Quantum Monte Carlo (QMC) Simulations within the Dynamical Mean-field Theory (DMFT)

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TP6, WA Prof. van Dongen (KOMET337)

Outline

Introduction: Hubbard model, DMFT, self-energy

General Monte Carlo principles

Hirsch-Fye QMC algorithm; error bars

Mott Insulator (1 band): QMC vs. ePT and SFT/DIA

LDA+DMFT(QMC) for $La_{1-x}Sr_xTiO_3$; MEM

Summary and Preview

Introduction: Hubbard model, DMFT

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

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Born-Oppenheimer approximation $\downarrow$

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

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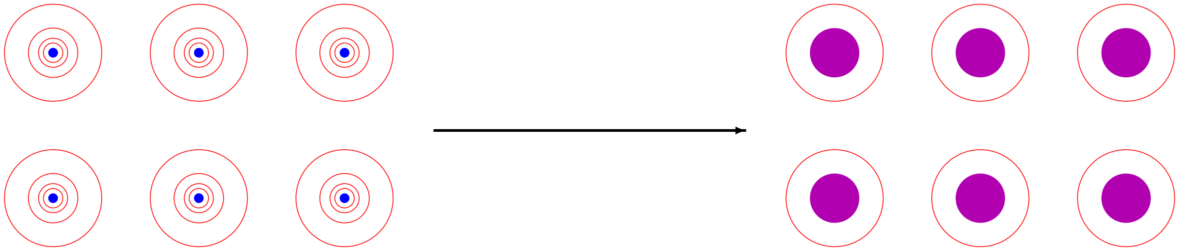
reduction to valence electrons ↓

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



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occupation number formalism, 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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← **density functional theory (DFT)**

reduction to valence electrons ↓

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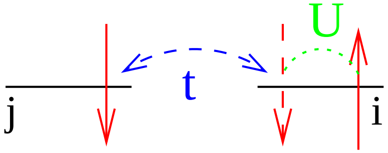
Hubbard model

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



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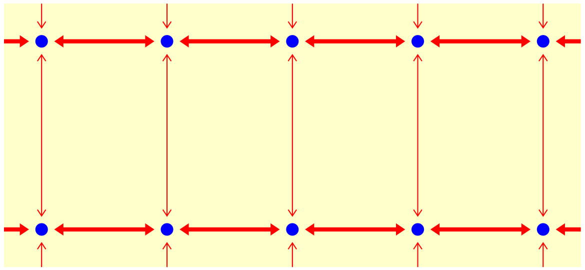
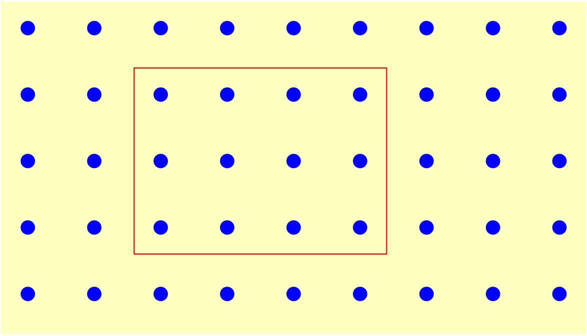
$d = 1$: Bethe ansatz, DMRG



Perturbation theory, e.g.

- $U \longrightarrow 0$: Hartree-Fock (uncorrelated)
- $t/U \longrightarrow 0$: half filling $(n = 1)$ $\rightsquigarrow$ Heisenberg model
- $T \longrightarrow \infty$, $n \longrightarrow 0$
- ($V_{\text{ion}} \longrightarrow 0$ $\rightsquigarrow$ jellium model $\rightsquigarrow$ LDA)

finite clusters: ED, QMC



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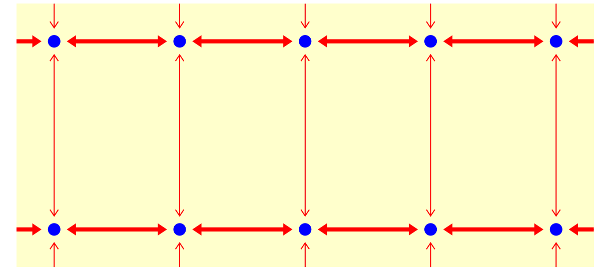

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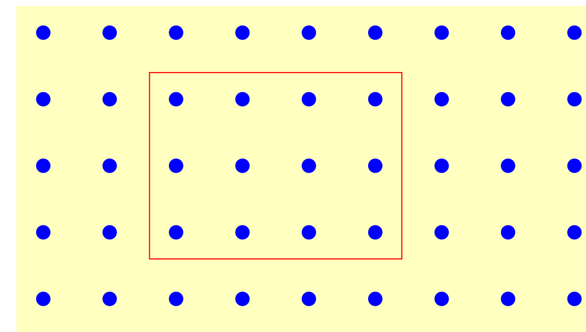
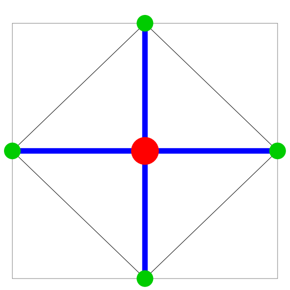
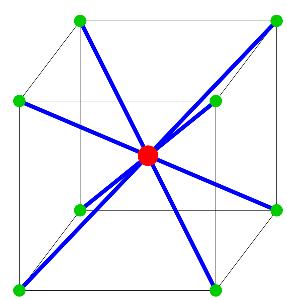


Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$

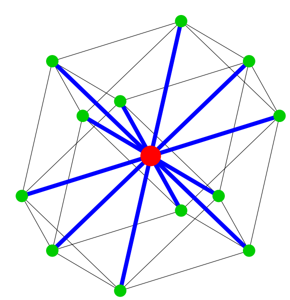
+ non-perturbative
  $\rightsquigarrow$ valid at MIT
+ dynamical on-site
  correlations preserved
+ exact for $Z \longrightarrow \infty$
+ in thermodynamic limit



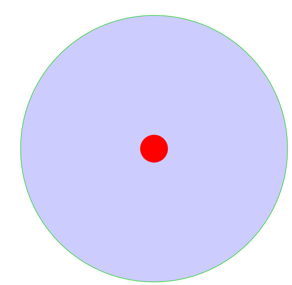
d=2: $Z = 4$



bcc: $Z = 8$



fcc: $Z = 12$

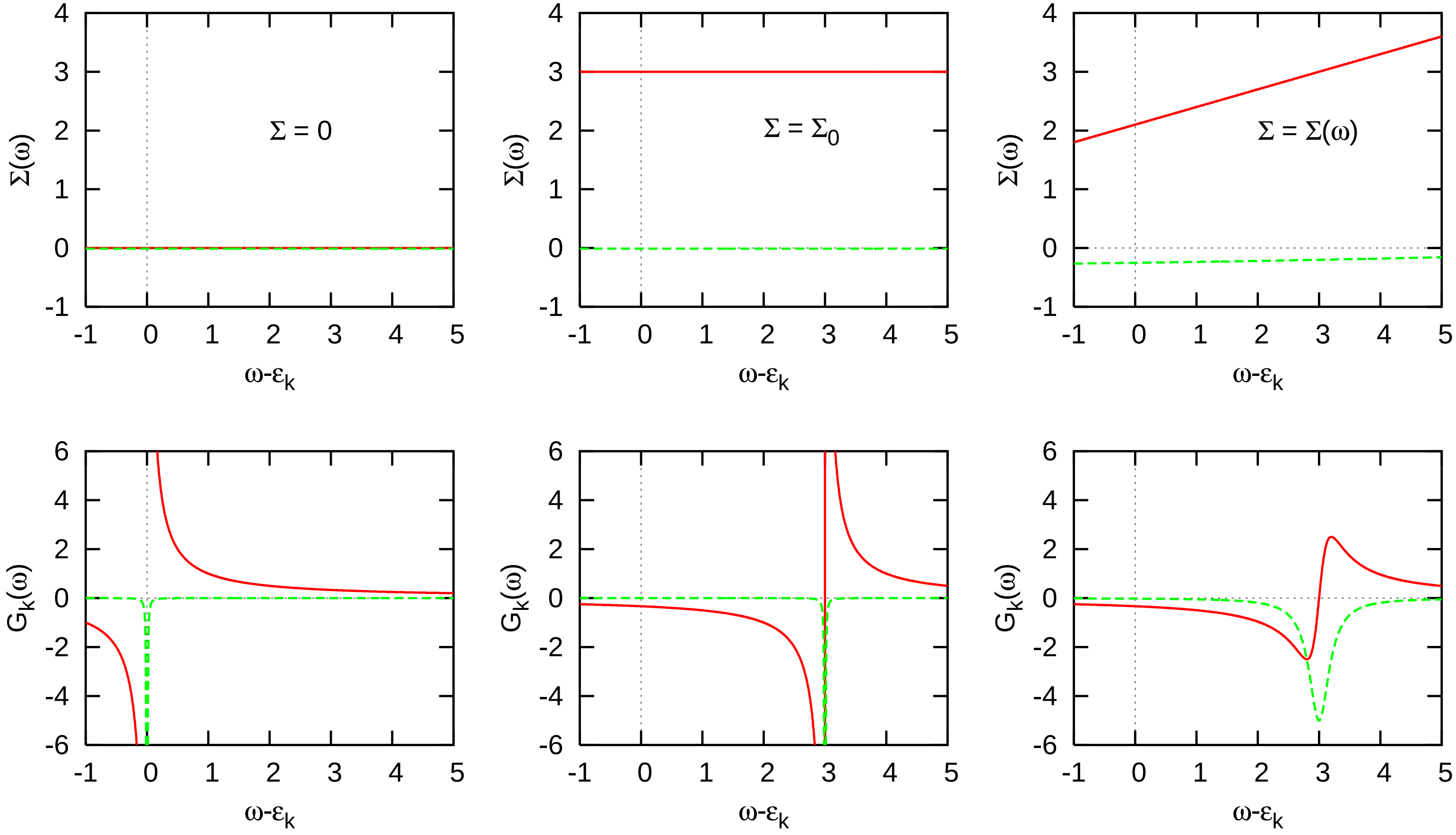


DMFT: $Z = \infty$

Excursus: Green function and self-energy

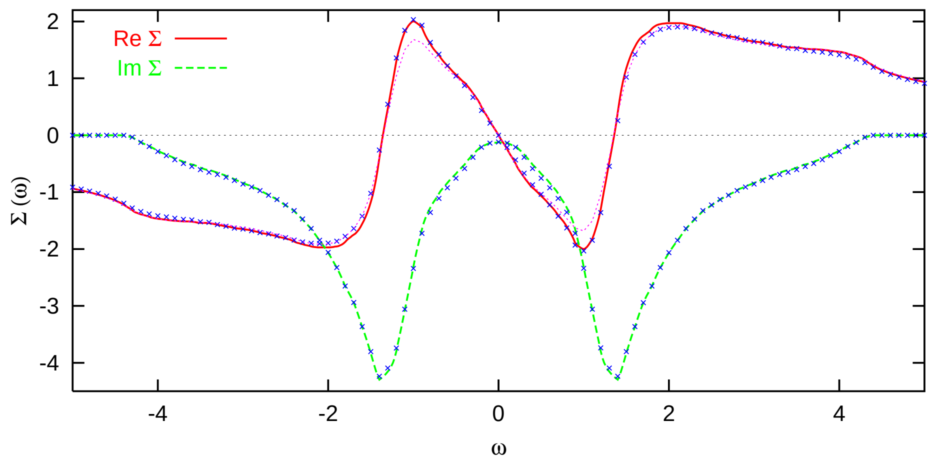
Noninteracting (1-band) system: dispersion $\epsilon_{\boldsymbol{k}}$, density of states $\rho(\epsilon) = \frac{1}{V_{\text{B}}} \int d^3k\, \delta(\epsilon - \epsilon_{\boldsymbol{k}})$

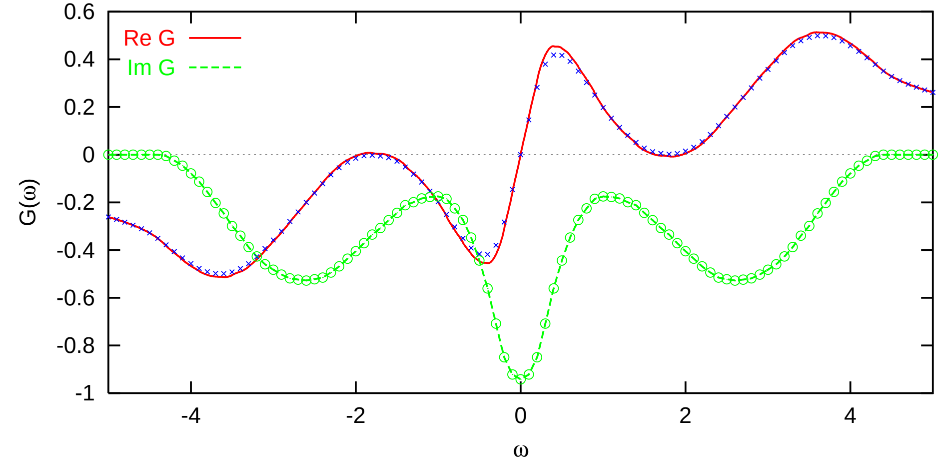
Green function (within DMFT for $\mu = 0$): $G_{\boldsymbol{k}}(\omega) = \dfrac{1}{\omega - \epsilon_{\boldsymbol{k}} - \Sigma(\omega)} = \dfrac{(\omega - \epsilon_{\boldsymbol{k}} - \Sigma') + i\Sigma''}{(\omega - \epsilon_{\boldsymbol{k}} - \Sigma')^2 + \Sigma''^2}$

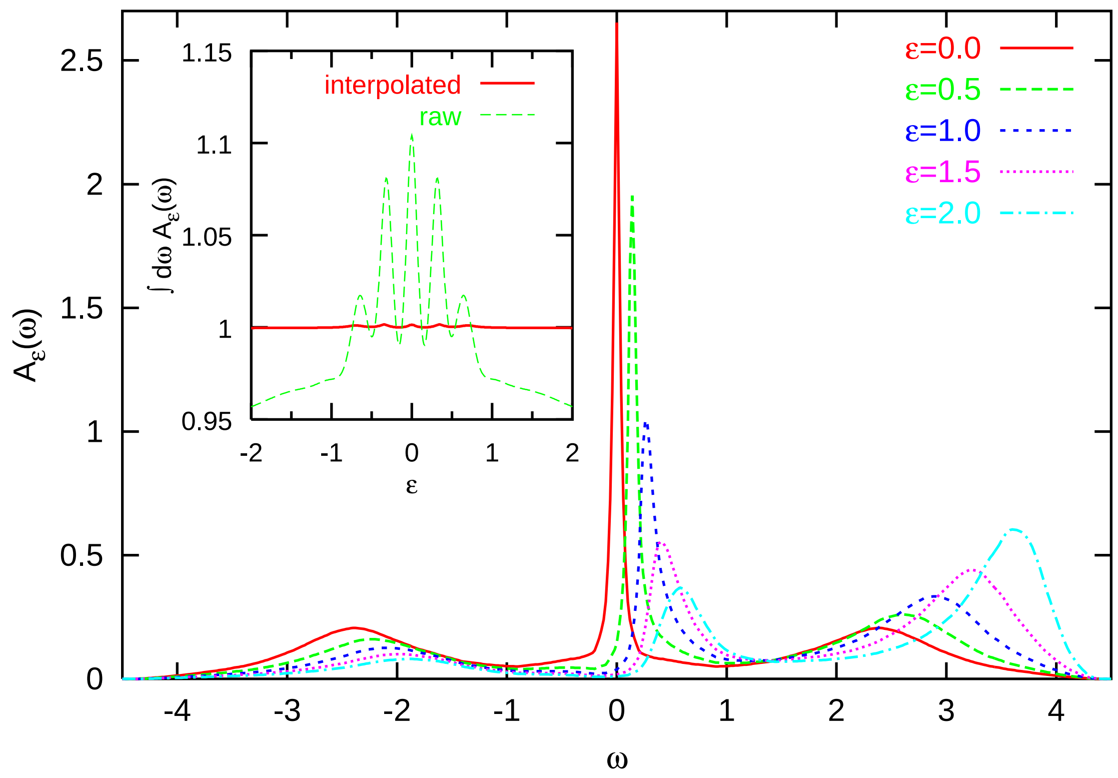


$$A(\omega) = -\frac{1}{\pi}\text{Im}G(\omega + i0^+) \xrightarrow{\Sigma\to 0} \rho(\omega); \qquad G(\omega) \equiv G_{ii}(\omega) = \int d\epsilon\, \frac{\rho(\epsilon)}{\omega - \epsilon - \Sigma(\omega)}$$

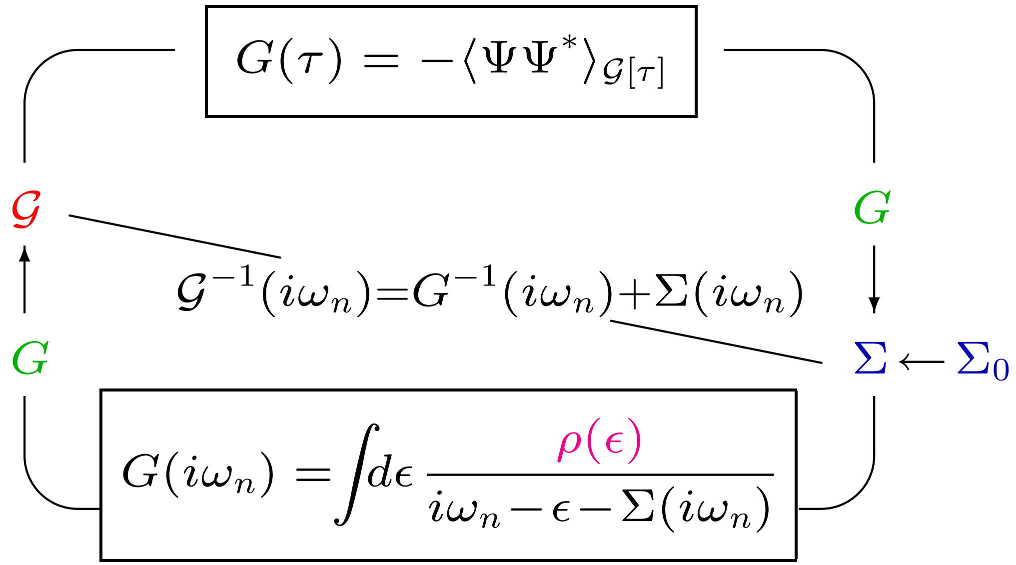
Example: half-filled frustrated Hubbard model, U=W=4, T=0.05





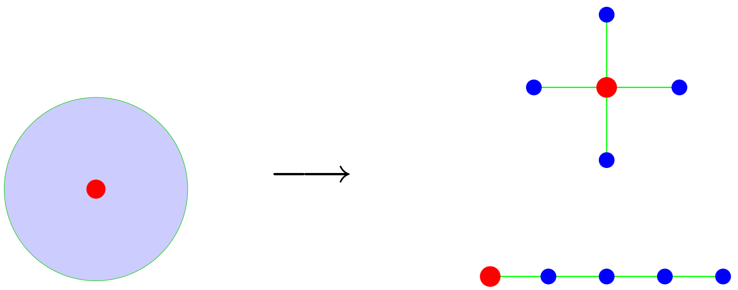


Iterative solution of DMFT equations



Impurity solver:

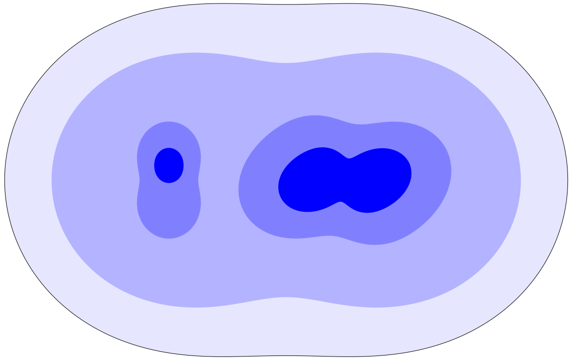
- Quanten-Monte-Carlo (QMC)
- Iterative perturbation theory (IPT; not controlled)
- Non-crossing approximation (NCA; not controlled)
- Exact diagonalization (ED; large finite-size errors)
- Numerical renormalization group (NRG; 1-2 bands)
- Density matrix renormalization group (DMRG)
- Self-energy functional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



Direct $d = \infty$ solution: PT, ePT

Excursus: Monte-Carlo Principles

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



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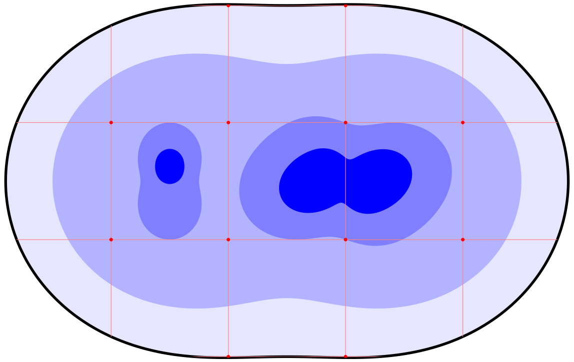

Deterministic: lattice + trapezoid rule
$N = V/(\Delta x)^d$ measurements

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

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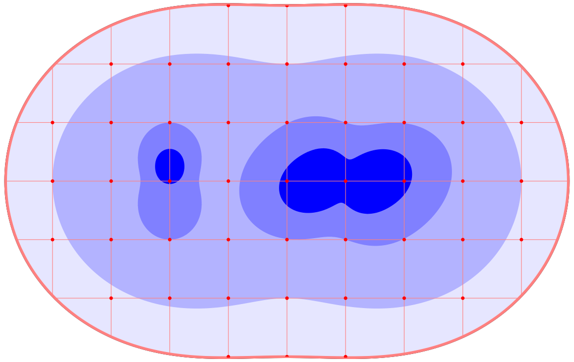

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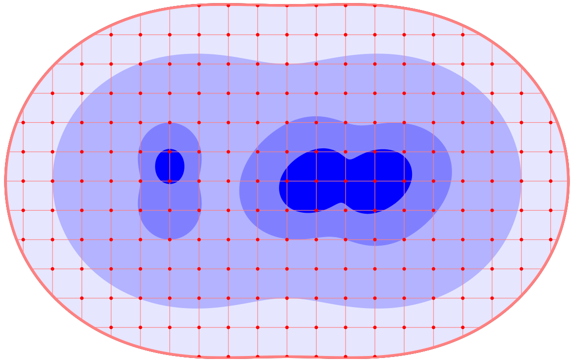

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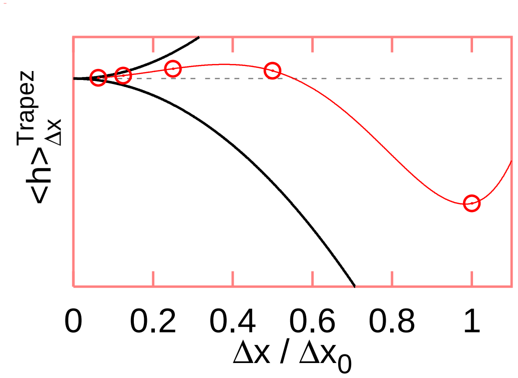

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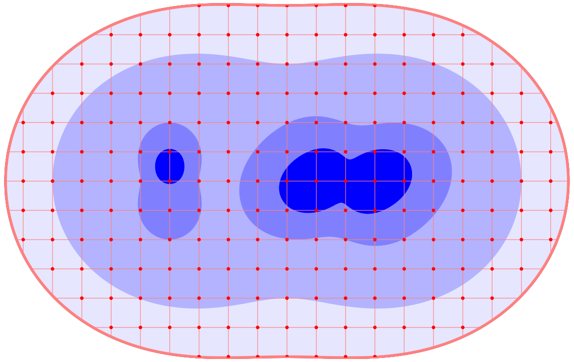

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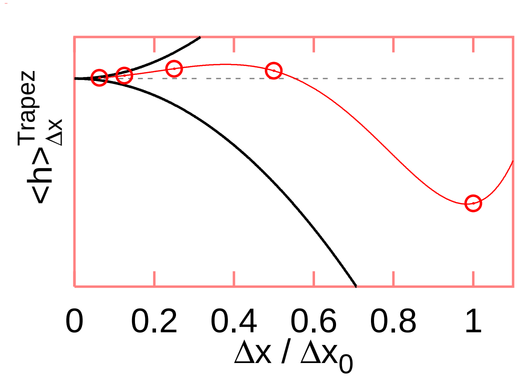
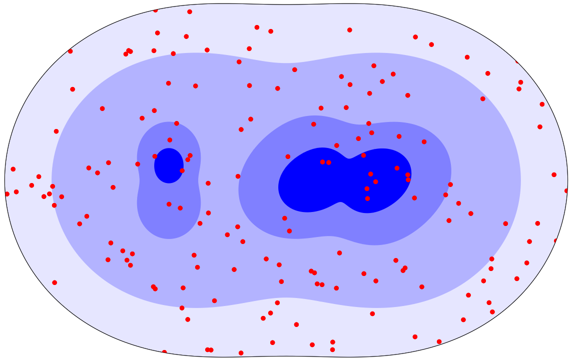
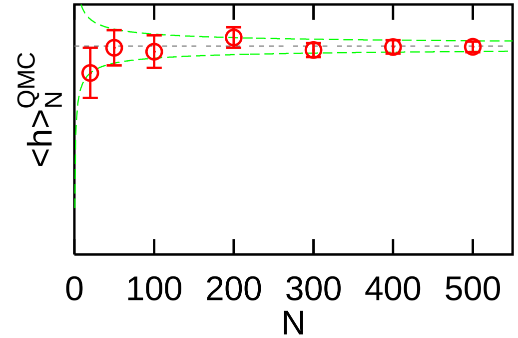




Stochastic: simple Monte-Carlo

N "configurations", equally probable

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



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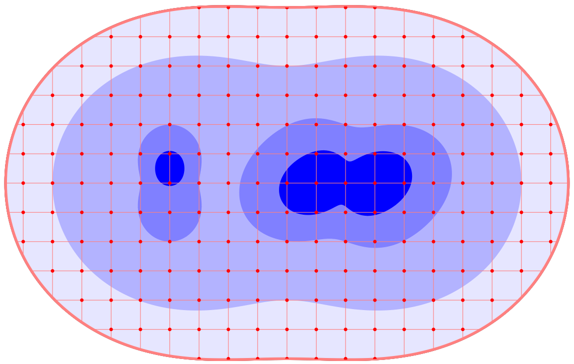

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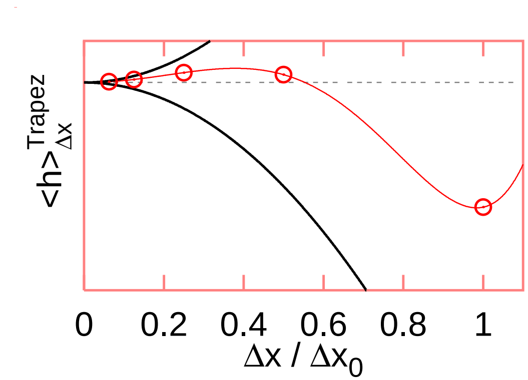

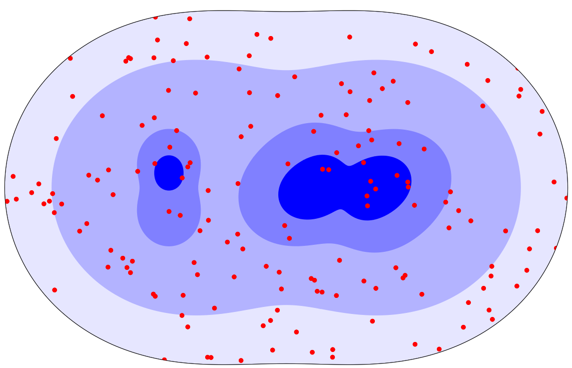

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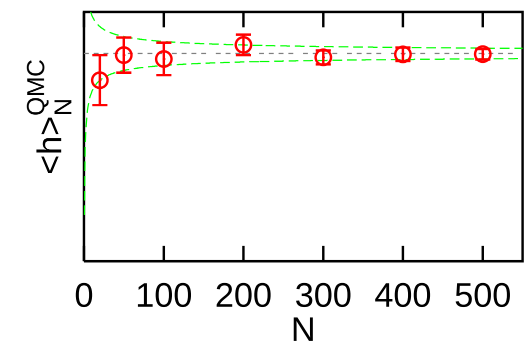
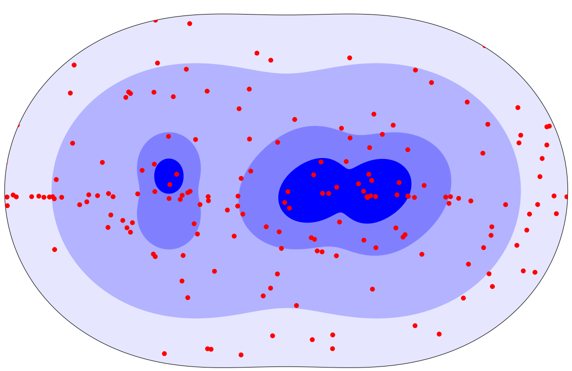


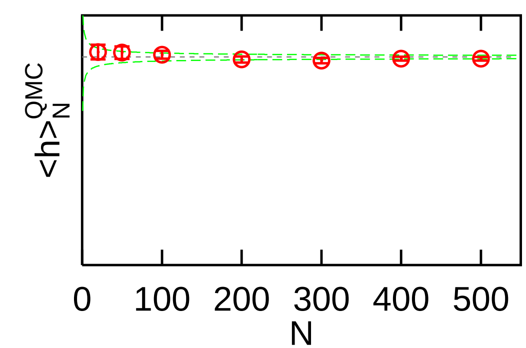


Stochastic: Importance sampling MC

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

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

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



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

Solution: generate probability distribution by *random walk*, e.g. using Metropolis algorithm:

$$P\{i \to j\} = \min\{p_j/p_i, 1\} \,, \quad p_j/p_i = e^{(E_j - E_i)/(k_\mathrm{B}T)}$$

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

+ Precise computation of observable averages $\langle O \rangle$

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

Hirsch-Fye QMC algorithm for DMFT impurity problem

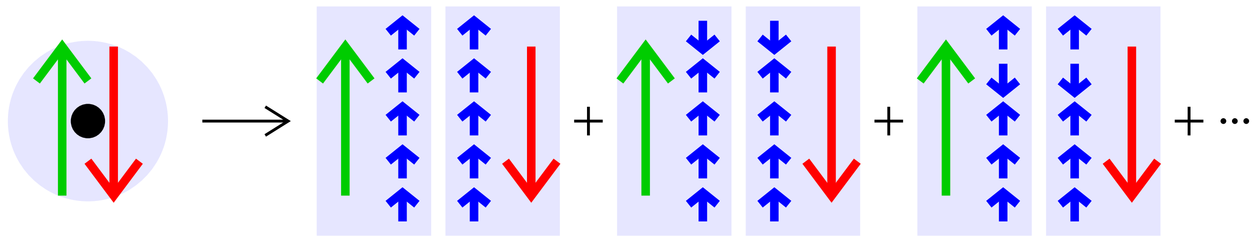
Wanted: Green-Funktion $G(\omega)$

Treatment in imaginary time using fermionic Grassmann variables ψ, ψ^*:

$$G_\sigma(\tau_2 - \tau_1) \equiv G_\sigma(\tau_1, \tau_2) = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\psi]\,\mathcal{D}[\psi^*]\;\psi_\sigma(\tau_1)\psi^*_\sigma(\tau_2)\;e^{\mathcal{A}},$$

$$\mathcal{A} = \mathcal{A}_0 - \frac{U}{2}\sum_{\sigma\sigma'}\int_0^\beta d\tau\,\psi^*_\sigma(\tau)\psi_\sigma(\tau)\psi^*_{\sigma'}(\tau)\psi_{\sigma'}(\tau)$$

discretization $\beta = \Lambda\,\Delta\tau$, Trotter decoupling, discrete Hubbard-Stratonovich transformation



Wick theorem:

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

Metropolis MC importance sampling over auxiliary Ising field, 2^Λ configurations, $50 \lesssim \Lambda \lesssim 400$

$+$ nonperturbative, numerically exact

$-$ effort scales as T^{-3}

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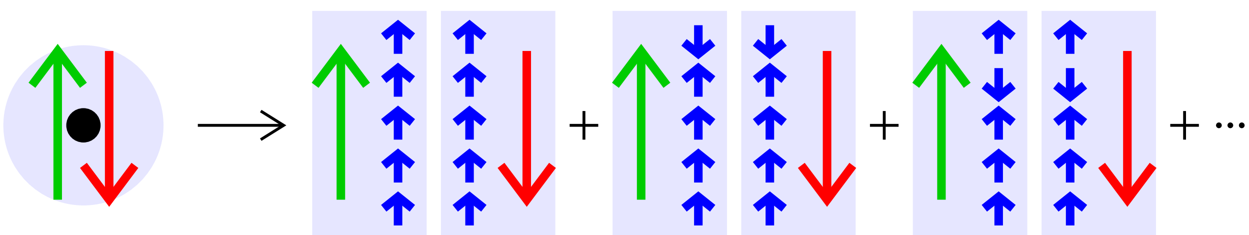


Wick theorem:

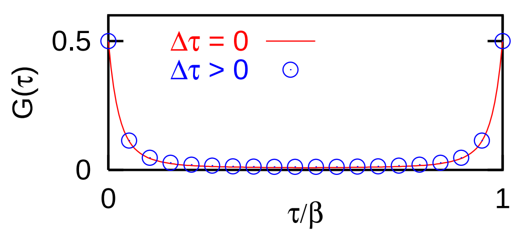
$$G = \frac{\sum M \det\{M\}}{\sum \det\{M\}}$$

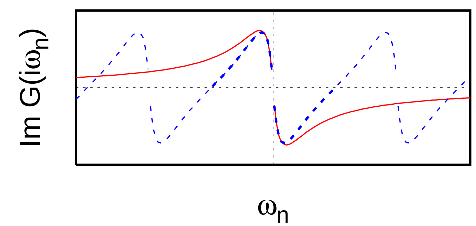
Metropolis MC importance sampling over auxiliary Ising field, 2^Λ configurations, $50 \lesssim \Lambda \lesssim 400$

+ nonperturbative, numerically exact

− effort scales as T^{-3}

− no information for $\omega \gtrsim \omega_{\text{Nyquist}}$

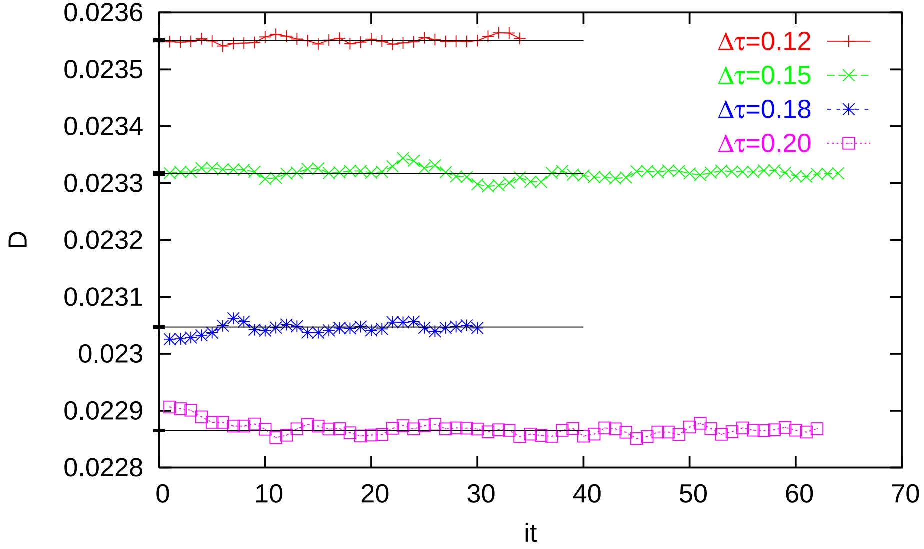


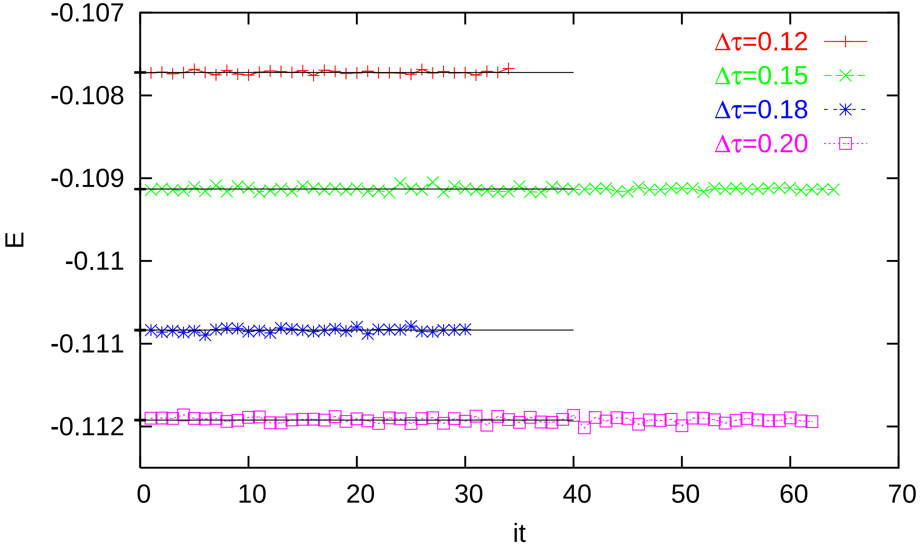


Contributions to DMFT-QMC error bars:

- statistical fluctuations + warm-up
- convergency (of self-consistency cycle)
- discretization (Trotter error and Fourier transform)

Example: half-filled frustrated Hubbard model, $U = 5$, $W = 4$, $T = 0.04$ (Mott insulator)





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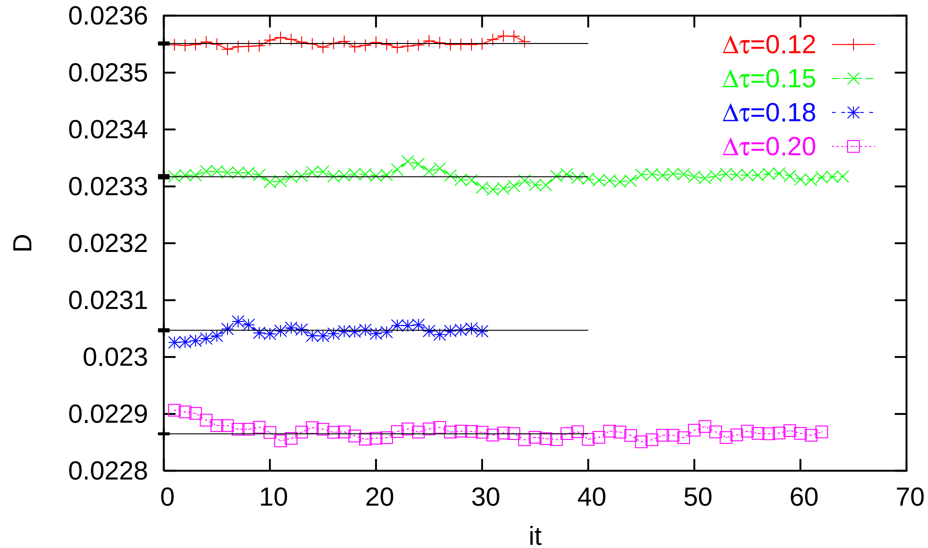
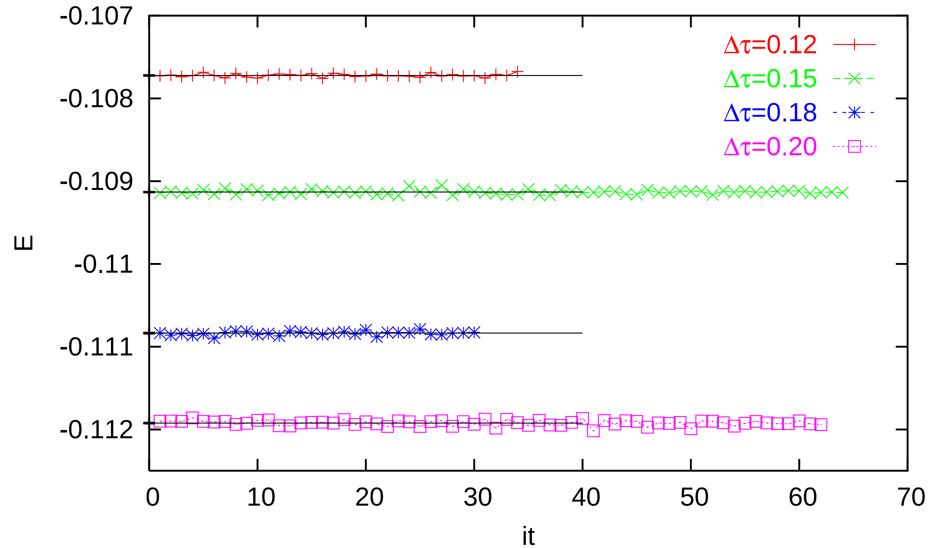
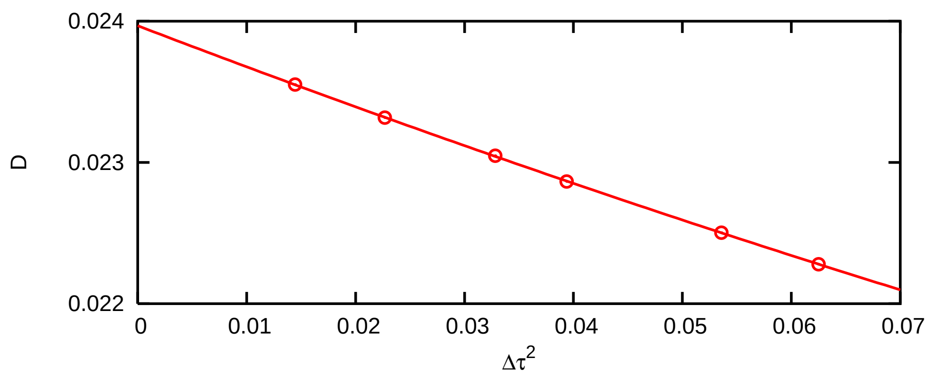
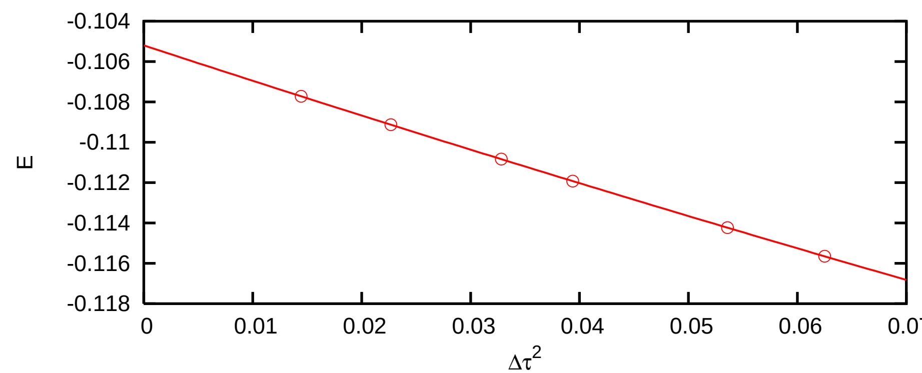








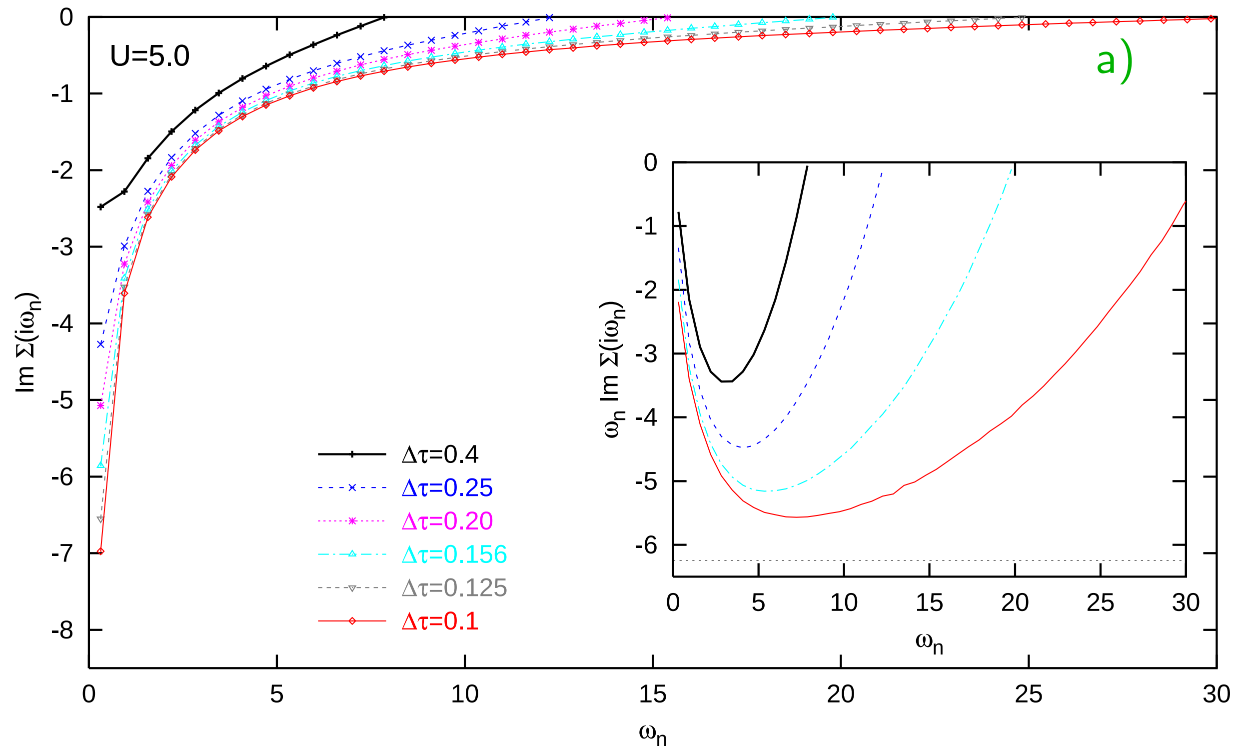
next: prerequisite for / proof of extreme precision

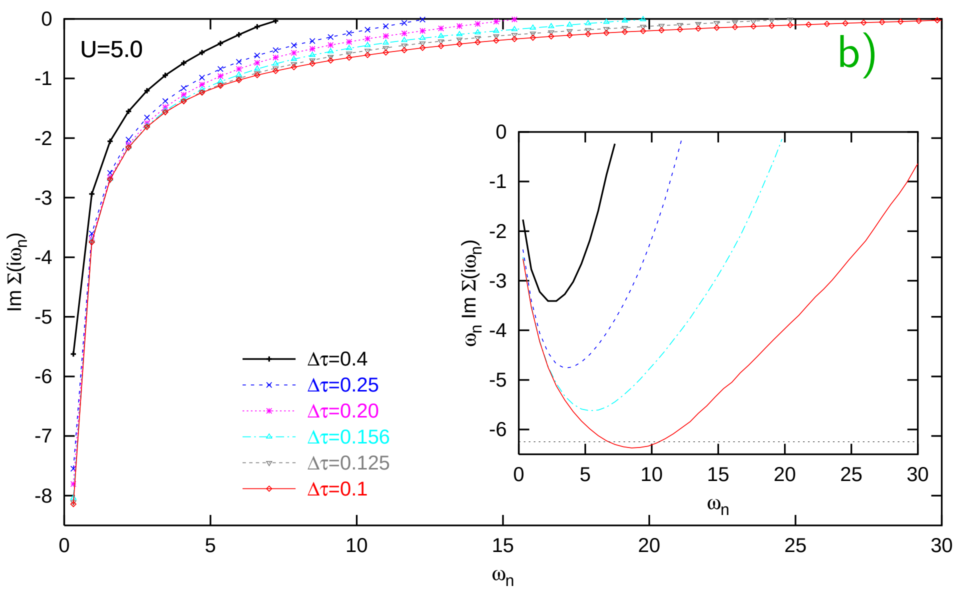
Fourier transformation schemes: self-energy ($T = 0.1$, $U = 5.0$)

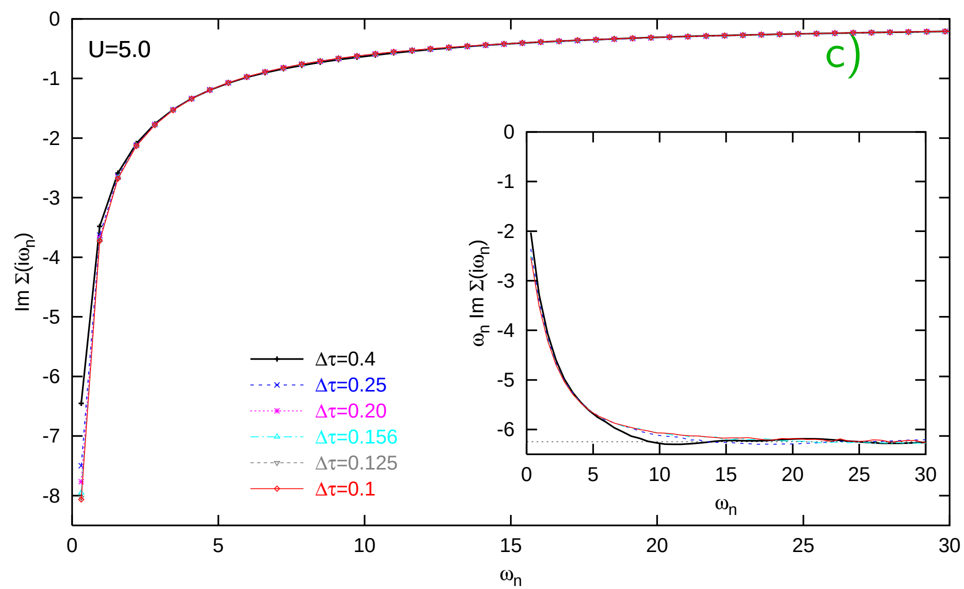
a) "Ulmke smoothing",
b) improved "Smoothing",
c) scheme with analytic high-frequency corrections

even stronger effects at lower T

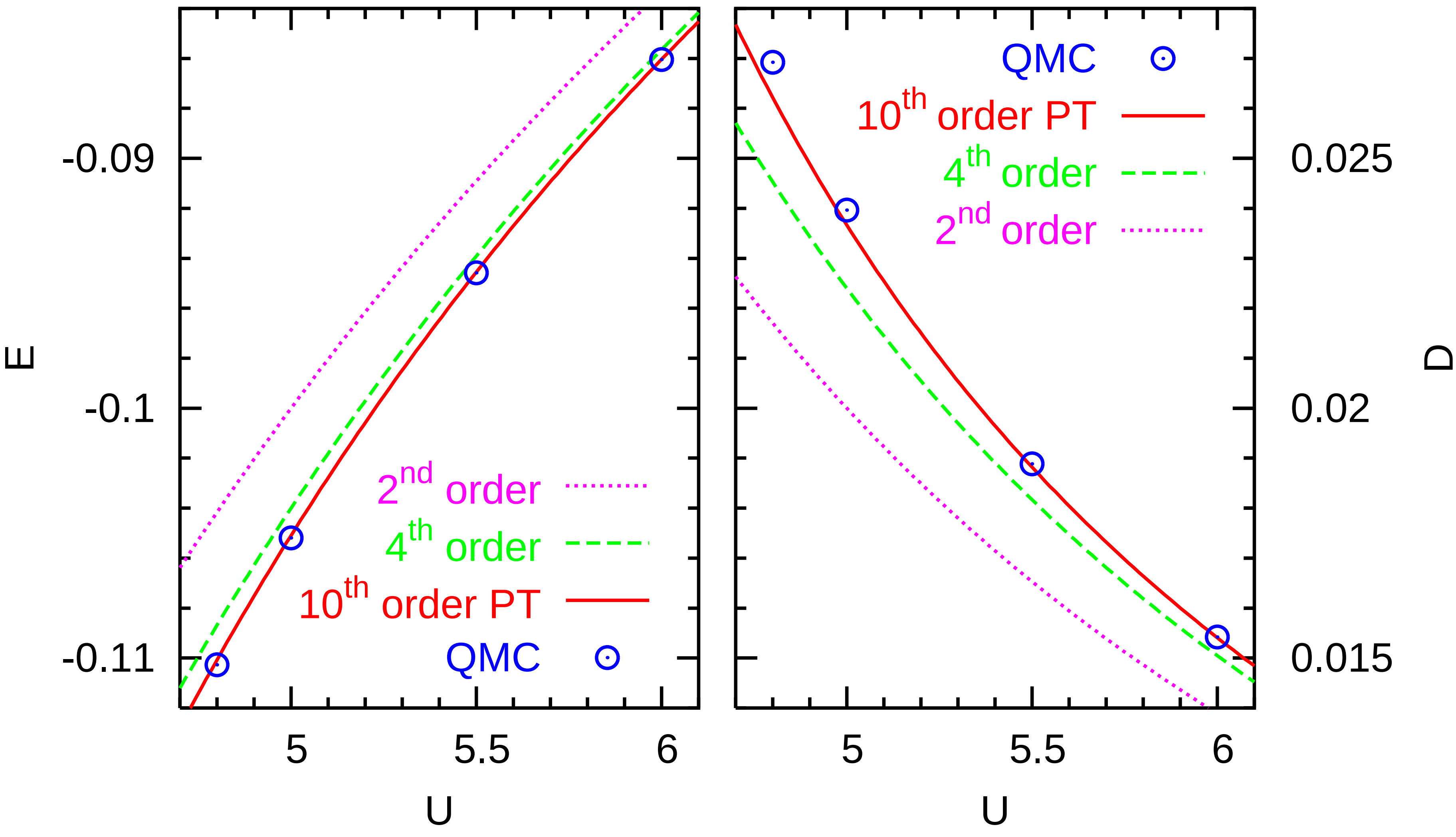
low-frequency errors of $\Sigma(\omega)$ small in b) und c)





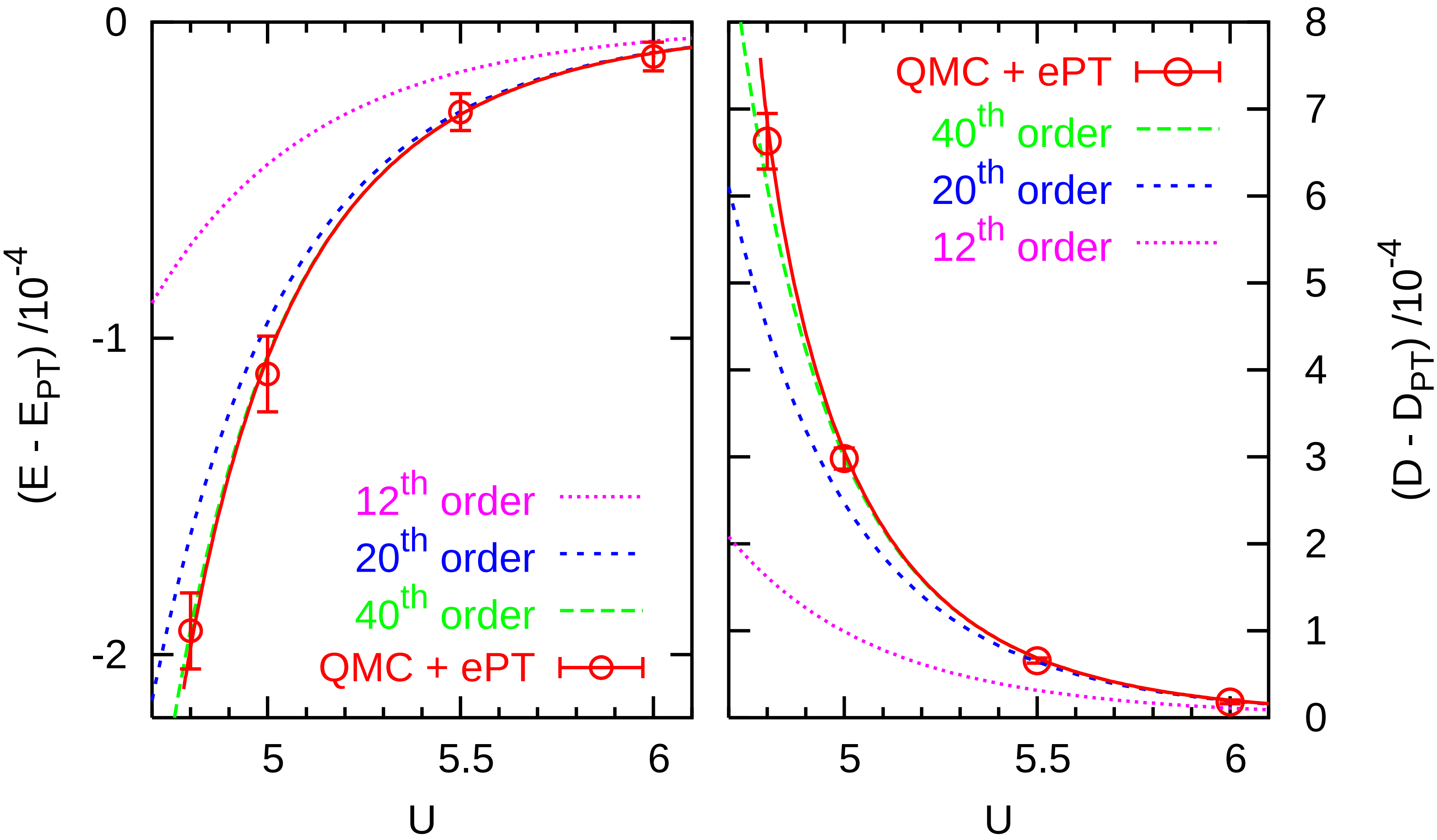


Mott insulator: energy + double occupancy I



Excellent agreement at $U = 6.0$.

Mott insulator: energy + double occupancy II



Mott insulator: U_{c1}, critical exponents, low-T parameter for $U_c(T)$

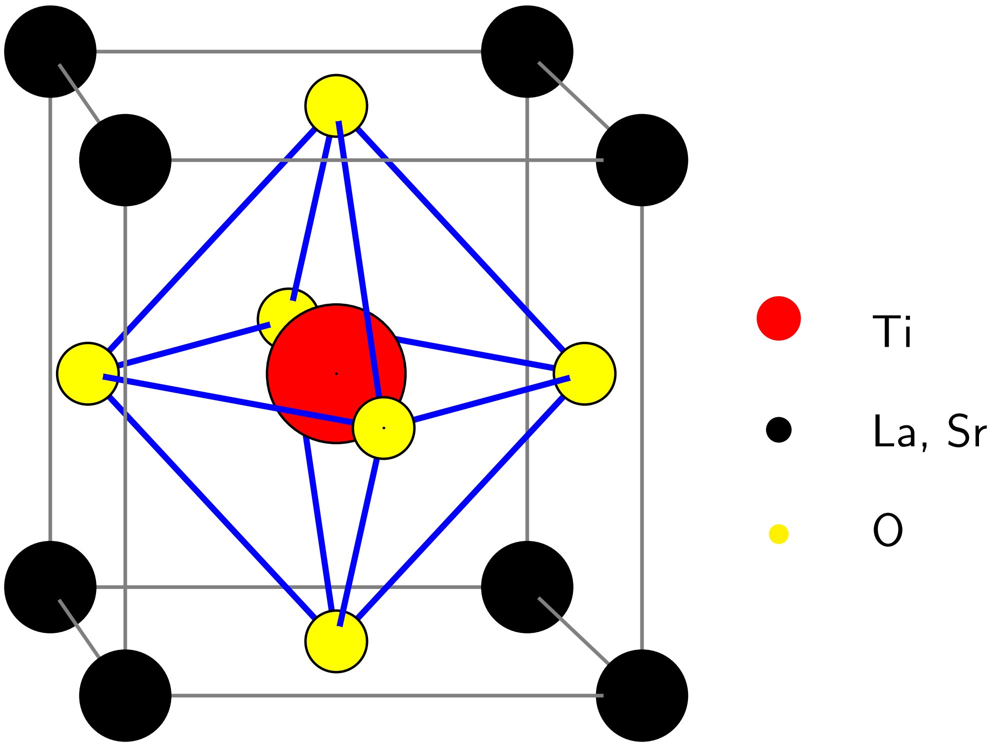
high-precision results for E, D at all U (parametrizations available) $\rightsquigarrow$ benchmark

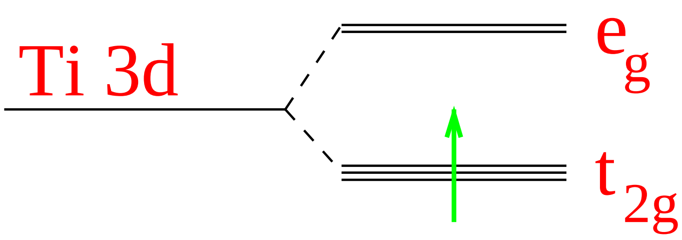
[Blümer, Kalinowski, cond-mat/0404568 (2004), cond-mat/0407442 (2004)]

Realistic LDA+DMFT(QMC) calculations

$La_{1-x}Sr_xTiO_3$

- perovskite structure
- $1-x$ t_{2g} electrons per site
- AF for $x \lesssim 0.05$
- strongly correlated metal
- density functional theory (LDA) fails





multi-band issues

$\dfrac{2M(2M-1)}{2}$ Hubbard-Stratonovich fields

approximation: Hund terms $J_{\alpha\alpha'}\, \boldsymbol{s}^{\alpha} \cdot \boldsymbol{s}^{\alpha'} \longrightarrow J_{\alpha\alpha'}\, s_z^{\alpha} s_z^{\alpha'}$ to avoid sign problem in QMC

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Analytic continuation

Aim: (ill-conditioned) inversion of $G(\tau) = \int d\omega \, \frac{\exp[-\tau\omega]}{1+\exp[-\beta\omega]} \, A(\omega)$

Maximum entropy method (MEM): introduce entropy function to find smoothest solution $A(\omega)$ compatible with $G(\tau)$

$G(\tau) \xrightarrow{\text{MEM}} \text{Im}G(\omega) \xrightarrow{\text{Kra-Kro}} \text{Re}G(\omega)$

MEM: not fully controlled; no $\Delta\tau$ extrapolation possible

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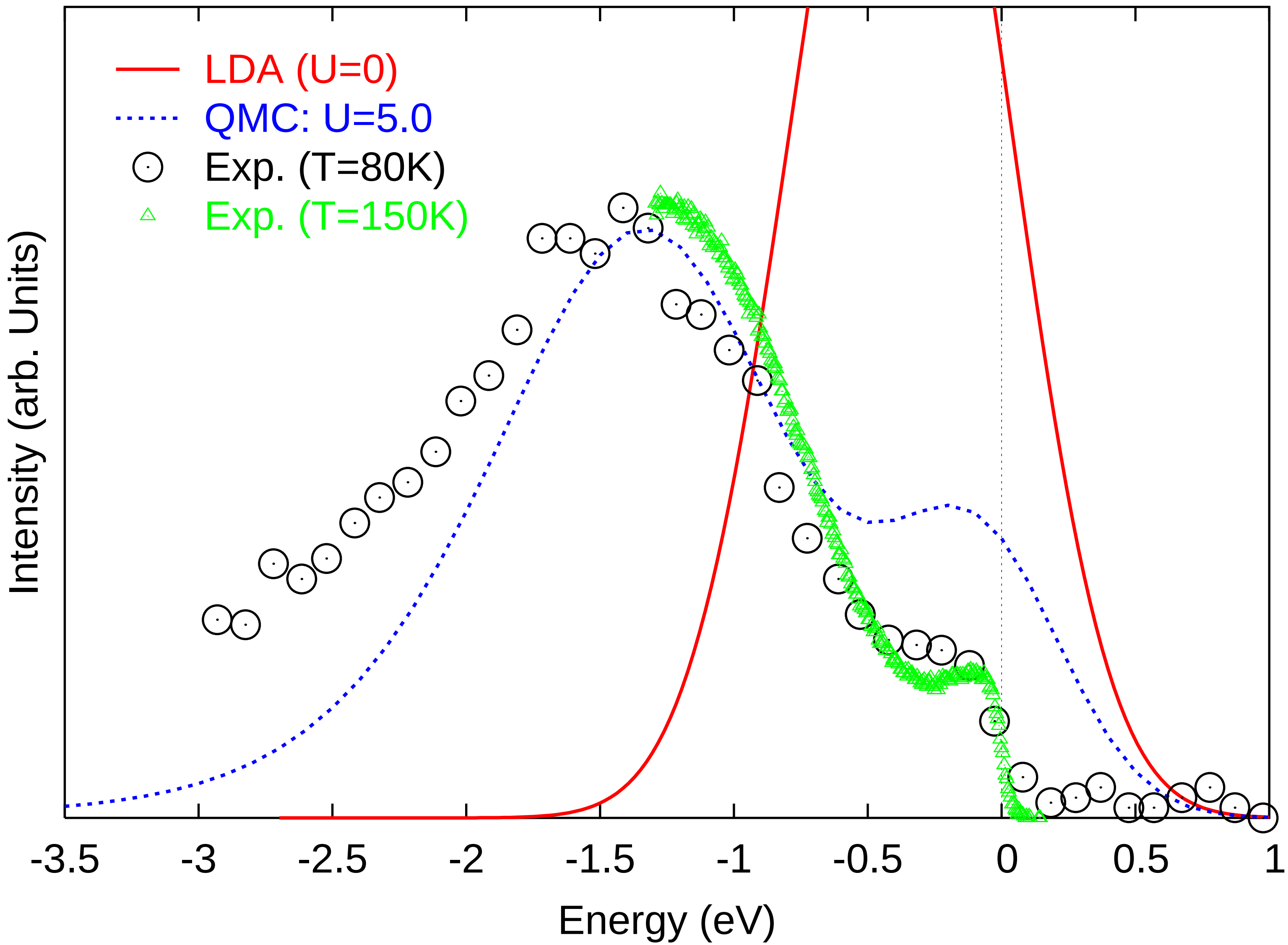
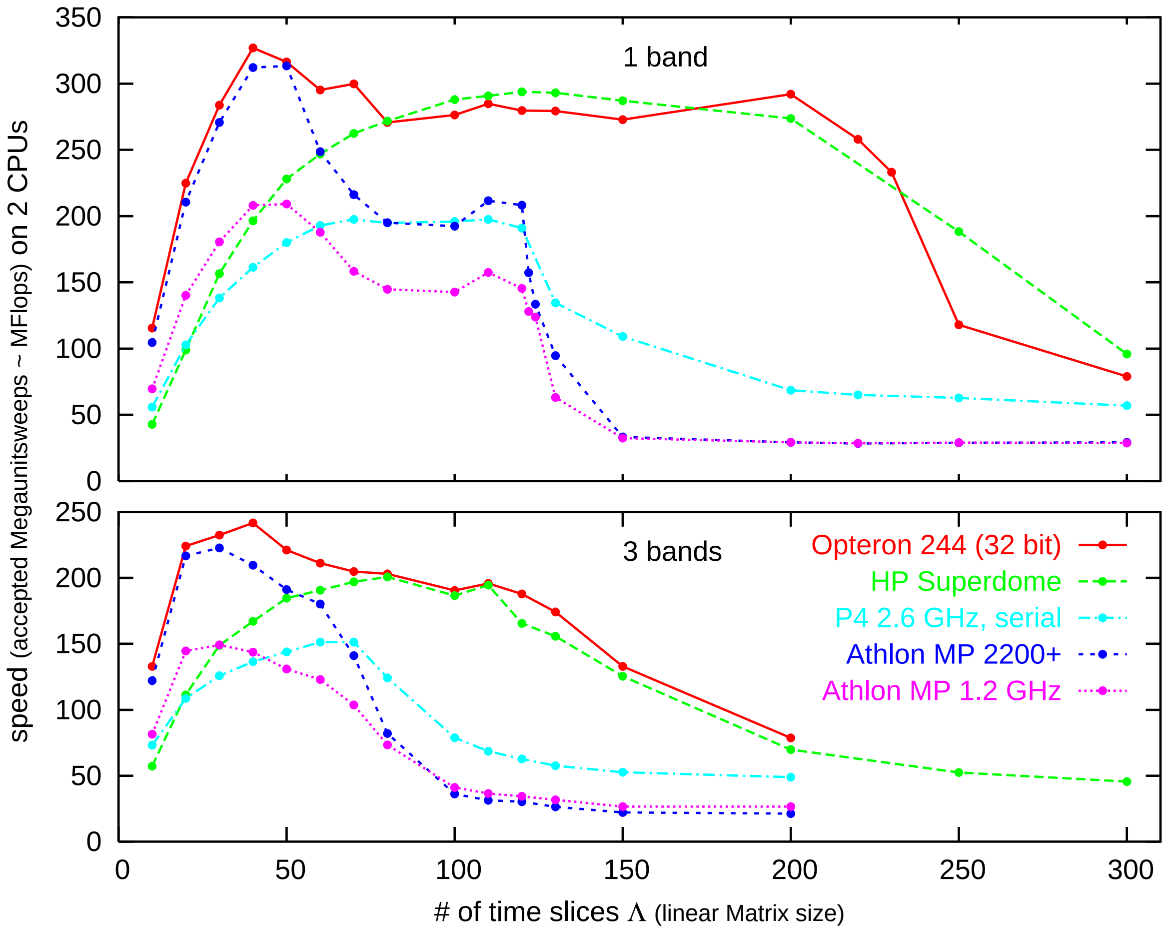
for ARPES, $\sigma(\omega)$: use 2-dimensional Newton scheme to invert Dyson equation for $G(\omega) \longrightarrow \Sigma(\omega)$

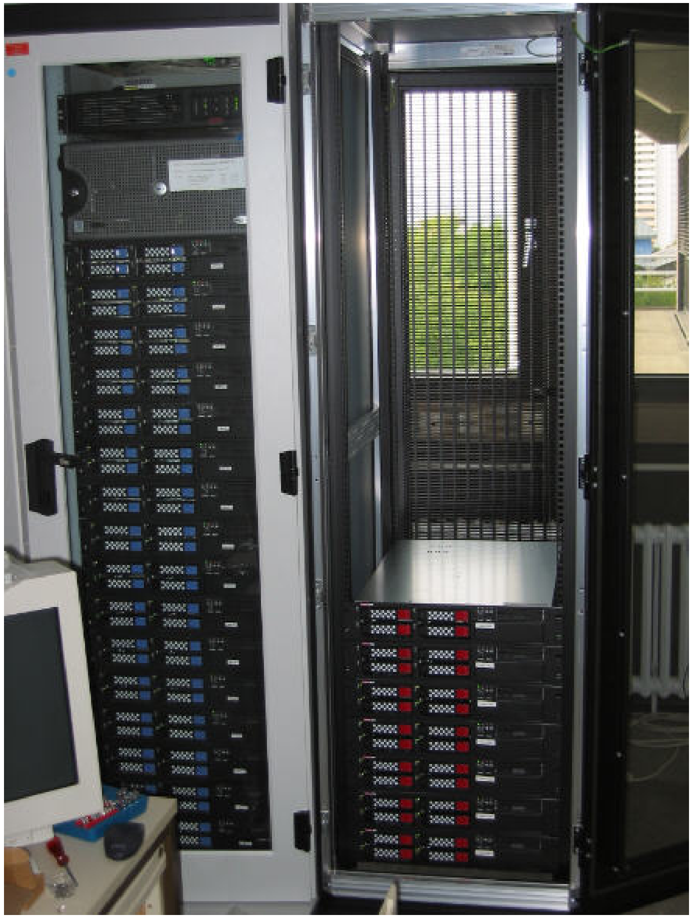
Photoemission spectra for $La_{1-x}Sr_xTiO_3$ (x=0.06)



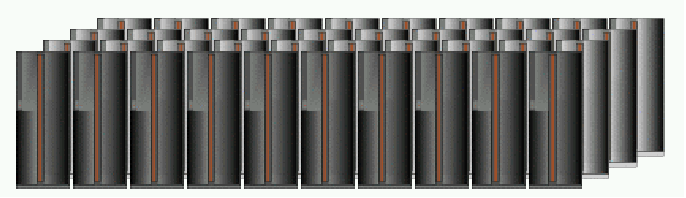
[Nekrasov, Held, Blümer, Poteryaev, Anisimov, Vollhardt, EPJB **18**, 55 (2000)]

Computers





Group cluster (2nd stage)



JUMP cluster (NIC Jülich)

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"derivation" of (1-band/multi-band) Hubbard model

characterization of DMFT

role of self-energy

Monte Carlo principles

QMC: principles and caveats (convergency, $\Delta\tau$ extrapolation)

extreme-precision QMC results for 1-band model (vs. ePT, SFT/DIA)

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LDA+DMFT: significant improvements for PES of $La_{1-x}Sr_xTiO_3$

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Further talks:
- DMFT for double perowskite models
- high-frequency corrected QMC (multi-band); observables
- MEM and LDA+DMFT