Quantum Monte Carlo simulations of strongly correlated fermions within dynamical mean-field theory

Nils Blümer, Univ. Mainz

Outline

Monte Carlo methods: principles and classical simulations

Systems with strong electronic (fermionic) correlations

Approaches for correlated electron systems

Auxiliary-field Hirsch-Fye QMC algorithm

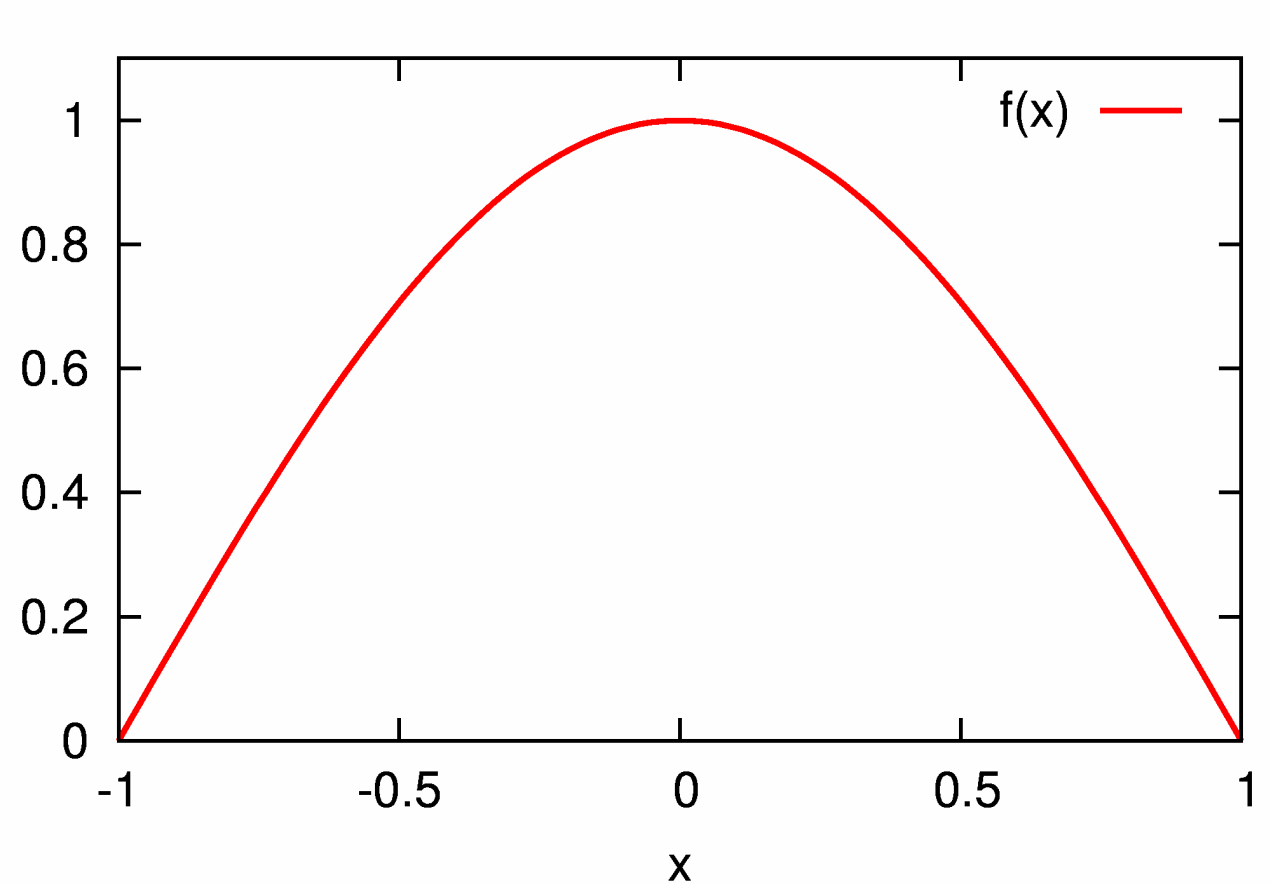
Multigrid Hirsch-Fye quantum Monte Carlo algorithm

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

Monte Carlo methods: principles and classical simulations

General task: evaluation of (high-dimensional) sums/integrals

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



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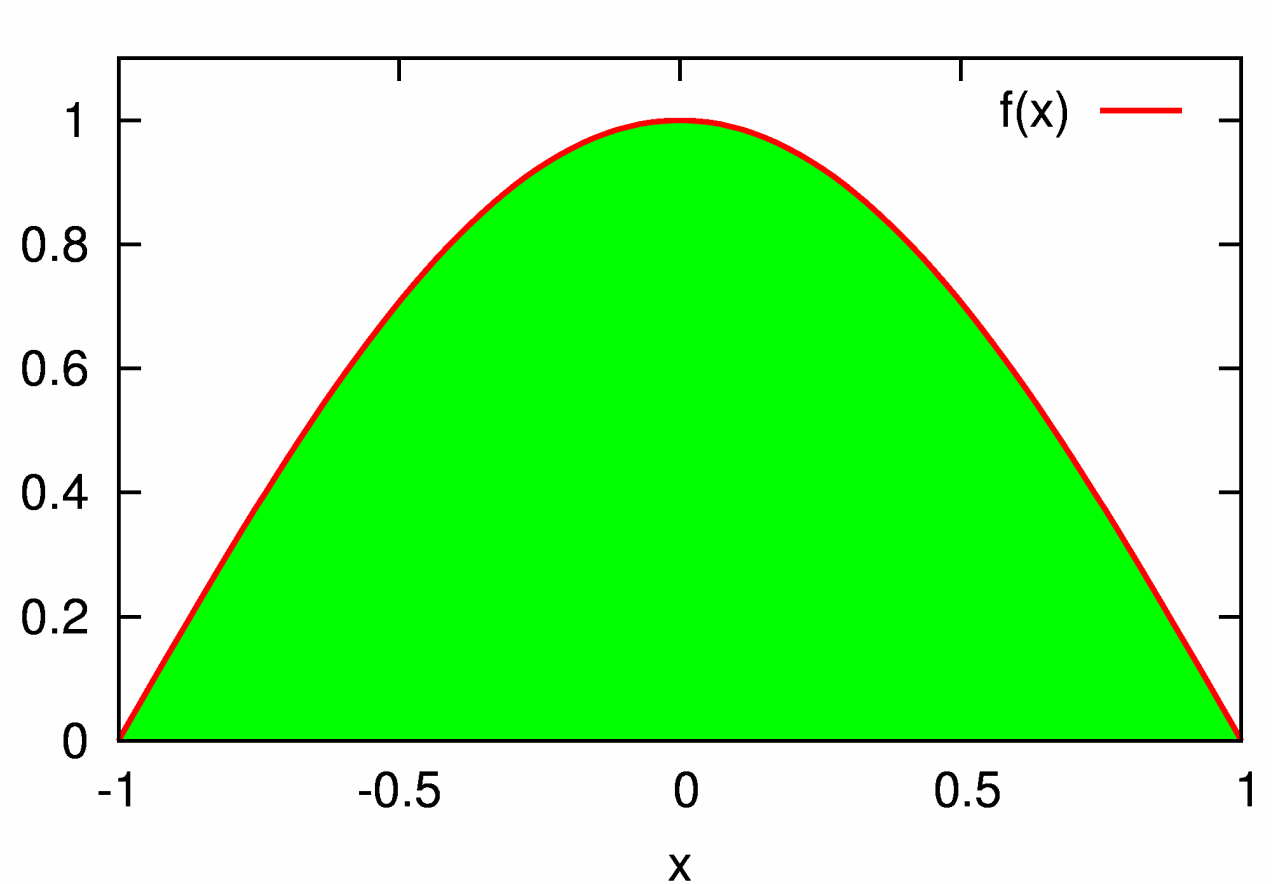

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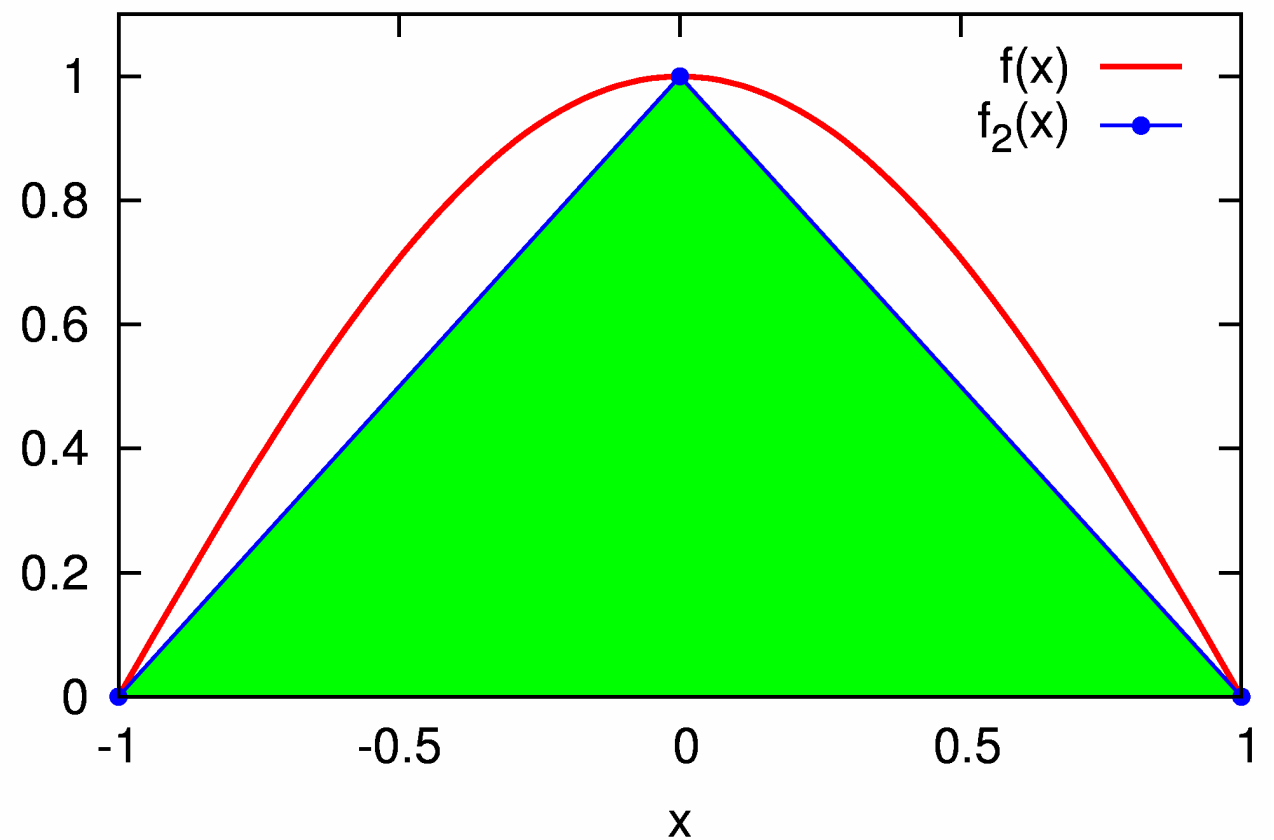

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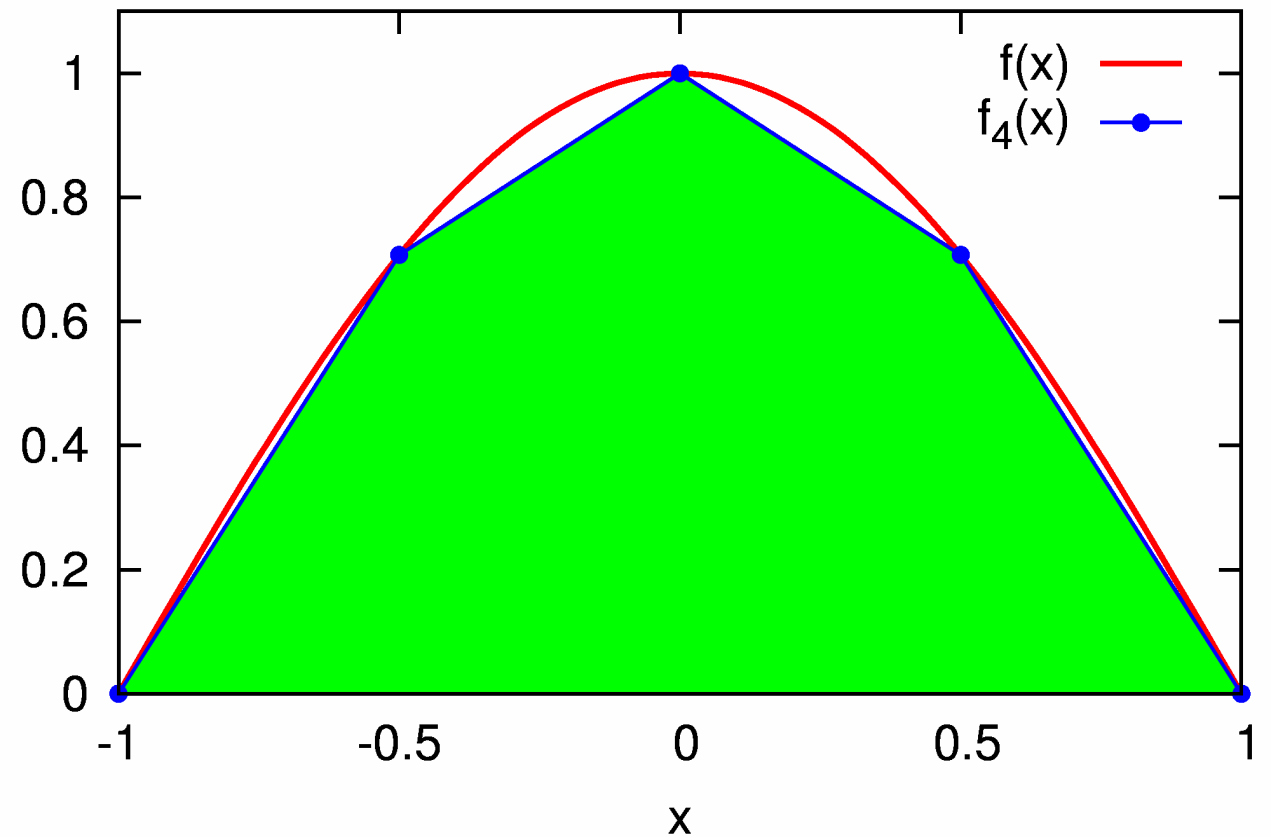

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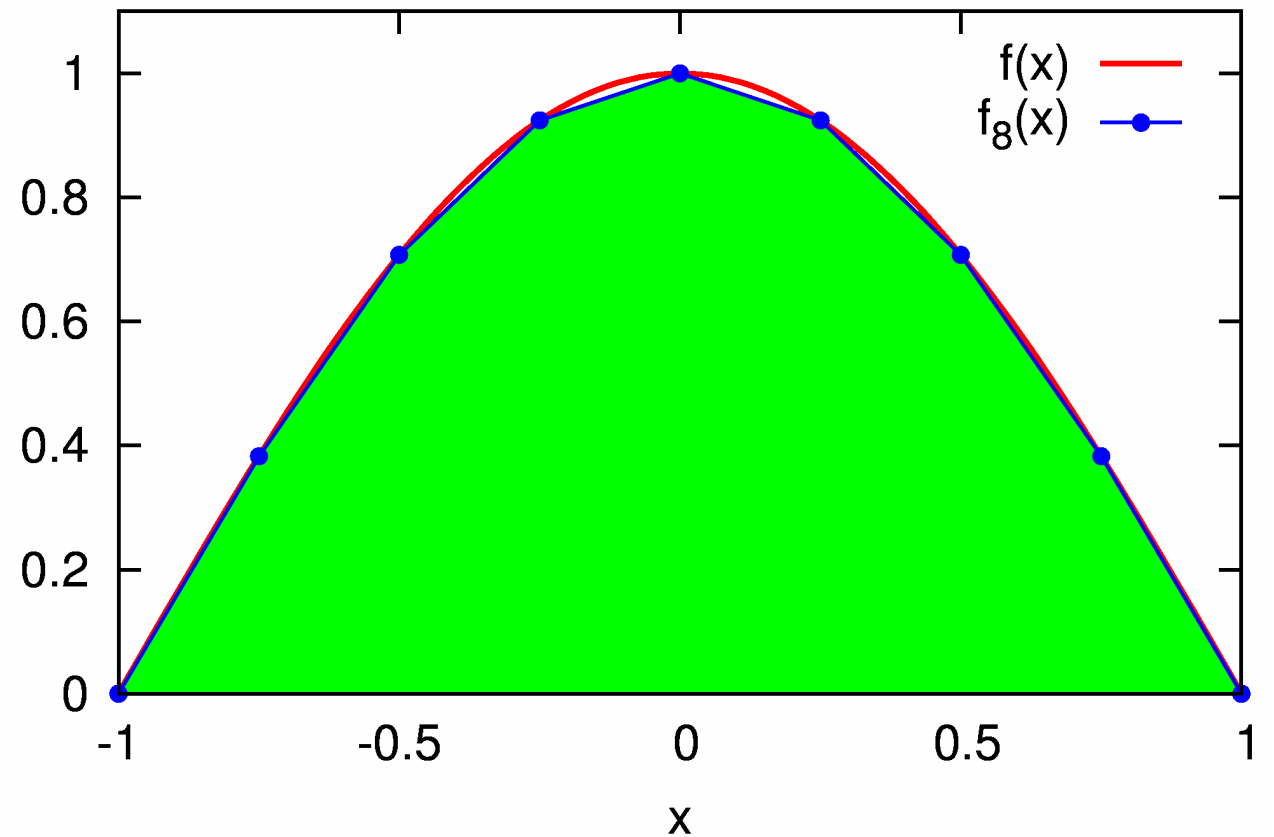

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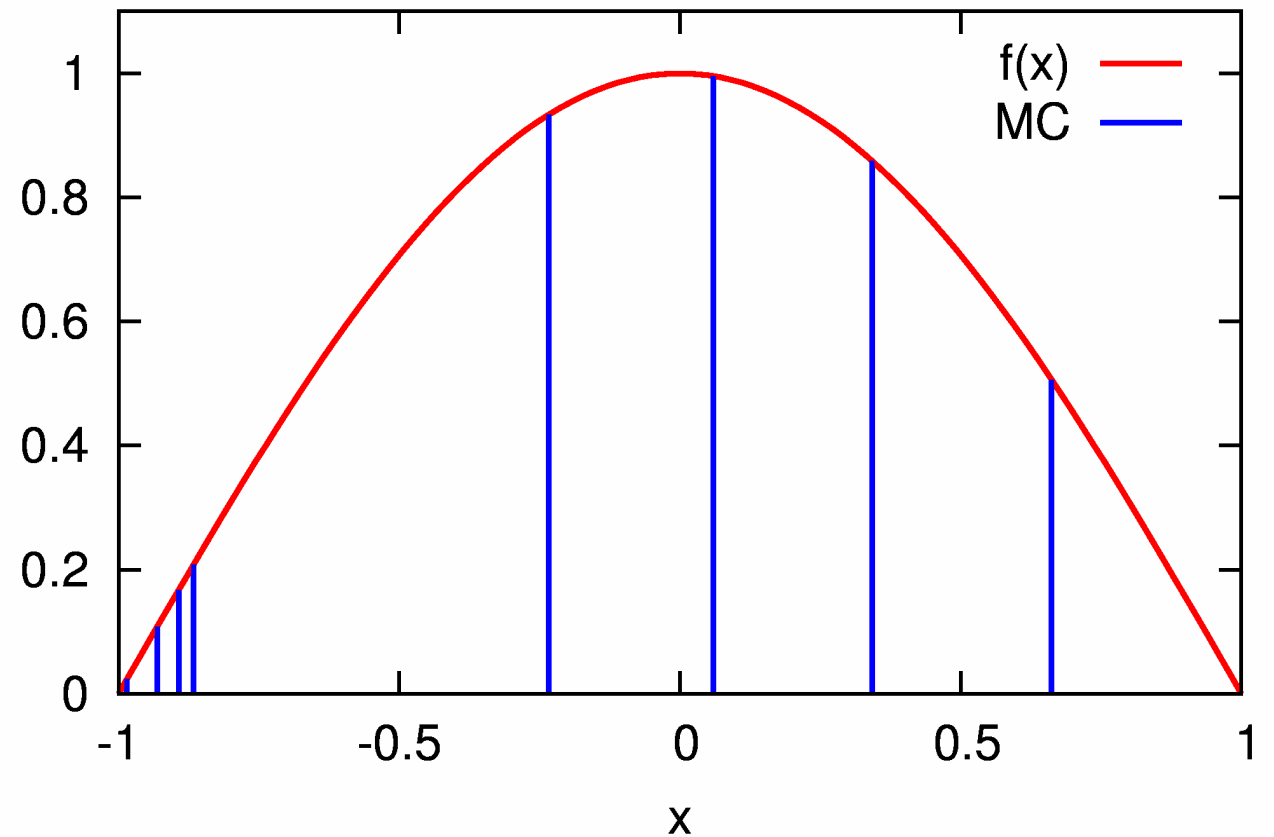

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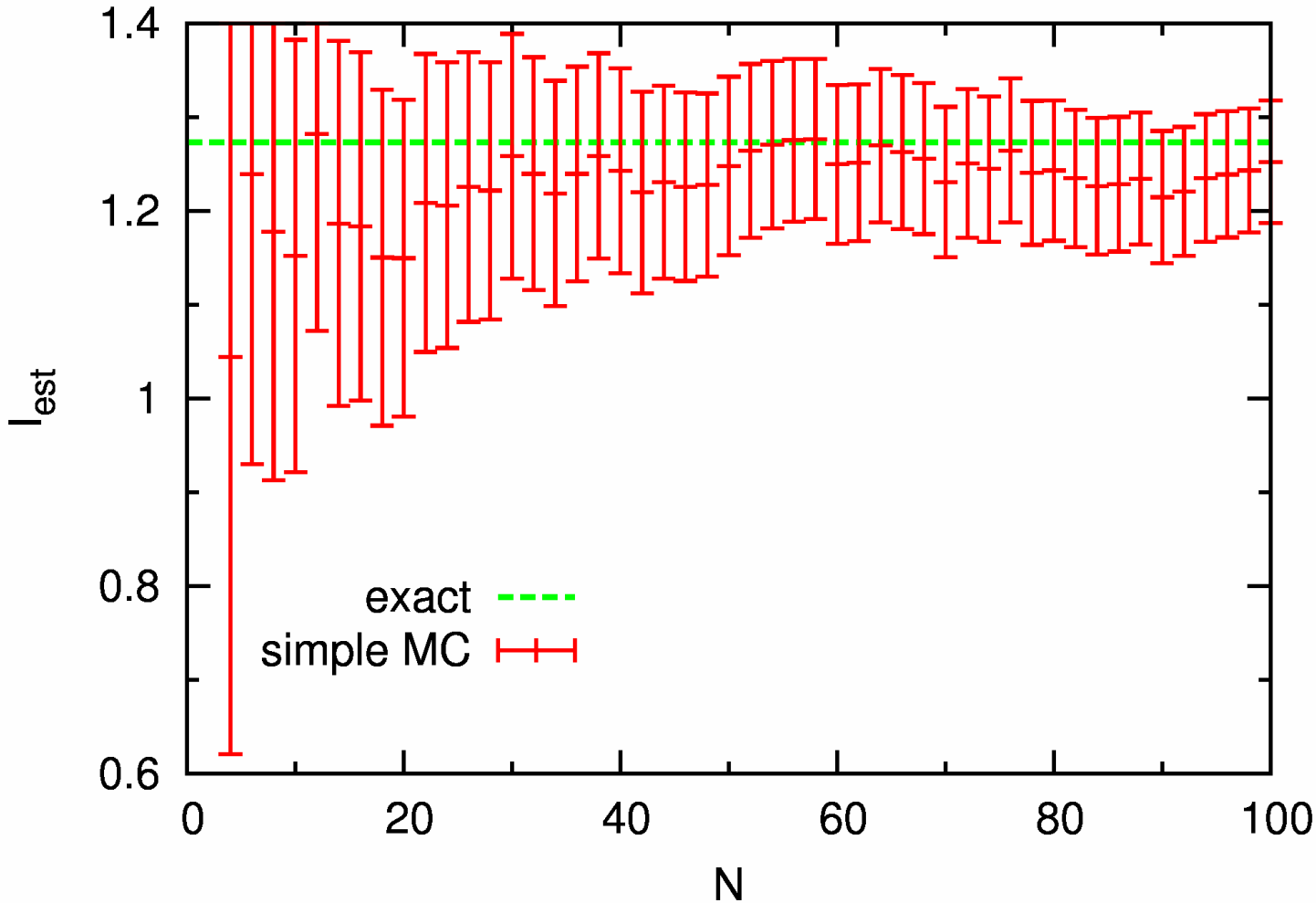
- discretization
- Monte Carlo

Convergence of results?



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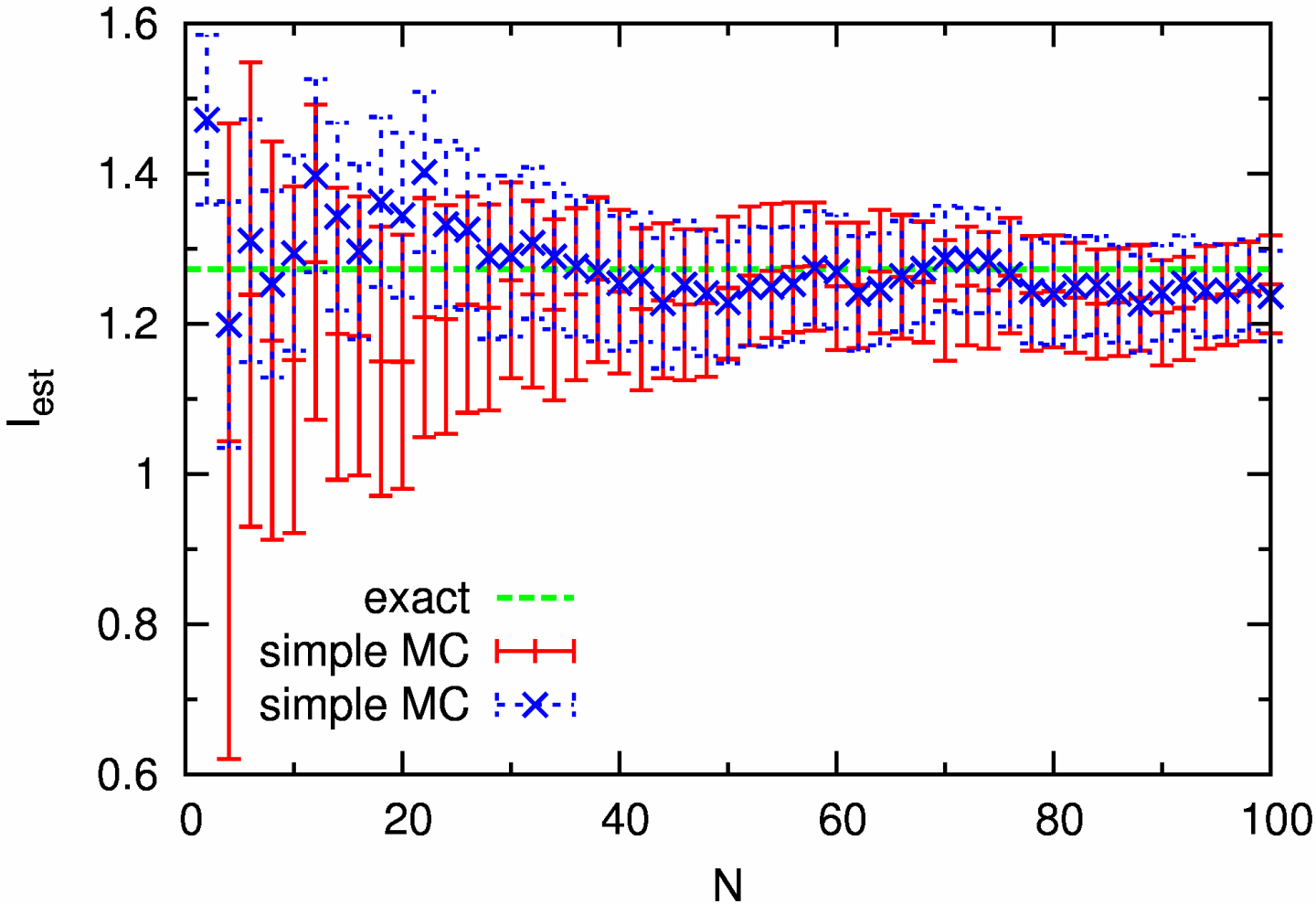

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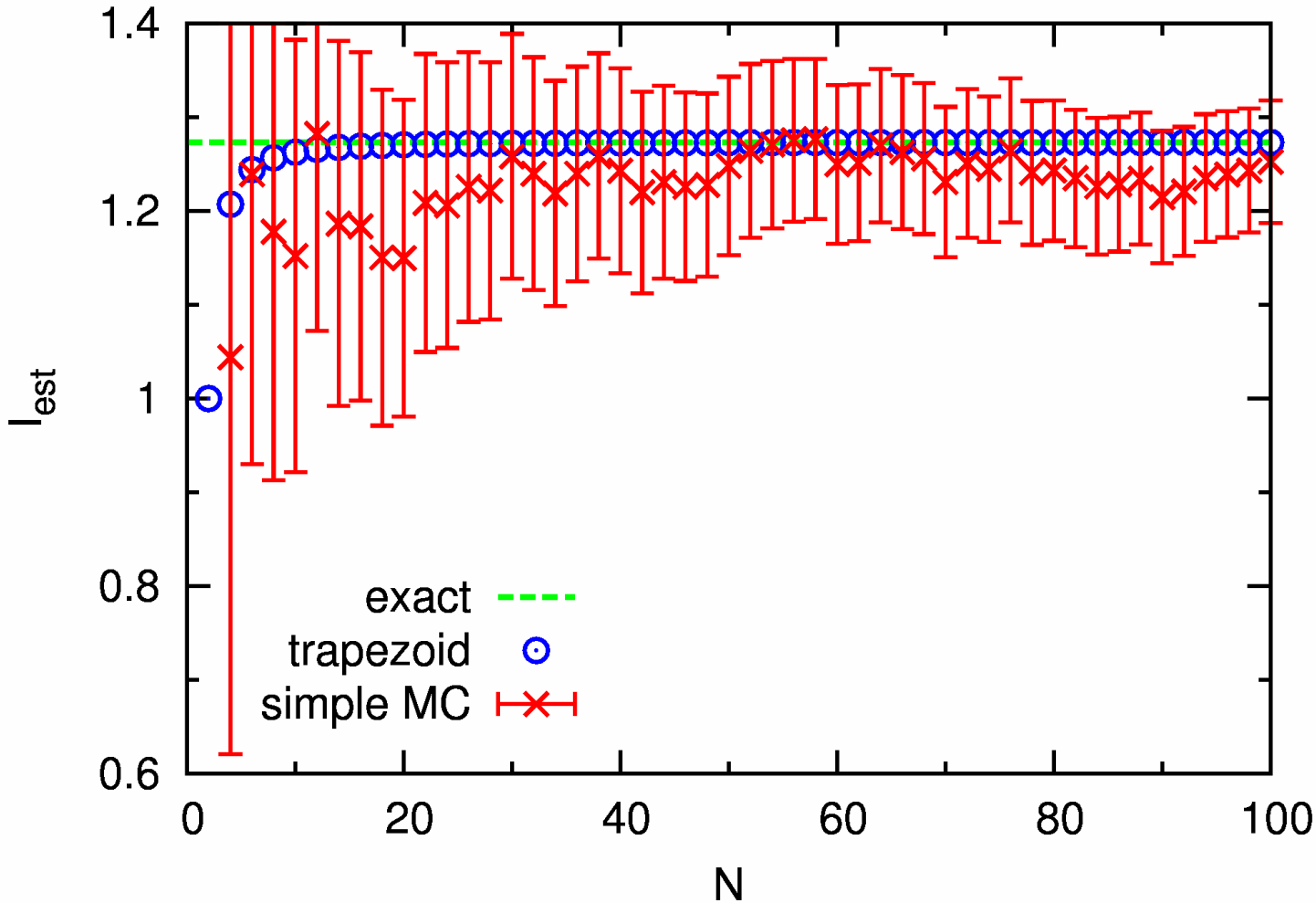

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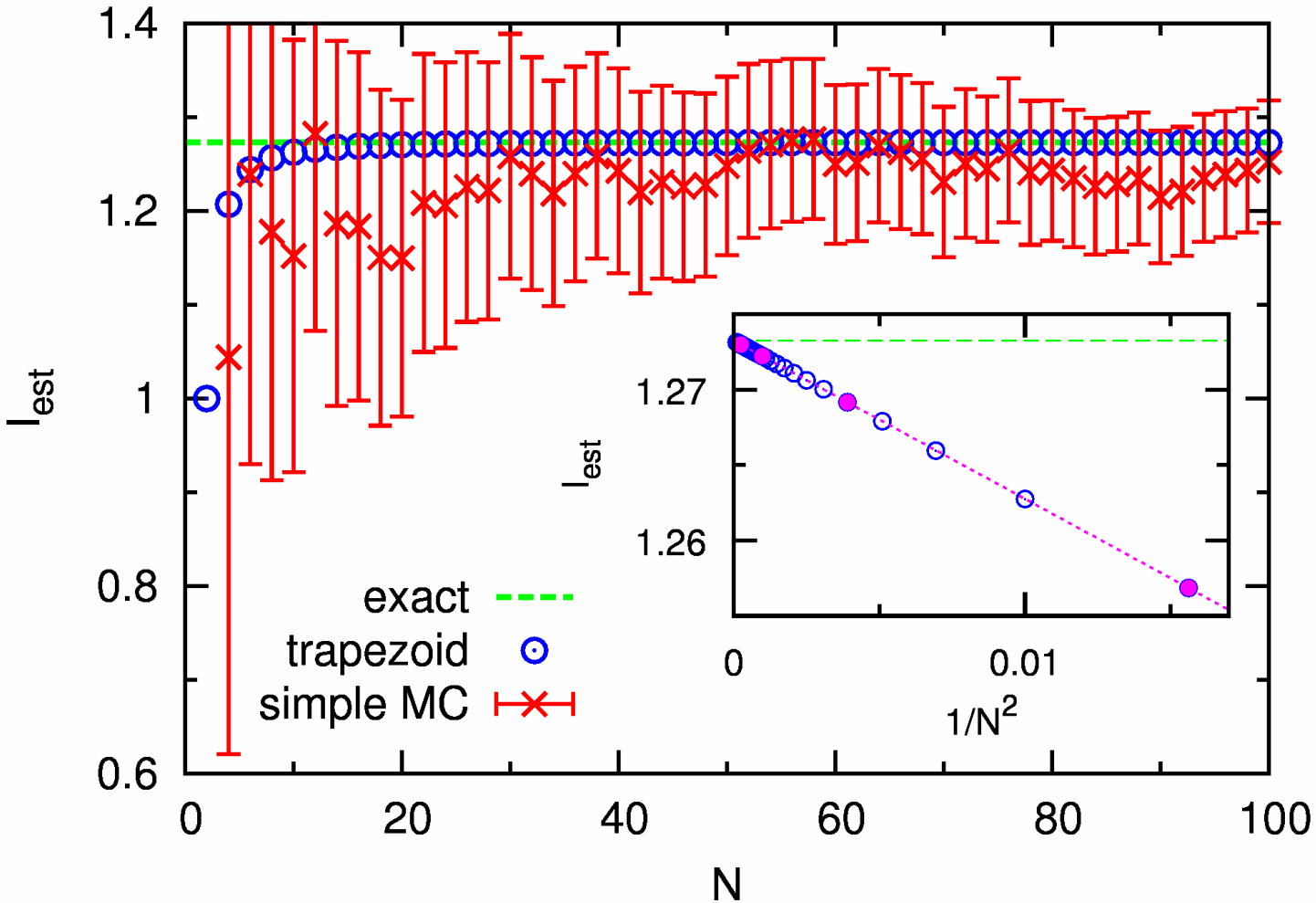
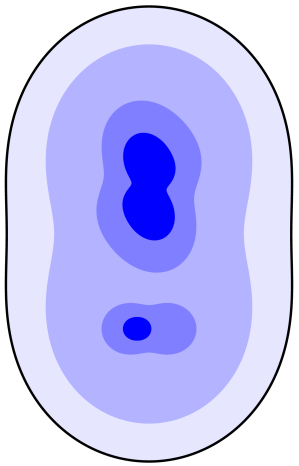


MC results are non-deterministic: only meaningful within statistical error bars!

In this case, the deterministic method converges much faster (and very regularly)

Second MC example: higher dimensions

Computation of average depth $\overline{h}$ of a lake from depth distribution $h(x_1, x_2)$



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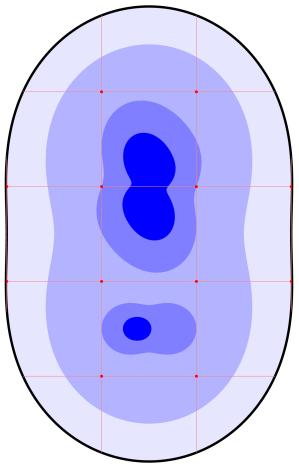

Deterministic: grid + trapezoid rule
$N = V/(\Delta x)^d$ measurements

$$\Delta h \propto (\Delta x)^2 \propto N^{-2/d}$$

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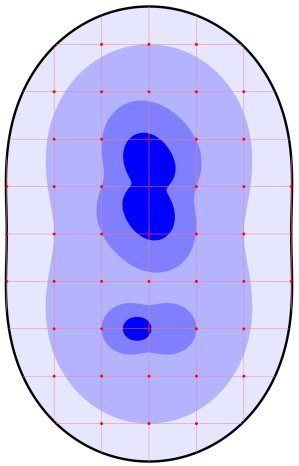

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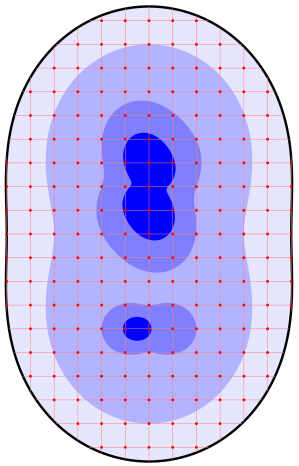

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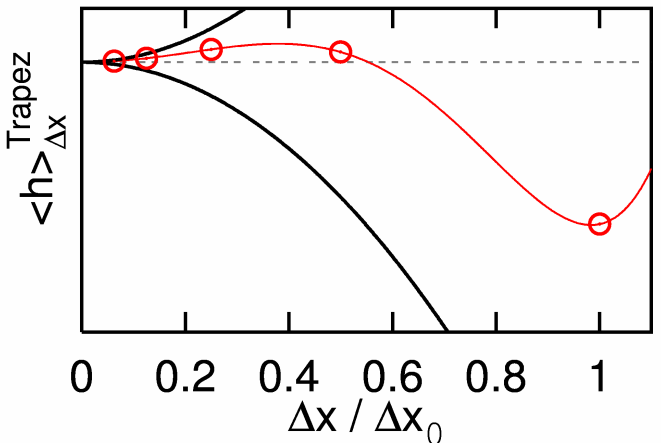

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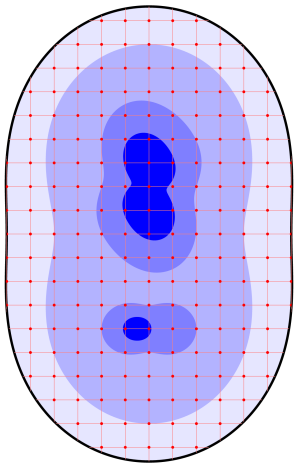

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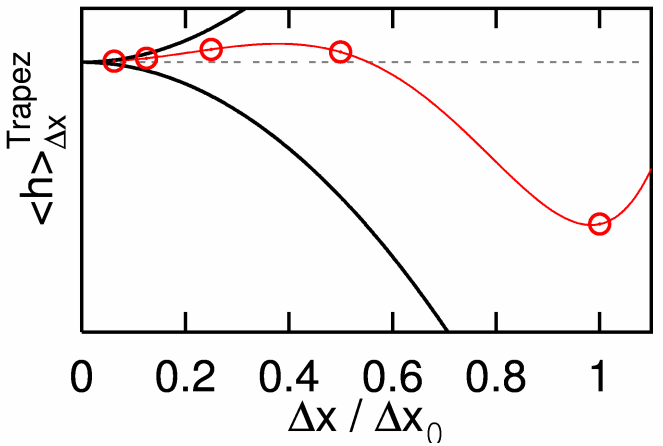
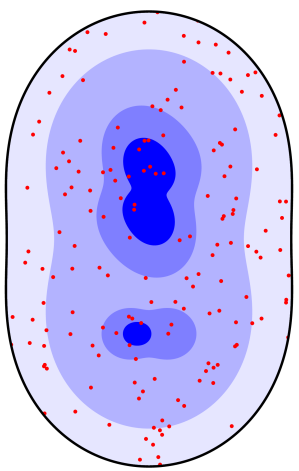


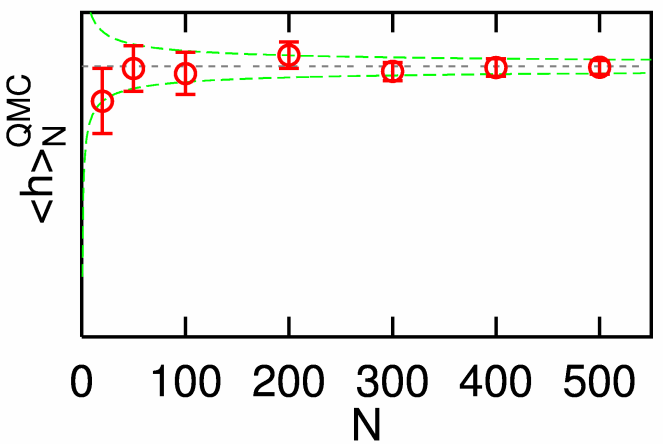


Stochastic: simple Monte-Carlo

N configurations $\vec{x}_i$, uniform probability

$$h_N^{\mathrm{QMC}} = \frac{1}{N}\sum_{i=1}^{N} h(\vec{x}_i)$$

$$\Delta h_N \lesssim \sqrt{\frac{\mathrm{var}\{h\}}{N}} \propto N^{-1/2}$$



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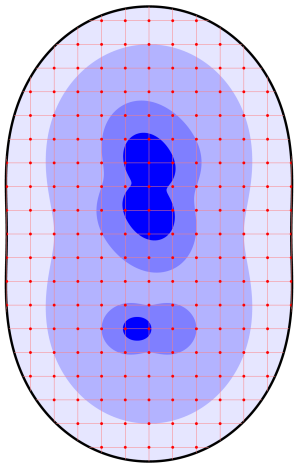

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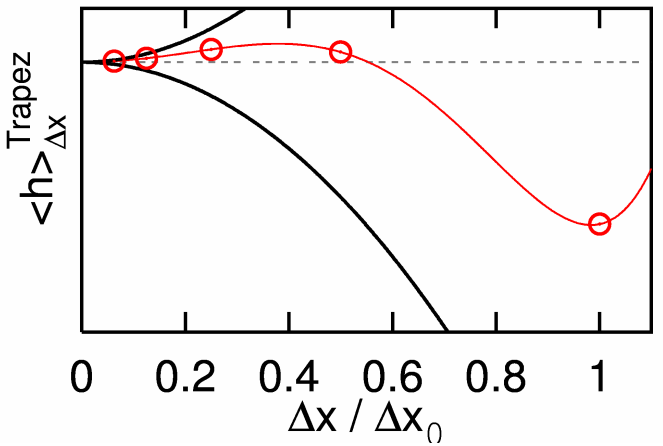

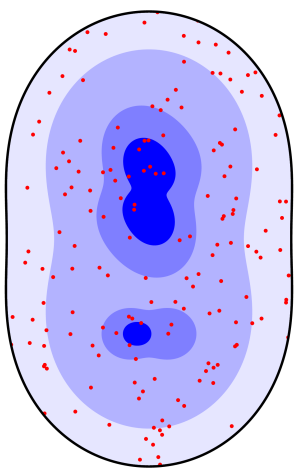

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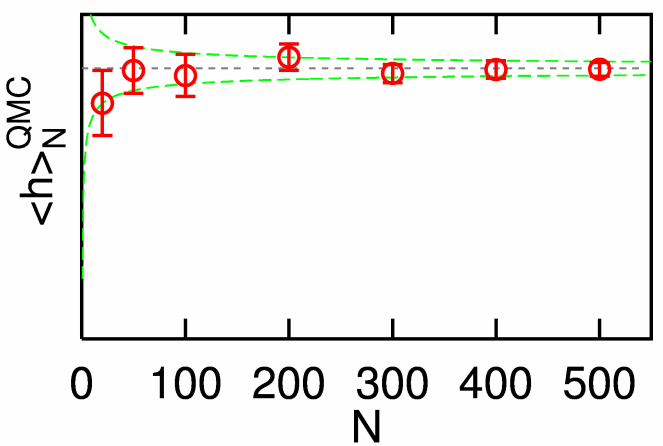
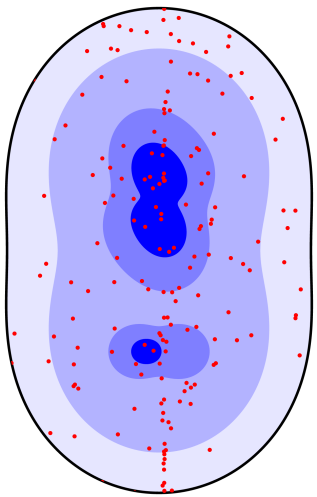


Central limit theorem

For which dimensionalities does MC "win"?

Advanced variant: Monte Carlo with importance sampling

Generate configurations $\vec{x}_i$ with optimized probability $p(\vec{x}_i)$: most important contributions are sampled more often.

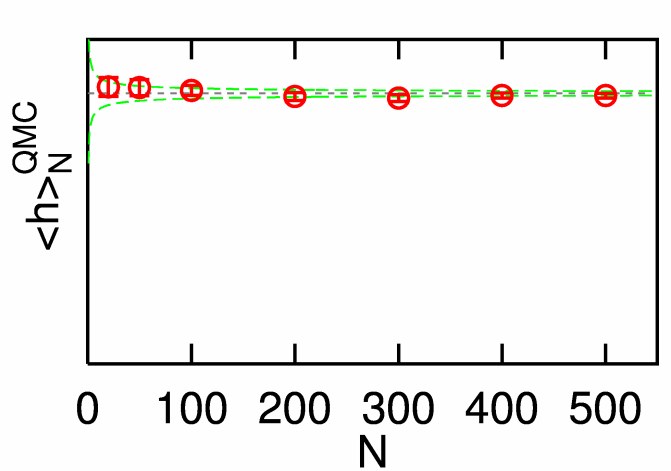


factorization: $h(\vec{x}) = p(\vec{x})\, o(\vec{x})$;

$p(\vec{x})$ normalized, $\mathrm{var}\{o\} \ll \mathrm{var}\{h\}$

$$h_N^{\mathrm{QMC}} = \frac{1}{N} \sum_{i=1}^{N} o(\vec{x}_i)$$

$$\Delta h \lesssim \sqrt{\frac{\mathrm{var}\{o\}}{N_{\mathrm{eff}}}} \propto N^{-1/2}$$



Ideal case: $\tilde{p}(\vec{x}) \approx |h(\vec{x})|$, but difficult to find good normalizable $\tilde{p}(\vec{x})$.

Application of Monte Carlo in Statistical Physics

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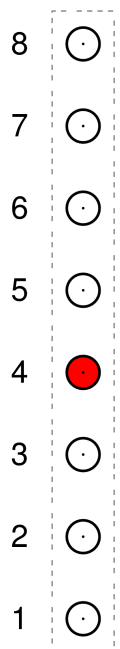

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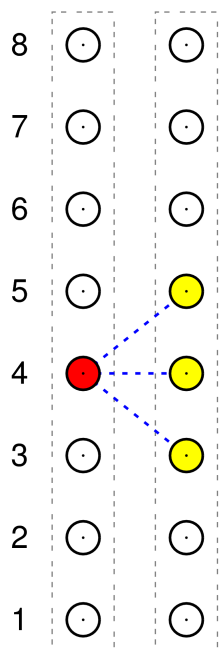

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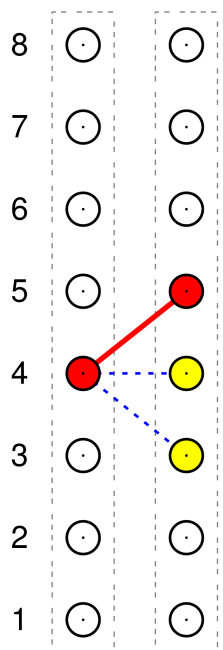

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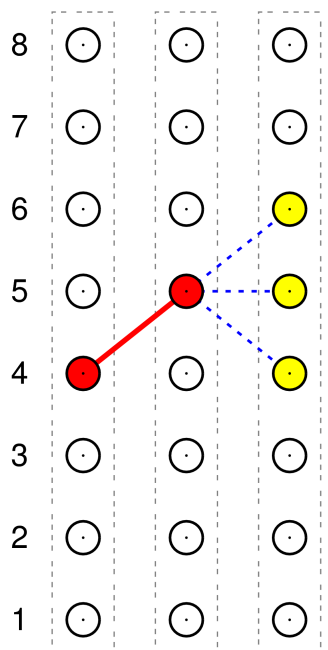

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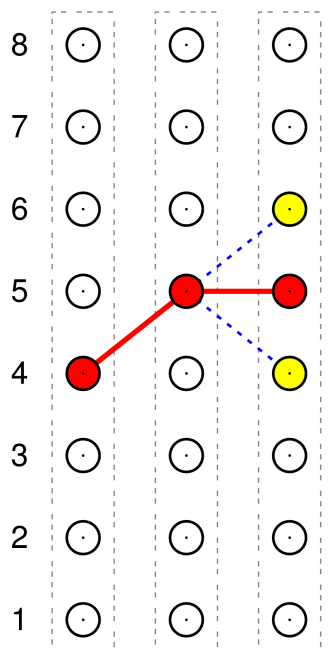

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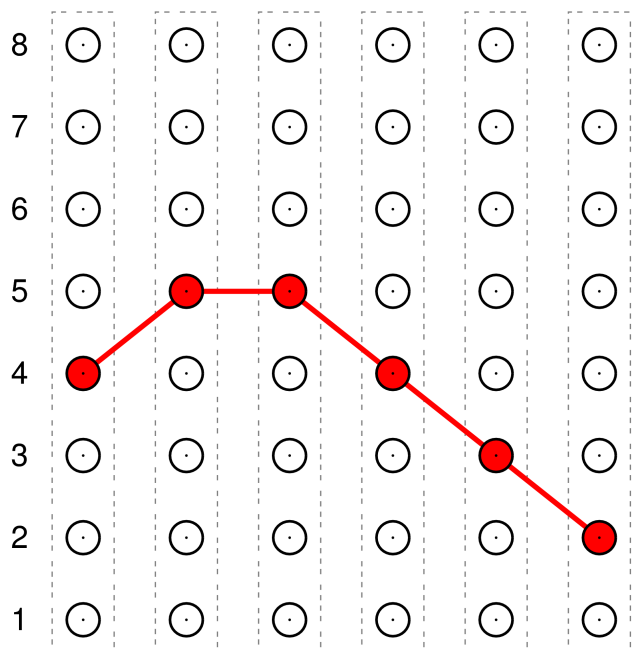

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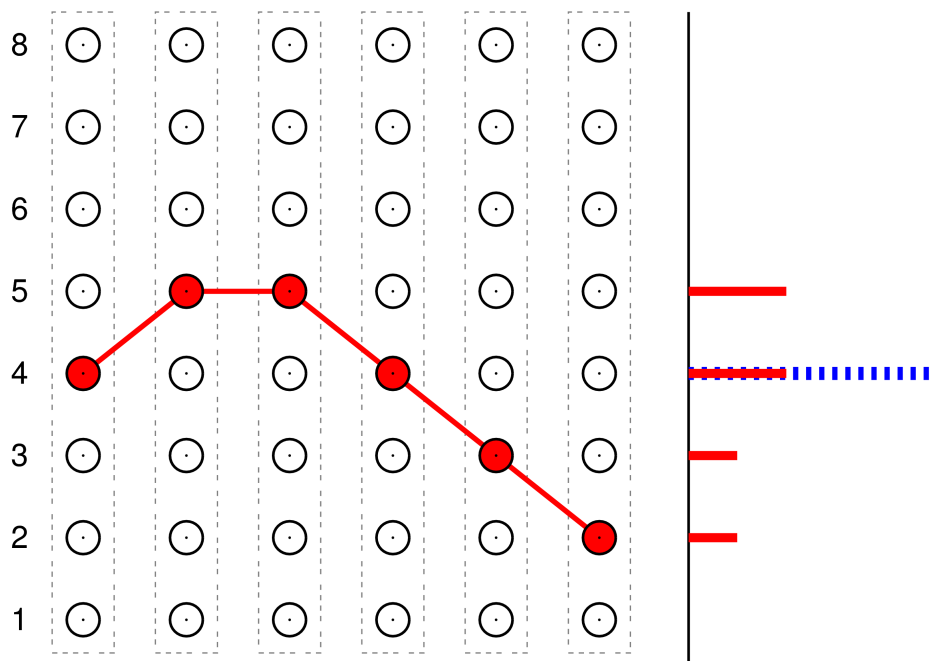

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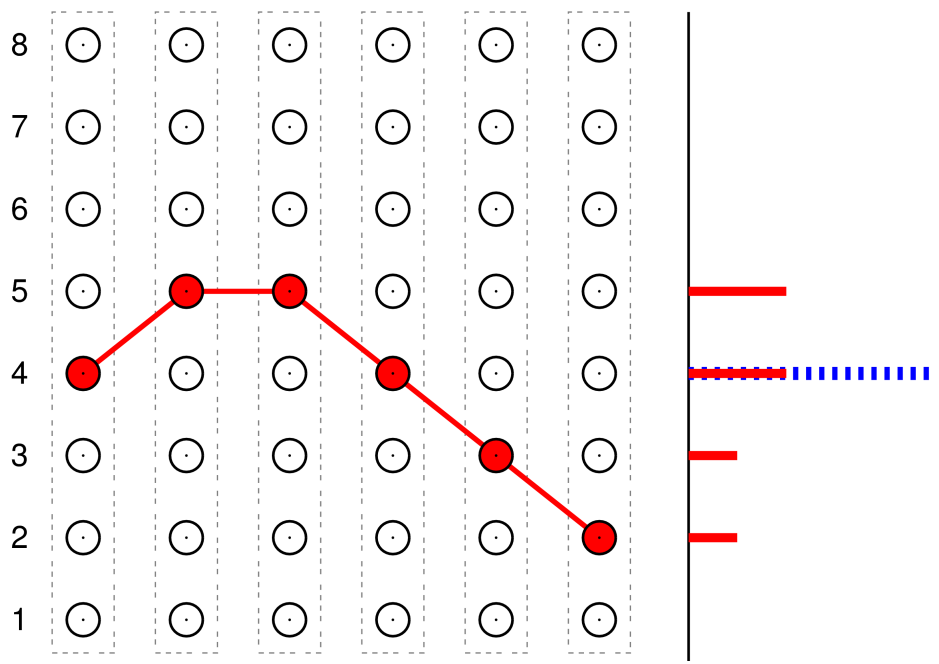

Ergodicity and detailed balance

$$p_i\, P\{i \to j\} = p_j\, P\{j \to i\}$$

$$\Rightarrow \quad P[\text{state } i \text{ after update } N] \overset{N\to\infty}{\longrightarrow} p_i$$

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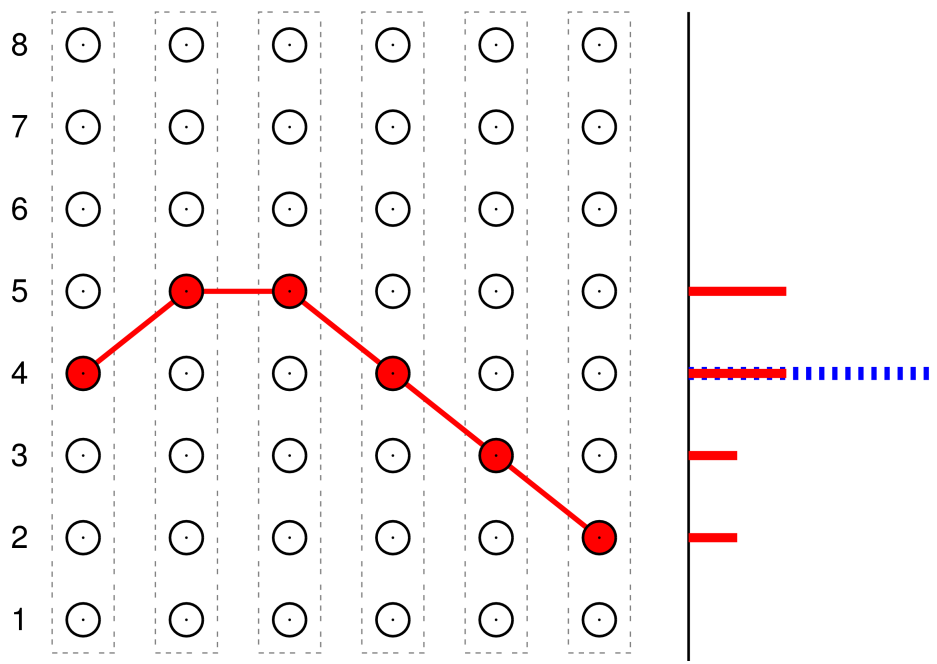

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Favorite choice: Metropolis rule

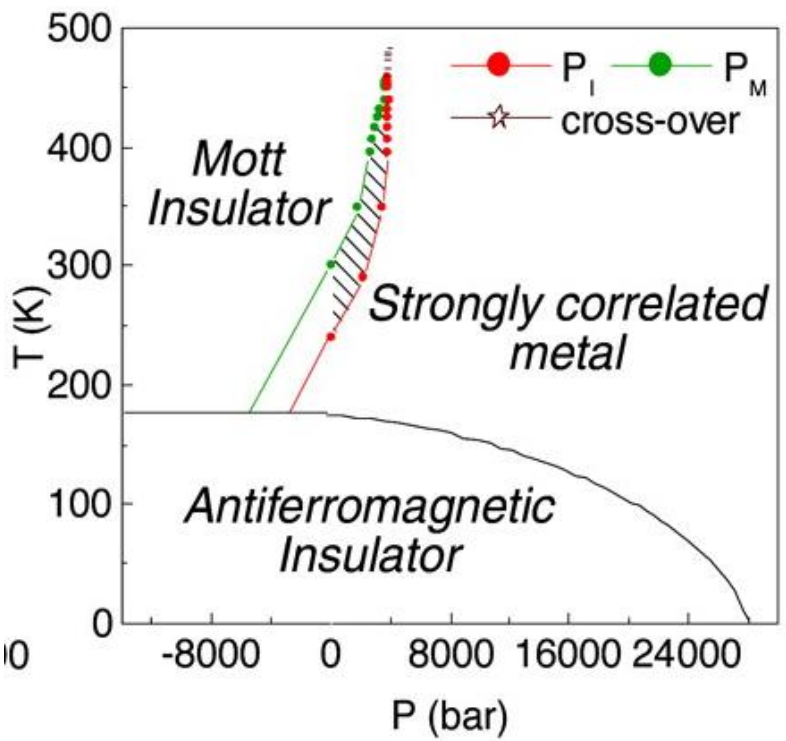
$$P\{i \to j\} = \min\left\{\frac{p_j}{p_i}, 1\right\}, \qquad \frac{p_j}{p_i} = e^{\Delta E/(k_B T)}$$

Systems with strong electronic/fermionic correlations

Mott metal-insulator transition

Prototype example: V_2O_3 doped
with Cr/Ti and/or under pressure

Phase diagram

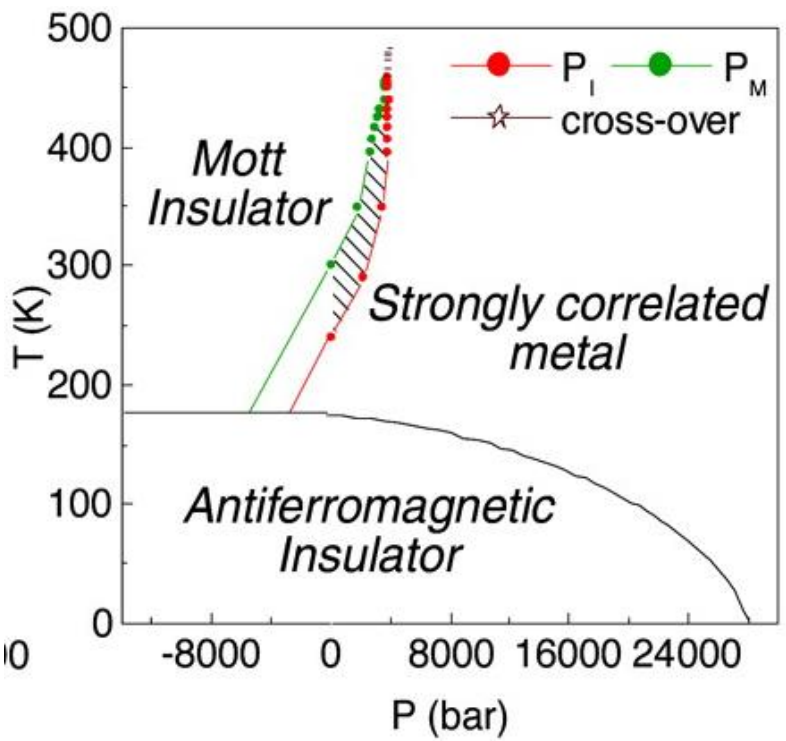


Systems with strong electronic/fermionic correlations

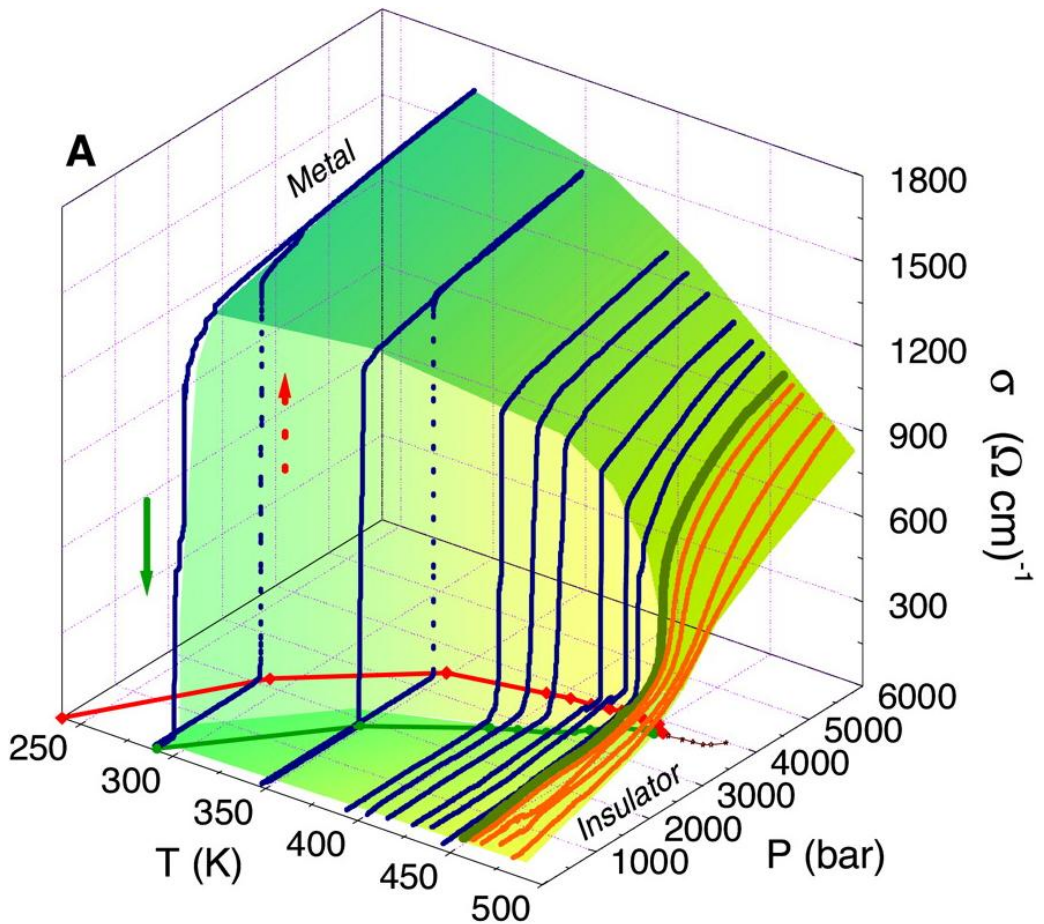
Mott metal-insulator transition

Prototype example: V_2O_3 doped with Cr/Ti and/or under pressure

Phase diagram



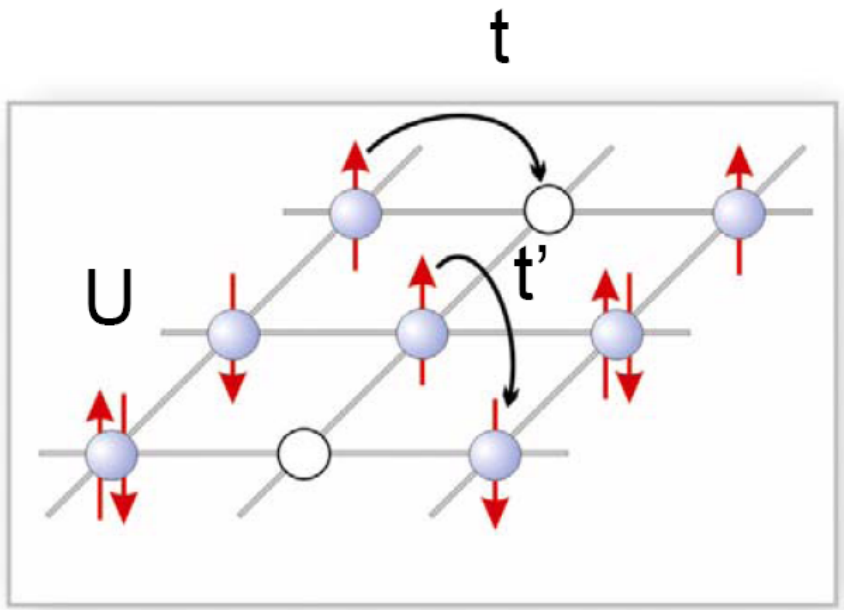
Electrical conductivity



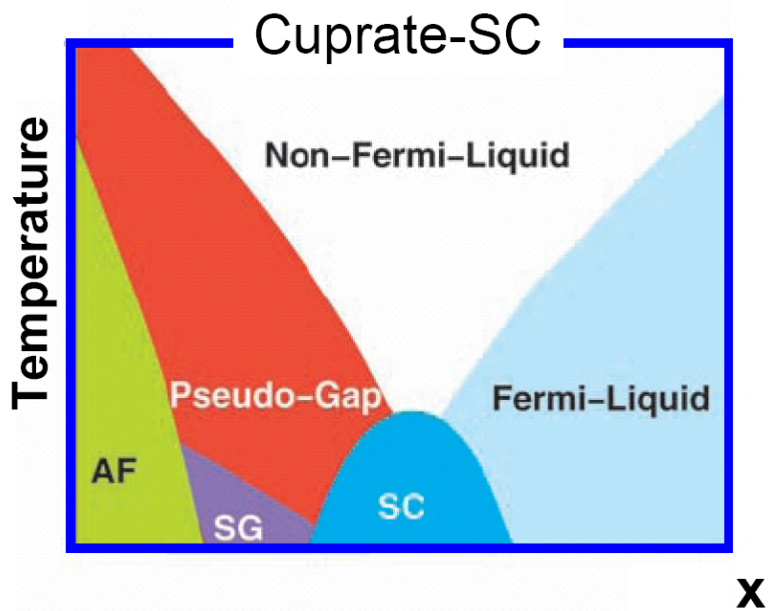
[Limelette et al., Science 302, 89 (2003)]

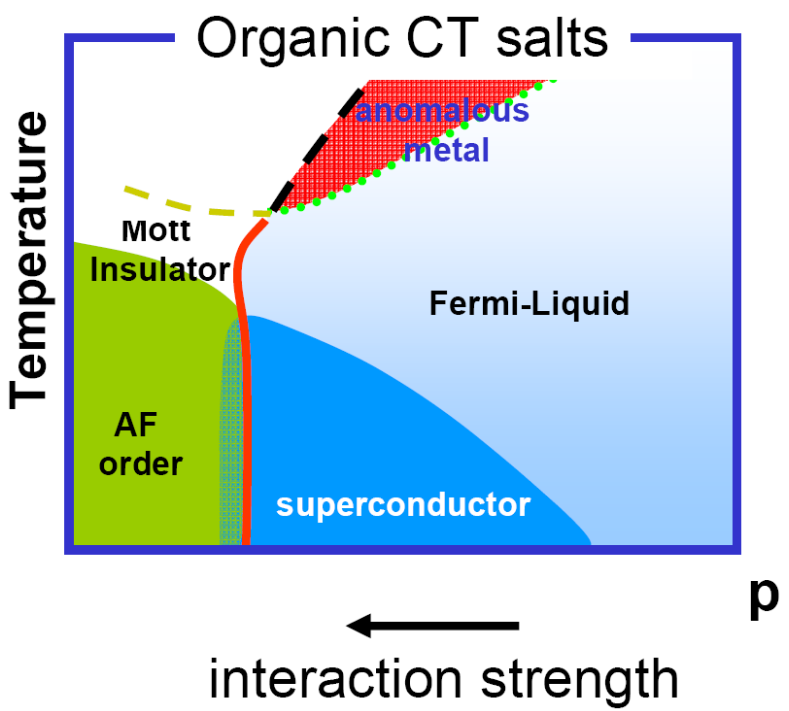
Complex phases of cuprate and organic superconductors

High-T_c physics contained in 2D Hubbard model?

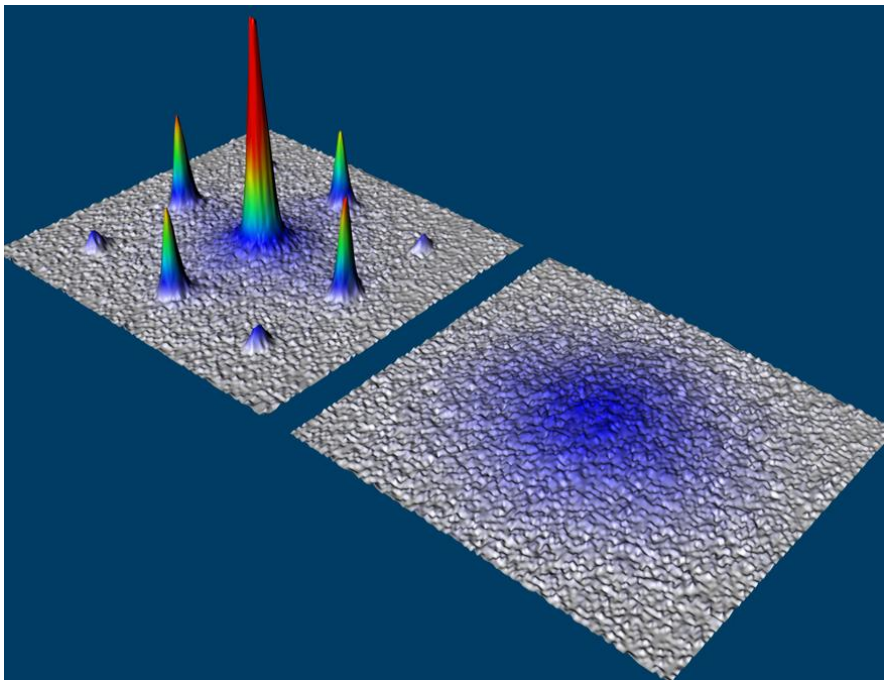


Are antiferromagnetic (AF) and Mott insulating phases essential for superconductivity?

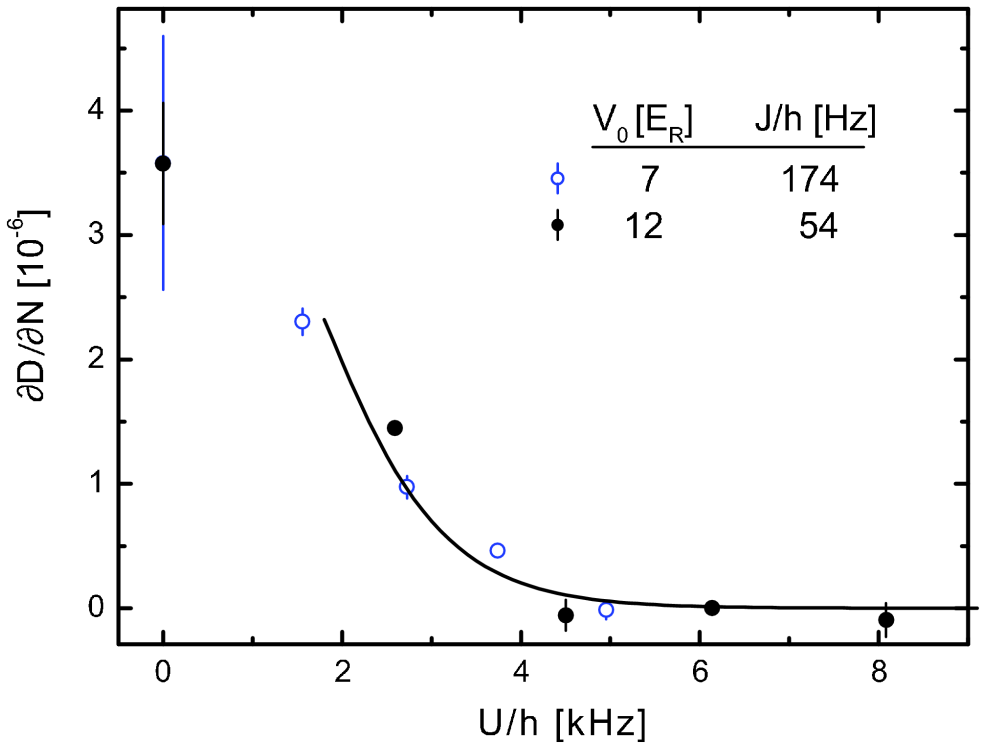




Correlated ultracold quantum gases on optical lattices



Localization (= decoherence) of ultracold bosons on optical lattice (Bloch group, 2002)



The transition to an incompressible phase for ultracold fermionic atoms [Jördens et al., Nature (2008)]

Also Bloch group [arXiv:0809.1464]

Approaches for correlated electron systems

General Hamiltonian for nuclei and electrons

$$H = \sum_{i=1}^{N_e} \frac{\boldsymbol{p}_i^2}{2m} + \sum_{k=1}^{L} \frac{\boldsymbol{P}_k^2}{2M_k} + \sum_{k<l} \frac{Z_k Z_l\, e^2}{|\boldsymbol{R}_k - \boldsymbol{R}_l|} - \sum_{i,k} \frac{Z_k\, e^2}{|\boldsymbol{r}_i - \boldsymbol{R}_k|} + \sum_{i<j} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$$

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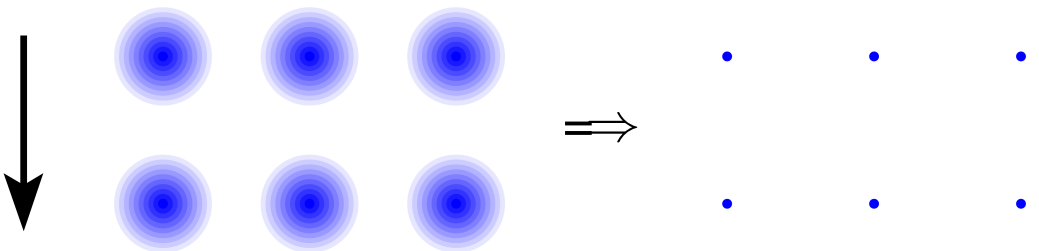
Born-Oppenheimer approximation (0^{th}order)



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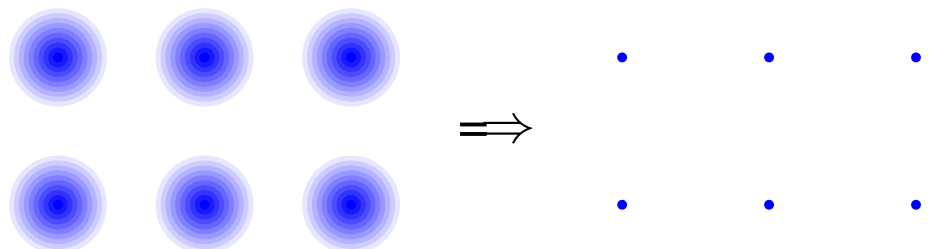

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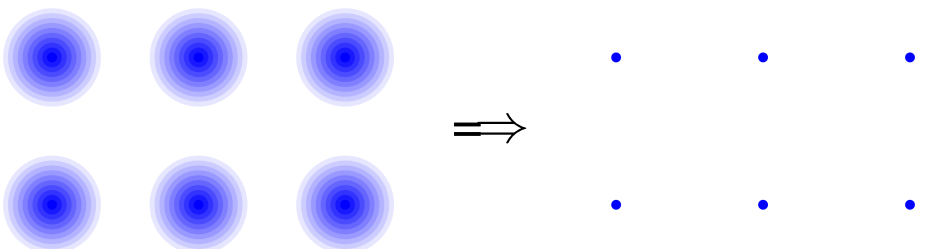

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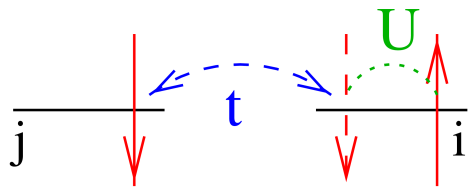
Classes of theoretical approaches for electronic problem

- continuum methods: density functional theory, variational+diffusion QMC, . . .
- methods for lattice electrons

Approaches for Hubbard-type models

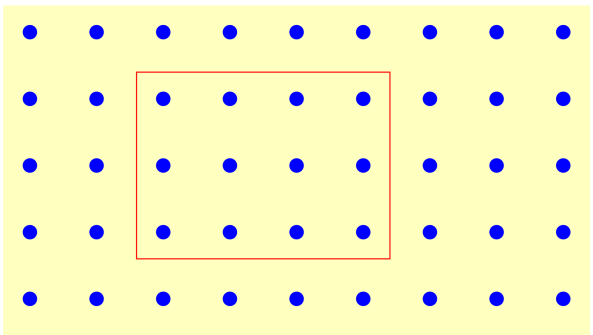
$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}\right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



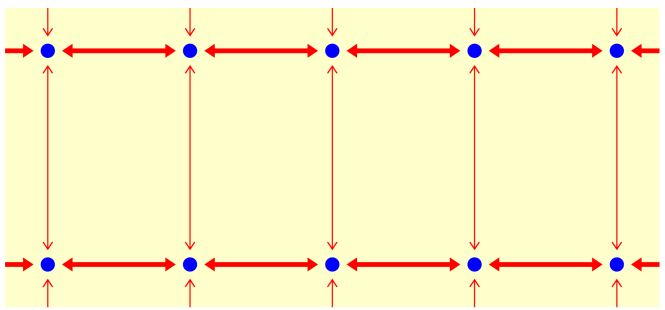
Perturbation theory

- $U \to 0$: 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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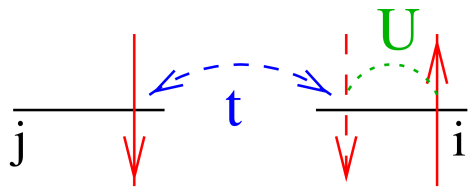

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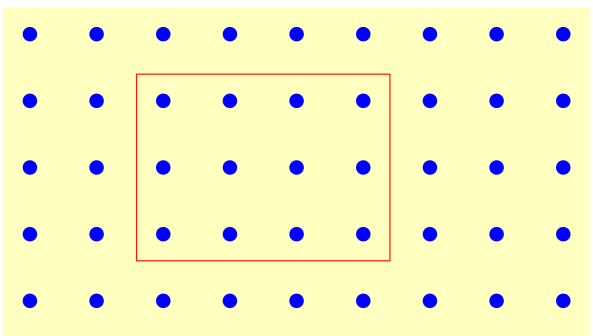

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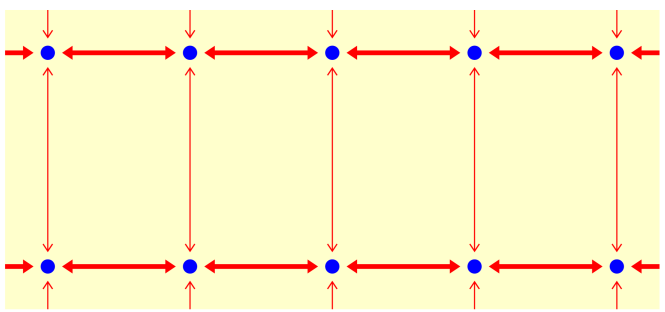


Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$

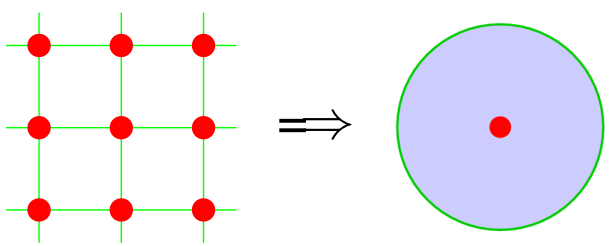
[Metzner, Vollhardt, PRL (1989), Georges, Kotliar, PRL (1992), Jarrell, PRL (1992)]

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

\+ dynamical on-site correlations preserved

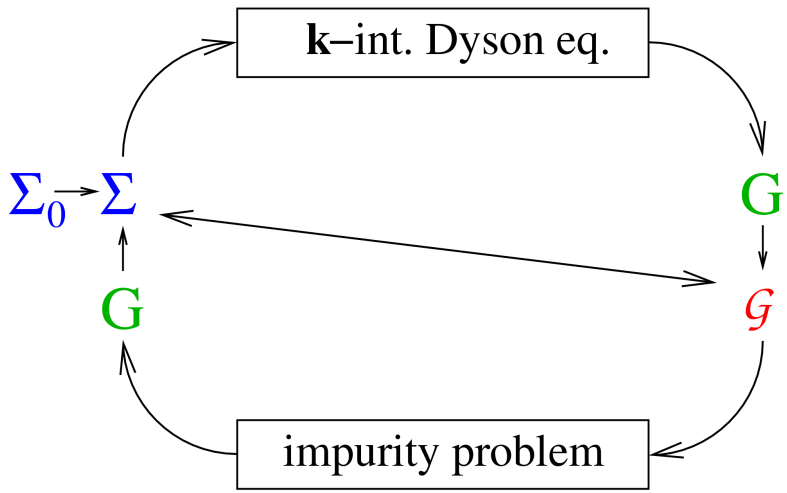
\+ in thermodynamic limit

+/− 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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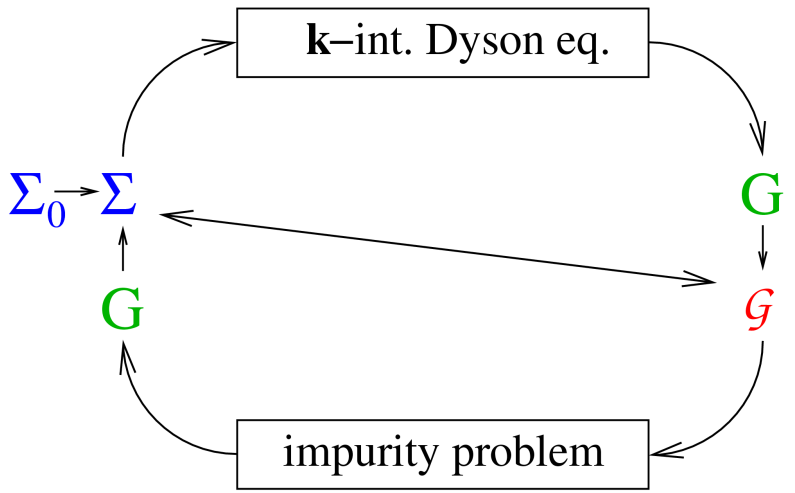

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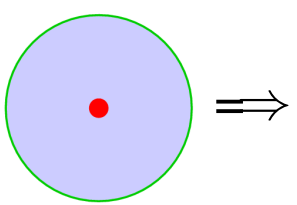
Impurity solver:

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



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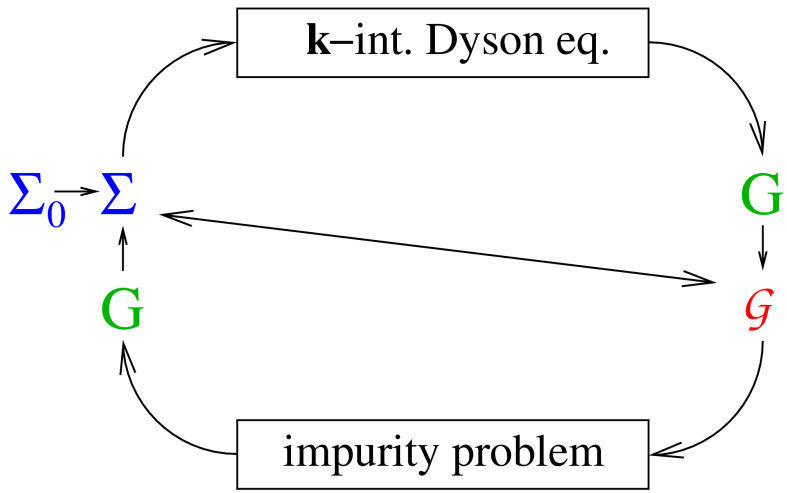

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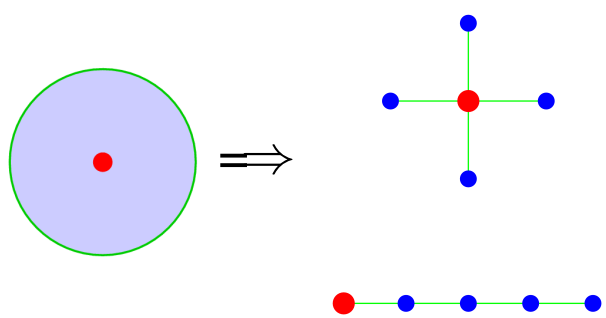

Auxiliary-field QMC algorithm [Hirsch, Fye (1986)]

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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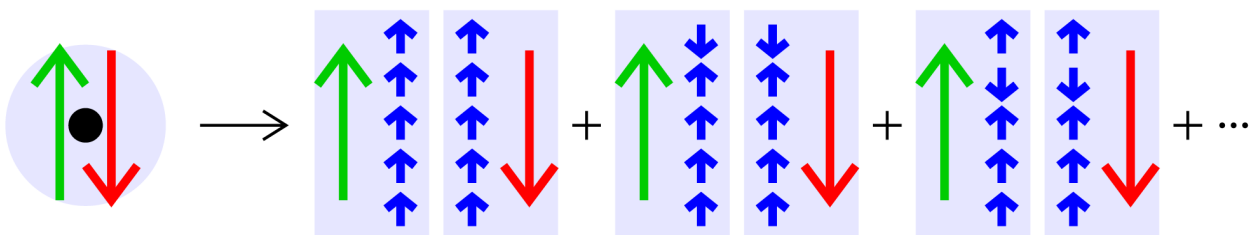

Wick theorem:

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

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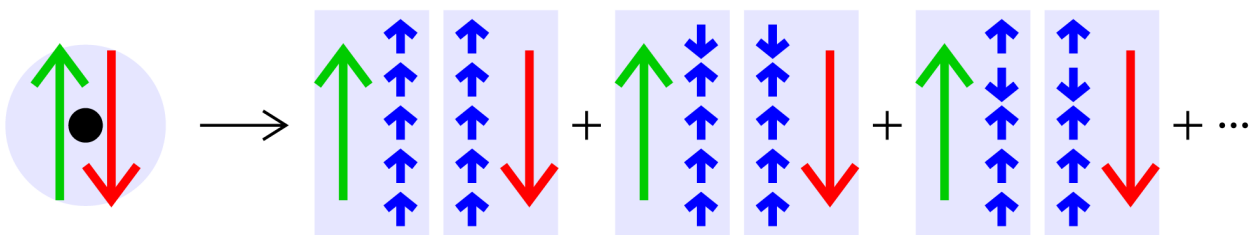

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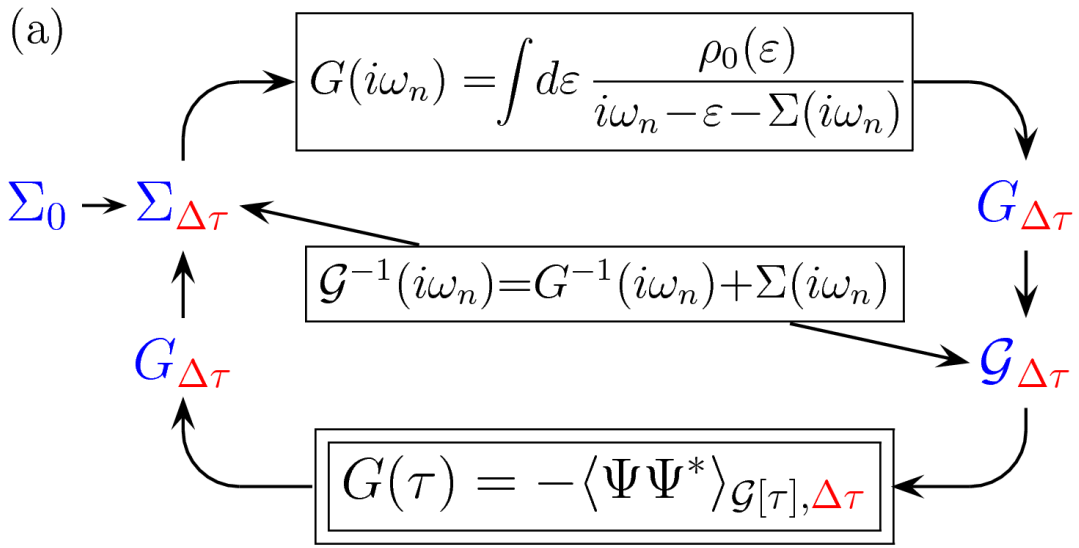
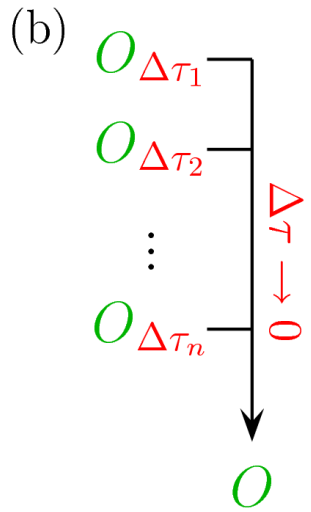
(iv) MC importance sampling over auxiliary Ising field $\{s\}$: 2^Λ configurations

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

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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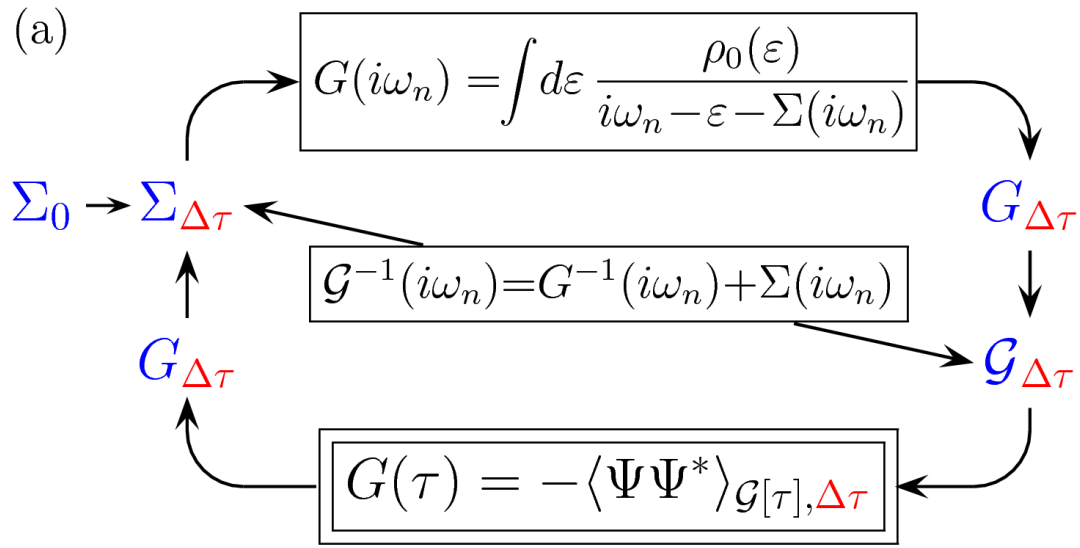

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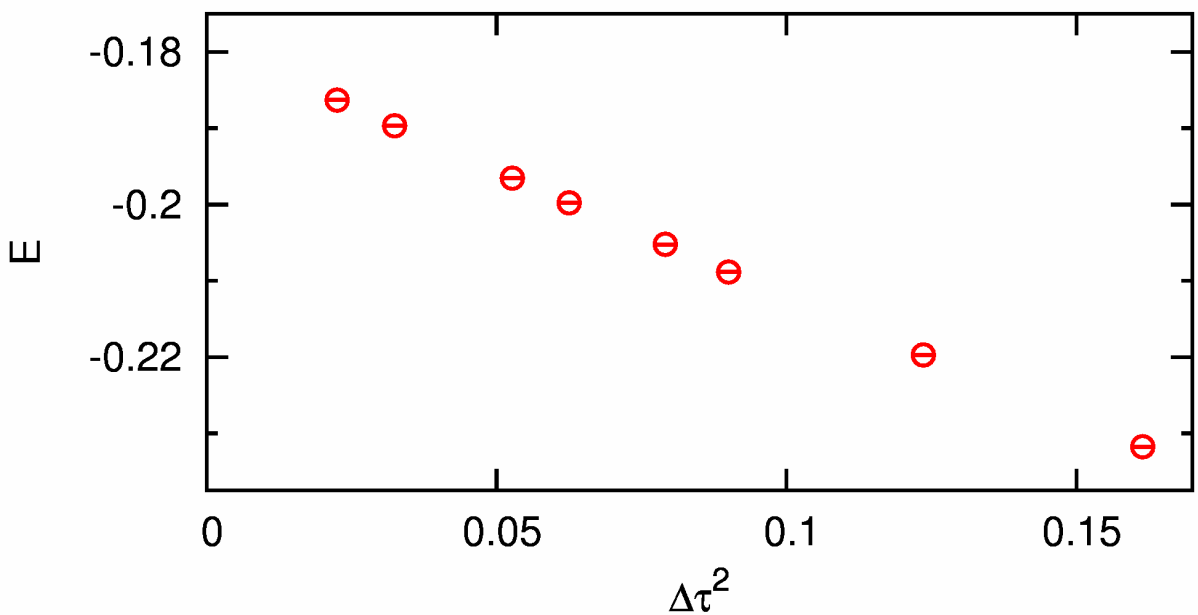
Example: energy E for $U = W = 4$ (Bethe DOS), $T = 1/45$

[NB, PRB (2007)]



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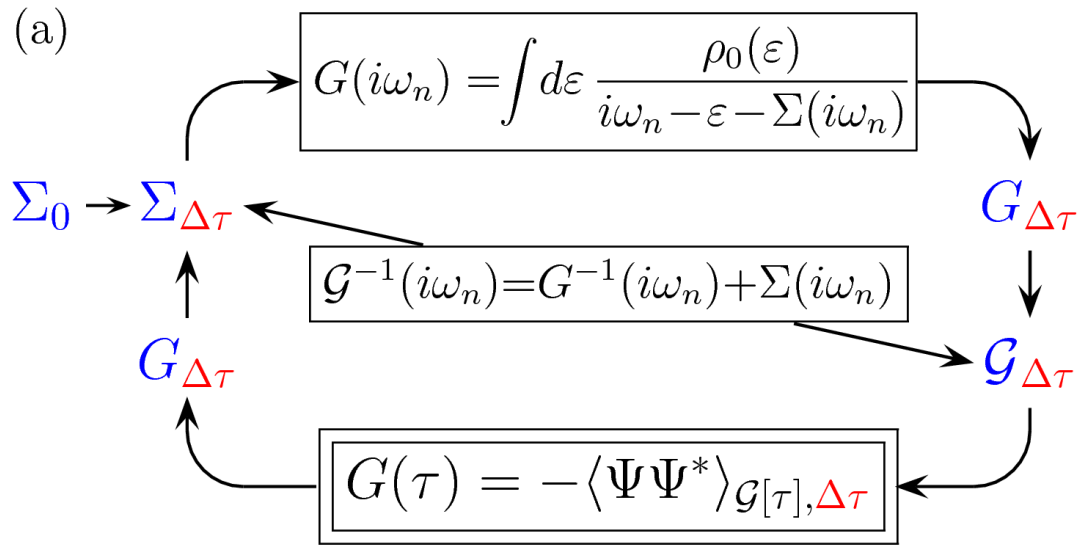

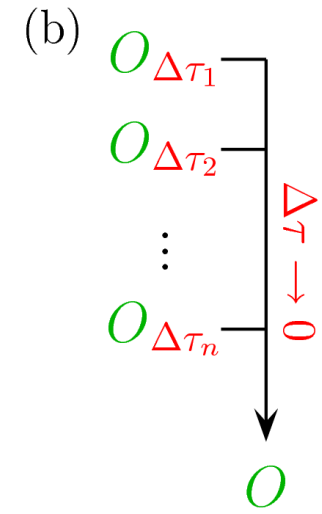

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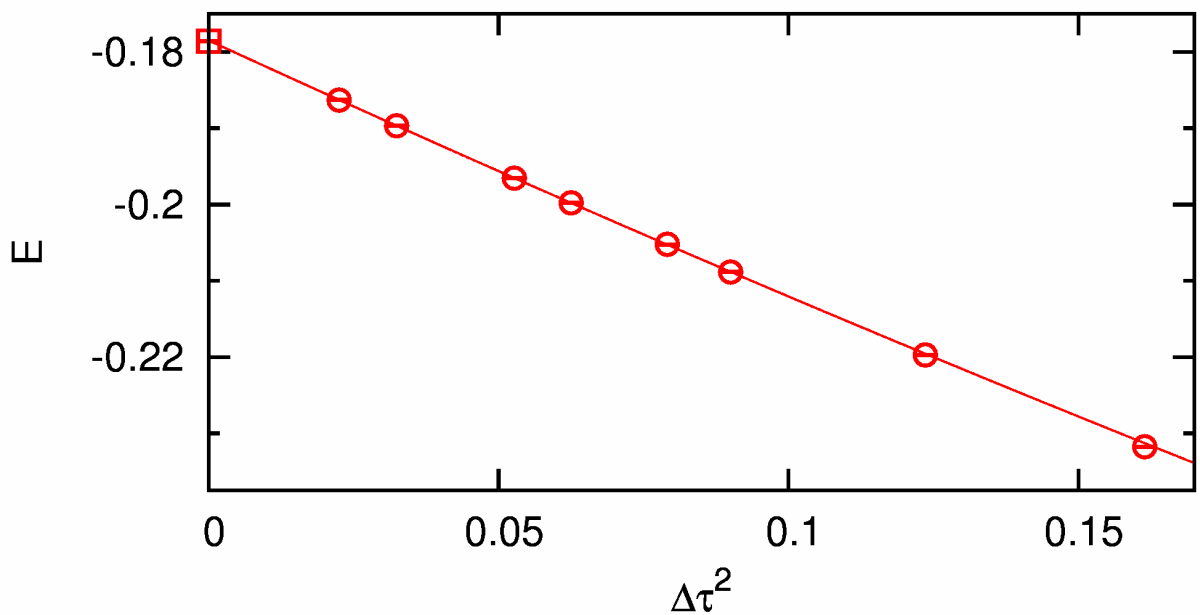
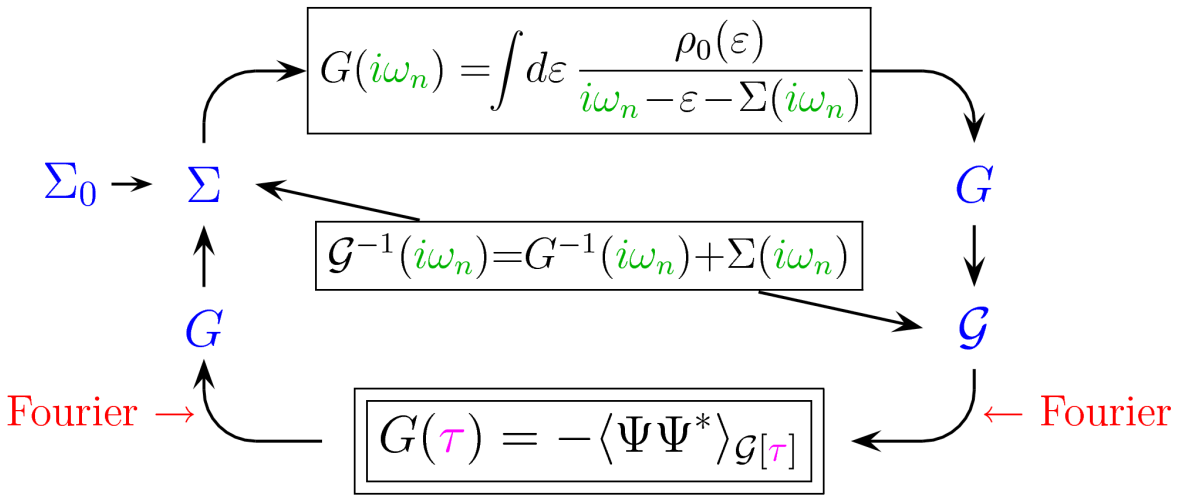


Special issue: Fourier transformations in DMFT-QMC cycle

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



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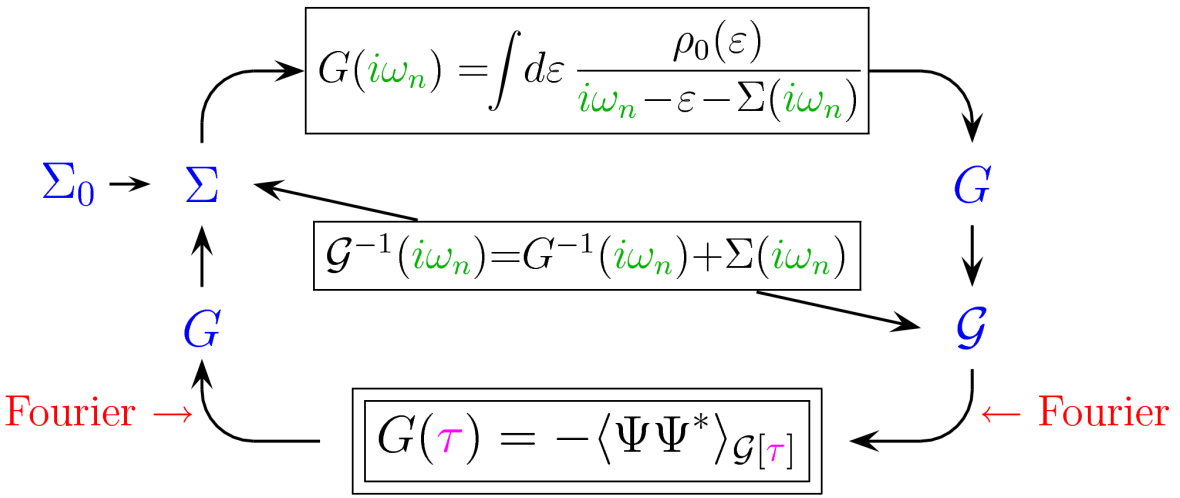
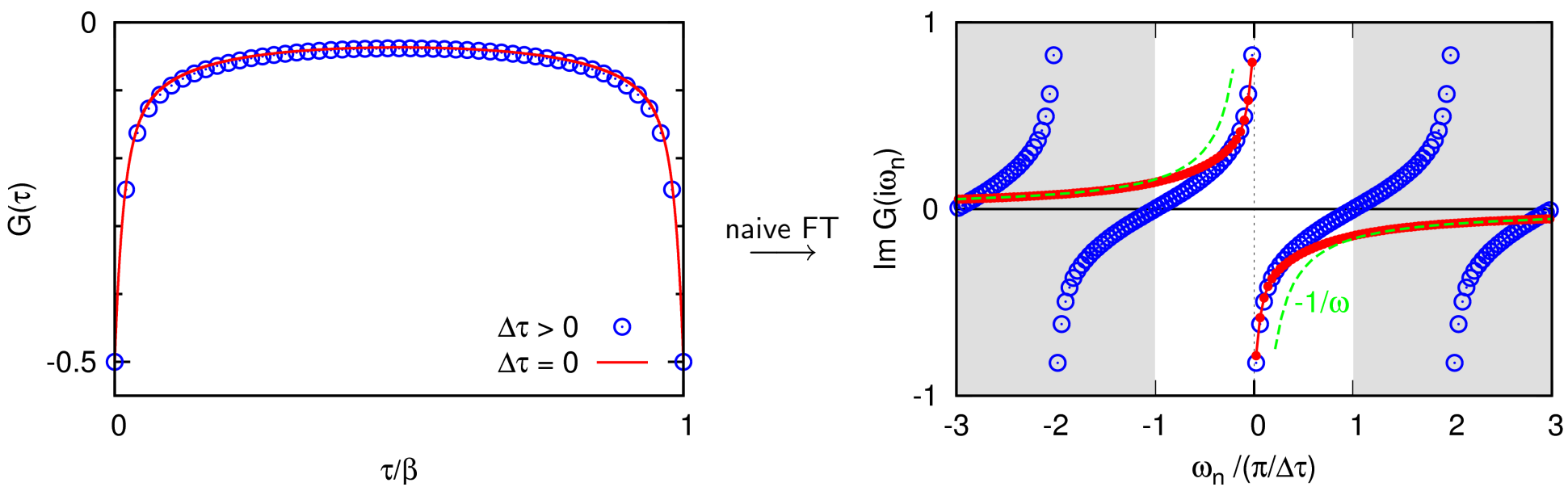


Naive discrete Fourier transformation $\rightsquigarrow$ oscillations (instead of $G(\omega) \overset{\omega\to\infty}{\longrightarrow} 1/\omega$)



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

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

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  [Oudovenko]

- spline-fit only
  difference w.r.t.
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  – IPT [Jarrell]

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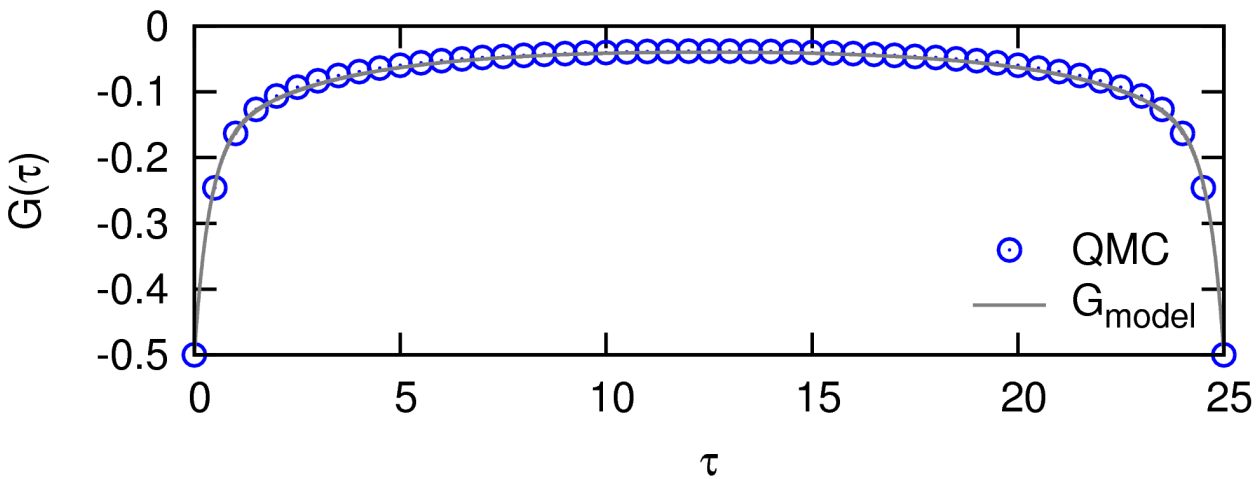

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Possible solution: interpolate $G_{\mathrm{QMC}}(\tau)$, e.g., by cubic splines [Jarrell, Krauth, Gull, . . .]

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

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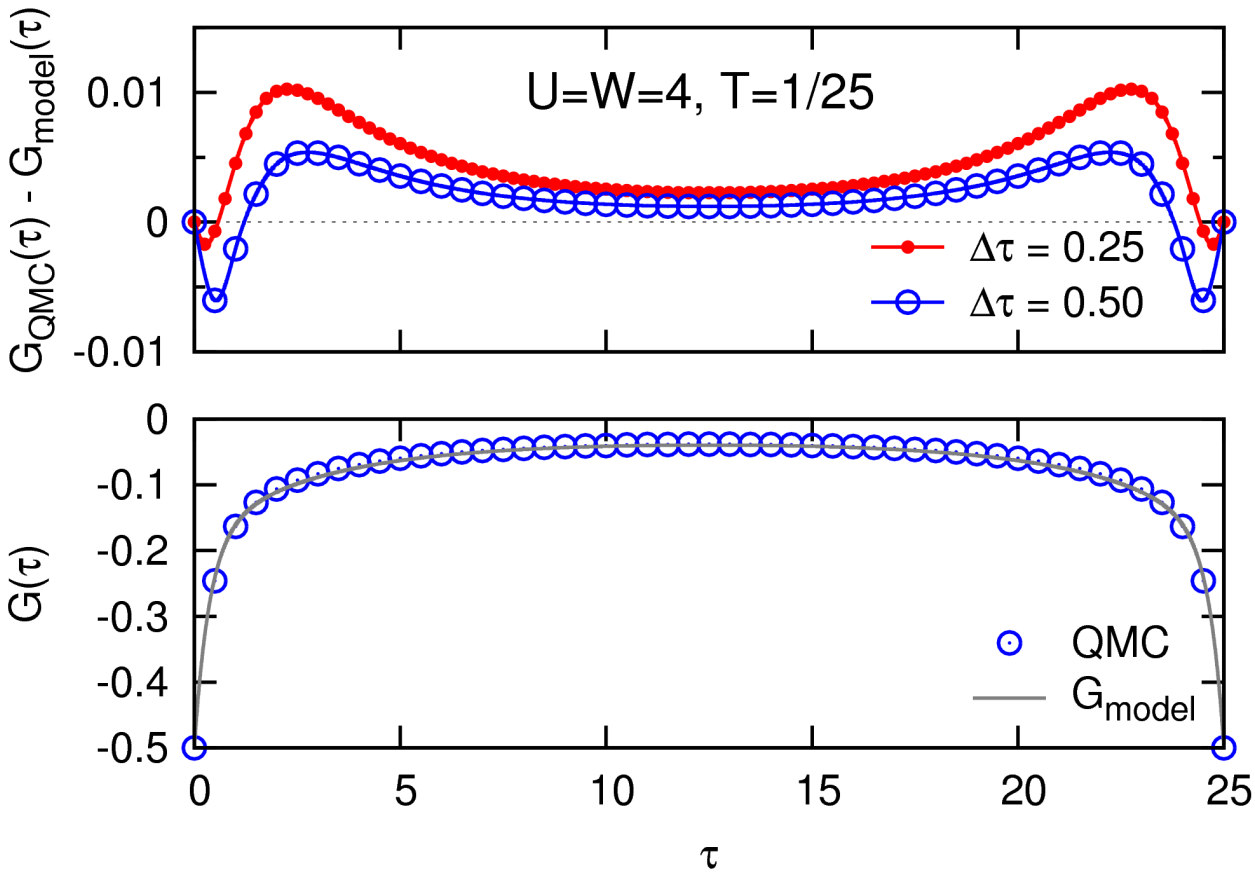

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multi-band case: additional terms

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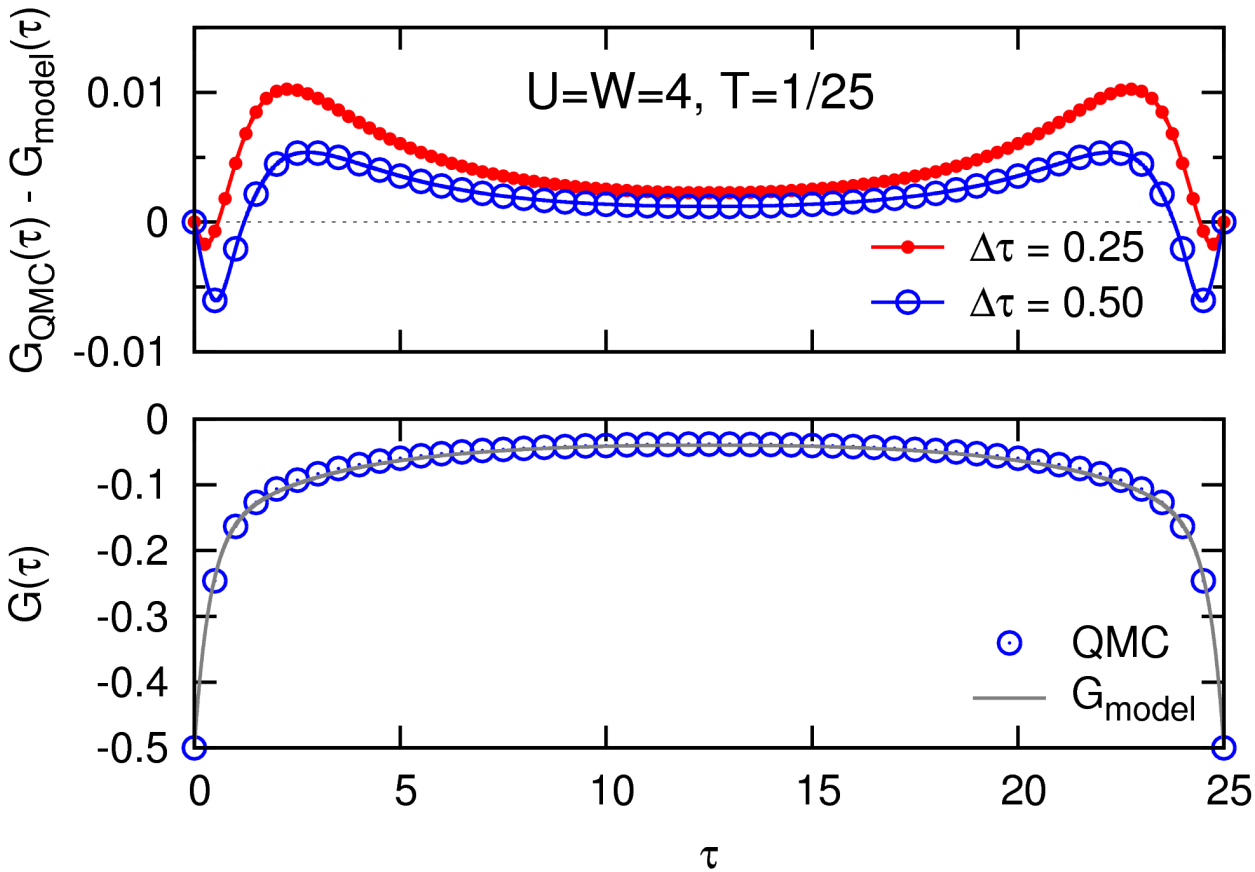

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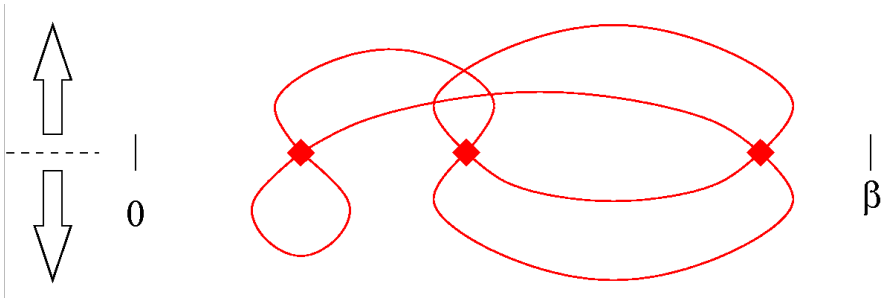
multi-band case: additional terms

Interdisciplinary project: replace spline interpolation by smooth fit!

New development: continuous-time QMC algorithms

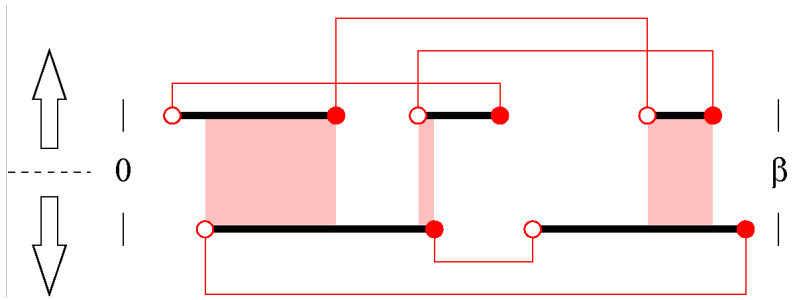
1. weak-coupling expansion

[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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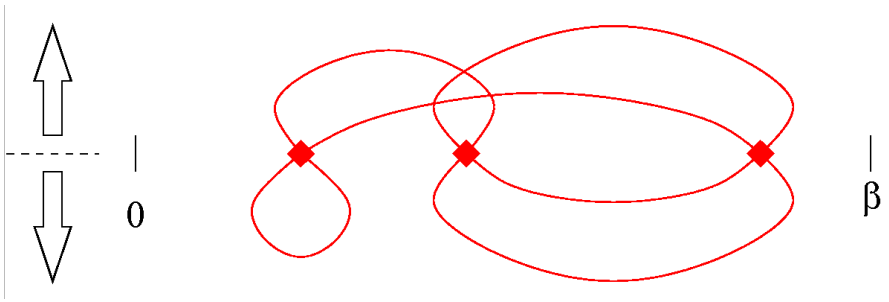

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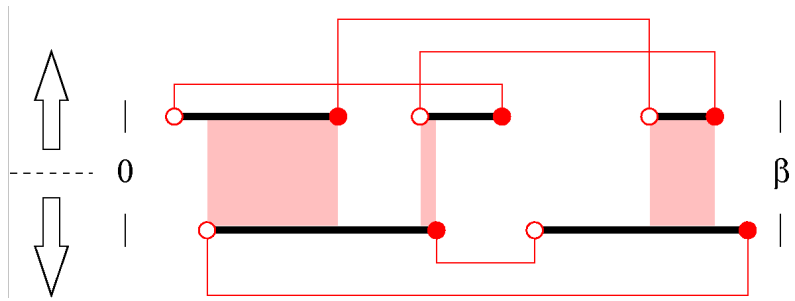
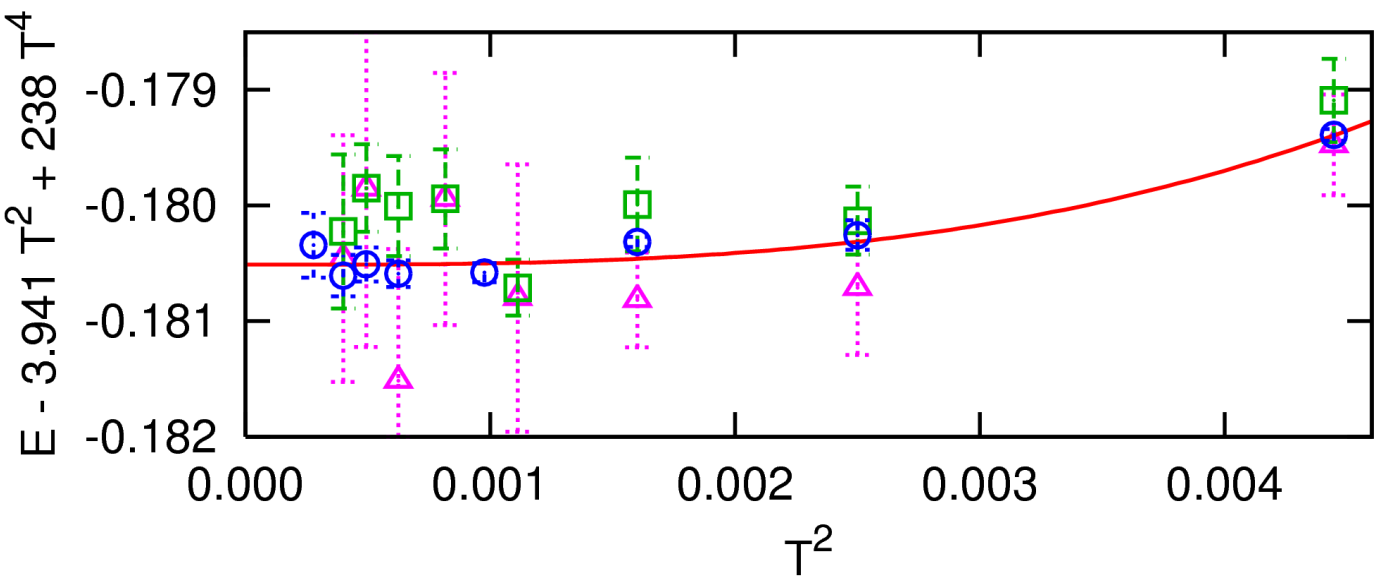


No systematic errors (in principle). Also more efficient than HF-QMC? No!



Test case:

1 band, $U = W = 4$

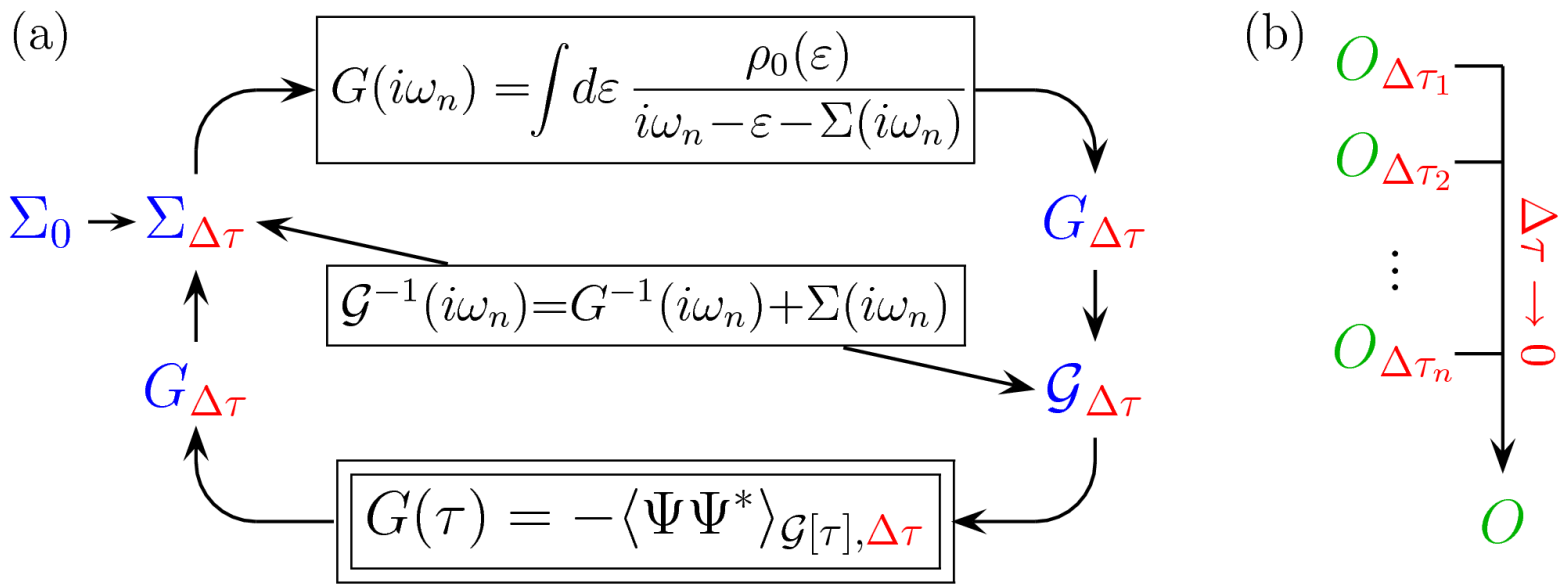
- ○ HF-QMC ($\Delta\tau \to 0$)
- □ weak-coupling CT-QMC
- △ hybridization CT-QMC

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

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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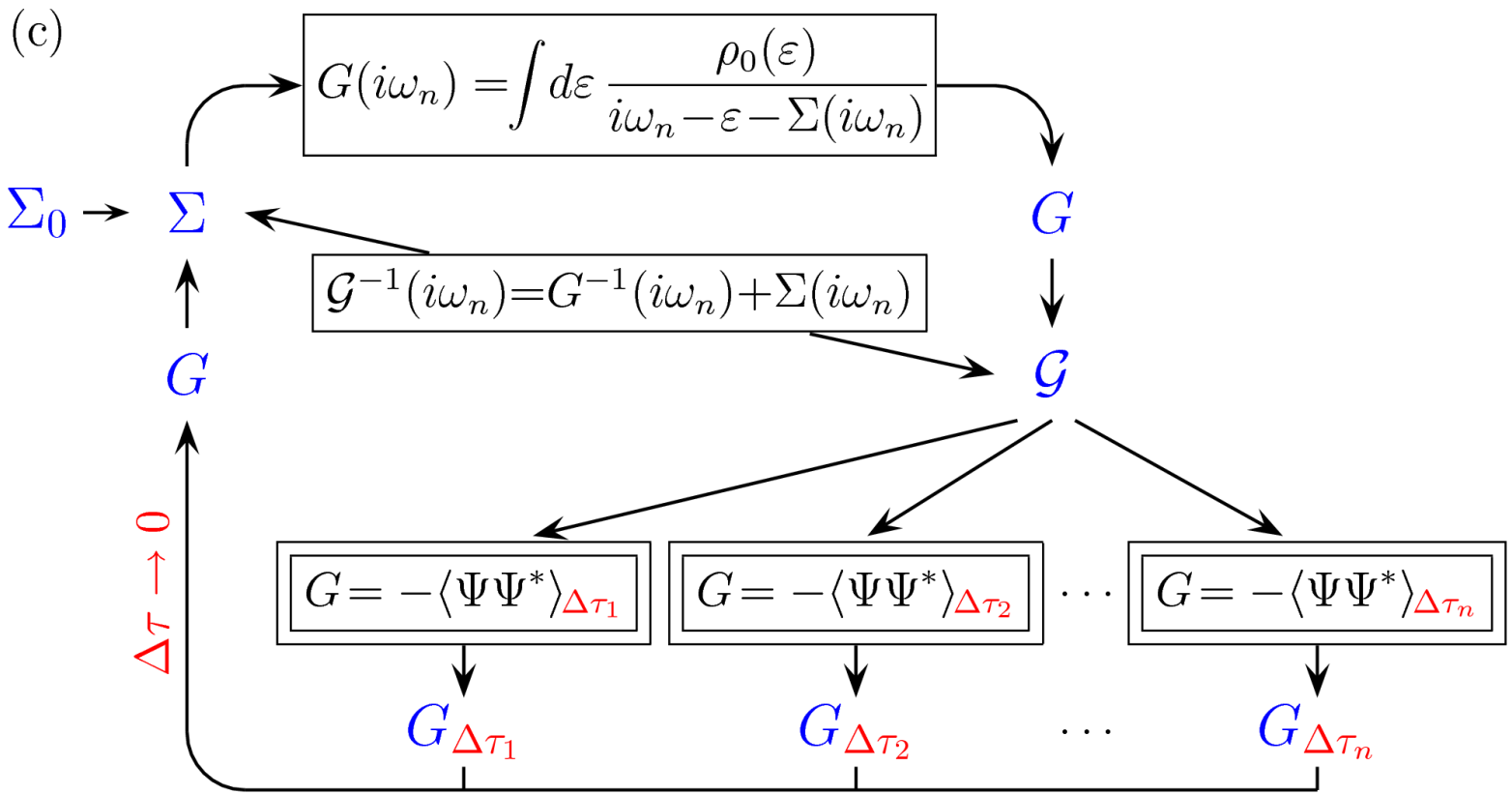
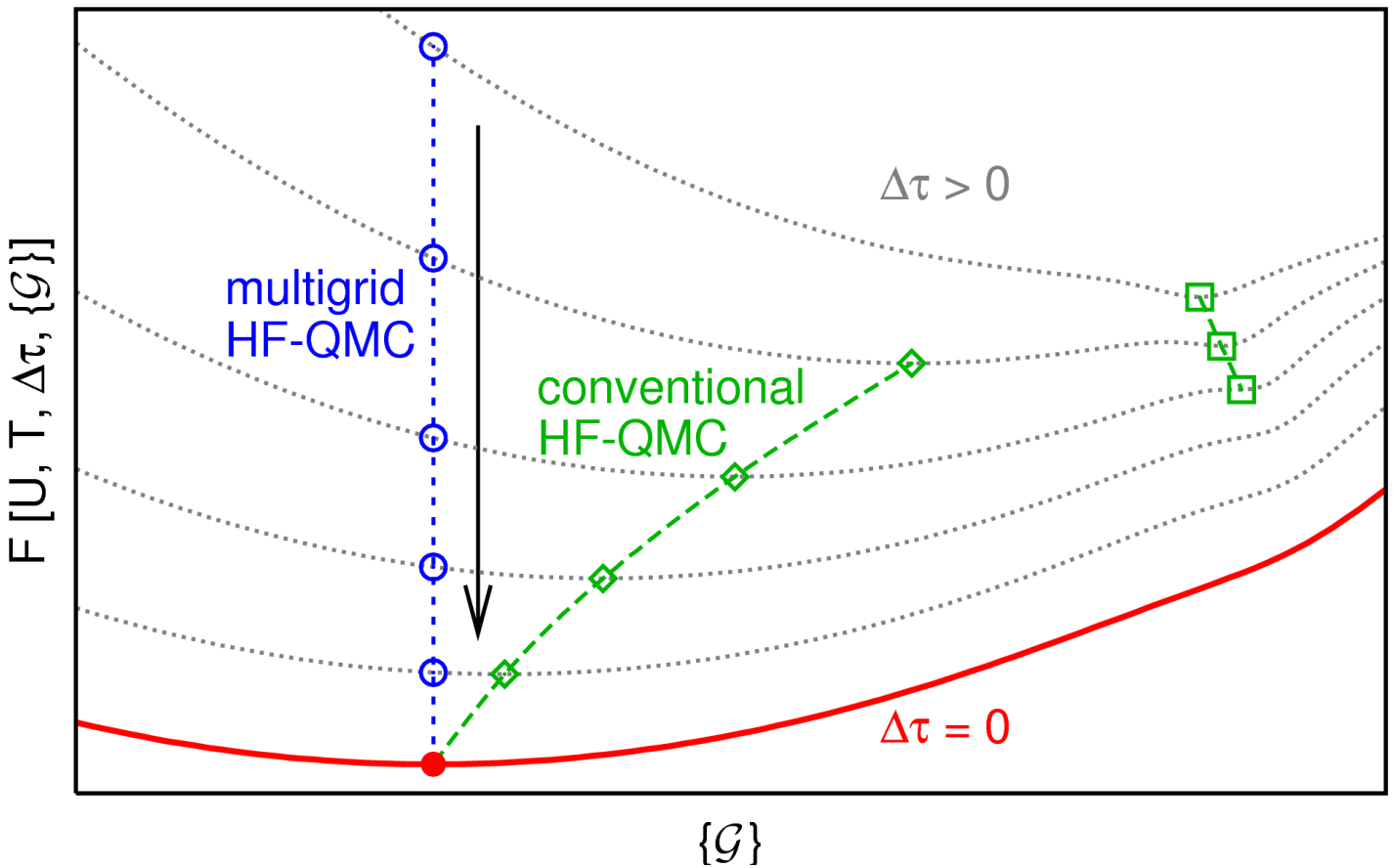


(c) Multigrid HF-QMC: internal elimination of Trotter error

$\rightsquigarrow$ 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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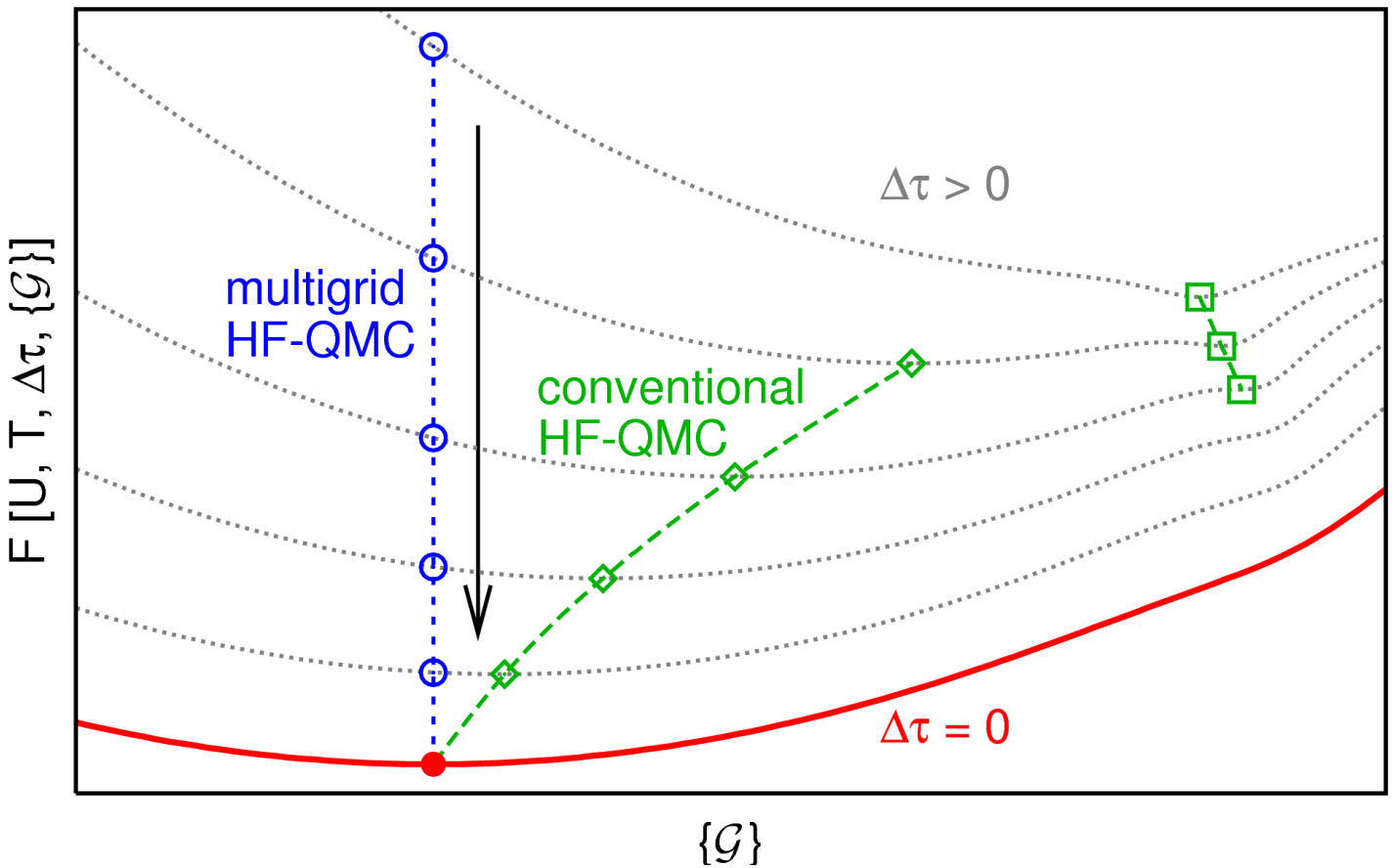
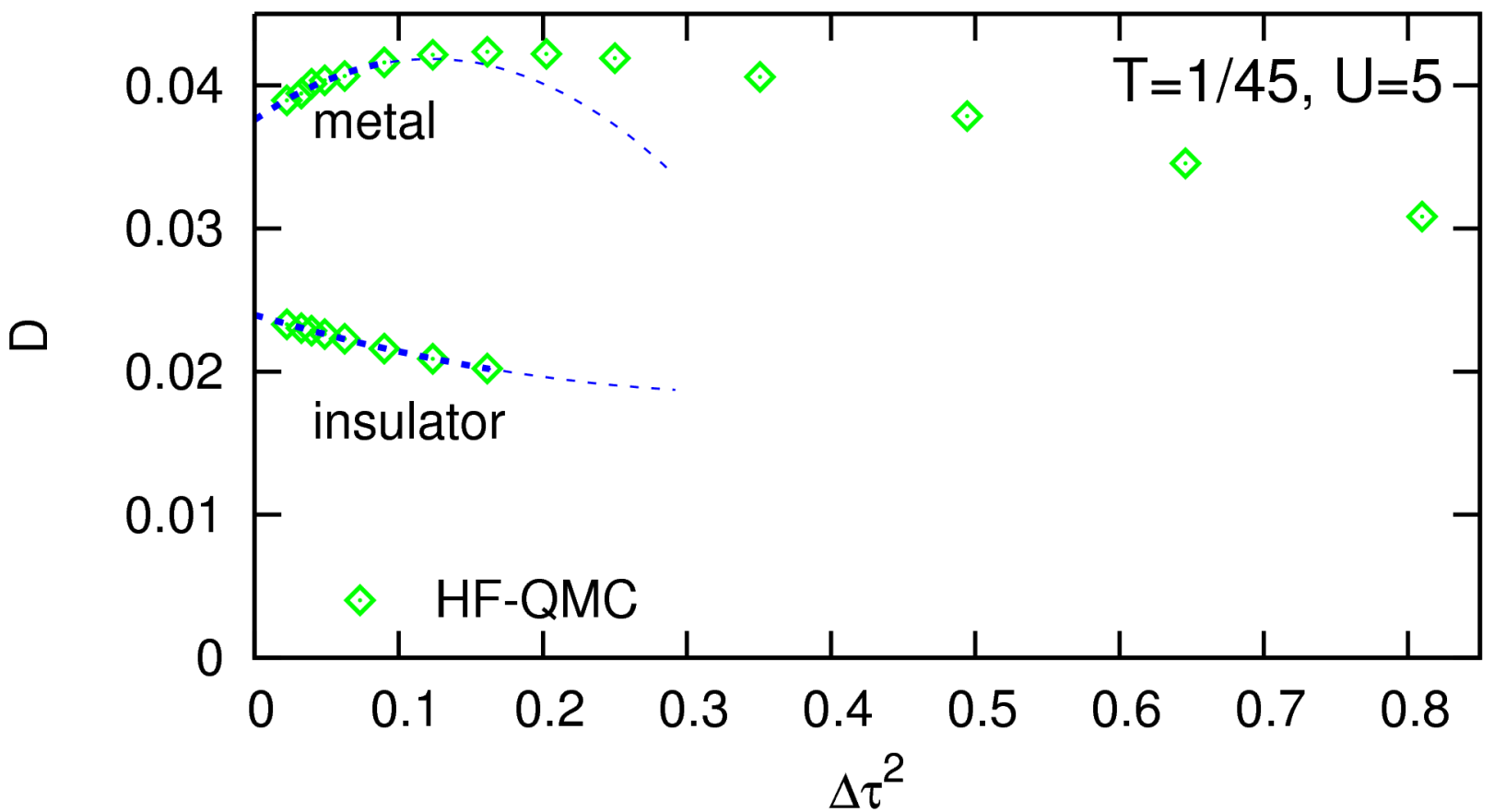


Conventional Hirsch-Fye QMC: DMFT fixed point shifts with $\Delta\tau$

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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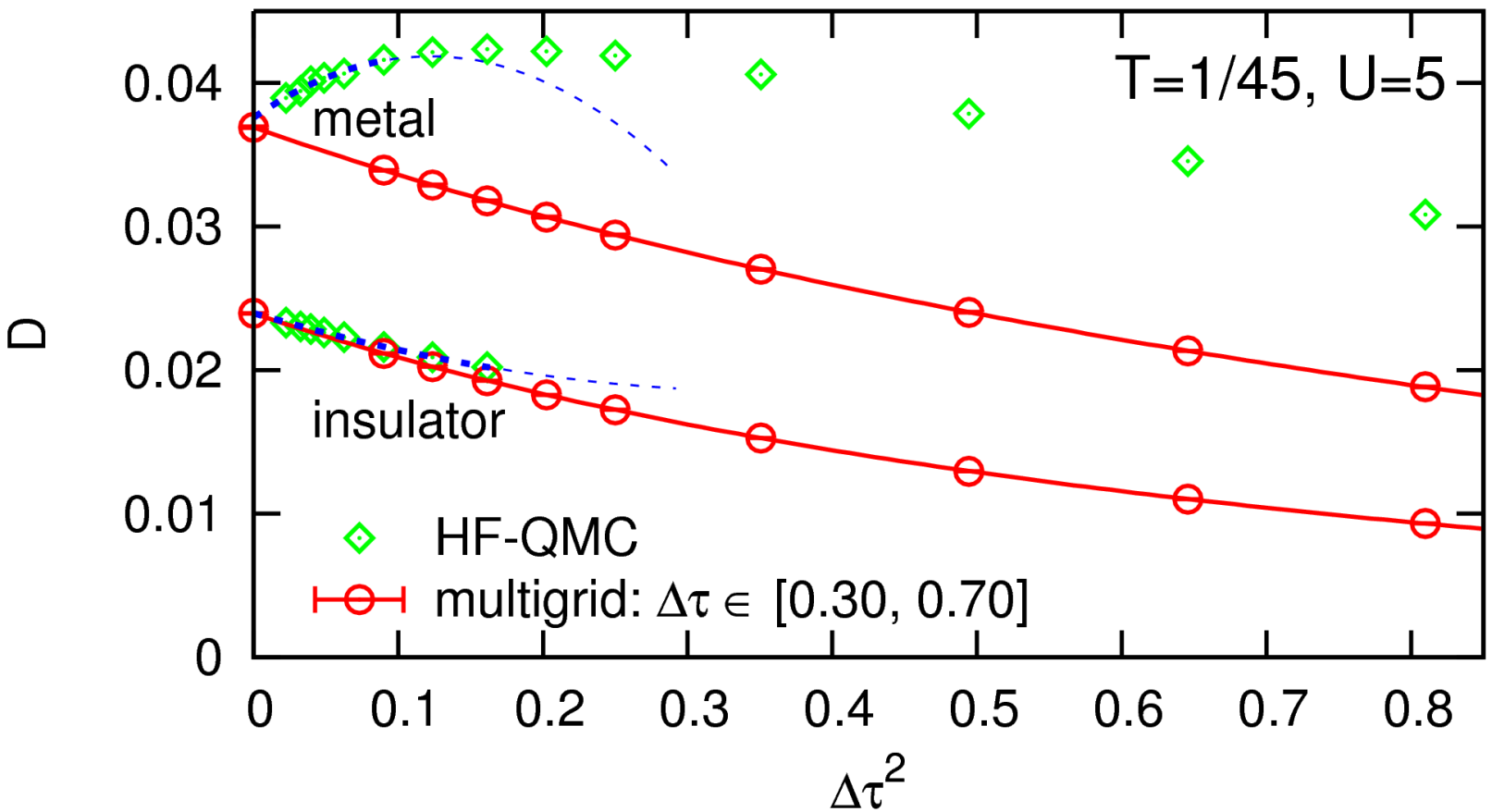

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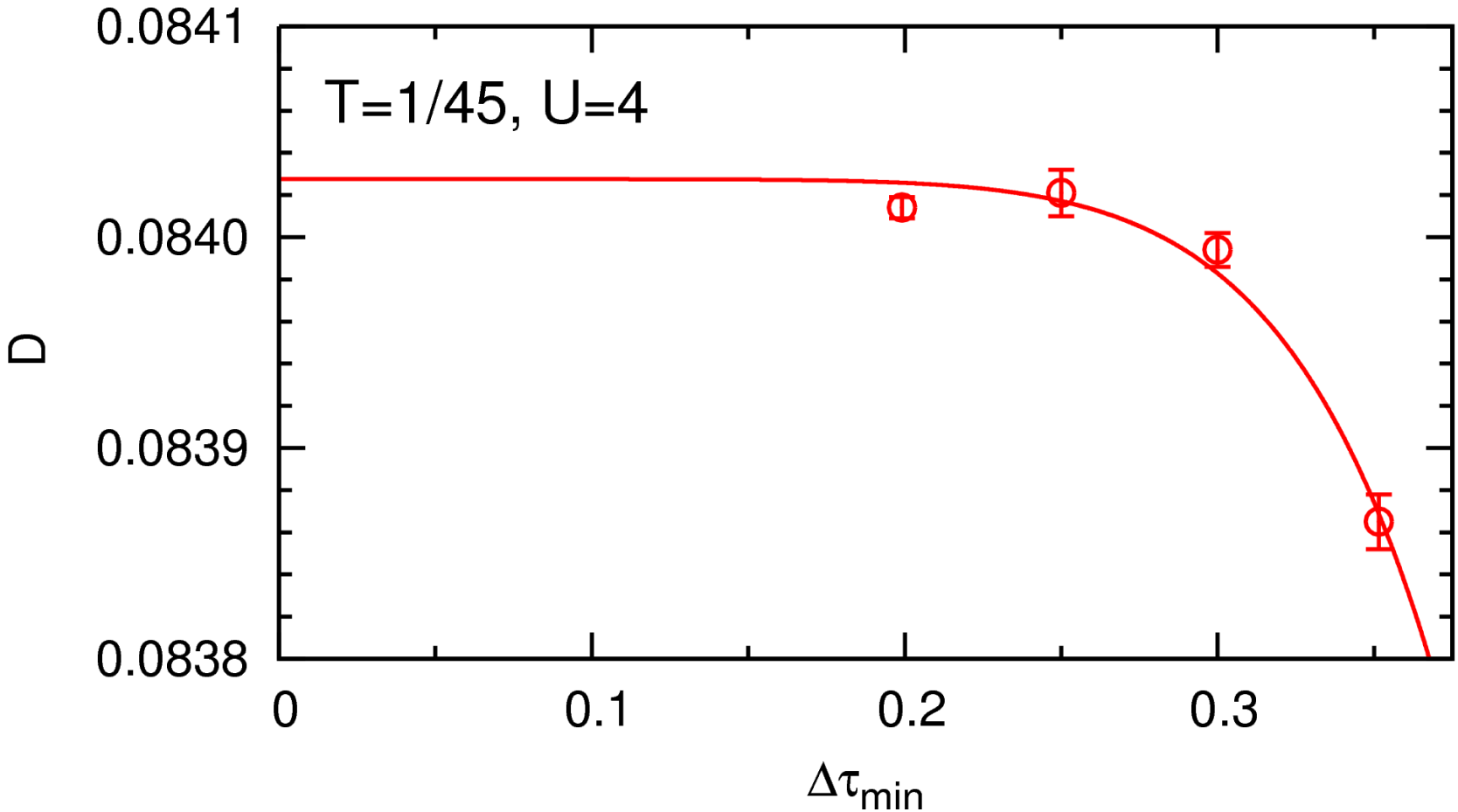
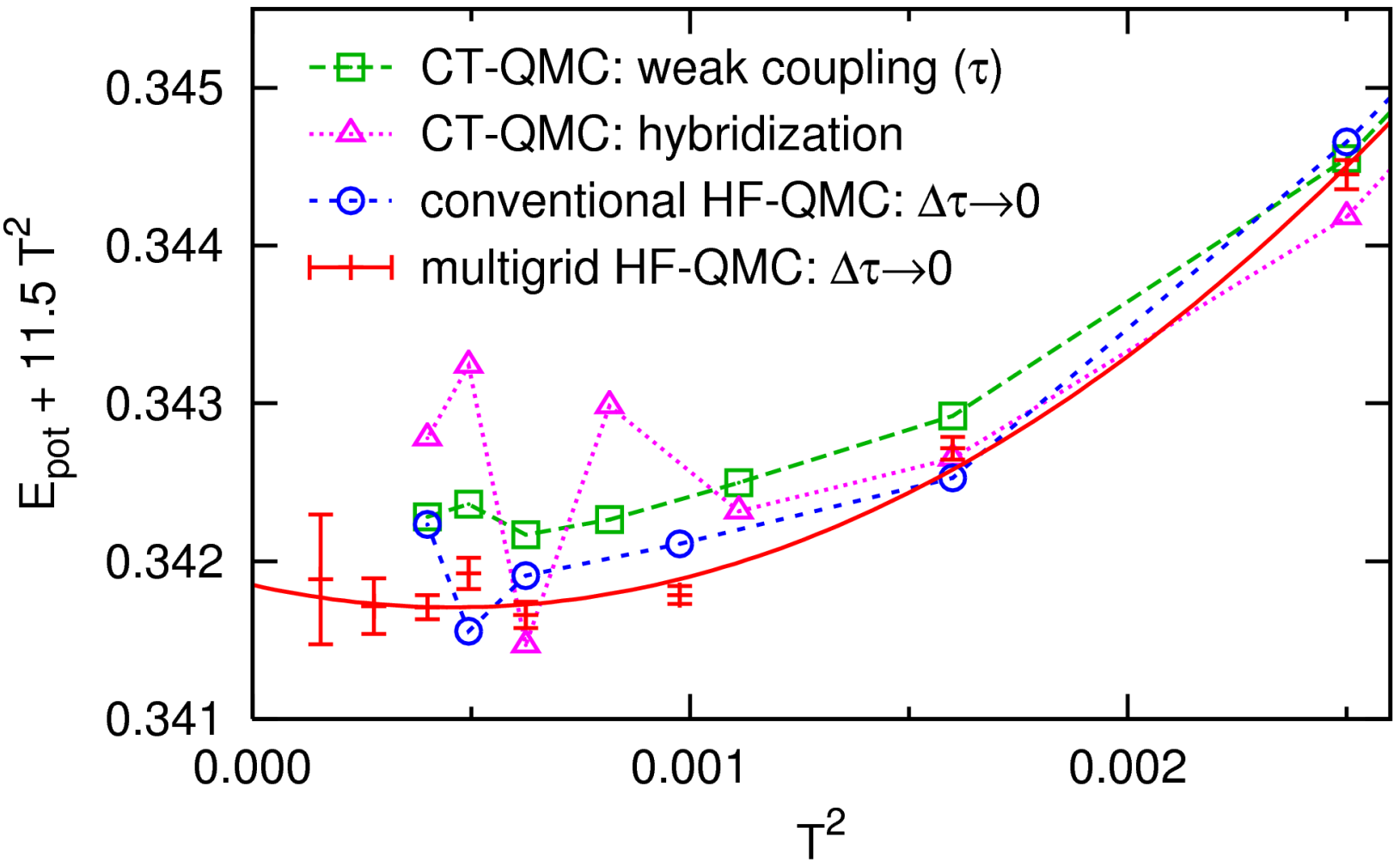
Multigrid HF-QMC: vastly larger useful range of $\Delta\tau$

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



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

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

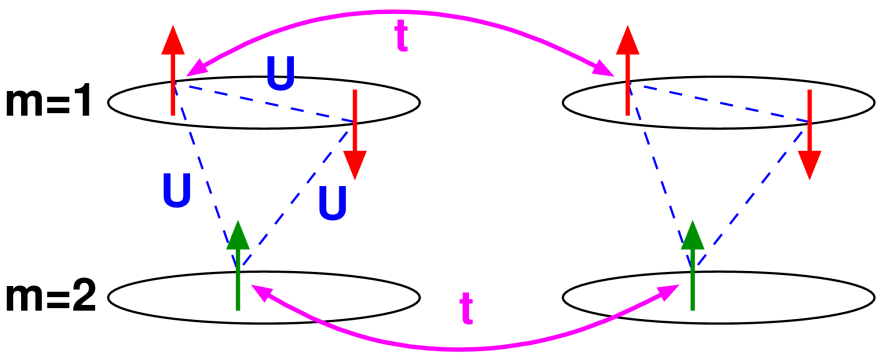


No more "difficult observables" for multigrid HF-QMC

Higher precision than CT-QMC methods at same effort

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

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



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no Hund exchange!

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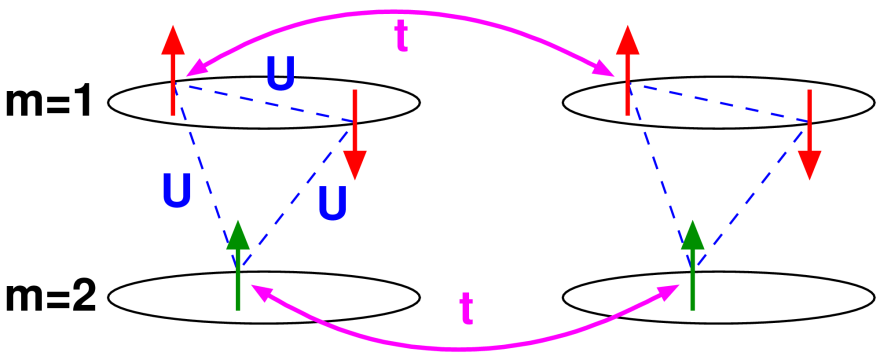

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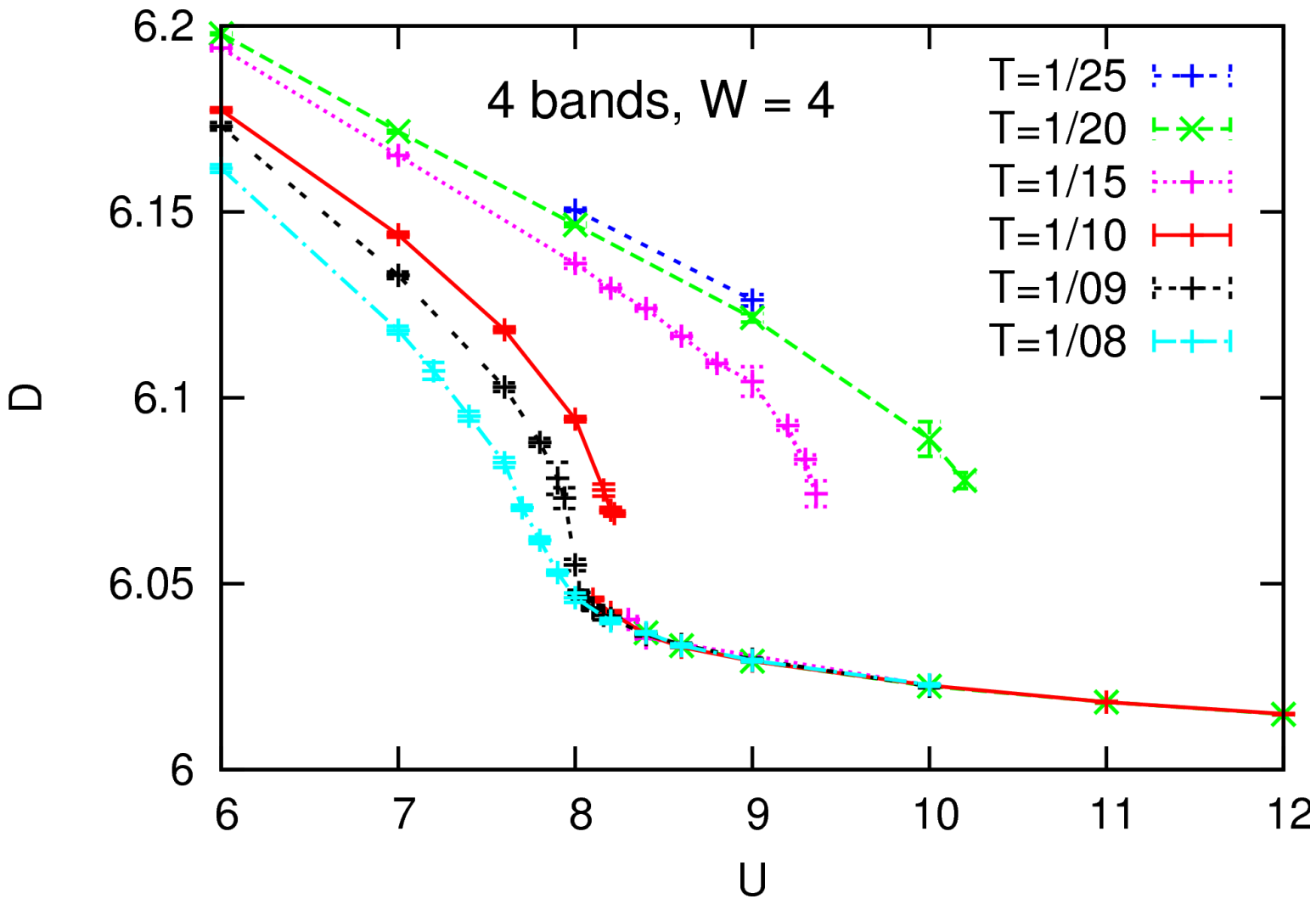
- Mott transition for any $M = 1, 2, ...$
- Analytic solutions for $M \to \infty$ [Florens et al., PRB (2002)]
- So far: only approximate numerical solution for $2 \leq M \leq 4$ [Inaba et al., PRB (2005)]

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

Multigrid HF-QMC: Double occupancy



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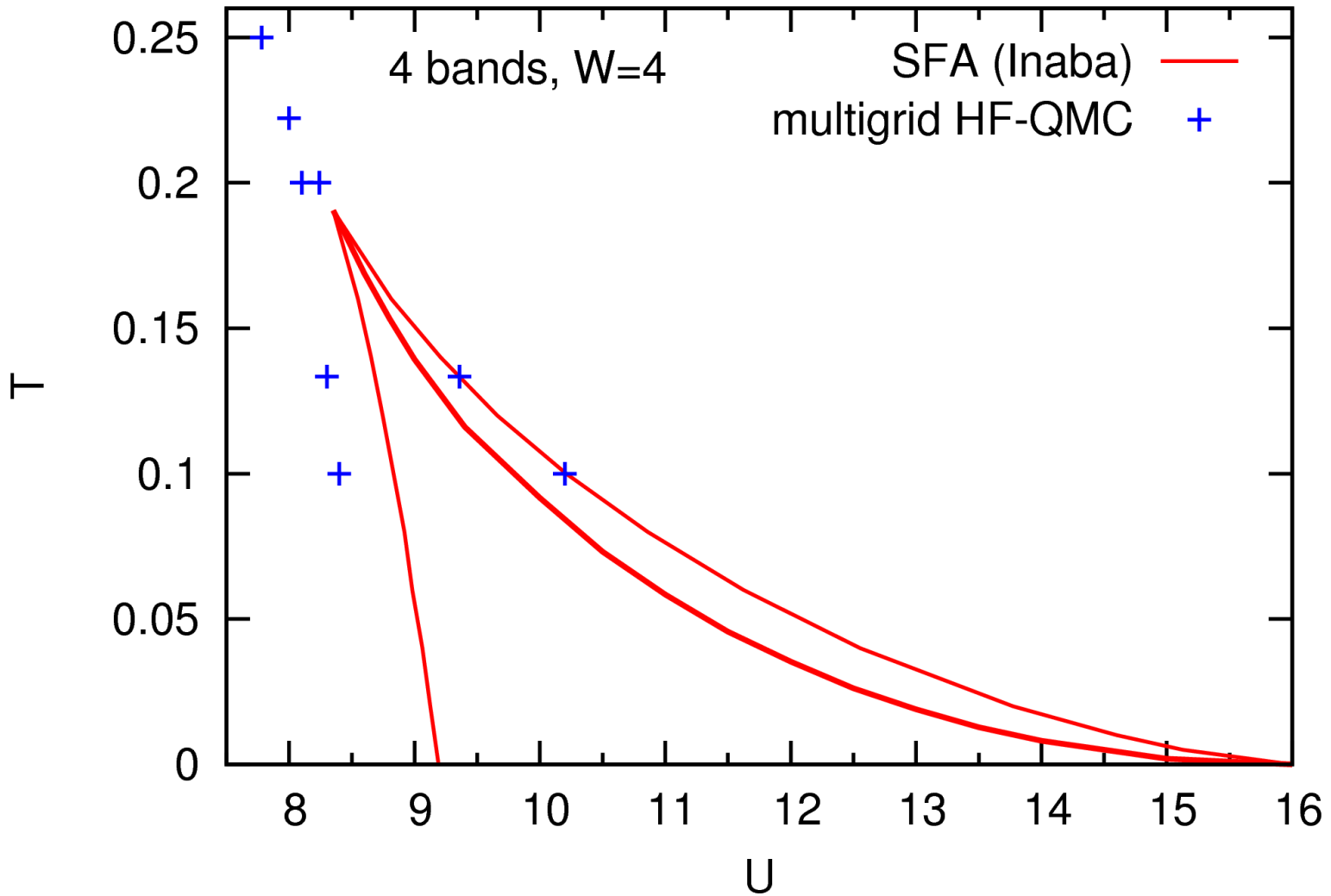
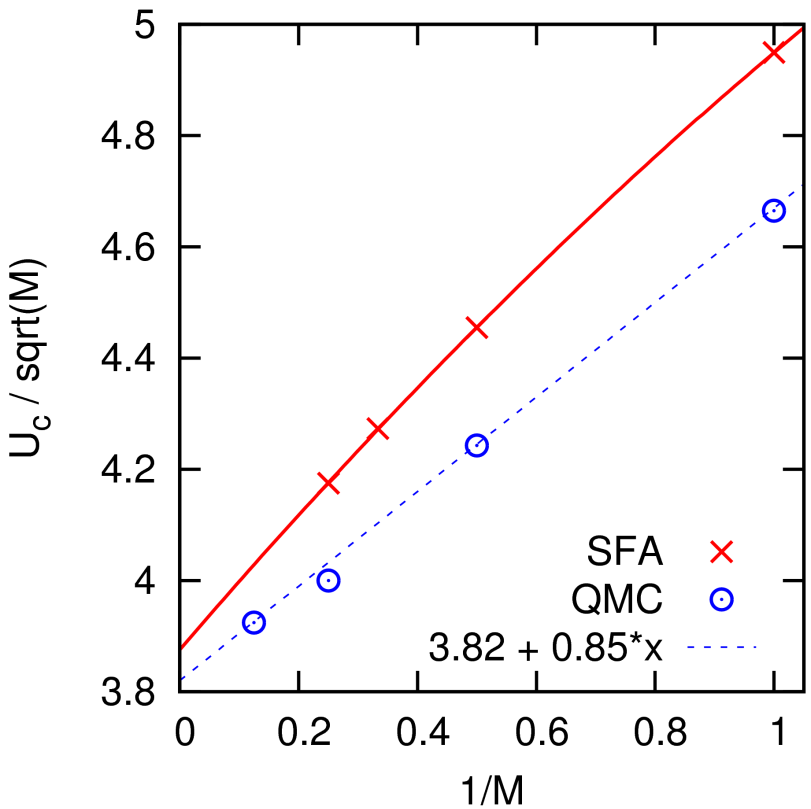
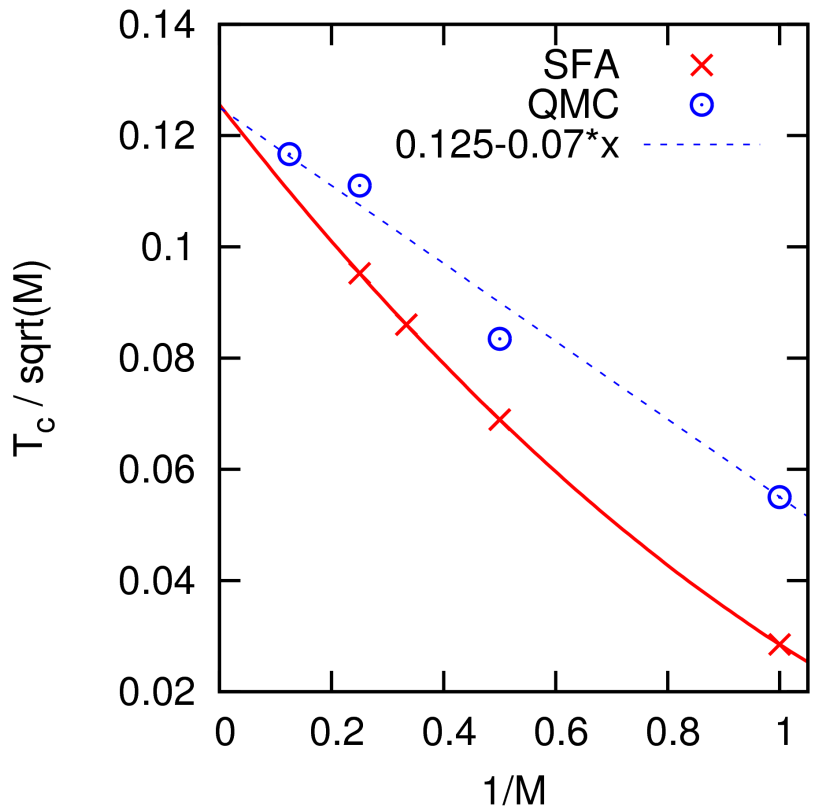


Phase diagram from multigrid HF-QMC: numerically exact results!

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

scaling of the critical parameters





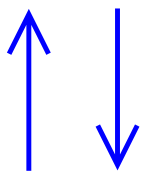
Multigrid HF-QMC: numerically exact results!

$\Longrightarrow$ Phase diagram for arbitrary M

Beyond electronic systems : Fermions with arbitrary spin multiplicity

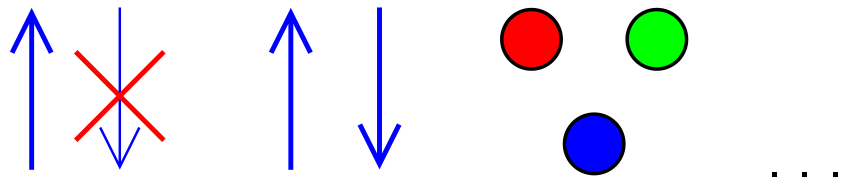
Condensed matter physics

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



Ultracold fermions

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

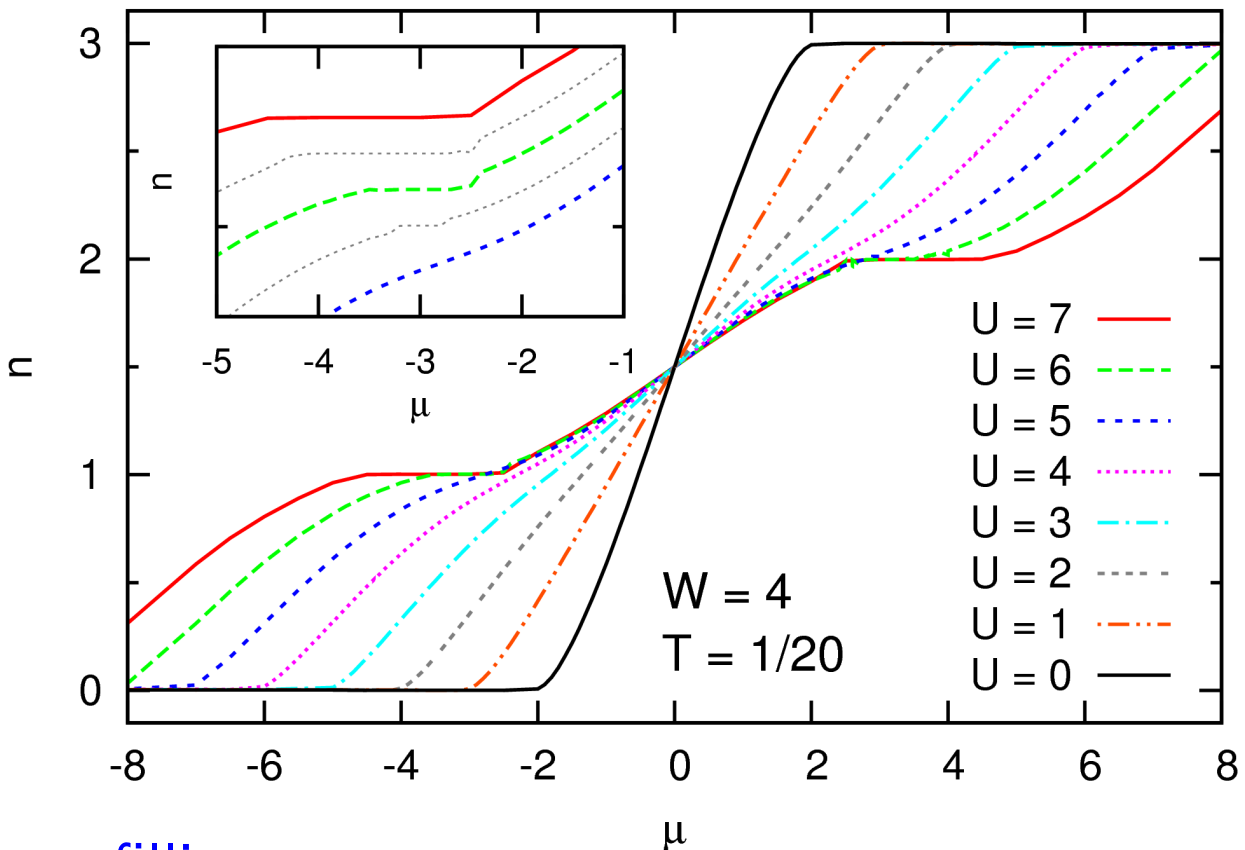


Example: ^{40}K
$|F = 9/2, m_F = -5/7, -7/2, -9/2\rangle$
[Regal, Jin, PRL (2003)]

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

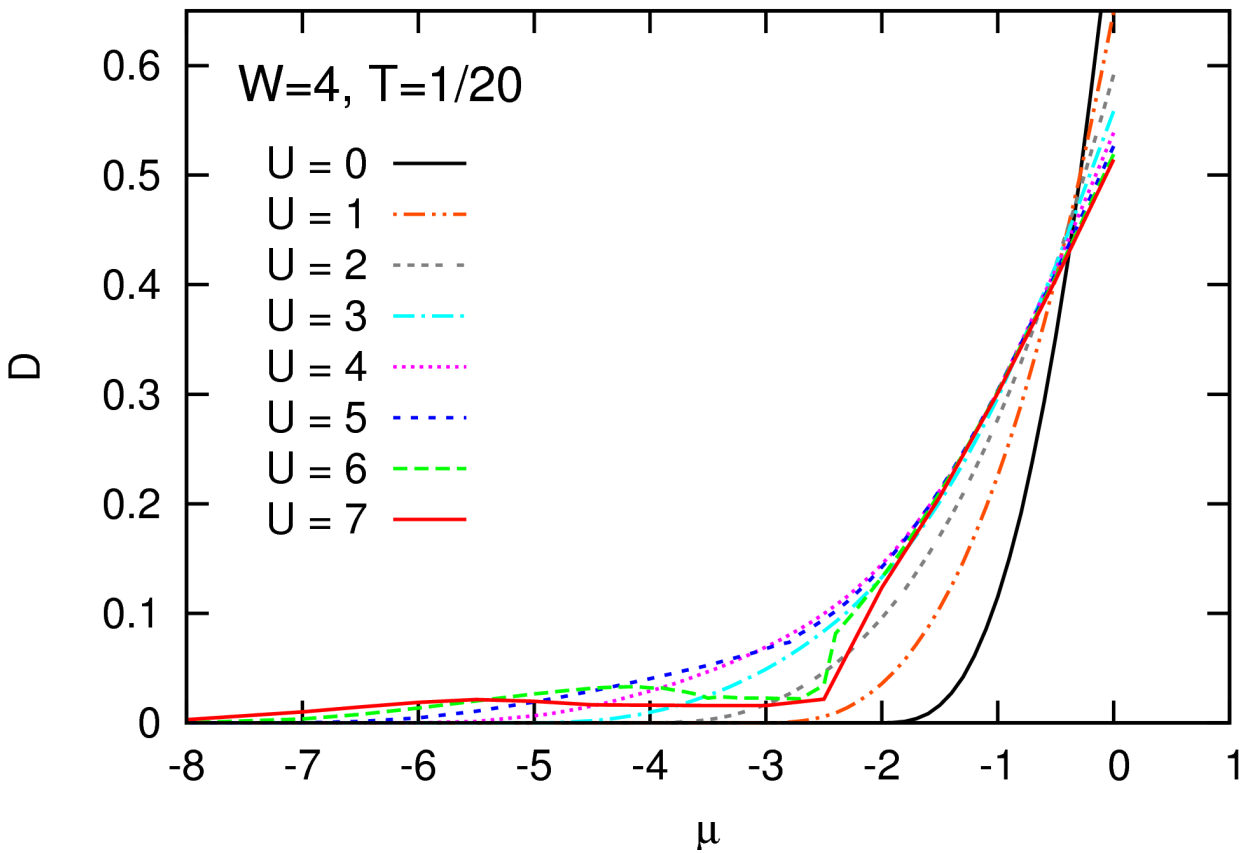


Density vs. filling

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

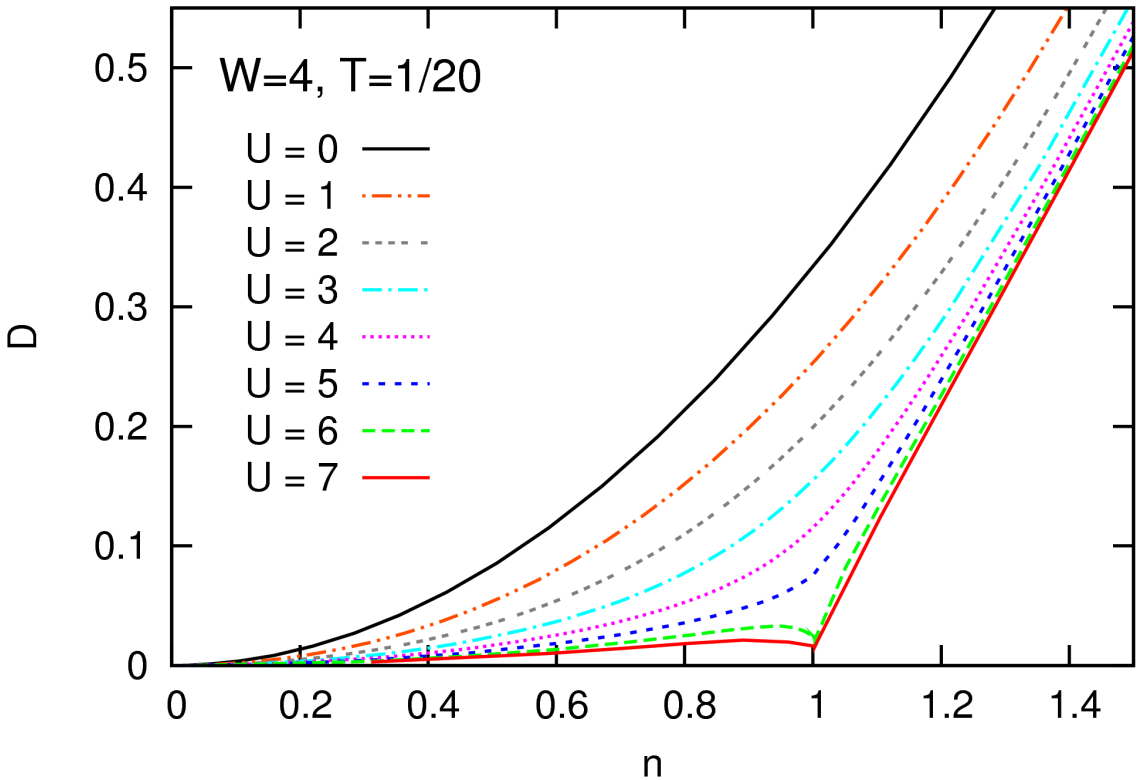
not at half-filling!

3-spin/flavor system in paramagnetic phase



Double occupancy vs. filling

Here mostly density effects



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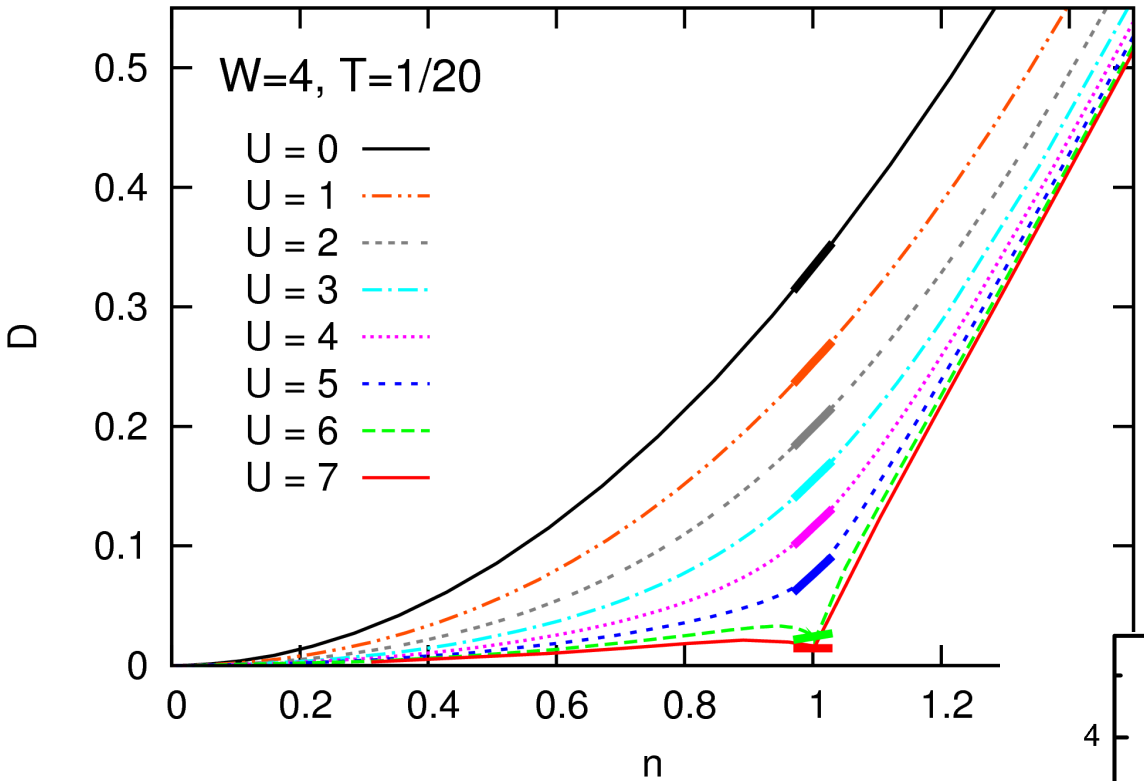


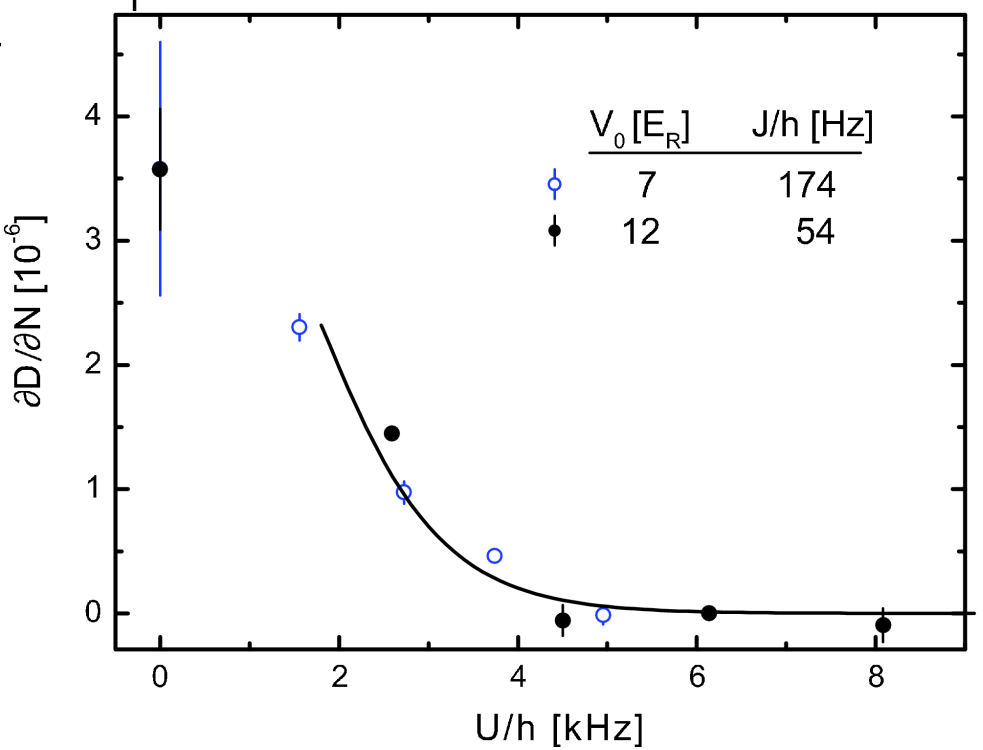
3-spin/flavor system:

Double occupancy vs. density

Experiment:2-spin system

Transition to an incompressible phase

[Jördens et al., Nature (2008)]



Summary

Monte Carlo methods: principles and classical simulations

Systems with strong electronic (fermionic) correlations

Approaches for correlated electron systems

Auxiliary-field Hirsch-Fye QMC algorithm

Multigrid Hirsch-Fye quantum Monte Carlo algorithm

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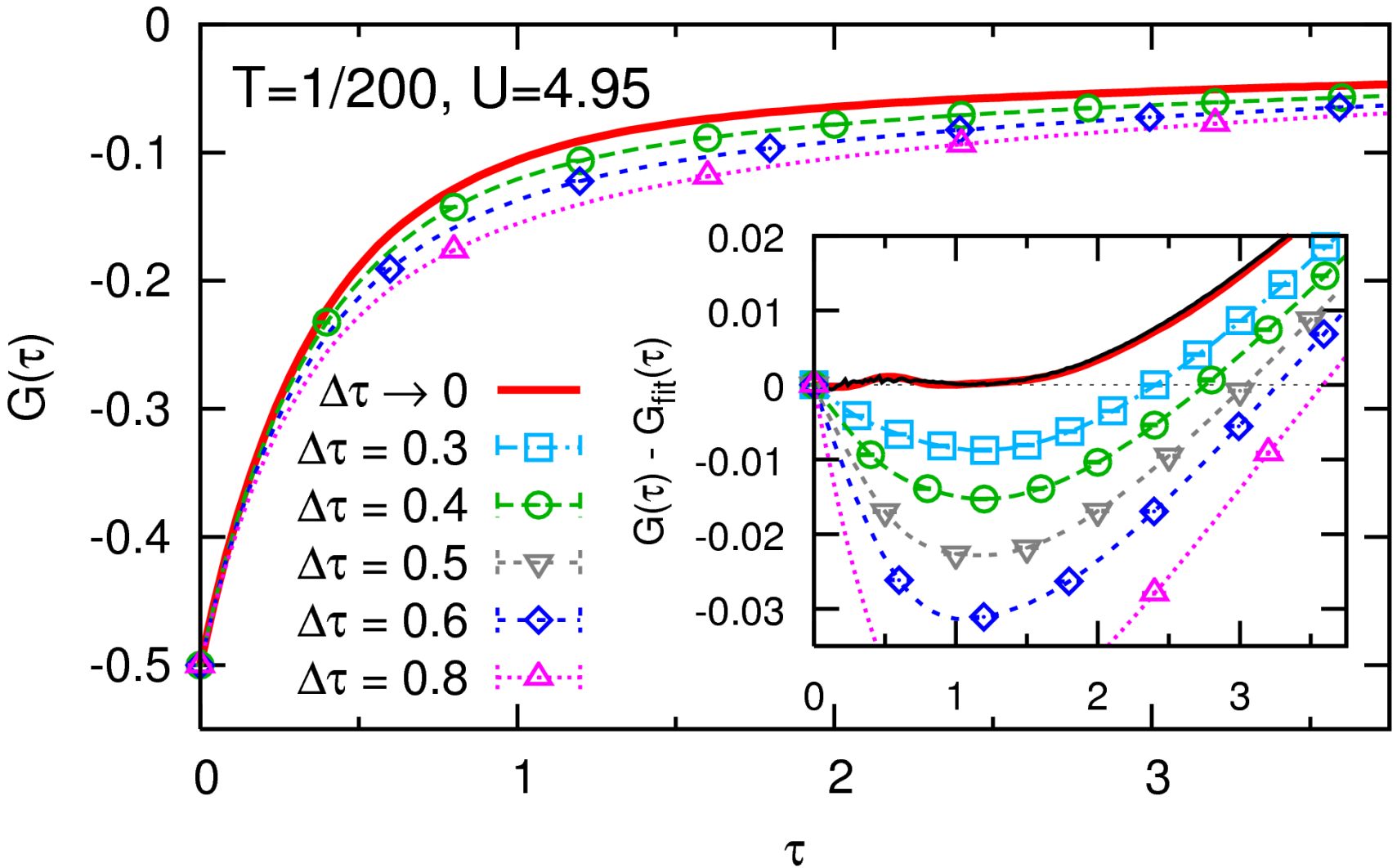
Technical issues: Green function fit (MEM?), Cache + BlueGene optimization, Analytic continuation

Acknowledgements: Carsten Knecht, **Elena Gorelik**, Eberhard Jacobi, Peter van Dongen; Funding by state RLP (Forschungsfonds 2007) and DFG (in SFB/TR 49)

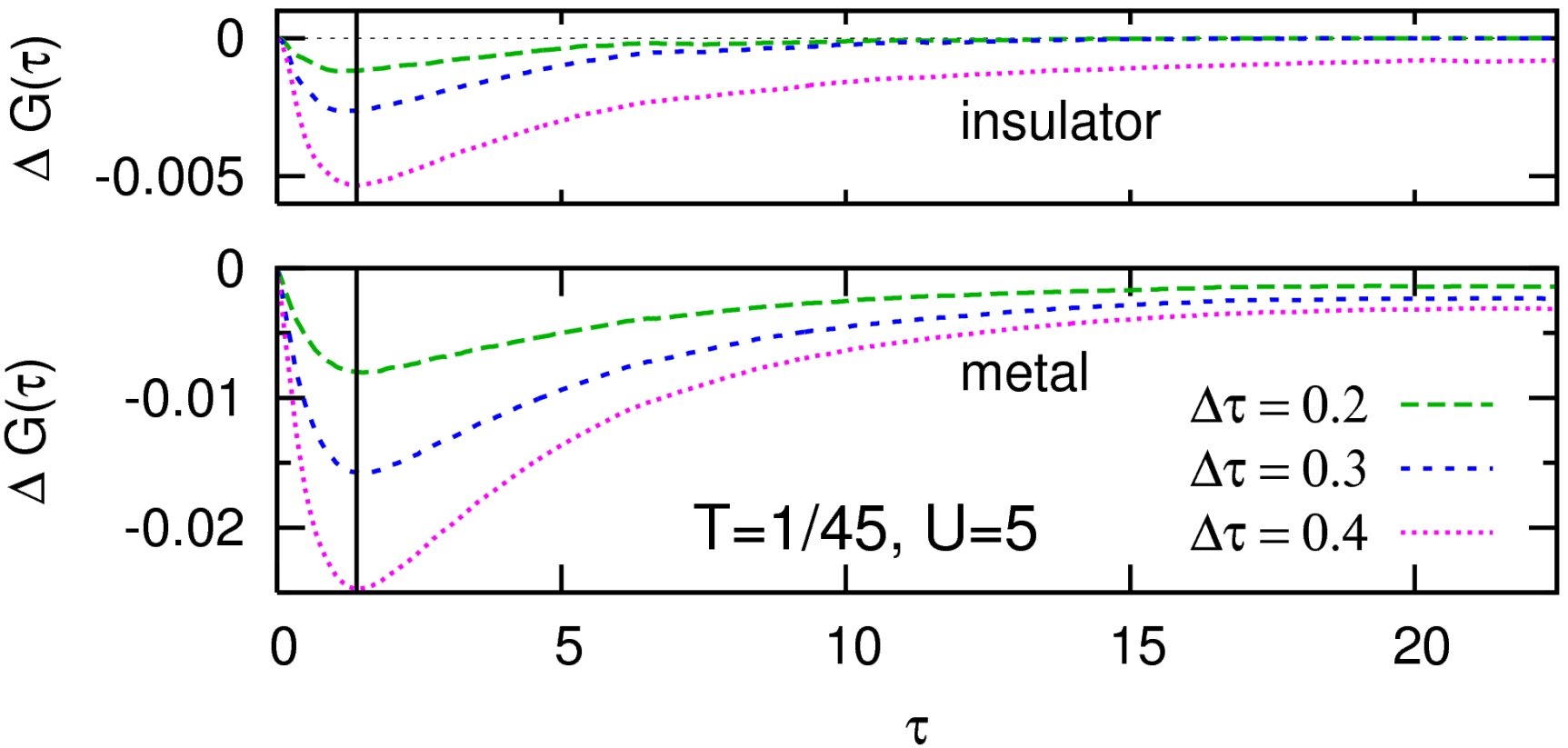
Illustration: interpolation and extrapolation of Green functions



[NB, arXiv:0712.1290]

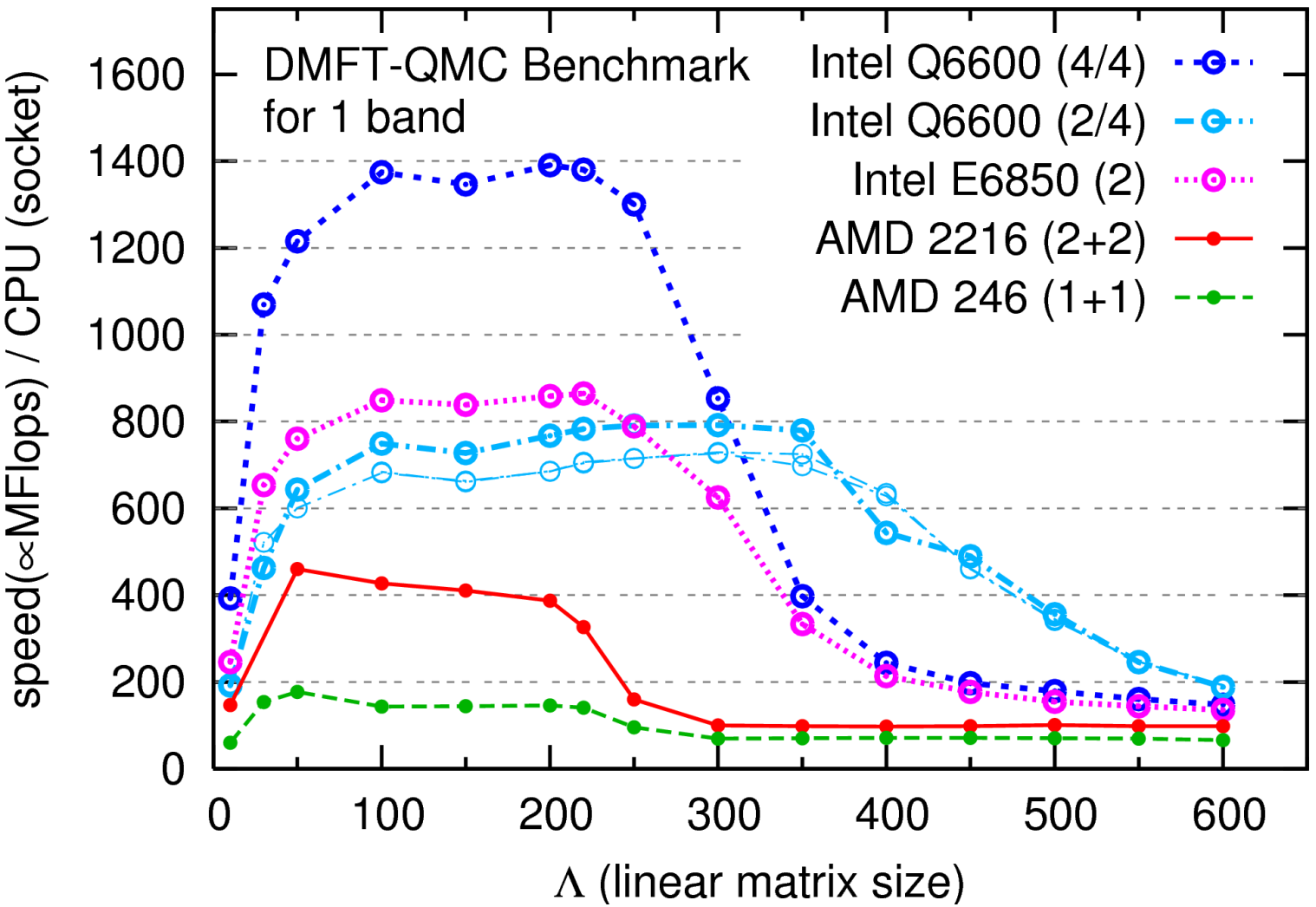
Excellent agreement with hybridization expansion CT-QMC [Werner et al., PRL (2006)]

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



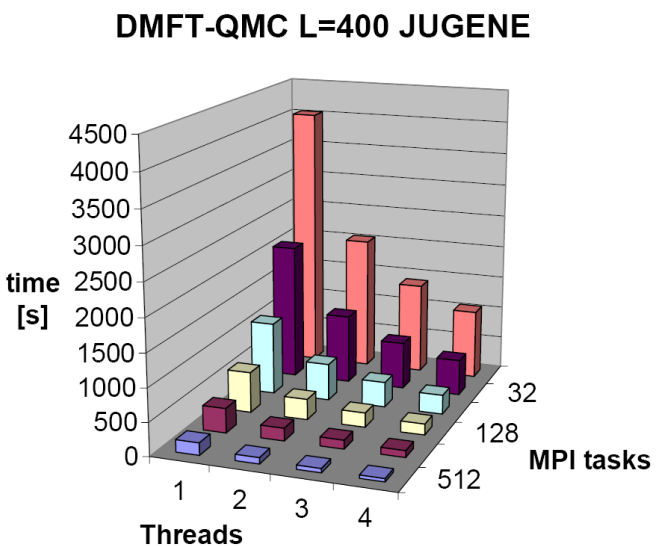
Uniform $\Delta\tau$ dependence, position of max. error independent of $\Delta\tau$ and phase!

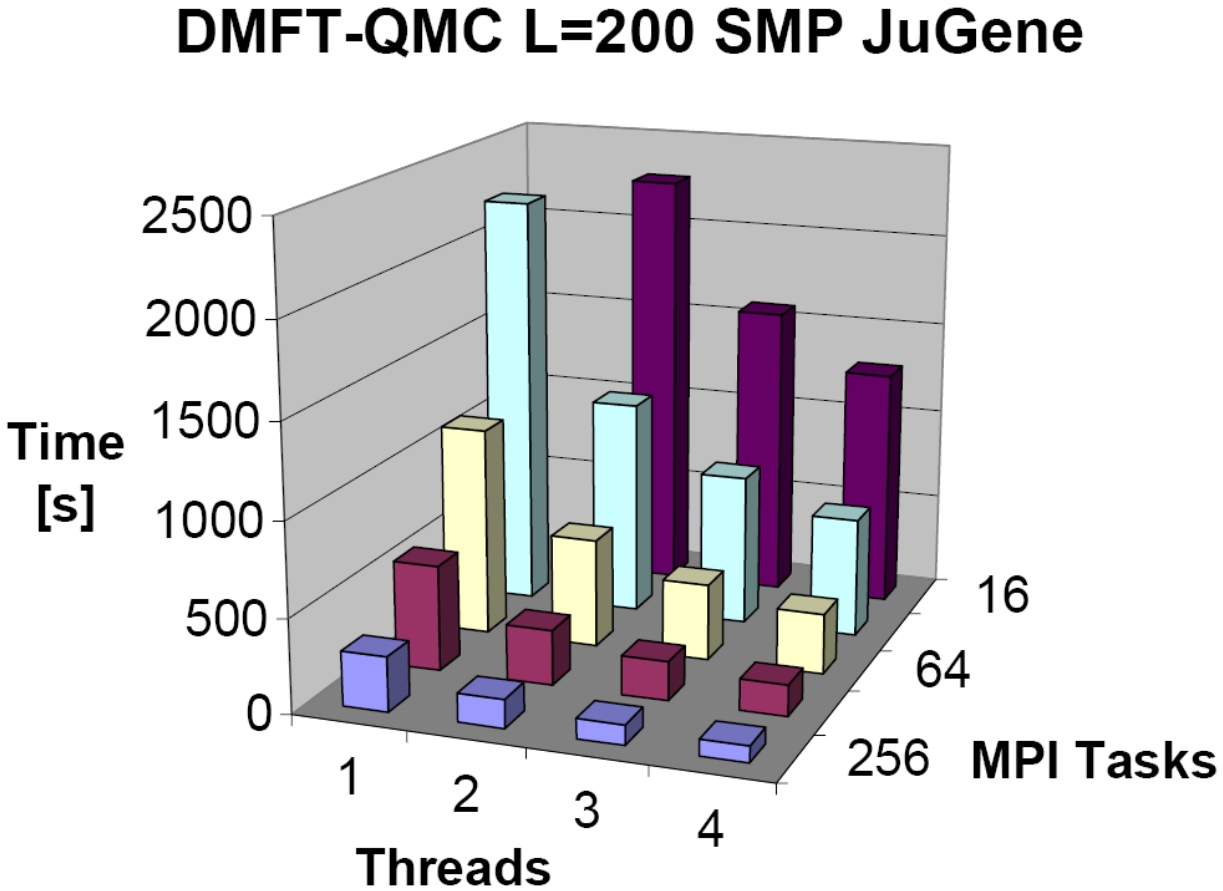
Benchmarks



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