

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

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## 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

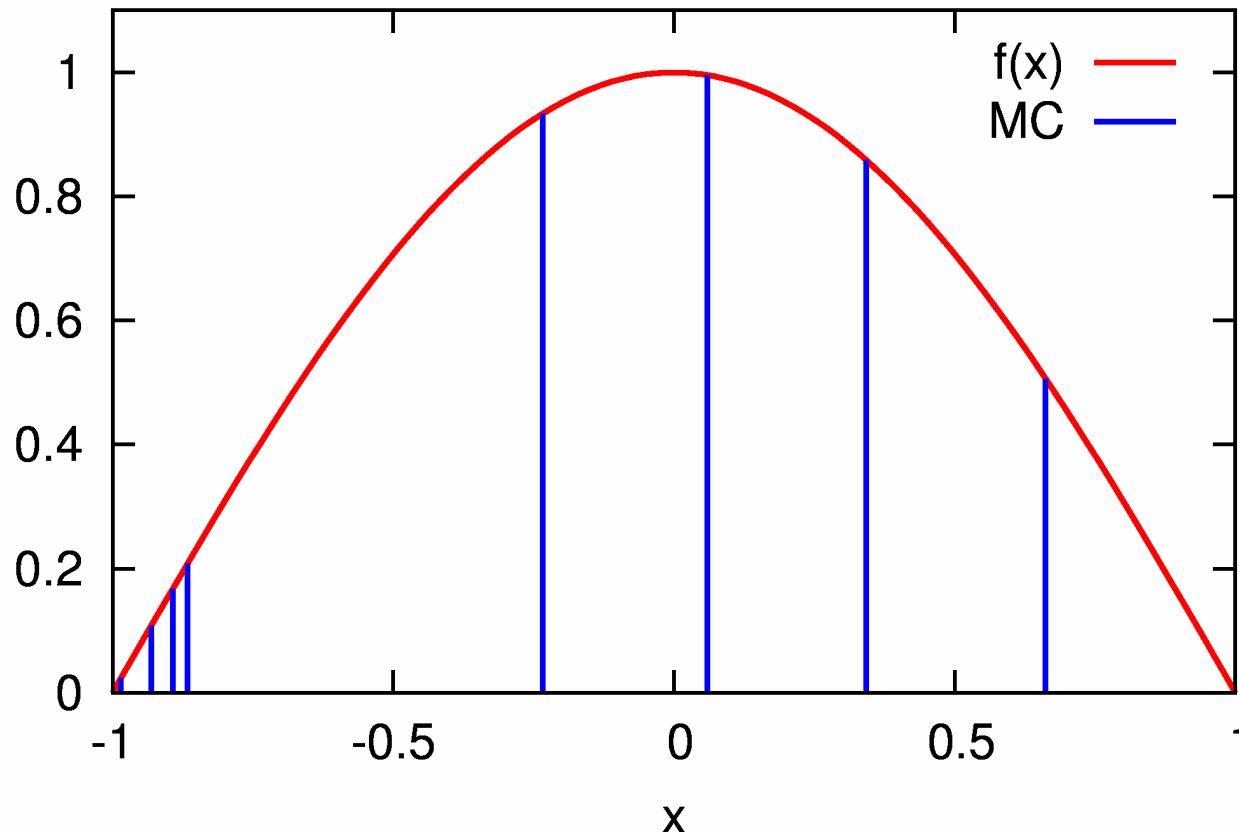
Multigrid Hirsch-Fye quantum Monte Carlo algorithm

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  $d = 1$ )

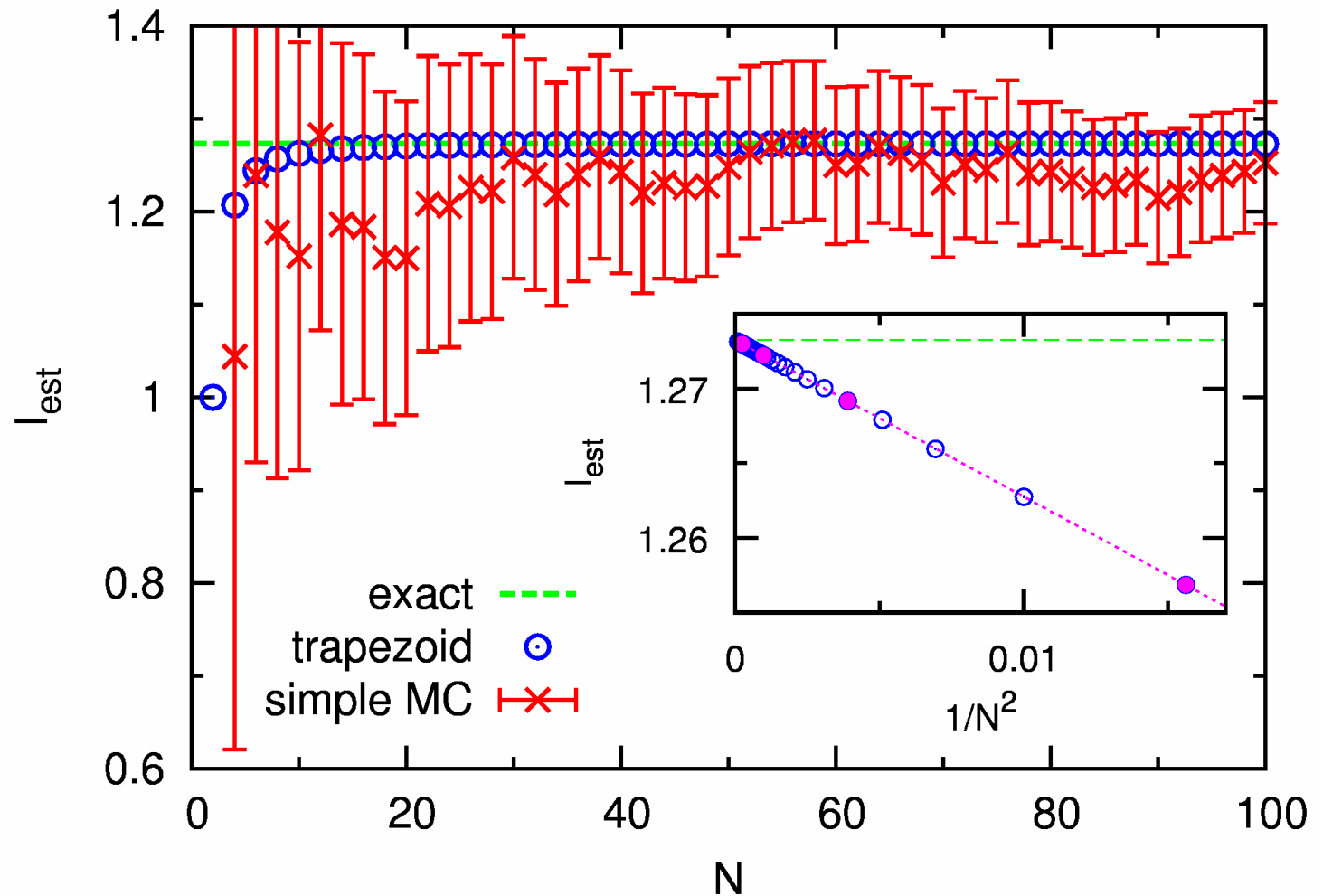


$$I = \int_a^b f(x) dx = ?$$

Numerical methods:

- discretization
- Monte Carlo

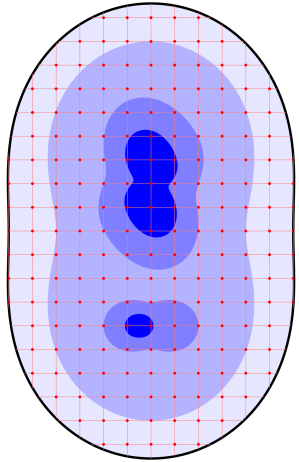
Convergence  
of results?



MC results are non-deterministic: only meaningful within **statistical error bars**!  
**In this case**, the deterministic method converges much faster (and very regularly)

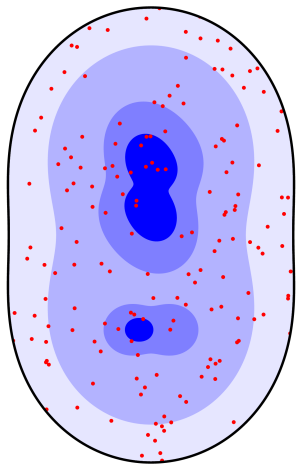
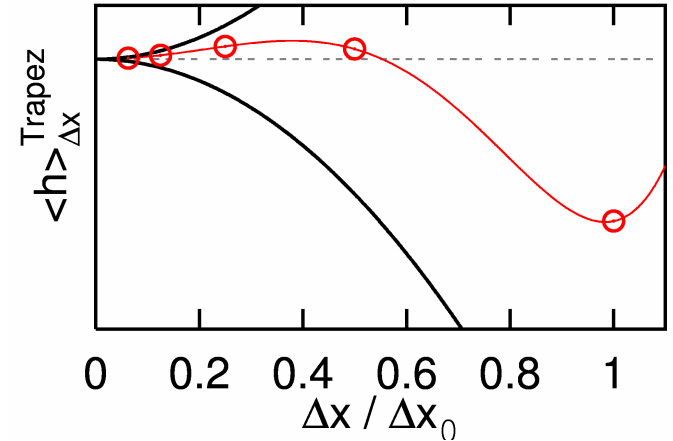
# Second MC example: higher dimensions

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



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

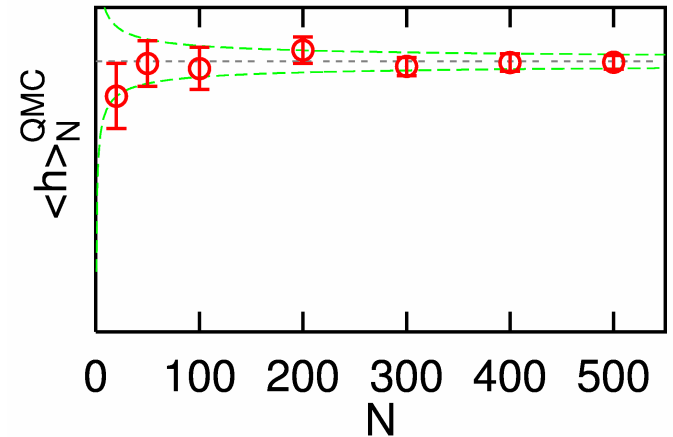
$$\Delta h \propto (\Delta x)^2 \propto N^{-2/d}$$



Stochastic: **simple Monte-Carlo**  
 $N$  configurations  $\vec{x}_i$ , uniform probability

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

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

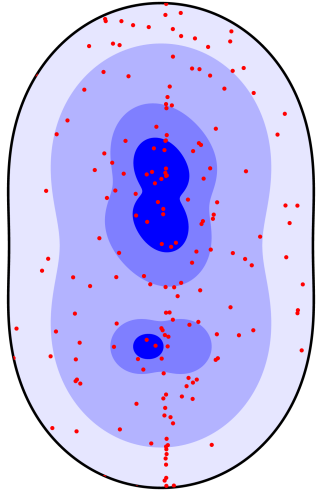


Central limit theorem

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.

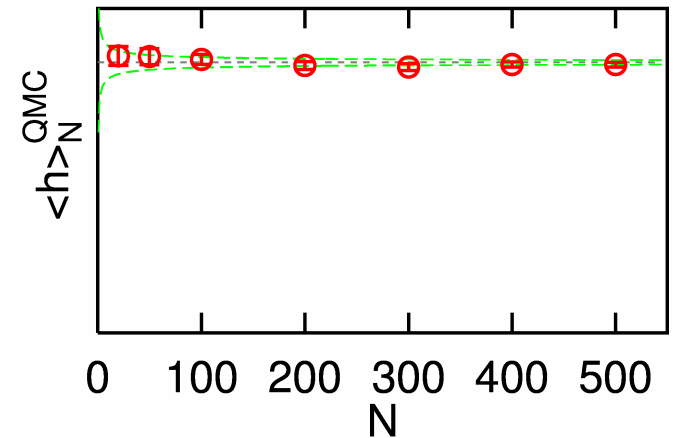


factorization:  $h(\vec{x}) = p(\vec{x}) o(\vec{x})$ ;

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

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

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



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

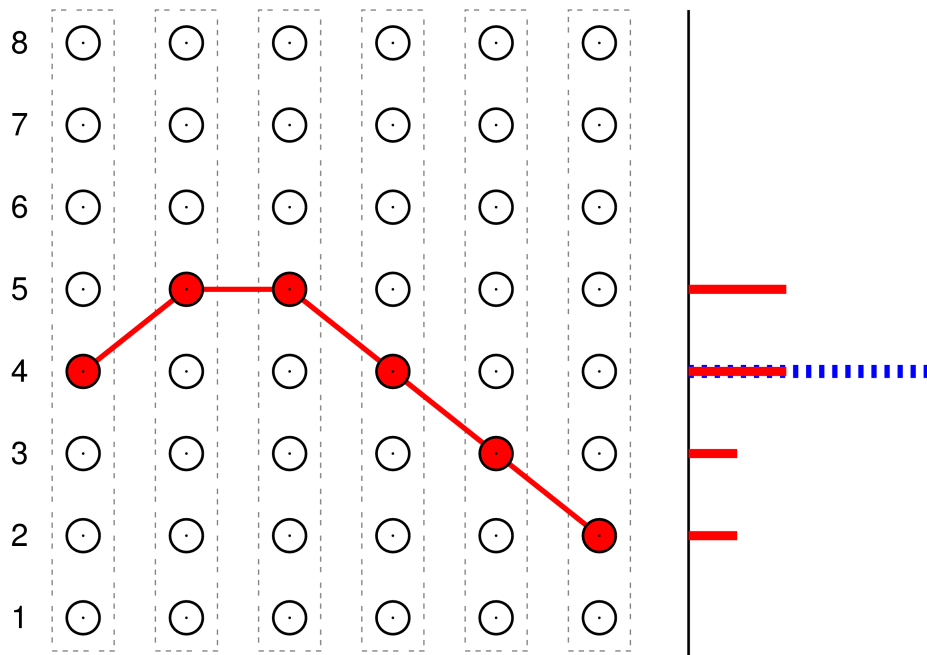
# Application of Monte Carlo in Statistical Physics

$$\langle O \rangle = \sum_i p_i O_i, \quad p_i = \frac{e^{-E_i/(k_B T)}}{\mathcal{Z}} \equiv \frac{\tilde{p}_i}{\mathcal{Z}}, \quad \mathcal{Z} = \sum_i e^{-E_i/(k_B T)}$$

**Simple Monte Carlo:** Estimation of both sums from a number  $N$  of equally probable configurations. **Problem:** typically  $\sqrt{\text{var}\{p\}} \gg \bar{p}$ .

**Importance Sampling MC:** Probability distribution given by Boltzmann weights  $p_i$ . **Problem:** Normalization  $1/\mathcal{Z}$  unknown.

**Solution:** approach target probability distribution by random walk (e.g.: 8 states)



Ergodicity and detailed balance

$$p_i P\{i \rightarrow j\} = p_j P\{j \rightarrow i\}$$

$$\Rightarrow P[\text{state } i \text{ after update } N] \xrightarrow{N \rightarrow \infty} p_i$$

Favorite choice: Metropolis rule

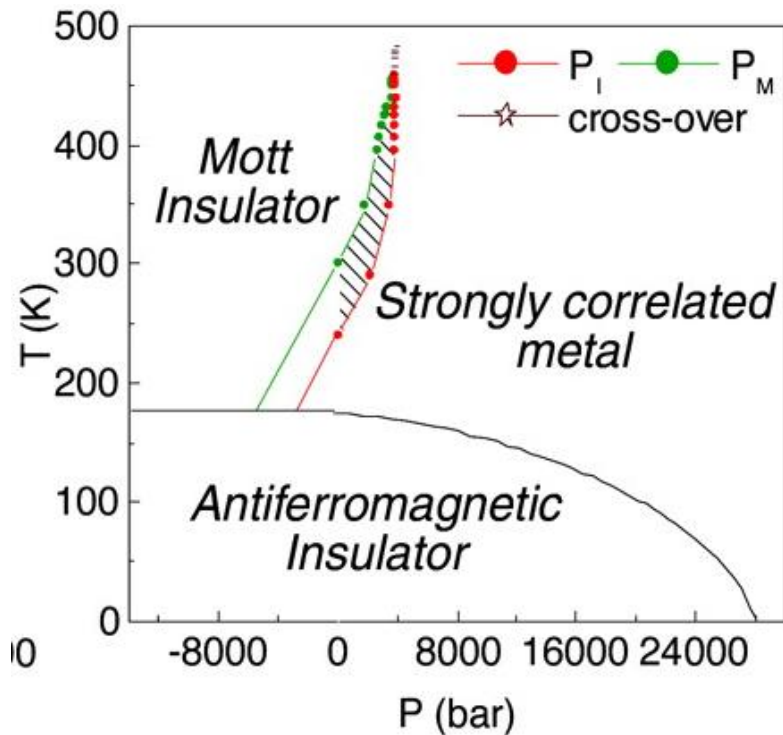
$$P\{i \rightarrow j\} = \min\left\{\frac{p_j}{p_i}, 1\right\}, \quad \frac{p_j}{p_i} = e^{\Delta E/(k_B T)}$$

# Systems with strong electronic/fermionic correlations

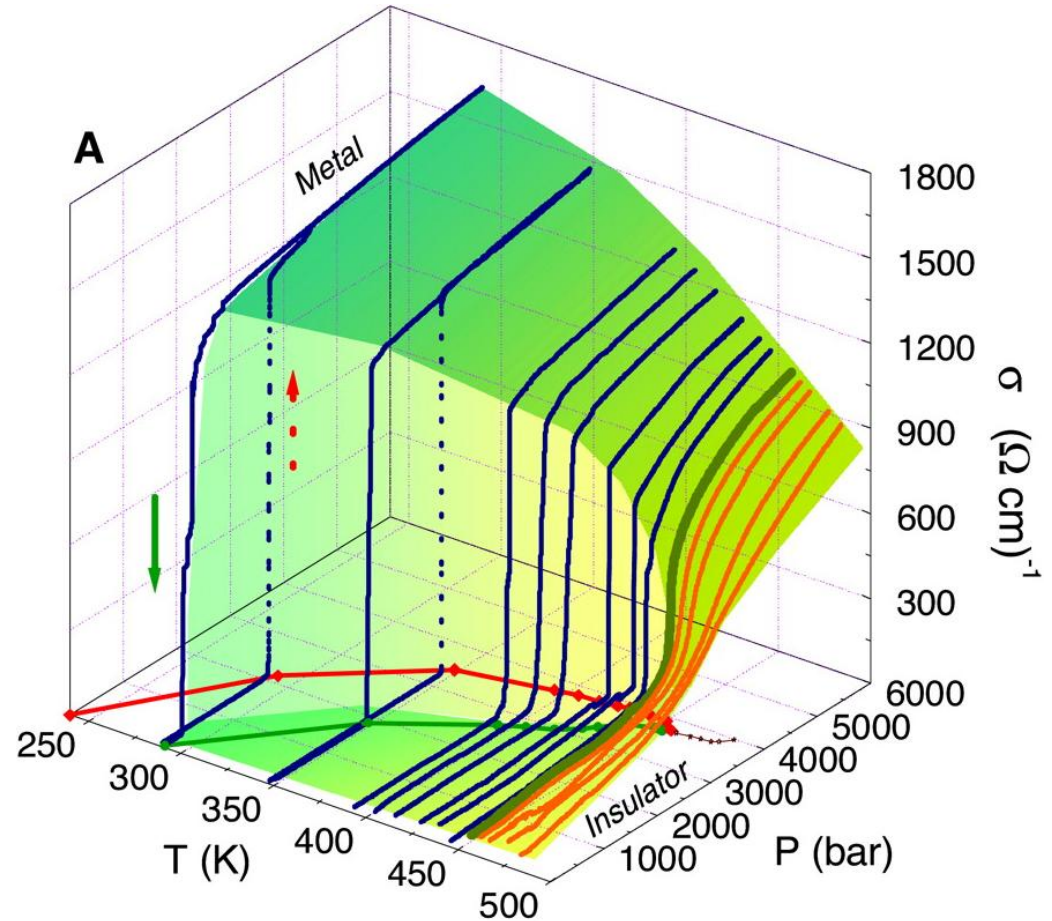
## Mott metal-insulator transition

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

## Phase diagram



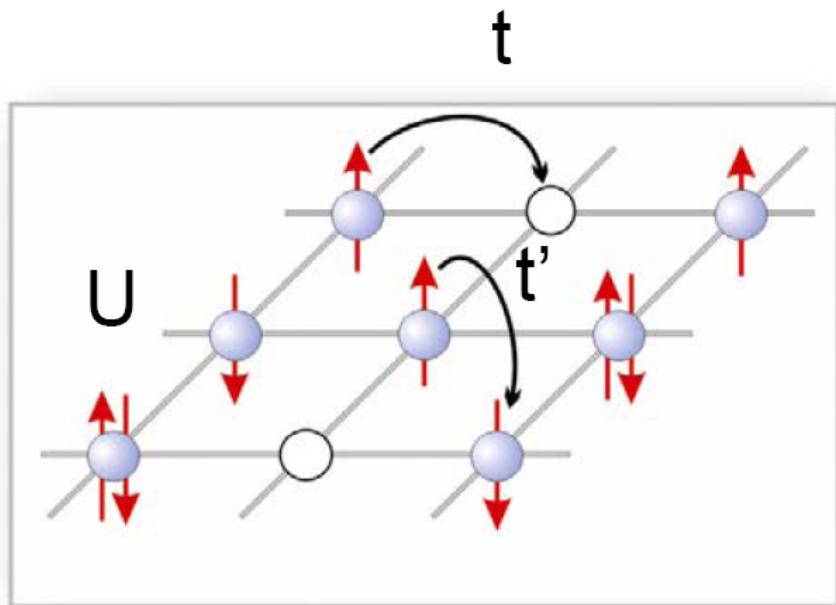
## Electrical conductivity



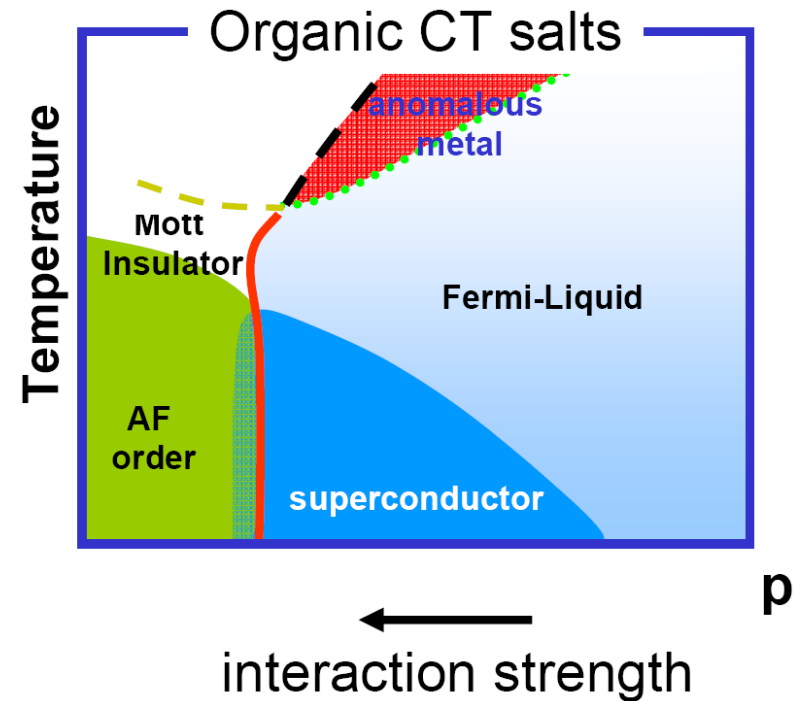
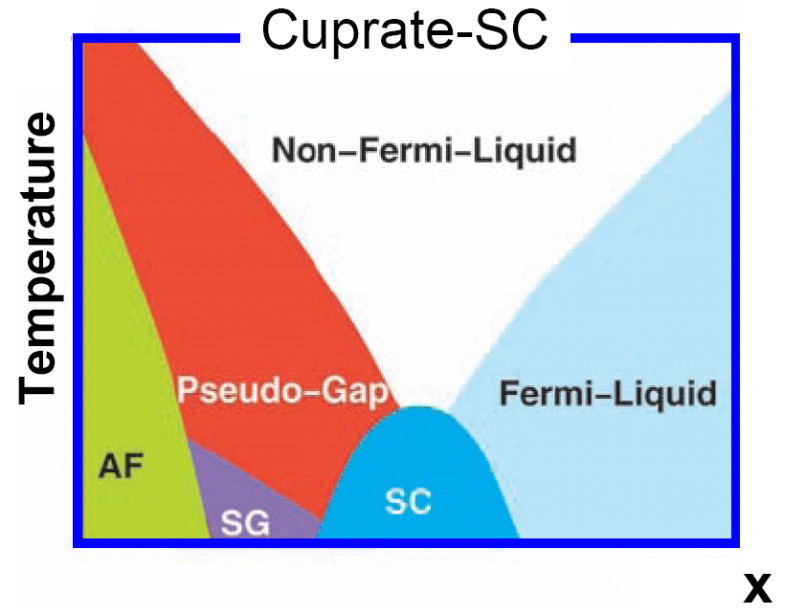
[Limelette et al., Science 302, 89 (2003)]

# Complex phases of cuprate and organic superconductors

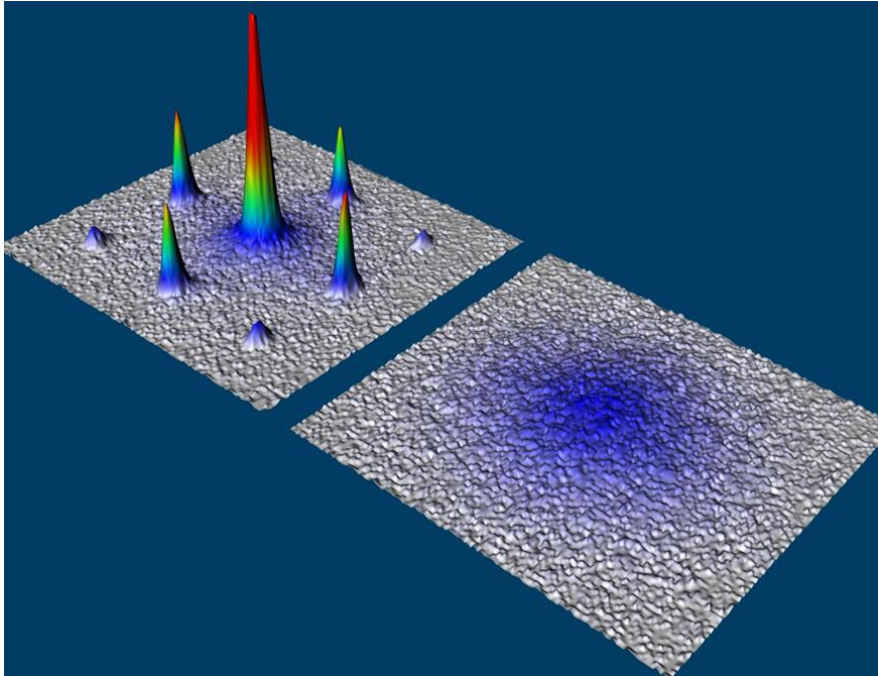
High- $T_c$  physics contained in 2D Hubbard model?



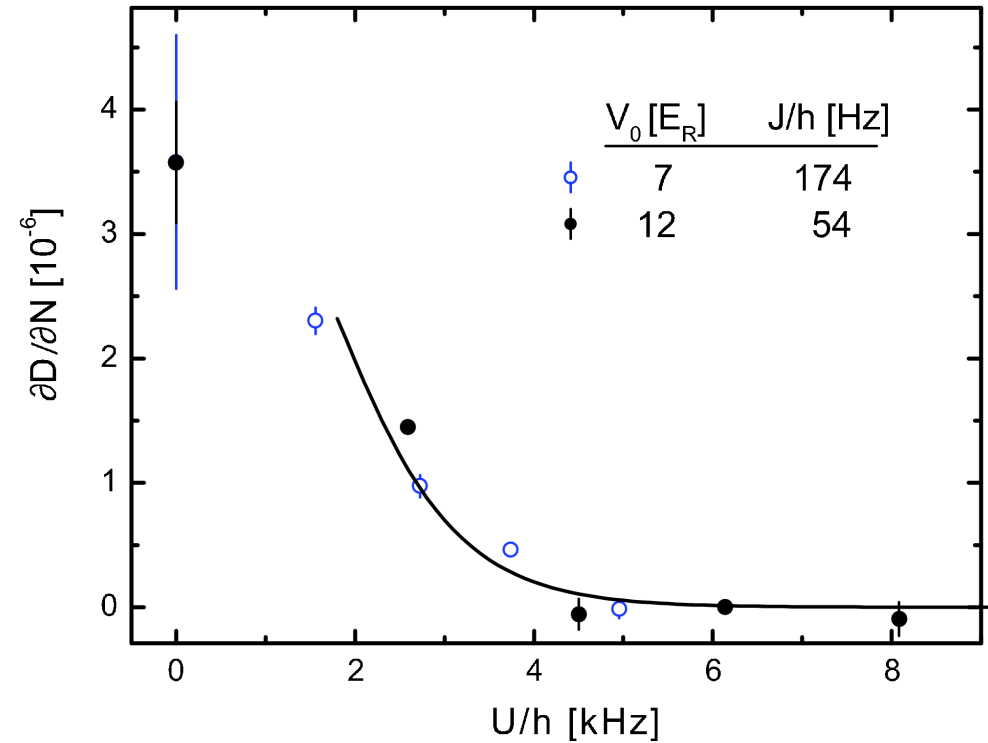
Are antiferromagnetic (AF) and Mott insulating phases essential for superconductivity?



# Correlated ultracold quantum gases on optical lattices



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



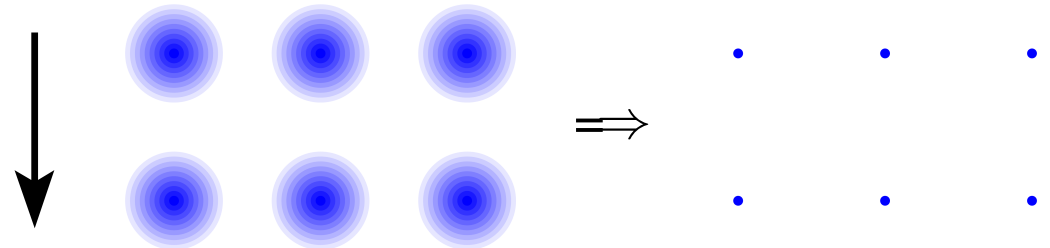
The transition to an incompressible phase for ultracold fermionic atoms [Jördens et al., Nature (2008)]  
Also Bloch group [arXiv:0809.1464]

# Approaches for correlated electron systems

## General Hamiltonian for nuclei and electrons

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

Born-Oppenheimer approximation (0<sup>th</sup> order)



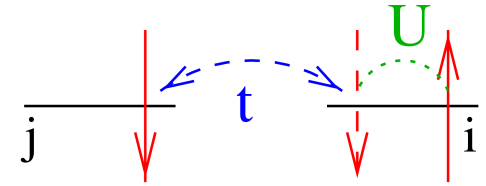
$$H = \sum_{i=1}^{N_e} \frac{\mathbf{p}_i^2}{2m} + \sum_i V(\mathbf{r}_i) + \sum_{i<j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

## Classes of theoretical approaches for electronic problem

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

# Approaches for Hubbard-type models

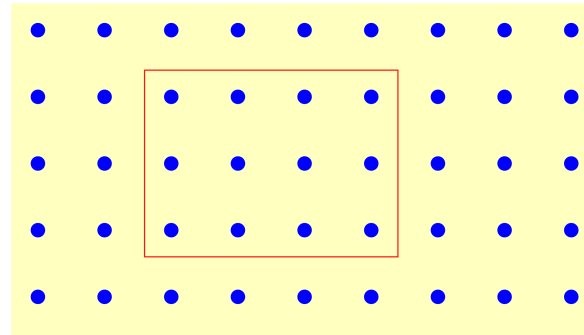
$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



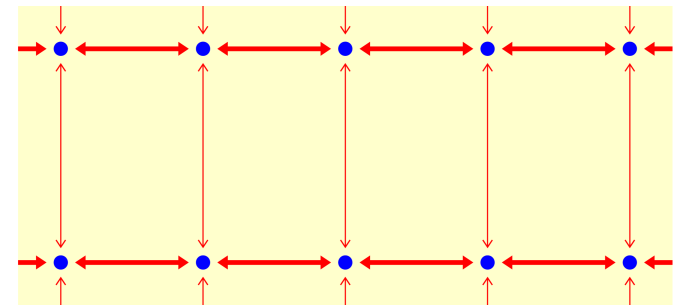
## Perturbation theory

- $U \rightarrow 0$ : Hartree-Fock  
2<sup>nd</sup> order PT, . . . .
- $t/U \rightarrow 0$  (for  $n = 1$ )  
 $\rightsquigarrow$  Heisenberg model

## finite clusters: ED, QMC



## $d \rightarrow 1$ : Bethe ansatz, DMRG



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

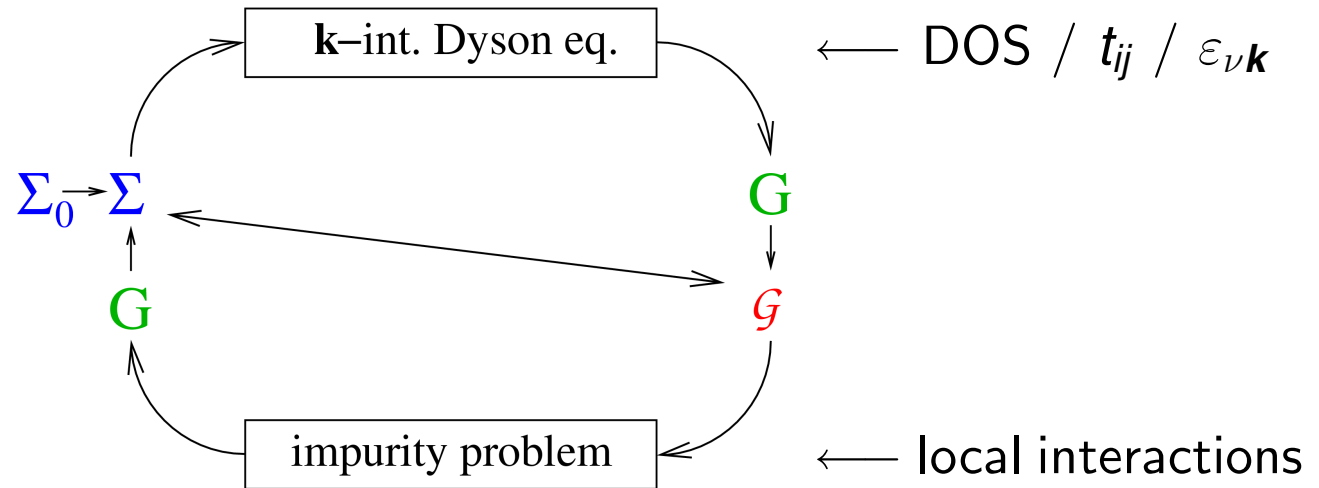
[Metzner, Vollhardt, PRL (1989), Georges, Kotliar, PRL (1992), Jarrell, PRL (1992)]

- + non-perturbative  $\rightsquigarrow$  valid at MIT
- + dynamical on-site correlations preserved
- + in thermodynamic limit
- +/- exact for coordination  $Z \rightarrow \infty$



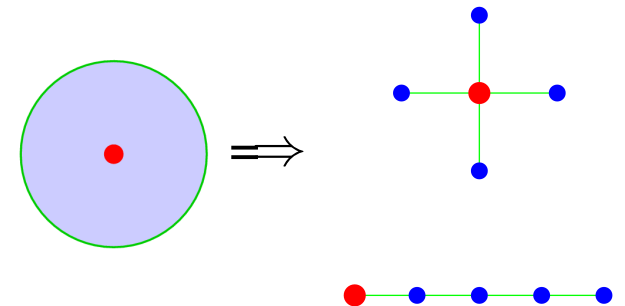
# Iterative solution of DMFT equations

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



## 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



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

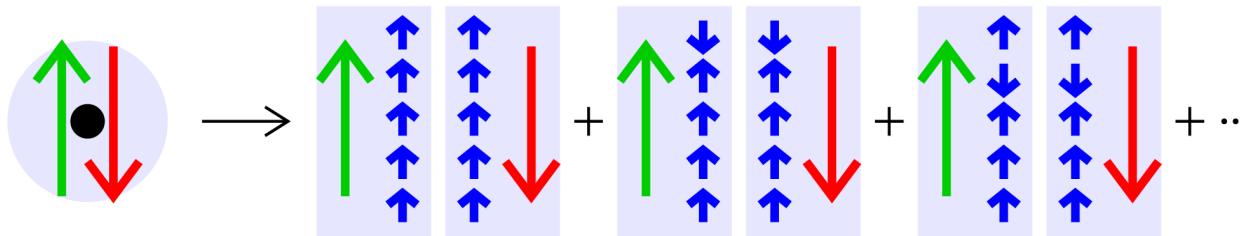
Green function  $G$  in imaginary time (fermionic Grassmann variables  $\psi, \psi^*$ ):

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

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

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

(iii) Hubbard-Stratonovich transformation



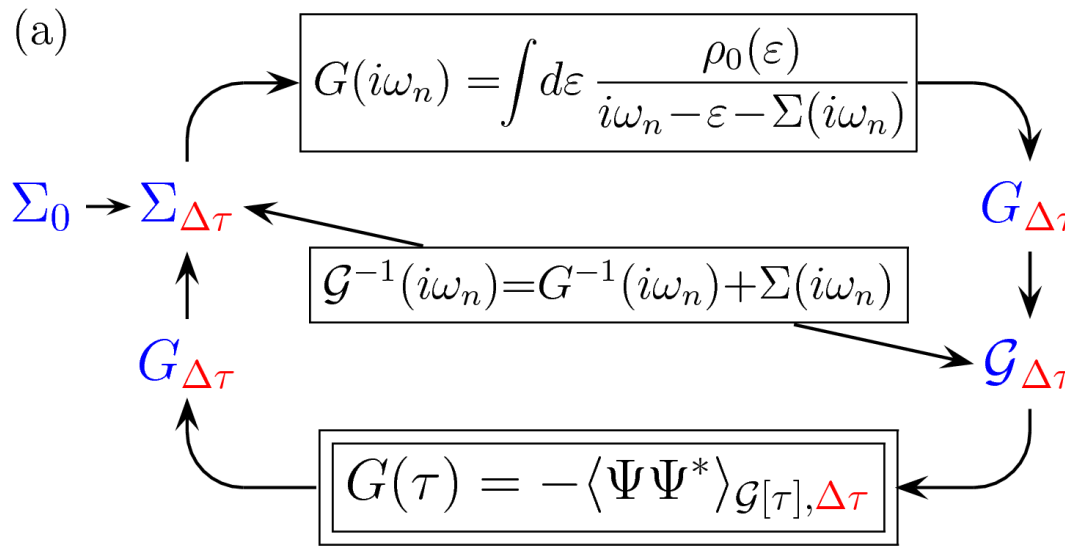
Wick theorem:

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

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

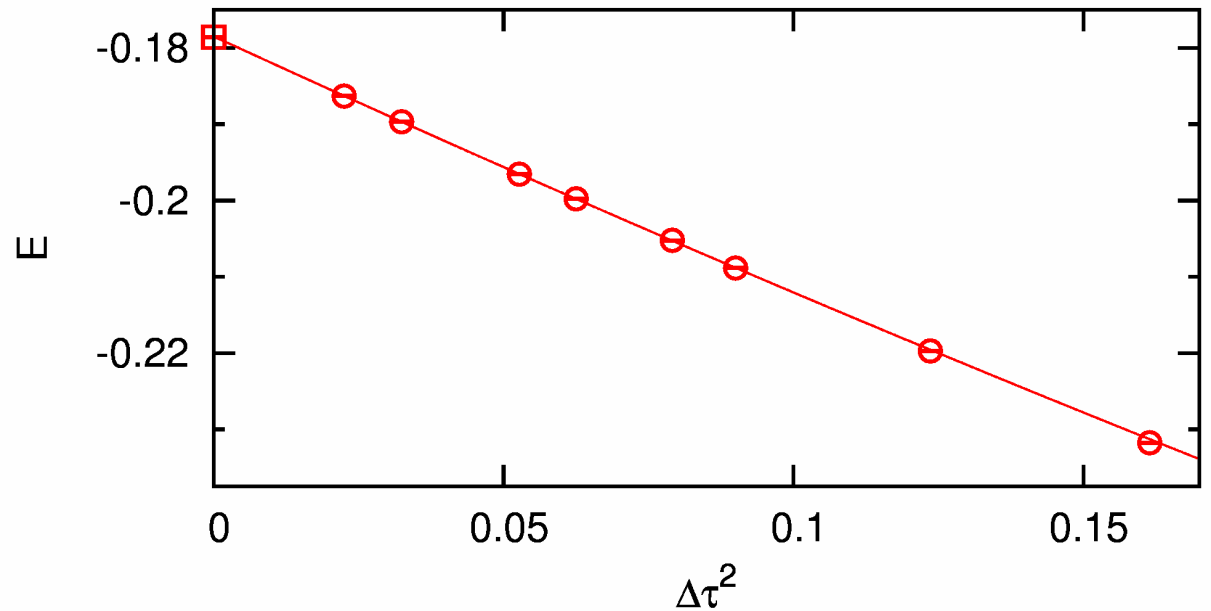
+ numerically exact, + no sign problem, – effort scales as  $T^{-3}$   
(density-type interactions)

Self-consistency cycle using conventional HF-QMC



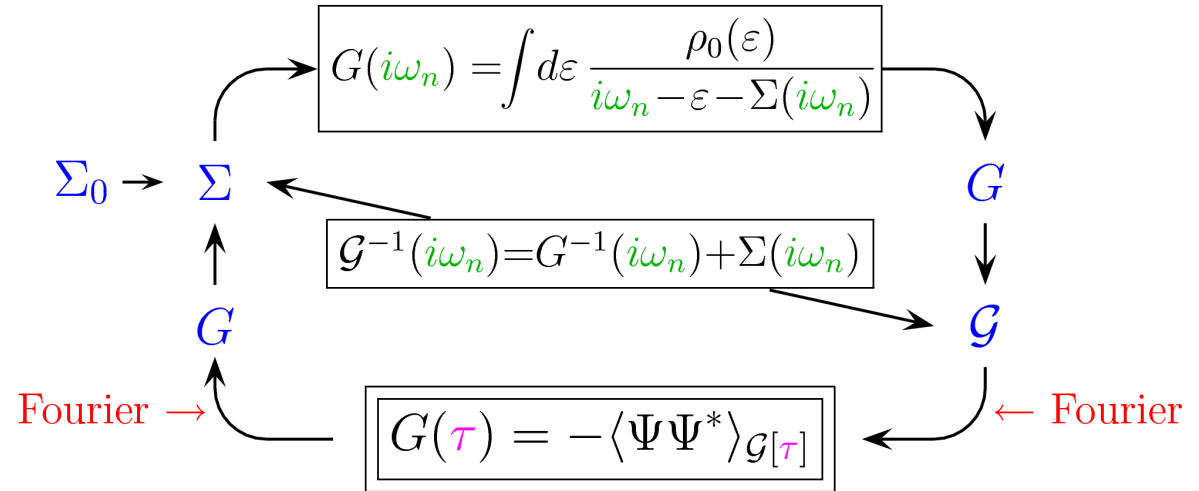
Extrapolation  $\Delta\tau \rightarrow 0$  can improve accuracy of observable estimates by several orders of magnitude ( $\sim$  same cost)

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

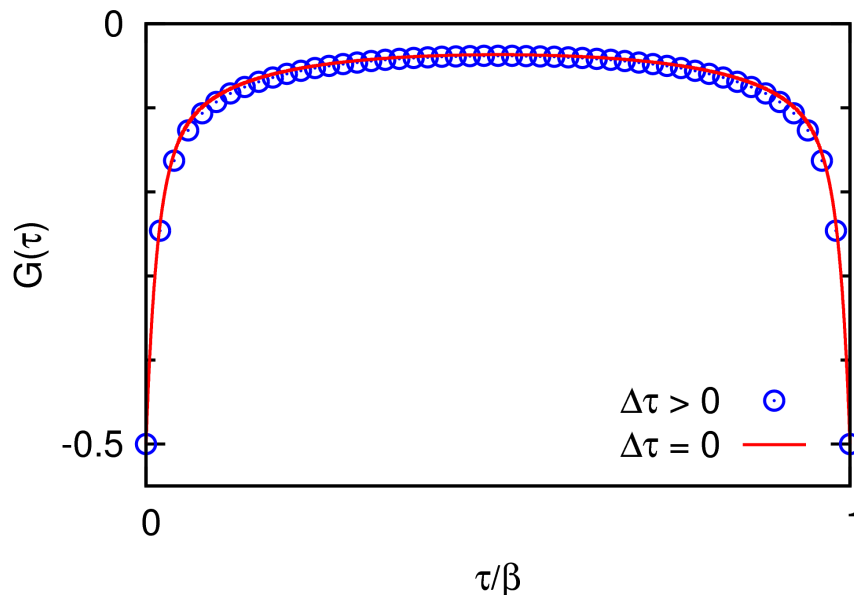


# Special issue: Fourier transformations in DMFT-QMC cycle

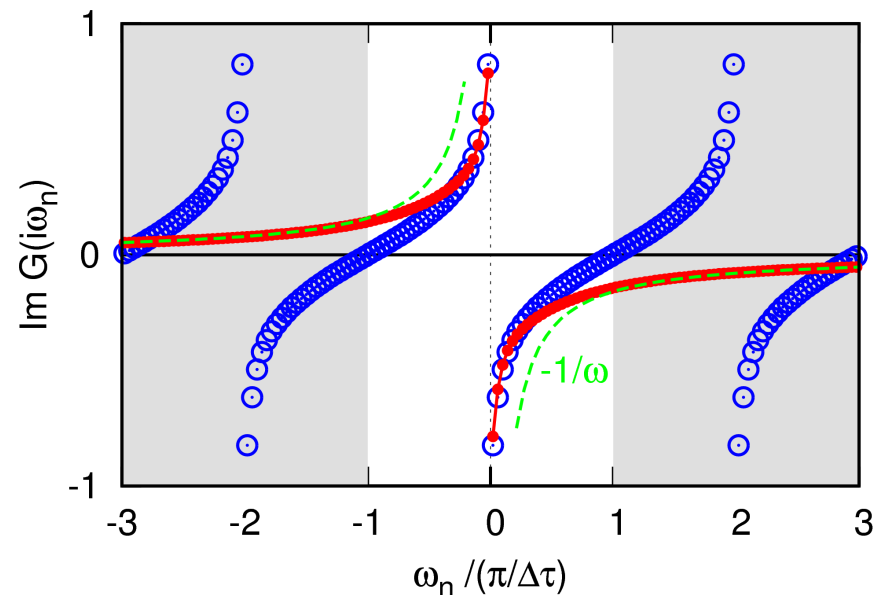
Iterative solution of DMFT equations (for imaginary-time impurity solver)



Naive discrete Fourier transformation  $\rightsquigarrow$  oscillations (instead of  $G(\omega) \xrightarrow{\omega \rightarrow \infty} 1/\omega$ )



naive FT  $\rightarrow$



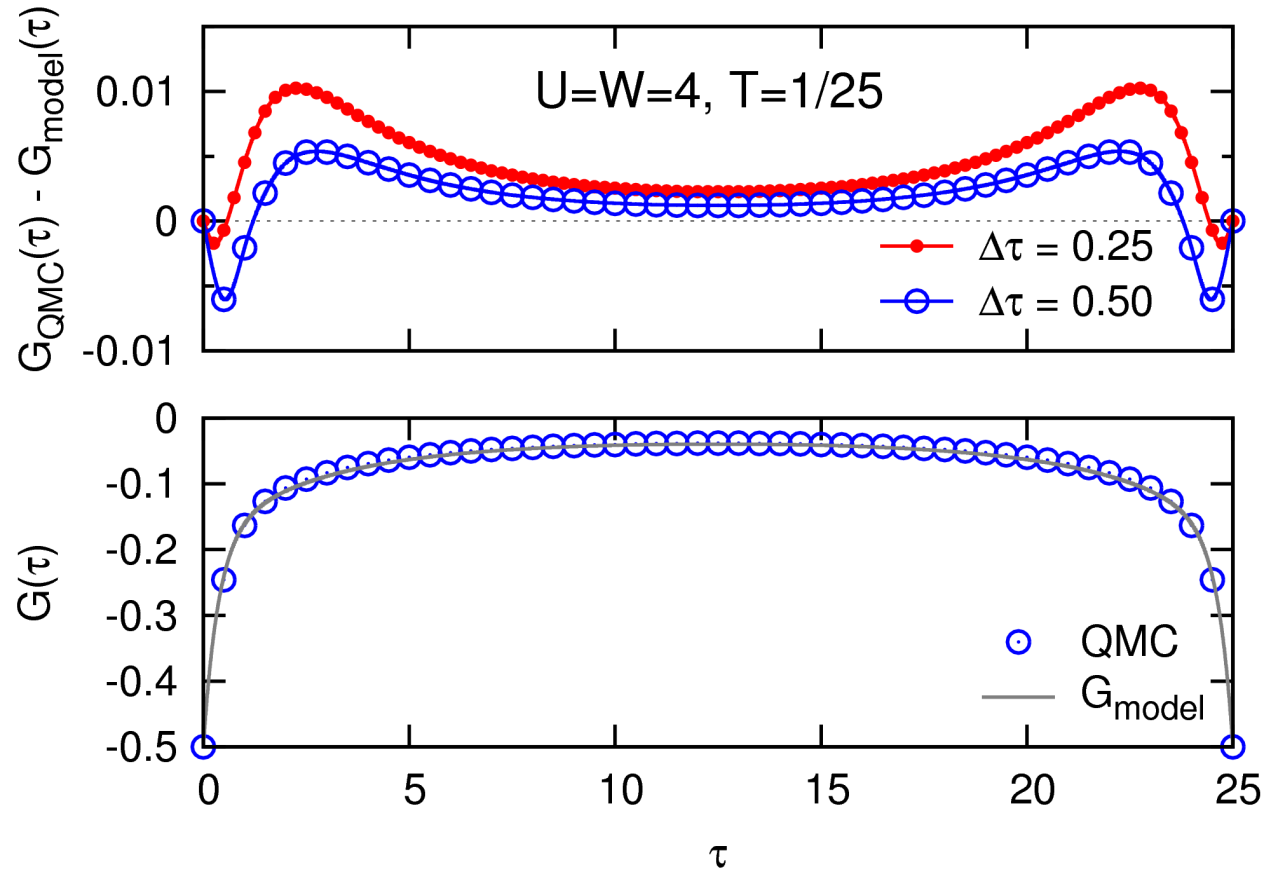
Possible solution: interpolate  $G_{\text{QMC}}(\tau)$ , e.g., by cubic splines [Jarrell, Krauth, Gull, . . .]

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

- adjust boundary cond. [Oudovenko]

- spline-fit only difference w.r.t. reference problem:

- IPT [Jarrell]
- high-frequency expansion for  $\Sigma(\omega)$  + param. [Knecht, NB]



$$\Sigma_{\sigma}(\omega) = U(\langle \hat{n}_{-\sigma} \rangle - \frac{1}{2}) \omega^0 + U^2 \langle \hat{n}_{-\sigma} \rangle (1 - \langle \hat{n}_{-\sigma} \rangle) \omega^{-1} + \mathcal{O}(\omega^{-2})$$

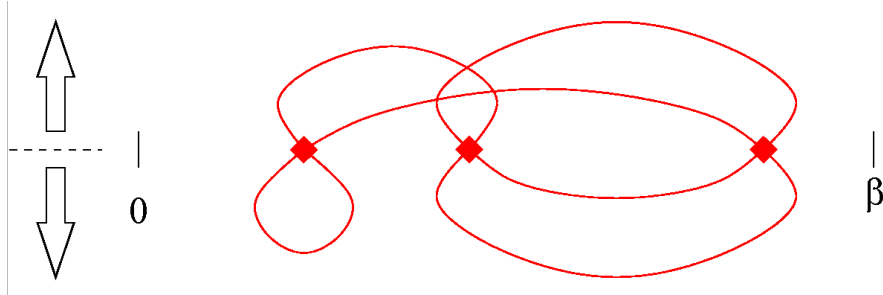
multi-band case:  
additional terms

Interdisciplinary project: replace spline interpolation by smooth fit!

# New development: continuous-time QMC algorithms

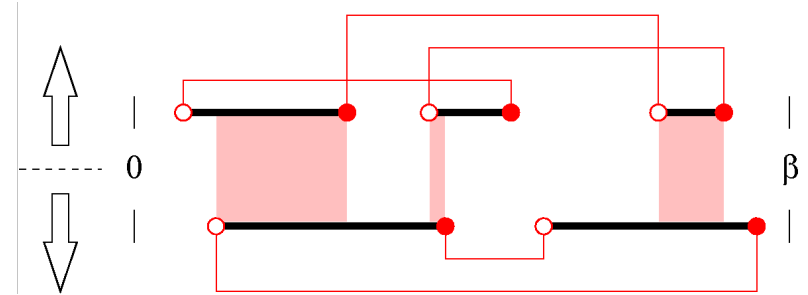
## 1. weak-coupling expansion

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

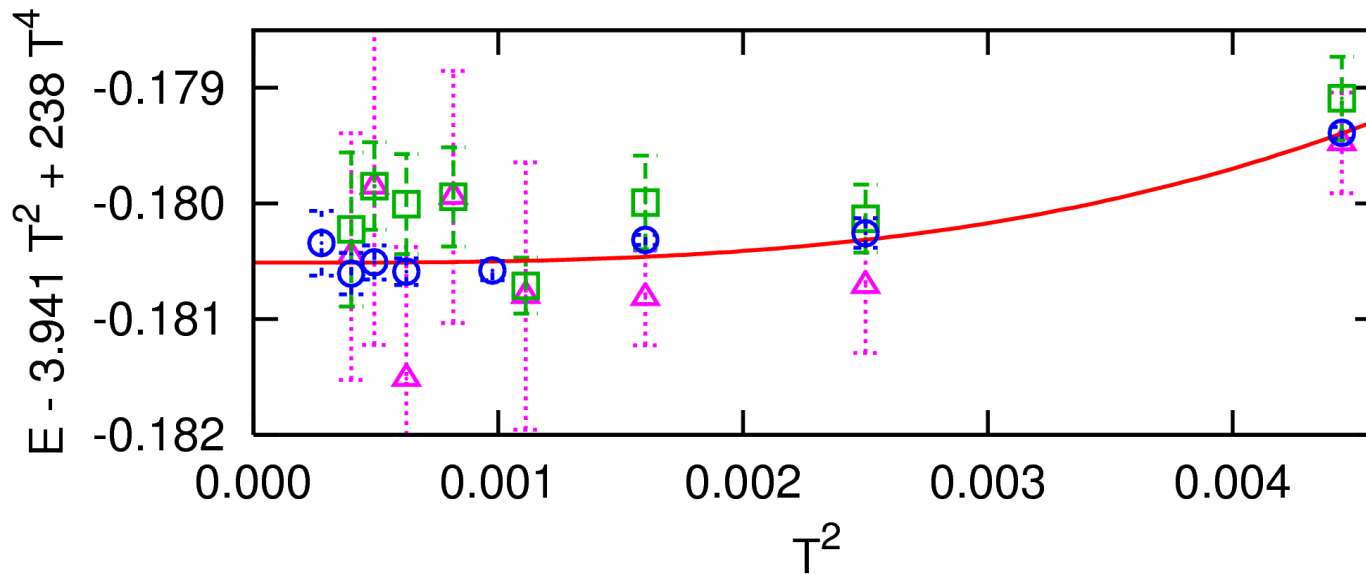


## 2. hybridization expansion

[Werner et al., PRL (2006)]



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



Test case:

1 band,  $U = W = 4$

○ HF-QMC ( $\Delta\tau \rightarrow 0$ )

□ weak-coupling CT-QMC

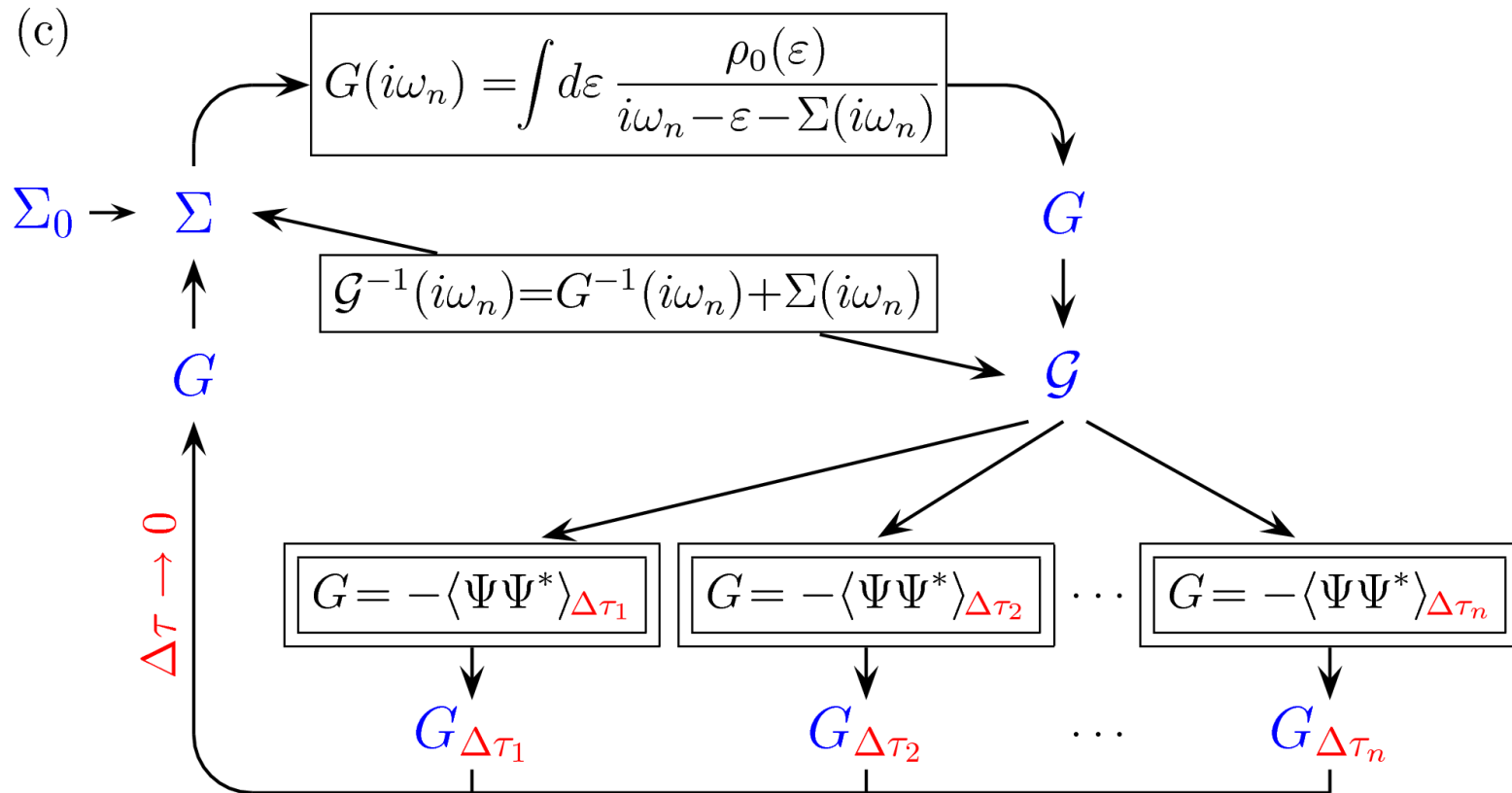
△ hybridization CT-QMC

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

# Multigrid Hirsch-Fye quantum Monte Carlo algorithm

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

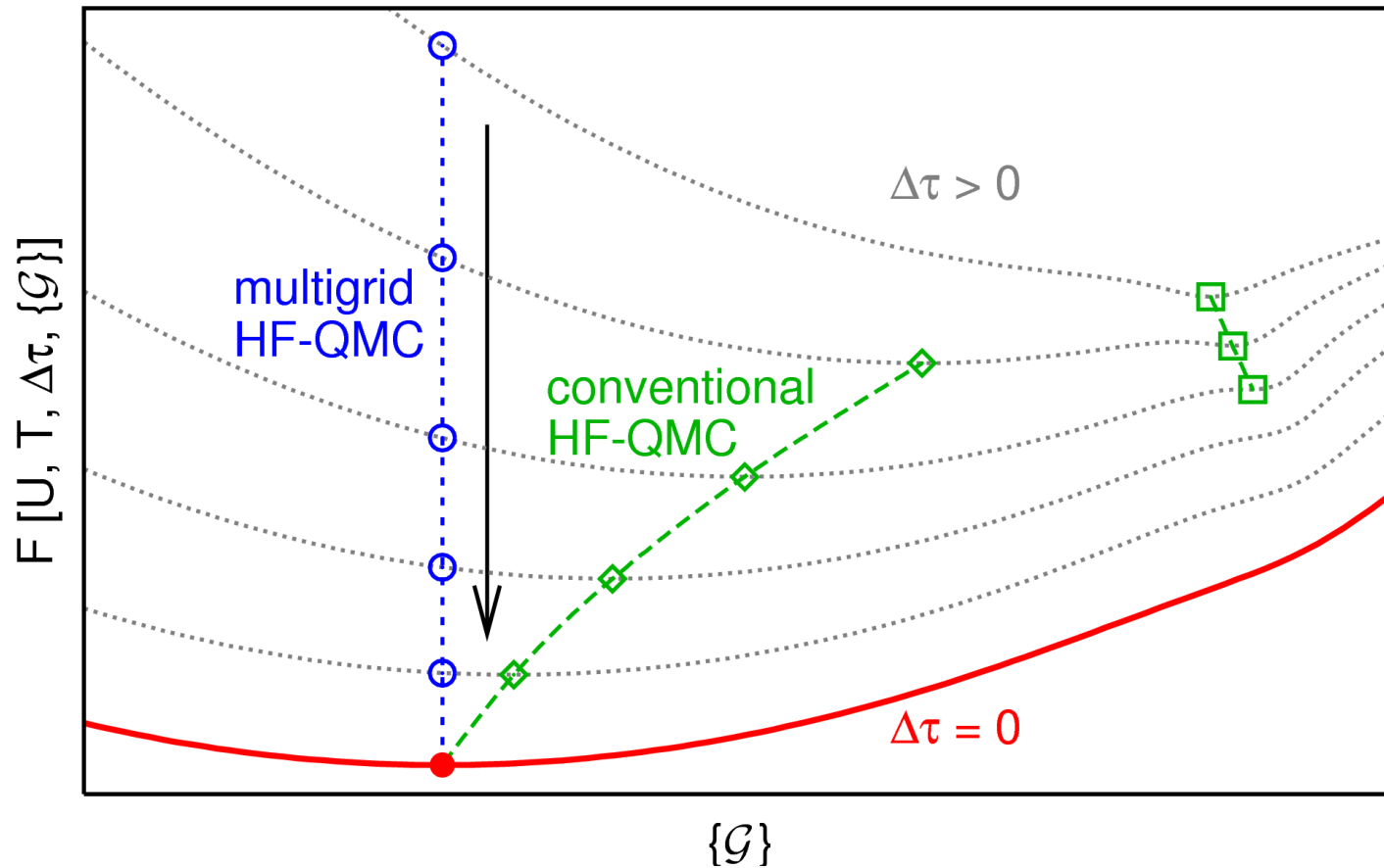
(b) *a posteriori* extrapolation of selected observables



(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

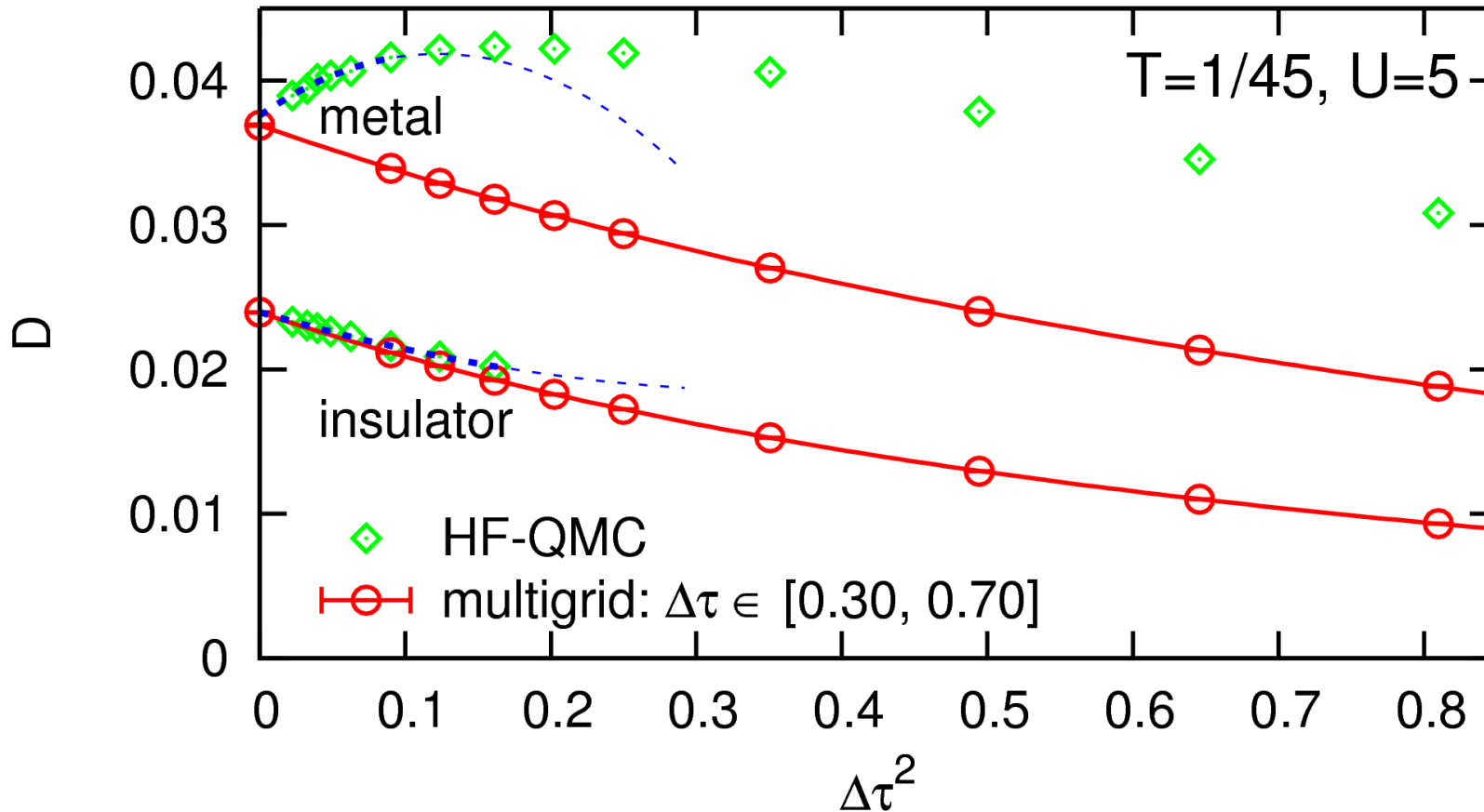


Conventional Hirsch-Fye QMC: DMFT fixed point shifts with  $\Delta\tau$

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

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

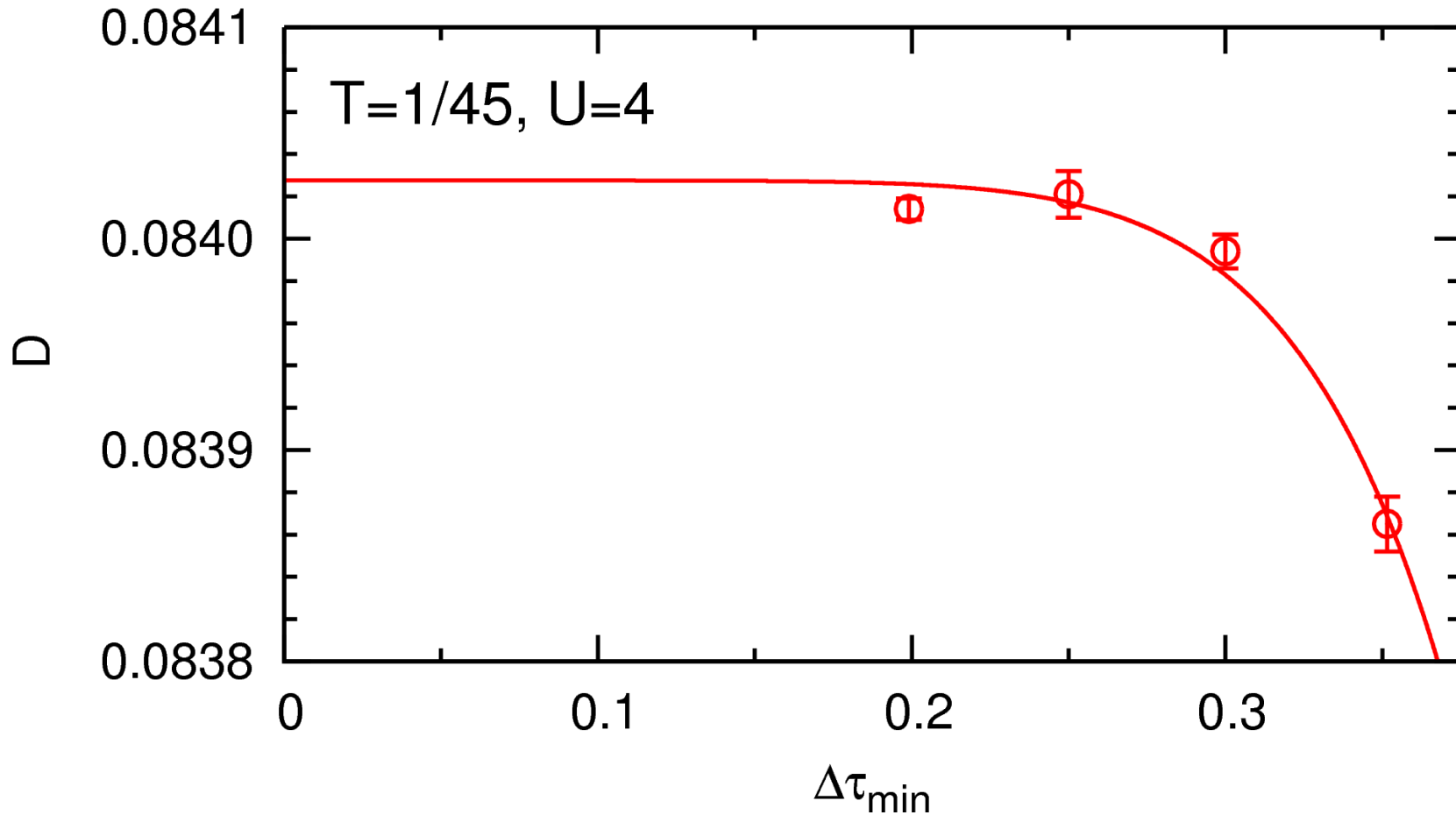
# Comparison: double occupancy $D = \langle n_{i\uparrow} n_{i\downarrow} \rangle$ near Mott transition



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

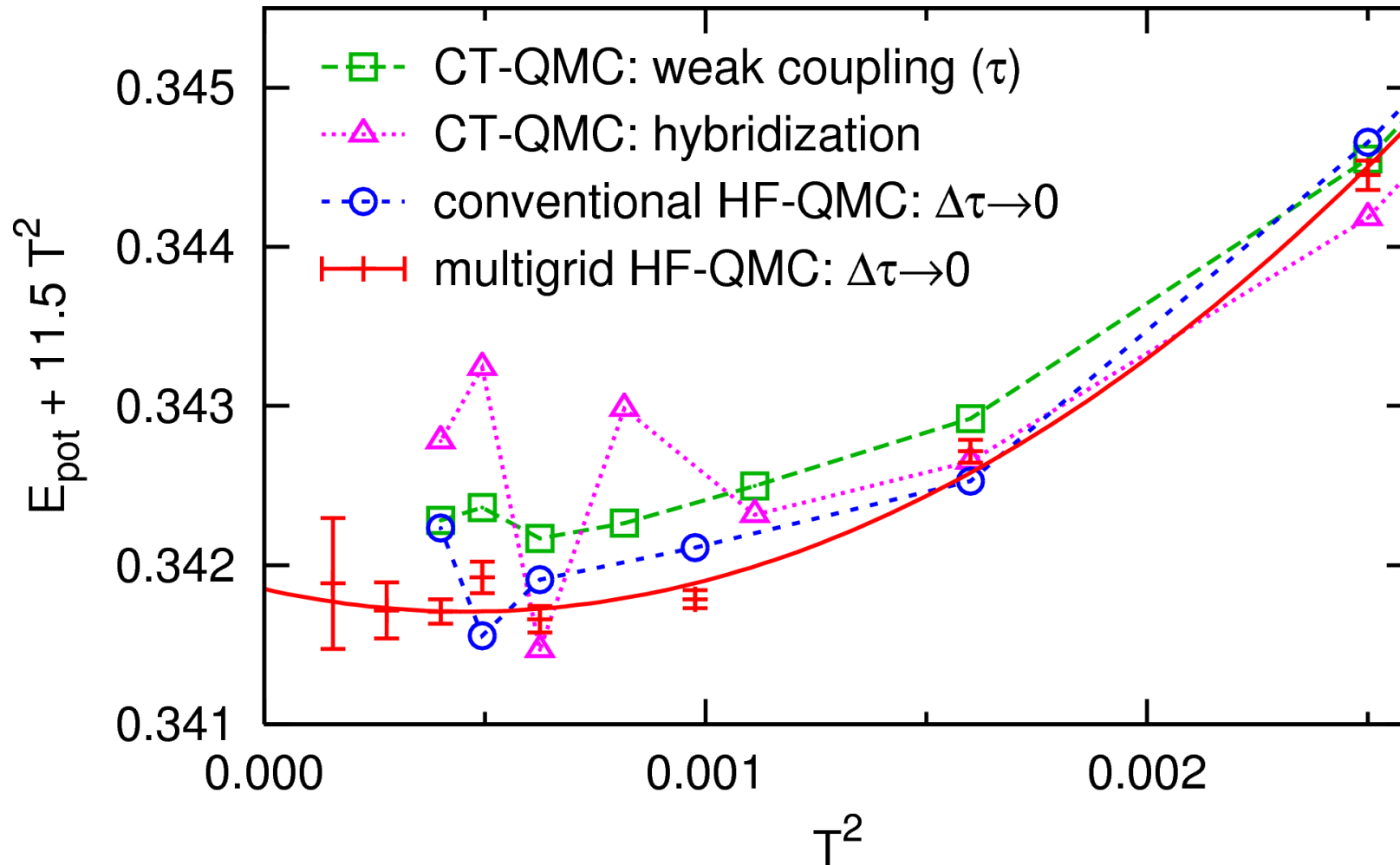
Multigrid HF-QMC: vastly larger useful range of  $\Delta\tau$

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



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

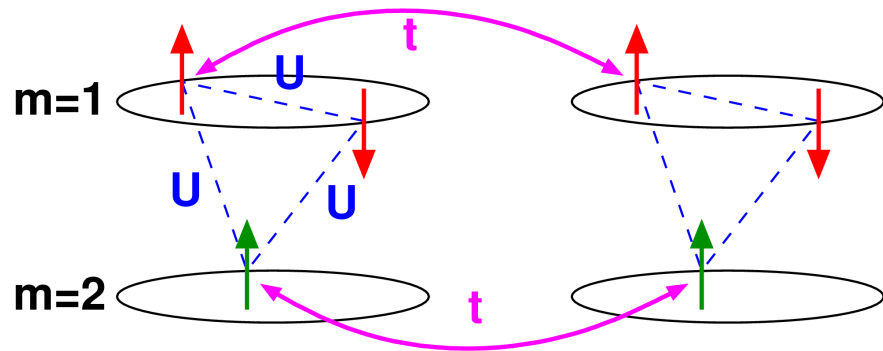
Efficiency: potential energy  $E_{\text{pot}} = UD$  (at  $U = W = 4$ )



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

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

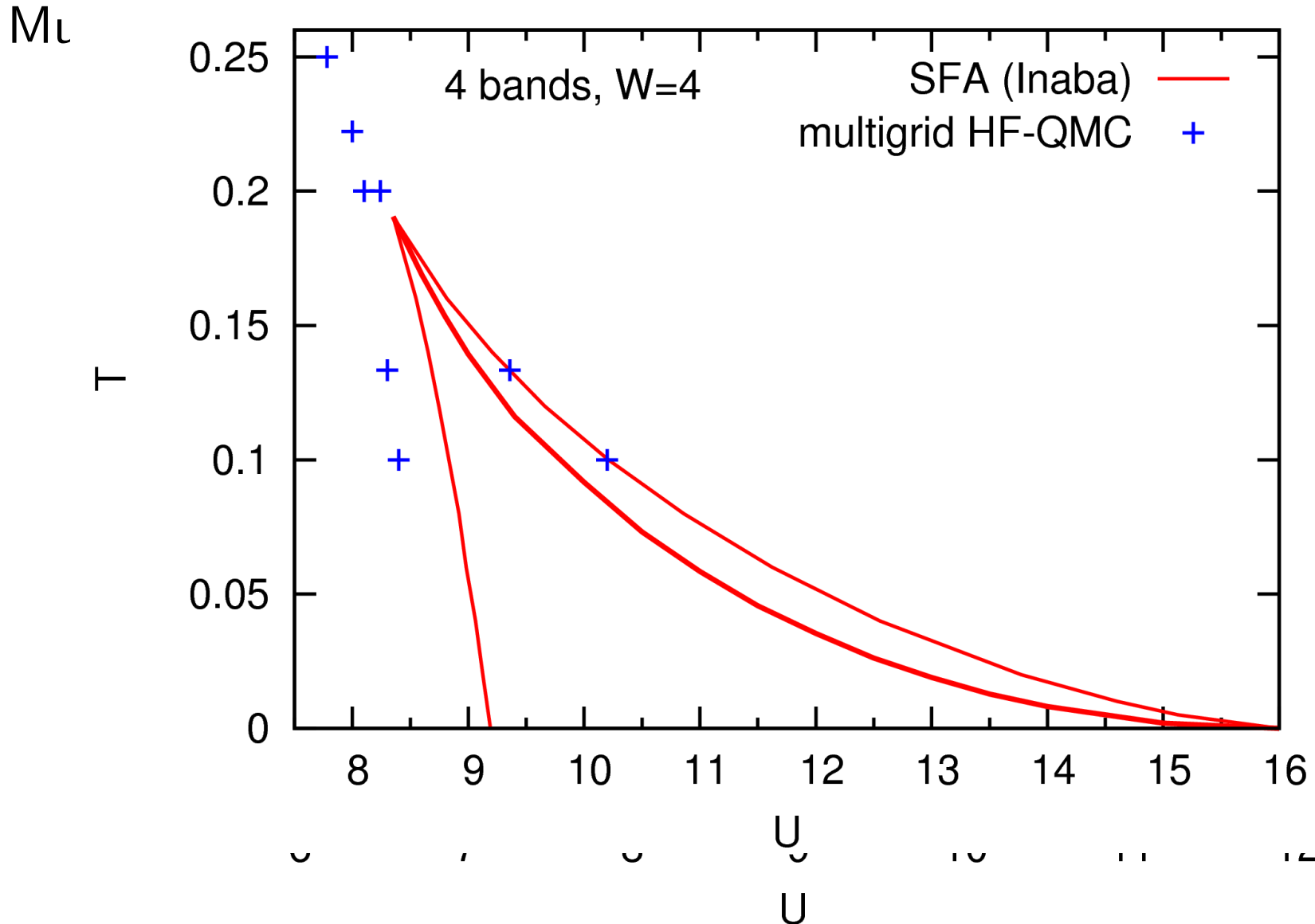


$$\alpha = (m, \sigma), \quad m = 1, \dots, M, \quad \sigma = \uparrow, \downarrow$$

no Hund exchange!

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

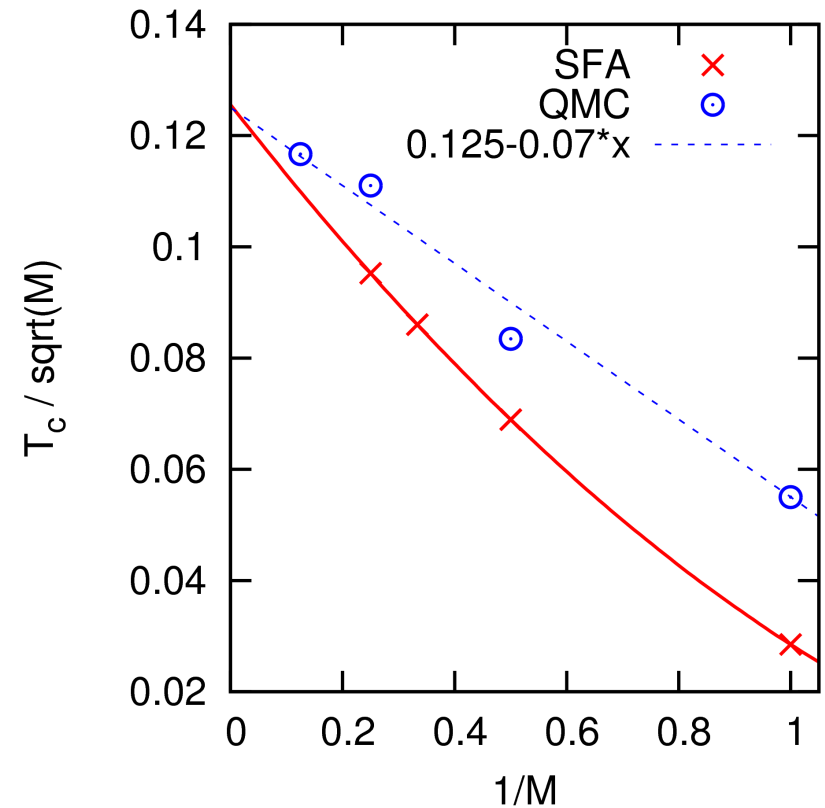
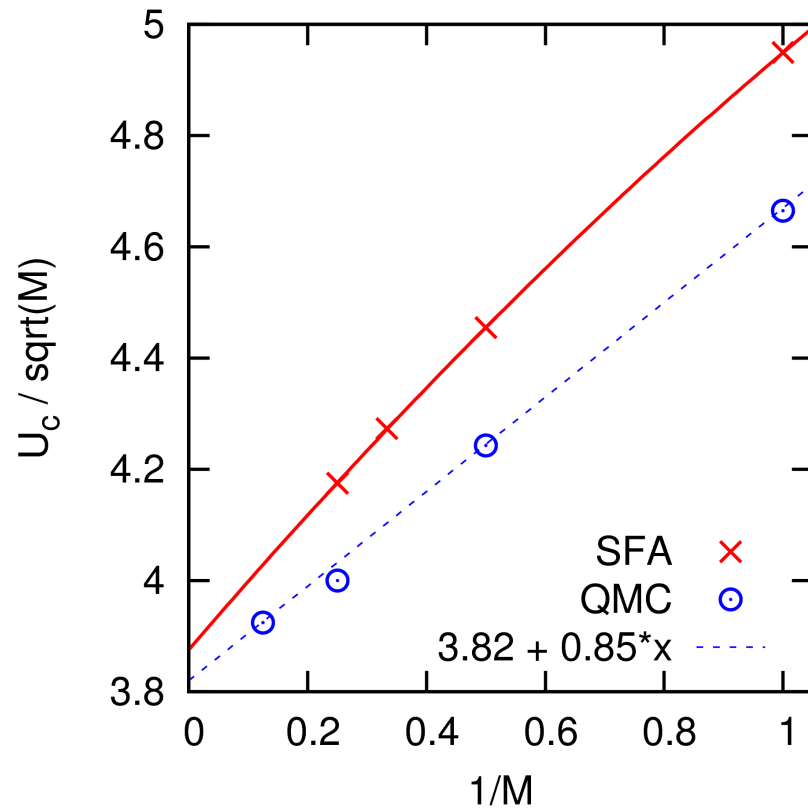
# Mott transition at variable degeneracy $SU(2M)$ : 4-band case



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!

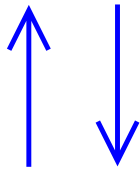
$\Rightarrow$  Phase diagram for arbitrary  $M$

# Beyond electronic systems : Fermions with arbitrary spin multiplicity

## Condensed matter physics

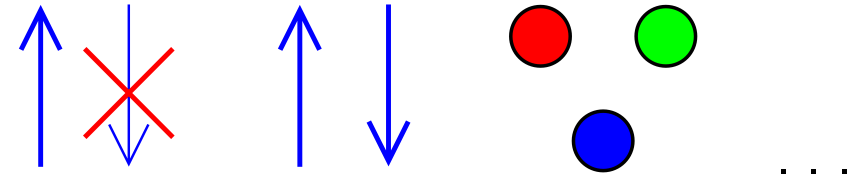
electronic systems

$SU(2)$  spin-rotational symmetry



## Ultracold fermions

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



Example:  $^{40}\text{K}$

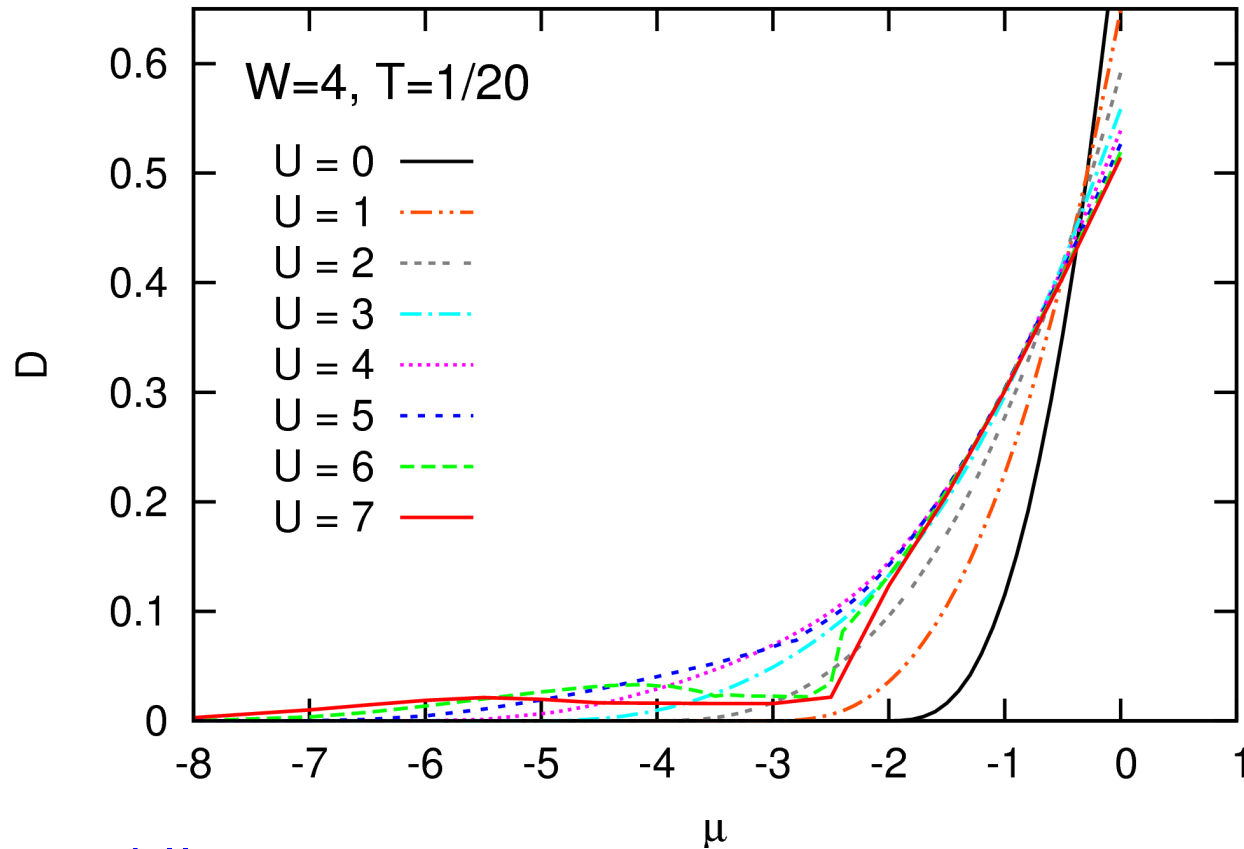
$|F = 9/2, m_F = -5/2, -7/2, -9/2\rangle$

[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

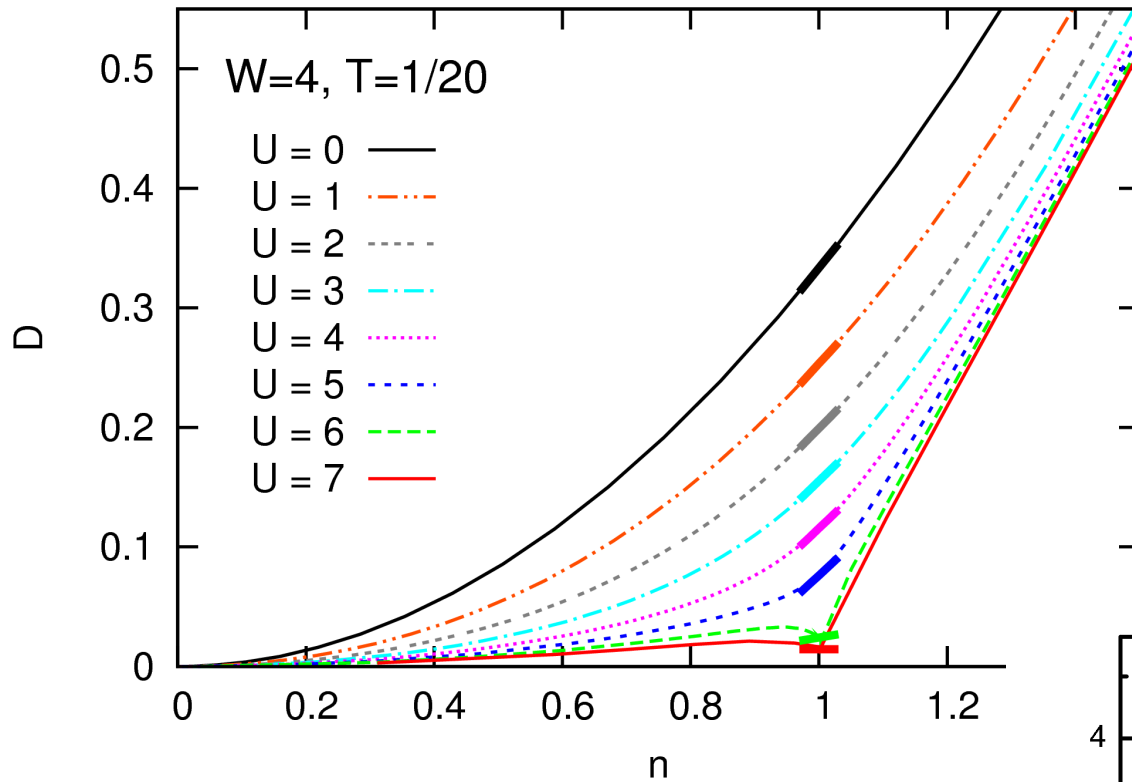
# 3-spin/ flavor system in paramagnetic phase



Density vs. filling  
Double occupancy vs. filling

Plateaus: incompressible Mott phase (for  $U \gtrsim 6$ )  
Here mostly density effects

not at half-filling!



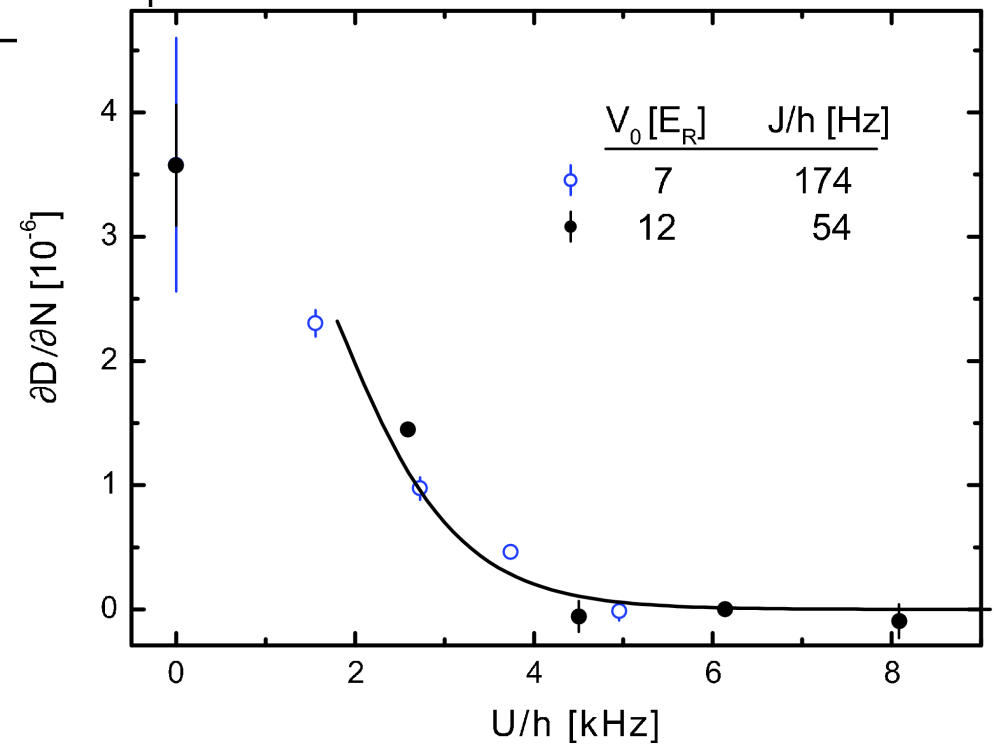
3-spin/3-flavor system:

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

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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

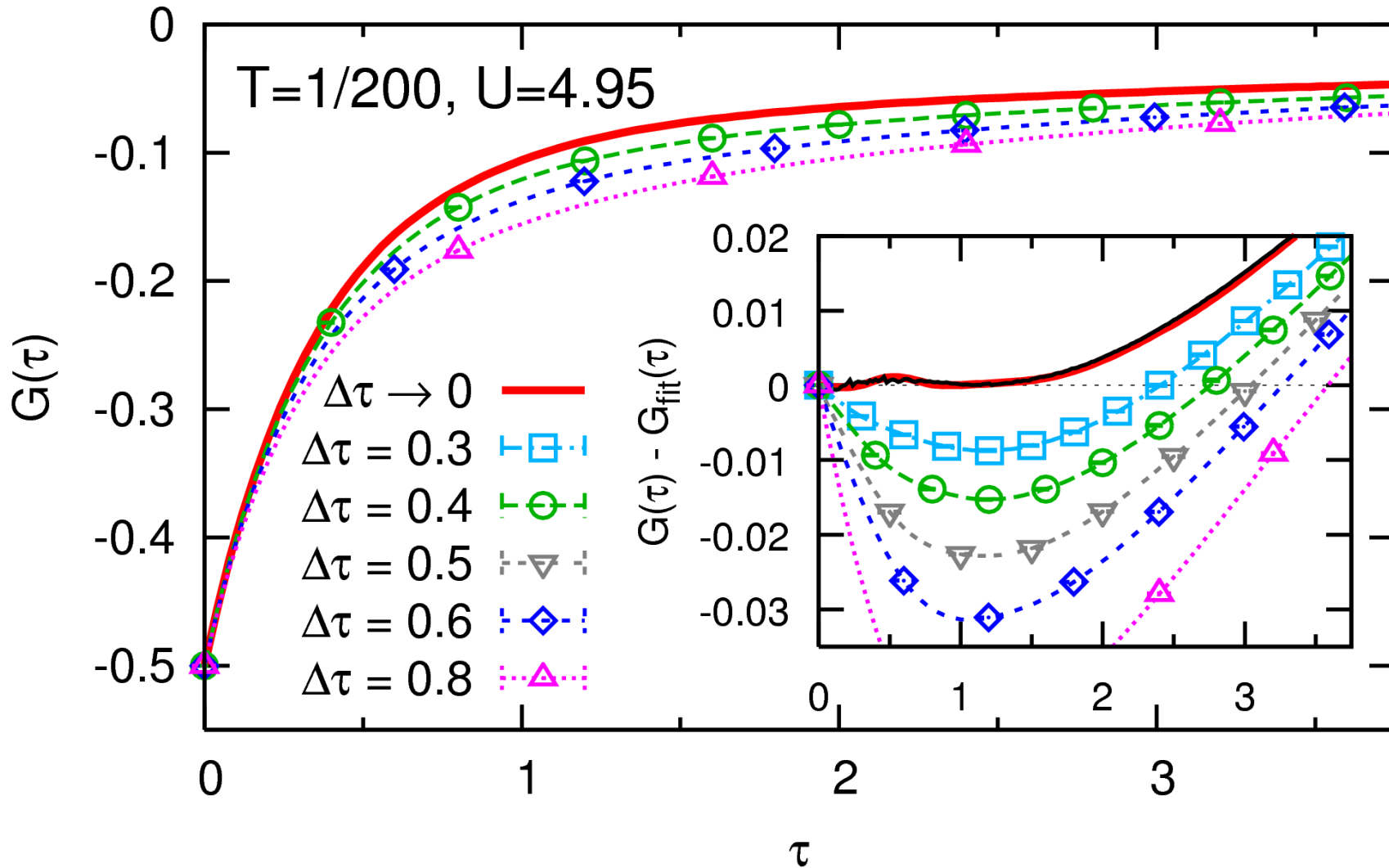
Not shown: unbiased spectra, LDA+DMFT, Superlinear MPI + OpenMP scaling

New project: real-space DMFT+QMC for ultracold atom clouds on optical lattices

**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)

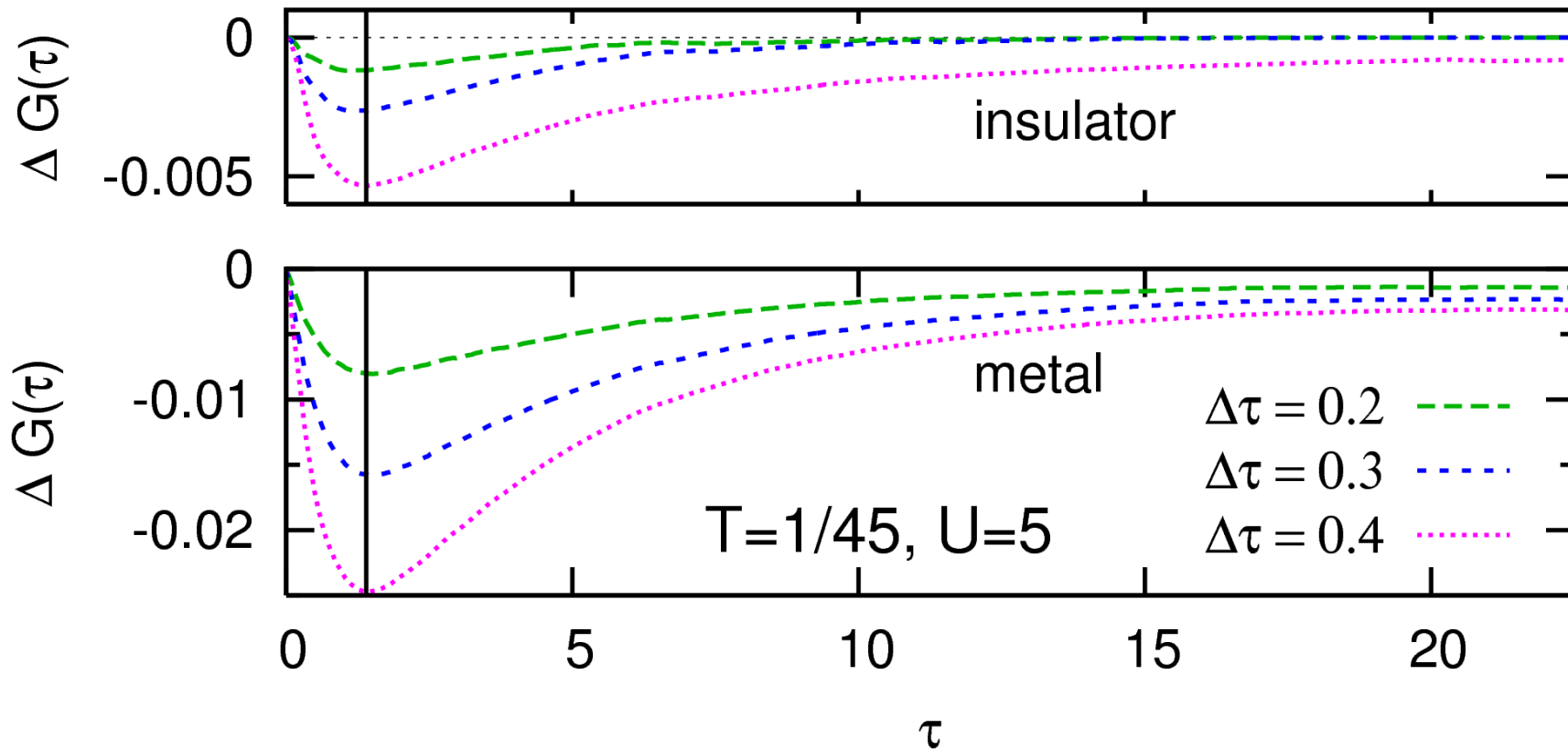
# Illustration: interpolation and extrapolation of Green functions



[NB, arXiv:0712.1290]

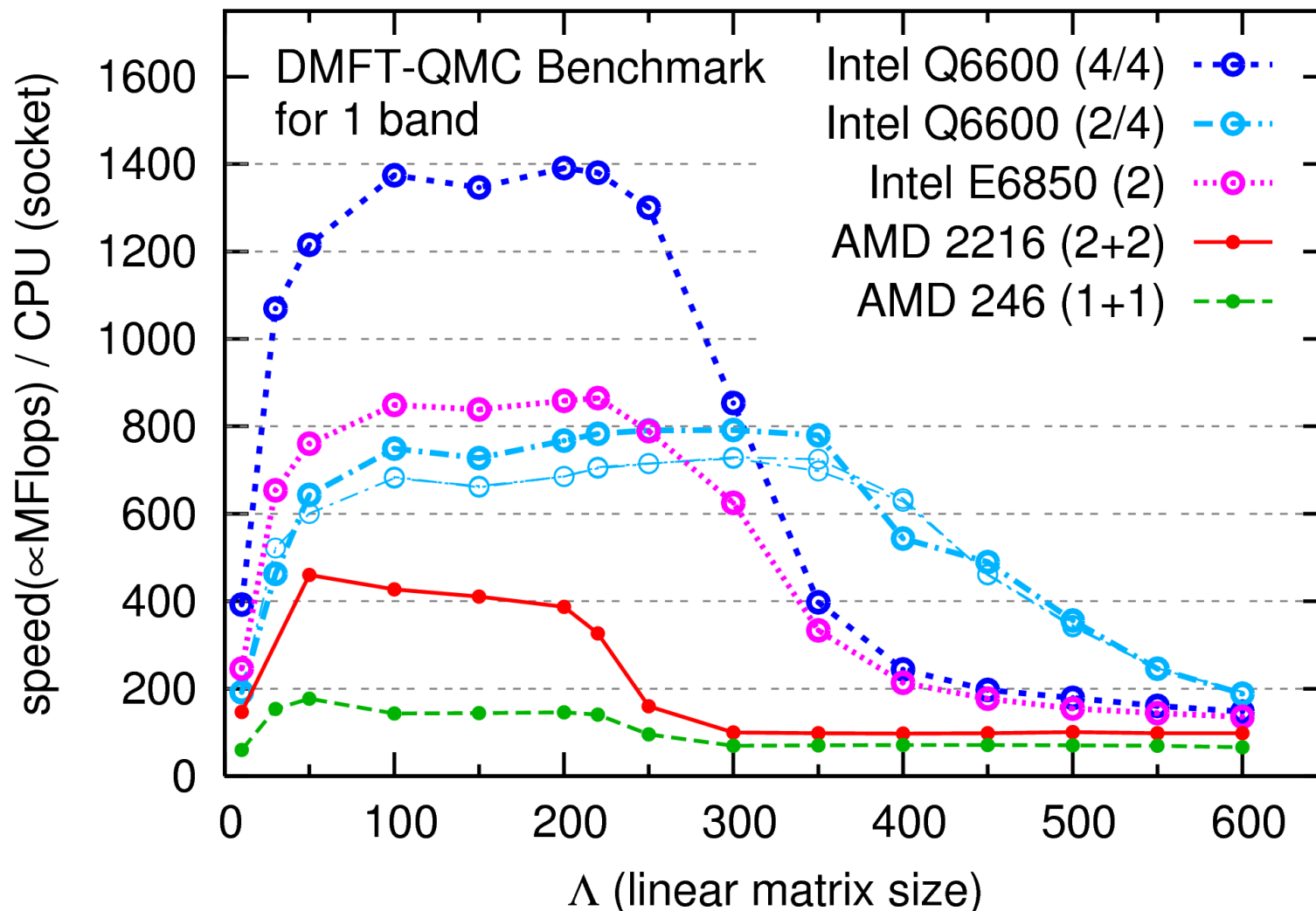
Excellent agreement with hybridization expansion CT-QMC [Werner et al., PRL (2006)]

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



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

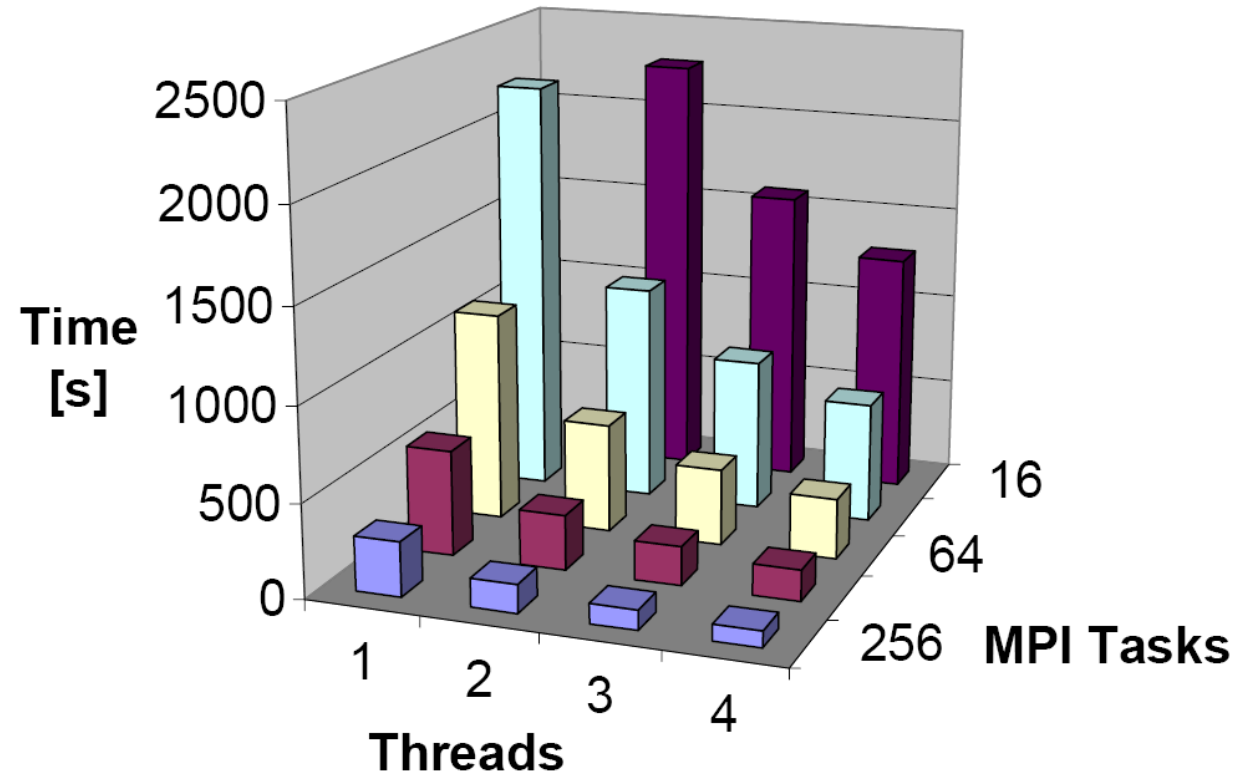
# Benchmarks



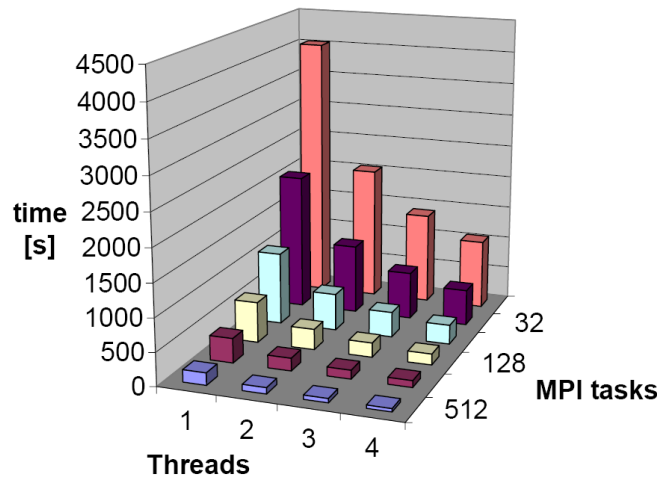
HF-QMC profits strongly from modern large-cache architectures

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

## DMFT-QMC L=200 SMP JuGene



DMFT-QMC L=400 JUGENE



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

# Superlinear scaling on JUMP

