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

Nils Blümer, Univ. Mainz

Outline

Introduction: Hubbard model, DMFT, HF-QMC

Efficiency of QMC DMFT solvers

Unbiased Green functions and spectra from HF-QMC

Multigrid Hirsch-Fye quantum Monte Carlo algorithm

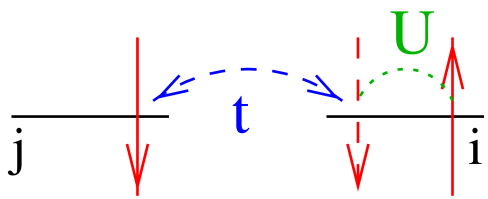
Applications: Mott transitions at large degeneracy / in 3-spin system

Summary and outlook

Introduction

Hubbard model

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



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 $\epsilon_{\boldsymbol{k}}$

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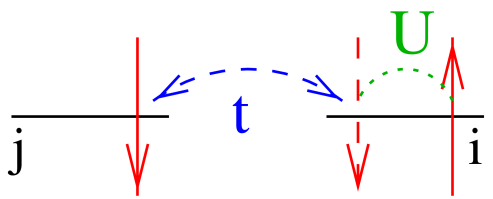

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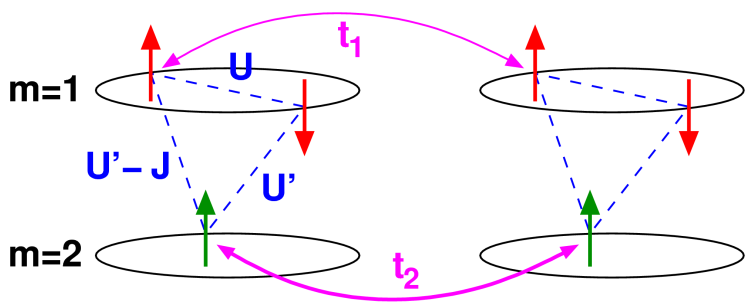

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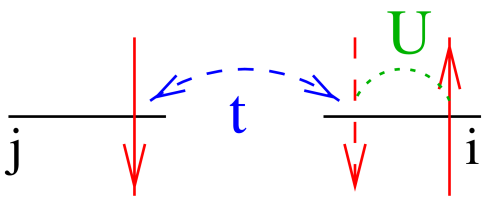

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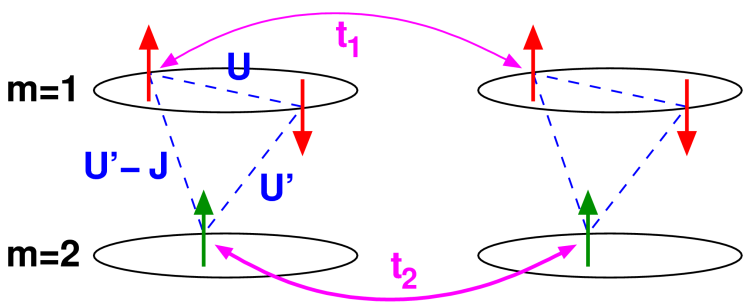

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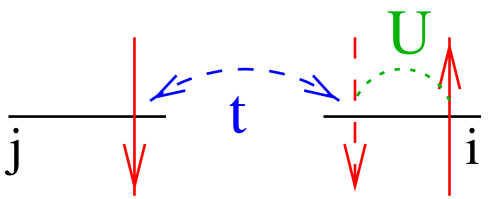

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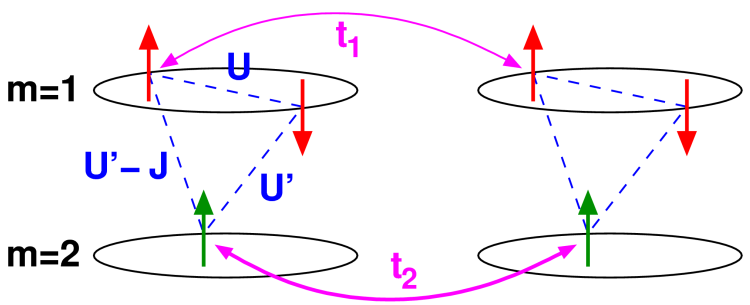

More complexity, more realistic: OSMT, spin+orbital order, LDA+DMFT, . . .

Approaches for Hubbard-type models

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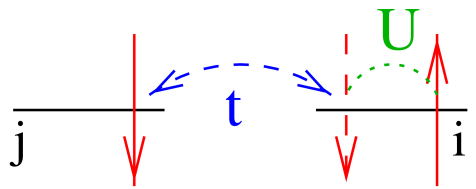
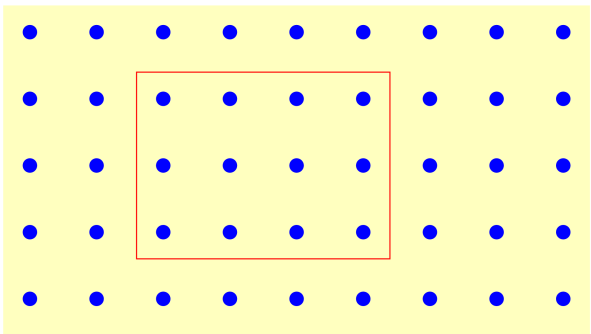


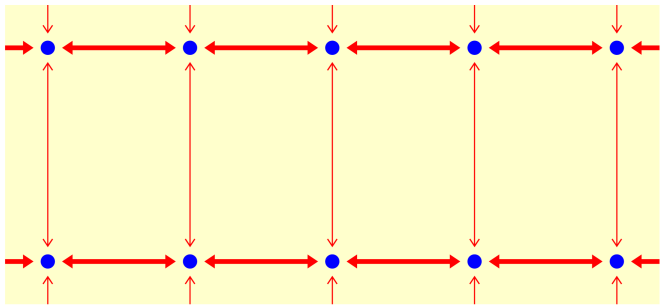
Perturbation theory

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

finite clusters: ED, QMC



$d \to 1$: Bethe ansatz, DMRG



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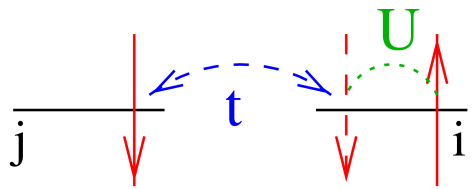

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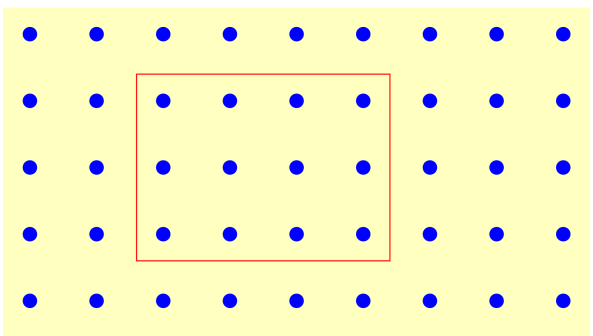

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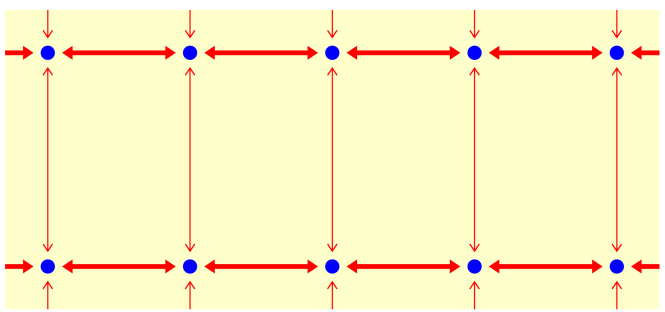


Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$

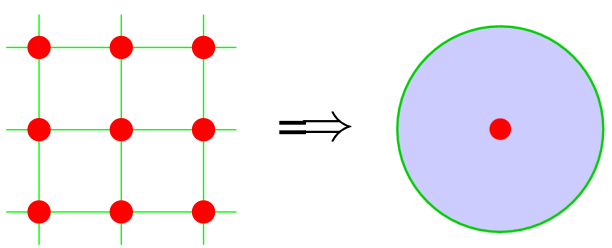
[Metzner, Vollhardt, PRL (1989), Georges, Kotliar, PRL (1992), Jarrell, PRL (1992)]

\+ non-perturbative $\rightsquigarrow$ valid at MIT

\+ dynamical on-site correlations preserved

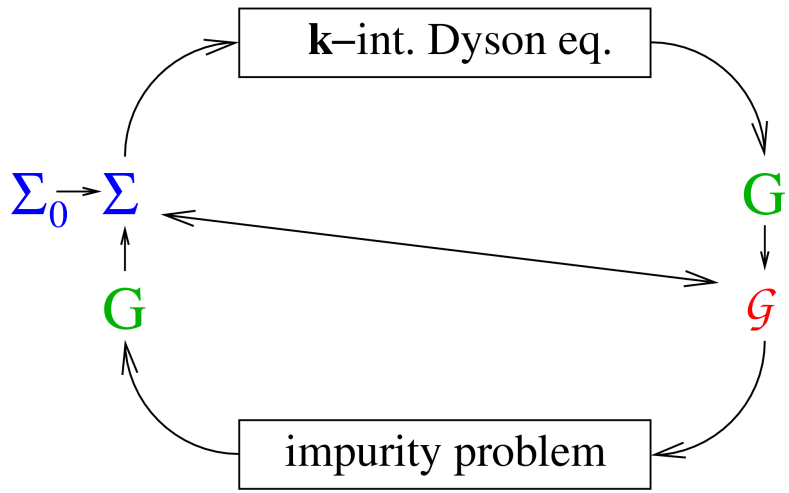
\+ in thermodynamic limit

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



Iterative solution of DMFT equations

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



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

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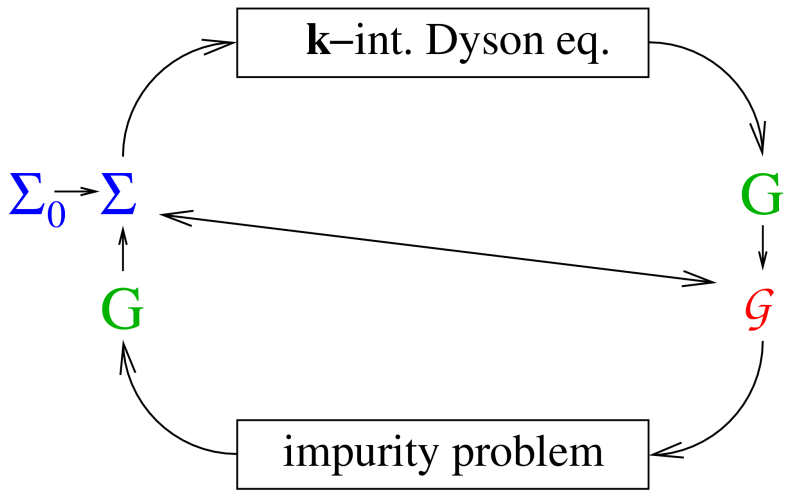

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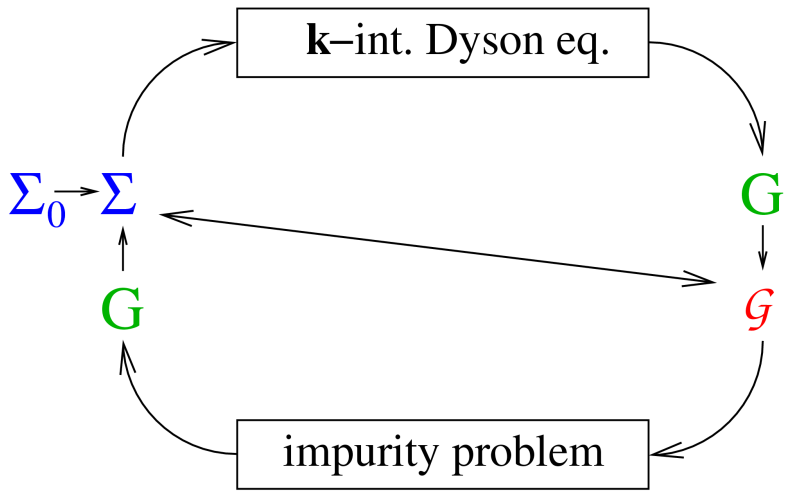

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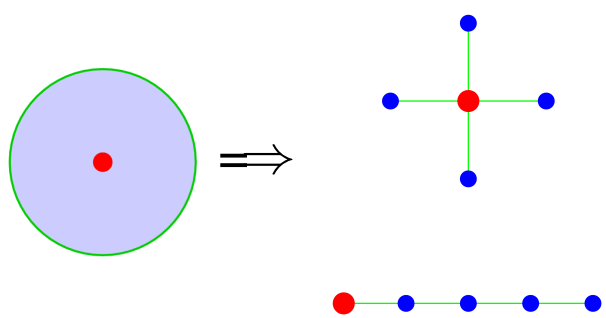
- Exact diagonalization (ED; large finite-size errors)
- Numerical renormalization group (NRG; 1-2 bands)
- Density matrix renormalization group (DMRG)
- Self-energy functional theory (SFT) + ED



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

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

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

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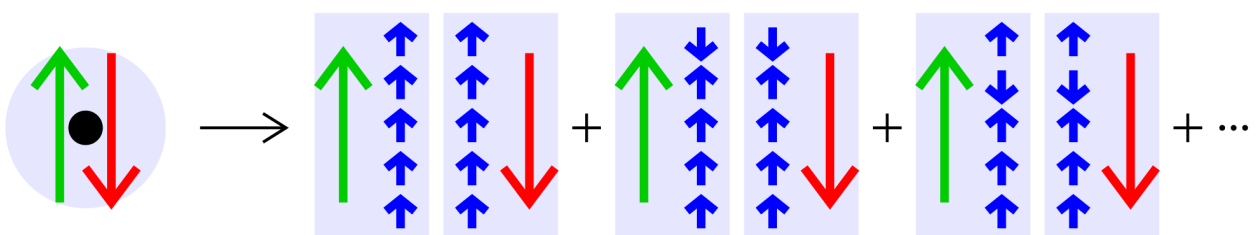

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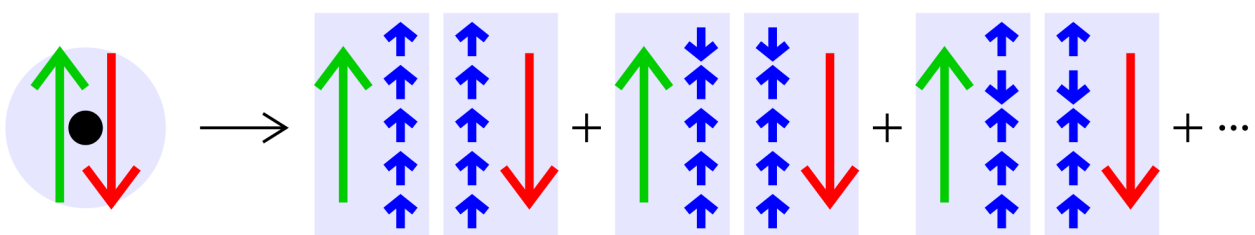

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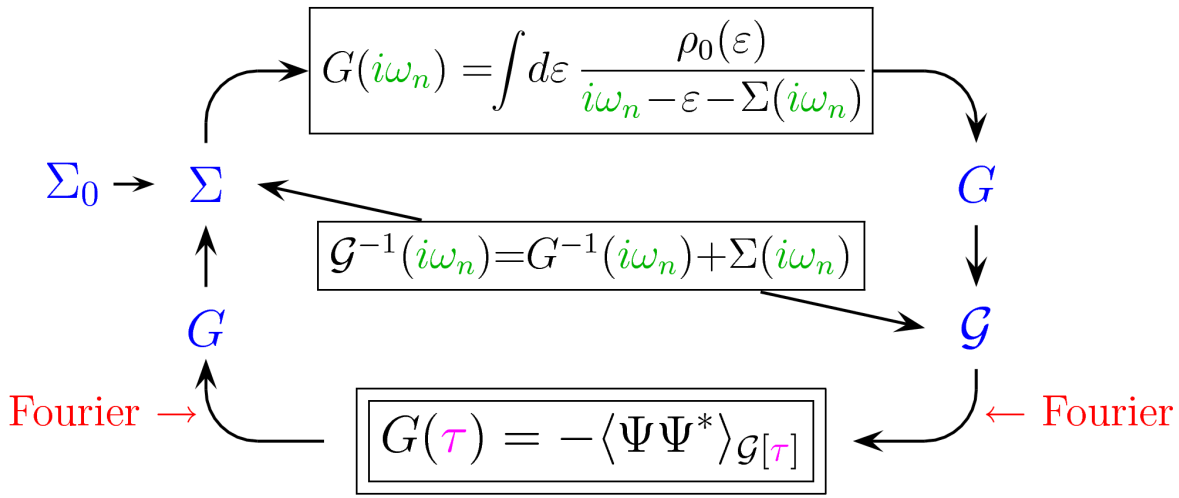
Metropolis MC importance sampling over auxiliary Ising field $\{s\}$: 2^Λ configurations

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

Special issue: Fourier transformations in DMFT-QMC cycle

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



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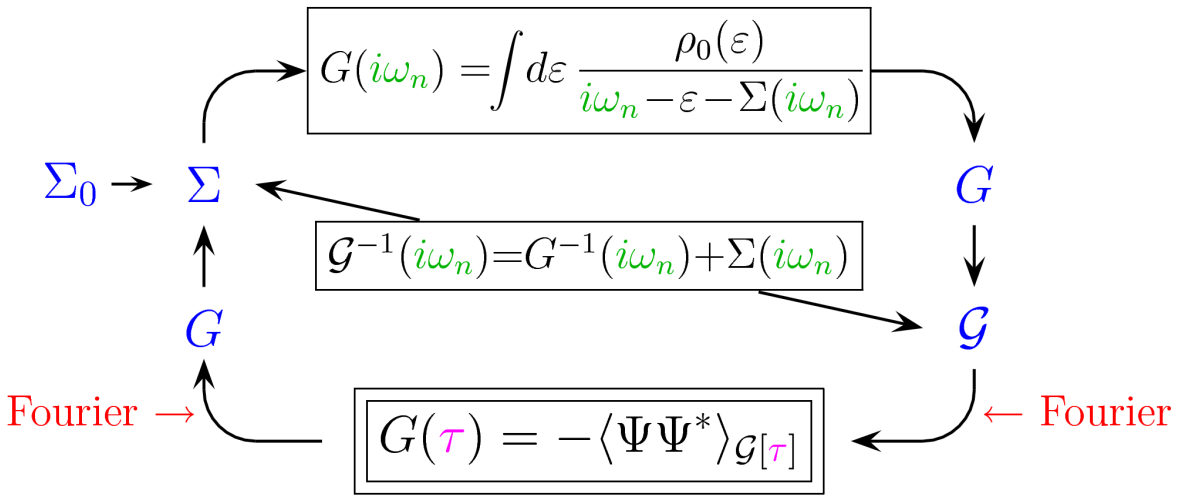
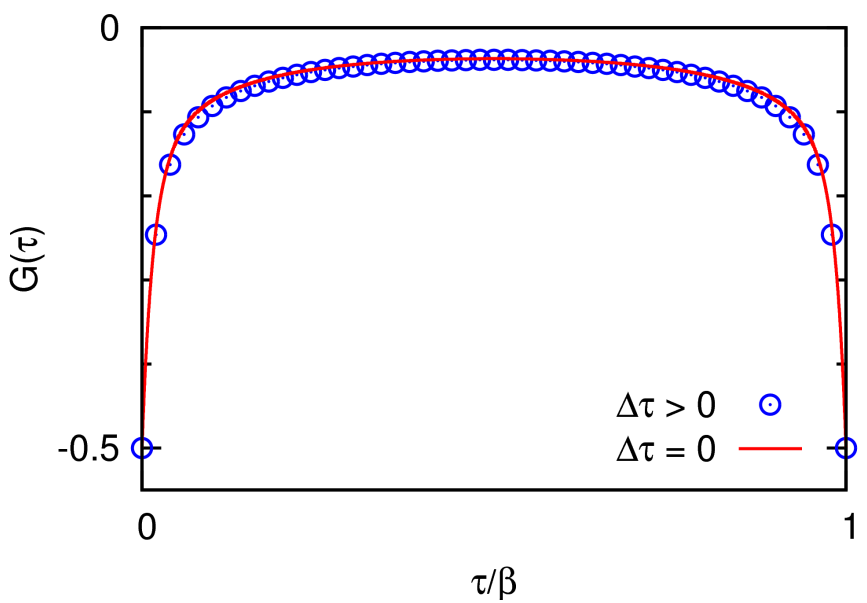
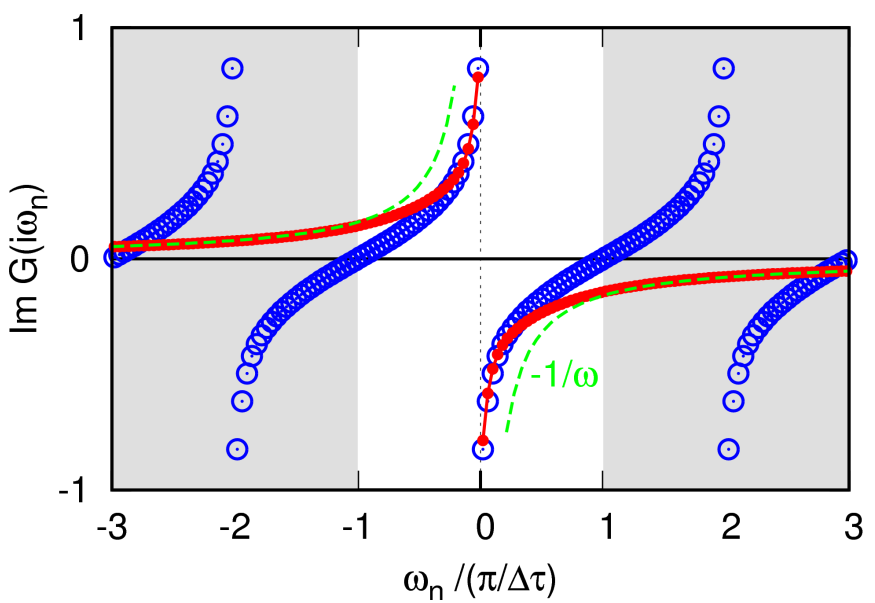


Naive discrete Fourier transformation $\rightsquigarrow$ oscillations (instead of $G(\omega) \overset{\omega\to\infty}{\longrightarrow} 1/\omega$)



naive FT $\longrightarrow$



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

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

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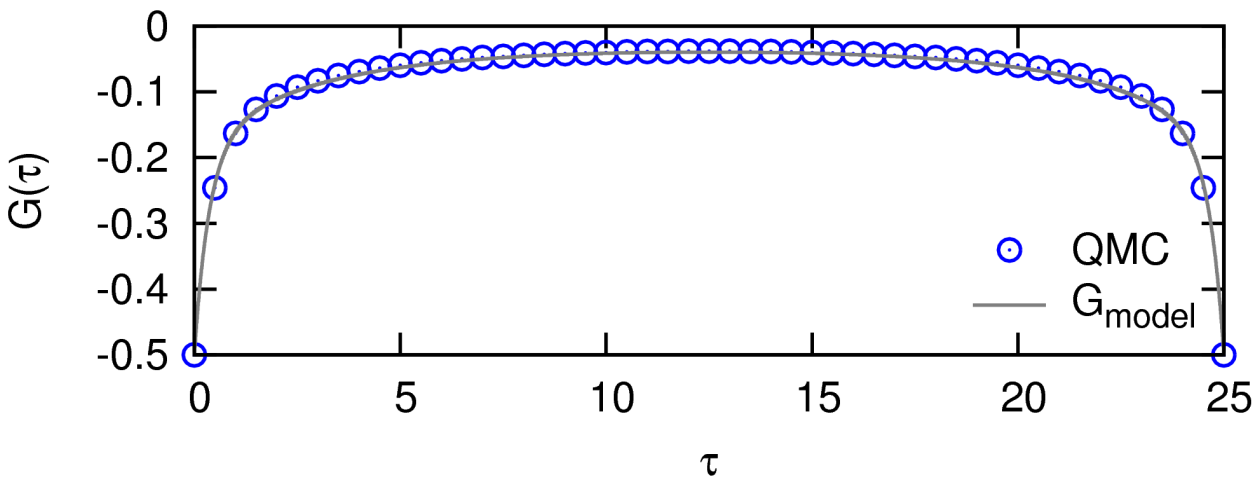

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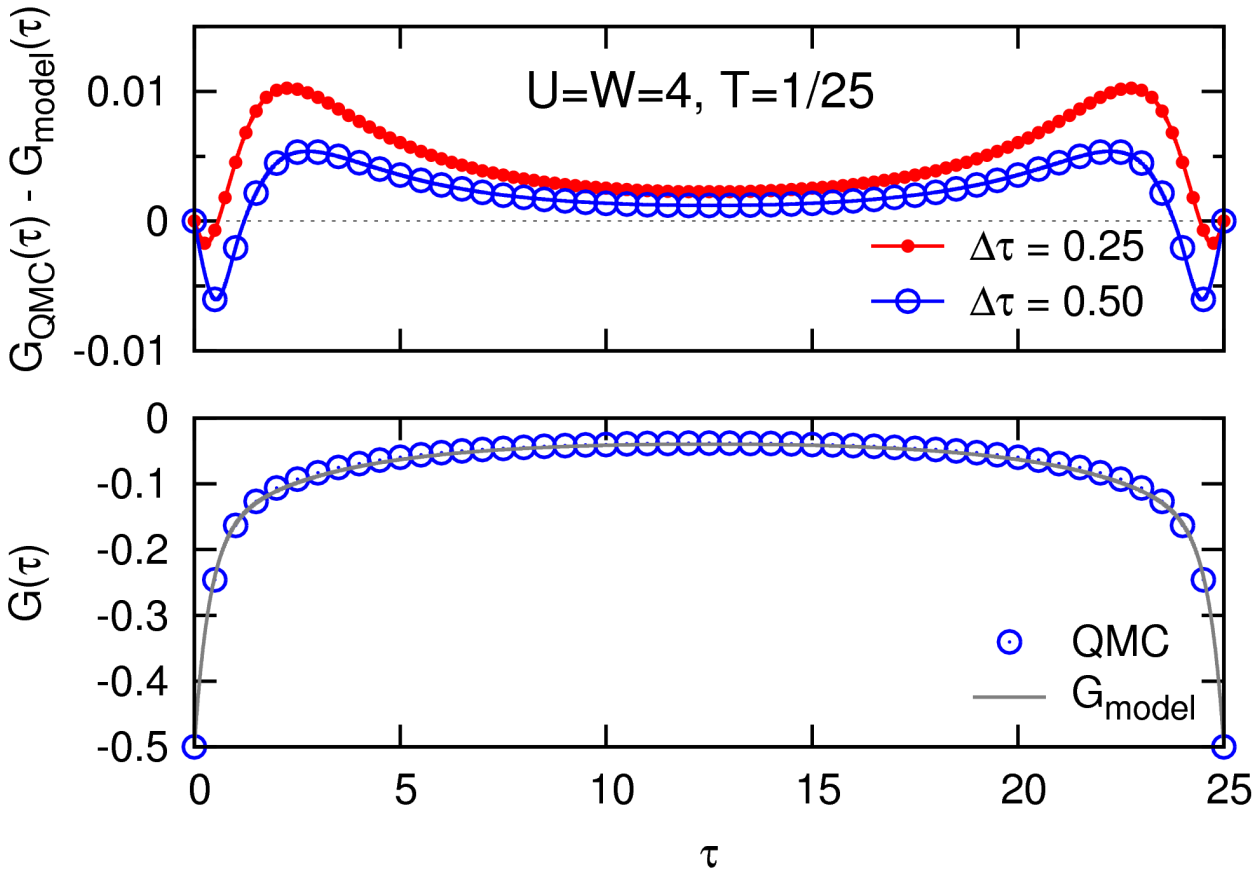

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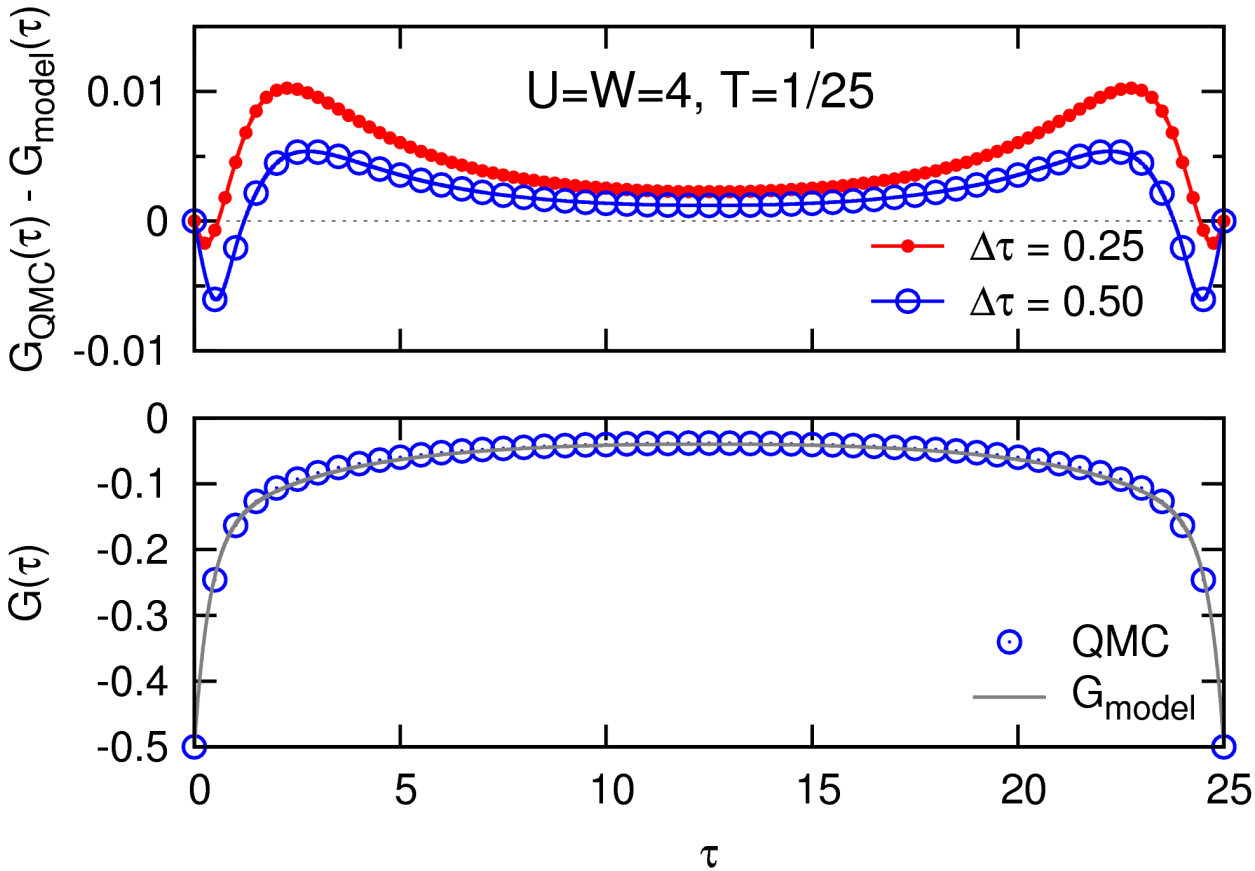

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Current project: replace spline interpolation by smooth fit!

Fourier trafo schemes: self-energy Σ ($T = 0.1$, $U = 5$)

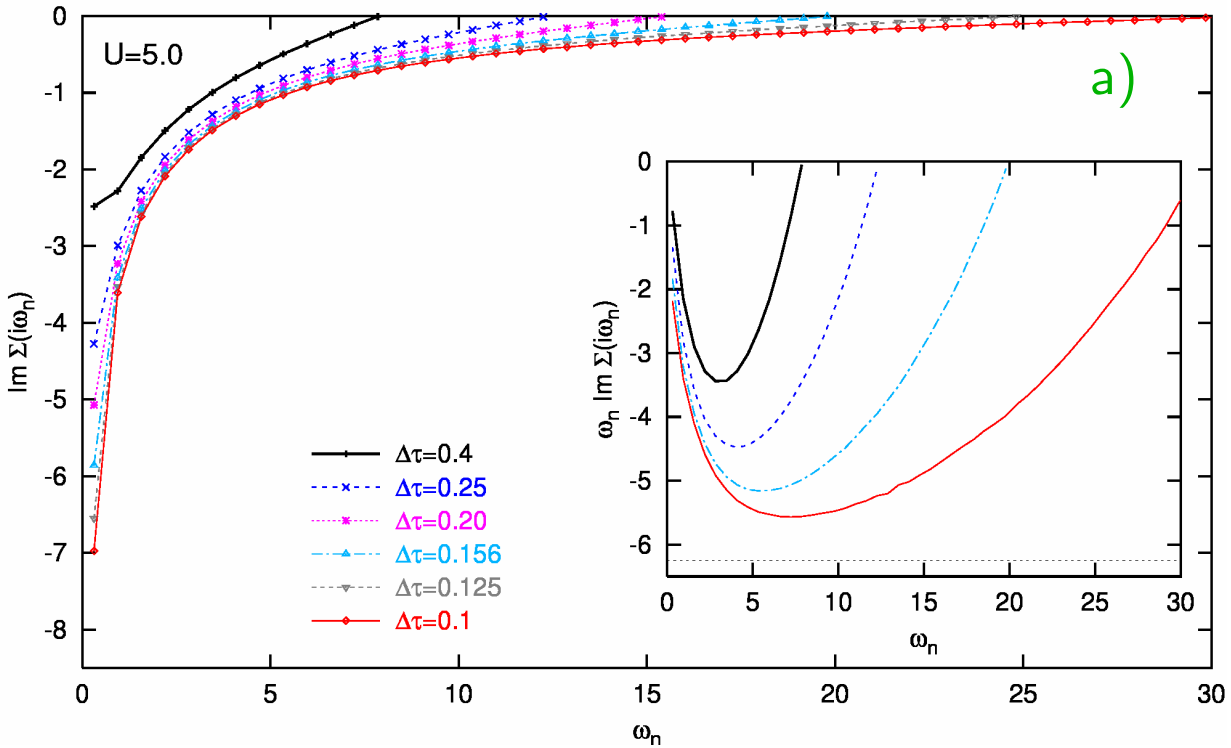
a) "Ulmke smoothing",

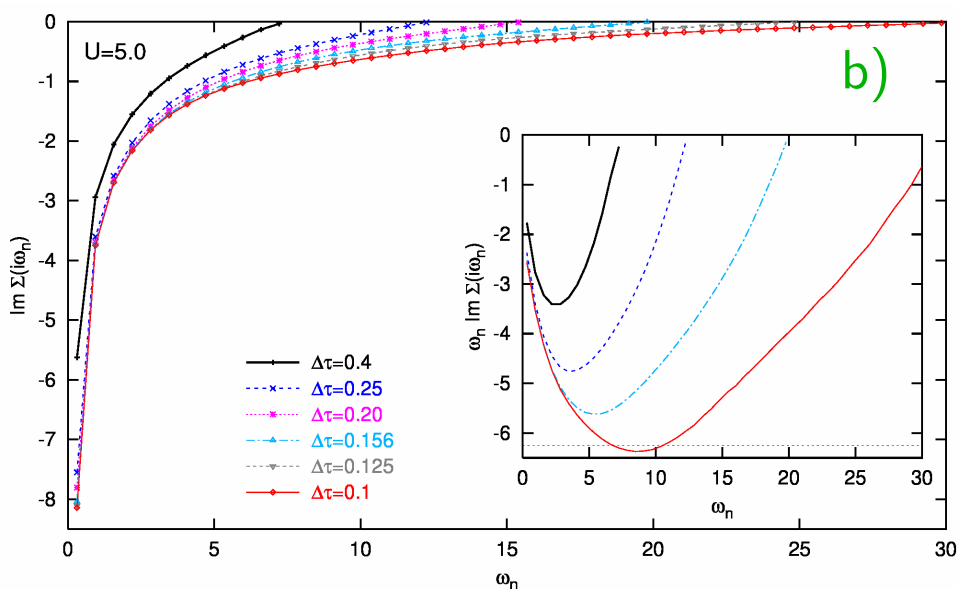
b) improved "smoothing",

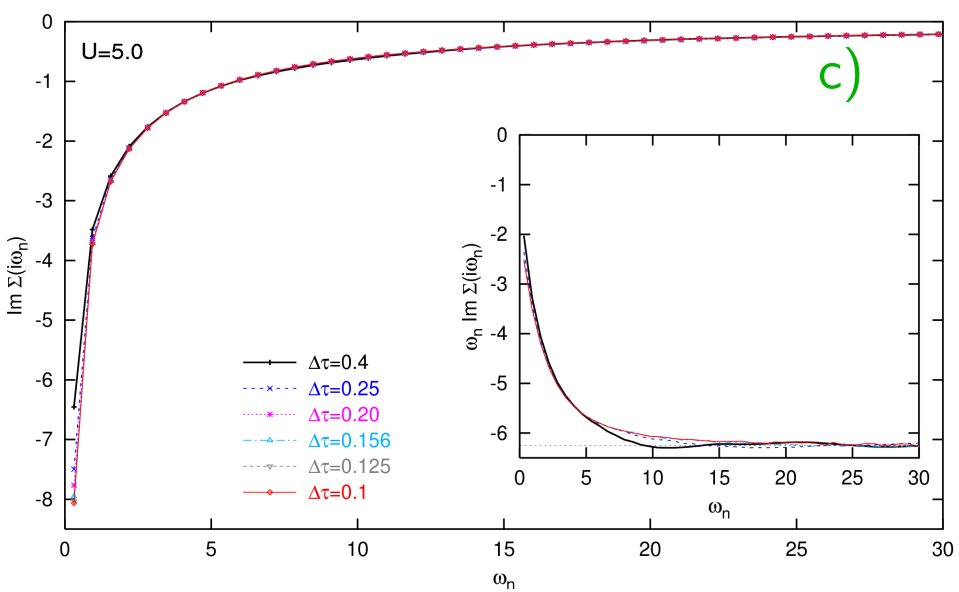
c) cubic spline + analytic high-frequency corrections

low-frequency errors of $\Sigma(\omega)$:

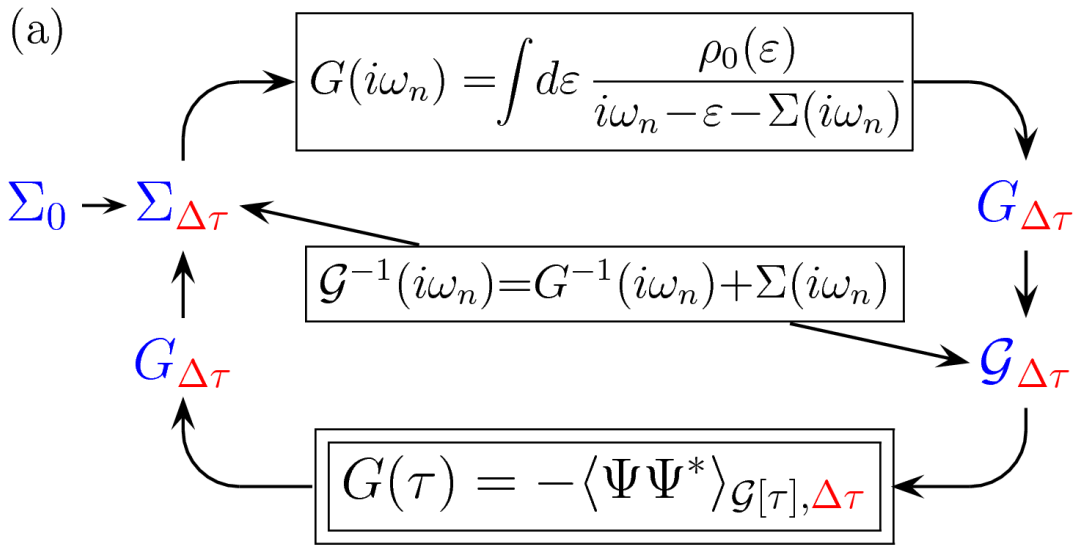
- large in a)
- small in b) and c)

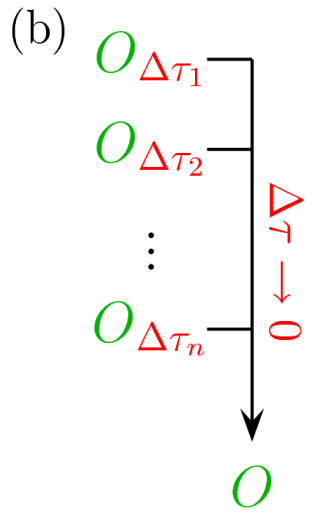






Self-consistency cycle using conventional HF-QMC





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

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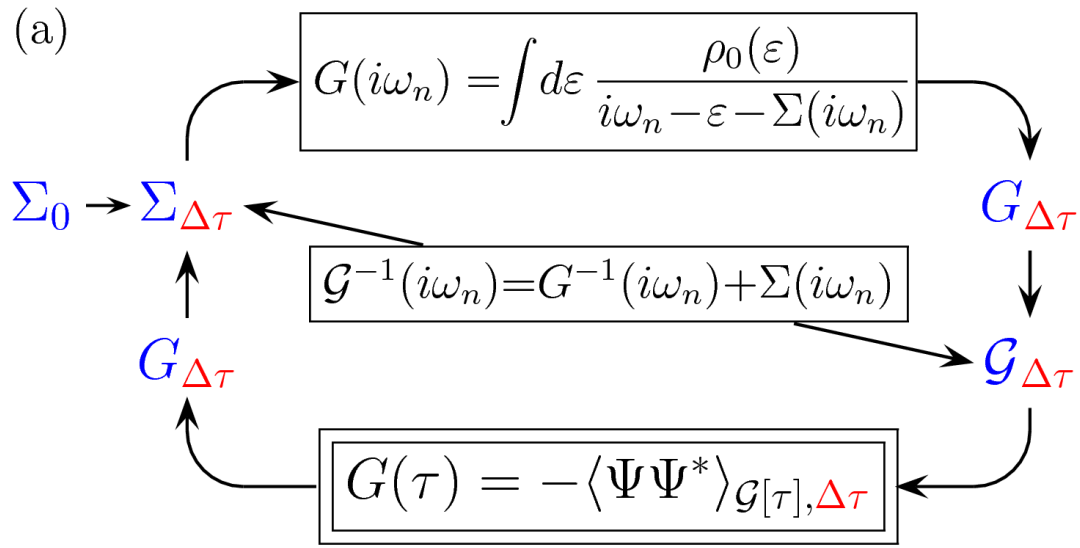

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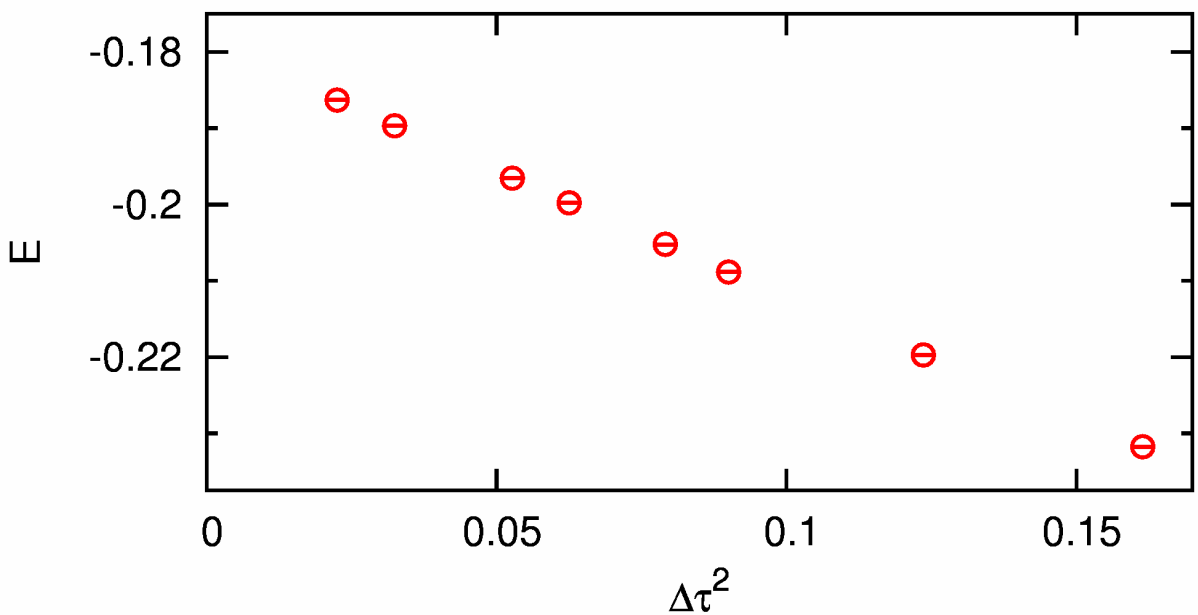
Example: energy E for $U = W = 4$ (Bethe DOS), $T = 1/45$

[NB, PRB (2007)]



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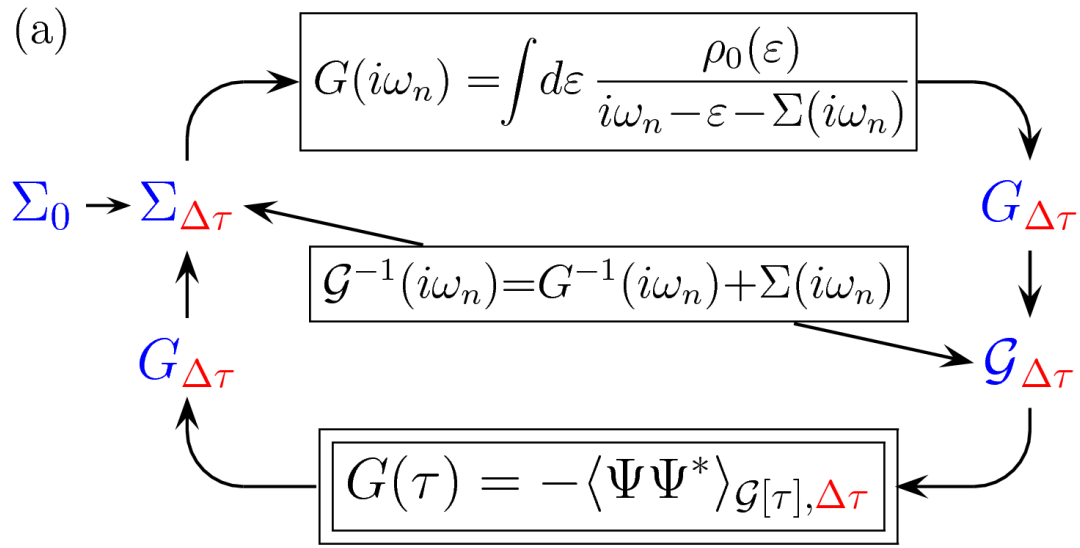

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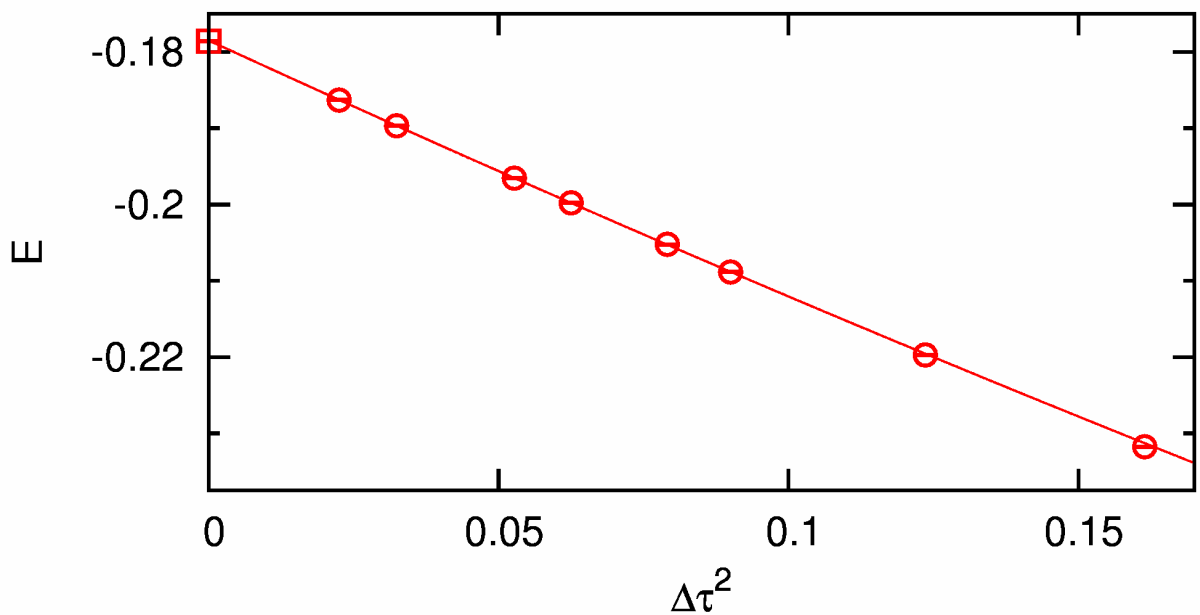


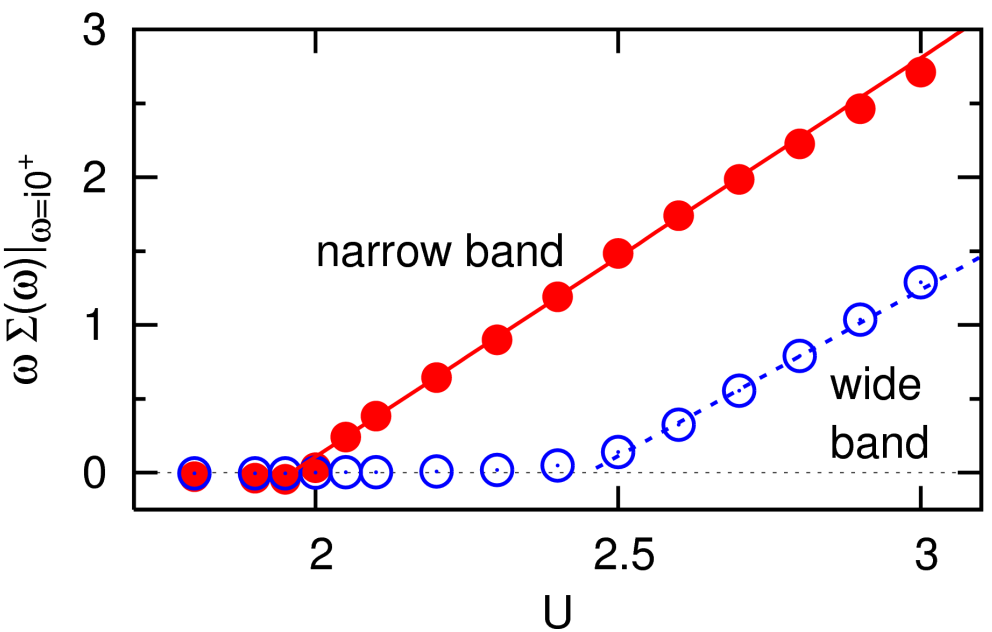
Selected applications

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



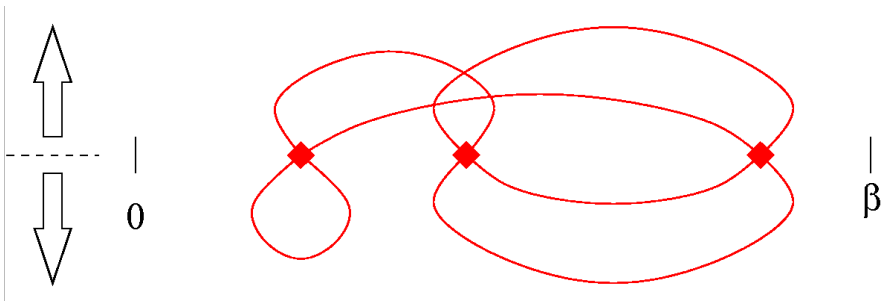
[C. Knecht, NB, and P.G.J. van Dongen, PRB 72, 081103(R) (2005)]

Efficiency of QMC DMFT solvers

New development: continuous-time QMC algorithms

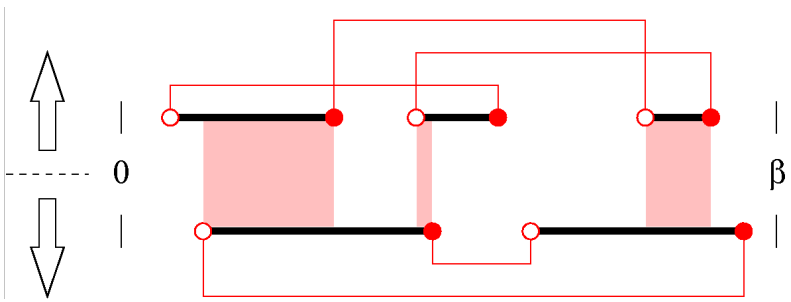
1. weak-coupling expansion

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



2. hybridization expansion

[Werner et al., PRL (2006)]



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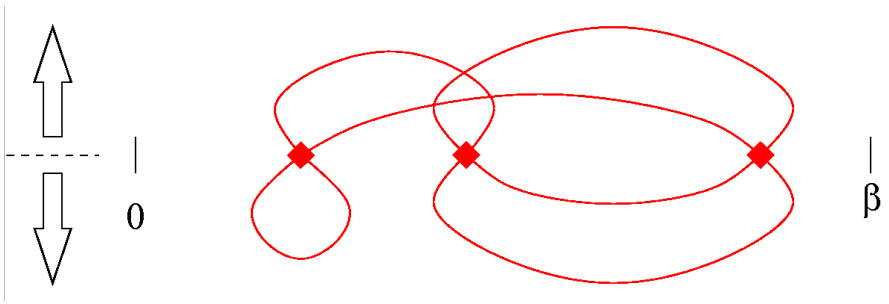

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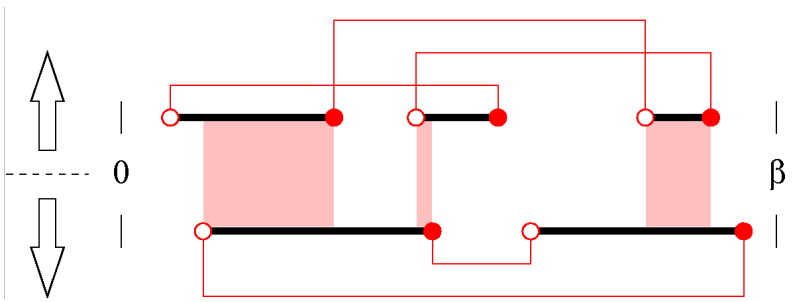
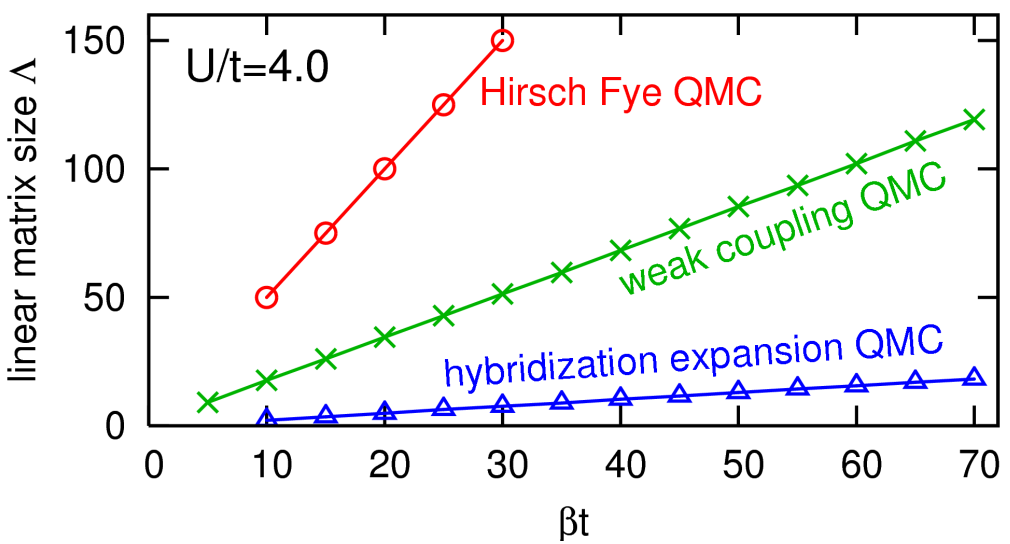


CT-QMC methods: smaller matrices

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



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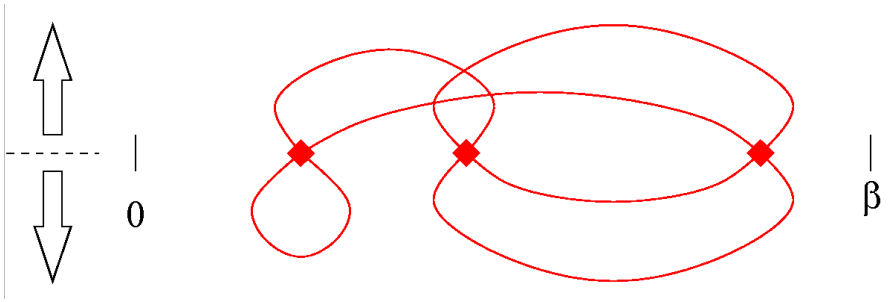

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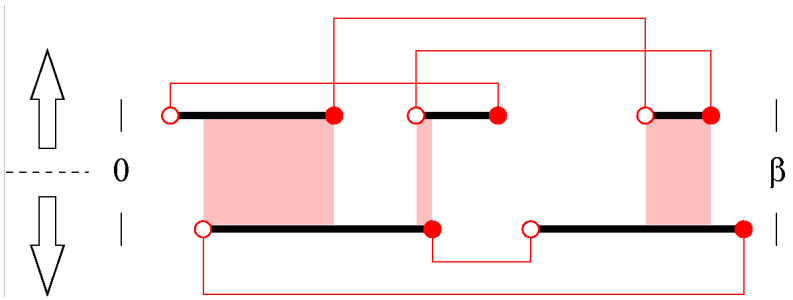

CT-QMC methods: smaller matrices

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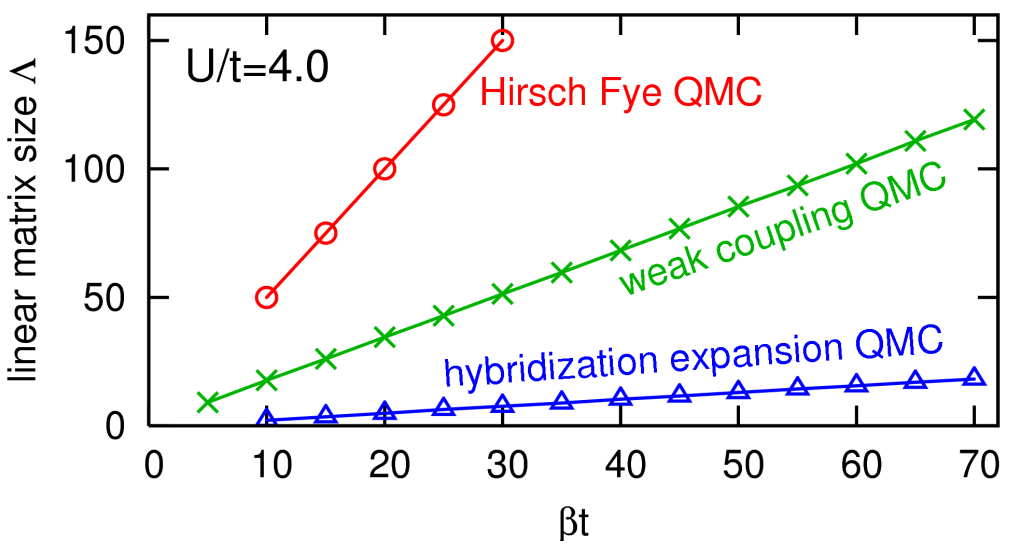
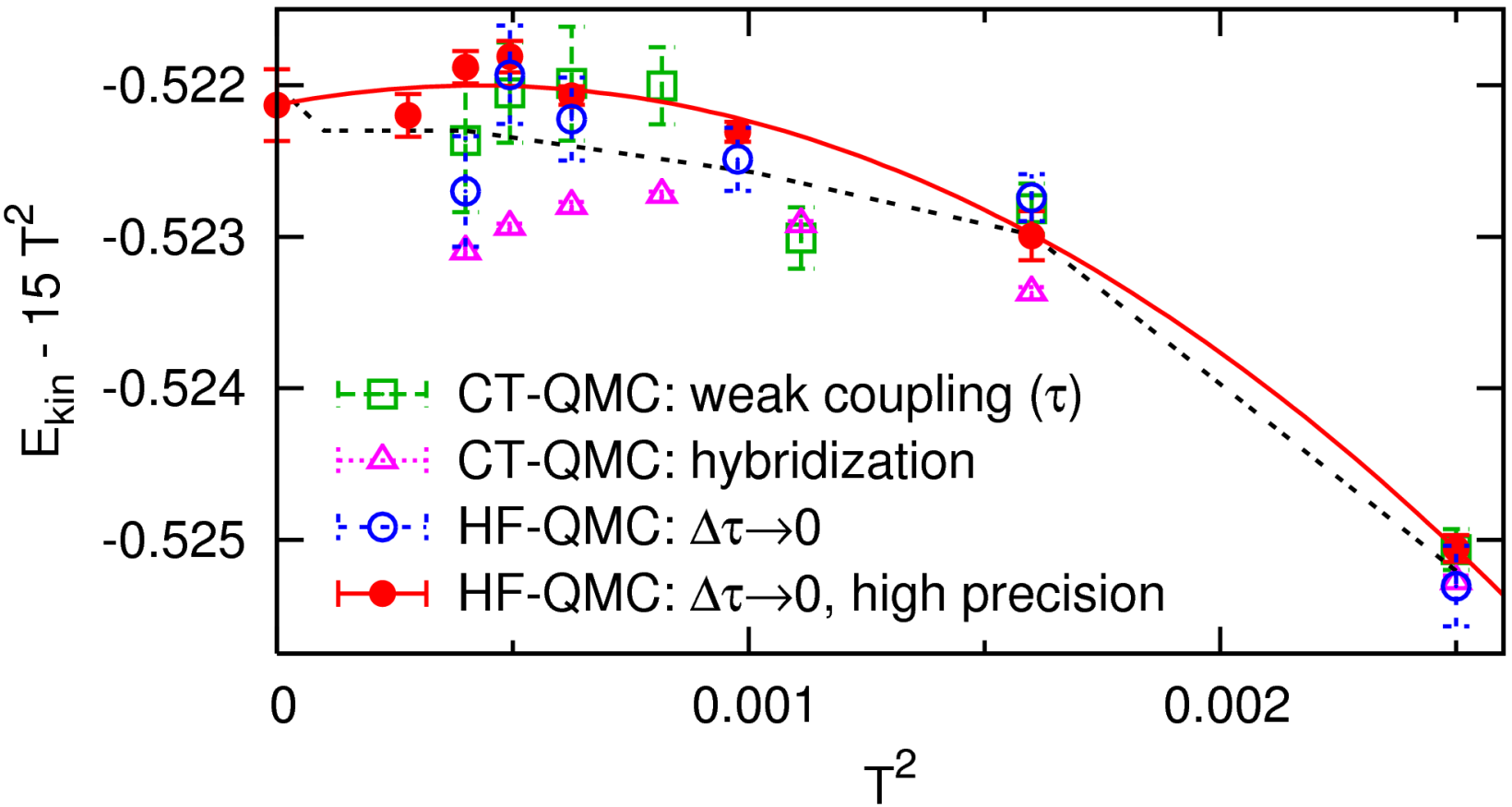
Claim [Troyer (2006)]:
"CT-QMC more efficient than HF-QMC by orders of magnitude"



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

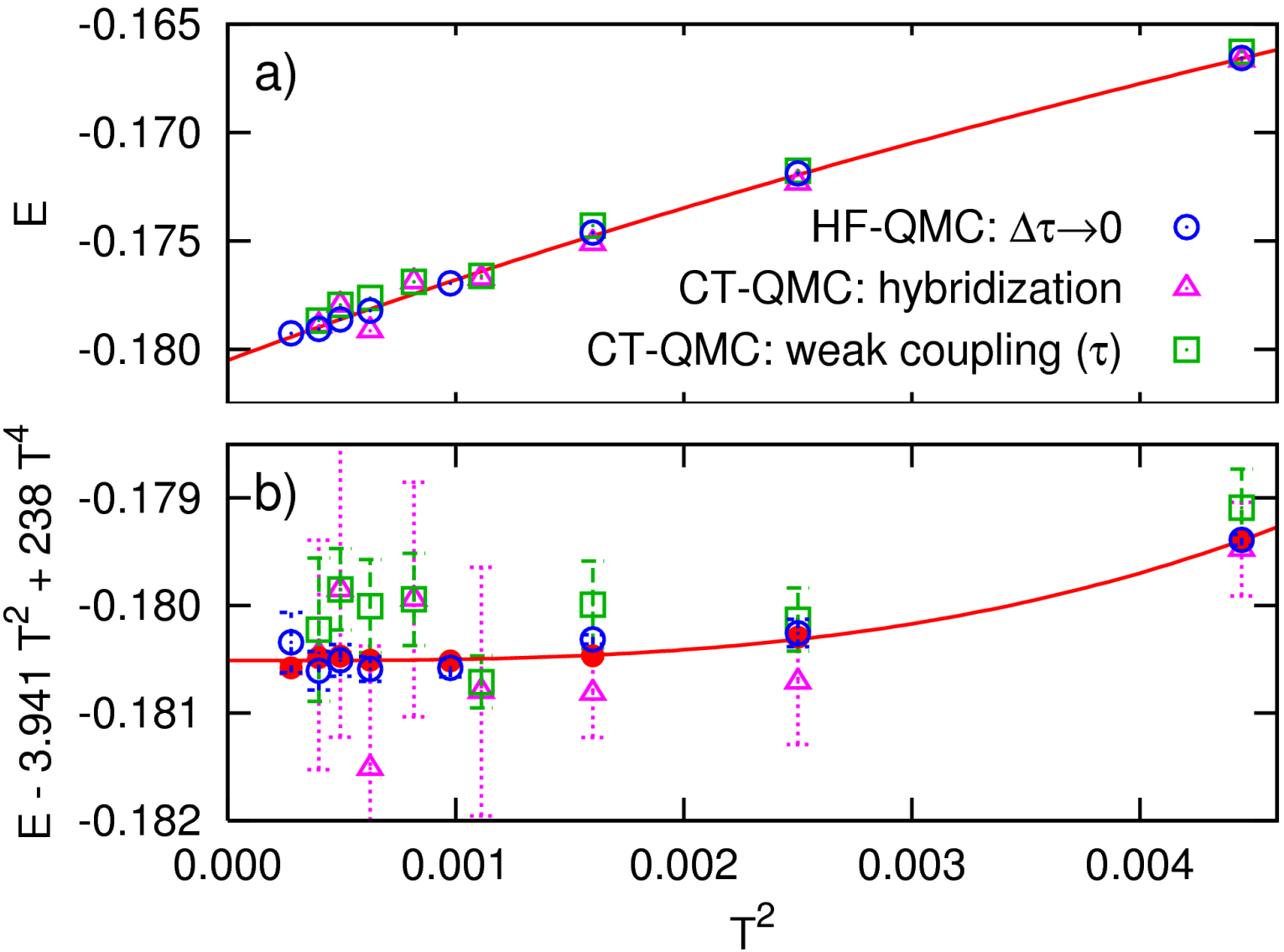
140 CPU hours on AMD Opteron 244 (serial) / mix of Opterons (parallel)



Similar precision for HF-QMC and weak-coupling CT-QMC

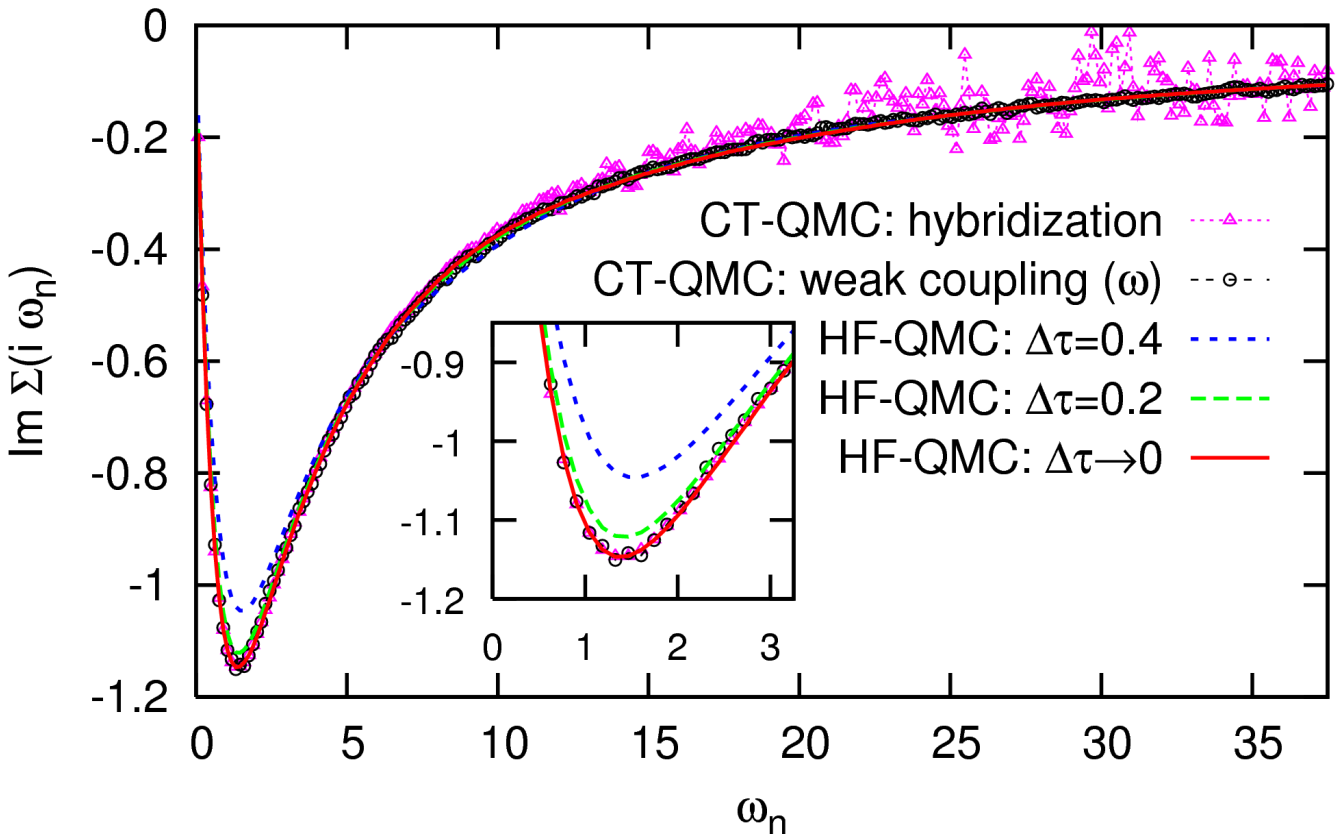
Systematic errors in hybridization CT-QMC data! [NB, PRB **76**, 205120 (2007)]

Comparison for 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

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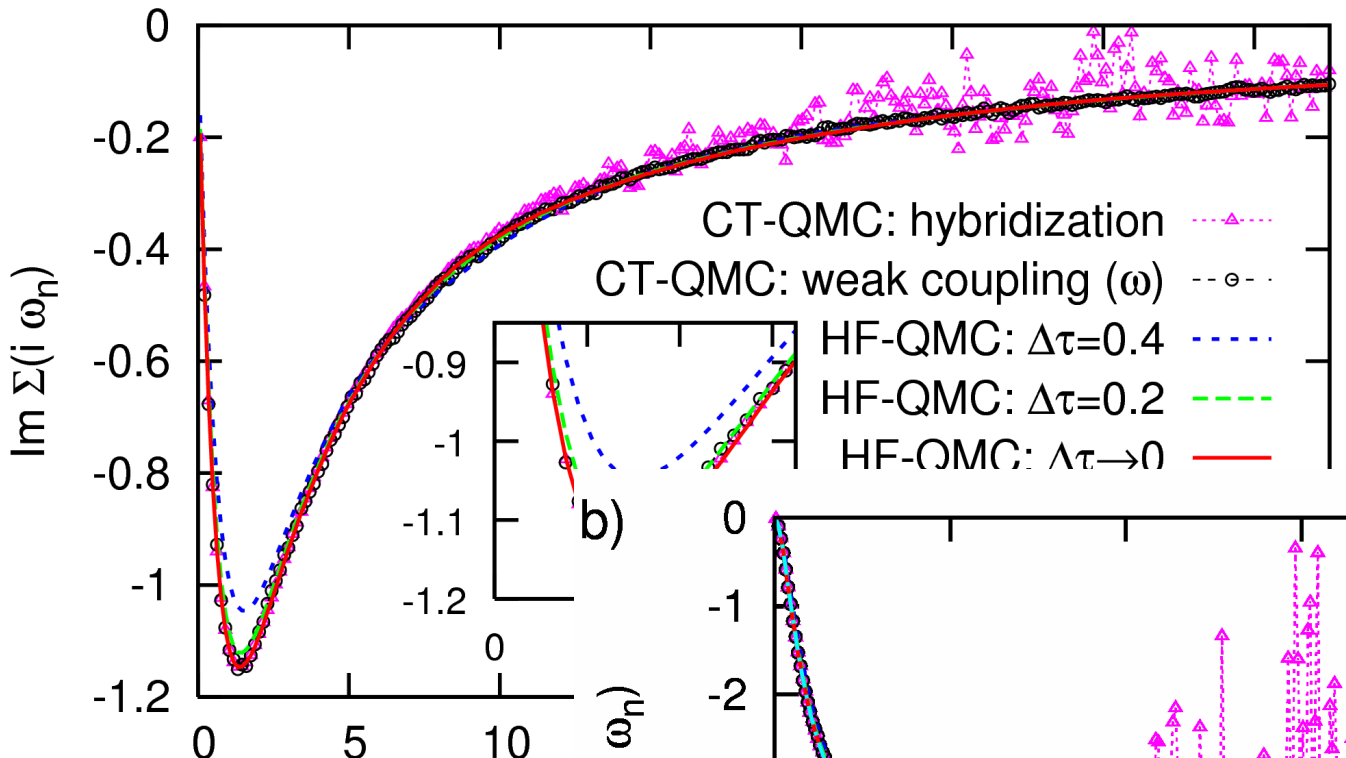
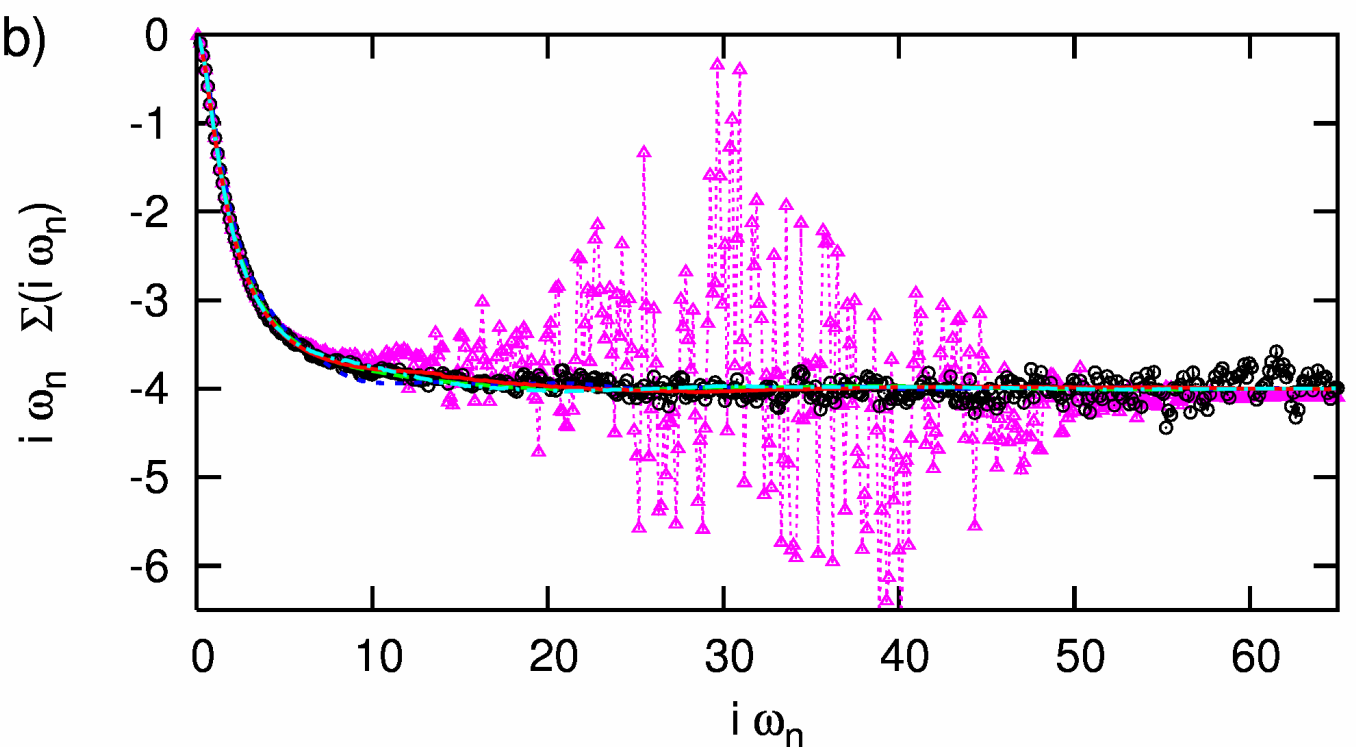
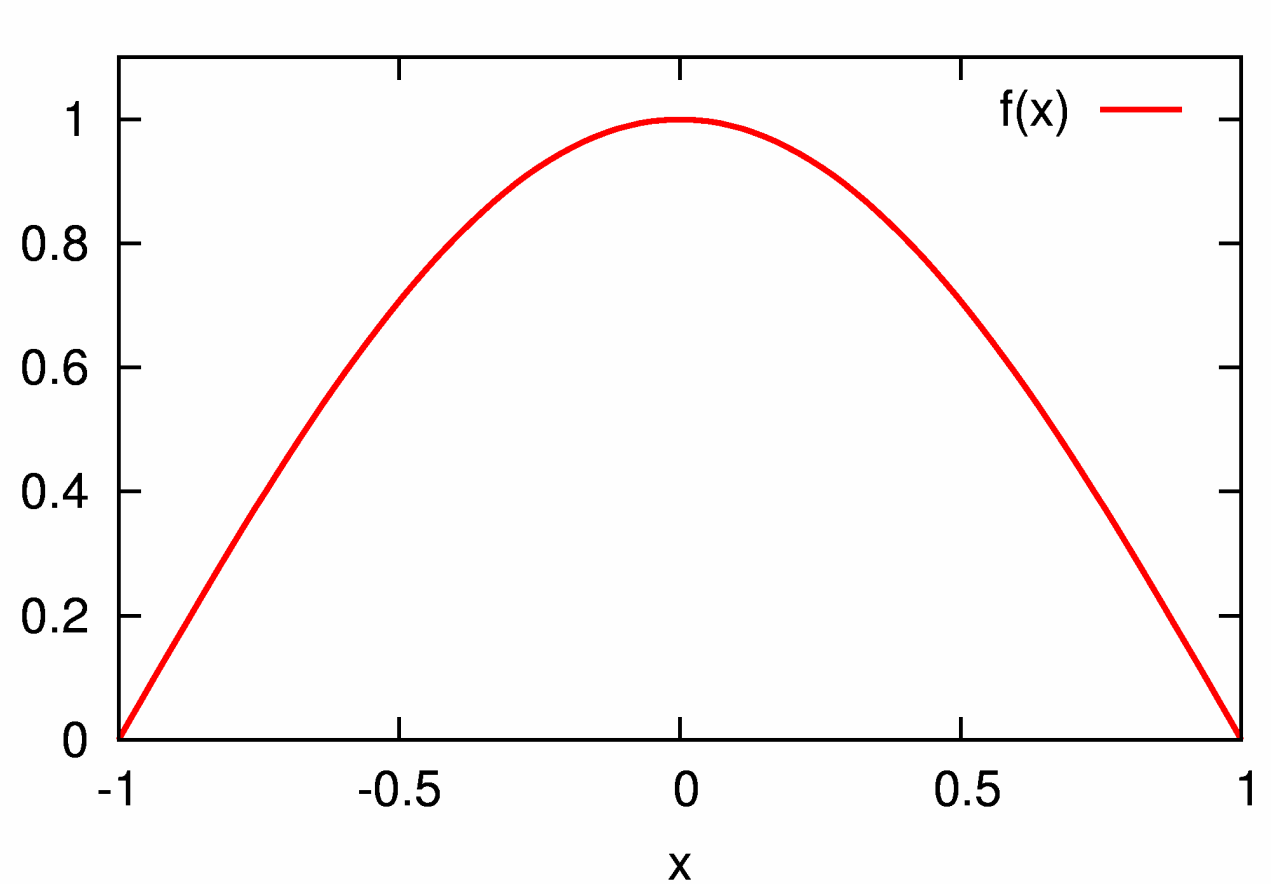


b)



large fluctuations in CT-QMC

Excursion: numerical quadrature of a convex function (in $d = 1$)



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

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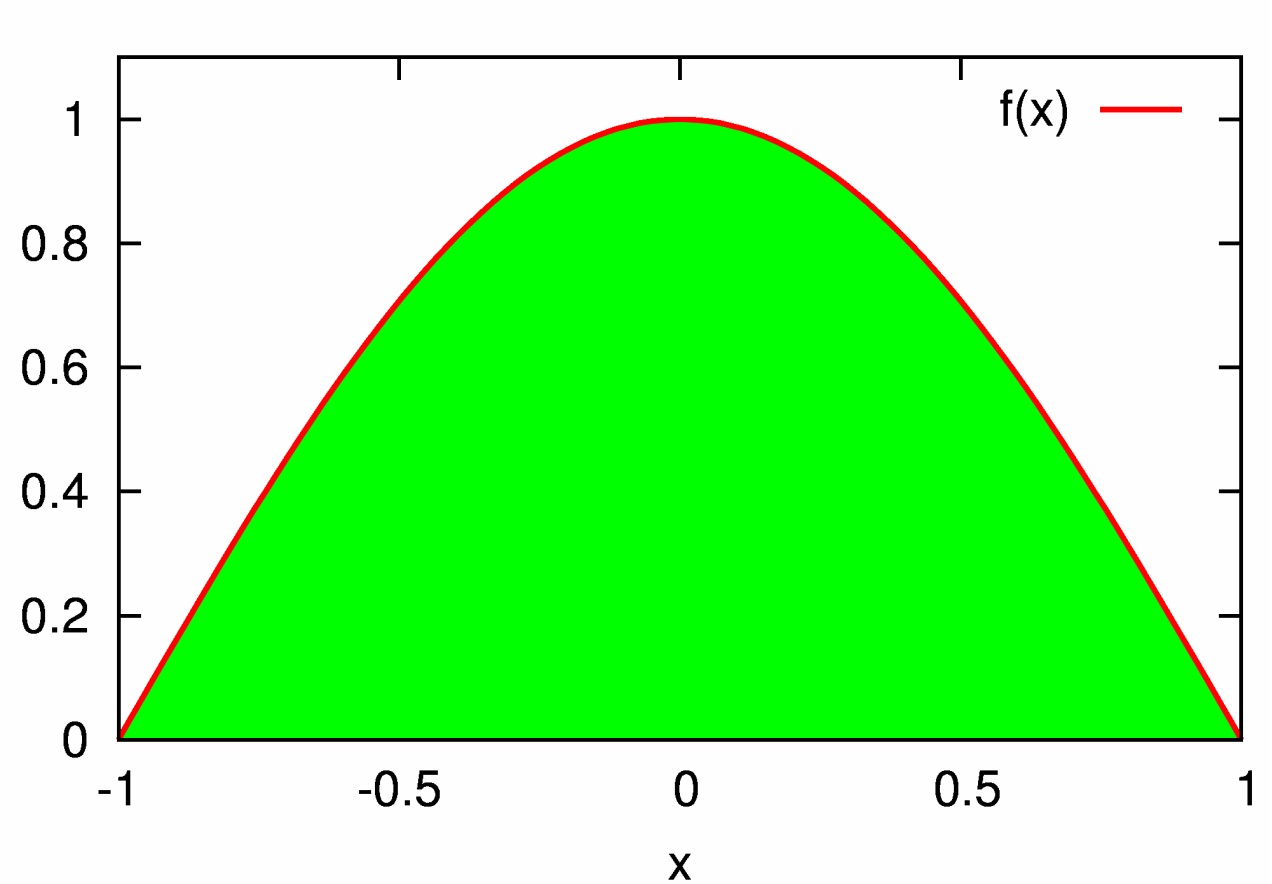

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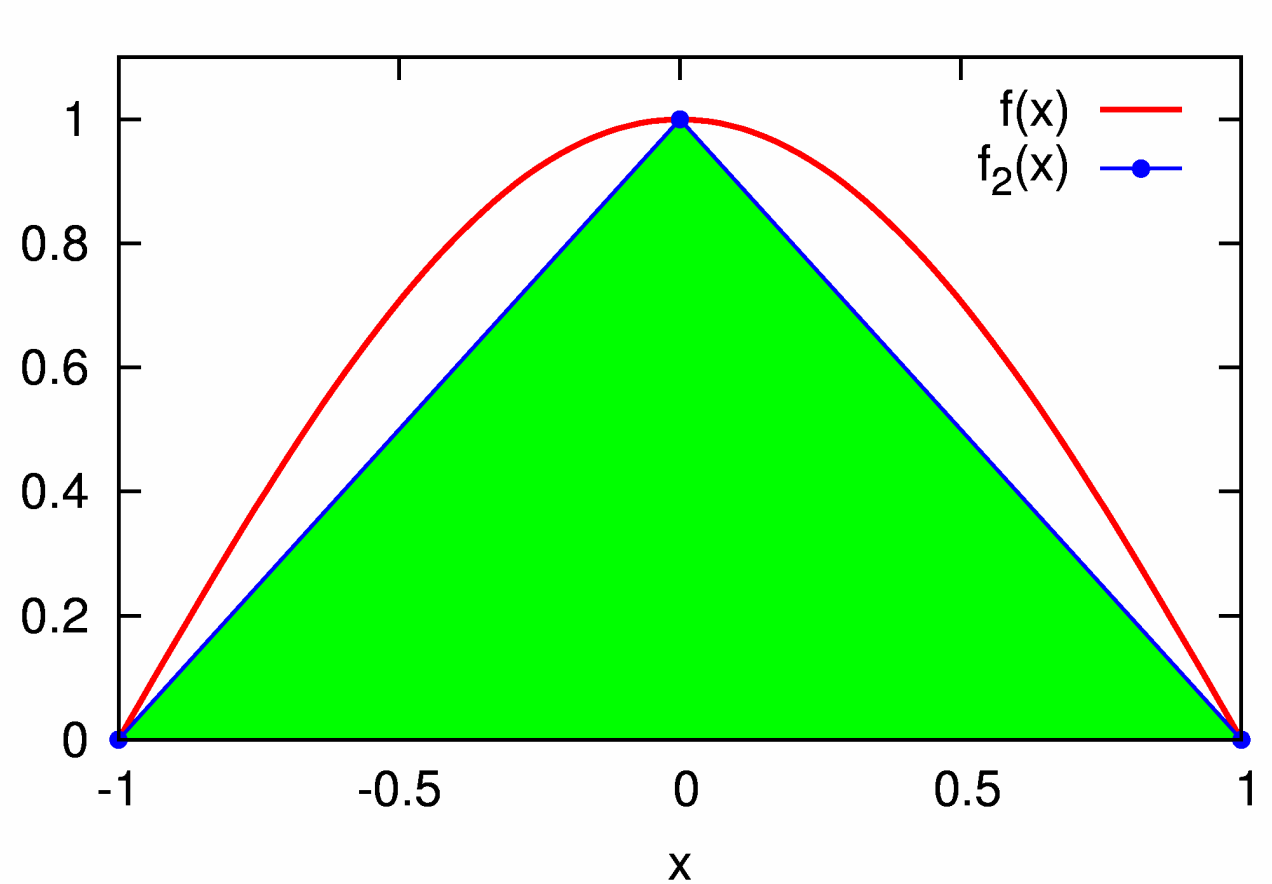

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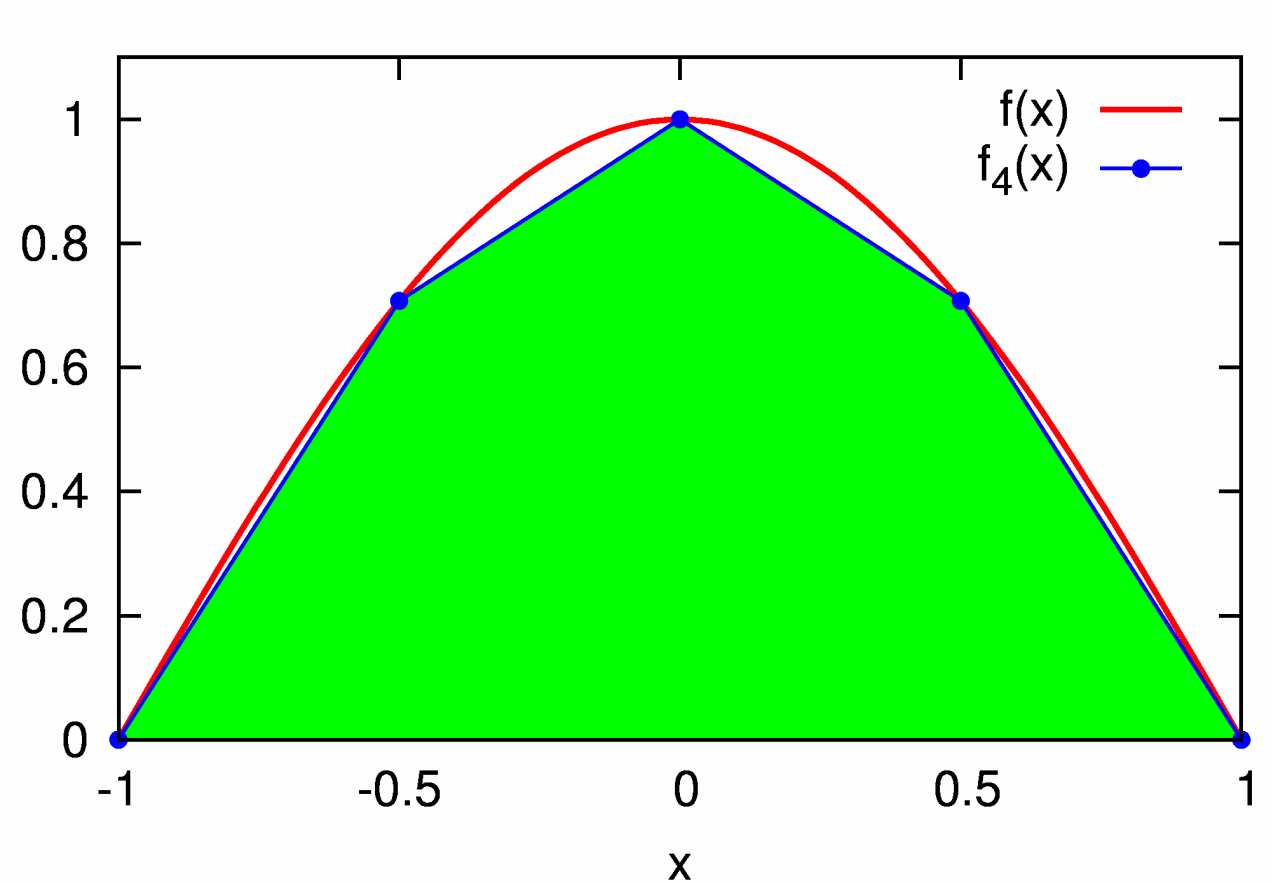

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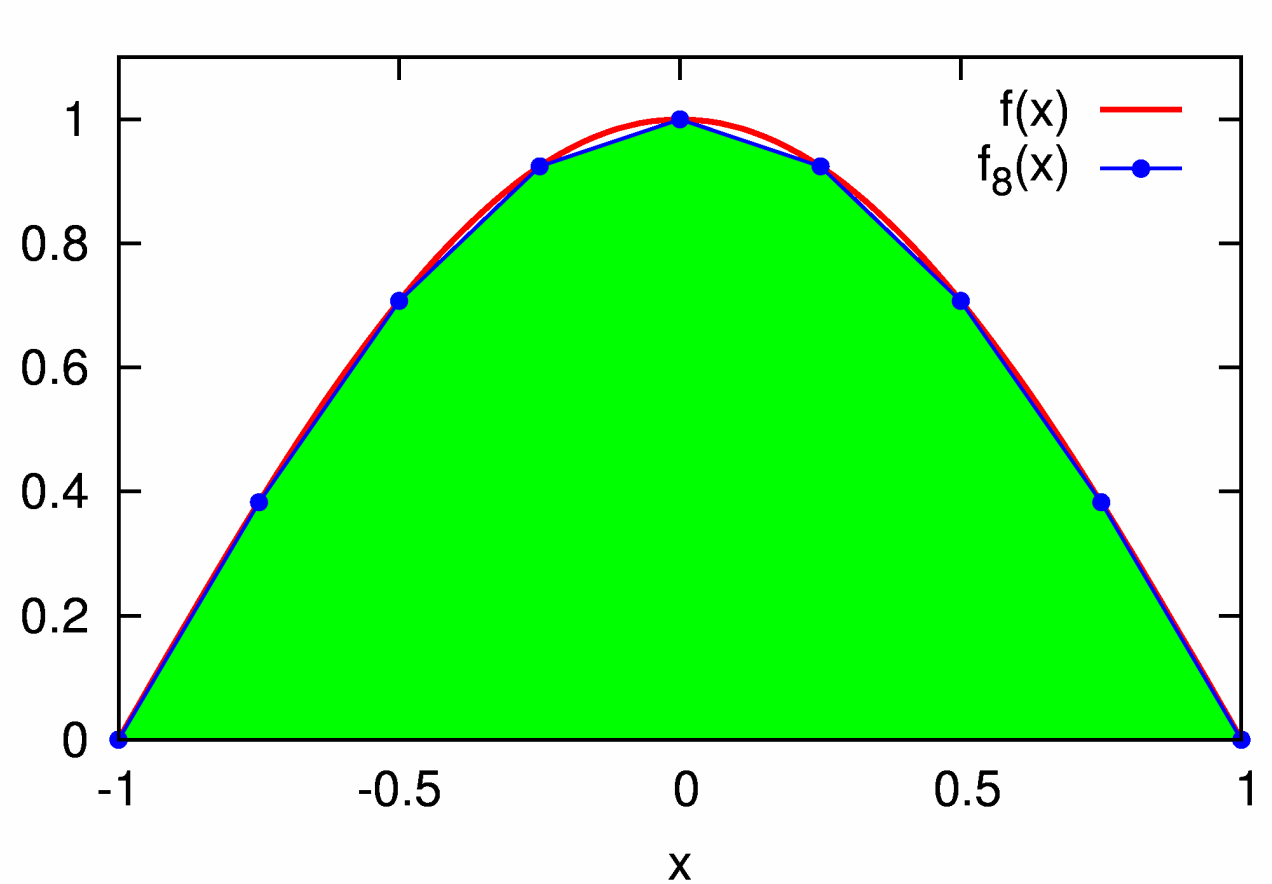

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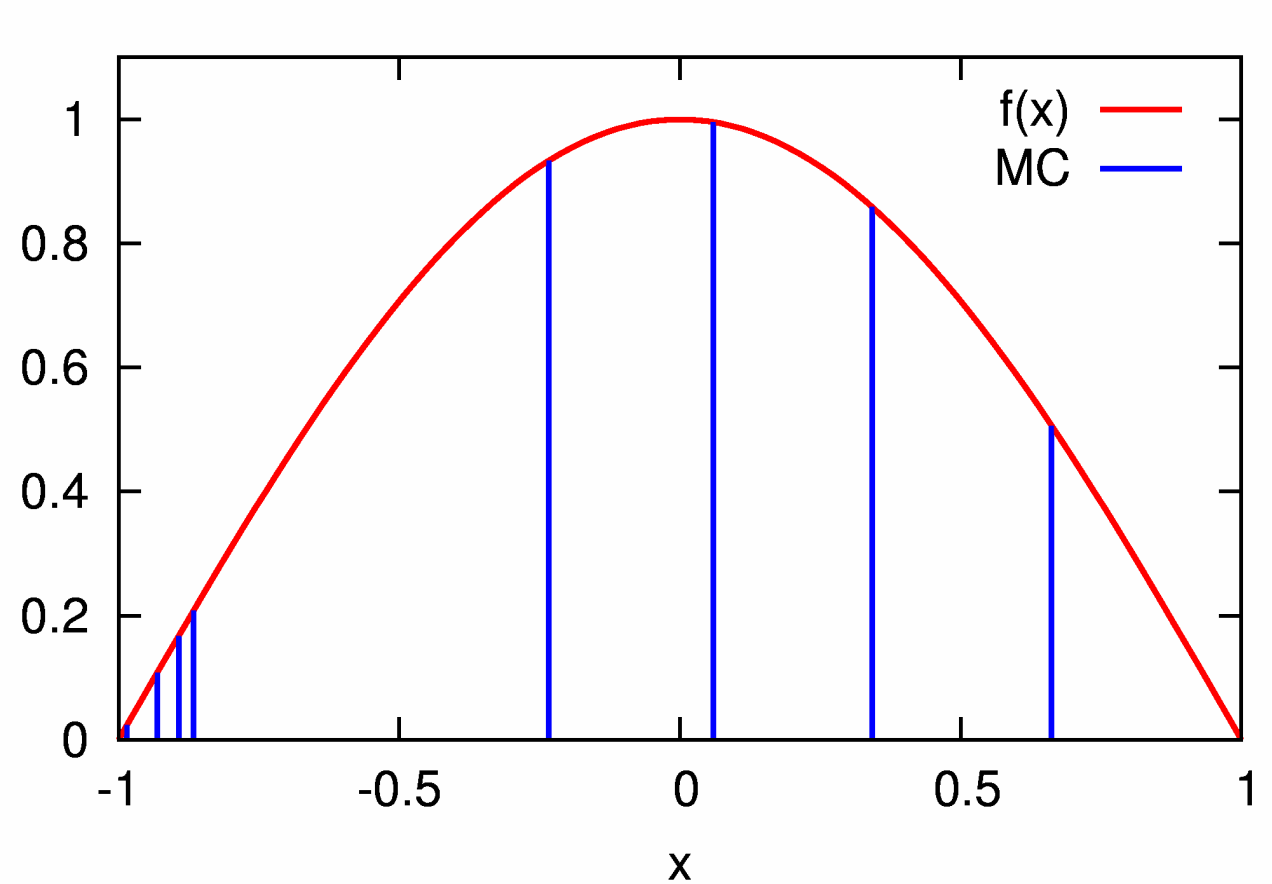

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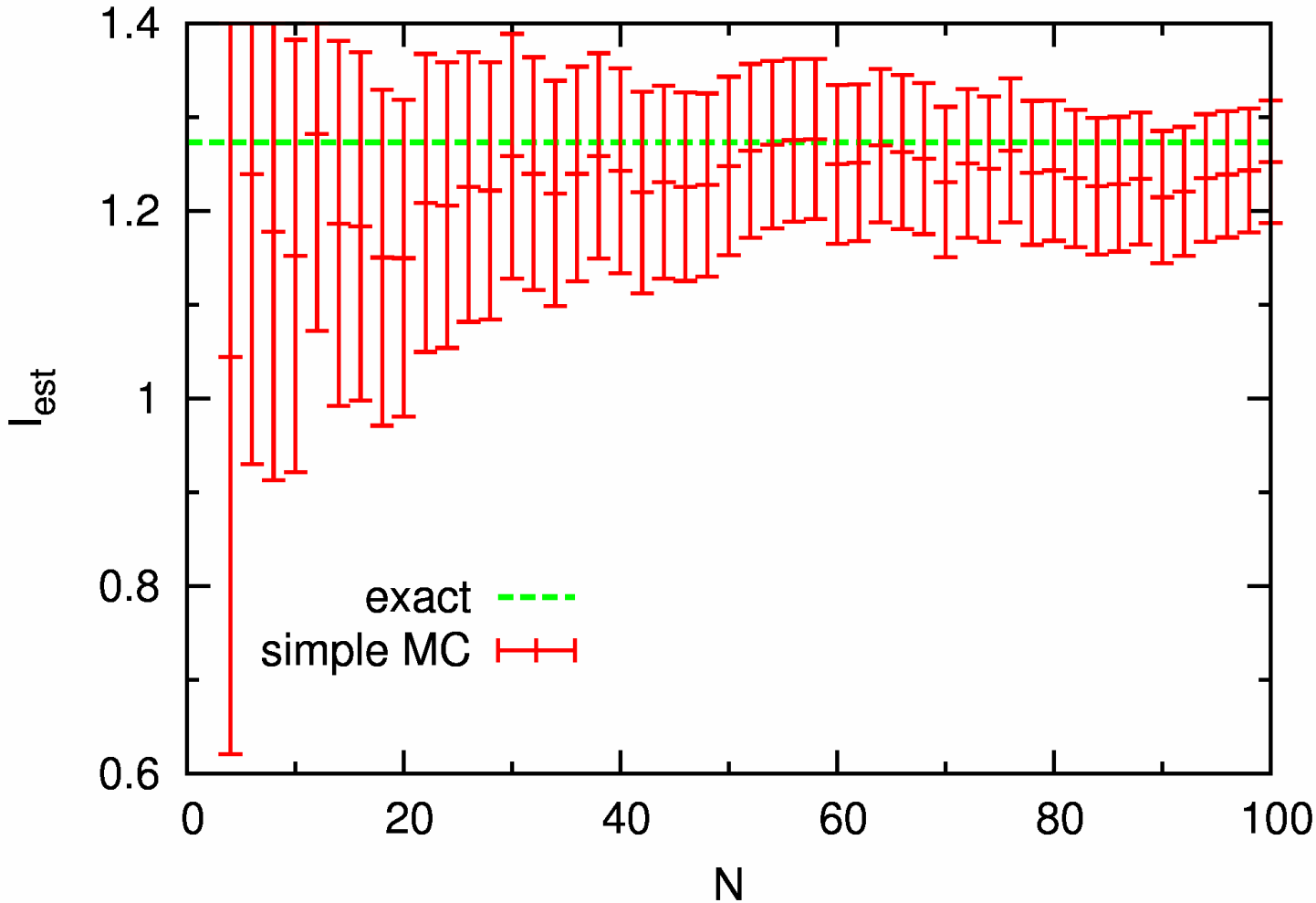
Numerical methods:

- discretization
- Monte Carlo

Convergence of results?



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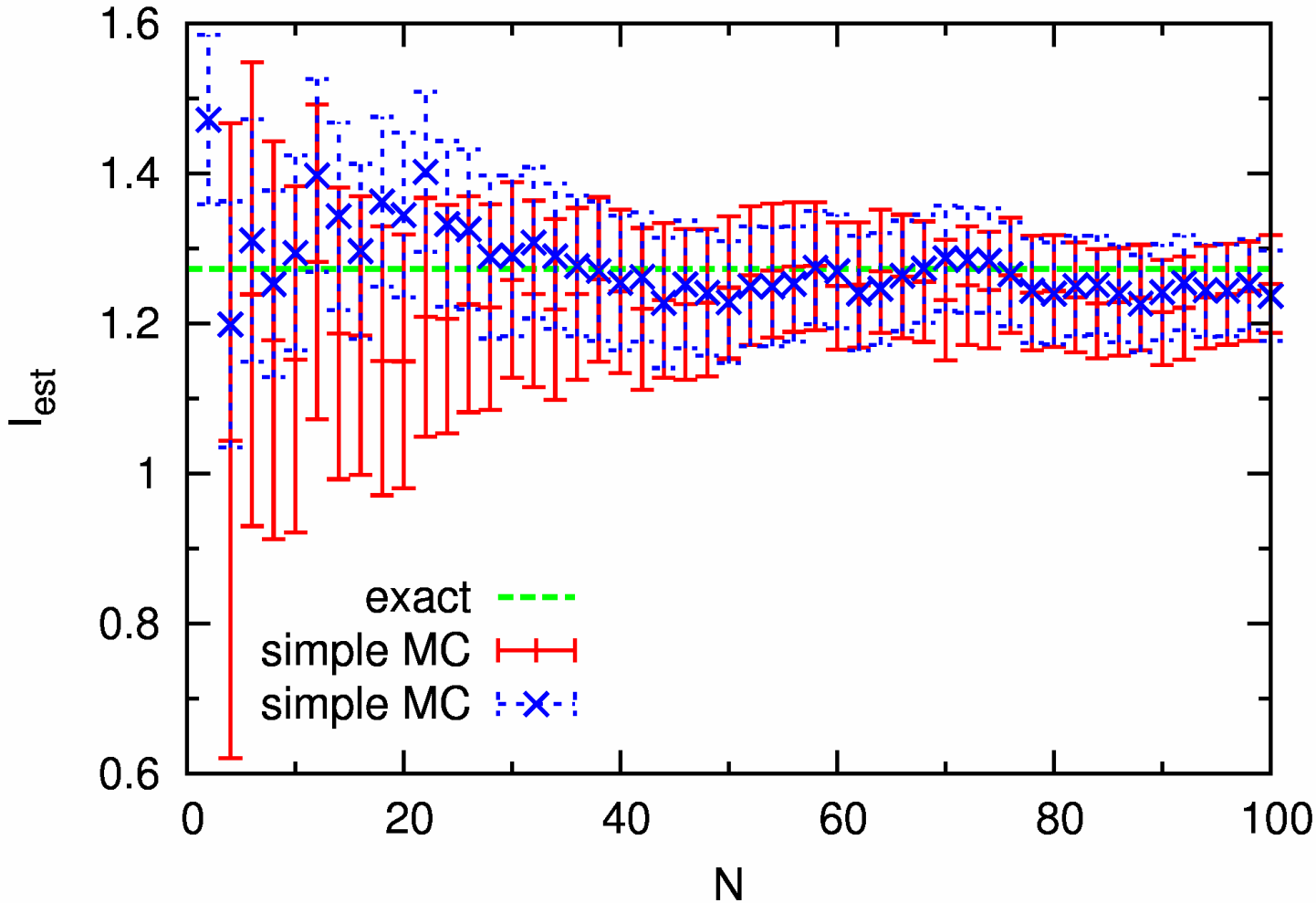

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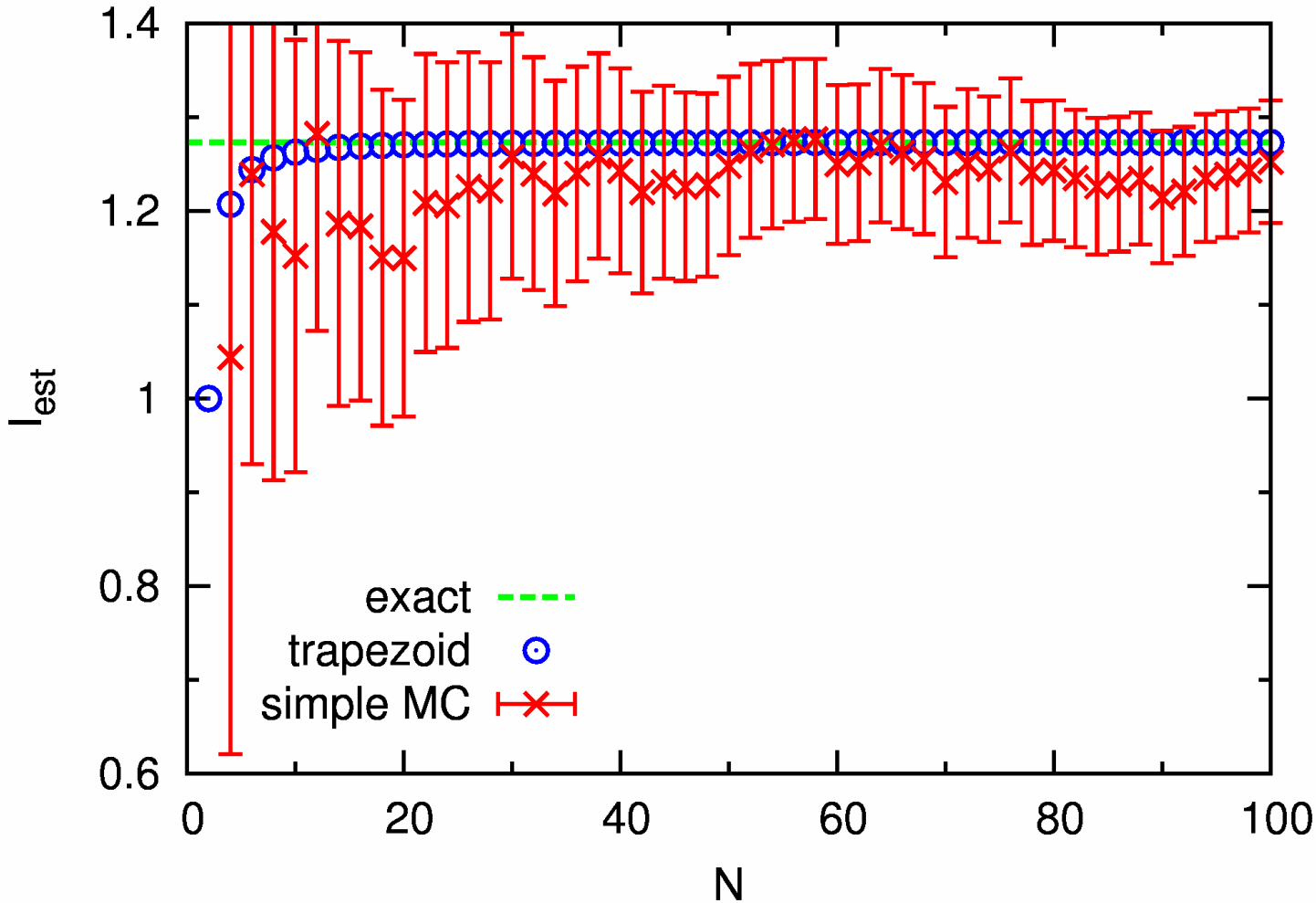

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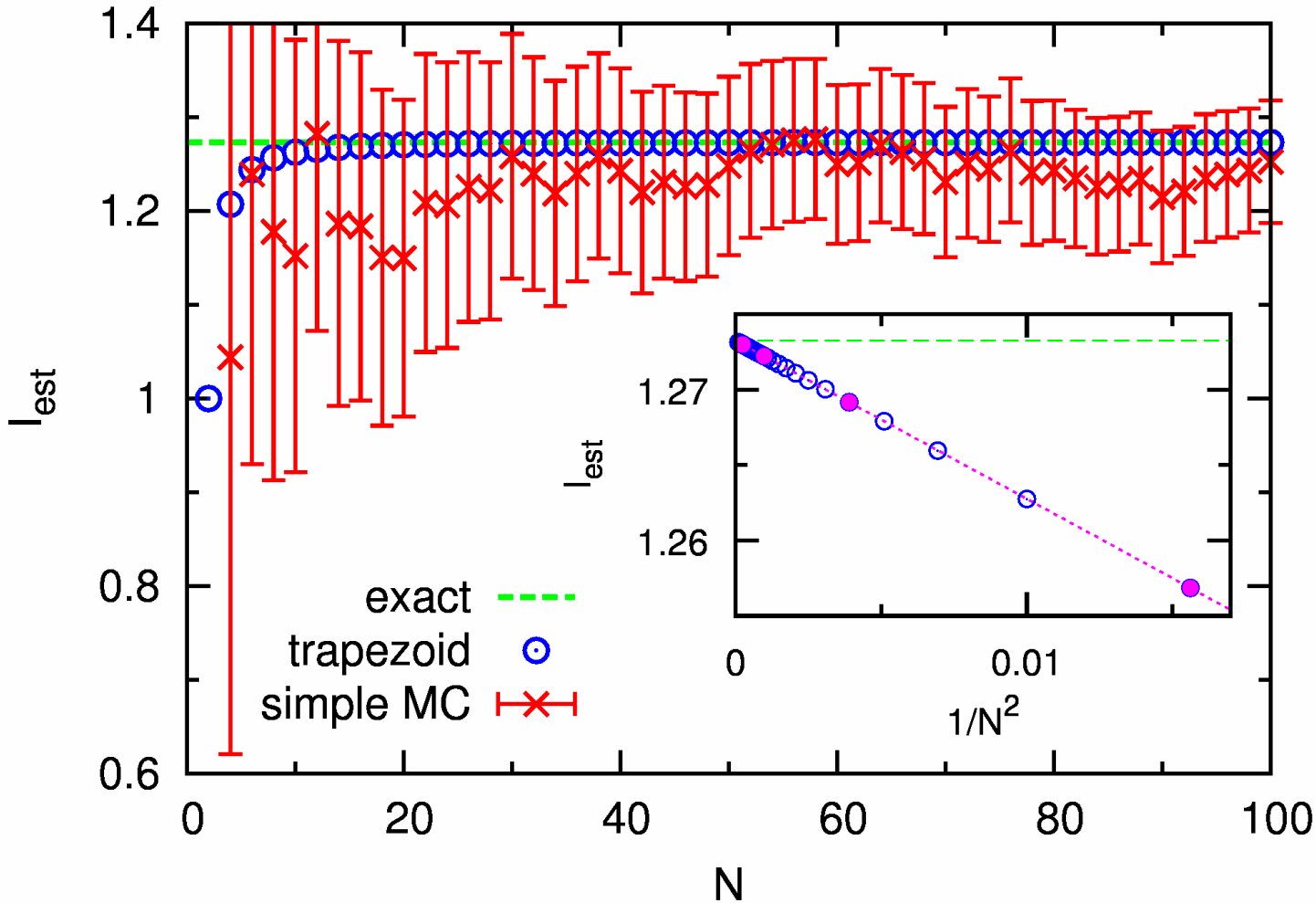

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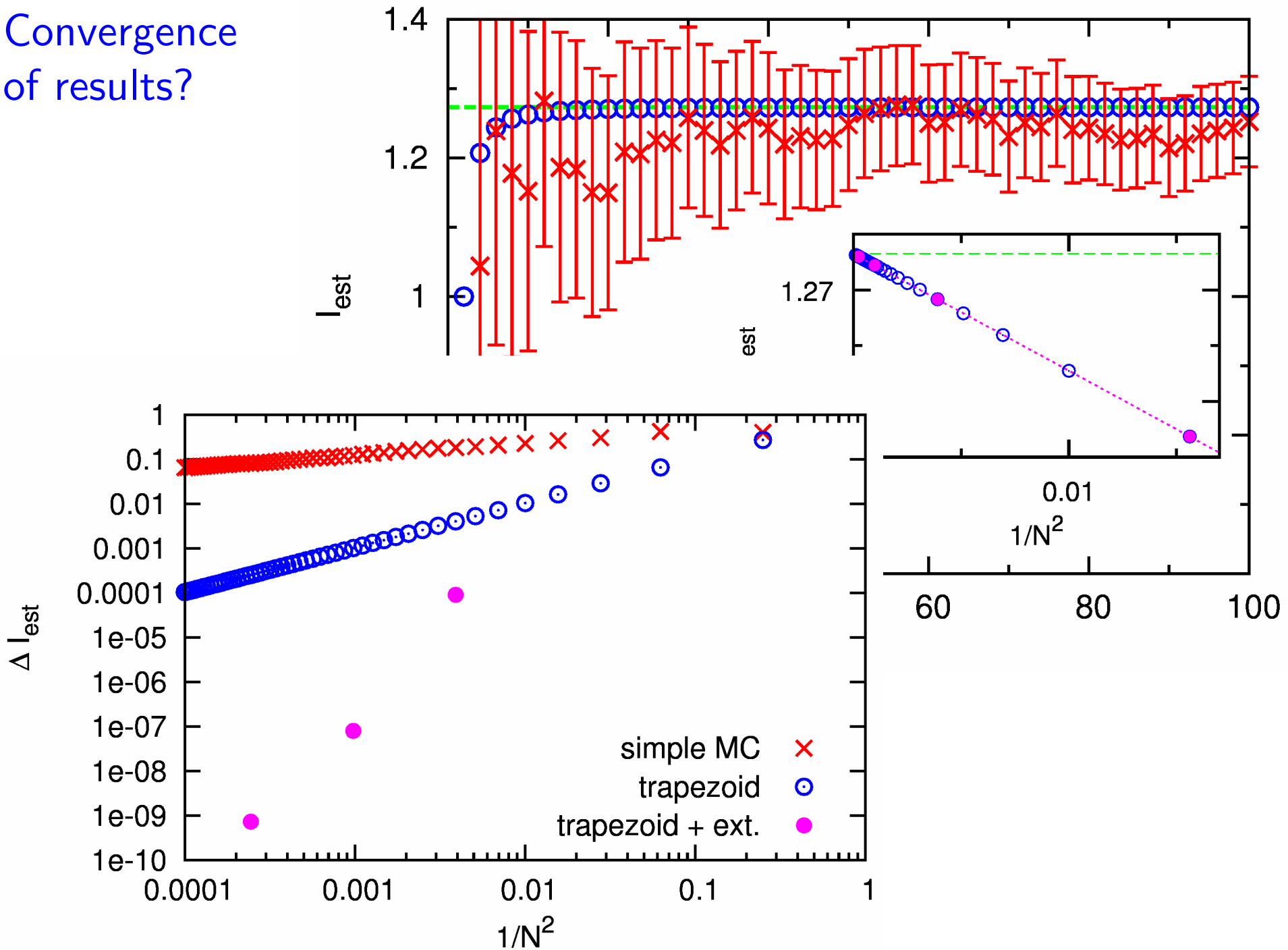

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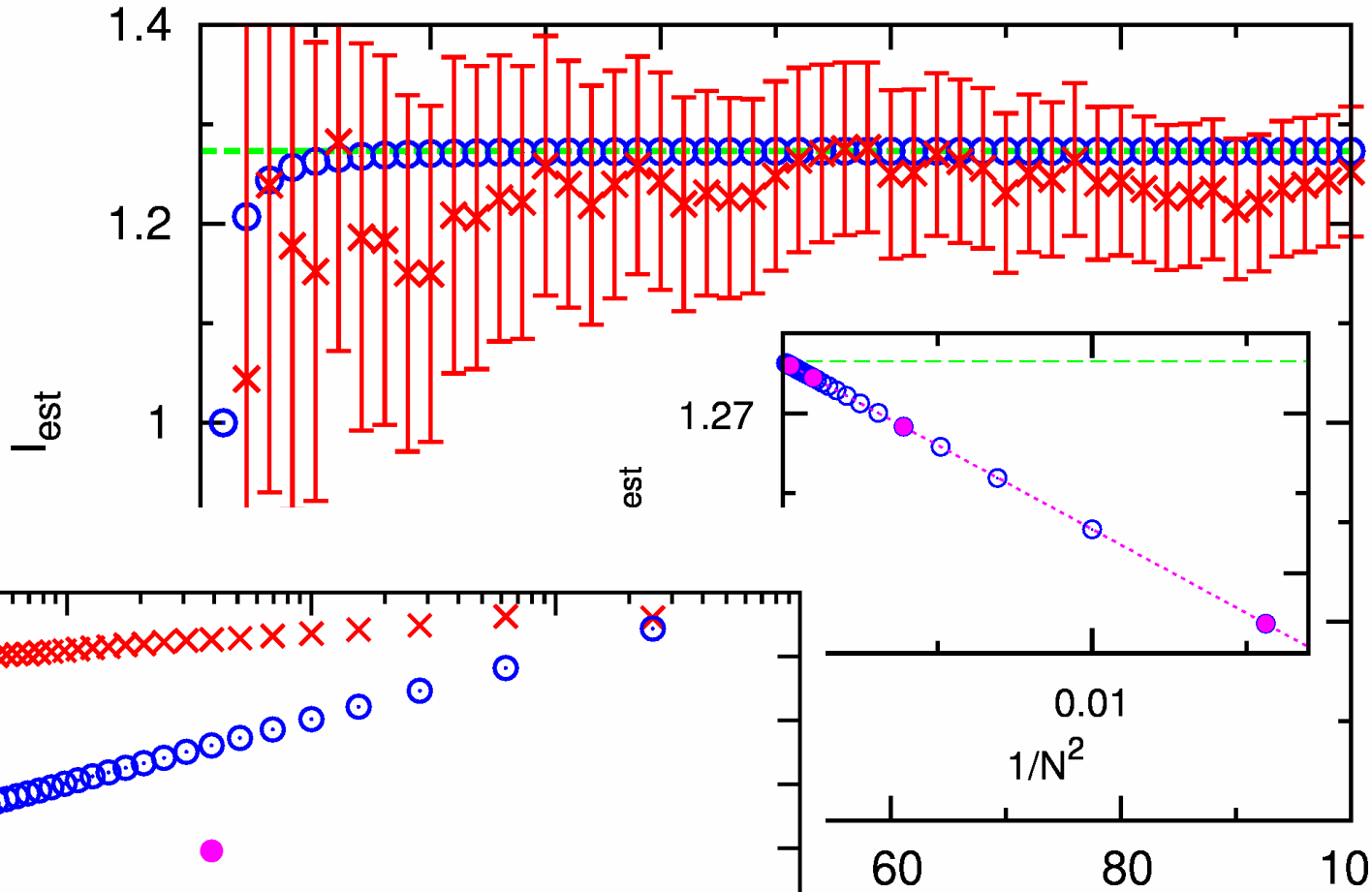

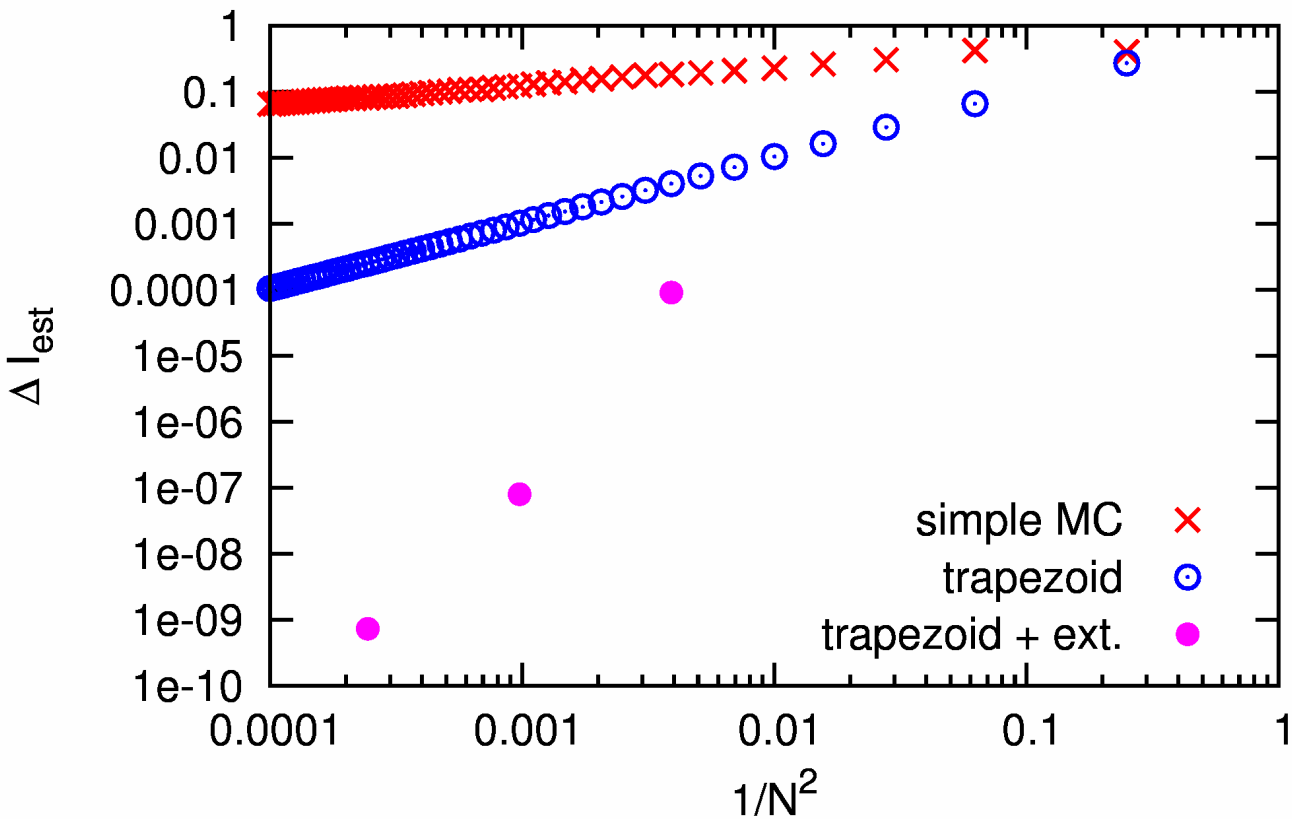

Many orders of magnitude gained by extrapolation

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

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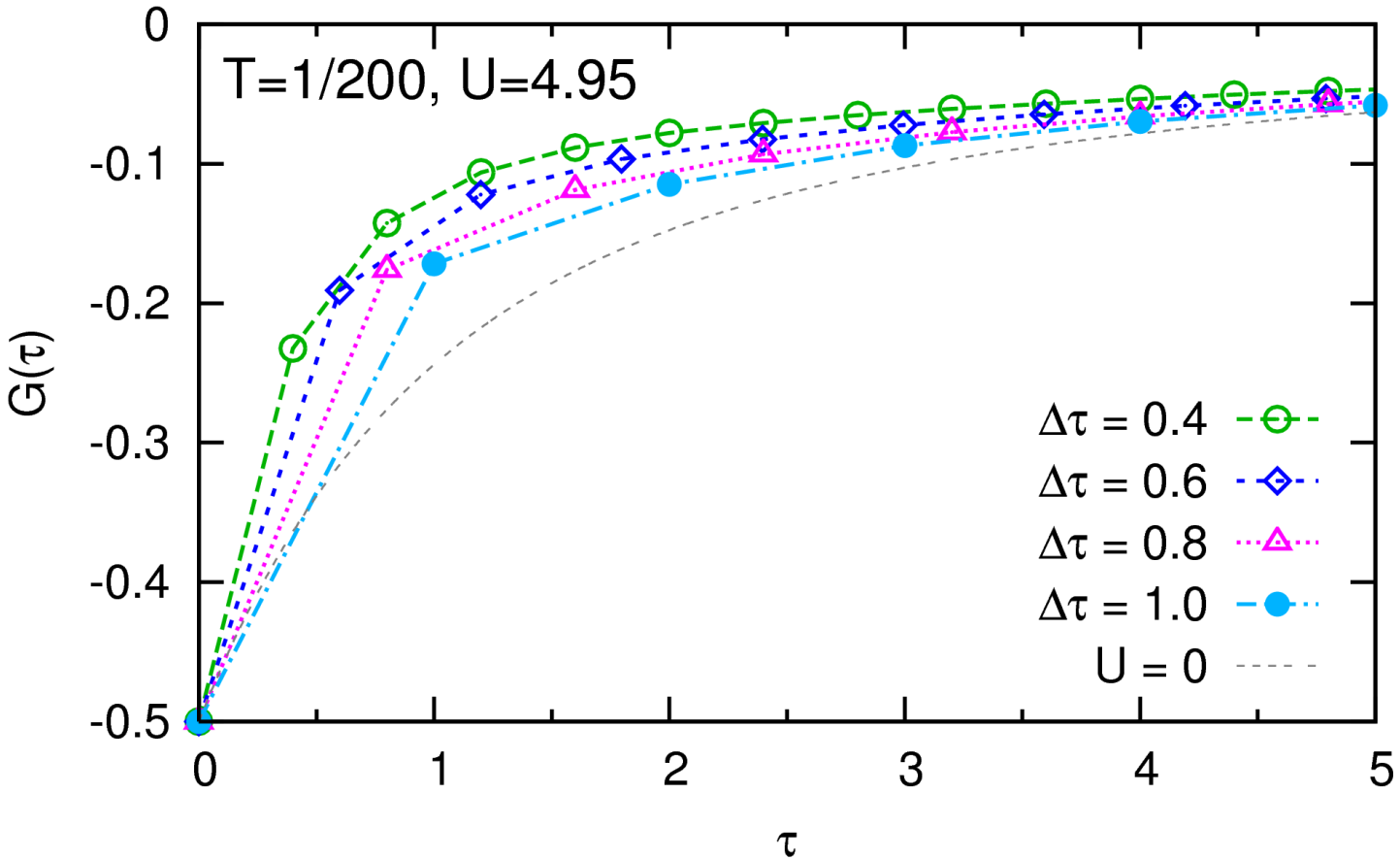
Reason: no obvious extrapolation scheme for $G(\tau)$



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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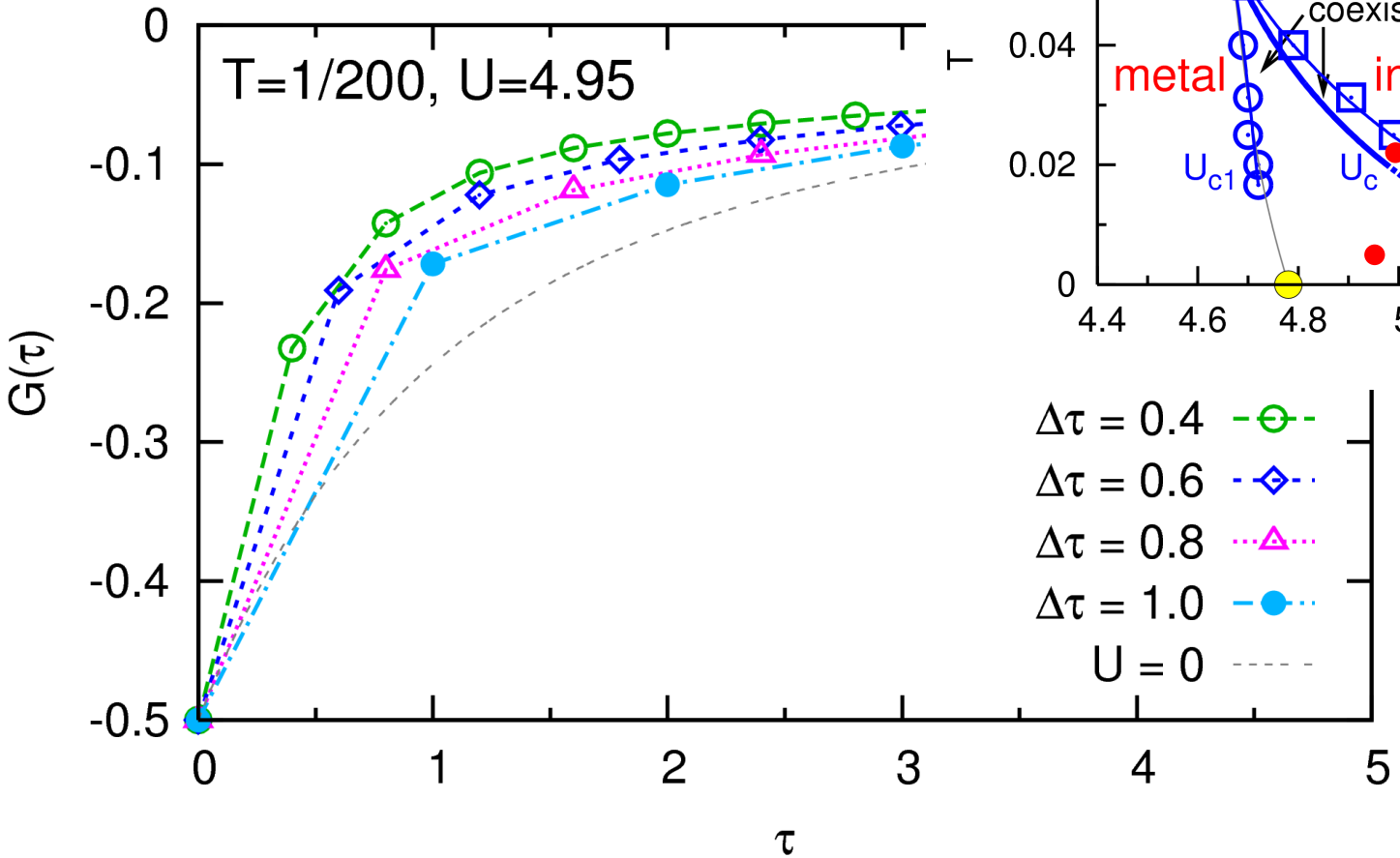

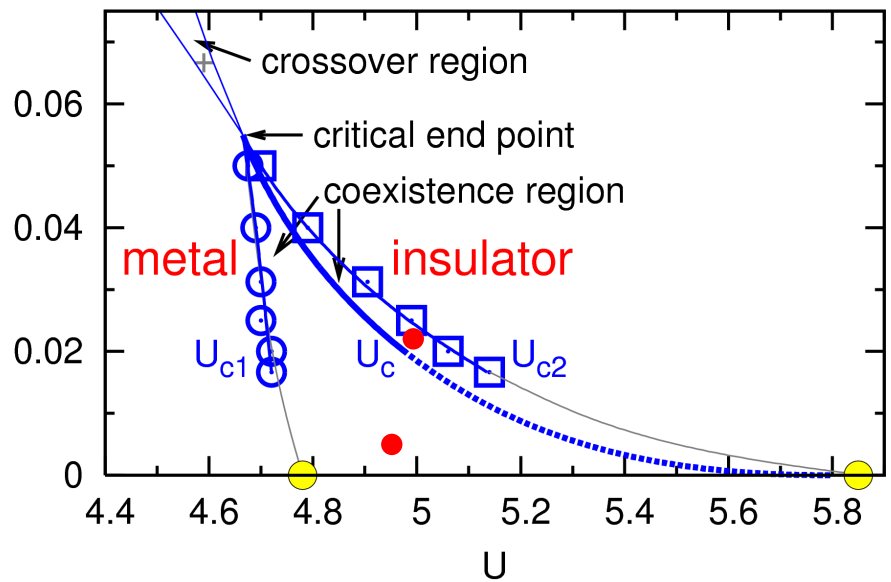

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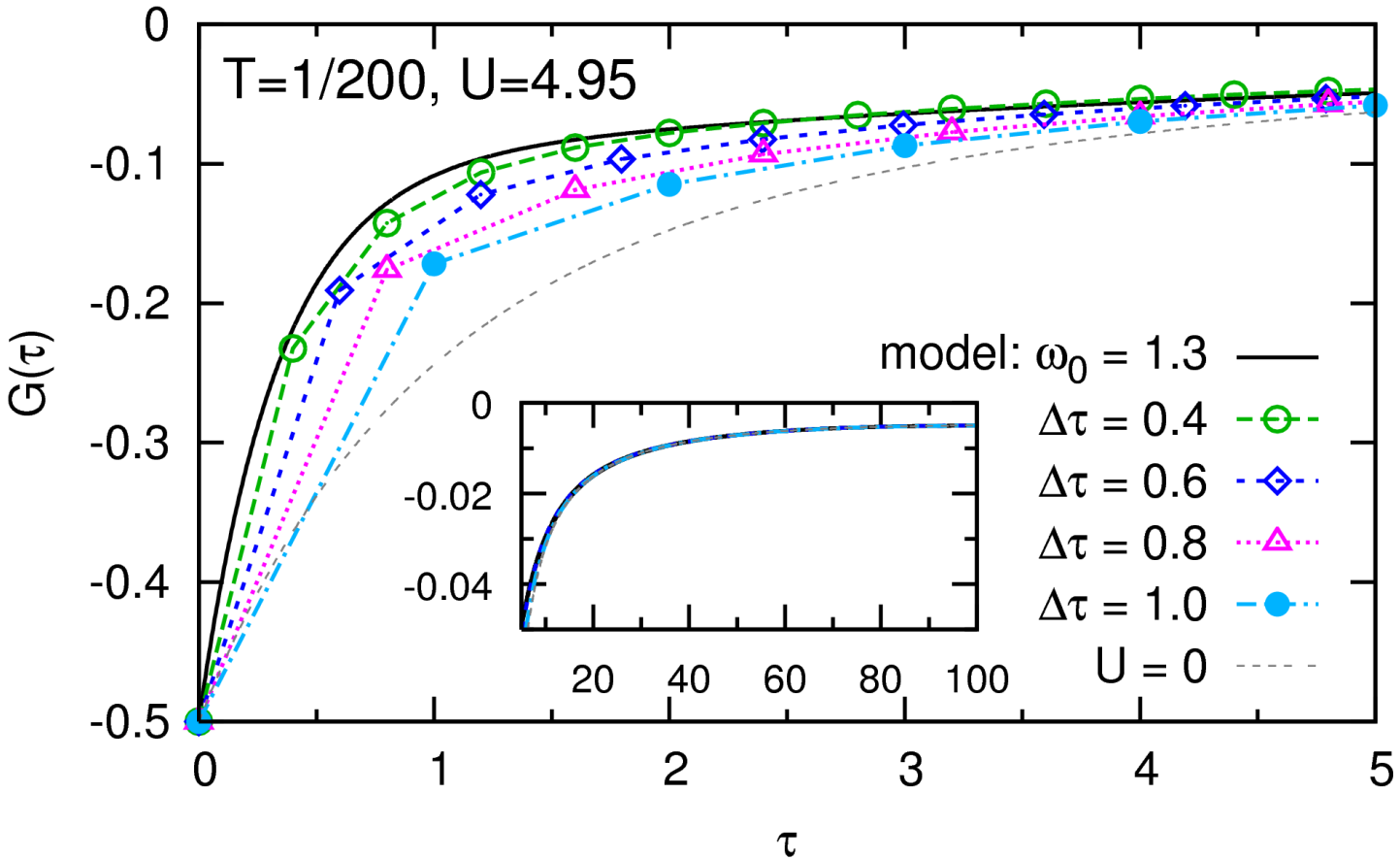

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New Green function extrapolation scheme

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

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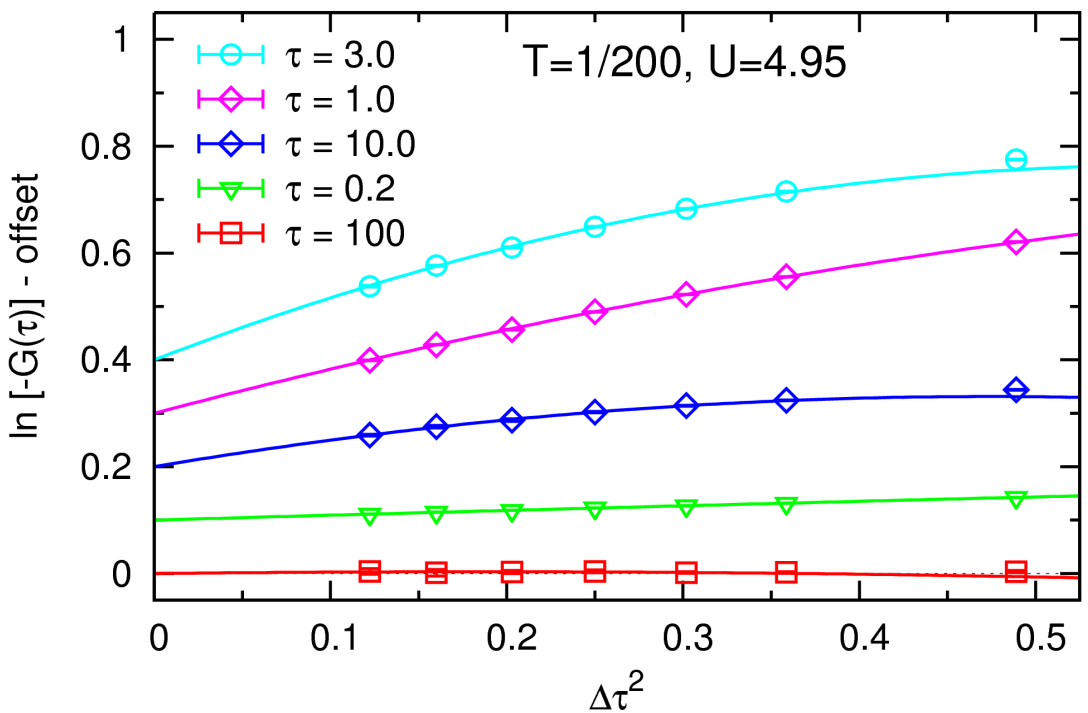
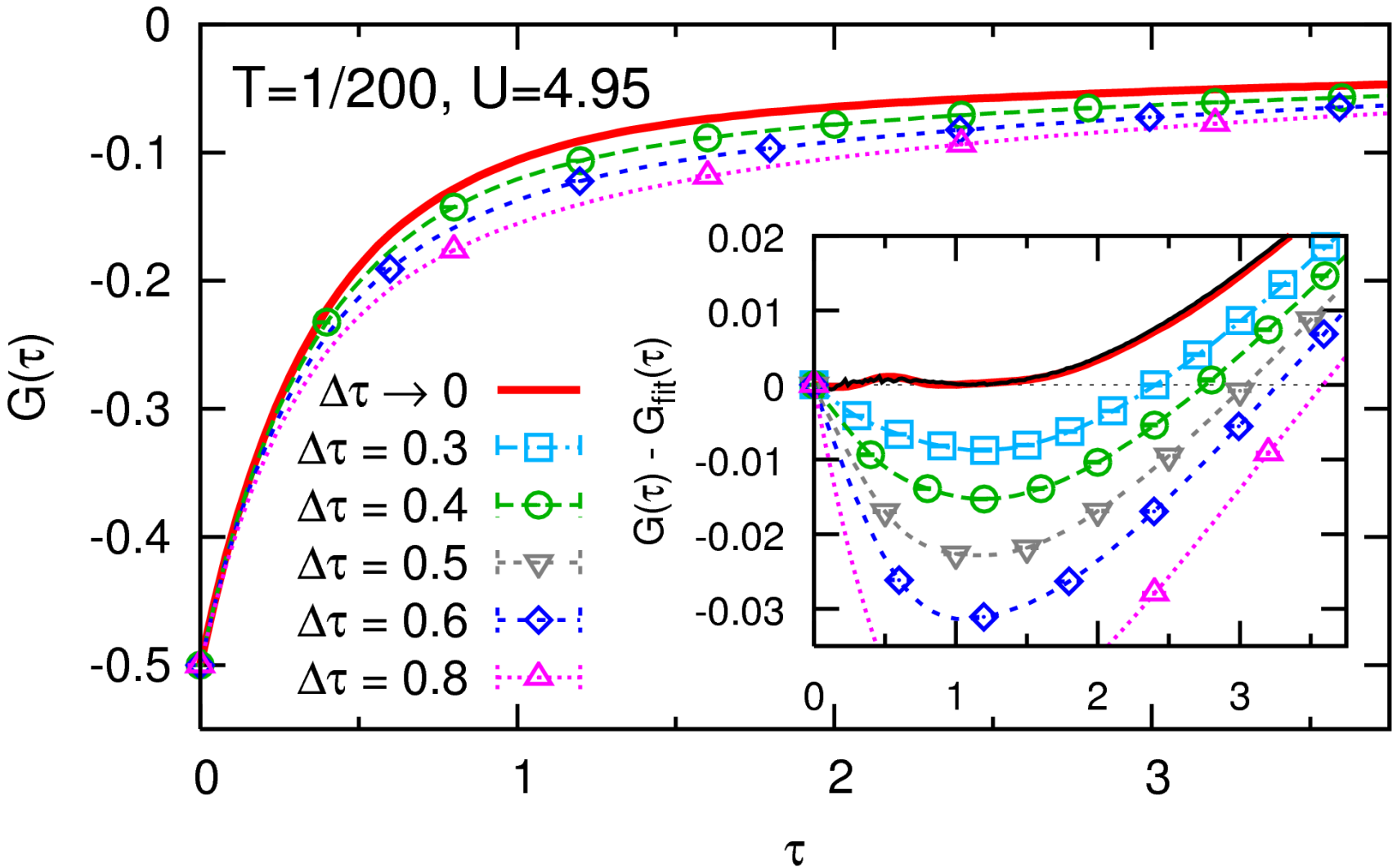
- Extrapolate $\log[-G(\tau)]$ using cubic least-squares fits, overweighting low $\Delta\tau$



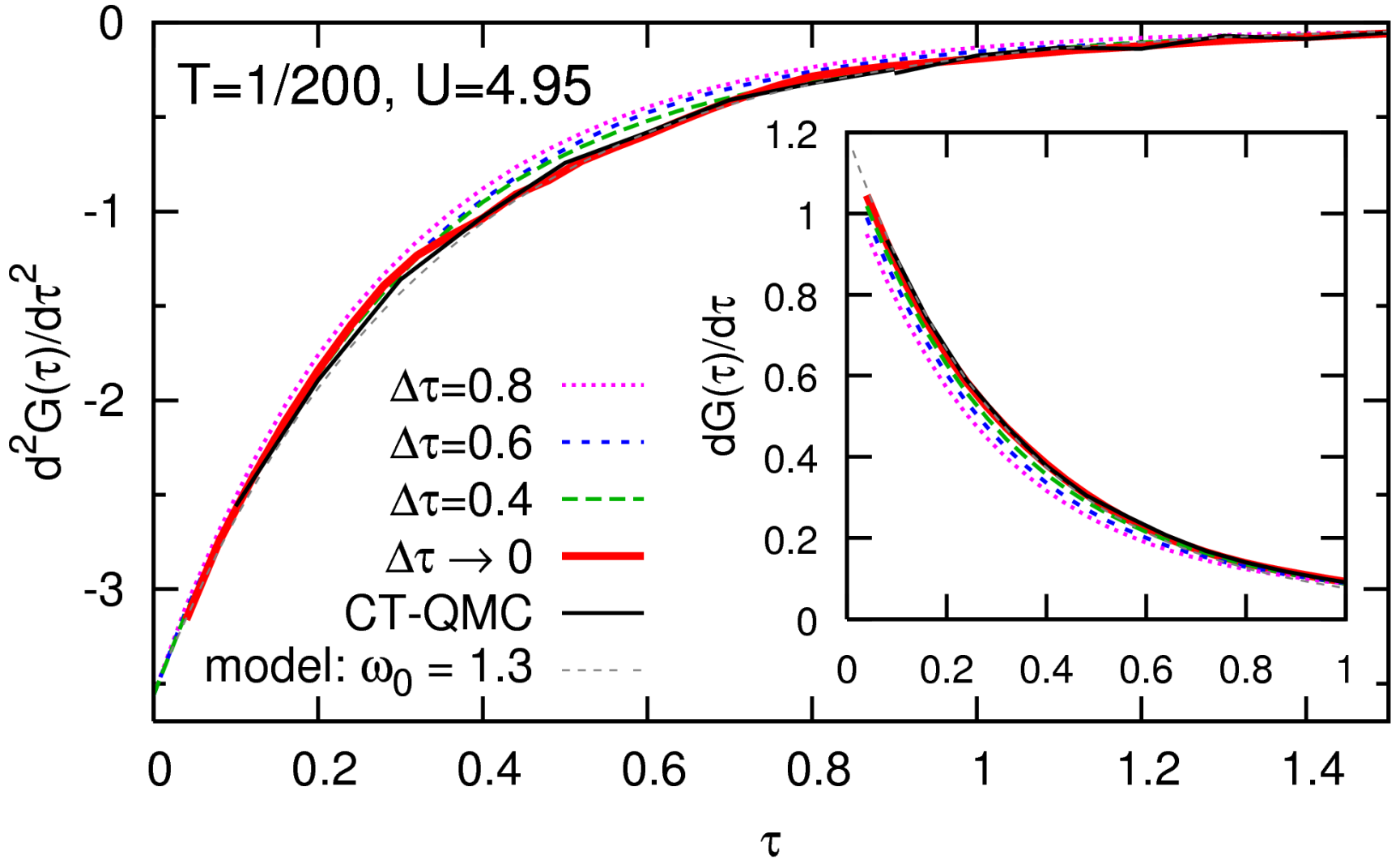
Result: unbiased, numerically exact Green function



[NB, arXiv:0712.1290]

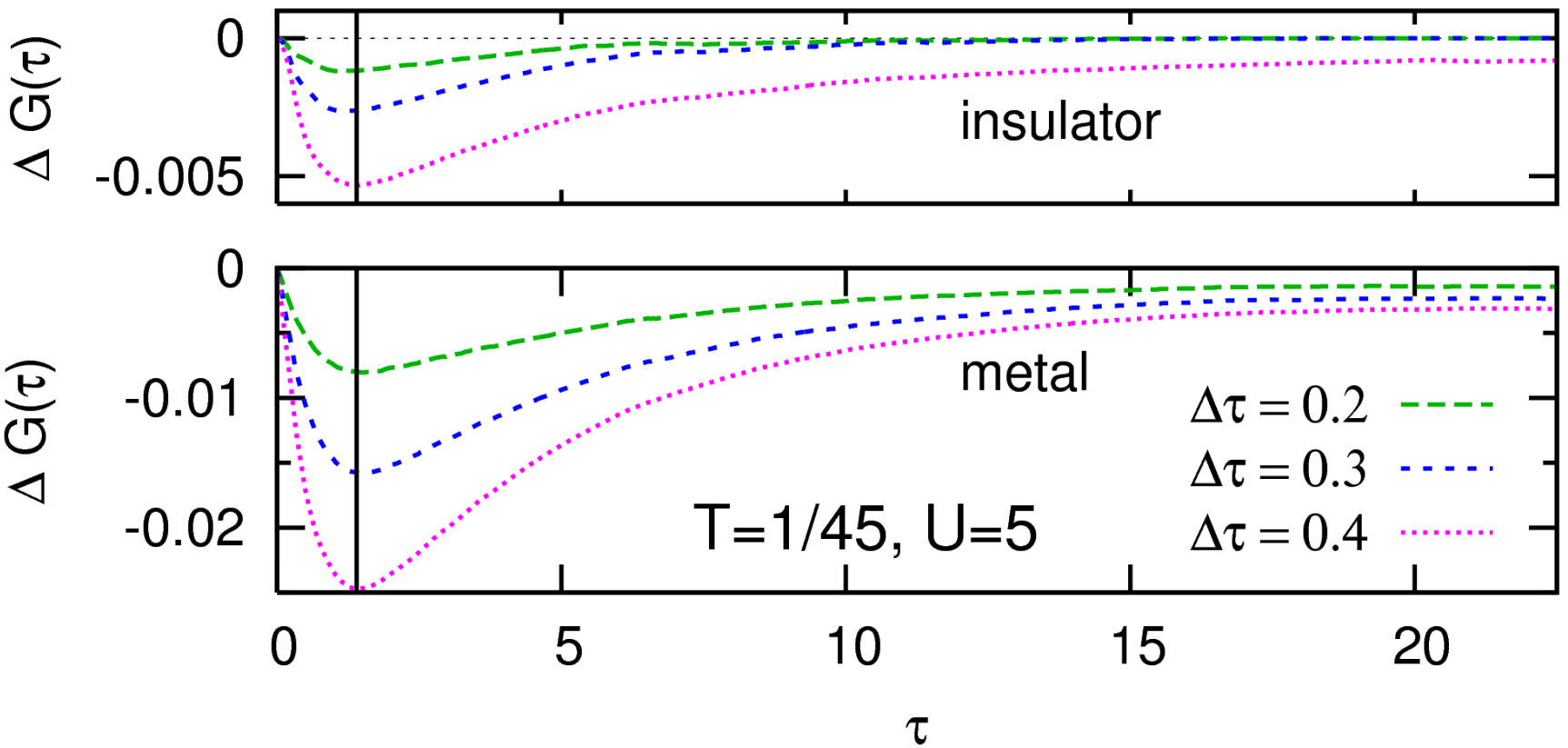
Excellent agreement with hybridization expansion CT-QMC [Werner et al., PRL (2006)]

2nd and 1st order derivatives of Green function



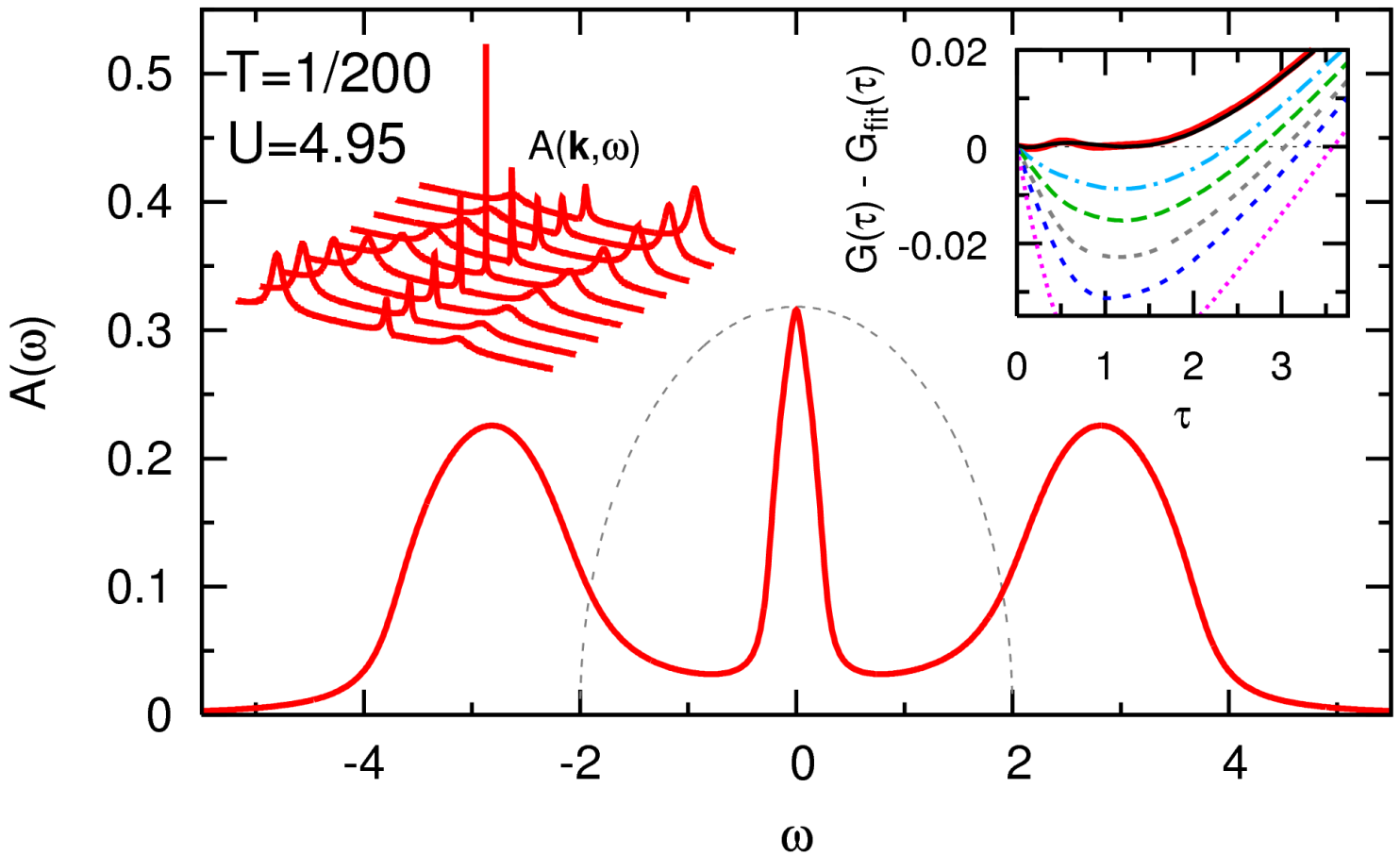
Exact asymptotics $\left.\frac{d^2G(\tau)}{d\tau^2}\right|_{\tau=0+} = -\frac{1}{2}\left(1+\frac{U^2}{4}\right)$; $\left.\frac{dG(\tau)}{d\tau}\right|_{\tau=0+}$ nonuniversal

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



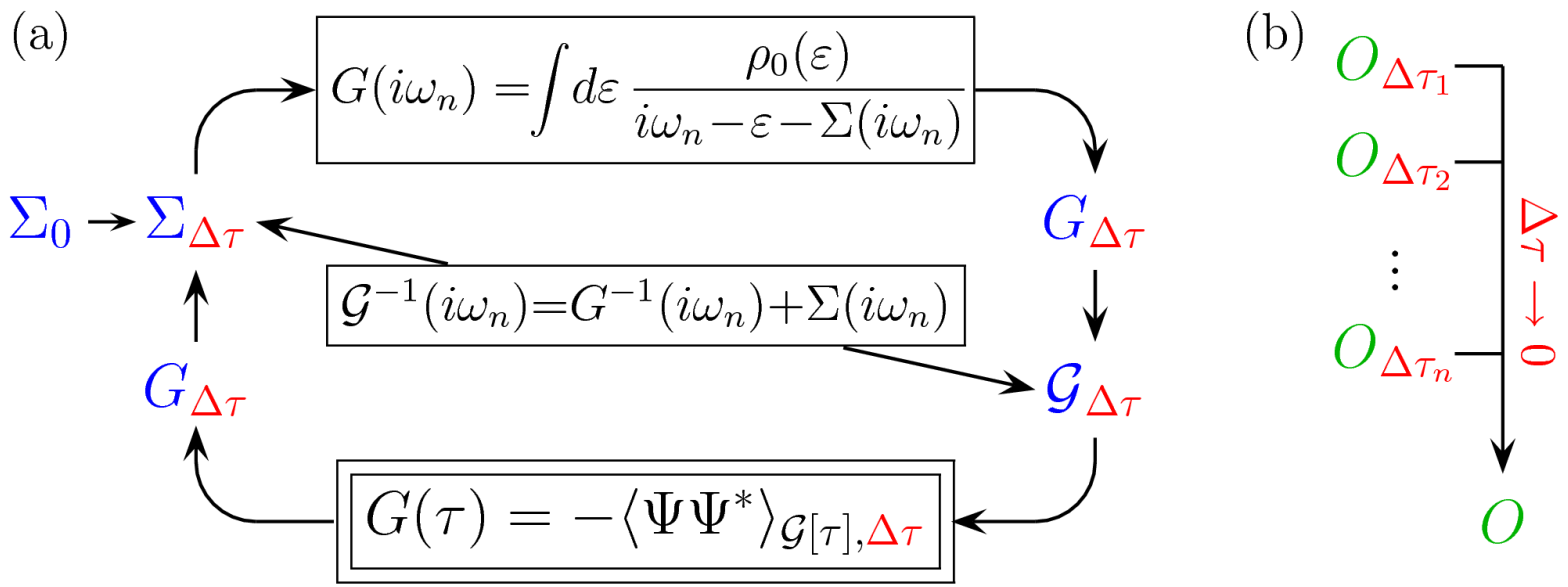
First spectra without discretization error from HF-QMC, at ultra-low T

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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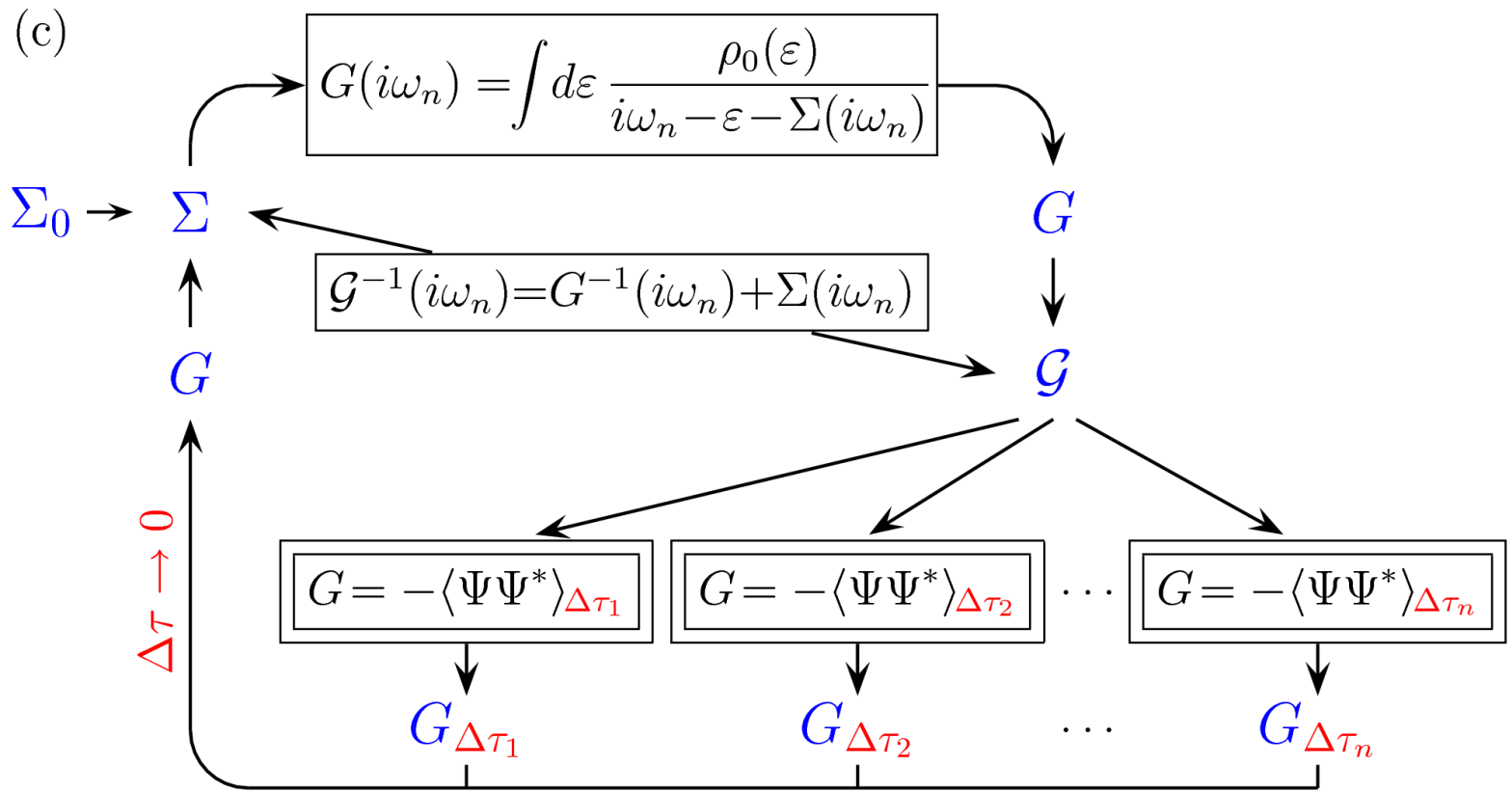
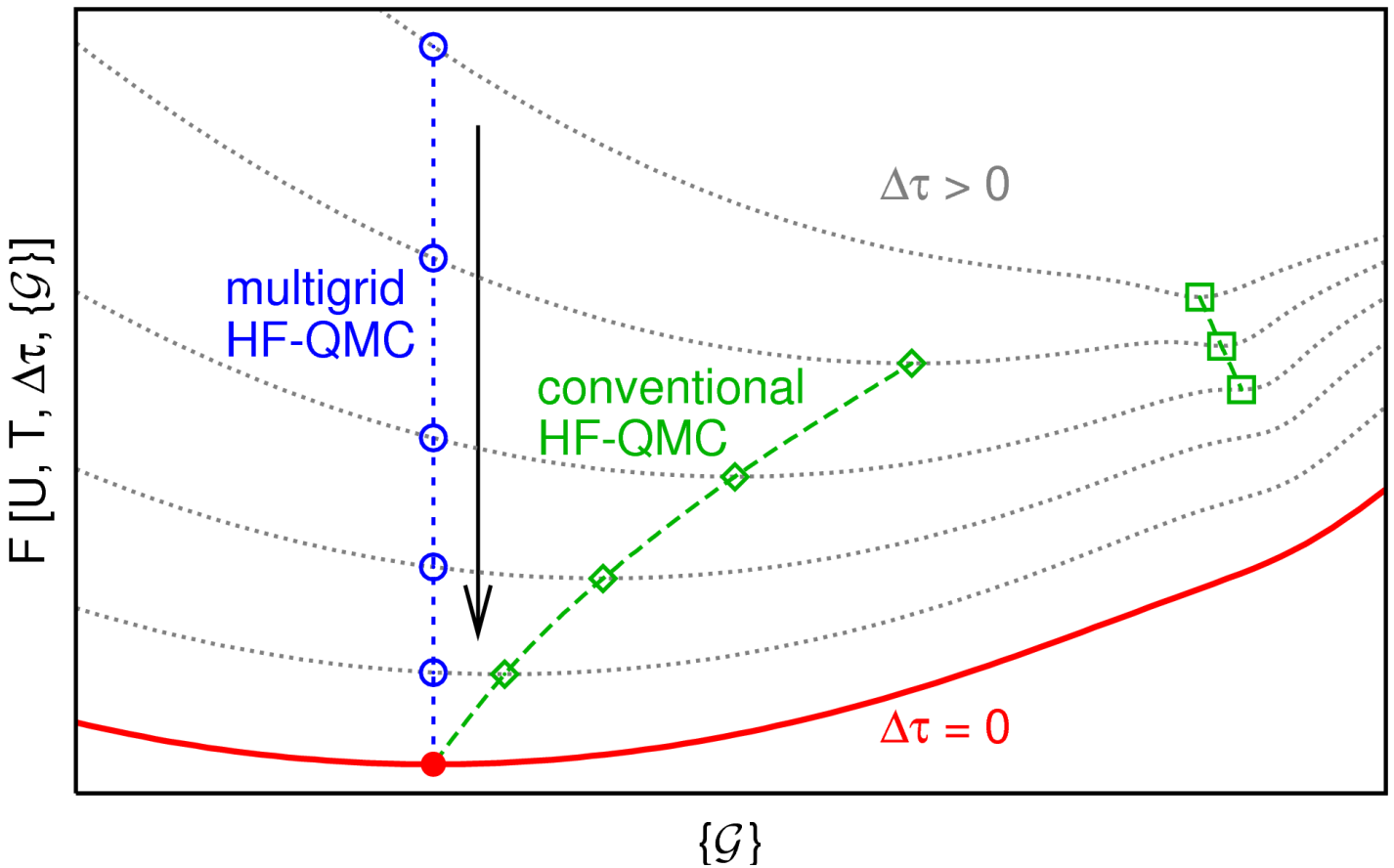


(c) Multigrid HF-QMC: internal elimination of Trotter error

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

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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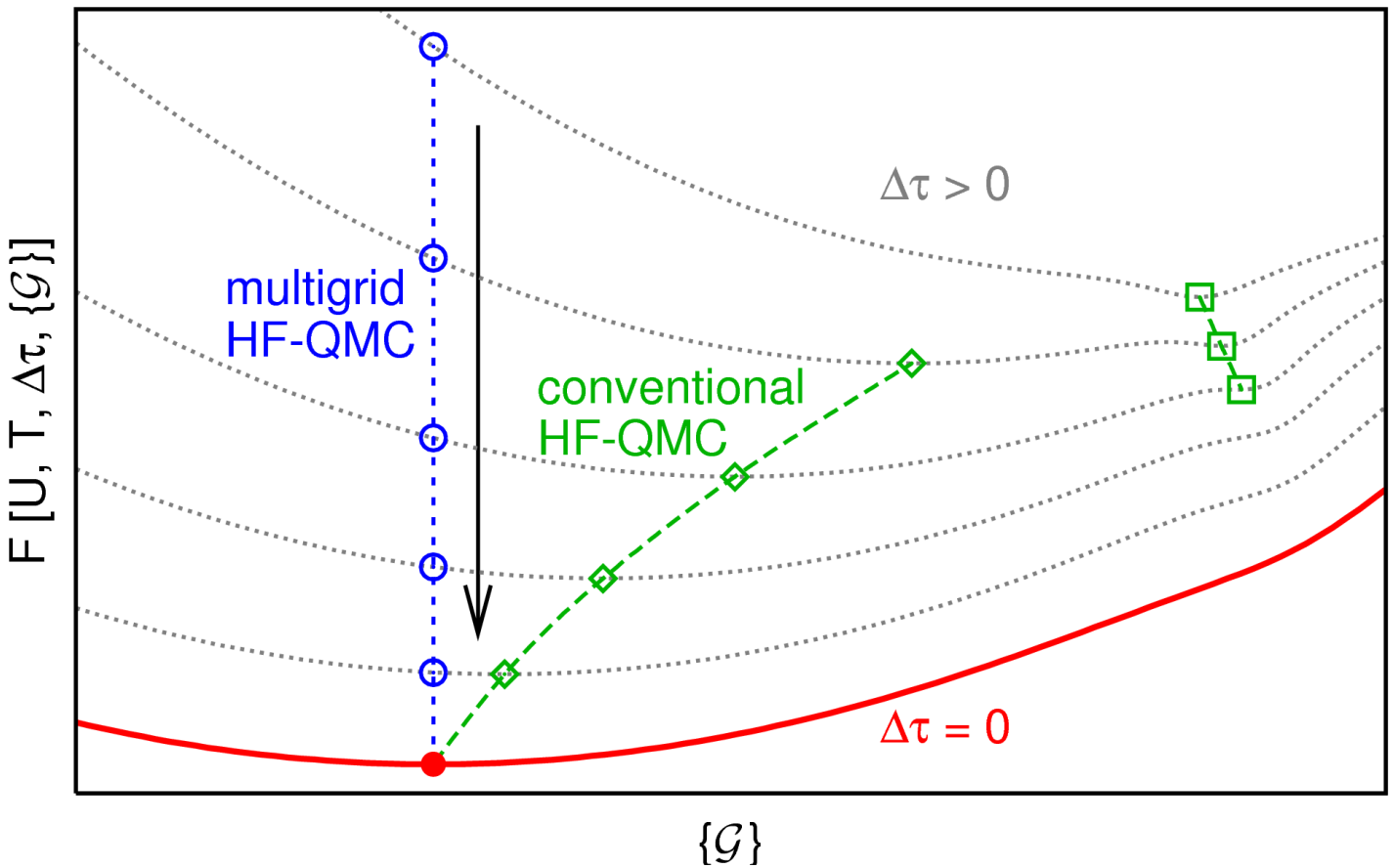
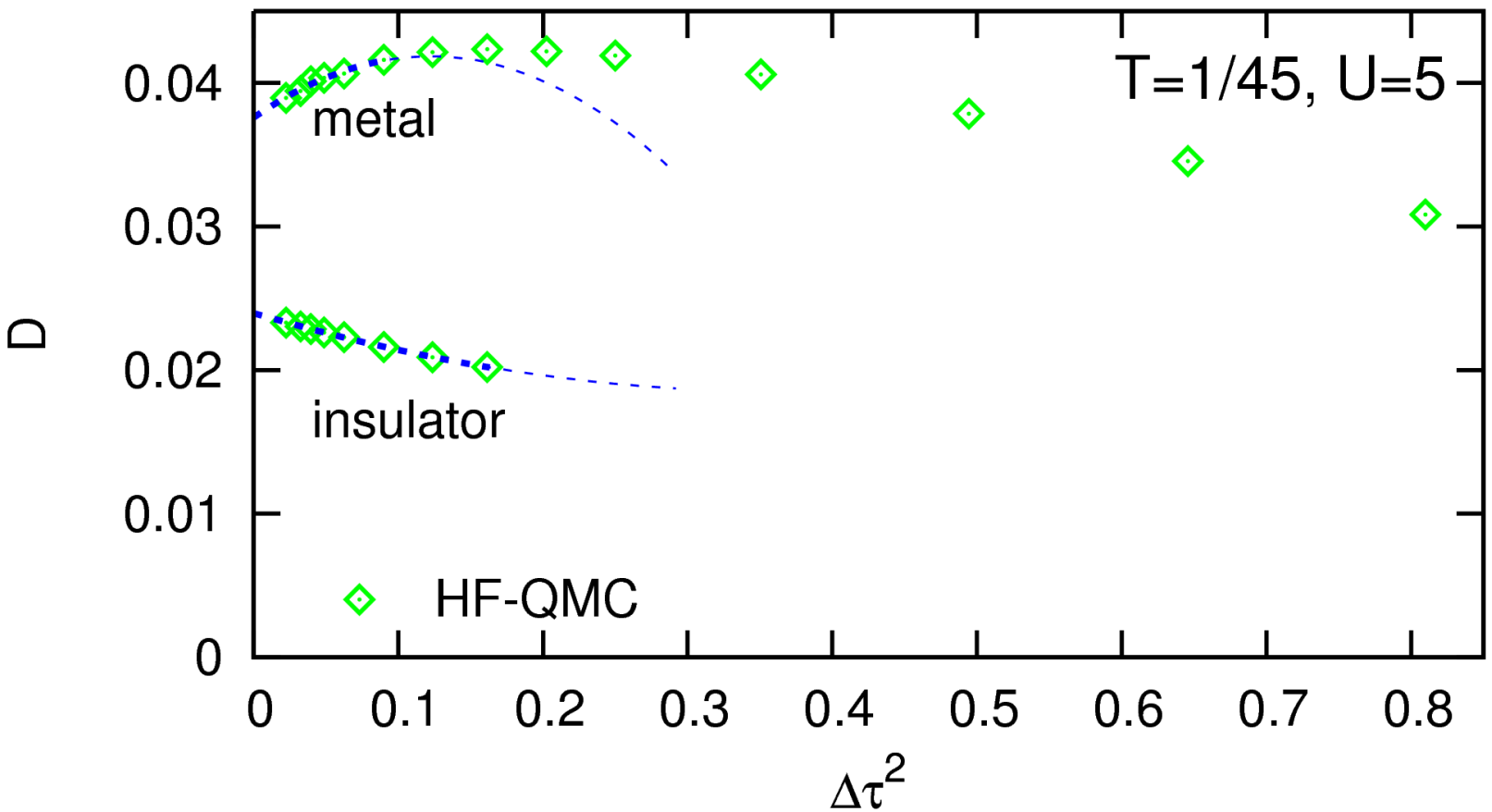


Conventional Hirsch-Fye QMC: DMFT fixed point shifts with $\Delta\tau$

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 $\Delta\tau \approx 0.3$

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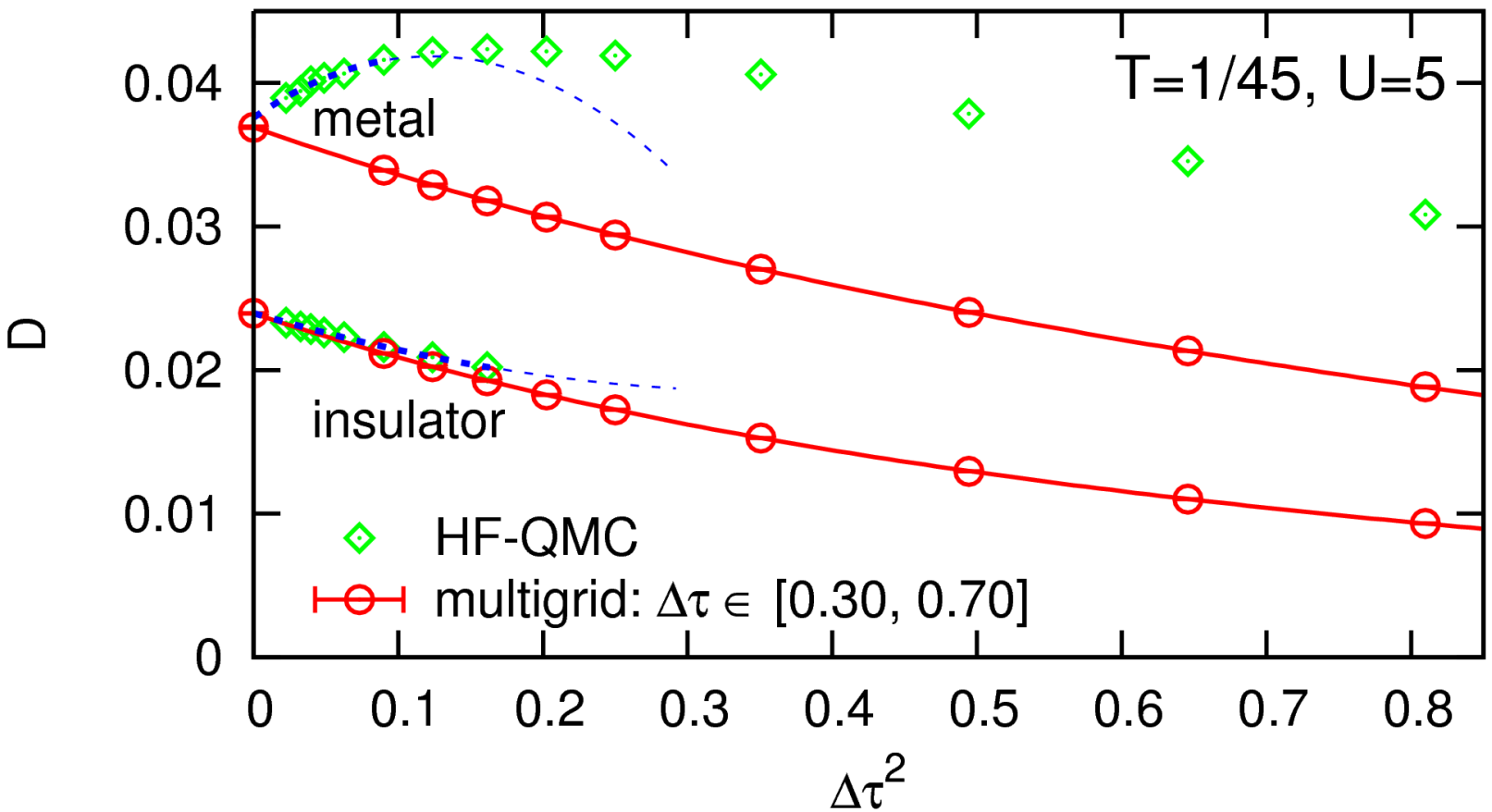
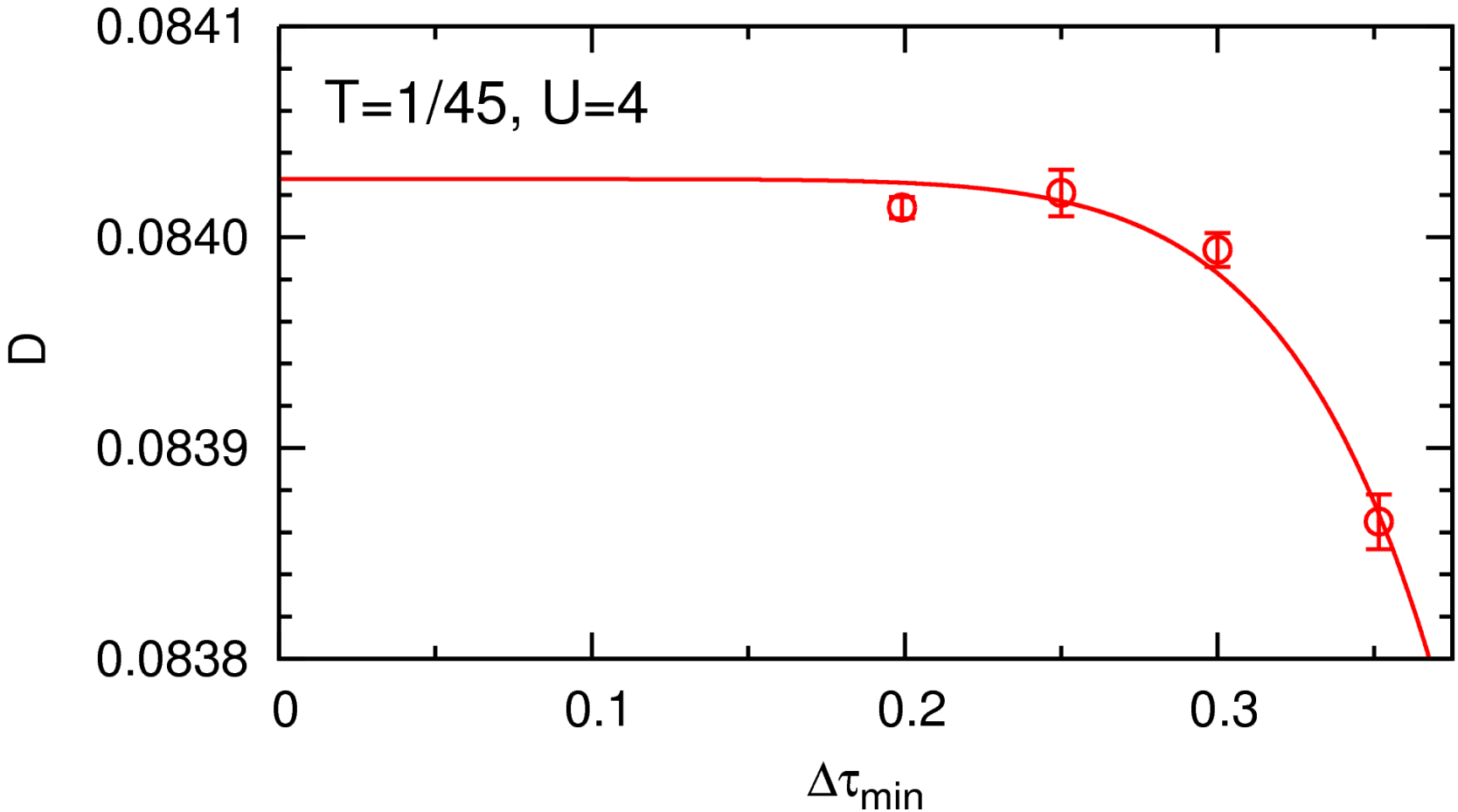


Conventional HF-QMC: no insulating solution for $\Delta\tau \gtrsim 0.4$

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

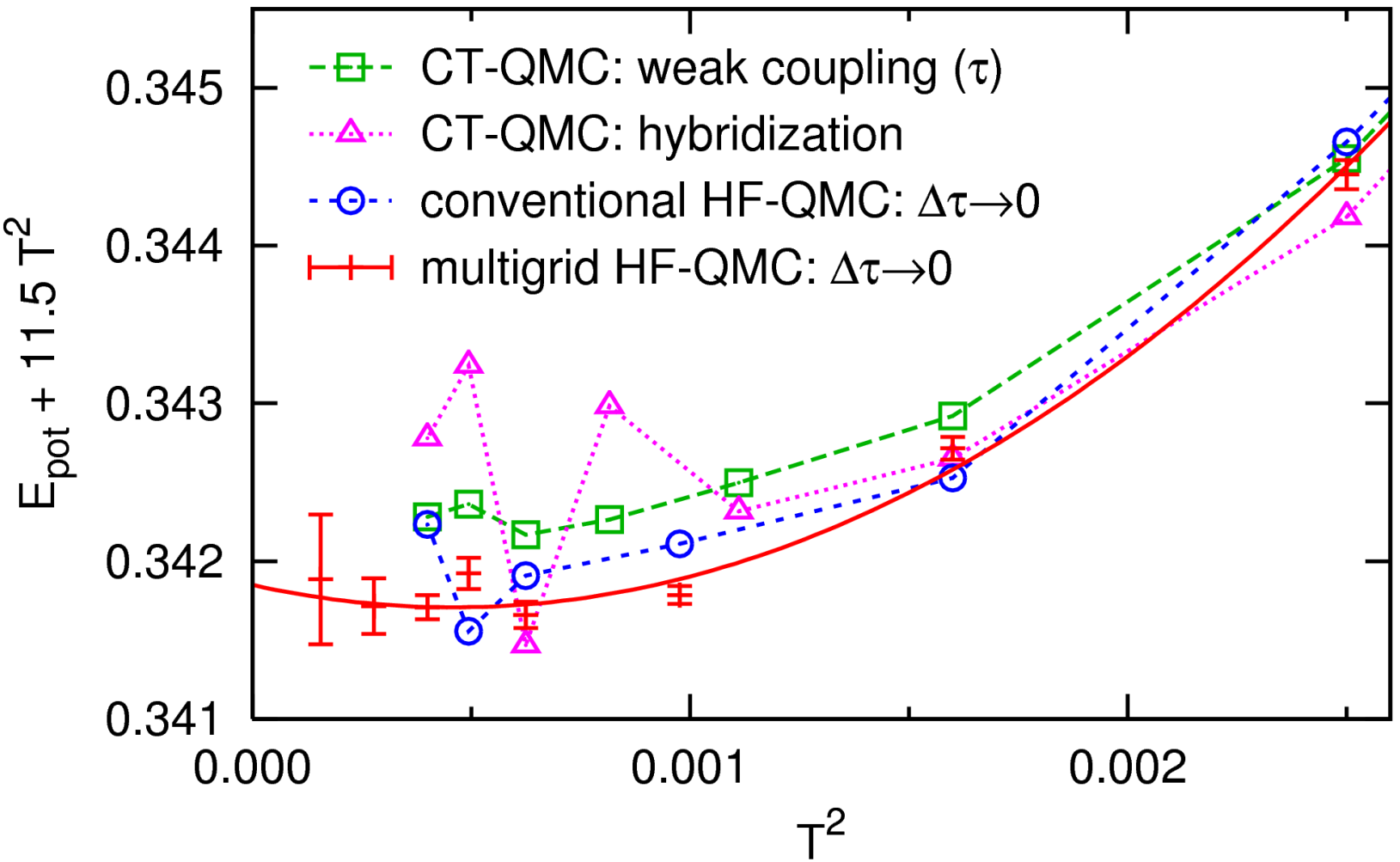
Multigrid HF-QMC: vastly larger useful range of $\Delta\tau$

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



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

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



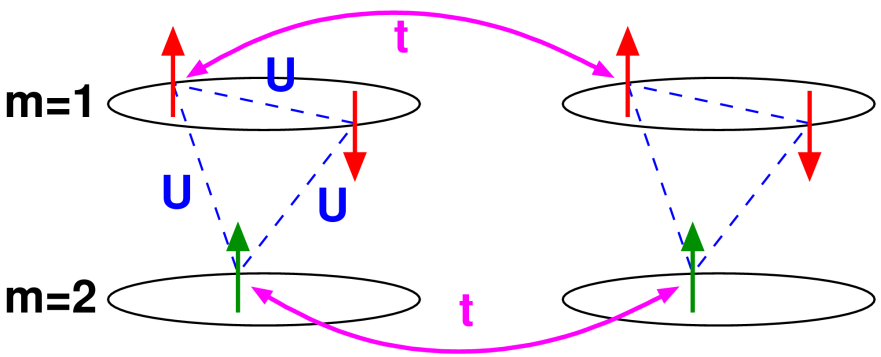
No more "difficult observables" for multigrid HF-QMC

Higher precision than CT-QMC methods at same effort

Applications

Mott transition at variable degeneracy $SU(2M)$: Motivation

$$H = -t \sum_{\langle ij \rangle} \sum_{\alpha} c^{\dagger}_{i\alpha} c_{j\alpha} + \frac{1}{2} U \sum_{i} \sum_{\alpha \neq \alpha'} n_{i\alpha} n_{i\alpha'}$$



$\alpha = (m, \sigma), \quad m = 1, ..., M, \quad \sigma = \uparrow, \downarrow$

no Hund exchange!

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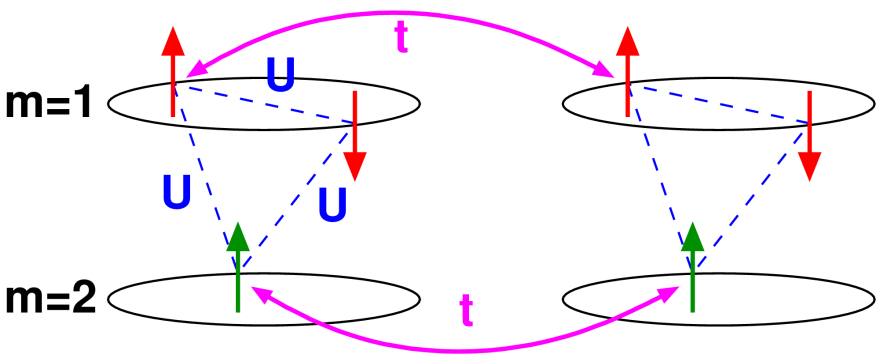

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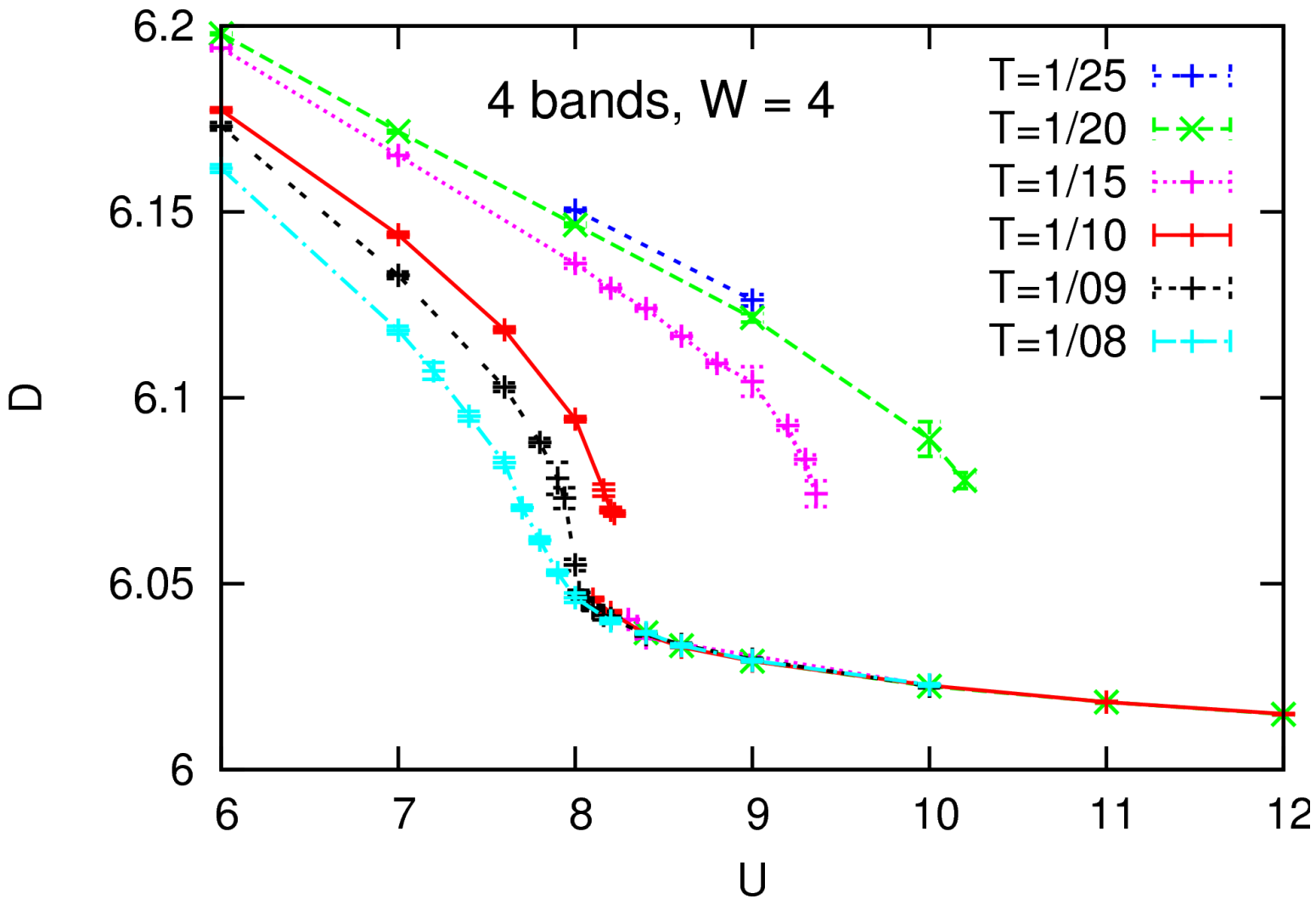
no Hund exchange!

- Mott transition for any $M = 1, 2, ...$
- Analytic solutions for $M \to \infty$ [Florens et al., PRB (2002)]
- So far: only approximate numerical solution for $2 \leq M \leq 4$ [Inaba et al., PRB (2005)]

Mott transition at variable degeneracy $SU(2M)$: 4-band case

Multigrid HF-QMC: Double occupancy



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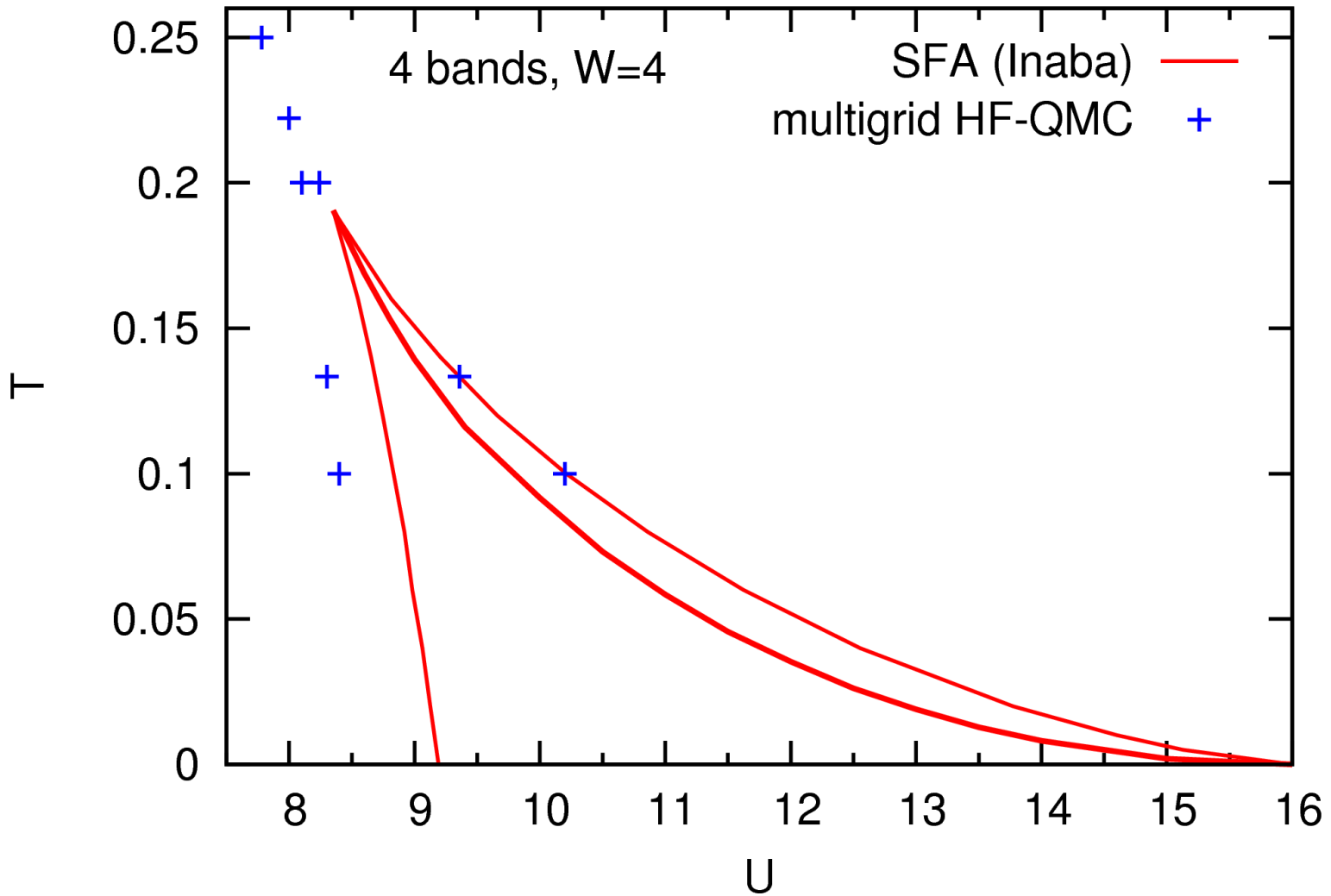
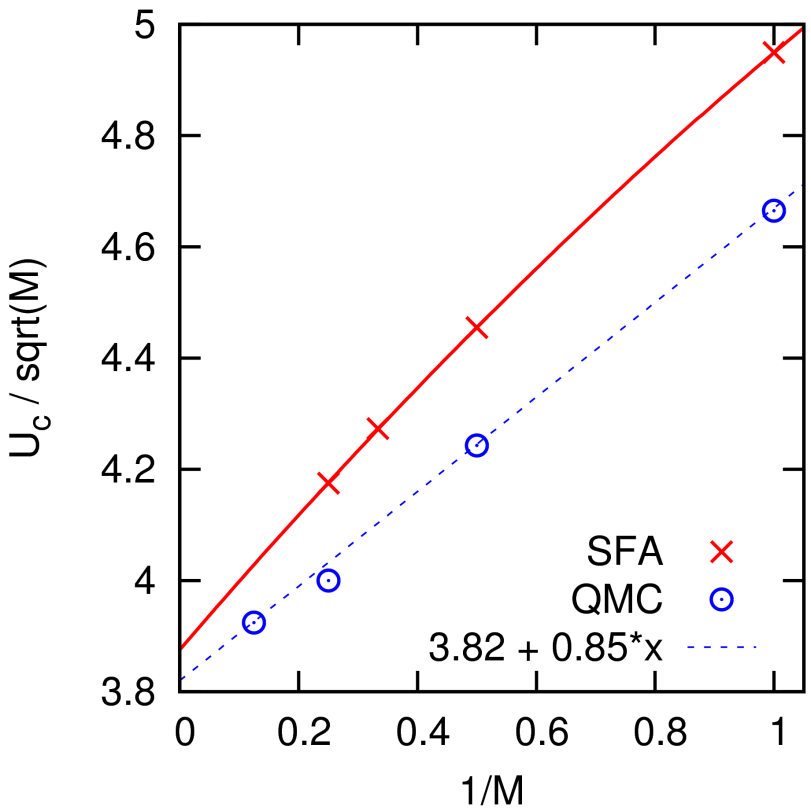
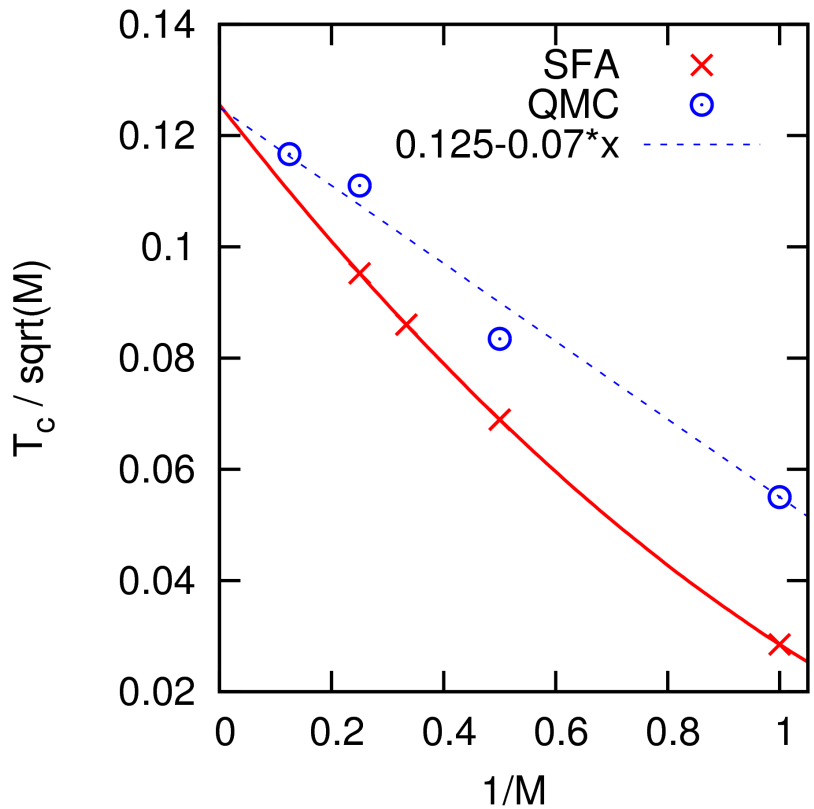


Phase diagram from multigrid HF-QMC: numerically exact results!

Mott transition at variable degeneracy $SU(2M)$:

scaling of the critical parameters





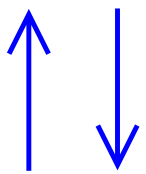
Multigrid HF-QMC: numerically exact results!

$\Longrightarrow$ Phase diagram for arbitrary M

Beyond electronic systems : Fermions with arbitrary spin multiplicity

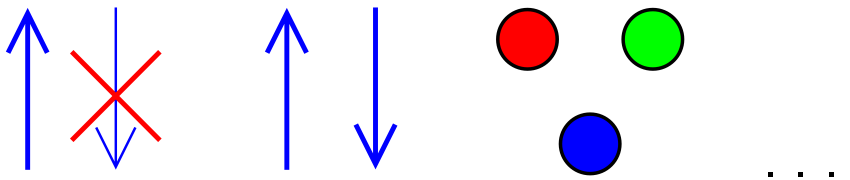
Condensed matter physics

electronic systems
$SU(2)$ spin-rotational symmetry



Ultracold fermions

combination of S and I into hyperfine state with angular momentum $F \geq 1/2$

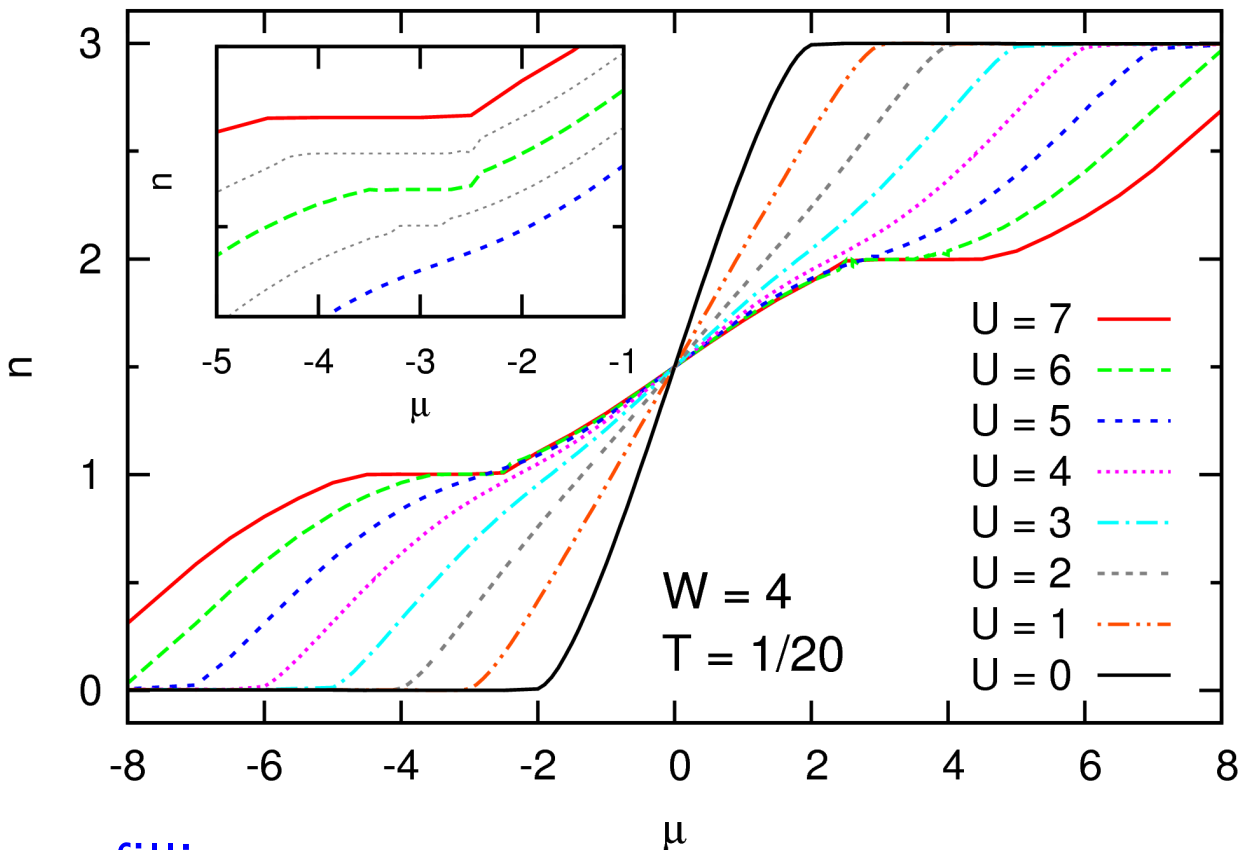


Example: ^{40}K
$|F = 9/2, m_F = -5/7, -7/2, -9/2\rangle$
[Regal, Jin, PRL (2003)]

QMC generalization for arbitrary spin multiplicity

- in principle straightforward, but changes in $\sim 50\%$ of code
- at this opportunity: cleaner solutions, documentation

3-spin/flavor system in paramagnetic phase

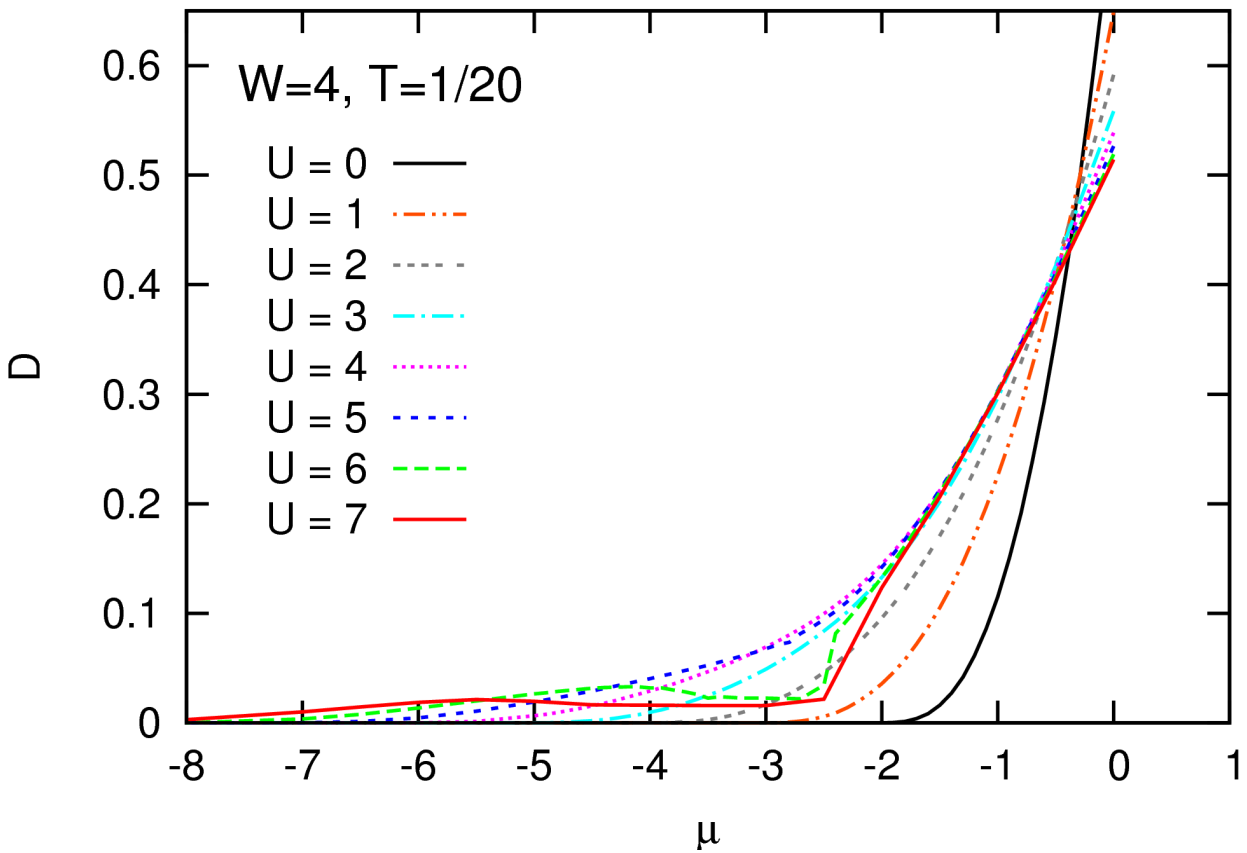


Density vs. filling

Plateaus: incompressible Mott phase (for $U \gtrsim 6$)

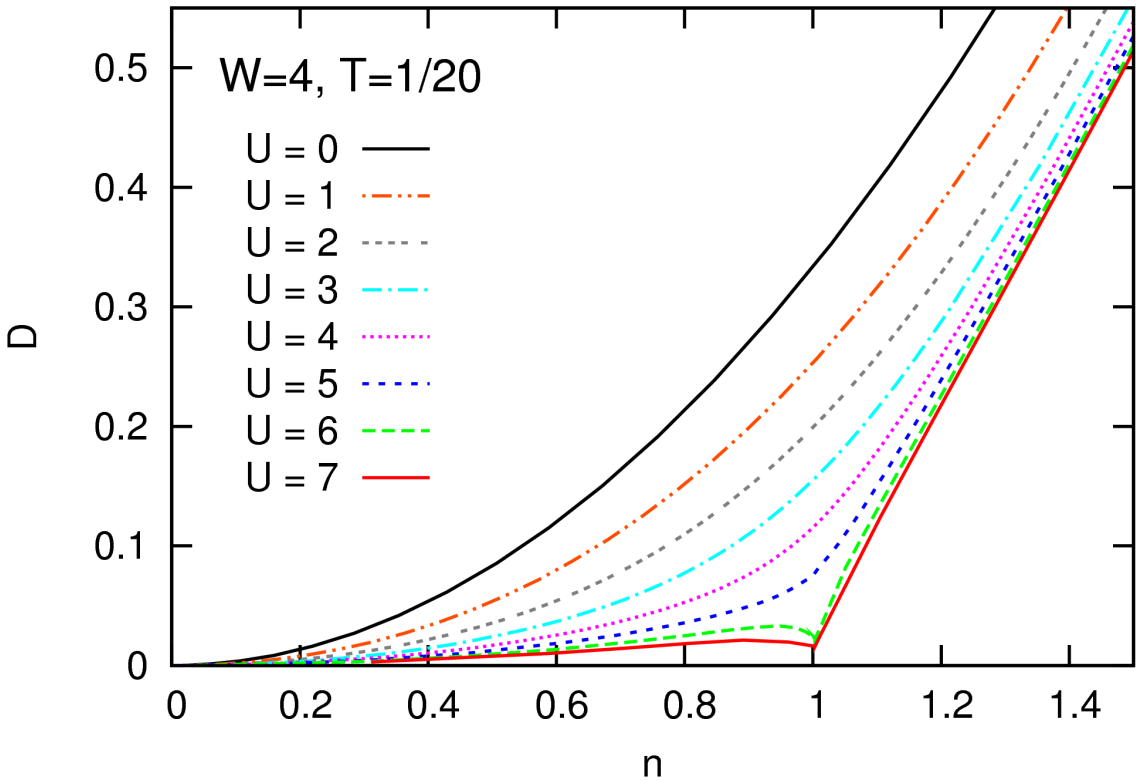
not at half-filling!

3-spin/flavor system in paramagnetic phase



Double occupancy vs. filling

Here mostly density effects



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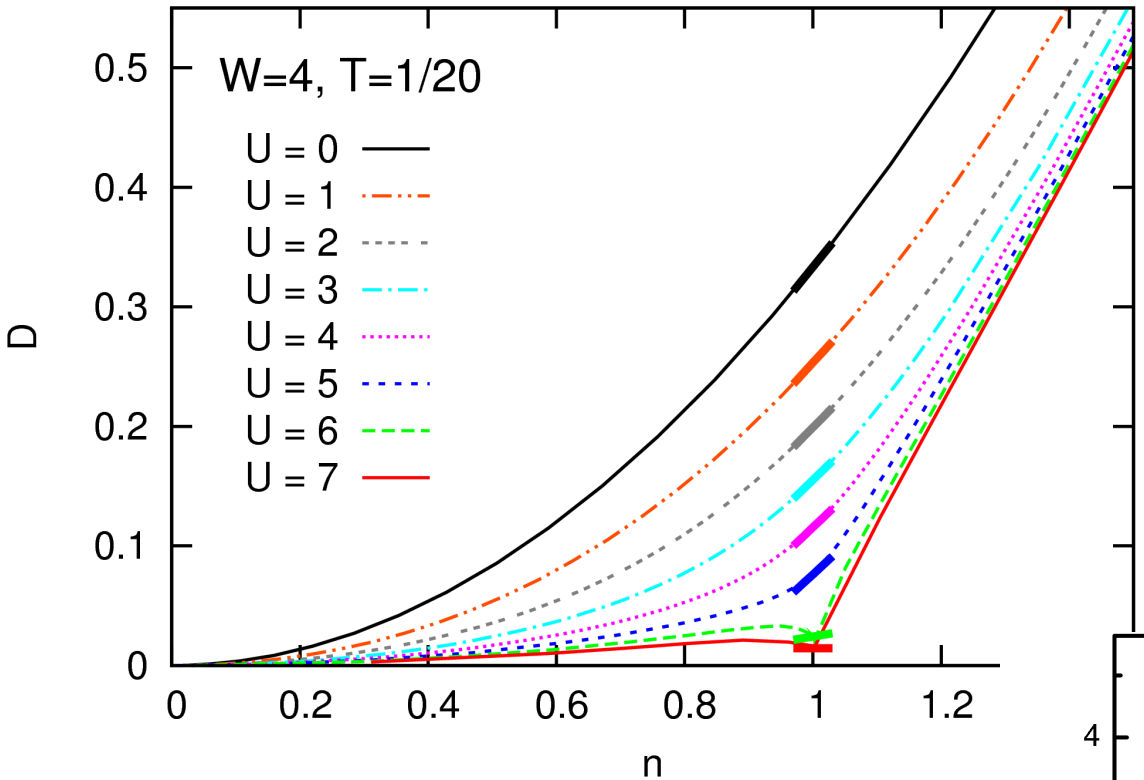


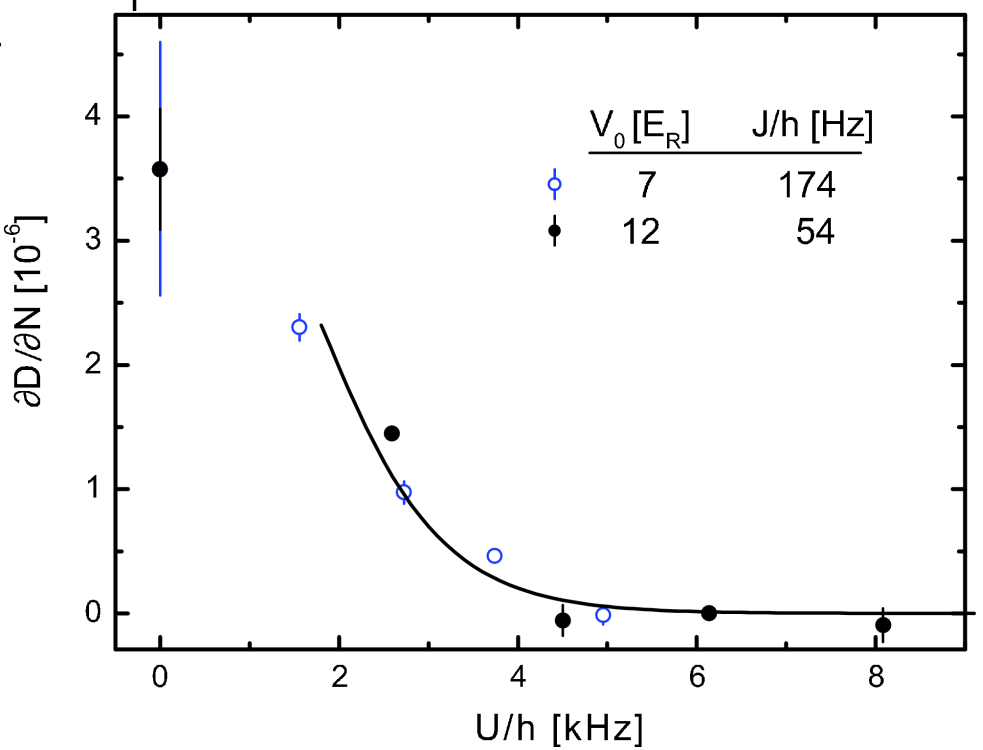
3-spin/flavor system:

Double occupancy vs. density

Experiment:2-spin system

Transition to an incompressible phase

[Jördens et al., Nature (2008)]



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

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Acknowledgements:

Carsten Knecht, **Elena Gorelik**, Eberhard Jacobi, Peter van Dongen;
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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?

Thermal breakdown of a Fermi liquid

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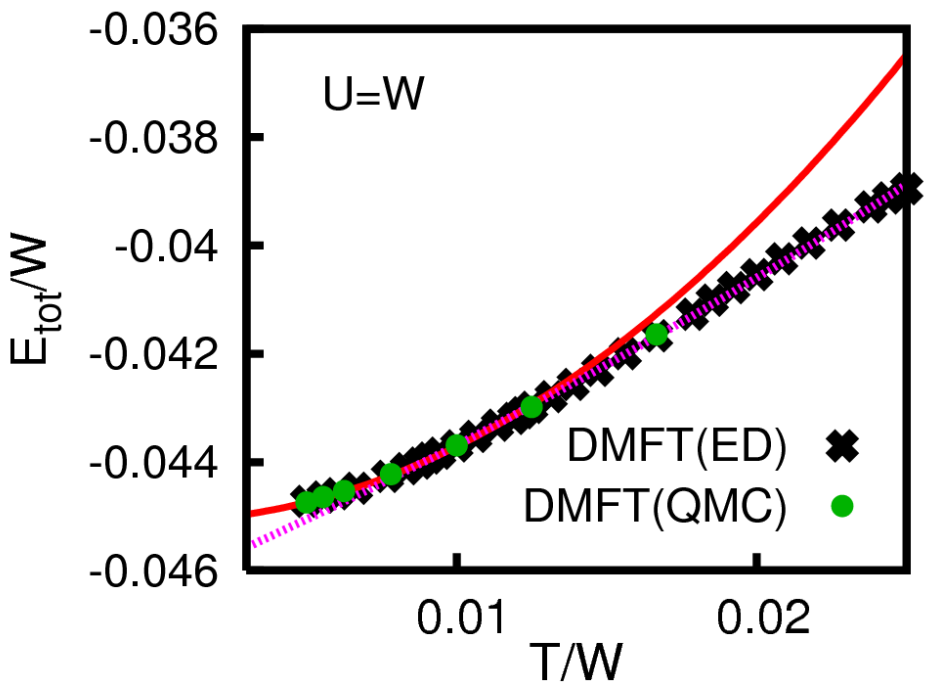
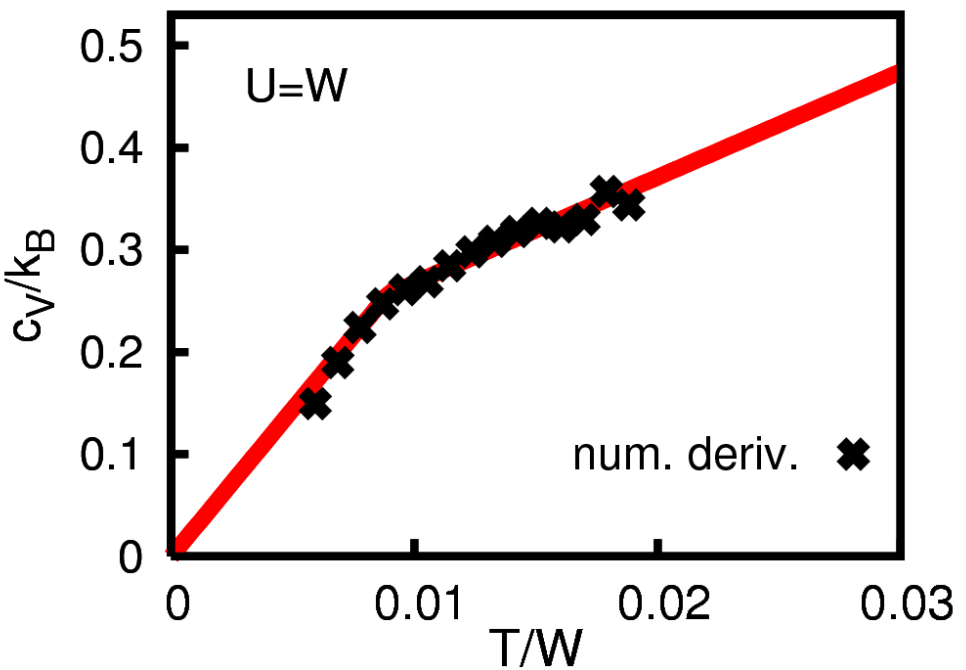
quadratic resistivity $\rho \propto T^2$ for "low enough" T

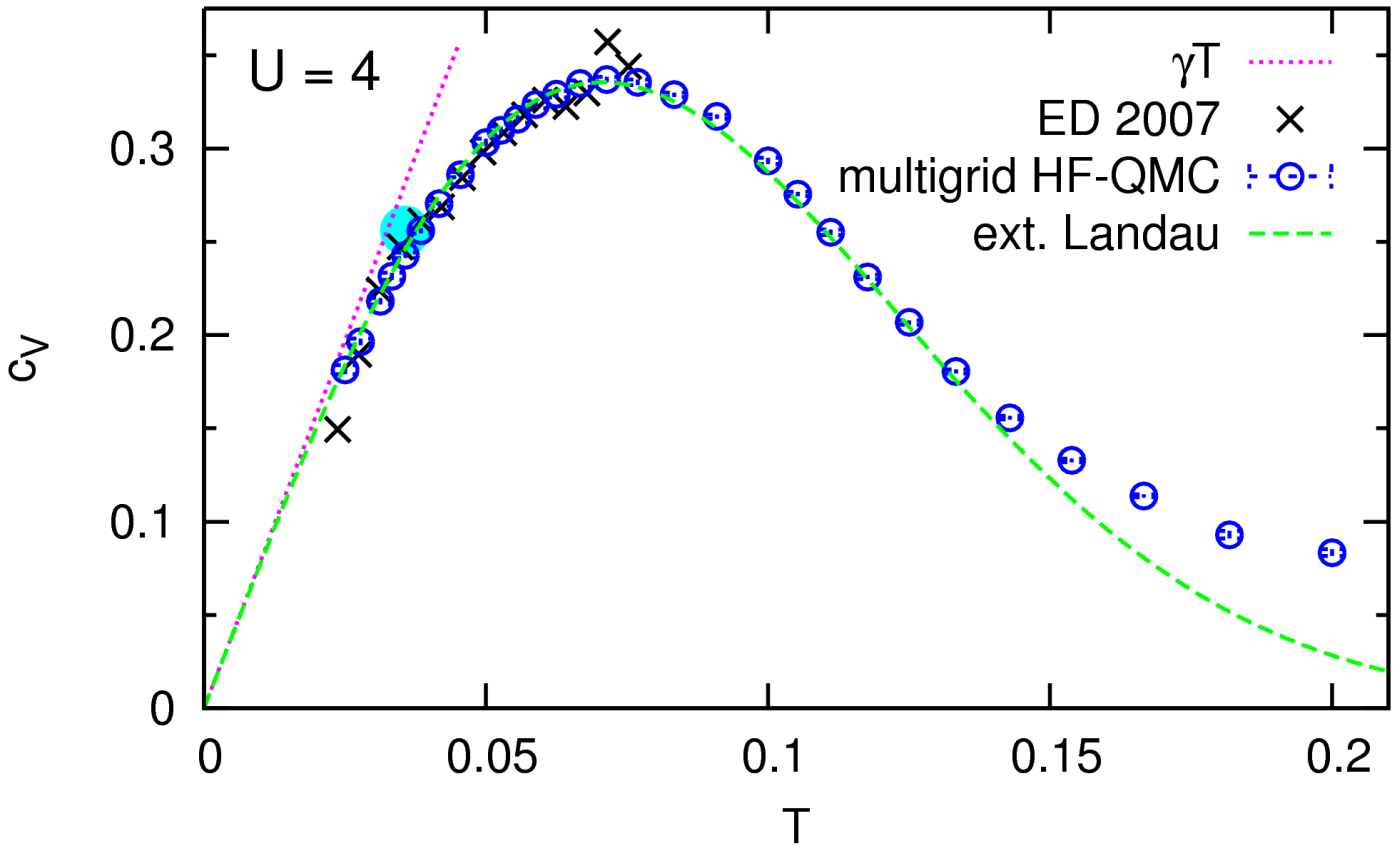
When/how do these laws break down?

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]

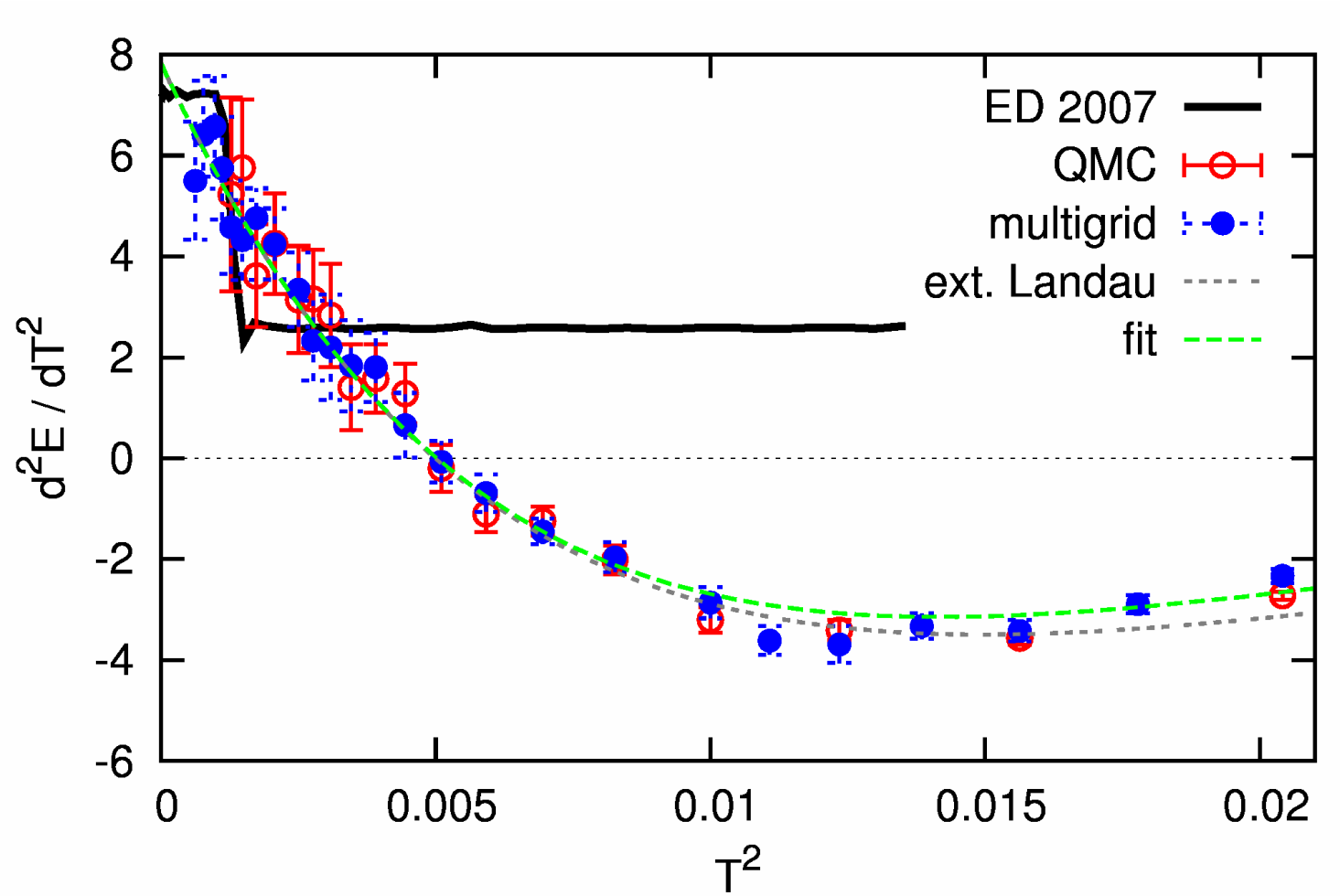


High-precision results $\rightsquigarrow$ no kink!

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

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

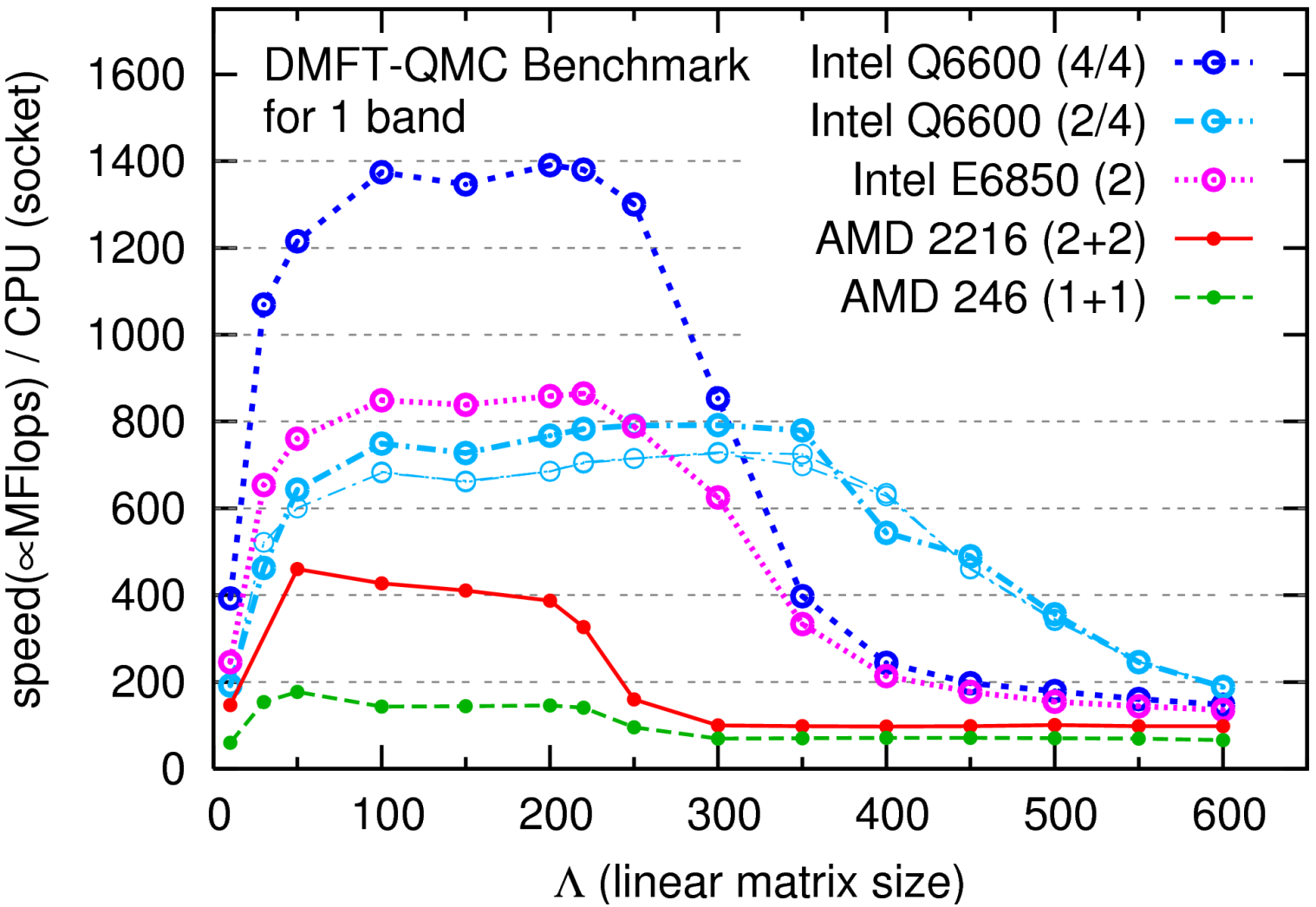
Direct measure of "kinkiness": energy curvature



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

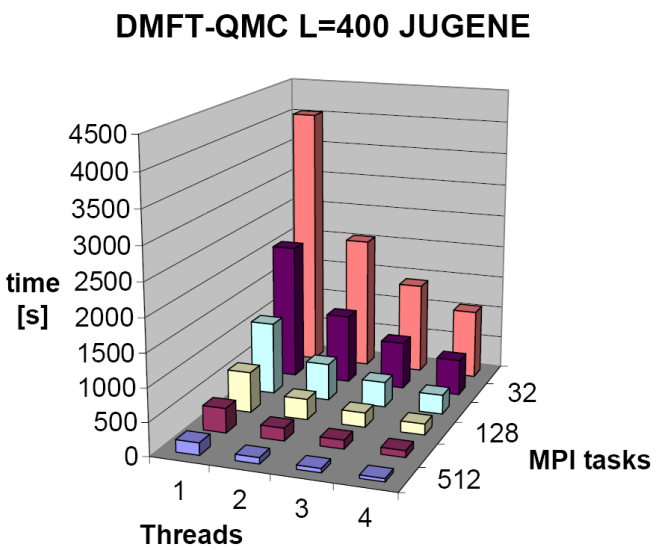
Initial slope: contributions from Sommerfeld expansion + T-dependence of $\Sigma(\omega)$

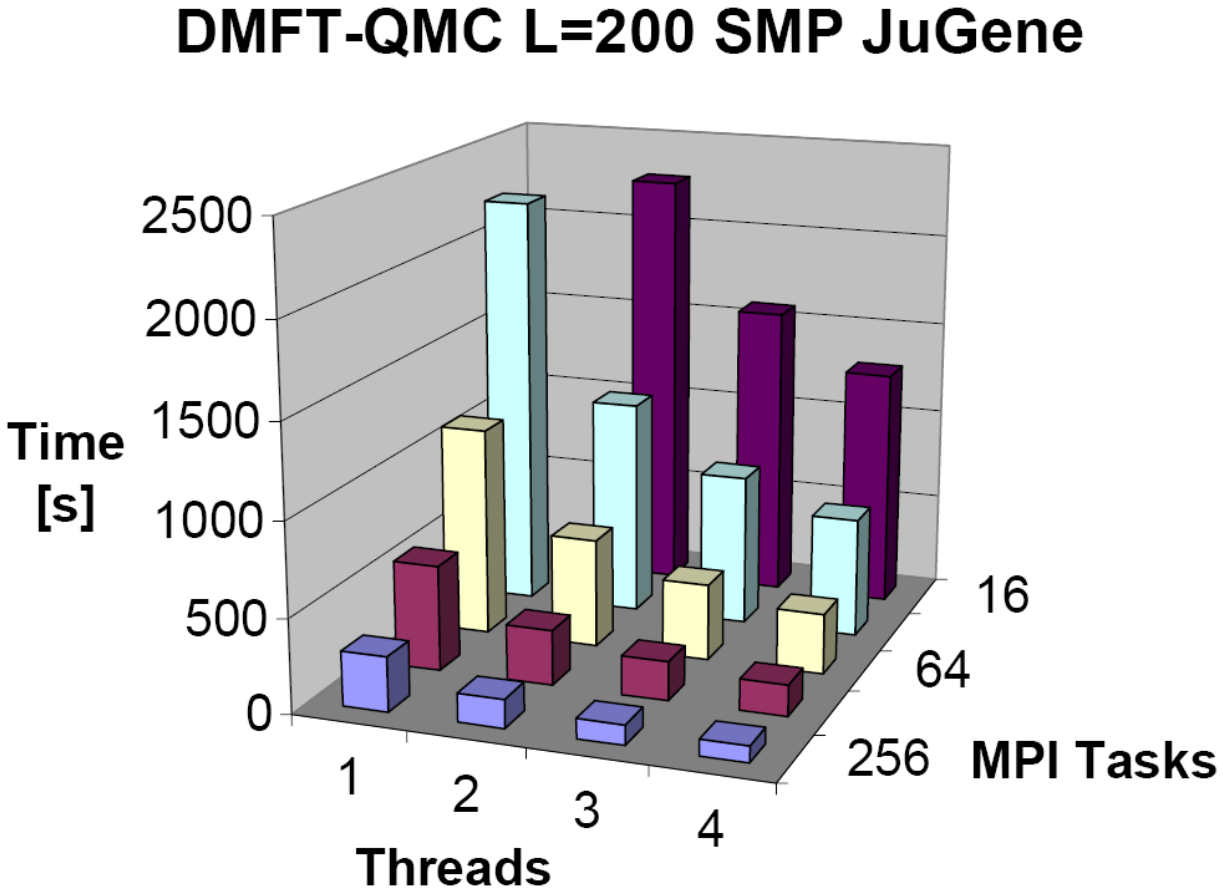
Benchmarks



HF-QMC profits strongly from modern large-cache architectures

New (4/2008): hybrid parallelization (MPI + OpenMP)





Very good scaling: speed roughly linear with number of CPU cores

Superlinear scaling on JUMP