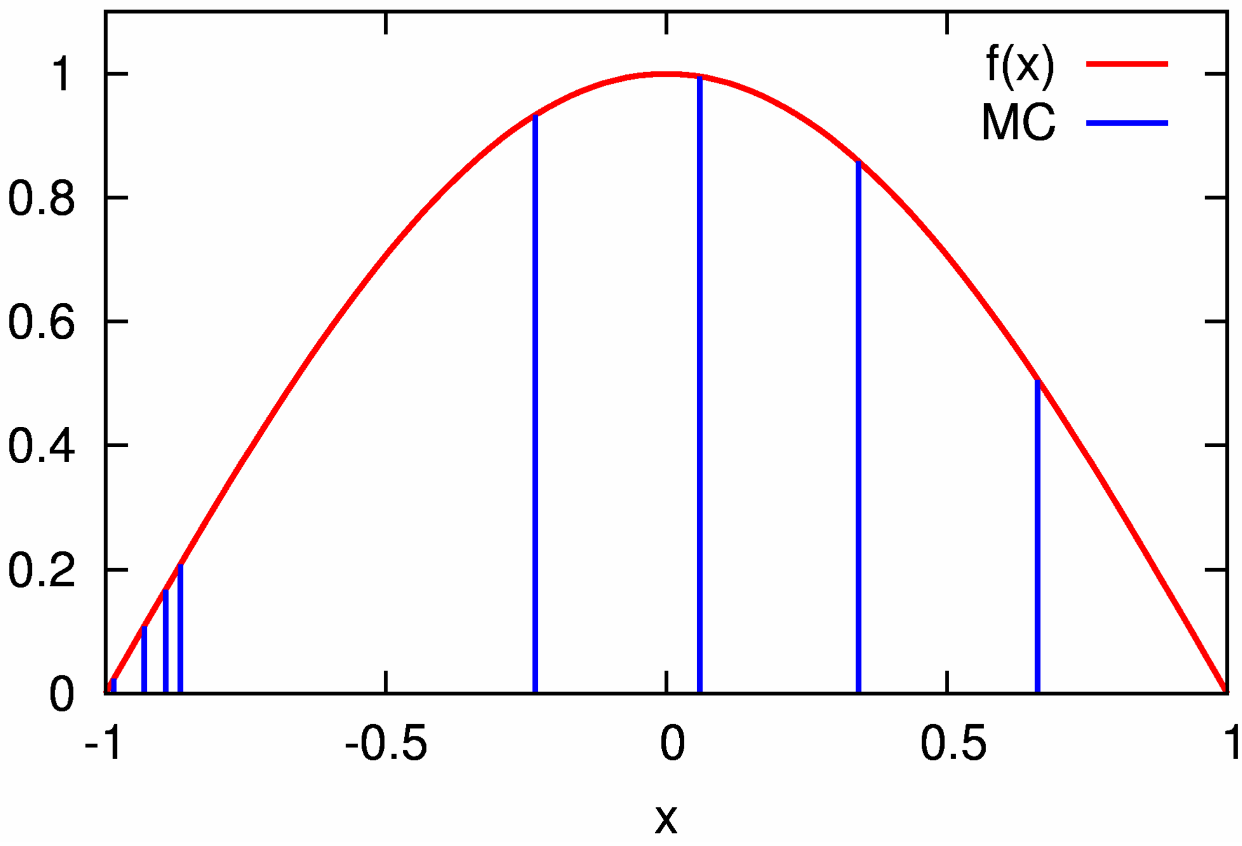
Numerical methods:

- discretization

A brief reminder

Simple example: quadrature of a convex function (in $d = 1$)

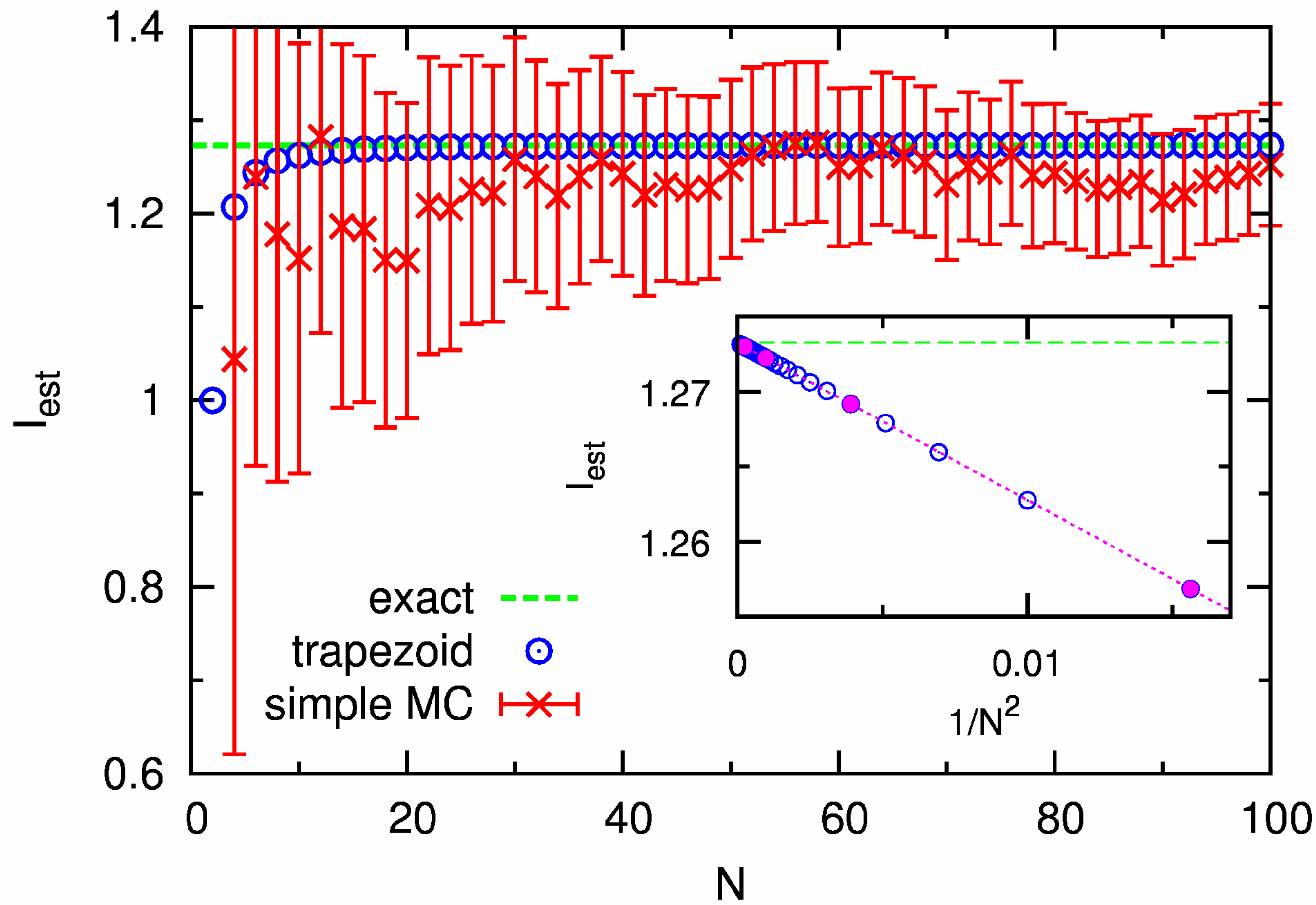


$$I = \int_a^b f(x)\,dx = ?$$

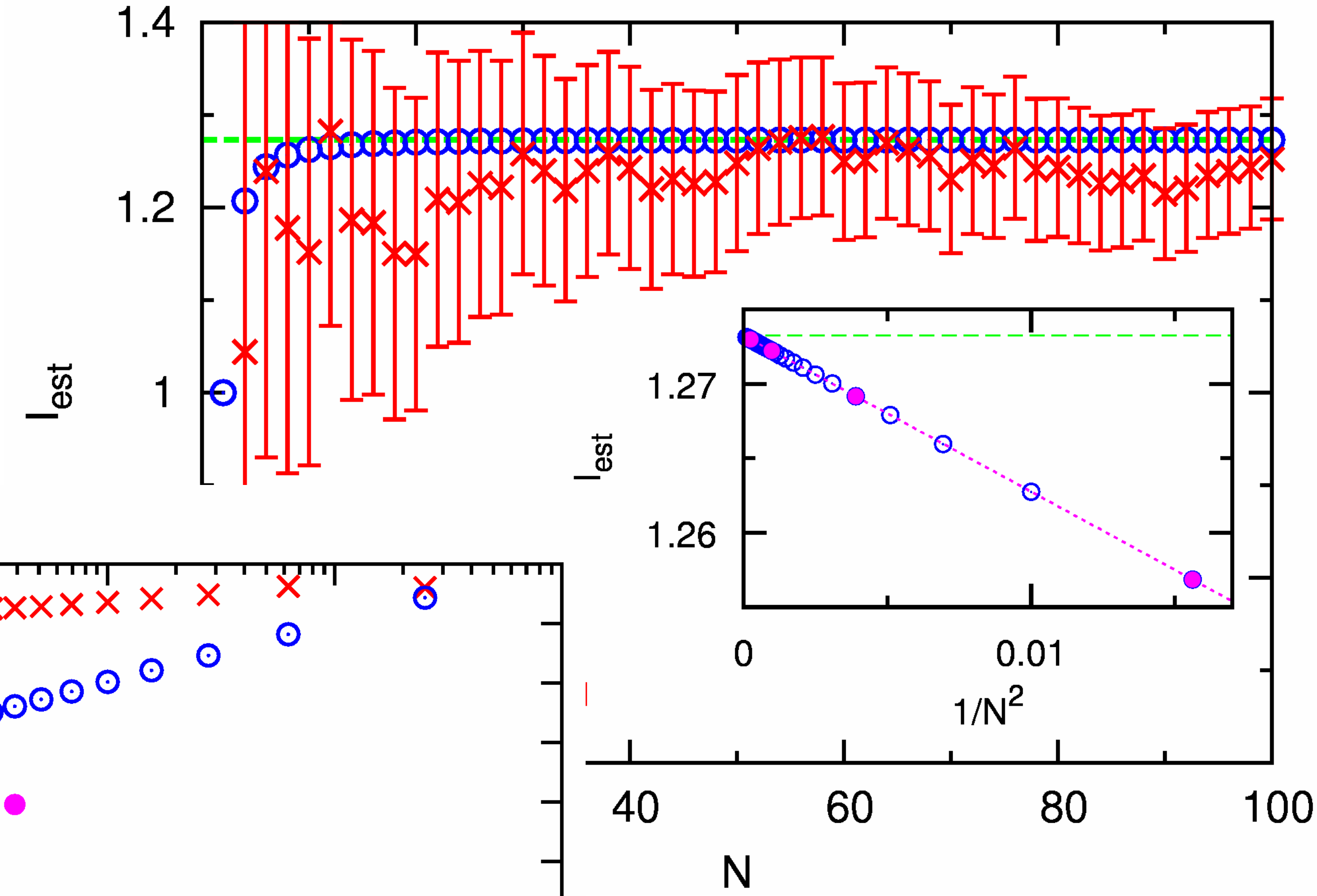
Numerical methods:

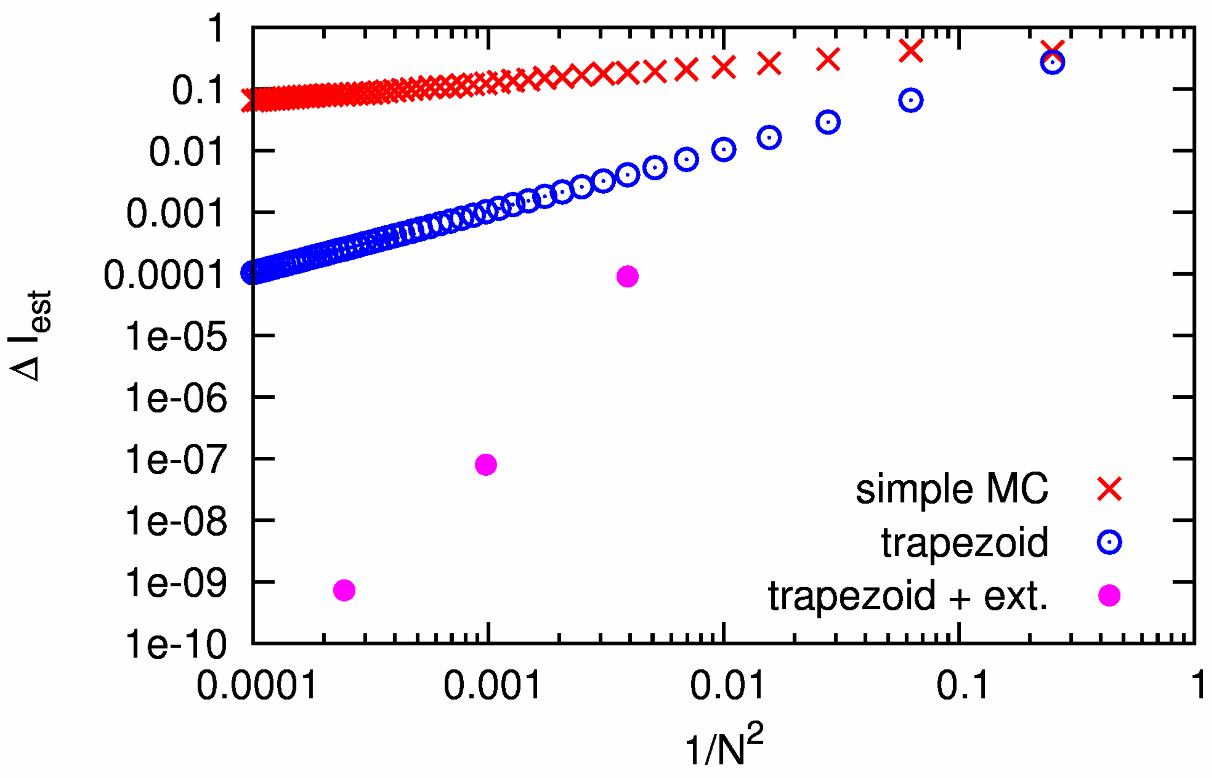
- discretization
- Monte Carlo

Convergence of results?

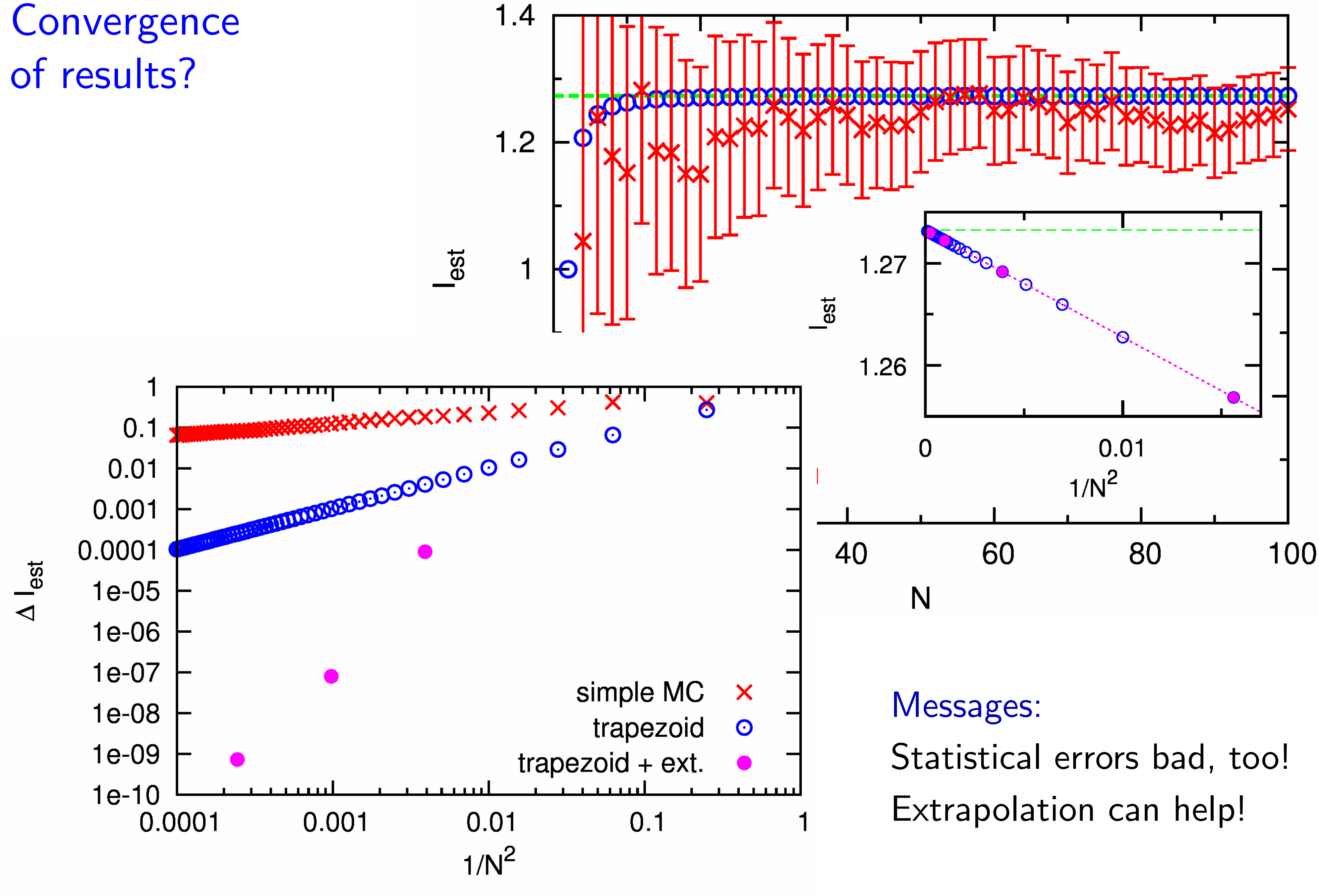


Convergence of results?





Convergence of results?



Messages:

Statistical errors bad, too!

Extrapolation can help!