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

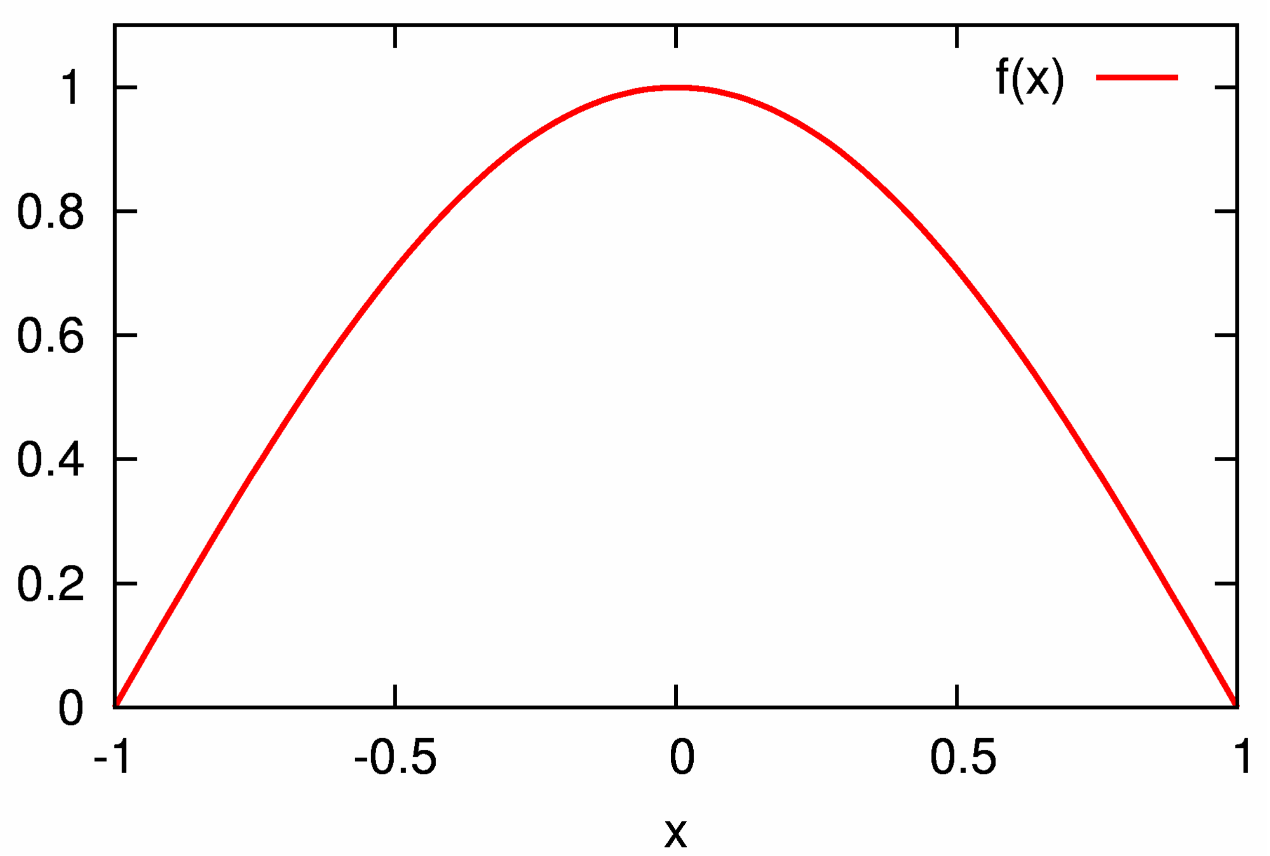
Multigrid Hirsch-Fye quantum Monte Carlo algorithm

Applications: spectral-weight transfer, specific heat

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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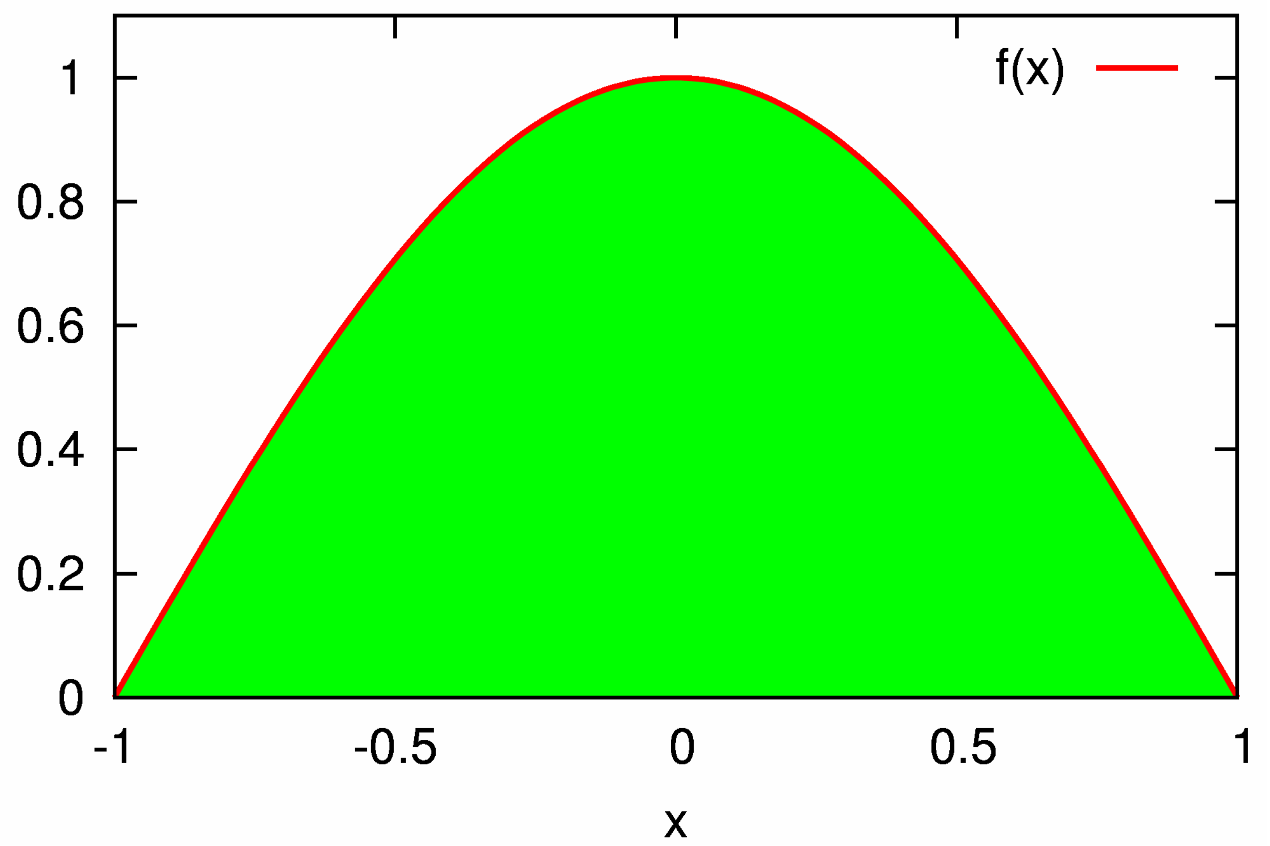

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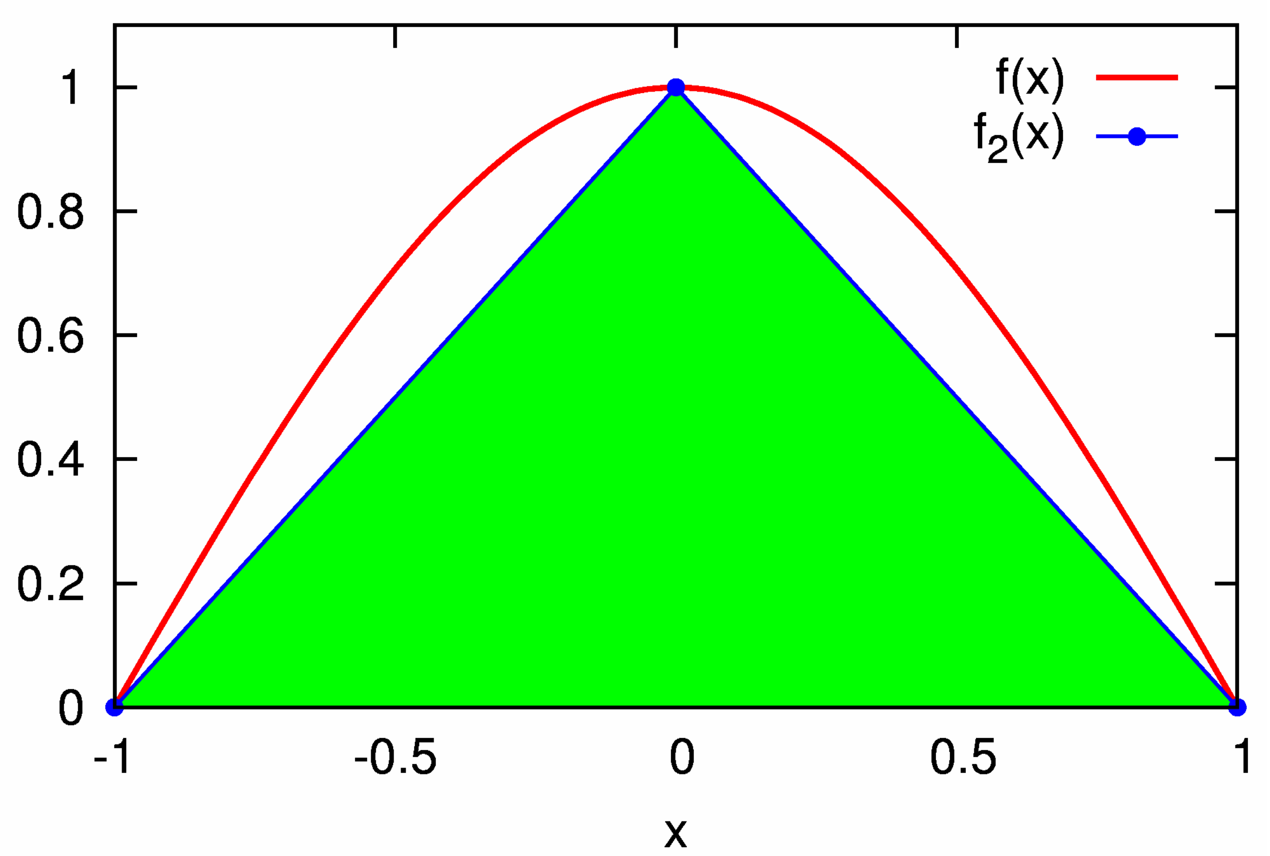

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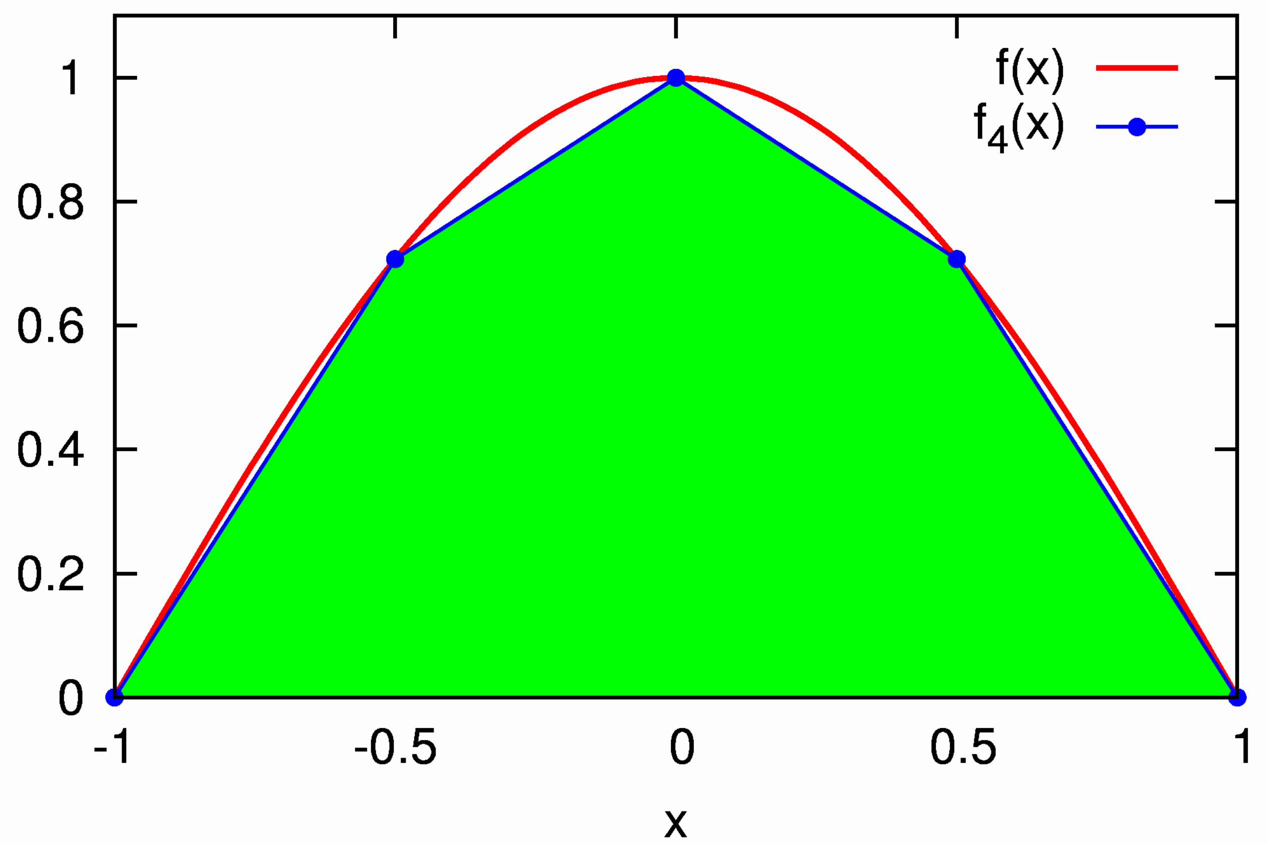

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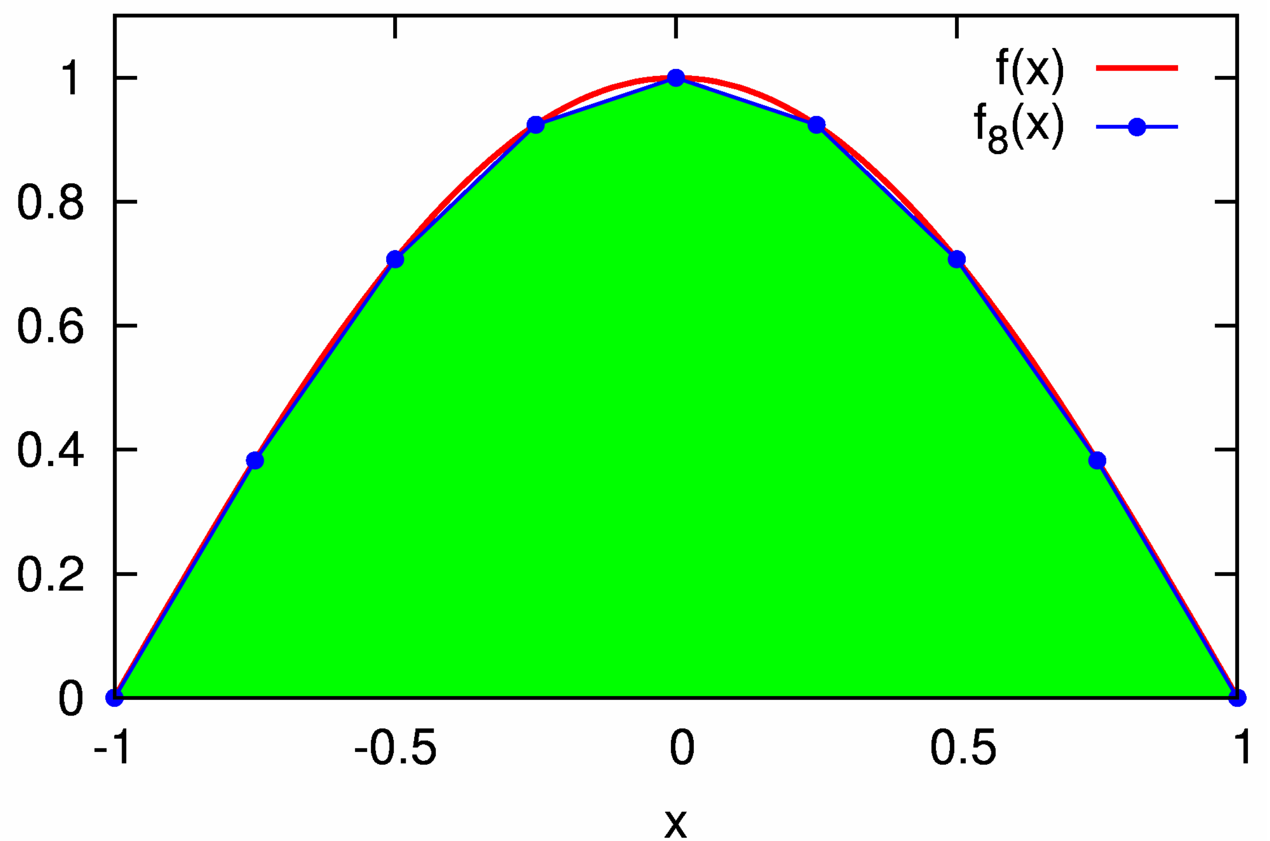

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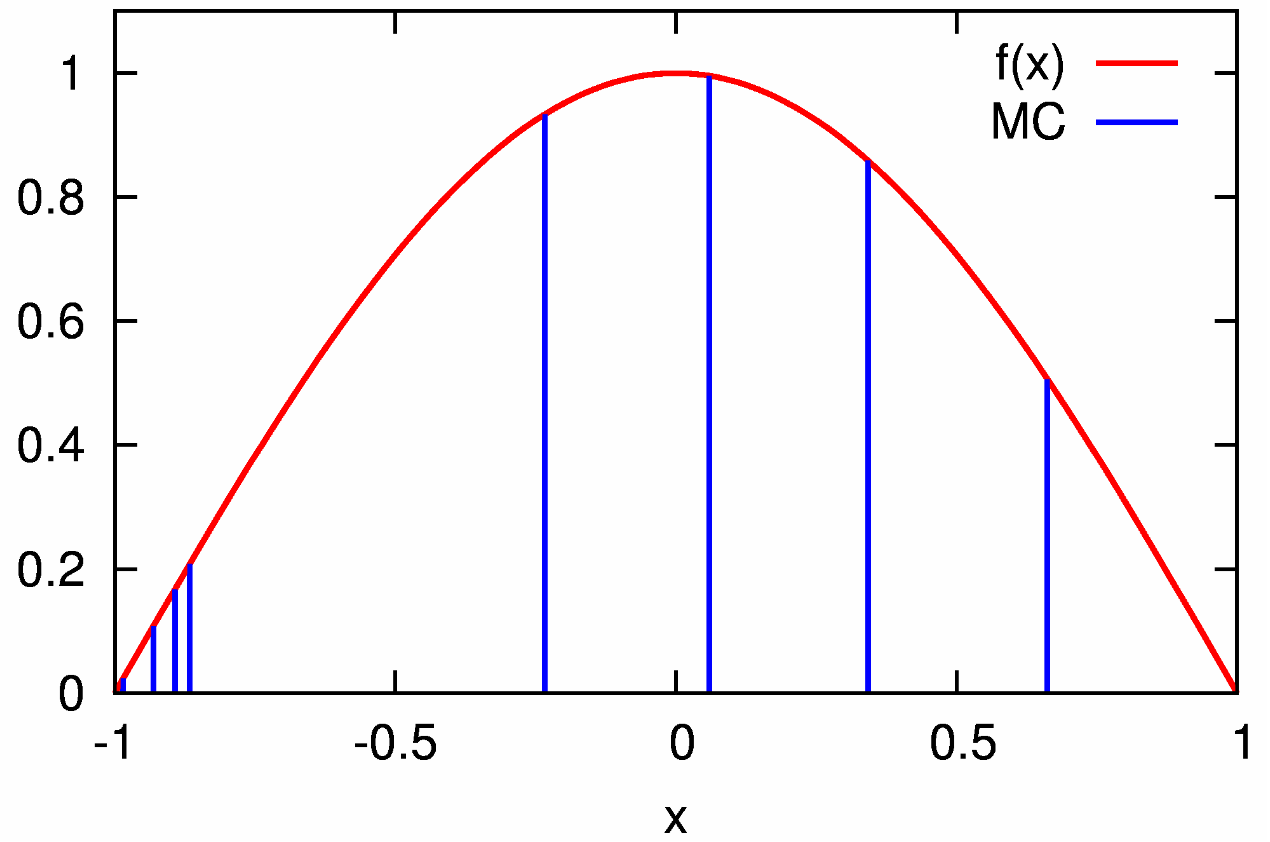

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- discretization
- Monte Carlo

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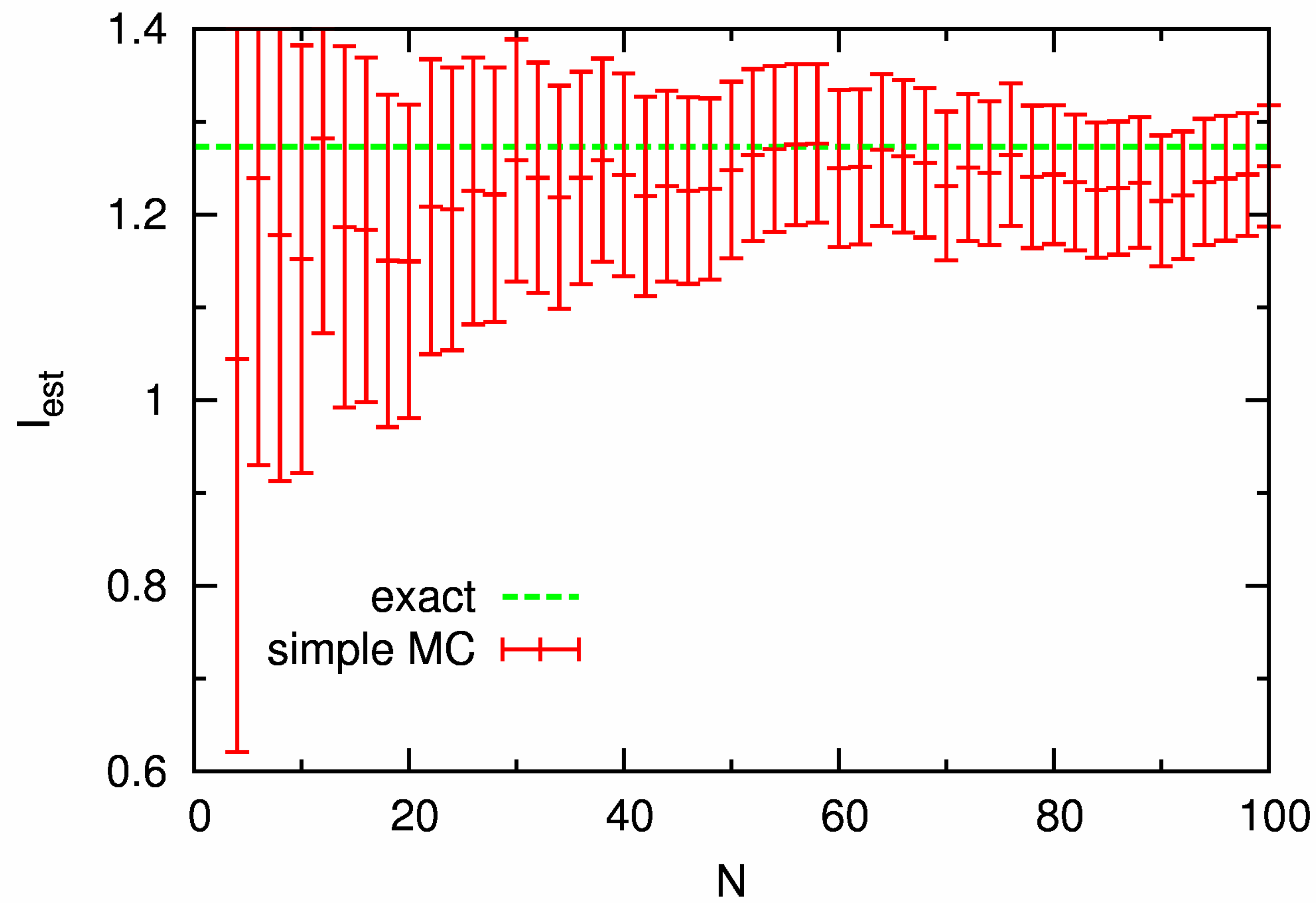

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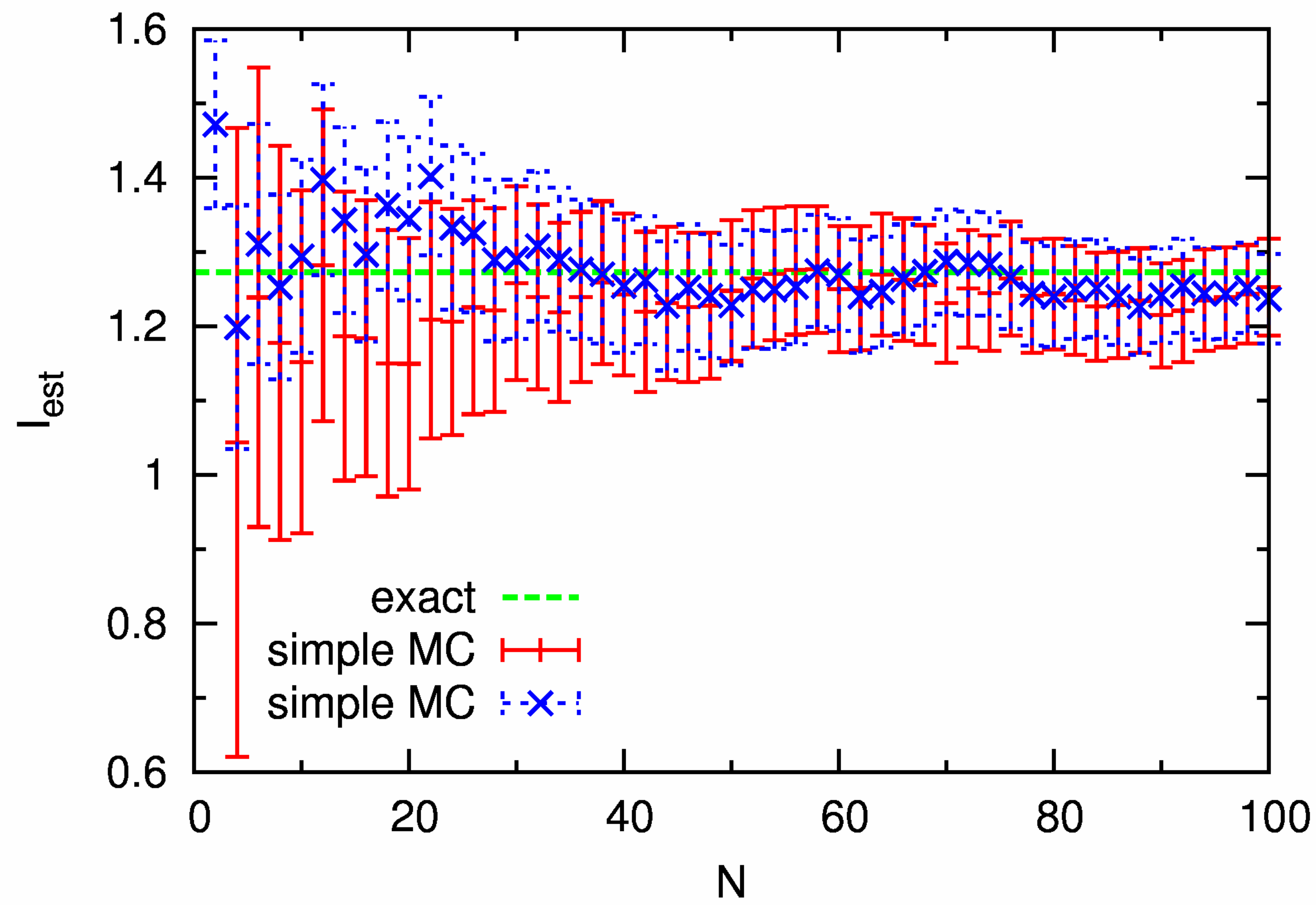

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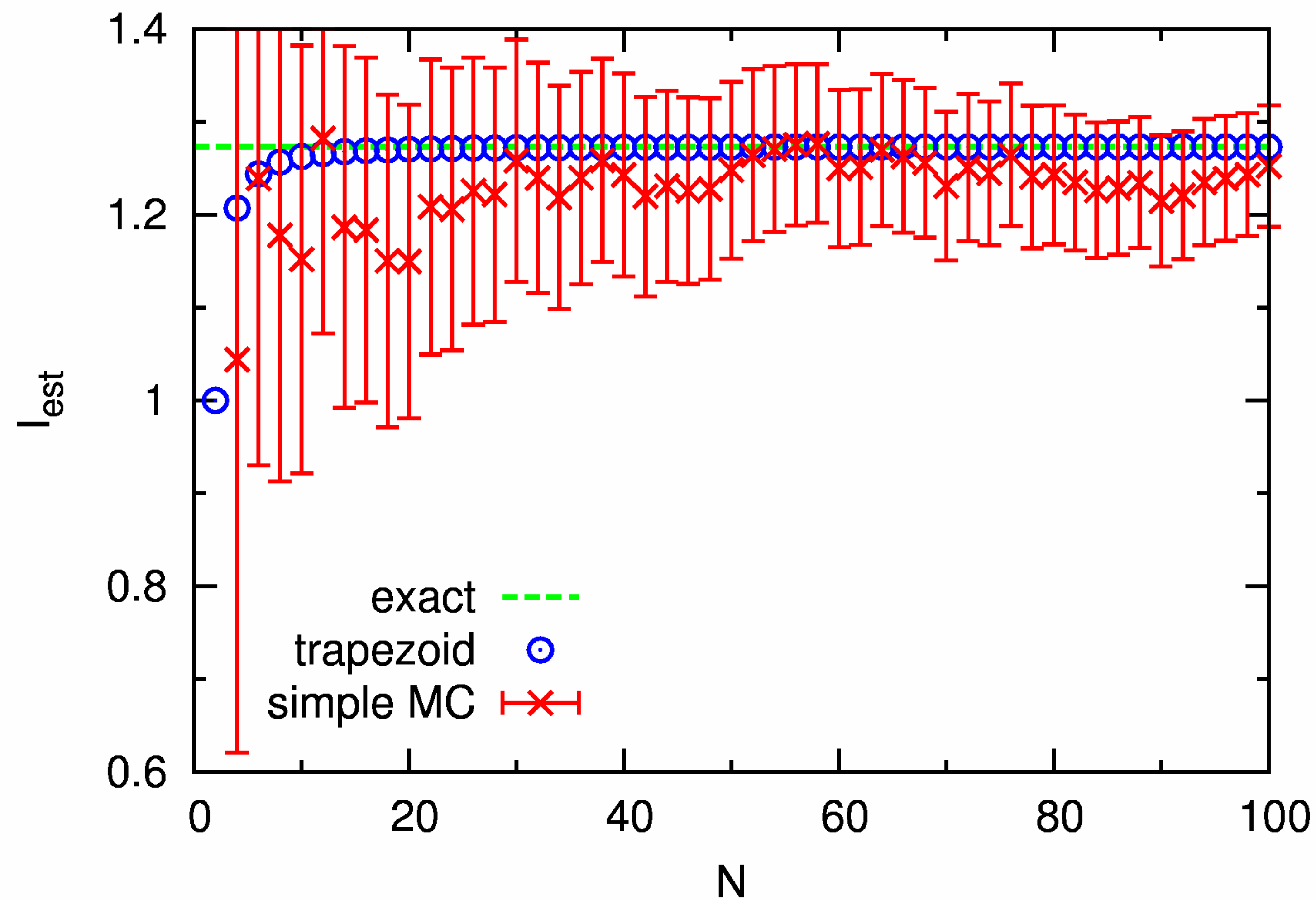

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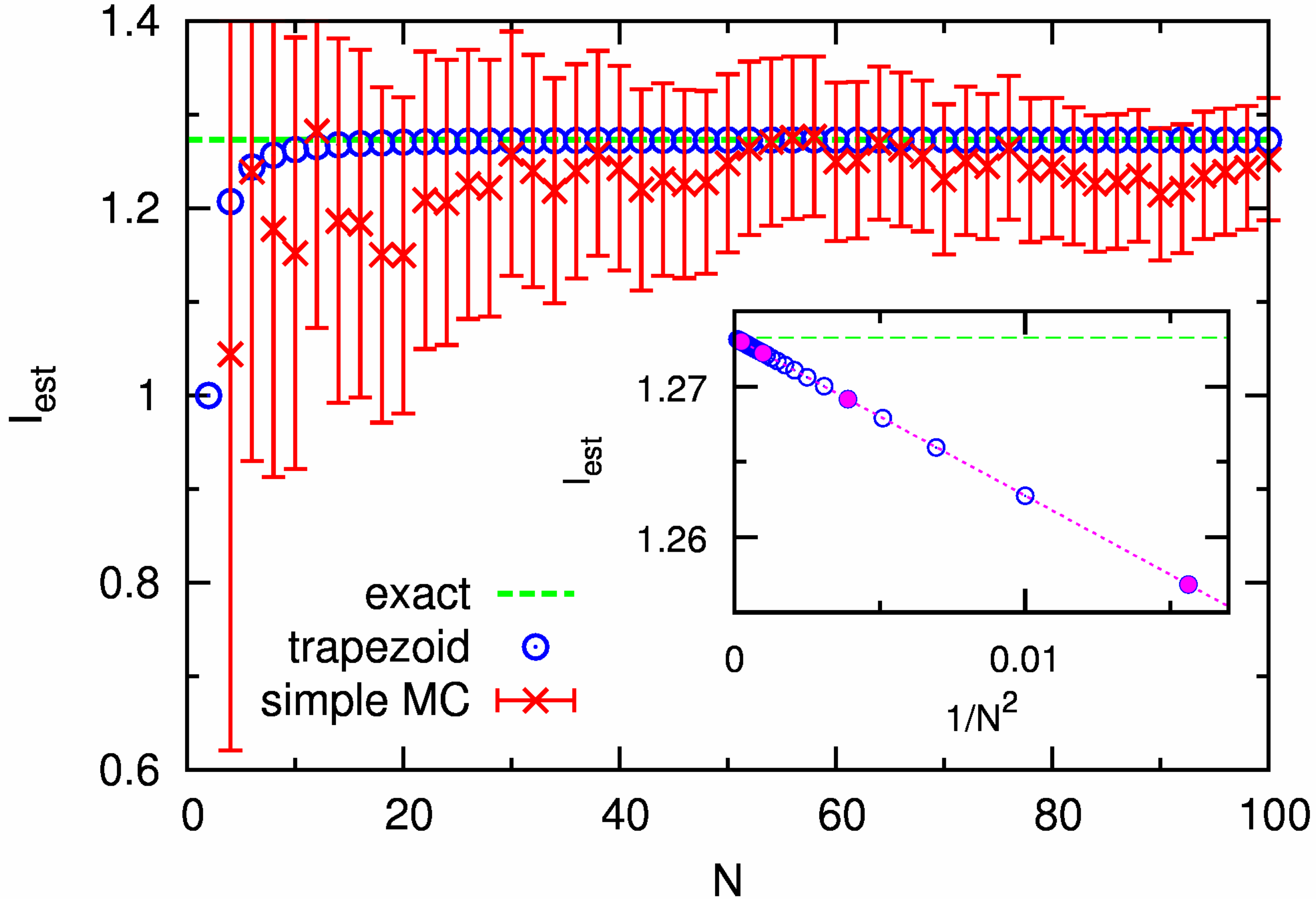

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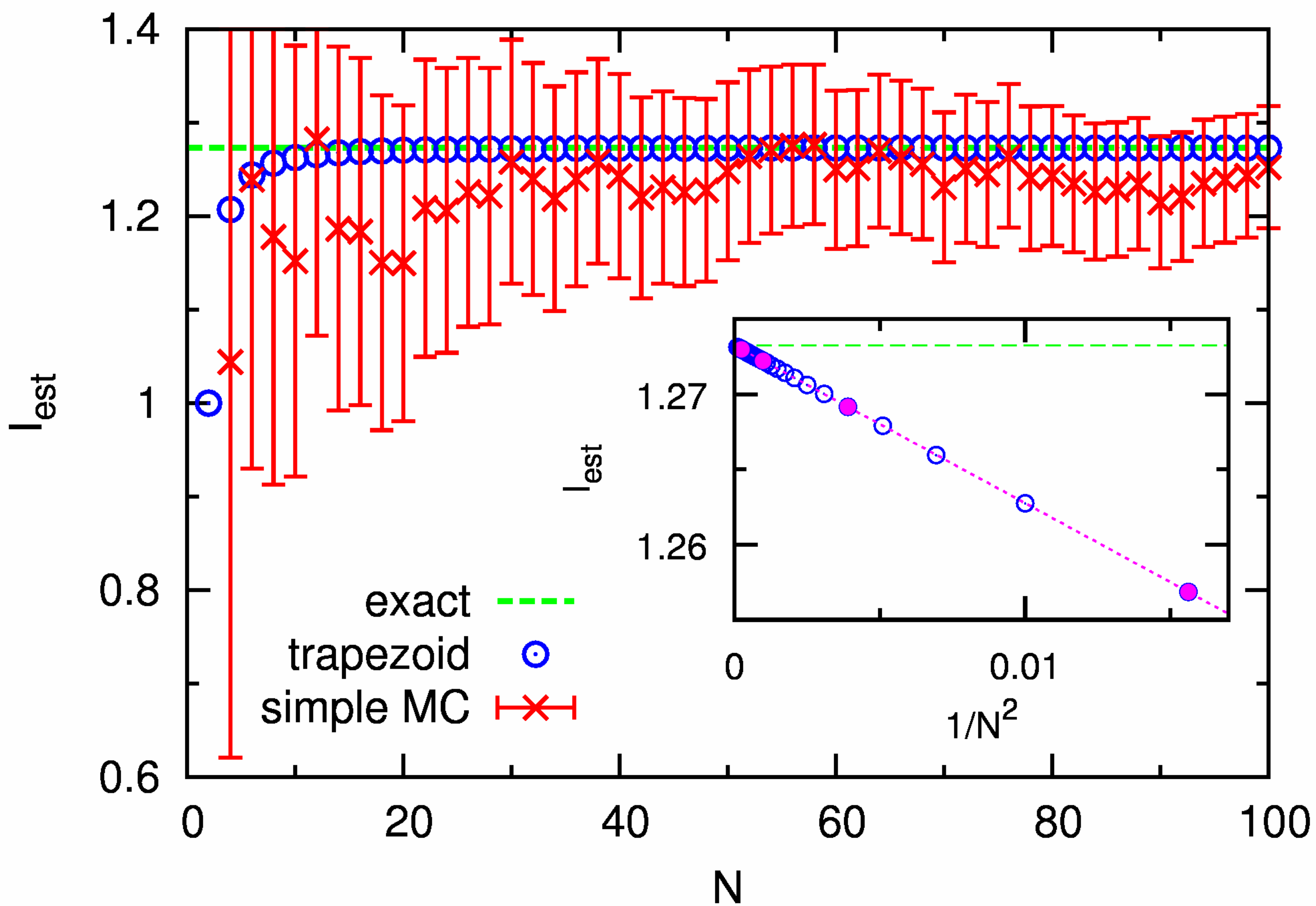
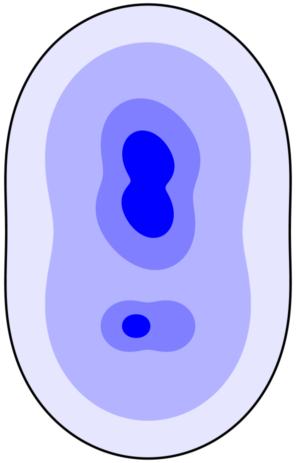


MC results are non-deterministic: only meaningful within statistical error bars!

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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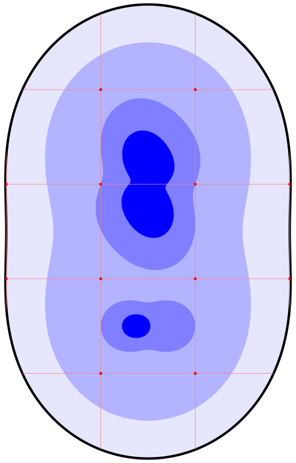

Deterministic: grid + trapezoid rule
$N = V/(\Delta x)^d$ measurements

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

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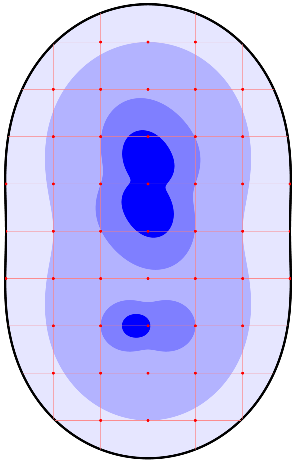

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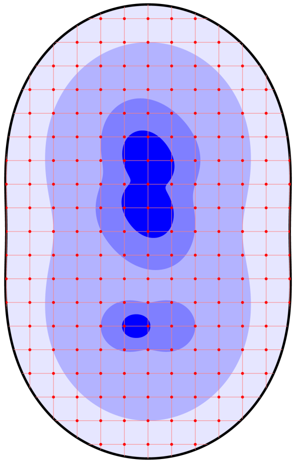

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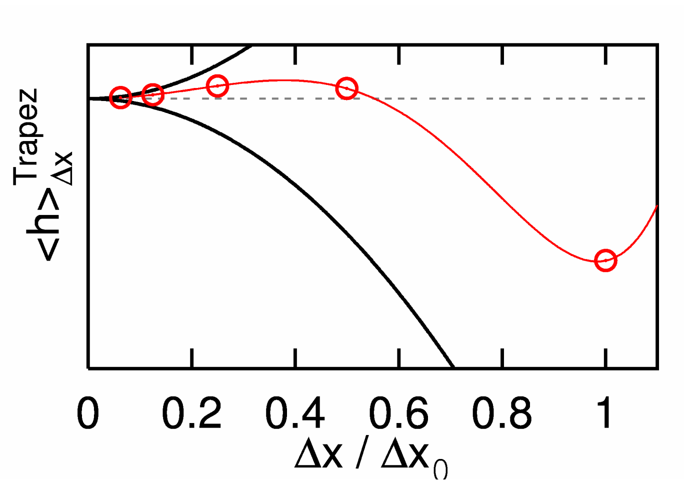

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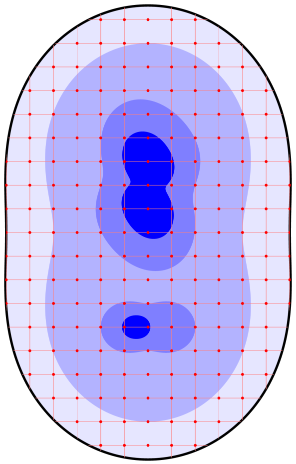

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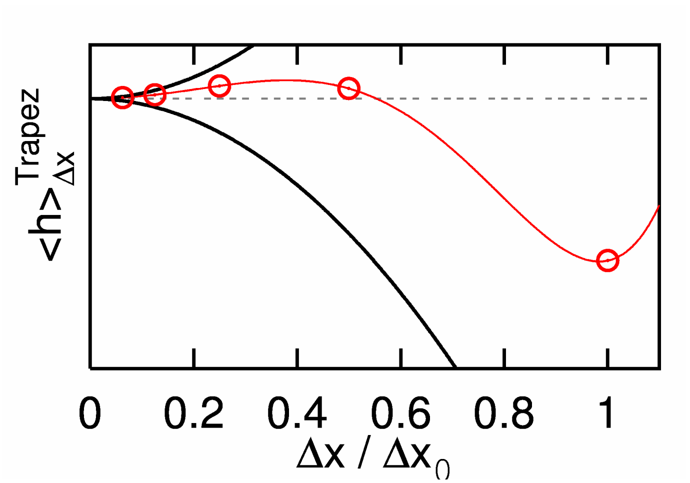
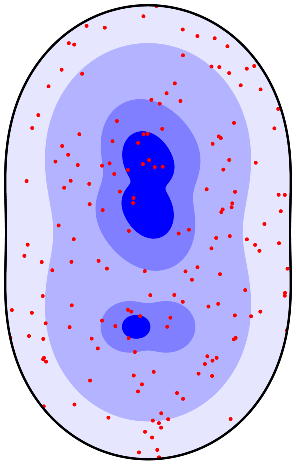


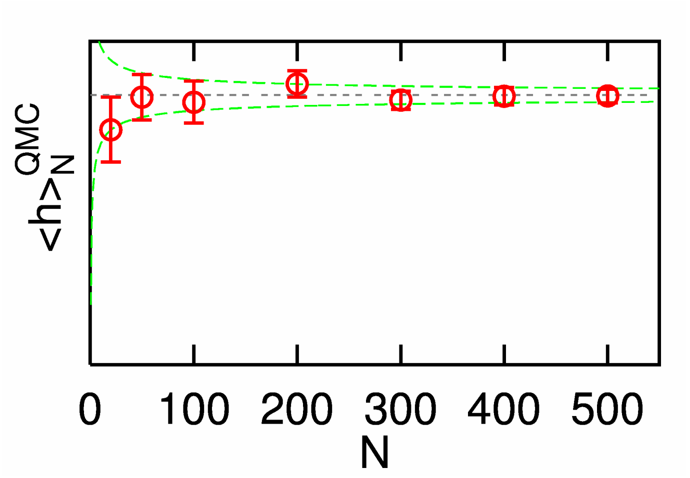


Stochastic: simple Monte-Carlo

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

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

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



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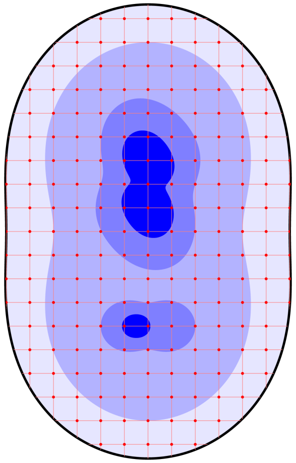

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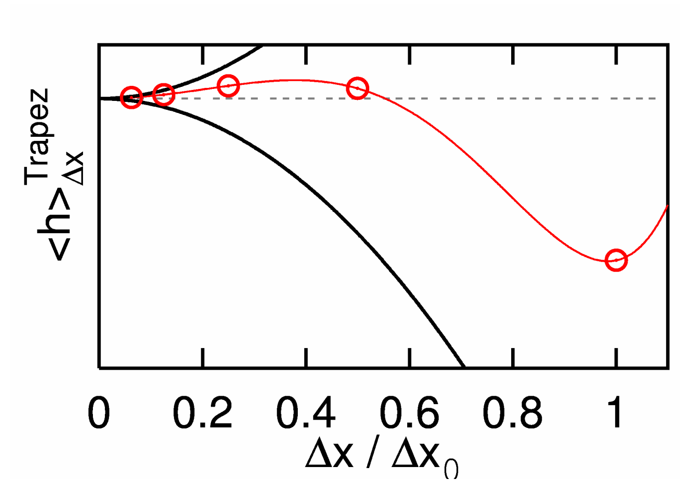

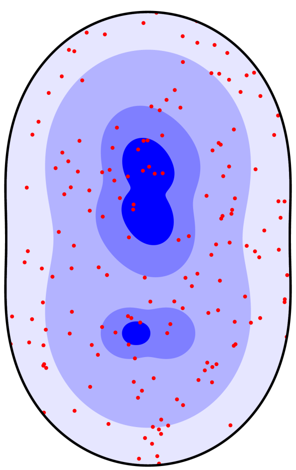

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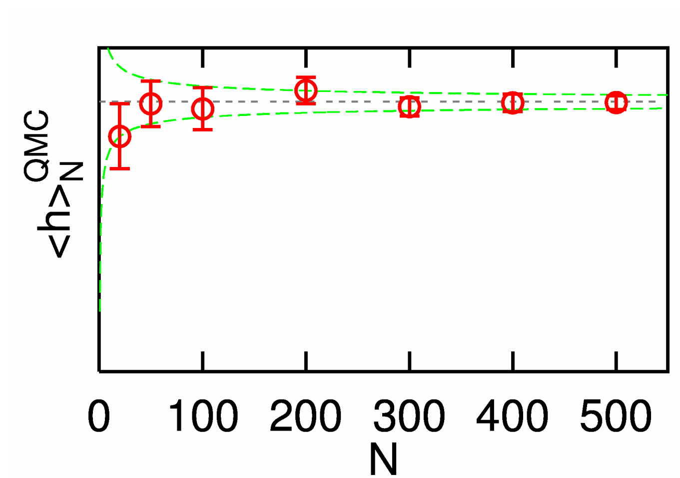
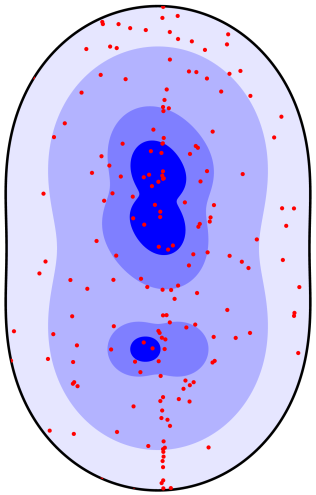


Central limit theorem

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.

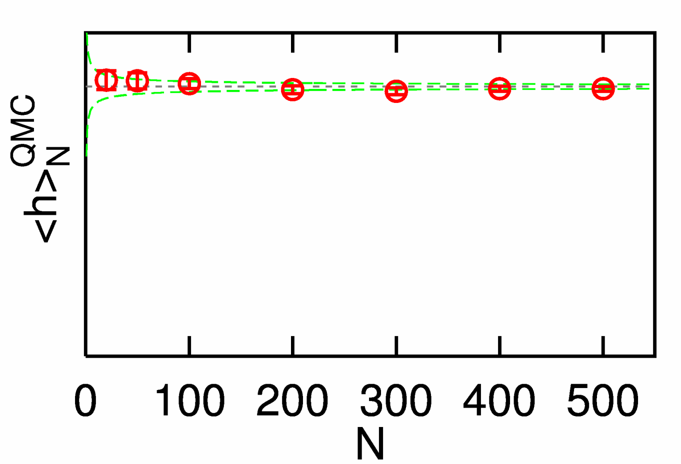


factorization: $h(\vec{x}) = p(\vec{x})\, o(\vec{x})$;

$p(\vec{x})$ 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

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

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

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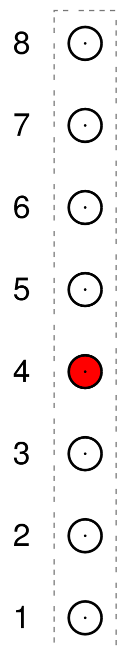
Solution: approach target probability distribution by random walk (e.g.: 8 states)



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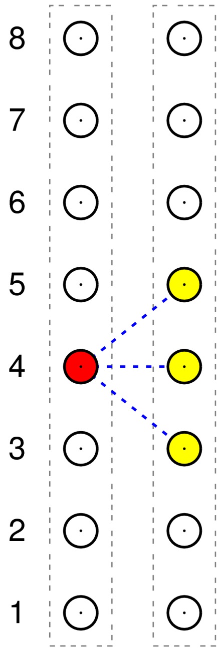

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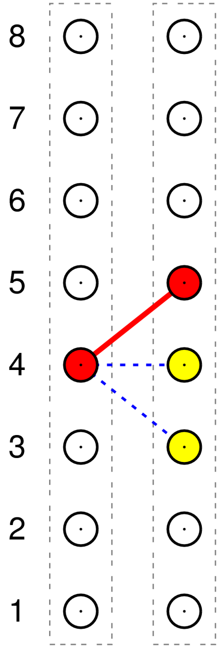

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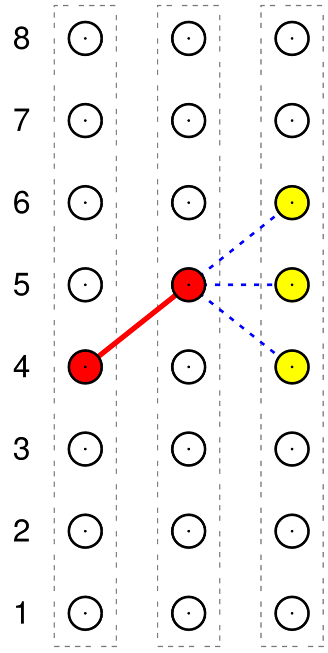

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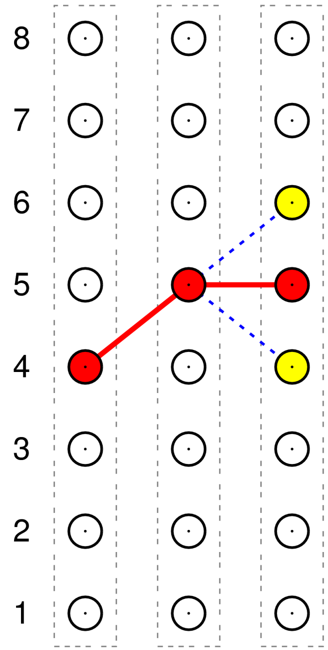

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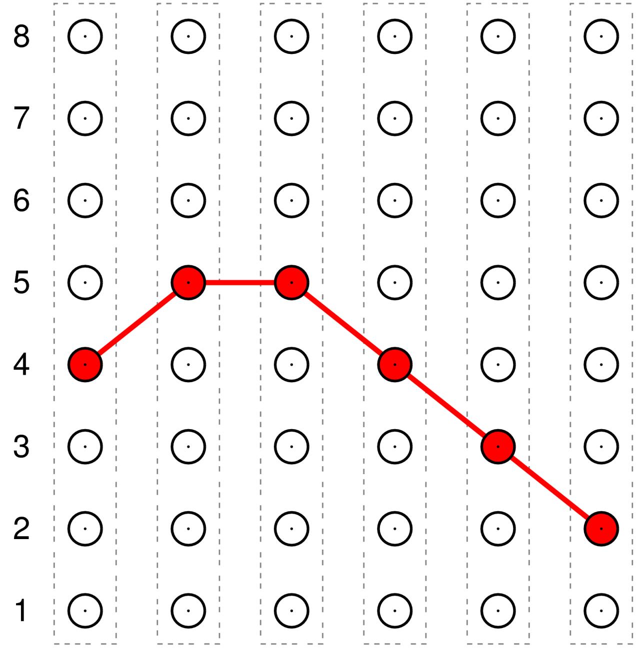

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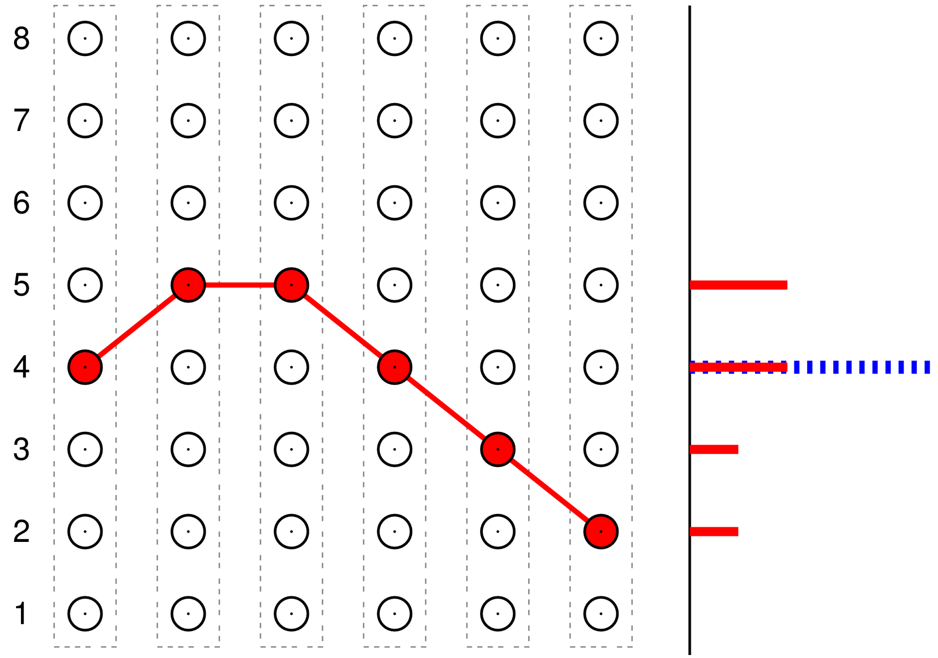

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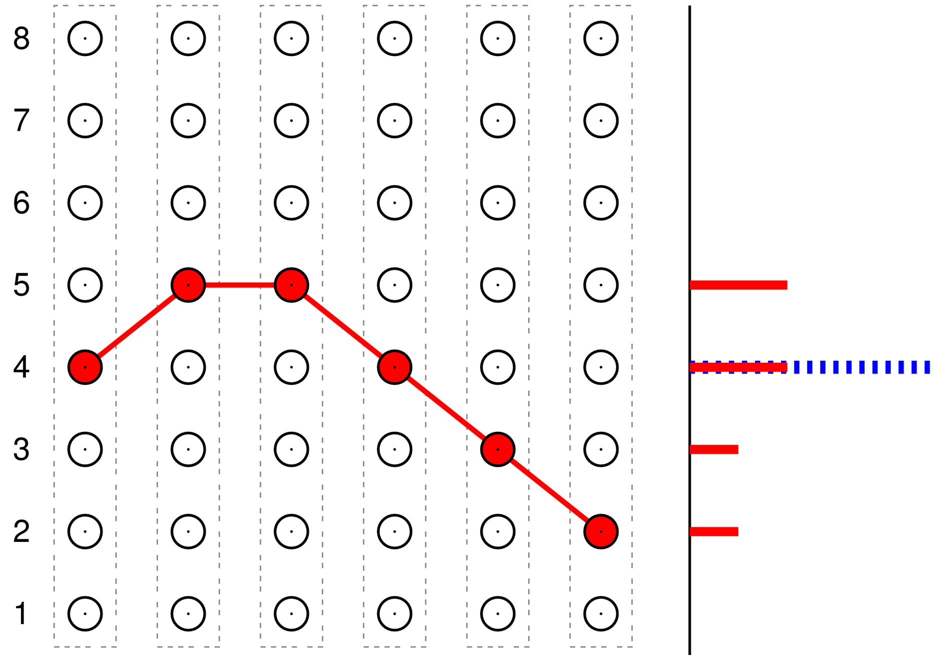

Ergodicity and detailed balance

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

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

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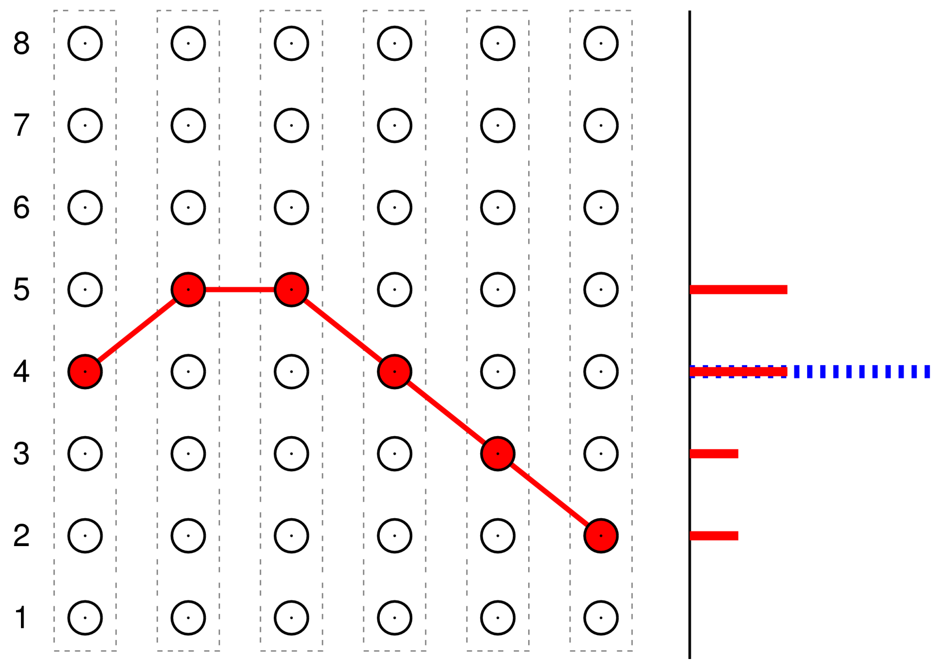

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Favorite choice: Metropolis rule

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

From the configurations of a long Markov Monte Carlo run, observables are estimated as

$$\langle O \rangle = \frac{\sum_i \tilde{p}_i O_i}{\sum_i \tilde{p}_i} \quad \longrightarrow \quad \langle O \rangle \approx \frac{1}{N} \sum_{n=N_0+1}^{N_0+N} O_{i_n}; \qquad \langle (\Delta O)^2 \rangle \propto \frac{\mathrm{var}\{O\}}{N}$$

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+ Precise computation of observable averages $\langle O \rangle$
+ Freedom in choosing transition rules

– Subsequent measurements O_{i_n} become correlated $\rightsquigarrow$ finite autocorrelation time

– Not accessible by construction: partition function $\mathcal{Z}$, free energy F

Important "classical" Monte Carlo application: Ising model

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j; \quad \sigma_i \in \{1, -1\} \equiv \{+, -\} \equiv \{\uparrow, \downarrow\}$$

Model for ferromagnets, "fruit fly" of statistical physics, $\sim$ lattice gas model, . . .

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Ground state: ferromagnetic ($\sigma_i = \sigma_j \; \forall \, i, j$)

Finite-temperature magnetic phase transition in dimensions $d \geq 2$

Exact solutions for $d = 1$ [Bethe, 1935] and $d = 2$ [Onsager, 1944: square lattice]

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Quantum model: discrete states, but trivial eigen basis ($\sim$ classical system)

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Exact solutions for $d = 1$ [Bethe, 1935] and $d = 2$ [Onsager, 1944: square lattice]

Quantum model: discrete states, but trivial eigen basis ($\sim$ classical system)

Natural updates: single-spin flips

$$\begin{matrix} + & + & + & - \\ - & - & - & + \\ - & + & + & - \\ + & + & - & + \end{matrix} \quad \longleftrightarrow \quad \begin{matrix} + & + & + & - \\ - & - & + & + \\ - & + & + & - \\ + & + & - & + \end{matrix}$$

Important "classical" Monte Carlo application: Ising model

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j; \quad \sigma_i \in \{1, -1\} \equiv \{+, -\} \equiv \{\uparrow, \downarrow\}$$

Model for ferromagnets, "fruit fly" of statistical physics, $\sim$ lattice gas model, . . .

Ground state: ferromagnetic ($\sigma_i = \sigma_j \; \forall \, i, j$)

Finite-temperature magnetic phase transition in dimensions $d \geq 2$

Exact solutions for $d = 1$ [Bethe, 1935] and $d = 2$ [Onsager, 1944: square lattice]

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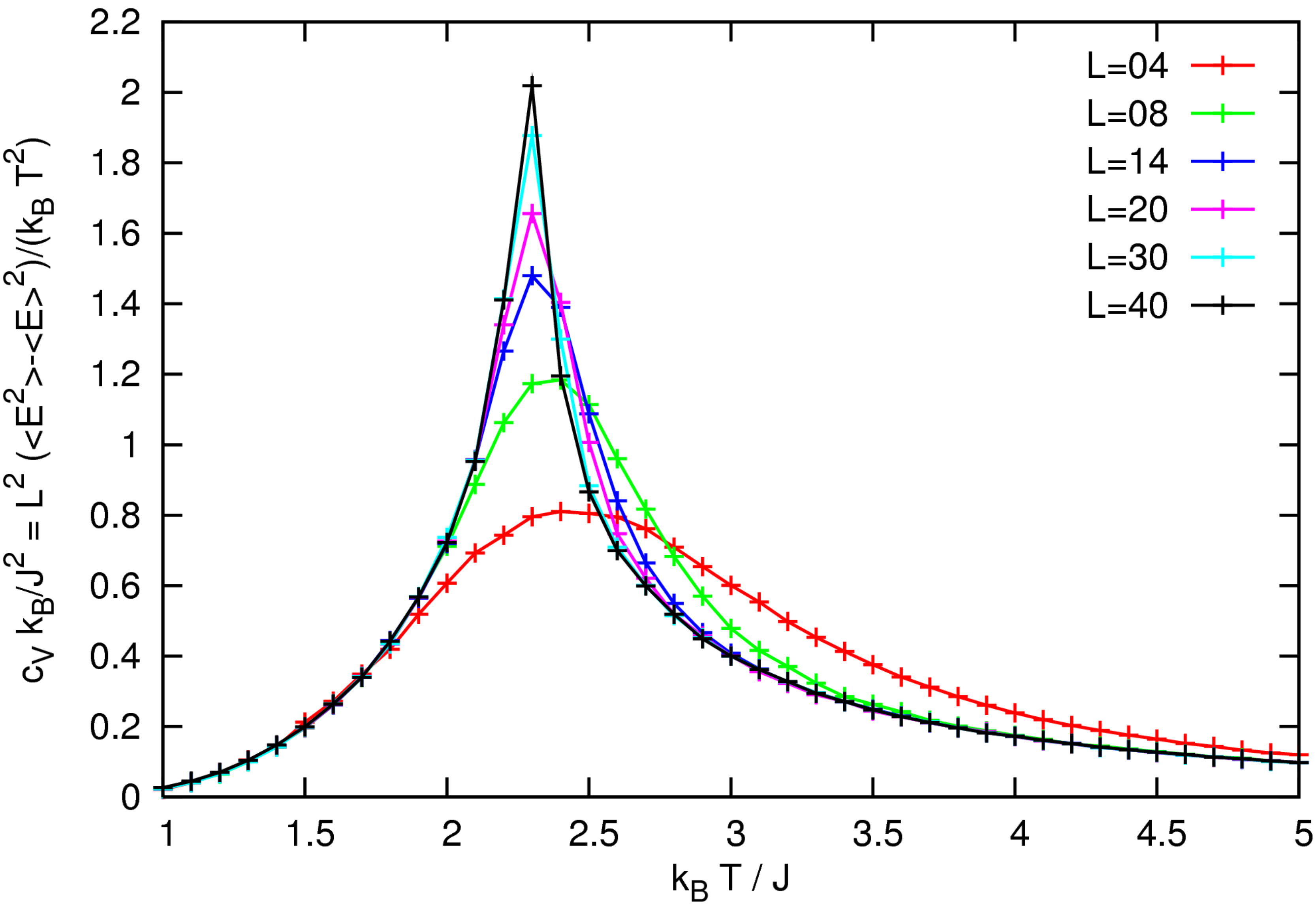
+	+	+	−		+	+	+	−
−	−	−	+	$\longleftrightarrow$	−	−	+	+
−	+	+	−		−	+	+	−
+	+	−	+		+	+	−	+

Java applet: `http://physics.ucsc.edu/~peter/java/ising/keep/ising.html`

Full lectures: e.g. `http://komet337.physik.uni-mainz.de/Bluemer/lectures_SS2008`

2-dimensional Ising model: specific heat (10^5 Wolff cluster updates)



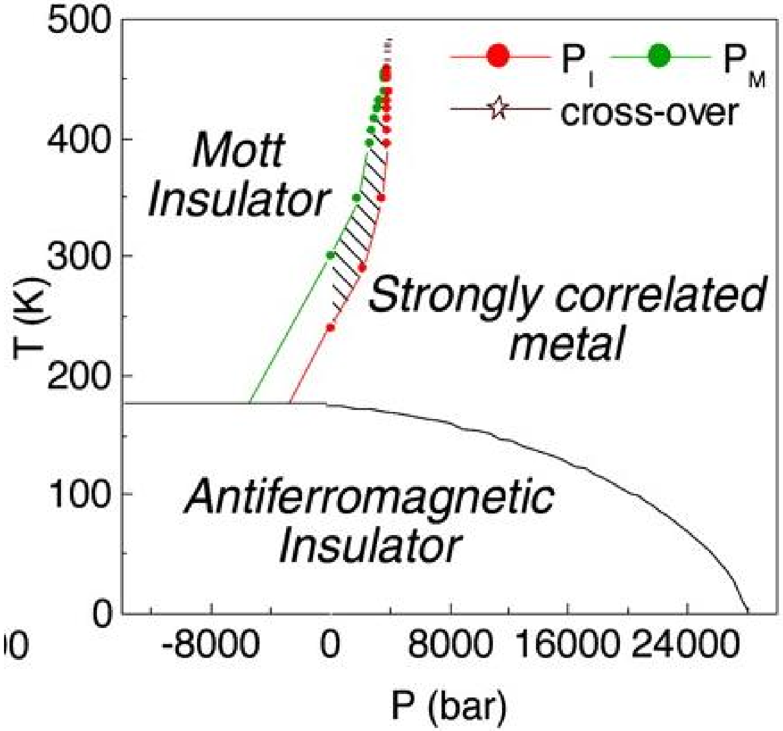
Finite-size analysis $\rightsquigarrow$ Curie temperature, critical exponents, . . .

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



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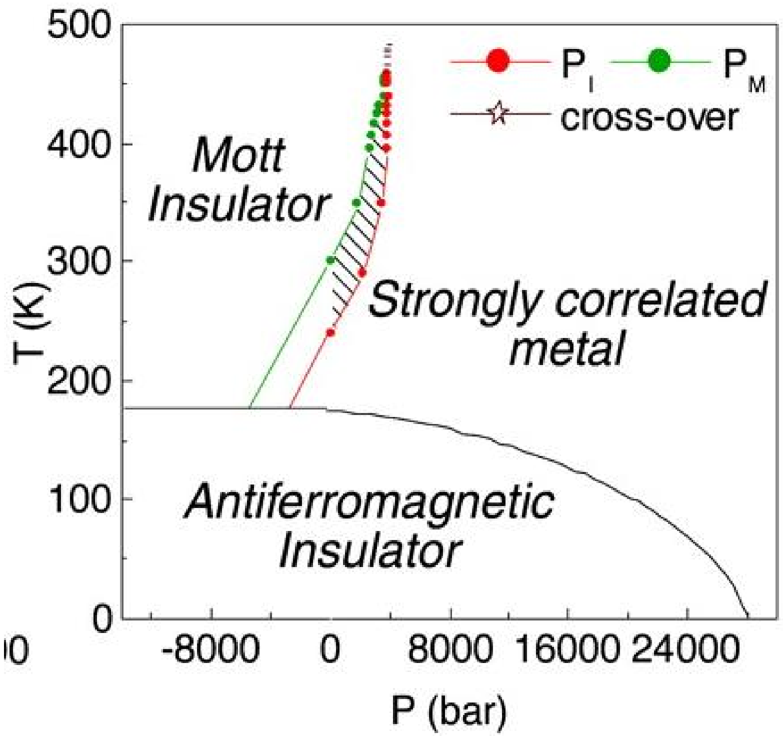
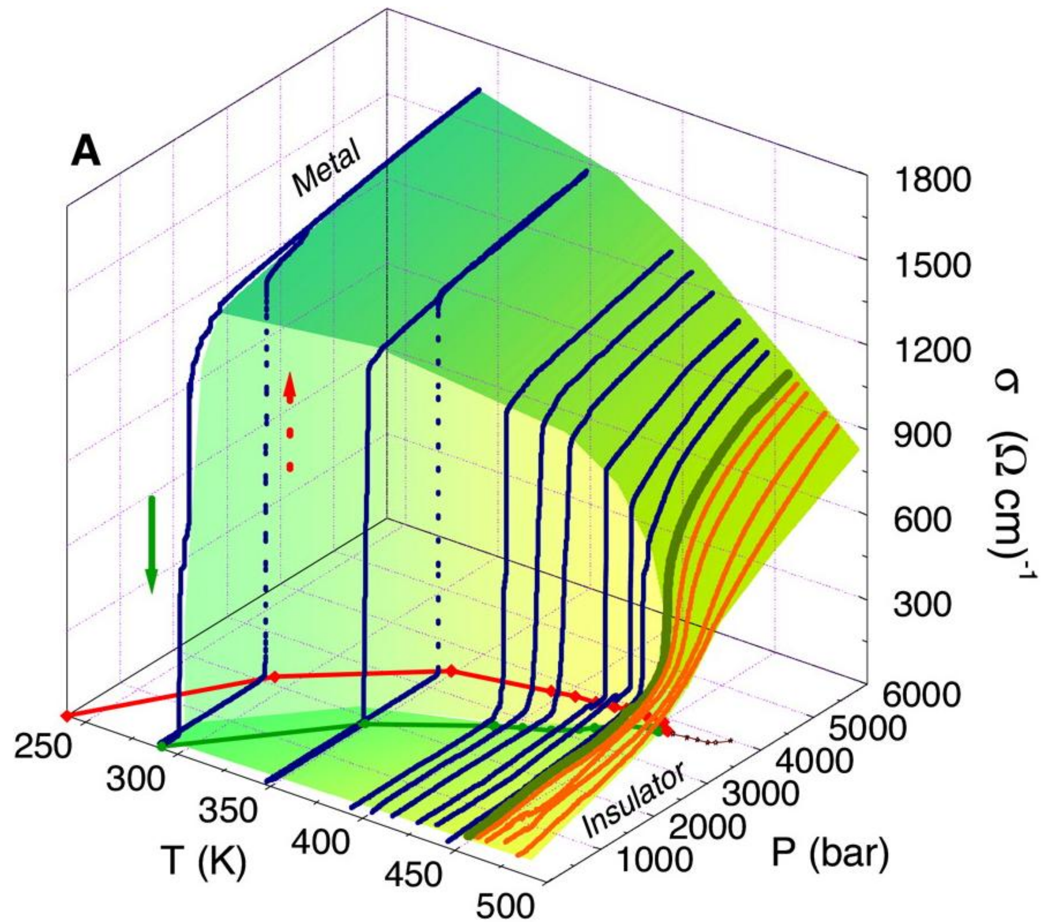
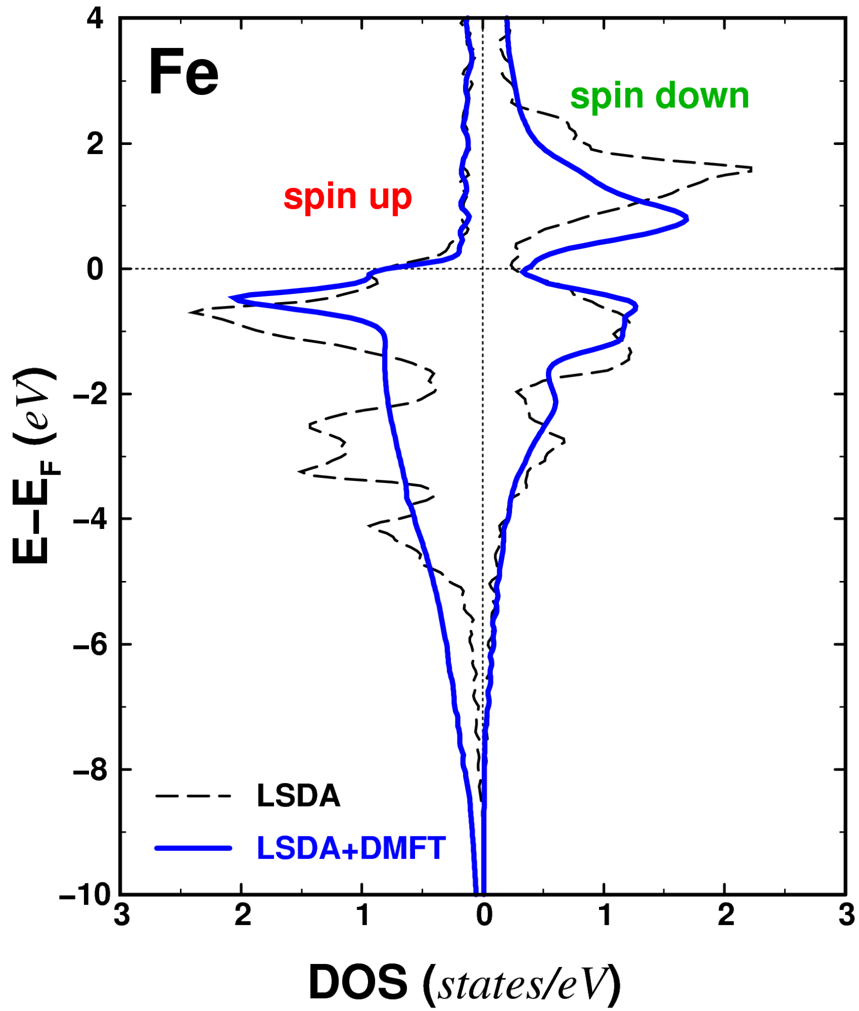


Electrical conductivity

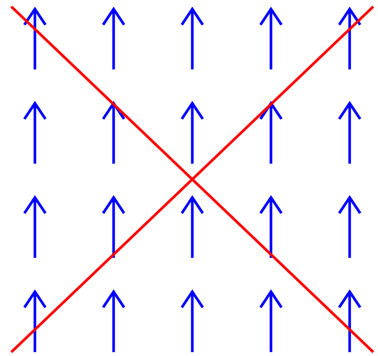


[Limelette et al., Science 302, 89 (2003)]

Itinerant ferromagnetism and half-metallicity

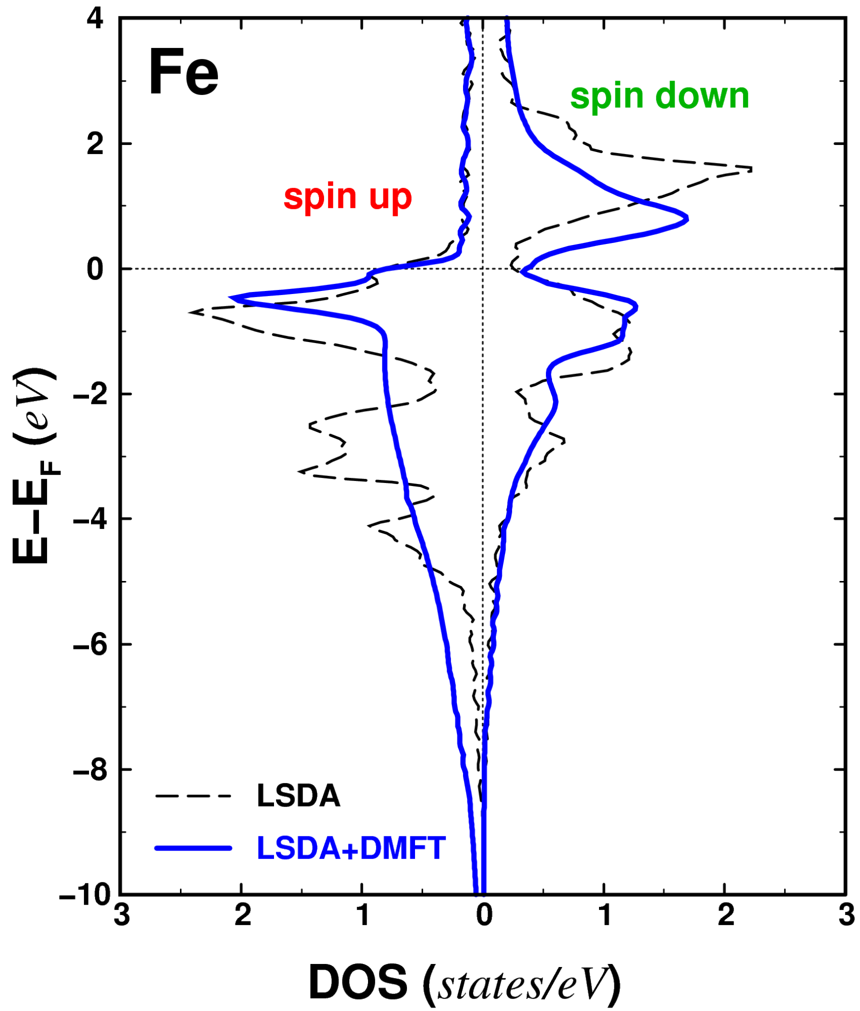


[Chioncel et. al, PRB (2003)]



Spin models insufficient

Itinerant ferromagnetism and half-metallicity



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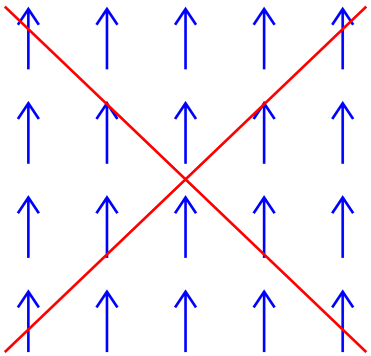
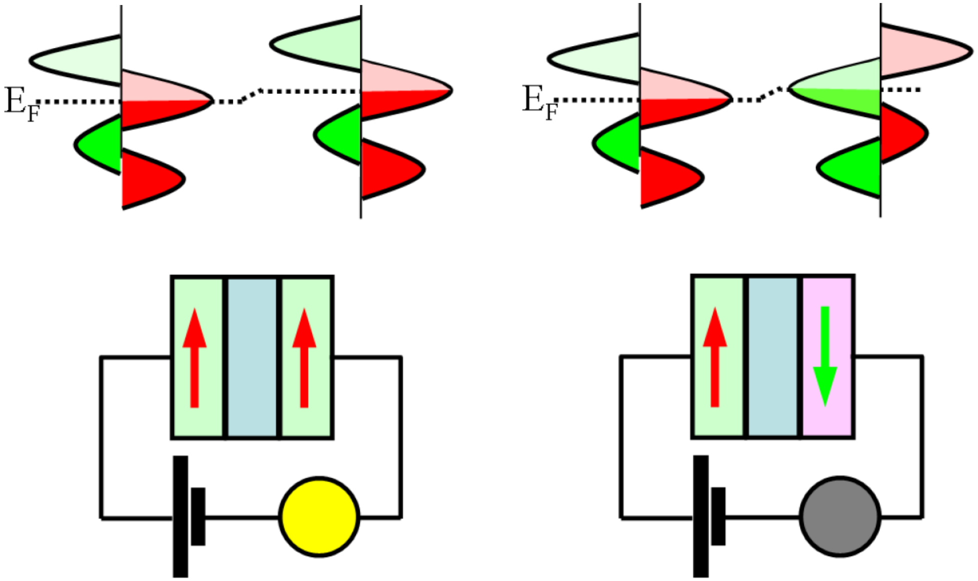


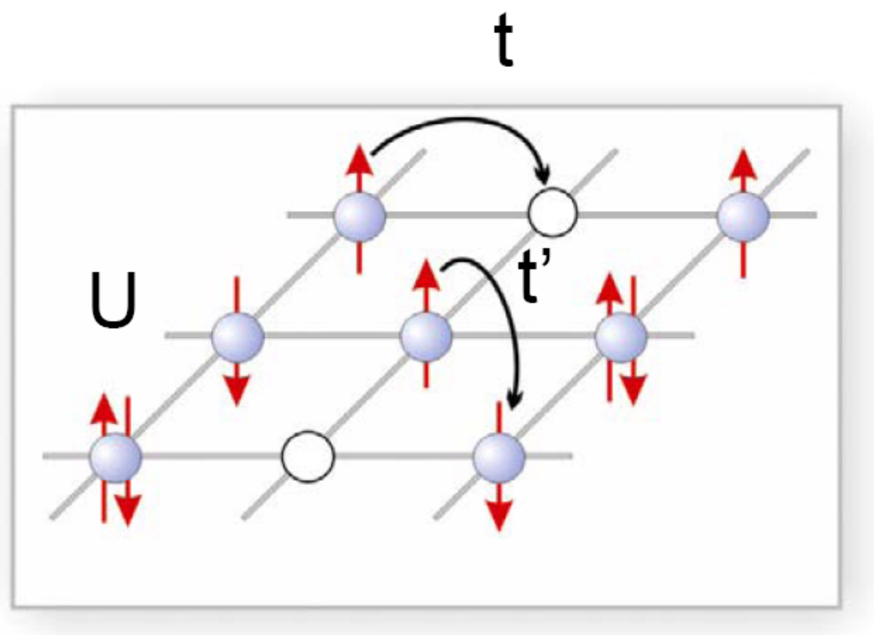
Spin models insufficient

Technological goal: TMR with half metals

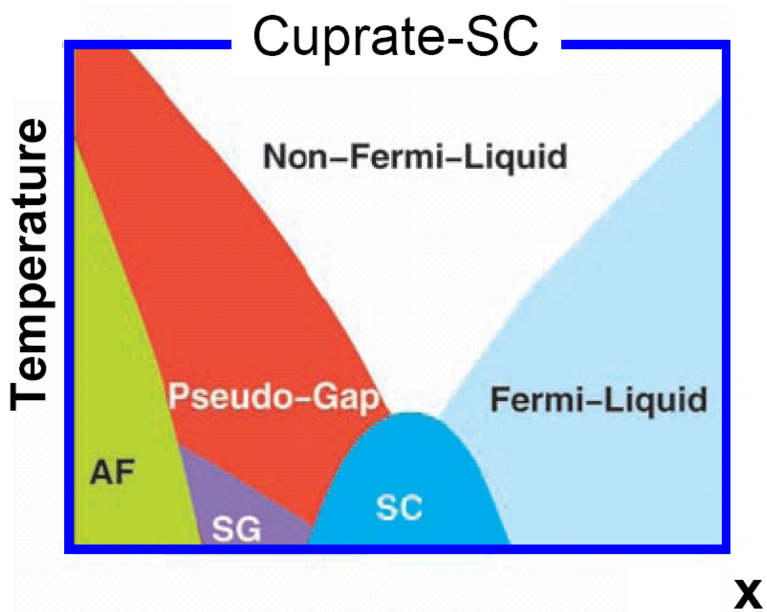


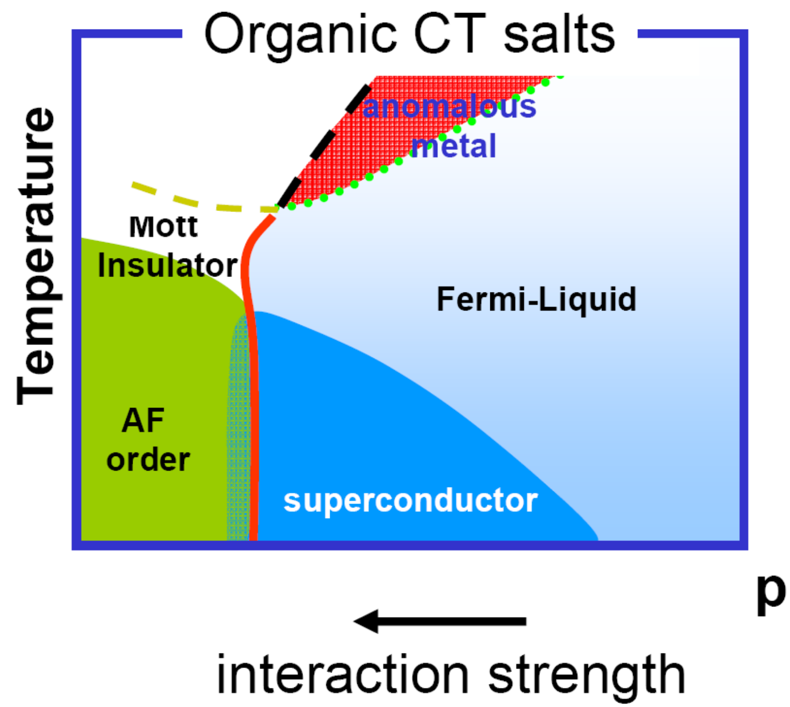
Complex phases of cuprate and organic superconductors

High-T_c physics contained in 2D Hubbard model?

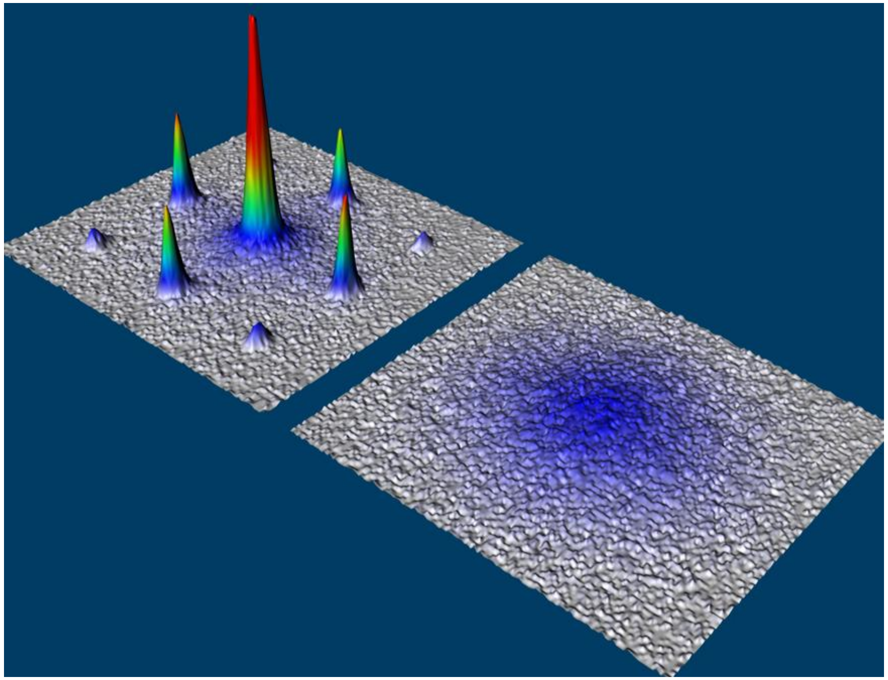


Are antiferromagnetic (AF) and Mott insulating phases essential for superconductivity?

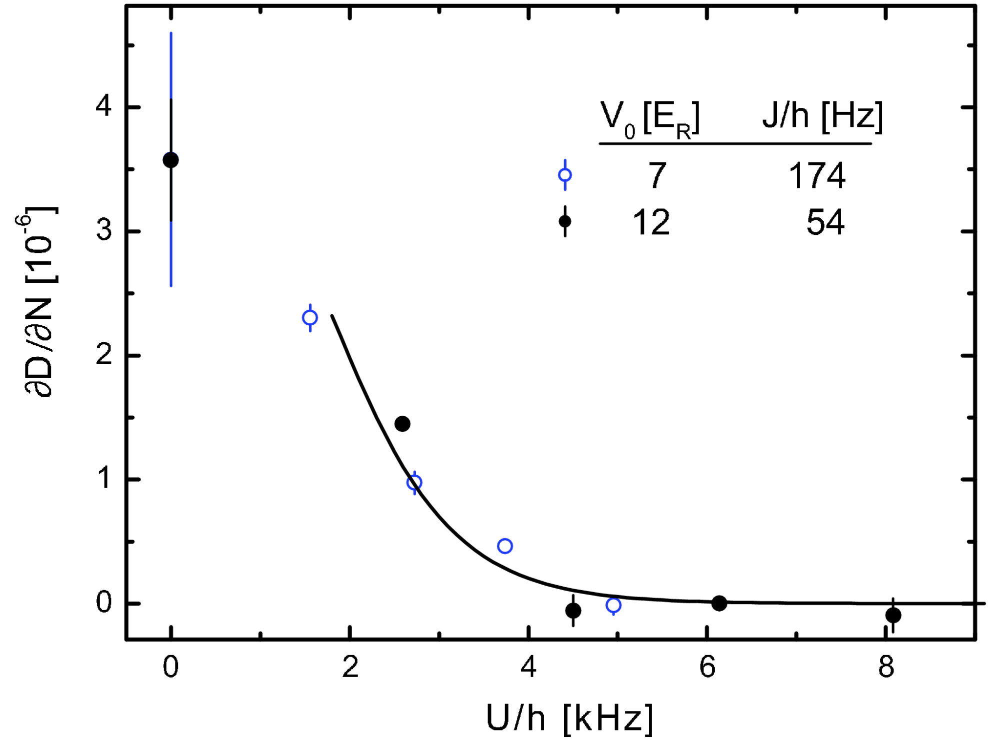




Correlated ultracold quantum gases on optical lattices



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)]

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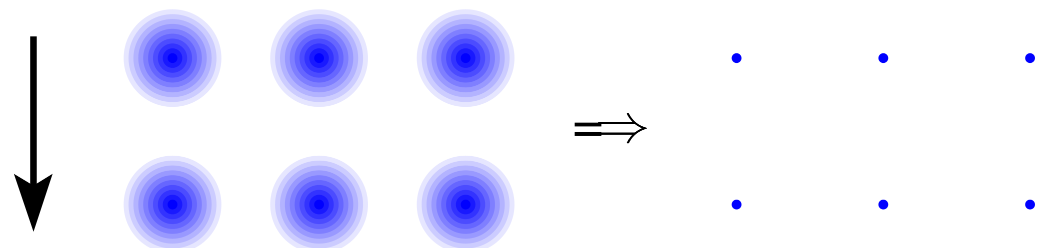
Born-Oppenheimer approximation (0^{th}order)



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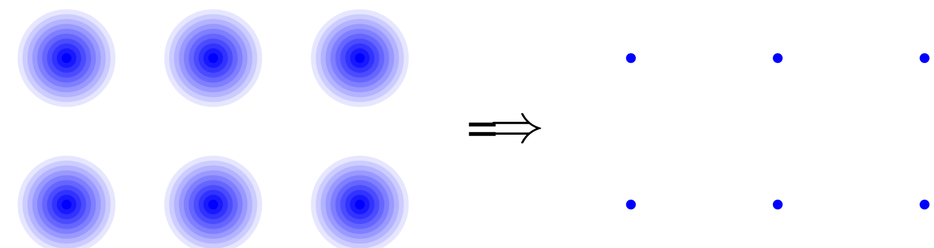
Born-Oppenheimer approximation (0^{th}order) $\downarrow$



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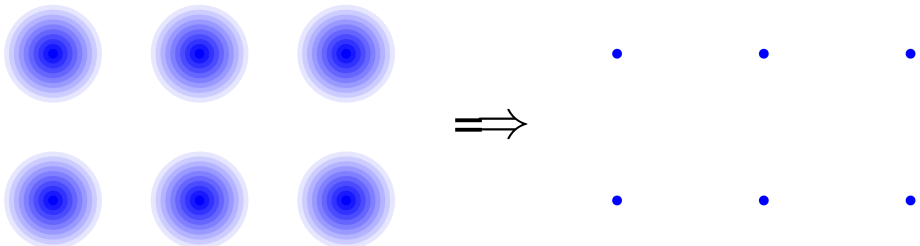

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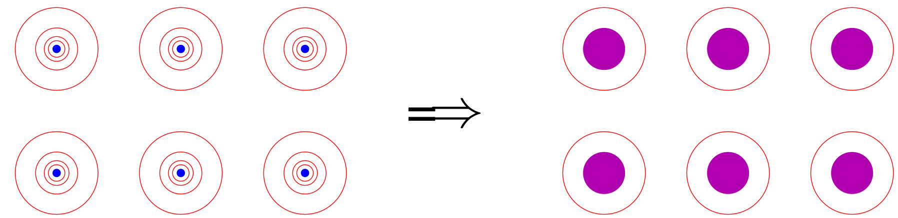
Classes of theoretical approaches for electronic problem

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

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

reduction to valence electrons ↓



$$H = \sum_{i=1}^{N_v} \frac{\boldsymbol{p}_i^2}{2m} + \sum_{i=1}^{N_v} V^{\text{ion}}(\boldsymbol{r}_i) + \sum_{i=1}^{N_v-1} \sum_{j=i+1}^{N_v} V^{ee}(\boldsymbol{r}_i, \boldsymbol{r}_j)$$

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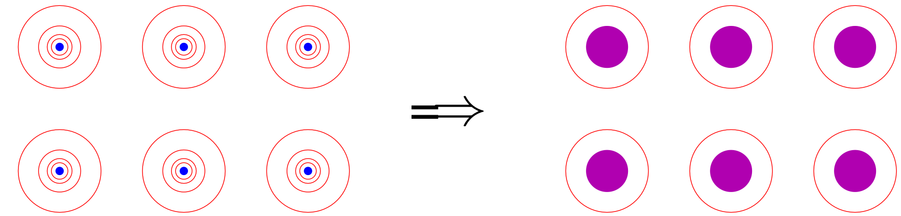

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occupation number formalism $\downarrow$ Wannier orbitals

$$\hat{H} = \sum_{i\nu j\sigma} t_{ij}^{\nu}\, \hat{c}_{i\nu\sigma}^{\dagger}\, \hat{c}_{j\nu\sigma} + \frac{1}{2} \sum_{\nu\nu'\mu\mu'} \sum_{ijmn} \sum_{\sigma\sigma'} \mathcal{V}_{ijmn}^{\nu\nu'\mu\mu'}\, \hat{c}_{i\nu\sigma}^{\dagger}\, \hat{c}_{j\nu'\sigma'}^{\dagger}\, \hat{c}_{n\mu'\sigma'}\, \hat{c}_{m\mu\sigma}$$

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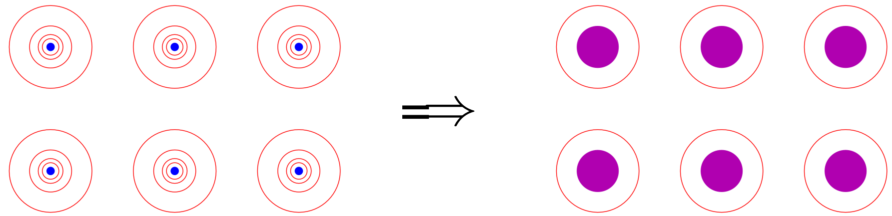

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Advantage of 2^{nd} quantization?

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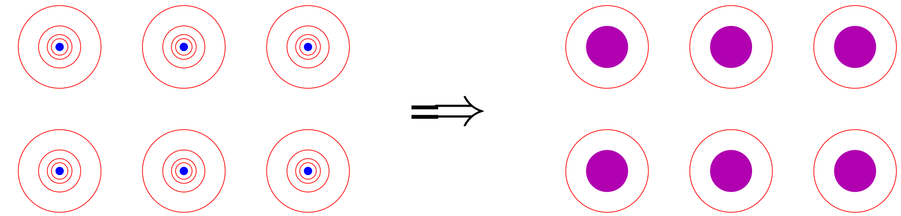

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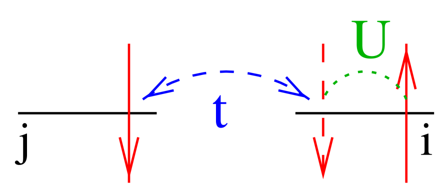
Advantage of 2nd quantization?

Hubbard model

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



Approaches for Hubbard-type models

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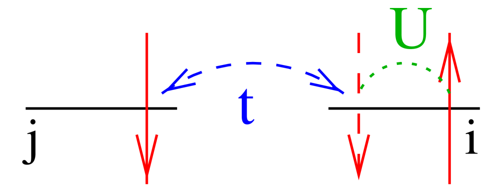
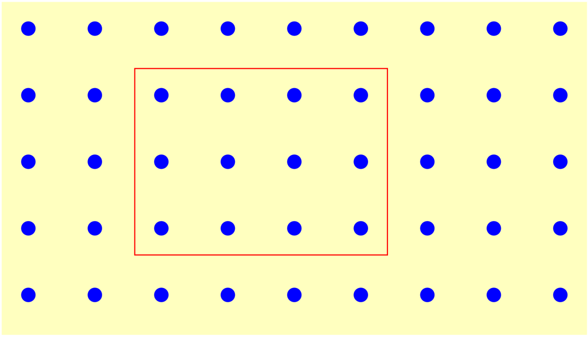


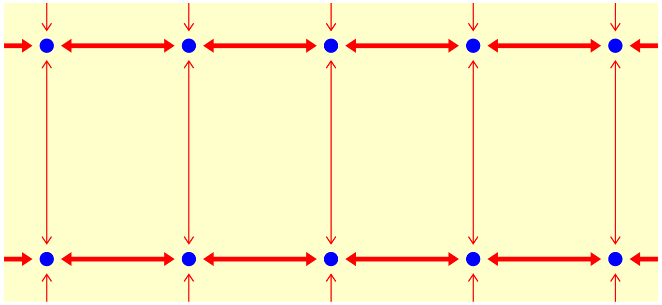
Perturbation theory

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

finite clusters: ED, QMC



$d \rightarrow 1$: Bethe ansatz, DMRG



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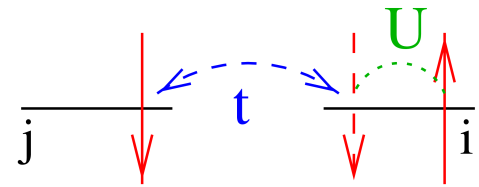

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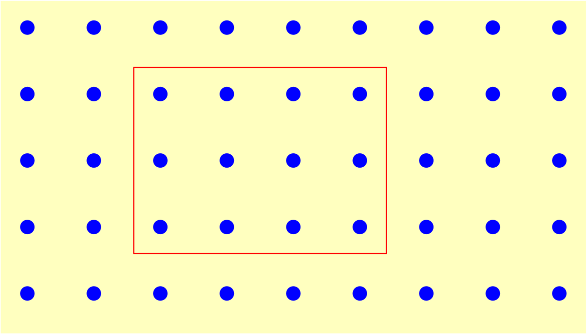

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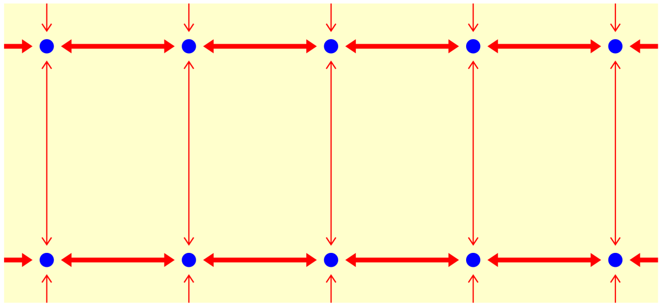
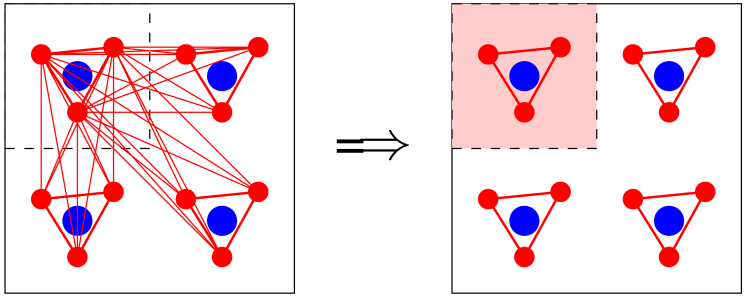


Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$

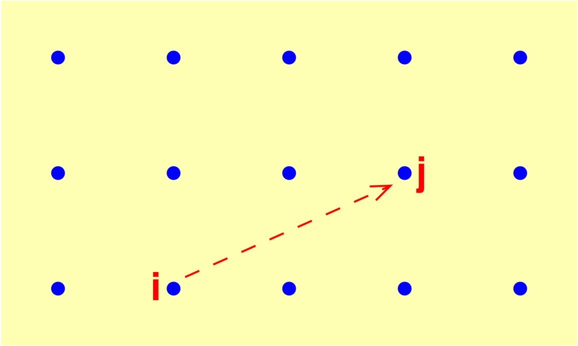
[Metzner, Vollhardt, PRL (1989), Georges, Kotliar, PRL (1992), Jarrell, PRL (1992)]

+ non-perturbative $\rightsquigarrow$ valid at MIT
+ dynamical on-site correlations preserved
+ in thermodynamic limit

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



Excursus: Green function and self-energy



Single-particle Green function (lattice sites i, j):

$$G_{ij}(t_1, t_2) = -\langle c_j\,(t_2)\, c_i^\dagger(t_1)\rangle$$

Translation invariance in space and time: $G_{ij}(t_1, t_2) \equiv G_{j-i}(t_2 - t_1) \xrightarrow{\text{Fourier}} G(\boldsymbol{k}, \omega)$

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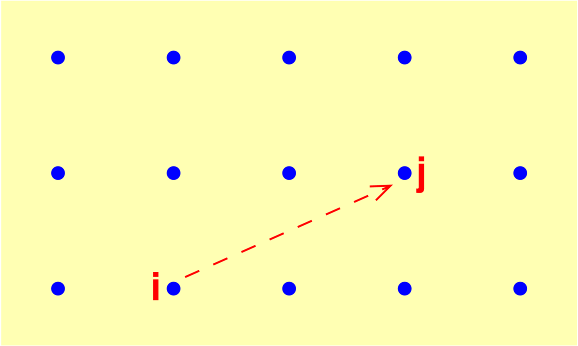

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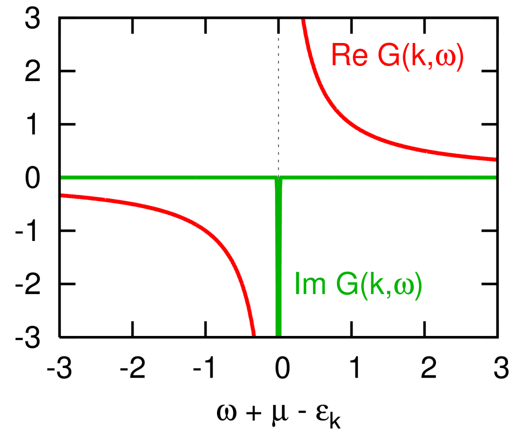
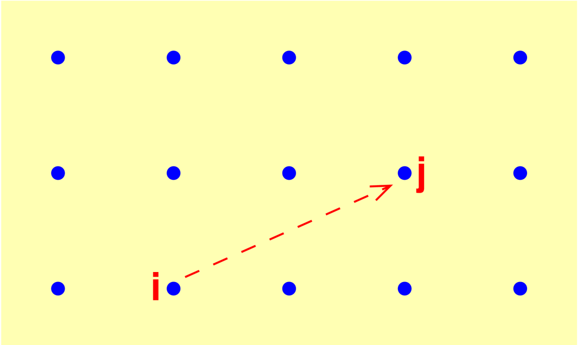
Noninteracting limit (dispersion $\varepsilon_{\boldsymbol{k}}$): $G^0(\boldsymbol{k}, \omega) = \dfrac{1}{\omega + \mu - \varepsilon_{\boldsymbol{k}}}$



Re $\Sigma(\boldsymbol{k}, \omega) \rightsquigarrow$ shift of energy levels

Im $\Sigma(\boldsymbol{k}, \omega) \rightsquigarrow$ broadening of energy levels

Excursus: Green function and self-energy



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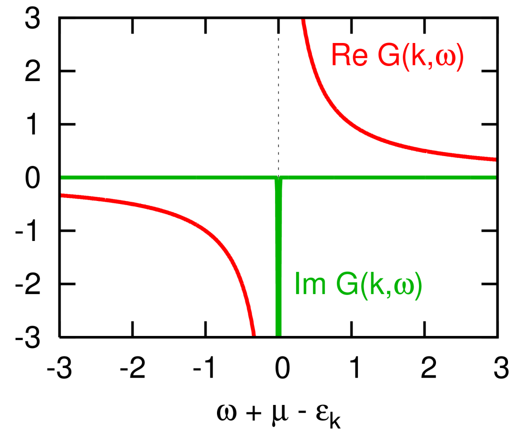


Self-energy Σ quantifies impact of interactions:

$$G(\boldsymbol{k}, \omega) = \frac{1}{\omega + \mu - \varepsilon_{\boldsymbol{k}} - \Sigma(\boldsymbol{k}, \omega)}$$

(lattice Dyson equation)

Re $\Sigma(\boldsymbol{k}, \omega) \rightsquigarrow$ shift of energy levels

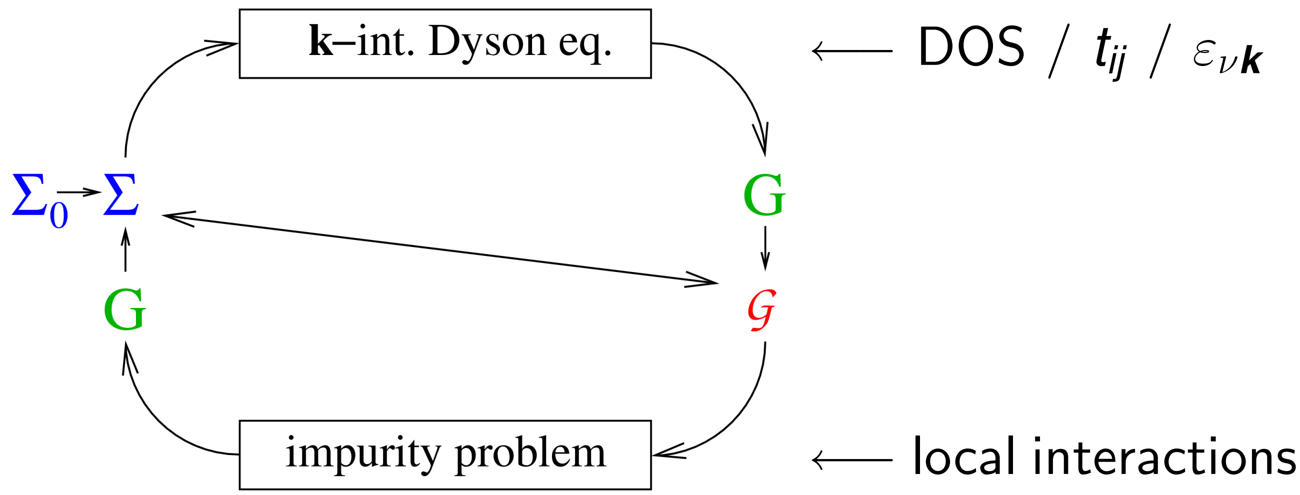
Im $\Sigma(\boldsymbol{k}, \omega) \rightsquigarrow$ broadening of energy levels

Iterative solution of DMFT equations

0. Initialize self-energy

1. Solve Dyson equation

2. Solve single impurity Anderson model (SIAM)



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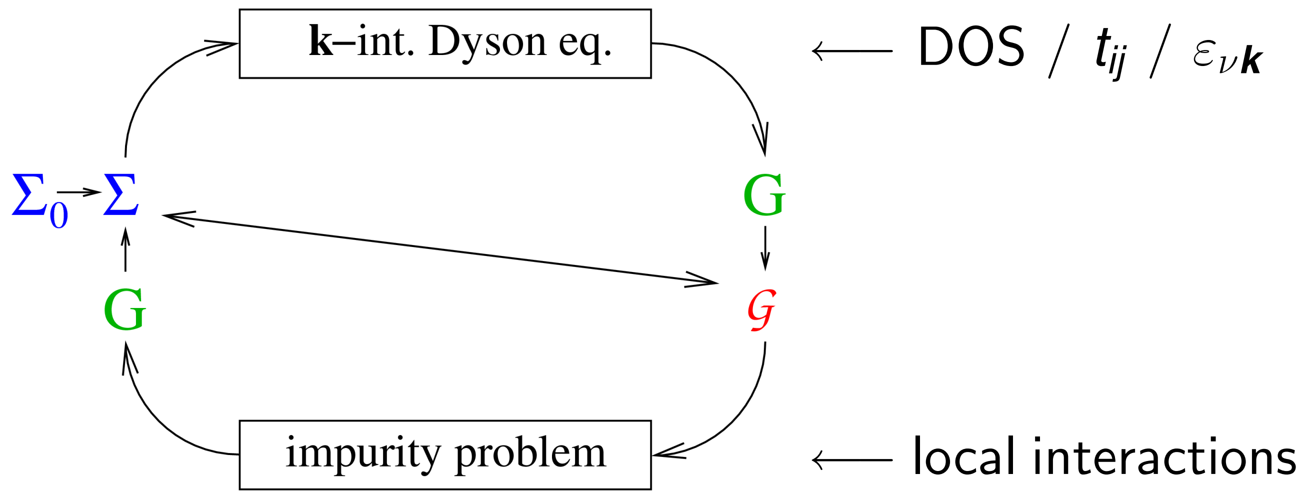

Impurity solver:

- Iterative perturbation theory (IPT; not controlled)
- Quantum Monte Carlo (QMC)

Iterative solution of DMFT equations

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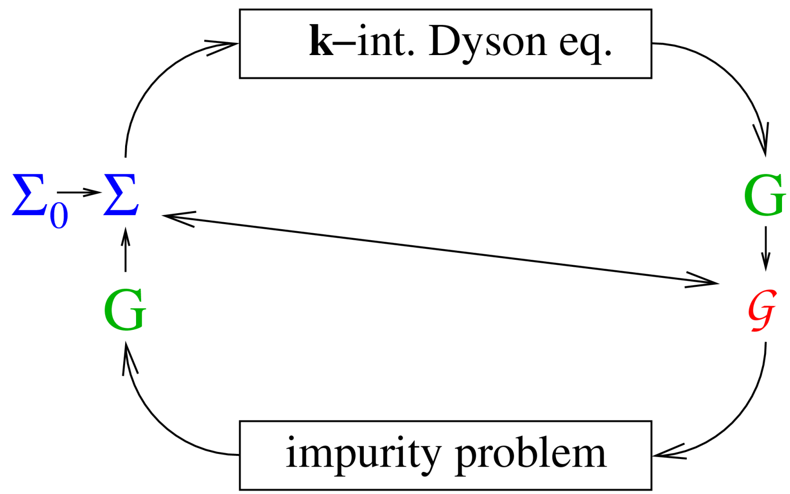
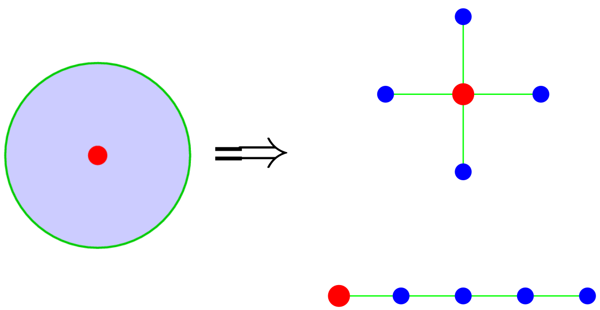


$\longleftarrow$ DOS / t_{ij} / $\varepsilon_{\nu\boldsymbol{k}}$

$\longleftarrow$ local interactions

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

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

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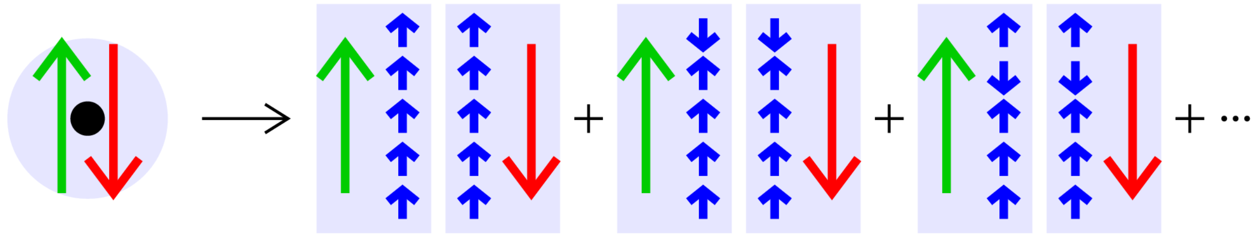
(iii) Hubbard-Stratonovich transformation



Wick theorem:

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

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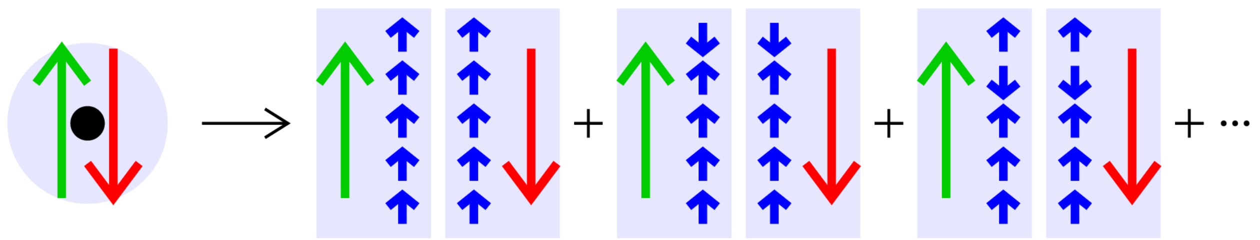


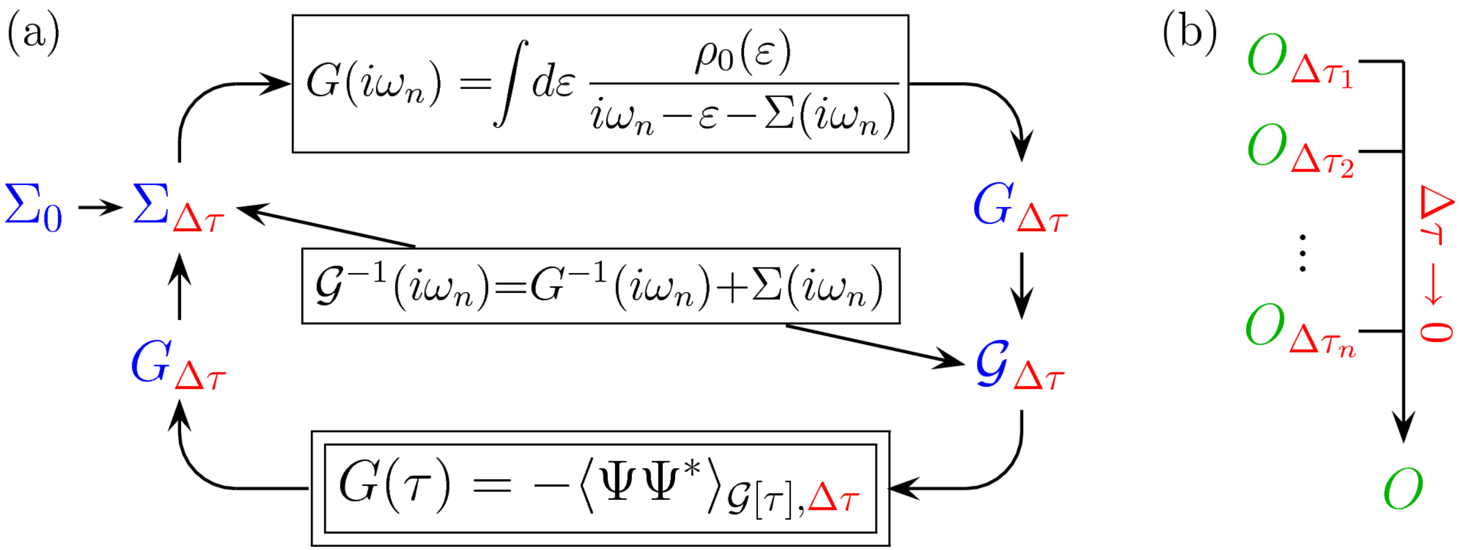
Wick theorem:

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

(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 (∼ same cost)

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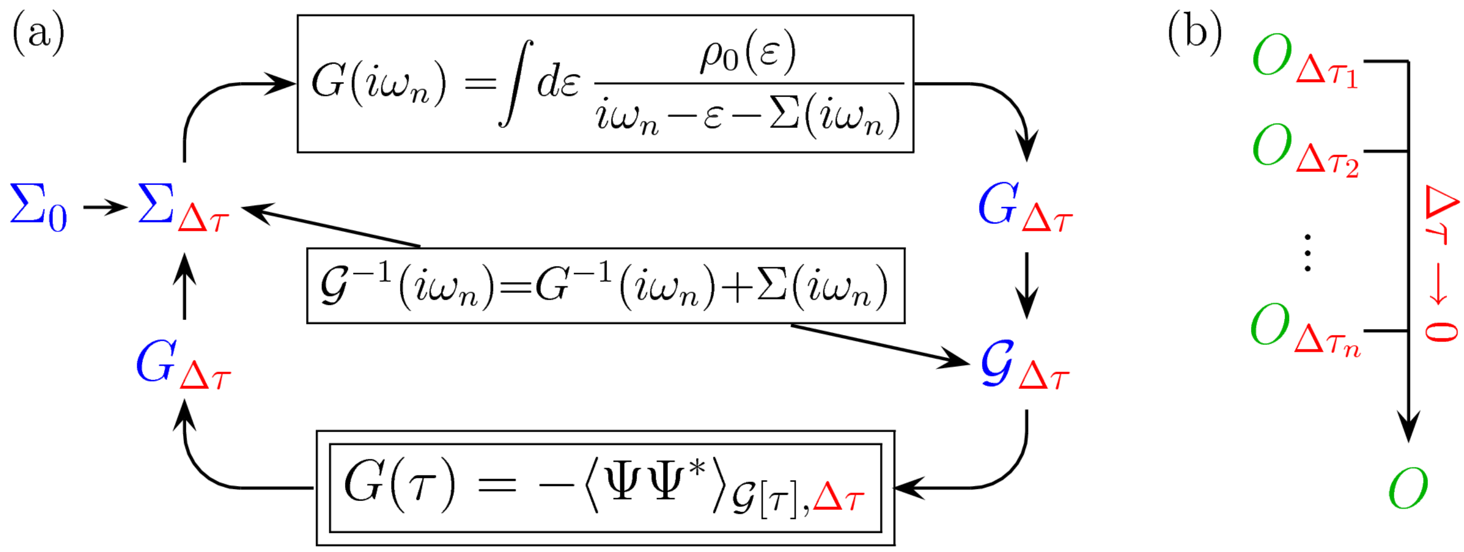

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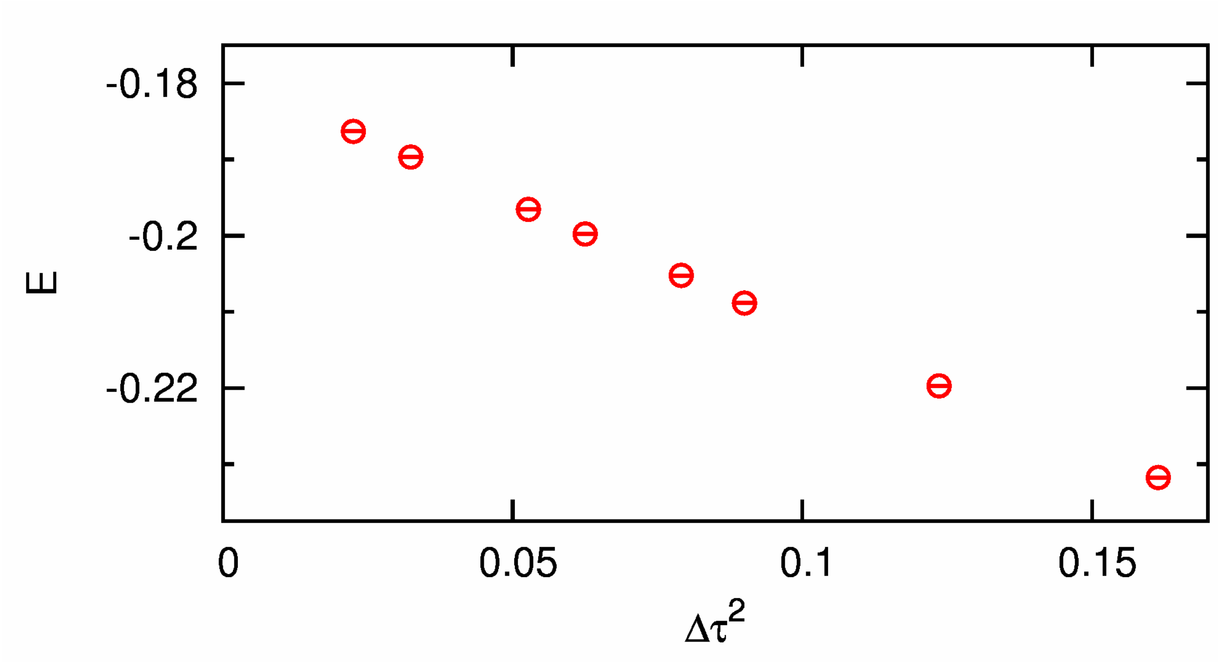
Example: energy E for $U = W = 4$ (Bethe DOS), $T = 1/45$ [NB, PRB (2007)]



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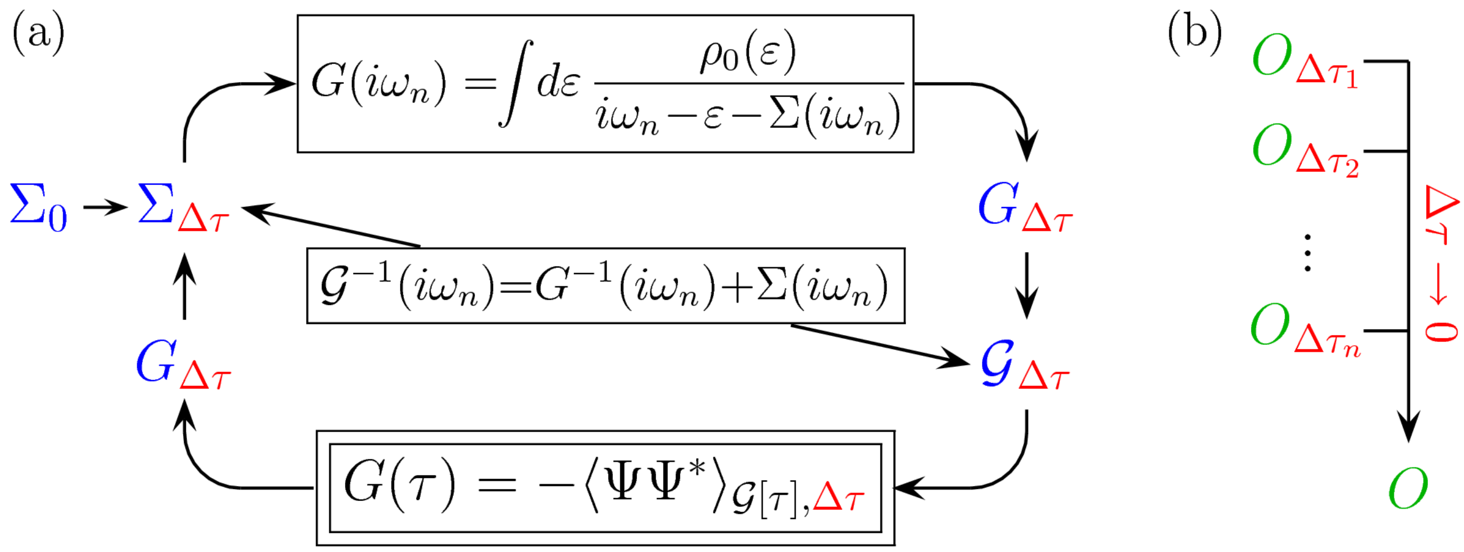

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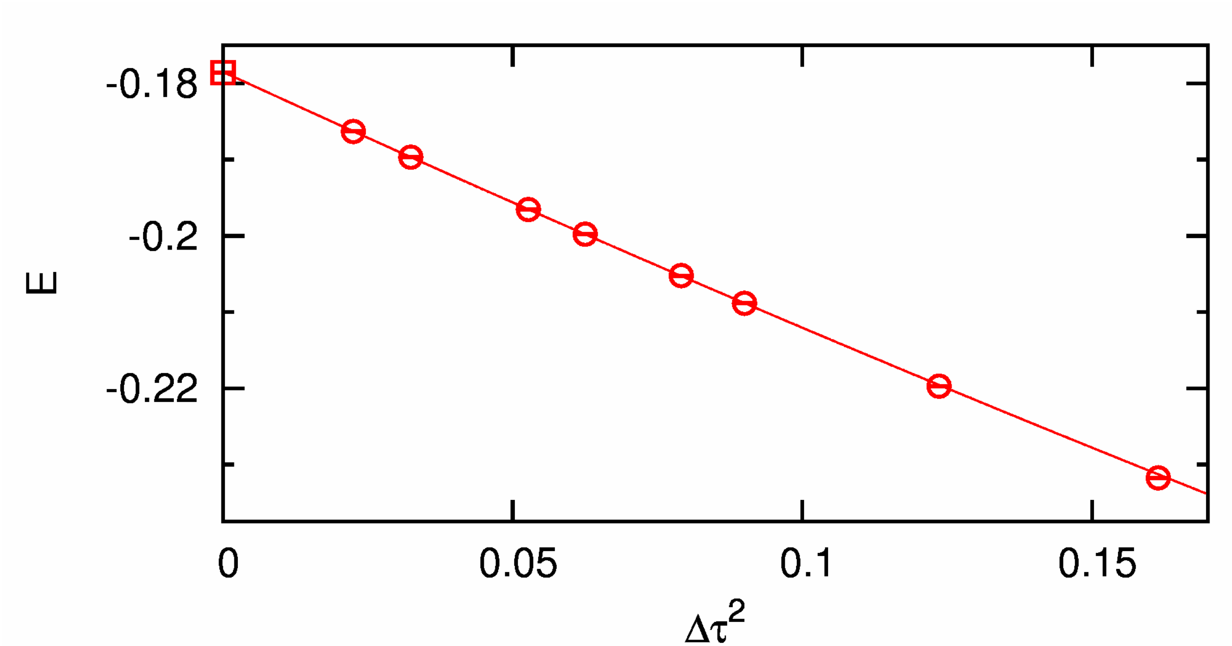
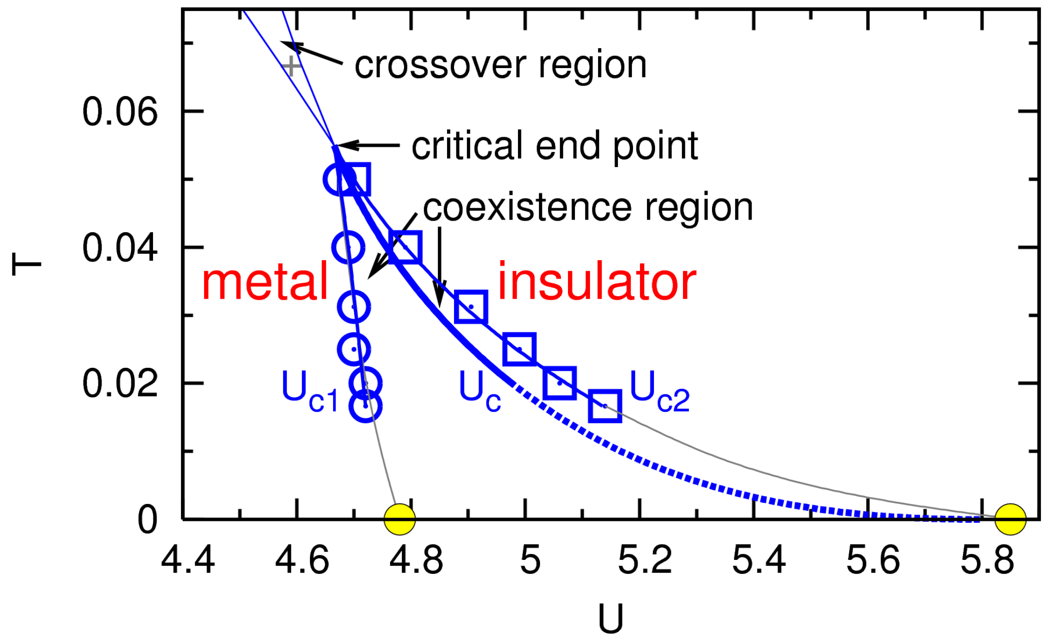


Mott transition within DMFT

Fully frustrated 1-band model,
energy scale: bandwidth $W = 4$



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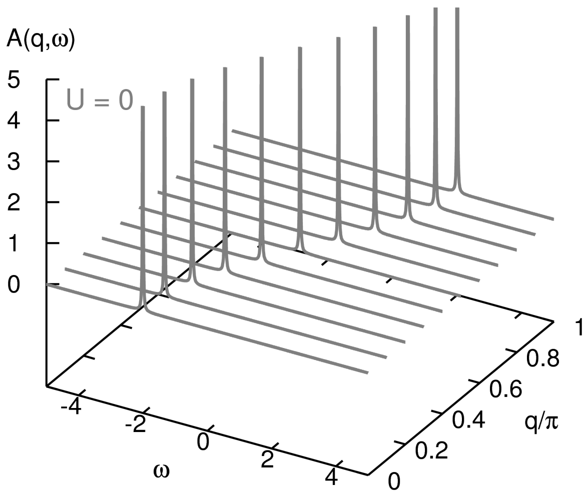
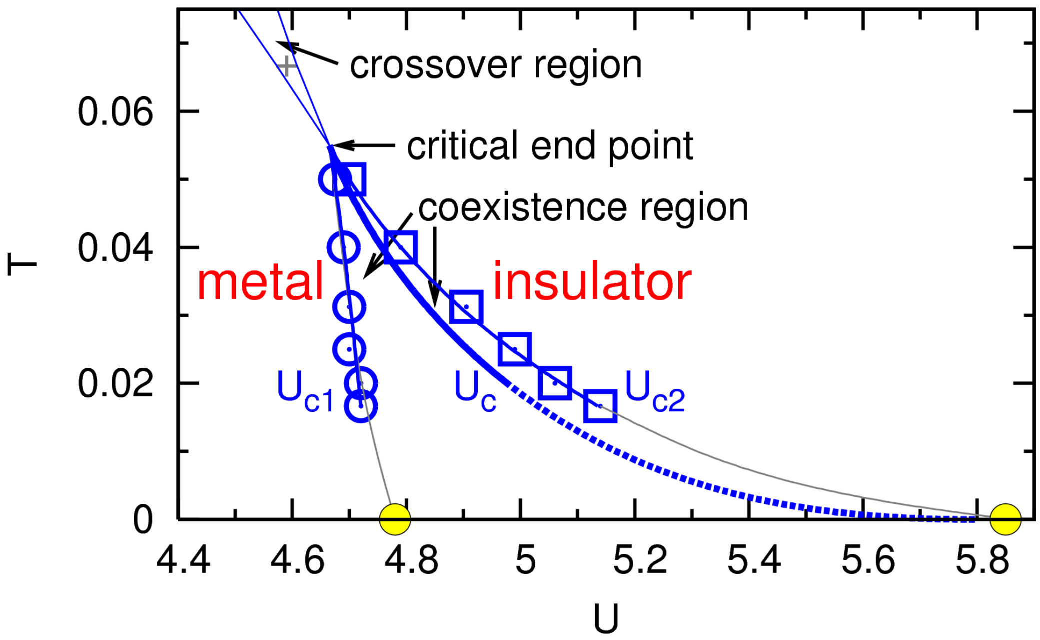
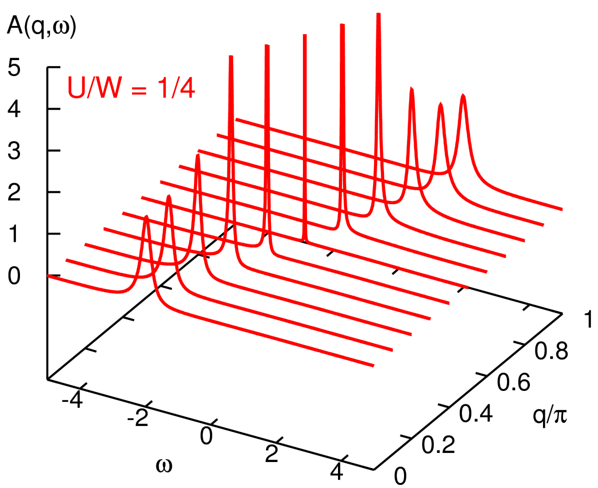
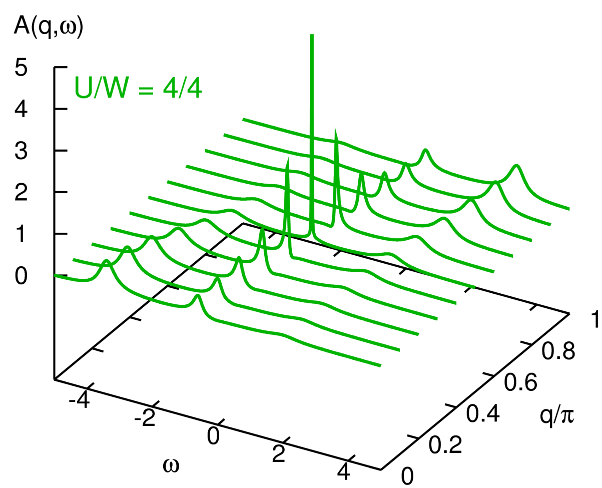
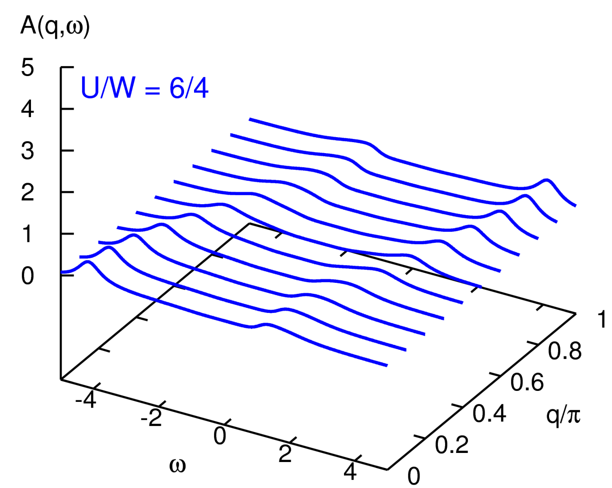






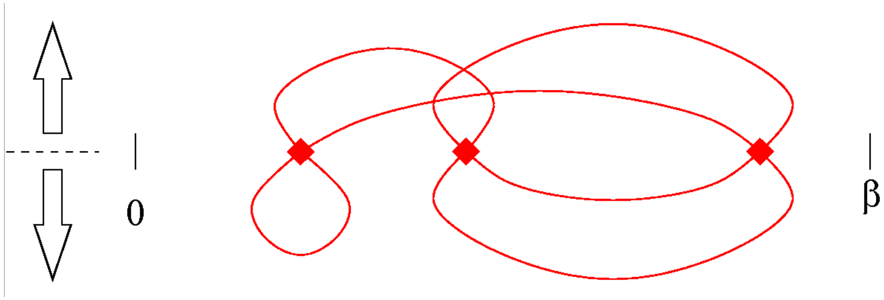




New development: continuous-time QMC algorithms

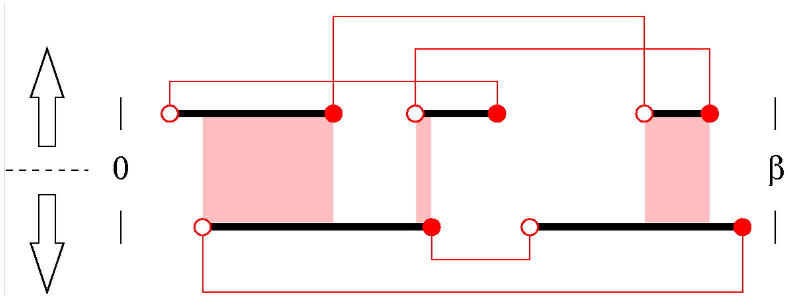
1. weak-coupling expansion

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



2. hybridization expansion

[Werner et al., PRL (2006)]



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

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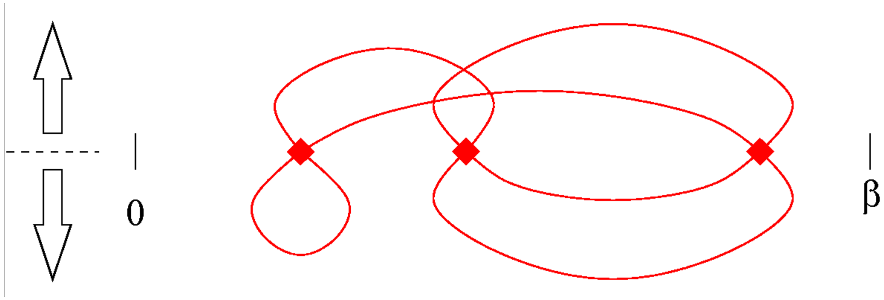

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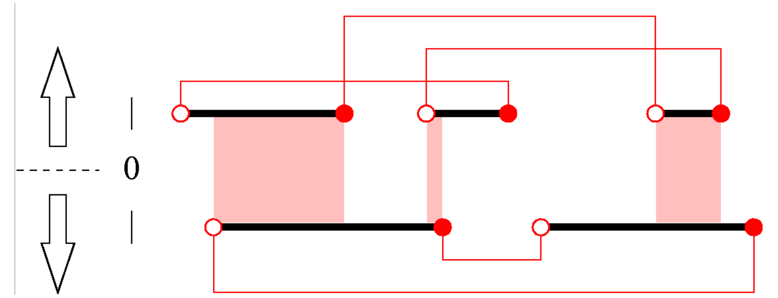
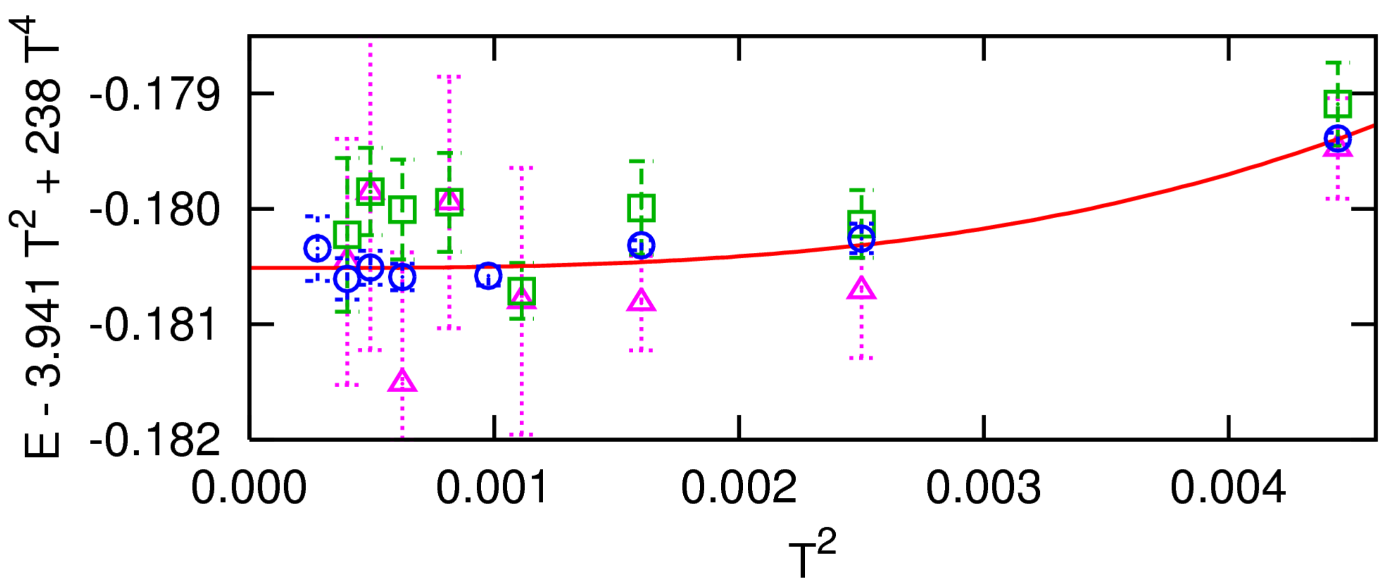


No systematic errors (in principle). Also more efficient than HF-QMC? No!



Test case:

1 band, $U = W = 4$

○ HF-QMC ($\Delta\tau \to 0$)

□ weak-coupling CT-QMC

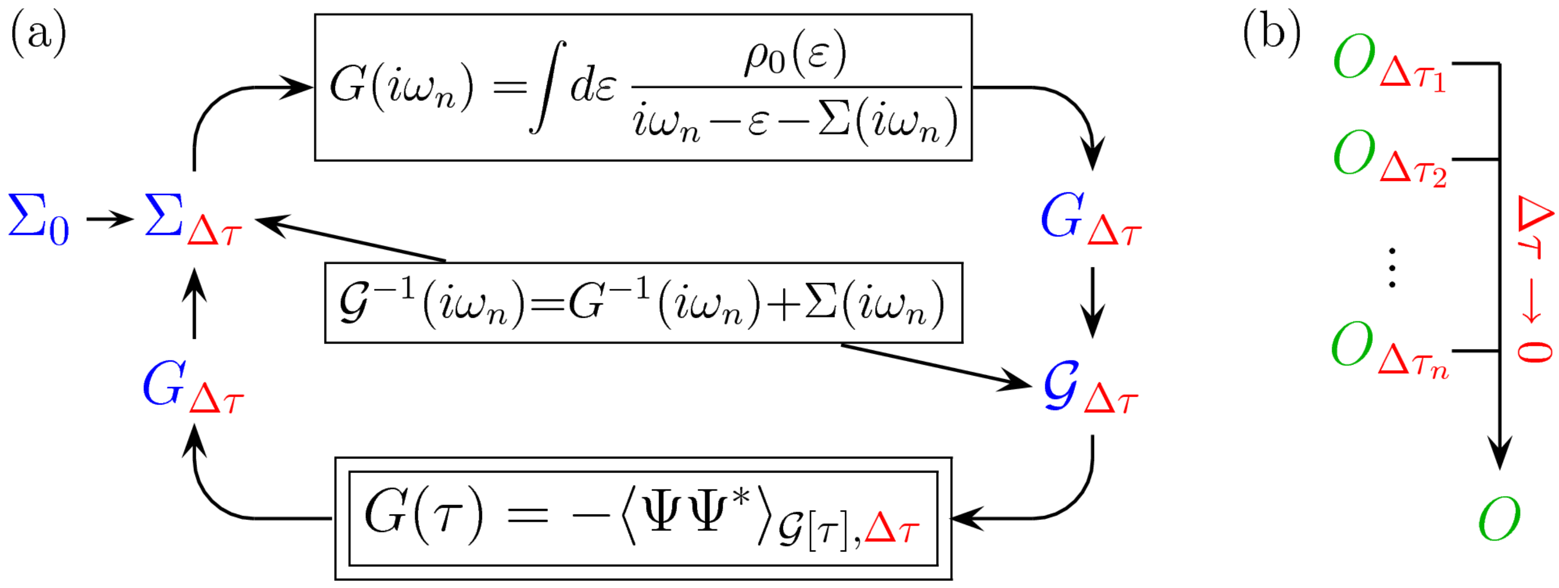
△ hybridization CT-QMC

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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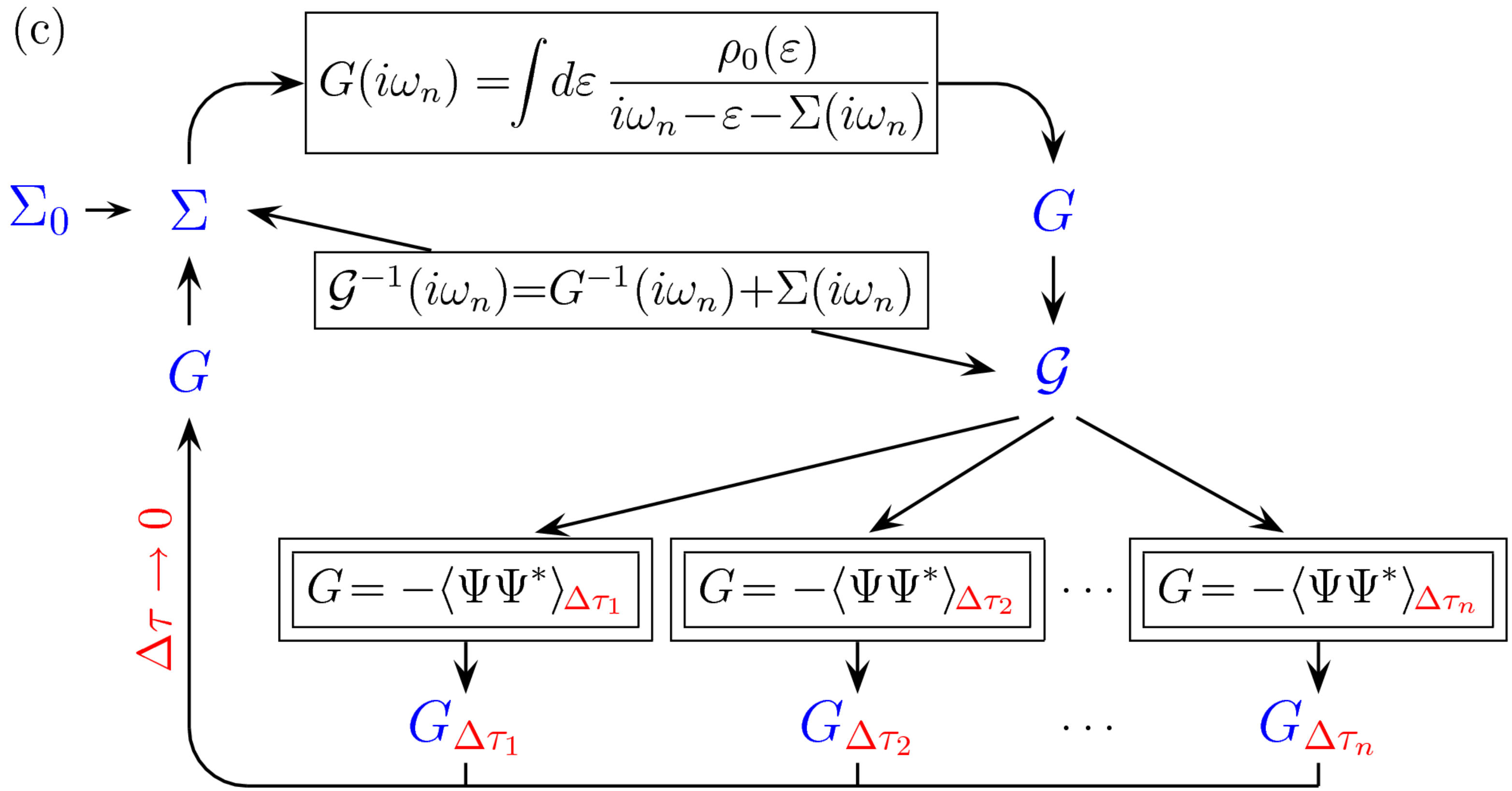
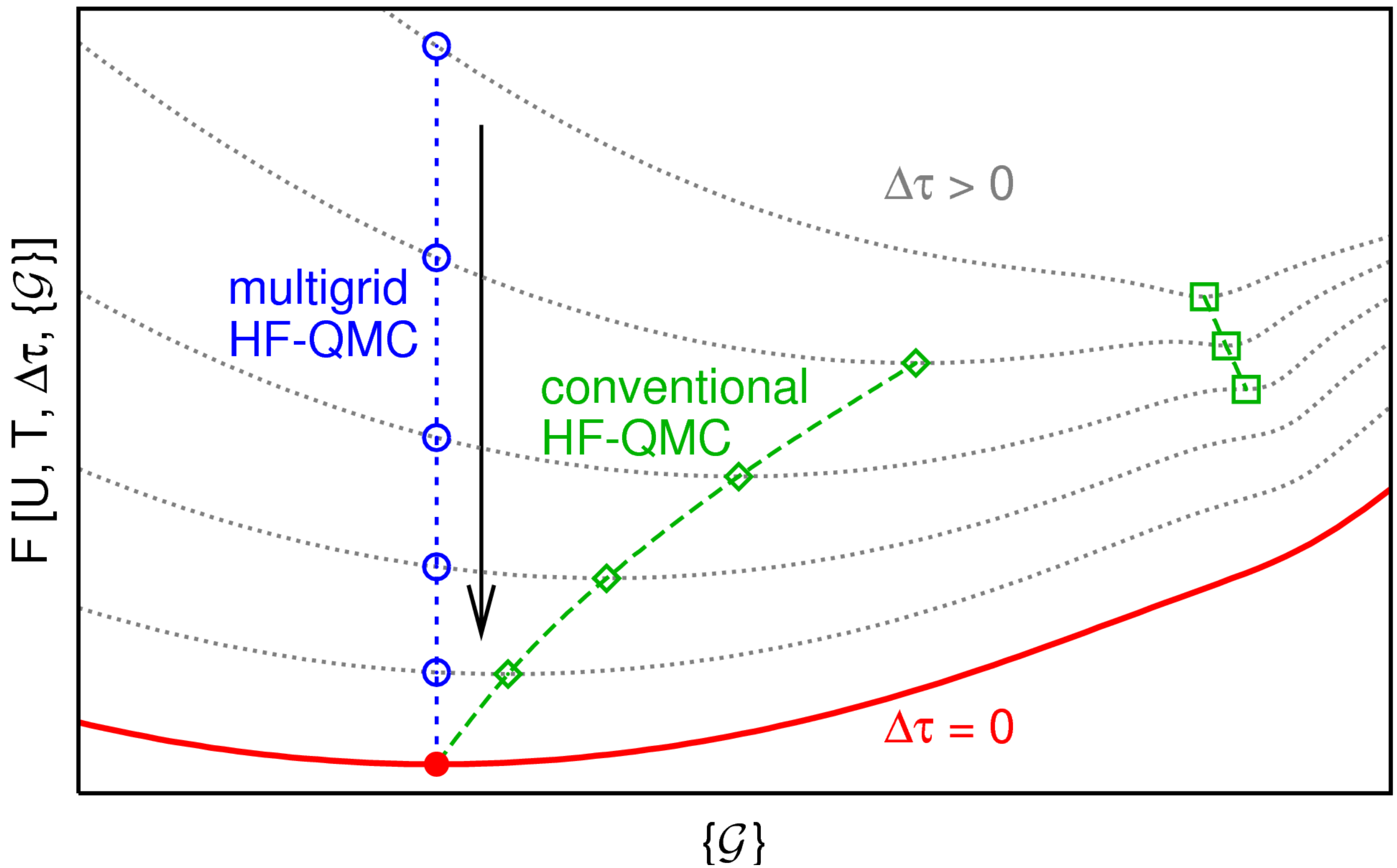


(c) Multigrid HF-QMC: internal elimination of Trotter error

$\rightsquigarrow$ 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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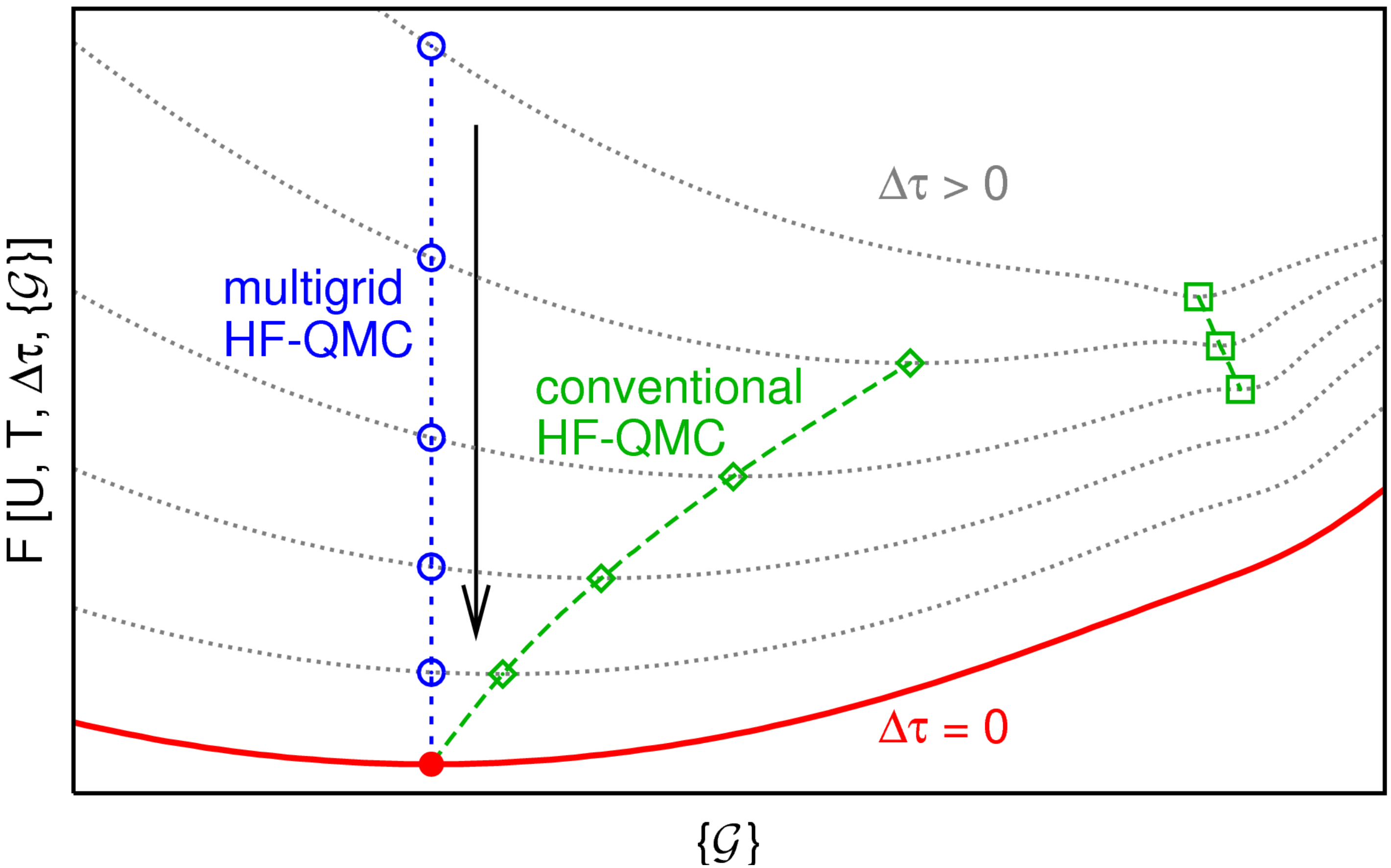

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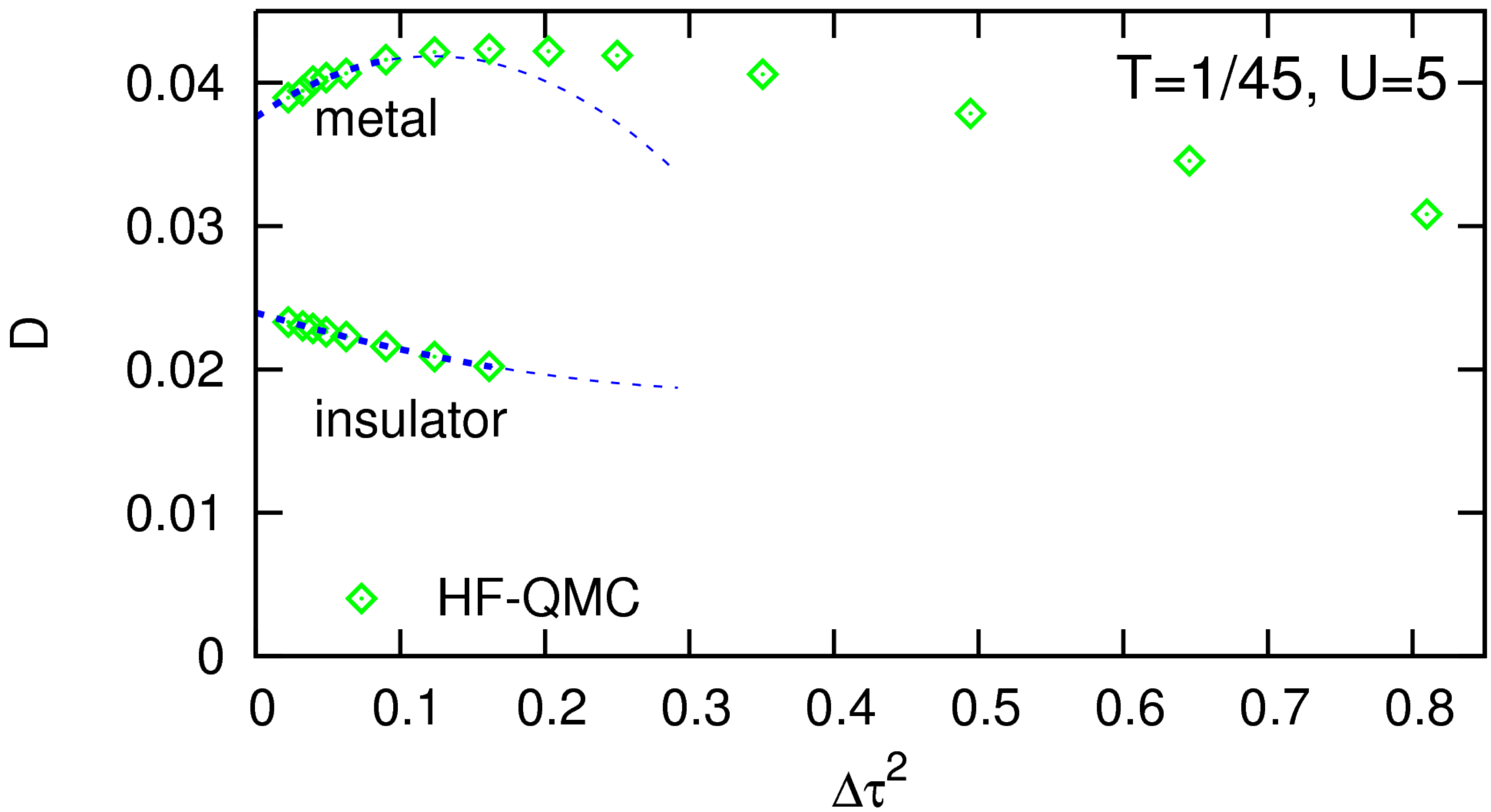
Implementation: Green function extrapolation, hierarchy of frequency scales

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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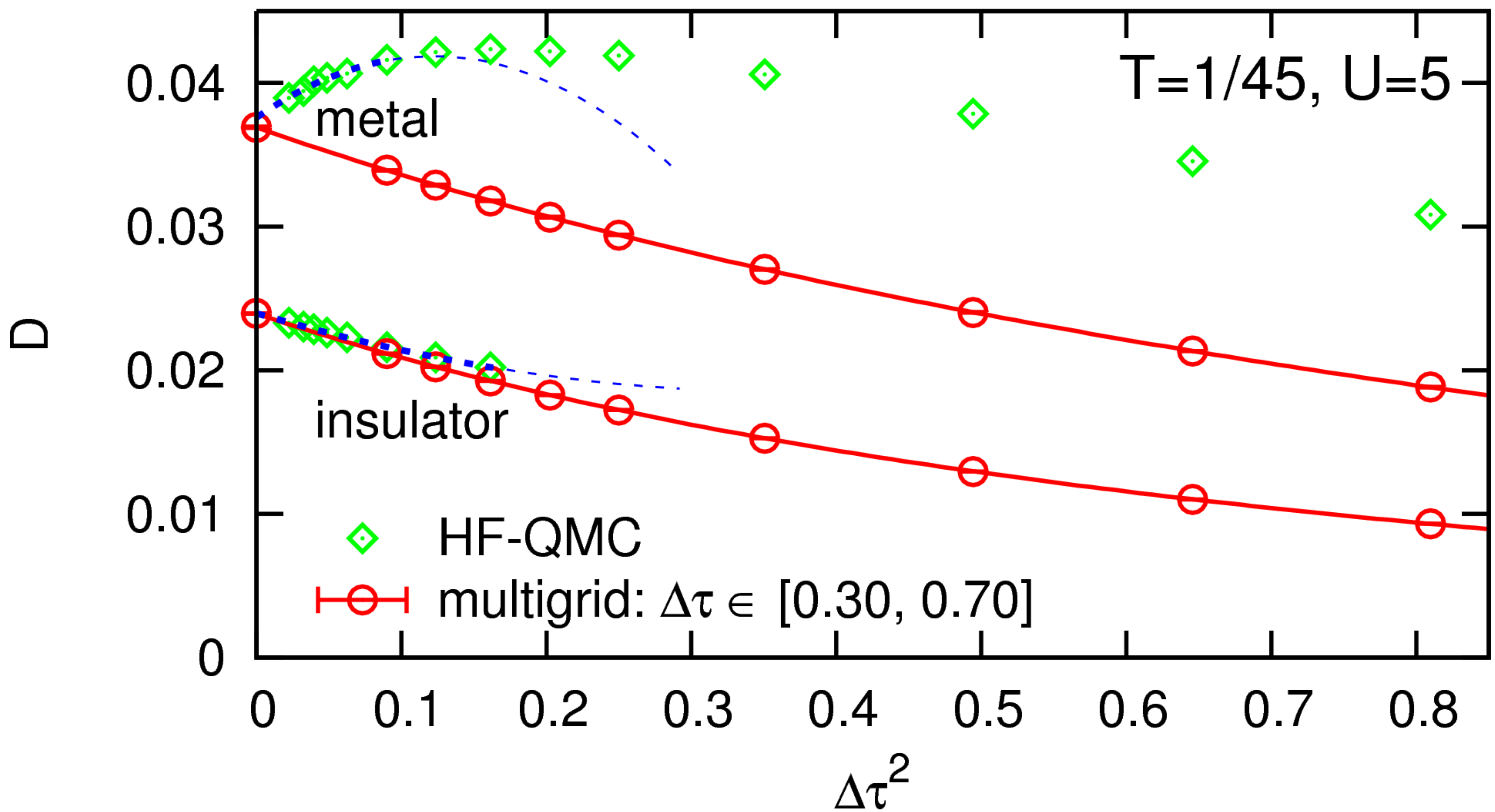
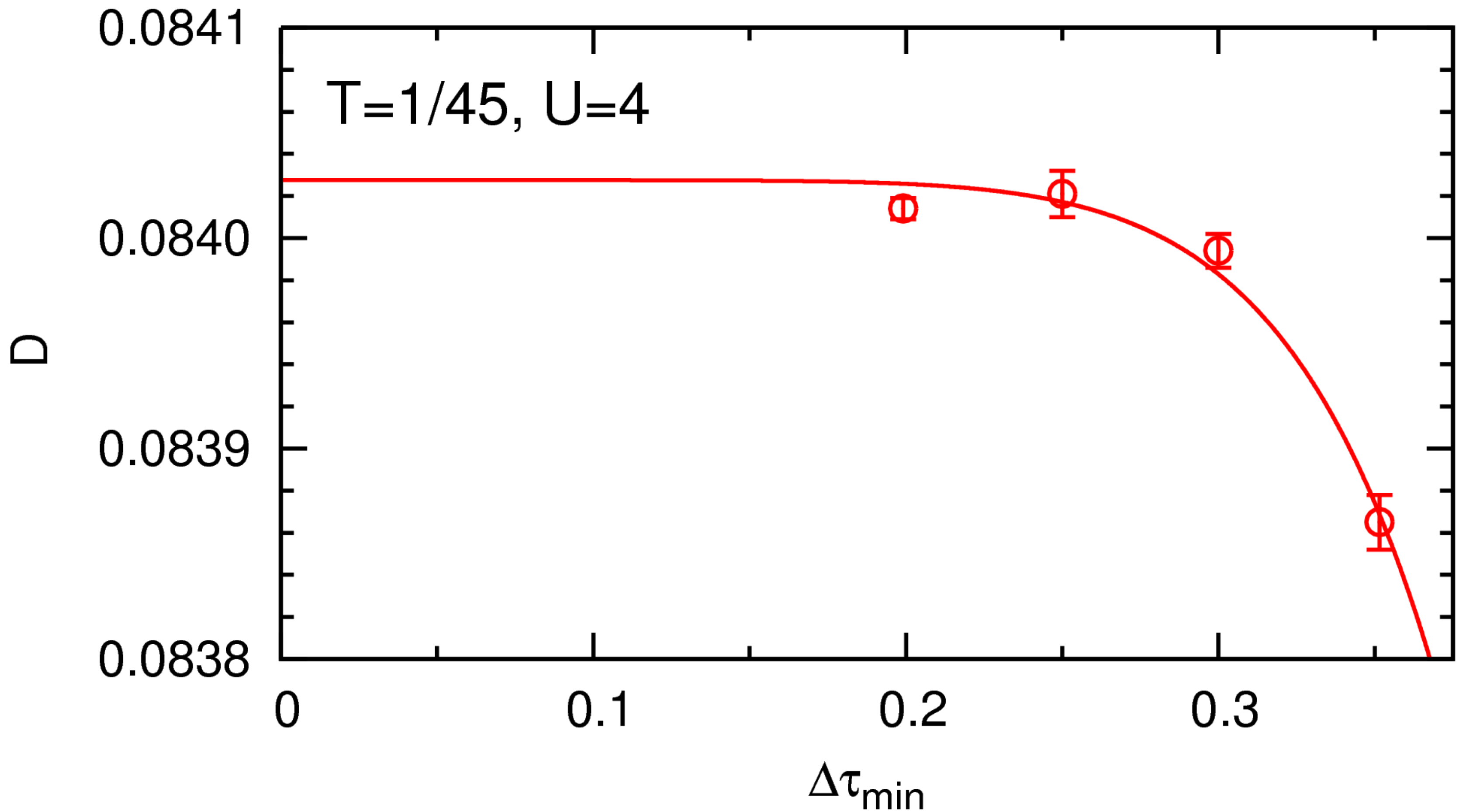


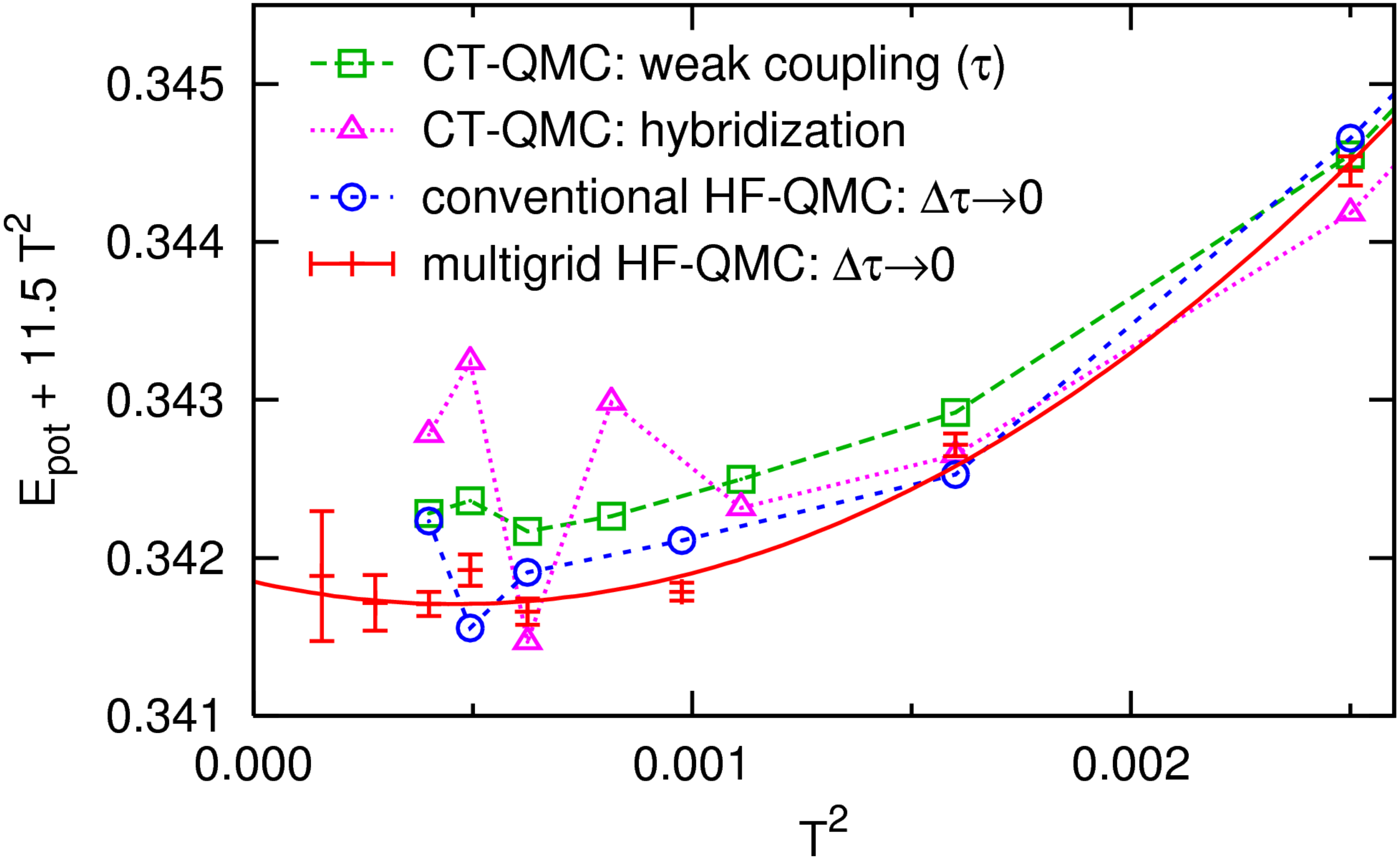
Conventional HF-QMC:	no insulating solution for $\Delta\tau \gtrsim 0.4$
	very irregular $\Delta\tau$ dependence beyond $\Delta\tau \approx 0.3$
Multigrid HF-QMC:	vastly larger useful range of $\Delta\tau$

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



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

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

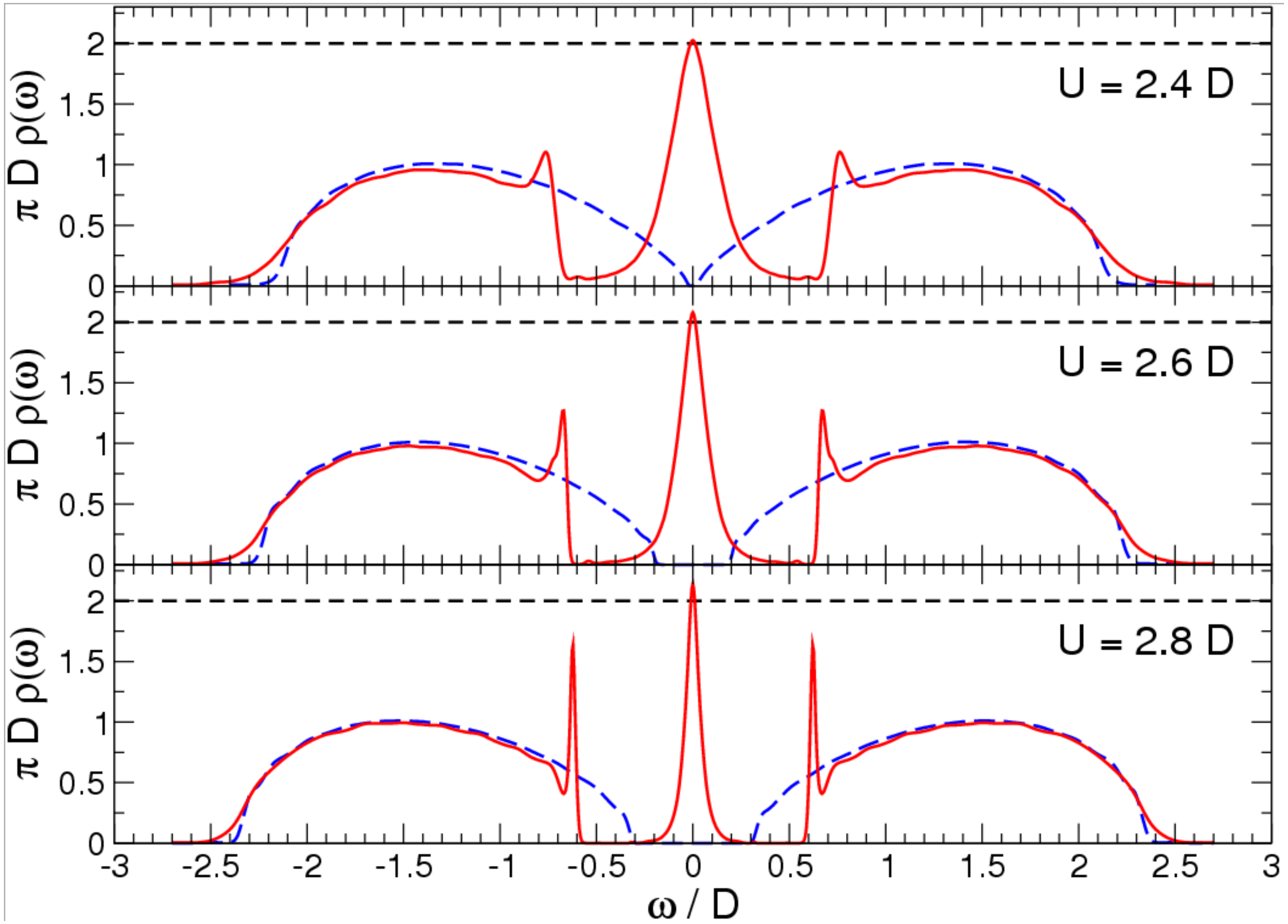


No more "difficult observables" for multigrid HF-QMC

Higher precision than CT-QMC methods at same effort

Spectral weight transfer at the Mott transition

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



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

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

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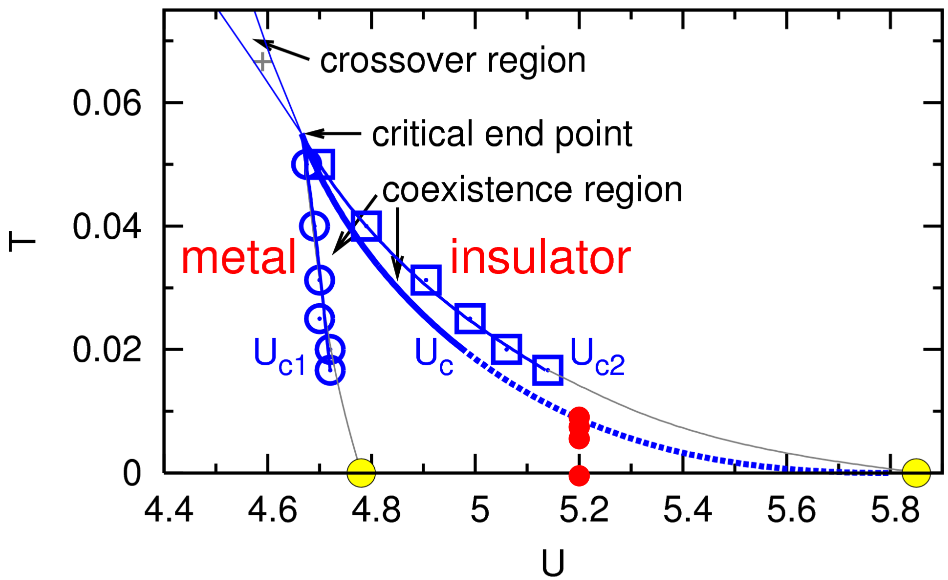

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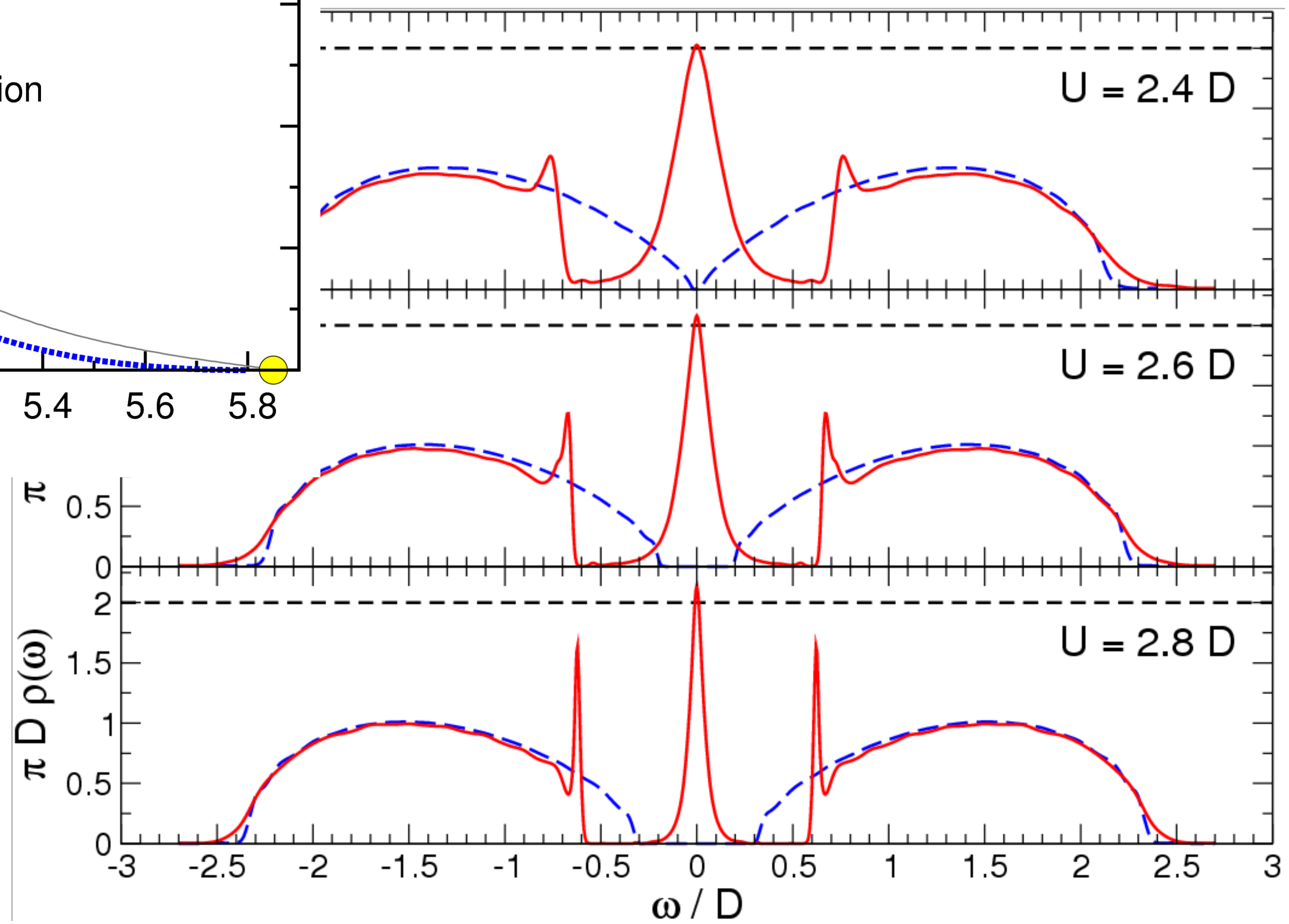
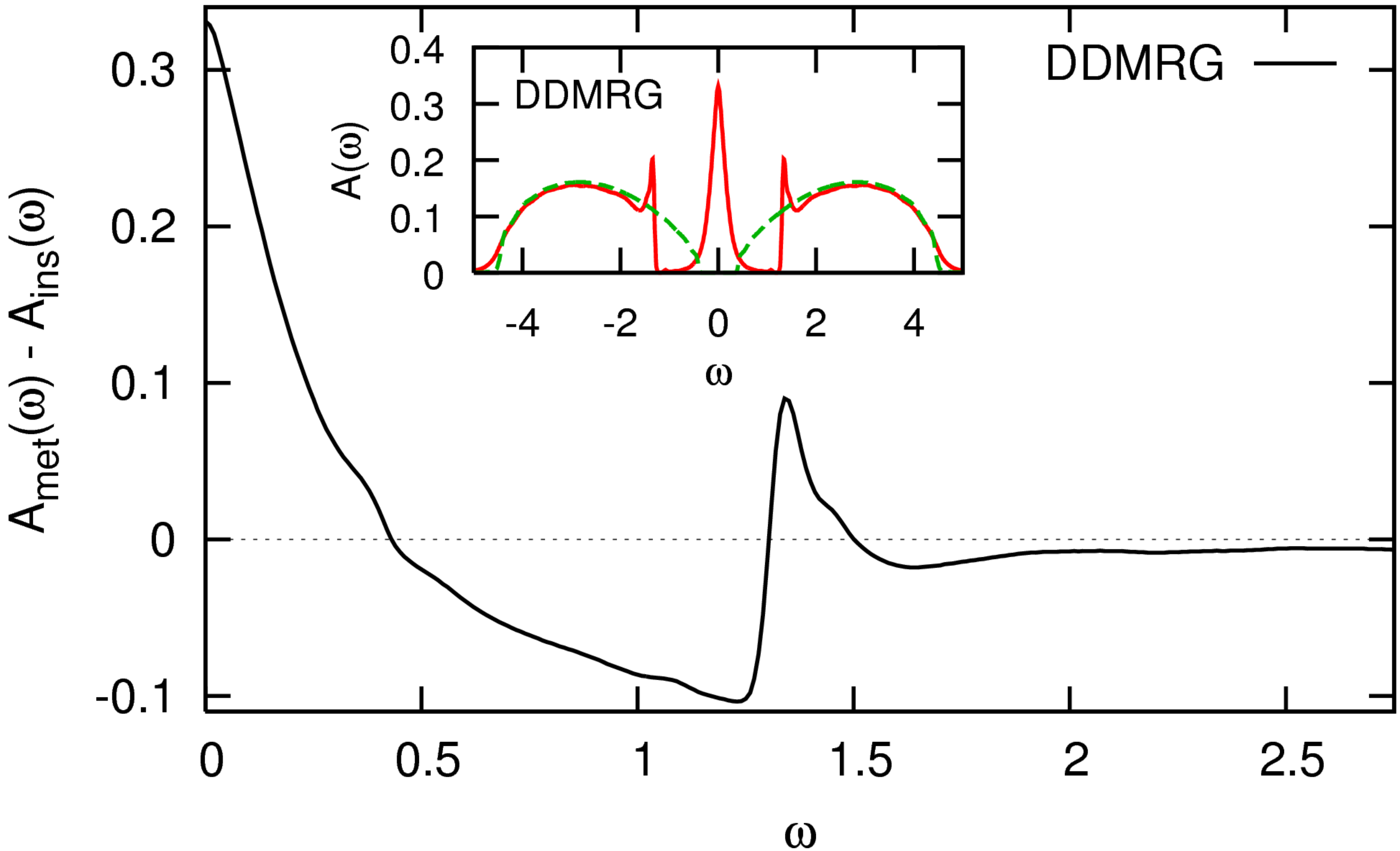


Dynamical DMRG $\rightsquigarrow$ Hubbard band subpeaks in metallic phase (at $T = 0$)

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

Check using multigrid HF-QMC. . .

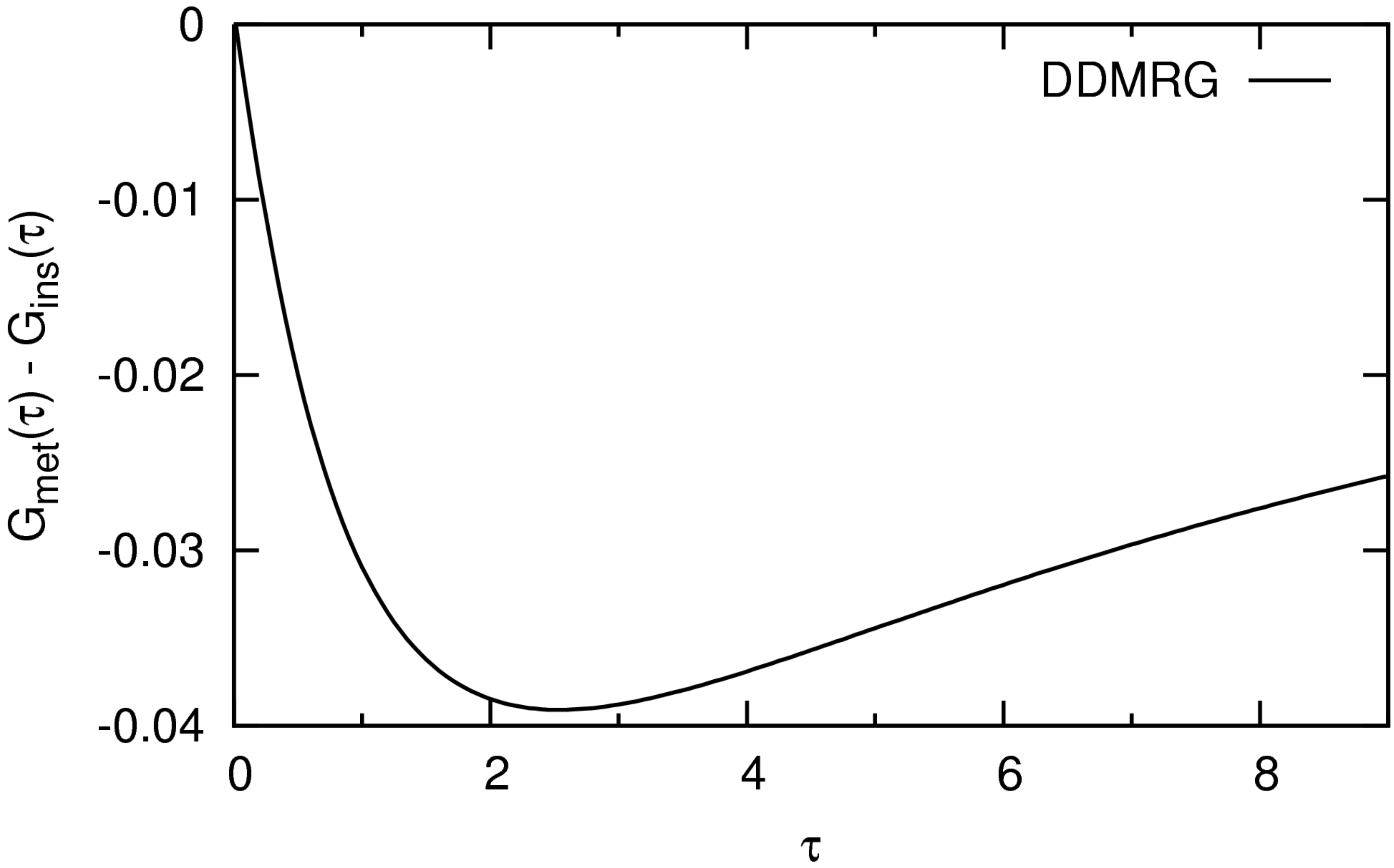
Analysis via difference of spectral functions (symmetric in ω) at $U = 5.2$



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

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

Difference Green functions in imaginary time



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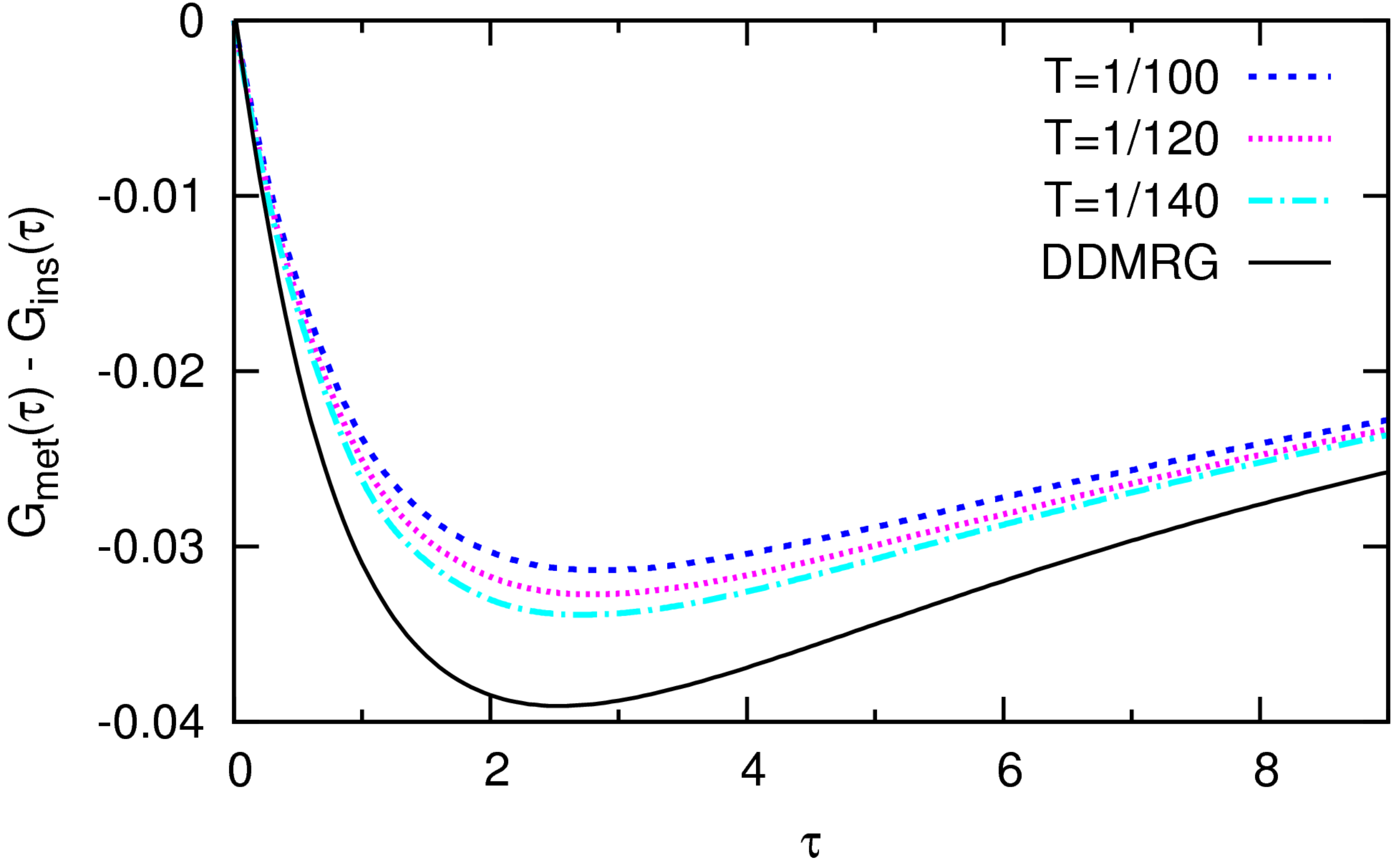

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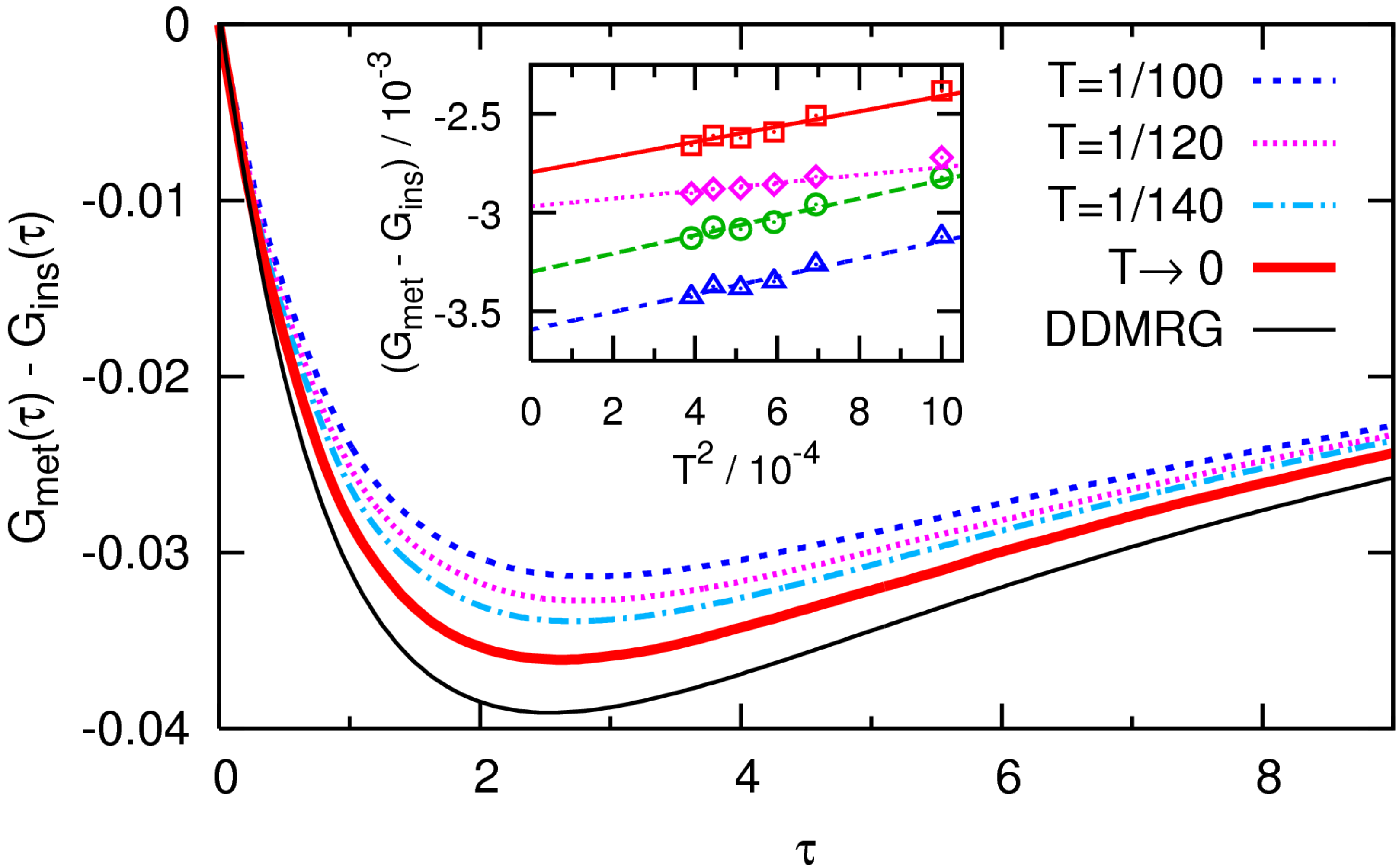
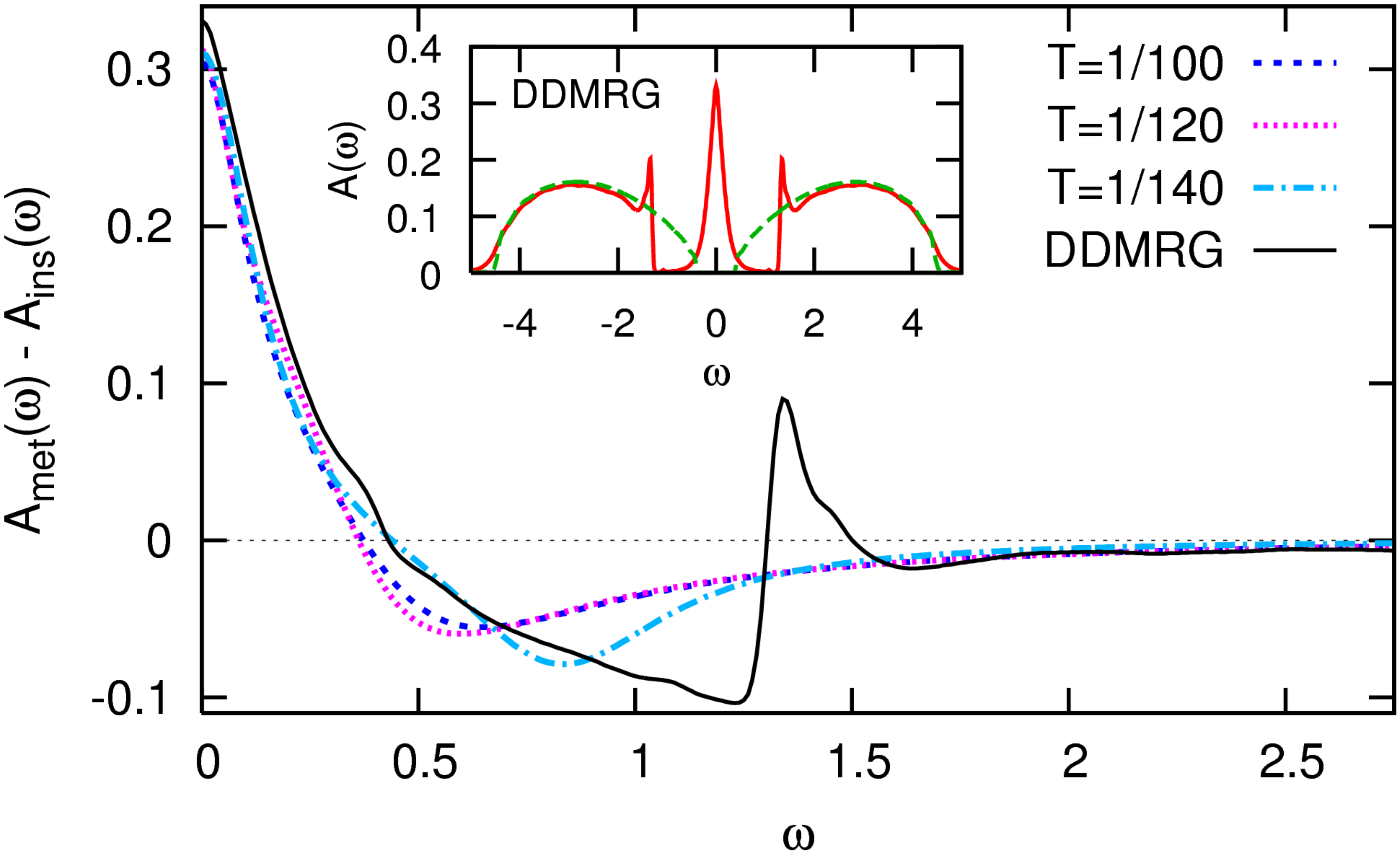


Multigrid HF-QMC data precise within linewidths [NB, arXiv:0801.1222]

DDMRG overestimates spectral weight transfer at $U = 5.2$ by about 10%!

Difference spectra



Similarities, but no indication for feature at $\omega = 1.3$ in QMC data [NB, arXiv:0801.1222]

Thermal breakdown of a Fermi liquid

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

When/how do these laws break down?

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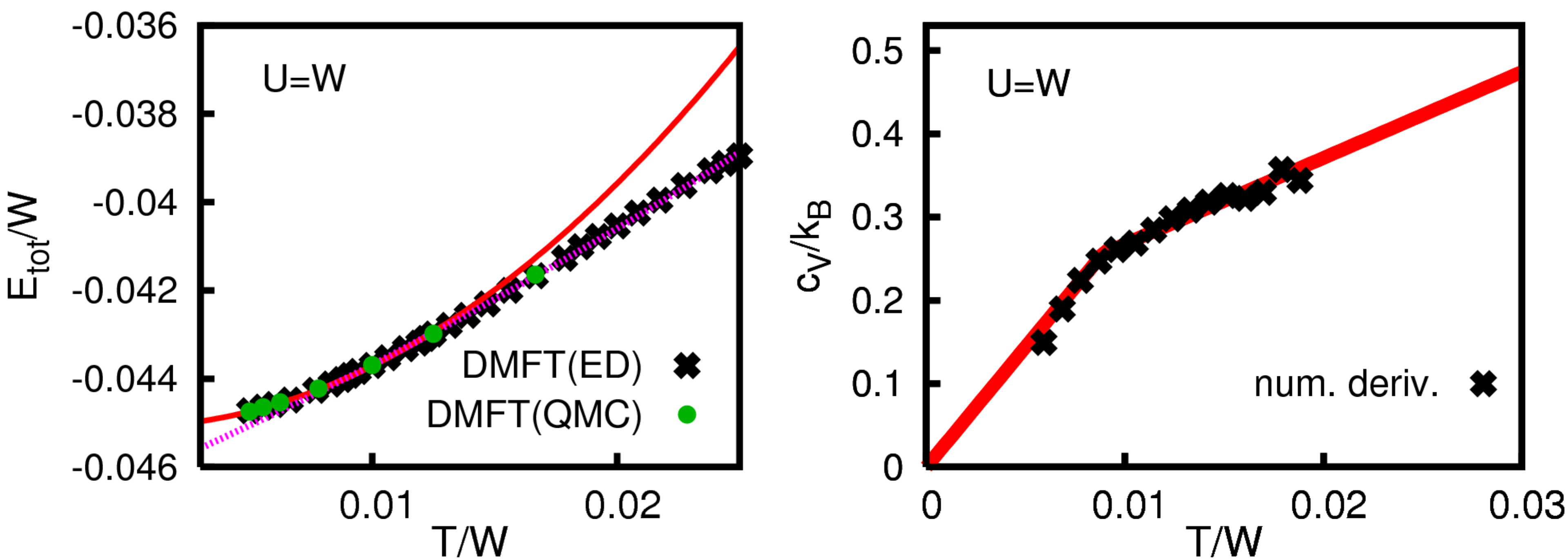
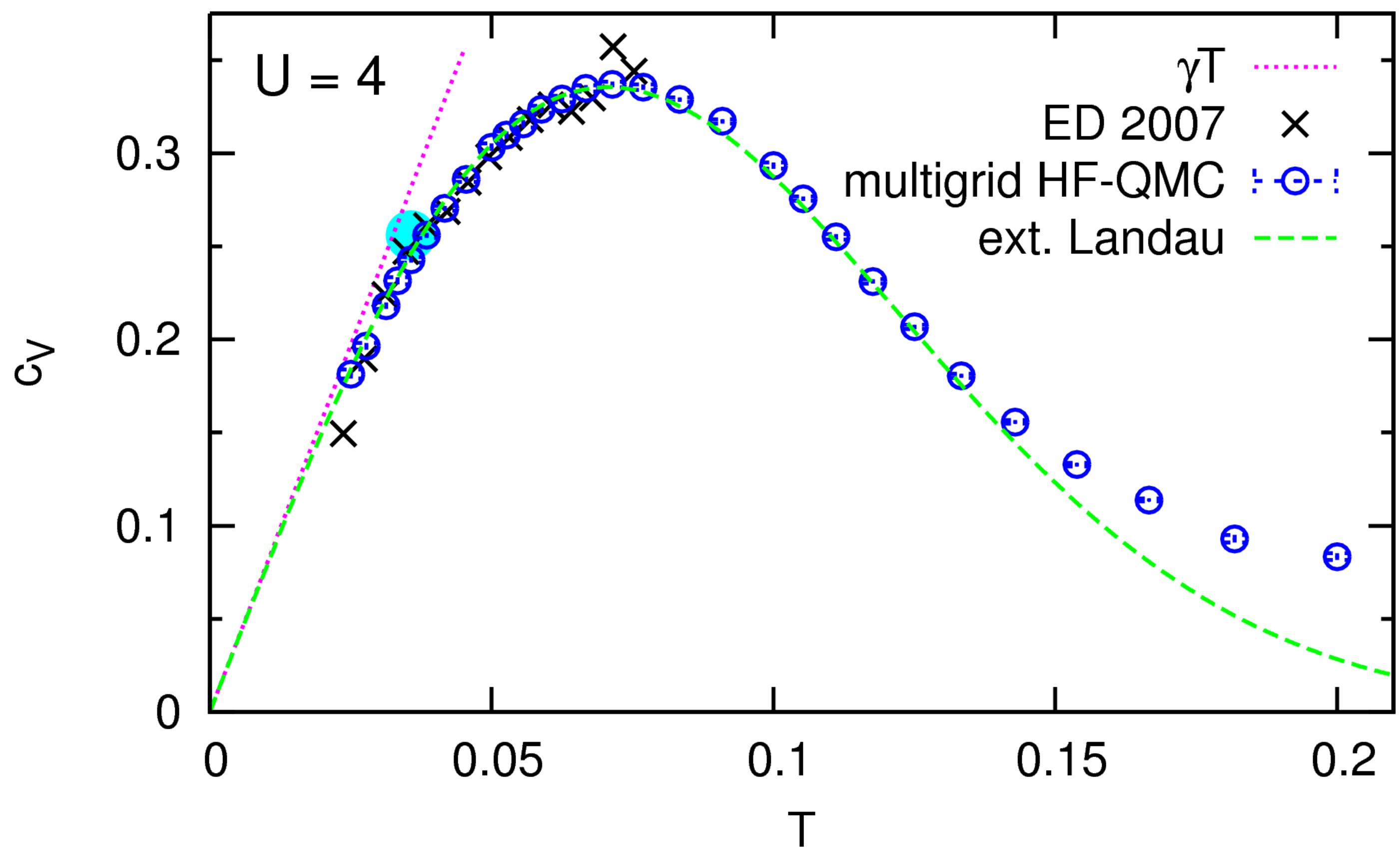
When/how do these laws break down?

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



Distinct kink in c_V! [A. Toschi, M. Capone, C. Castellani, K. Held, arXiv:0712.3723]

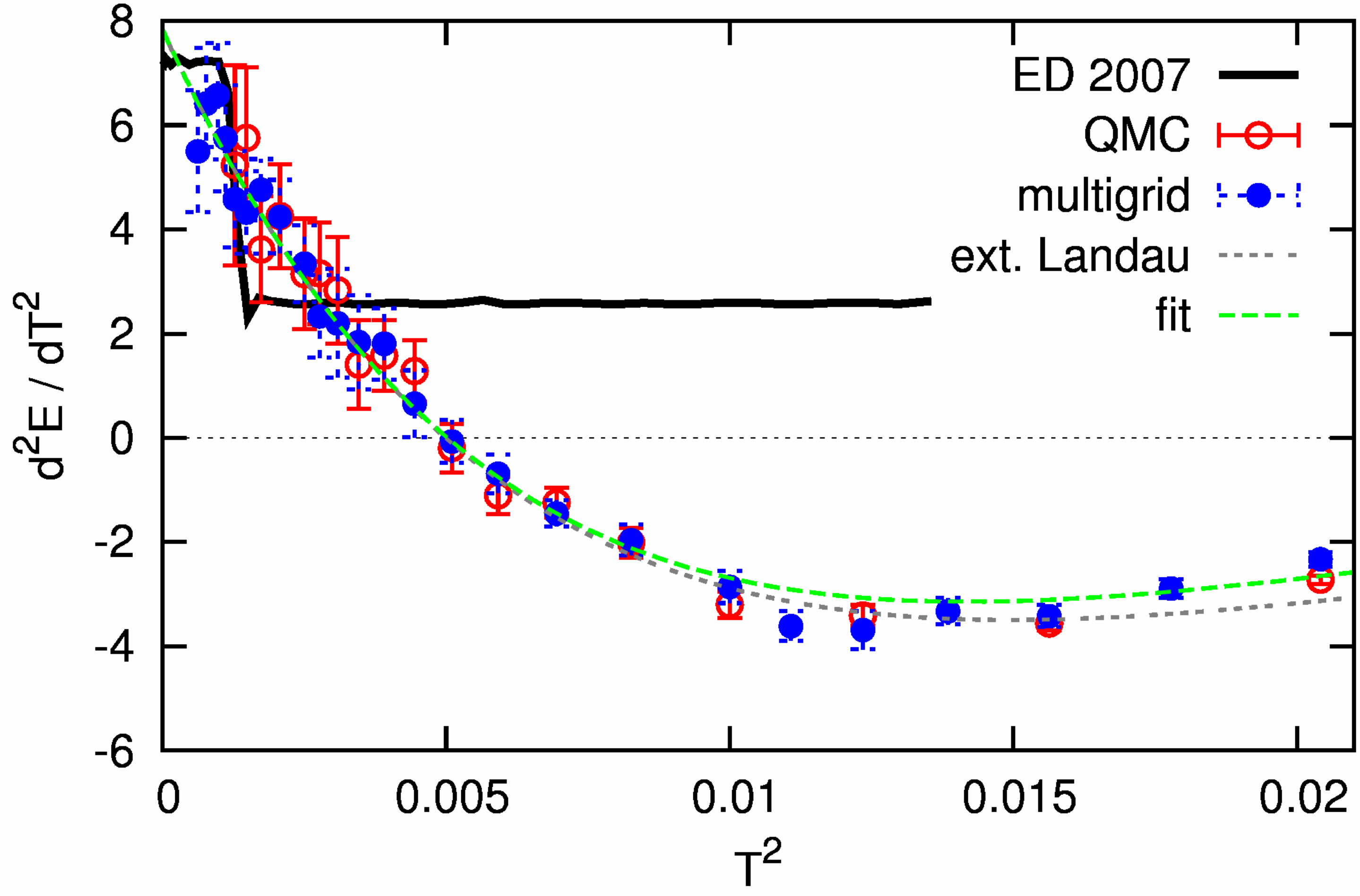


High-precision results ⇝ no kink!

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

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

Direct measure of "kinkiness": energy curvature



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

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

Summary

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: spectral-weight transfer, specific heat

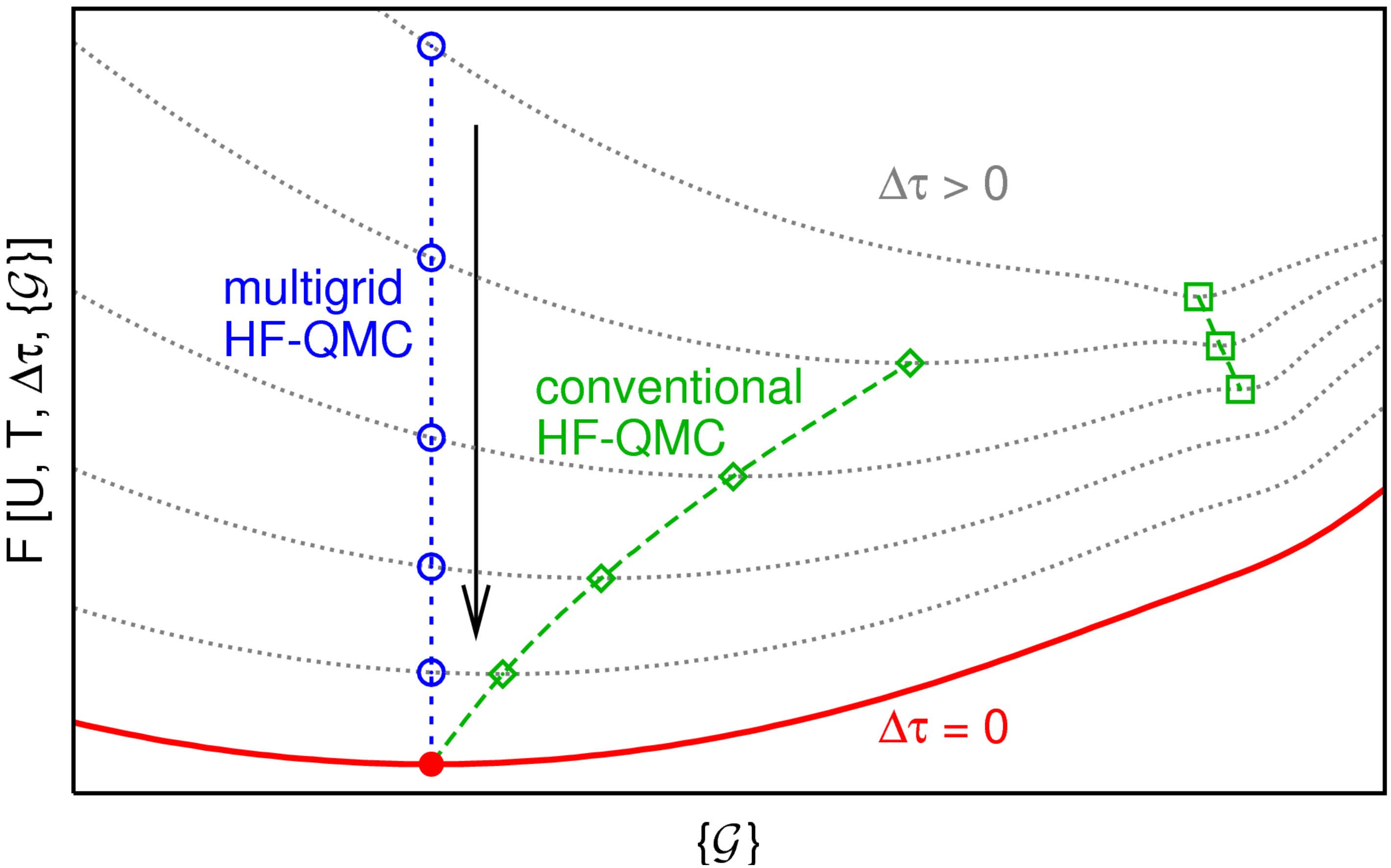
Not shown: arbitrary filling, multi-band [e.g. SU(2M) symmetric for M=1,2,4,8] . . .
3-spin/flavor systems ($\longrightarrow$ talk by E. Gorelik)

Acknowledgements

Carsten Knecht, Elena Gorelik, Eberhard Jacobi, Peter van Dongen

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

Schematic comparison via generalized Ginzburg-Landau functionals



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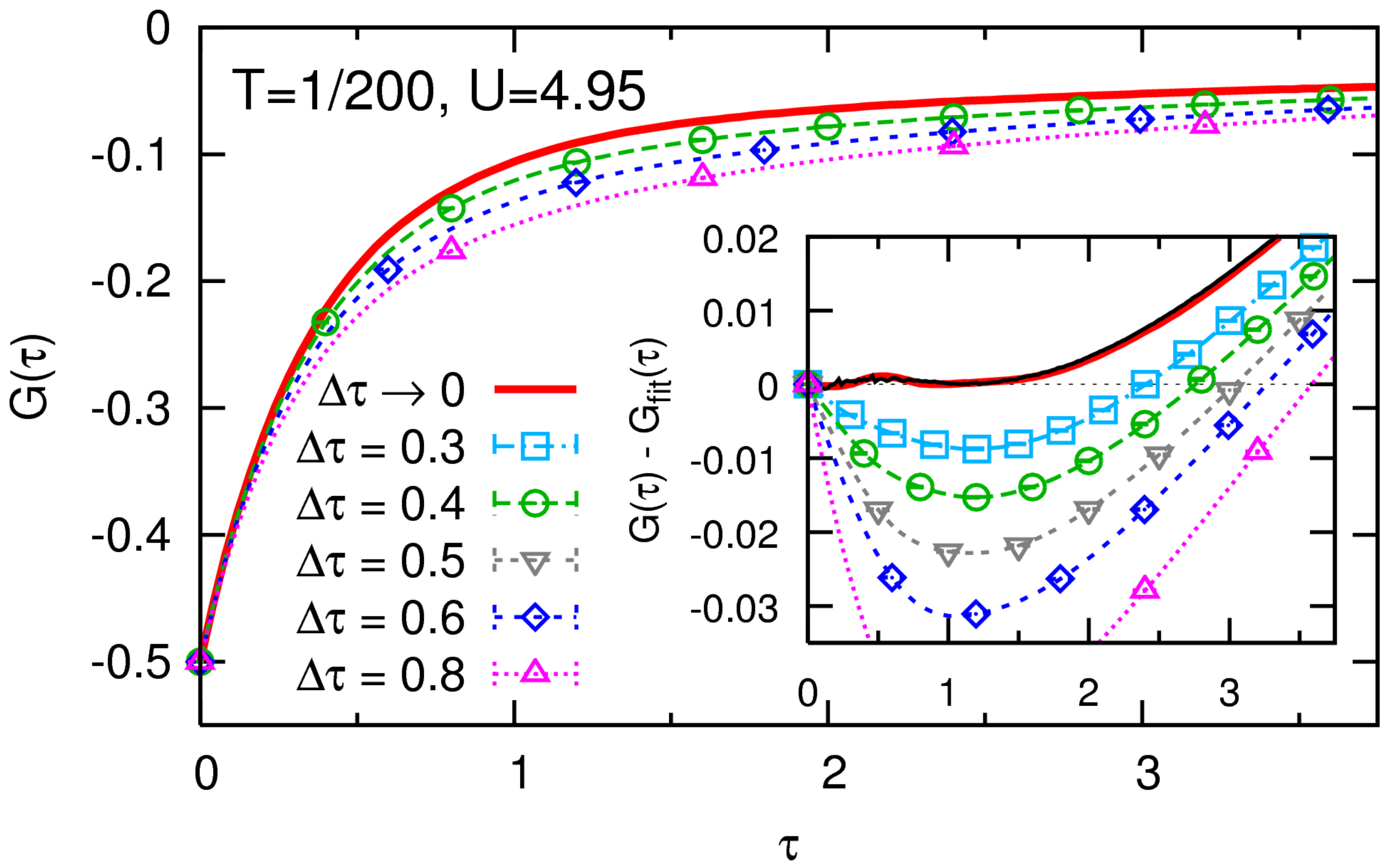
Multigrid Hirsch-Fye QMC: DMFT iteration towards exact fixed point

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

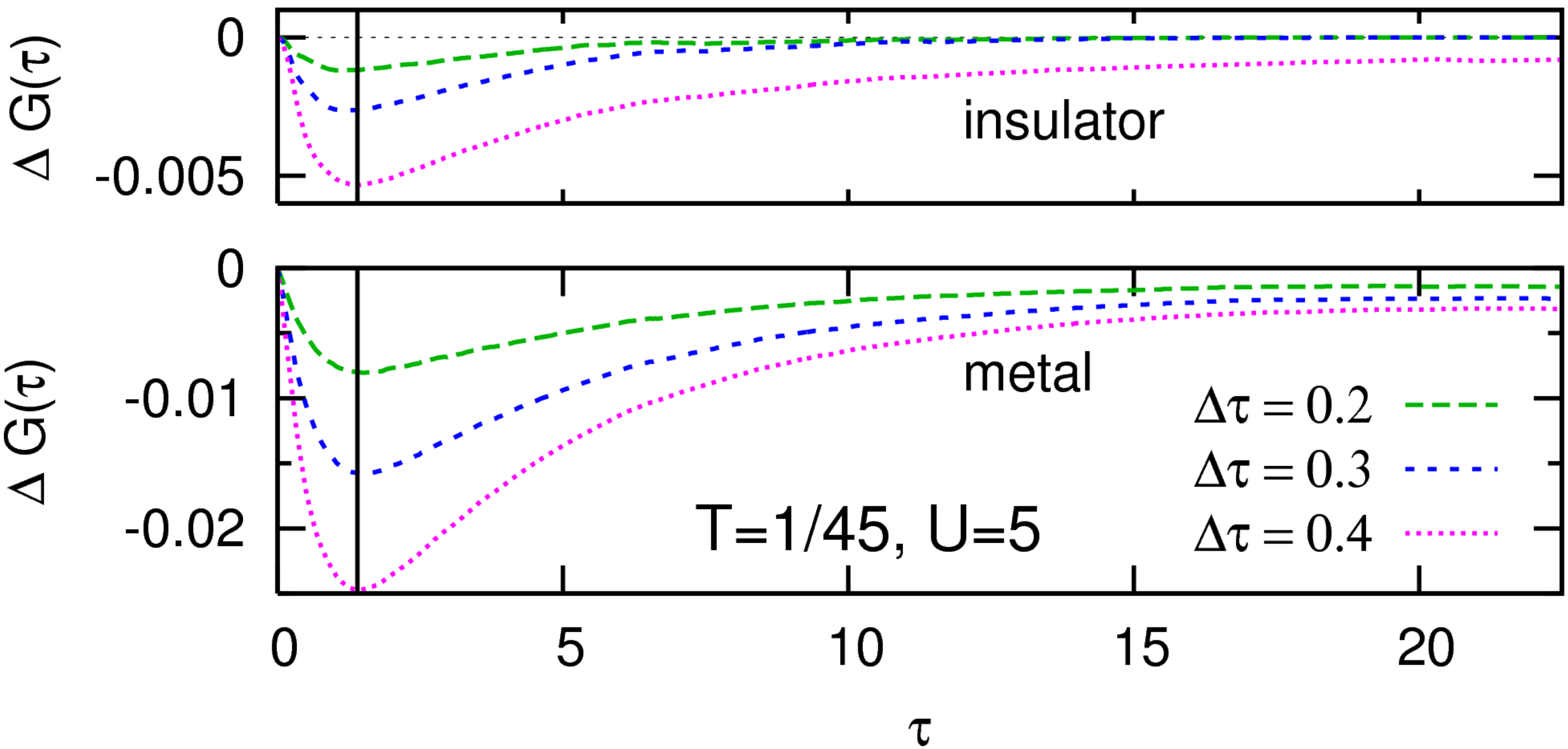
Example: interpolation and extrapolation of Green functions



[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!