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

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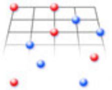
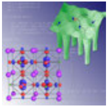


TR 49: *Condensed matter systems with variable many-body interactions*
Frankfurt / Kaiserslautern / Mainz

FOR 1346
LDA+DMFT
Augsburg *et al.*



Outline

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Introduction: Hubbard model and DMFT self-consistency

Hirsch-Fye QMC solution of the single-impurity Anderson model

Achieving DMFT self-consistency, extrapolation

Verification: comparison of DMFT results with determinantal QMC

[Gorelik, Paiva, Scalettar, Klümper, Blümer, arXiv:1105.3356]

Extension: real-space DMFT for ultracold fermions on optical lattices

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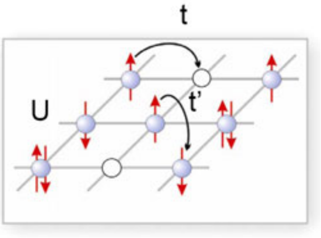
Tutorial: study Mott metal-insulator transition using HF-QMC

Hubbard model (arbitrary hopping, 1 band)

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

$$= \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}}\,\hat{n}_{\mathbf{k}\sigma} + U\sum_i \hat{D}_i; \qquad \hat{D}_i = \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$



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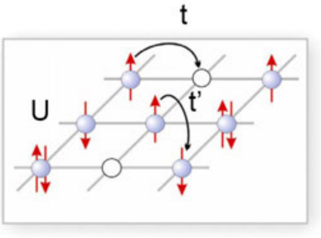
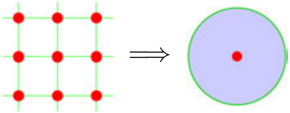


Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\mathbf{k},\omega) \equiv \Sigma(\omega)$

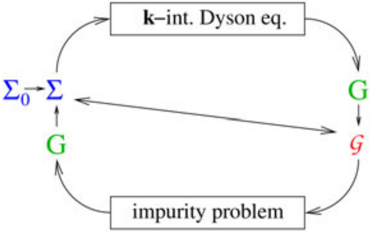
[Metzner, Vollhardt, PRL (1989), Georges, Kotliar, PRL (1992), Jarrell, PRL (1992)]

- $+$ non-perturbative $\rightsquigarrow$ valid at MIT
- $+$ in thermodynamic limit
- $+/-$ exact for coordination $Z \to \infty$
  (questionable for $d \leq 2 \rightsquigarrow$ DCA, CDMFT)



Iterative solution of DMFT self-consistency equations

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



$\longleftarrow$ DOS / t_{ij}^{ν} / $\epsilon_{\nu\mathbf{k}}$

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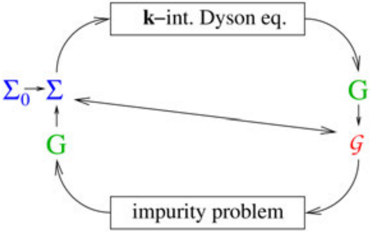

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Impurity solver:

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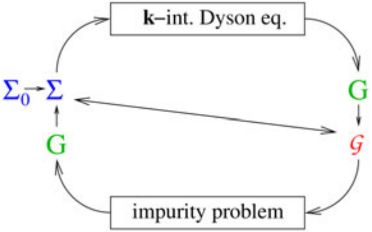

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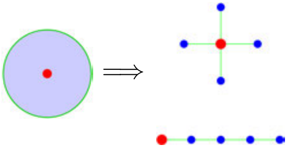
Impurity solver:

- Iterative perturbation theory (IPT; not controlled)
- Hirsch-Fye quantum Monte-Carlo (HF-QMC)
- Continuous-time quantum Monte-Carlo (CT-QMC)
- Exact diagonalization (ED; large finite-size errors)
- Numerical renormalization group (NRG; 1-2 bands)
- Density matrix renormalization group (DMRG)
- Determinantal quantum Monte Carlo (linear in $1/T$)



Hirsch-Fye quantum Monte Carlo method

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

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

$$G_\sigma(\tau) = -\frac{1}{\mathcal{Z}} \int \mathcal{D}[\psi, \psi^*] \underbrace{\psi_\sigma(\tau)\, \psi^*_\sigma(0)}_{\cong\, \hat{c}_\sigma \hat{c}^\dagger_\sigma} \exp\Big[\mathcal{A}_0 - U \int_0^\beta d\tau' \underbrace{\psi^*_\uparrow \psi_\uparrow \psi^*_\downarrow \psi_\downarrow}_{\cong\, \hat{n}_\uparrow \hat{n}_\downarrow}\Big]$$

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

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

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$$\hat{n}_\uparrow \hat{n}_\downarrow = \tfrac{1}{2}\left[\hat{n}_\uparrow + \hat{n}_\downarrow - \left(\hat{n}_\uparrow - \hat{n}_\downarrow\right)^2\right] \quad \rightsquigarrow \quad e^{-\Delta\tau\, U \hat{n}_\uparrow \hat{n}_\downarrow} = e^{-\Delta\tau\, U \hat{n}/2}\, e^{\Delta\tau\, U (\hat{n}_\uparrow - \hat{n}_\downarrow)^2/2}$$

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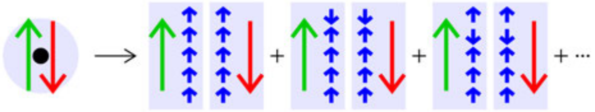
(iii) Hubbard-Stratonovich transform $\quad e^{\Delta\tau U (\hat{n}_\uparrow - \hat{n}_\downarrow)^2/2} = \frac{1}{2}\sum_{s=\pm 1} e^{\lambda s\,(\hat{n}_\uparrow - \hat{n}_\downarrow)}$

$\cosh(\lambda) = \exp(\Delta\tau U/2)$



Wick theorem:

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

Hirsch-Fye QMC: some more details (1/3) ...

Action $\mathcal{A}_0 - U\int_0^\beta d\tau'\,\psi_\uparrow^*\psi_\uparrow\psi_\downarrow^*\psi_\downarrow$ in discretized form:

$$\mathcal{A}_\Lambda[\psi,\psi^*,\mathcal{G},U] = (\Delta\tau)^2\sum_\sigma\sum_{l,l'=0}^{\Lambda-1}\psi_{\sigma l}^*(\boldsymbol{\mathcal{G}}_\sigma^{-1})_{ll'}\,\psi_{\sigma l'} - \Delta\tau\,U\sum_{l=0}^{\Lambda-1}\psi_{\uparrow l}^*\,\psi_{\uparrow l}\,\psi_{\downarrow l}^*\,\psi_{\downarrow l} \quad (11)$$

Matrix $\boldsymbol{\mathcal{G}}_\sigma$ consists of elements $\mathcal{G}_{\sigma ll'} \equiv \mathcal{G}_\sigma(l\Delta\tau - l'\Delta\tau)$; $\quad \psi_{\sigma l} \equiv \psi_\sigma(l\Delta\tau)$.

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The Trotter decomposition yields to lowest order

$$\exp\left(\mathcal{A}_\Lambda[\psi,\psi^*,\mathcal{G},U]\right) = \prod_{l=0}^{\Lambda-1}\Bigg[\exp\left((\Delta\tau)^2\sum_\sigma\sum_{l'=0}^{\Lambda-1}\psi_{\sigma l}^*(\boldsymbol{\mathcal{G}}_\sigma^{-1})_{ll'}\,\psi_{\sigma l'}\right) \times \exp\left(-\Delta\tau\, U\,\psi_{\uparrow l}^*\,\psi_{\uparrow l}\,\psi_{\downarrow l}^*\,\psi_{\downarrow l}\right)\Bigg]. \quad (12)$$

Hirsch-Fye QMC: some more details (2/3) ...

Hubbard-Stratonovich transformation (+ Trotter again) yields

$$G_{\sigma l_1 l_2} = \frac{1}{\mathcal{Z}} \sum_{\{s\}} \int \mathcal{D}[\psi]\, \mathcal{D}[\psi^*]\ \psi^*_{\sigma l_1} \psi_{\sigma l_2} \exp\Big(\sum_{\sigma, l, l'} \psi^*_{\sigma l} M^{s_l}_{\sigma l l'} \psi_{\sigma l'} \Big), \tag{14}$$

↑ 2^{Λ} HS field configurations

with*

$$M^{s_l}_{\sigma l l'} = (\Delta\tau)^2 (\mathcal{G}^{-1}_{\sigma})_{ll'} - \lambda \sigma \delta_{ll'} s_l$$

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$$M^{s_l}_{\sigma l l'} = (\Delta\tau)^2 (\mathcal{G}^{-1}_{\sigma})_{l l'} - \lambda \sigma \delta_{l l'} s_l \qquad (15)$$

Apply Wick's theorem $\rightsquigarrow$

$$G_{\sigma l l'} = \frac{1}{\mathcal{Z}} \sum_{\{s\}} \big(\mathbf{M}^{\{s\}}_{\sigma}\big)^{-1}_{l l'} \det \mathbf{M}^{\{s\}}_{\uparrow} \det \mathbf{M}^{\{s\}}_{\downarrow}, \qquad (16)$$

$$\mathcal{Z} = \sum_{\{s\}} \det \mathbf{M}^{\{s\}}_{\uparrow} \det \mathbf{M}^{\{s\}}_{\downarrow}.$$

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Computational cost of naive computation of each term:
matrix inverse: $\mathcal{O}(\Lambda^3)$ determinants worse than $\mathcal{O}(\Lambda^4)$

Hirsch-Fye QMC: fast update scheme

Gray code (or MC): flip single spin between subsequent configuration:

$$\mathbf{M}_\sigma \quad \stackrel{s_m \to -s_m}{\longrightarrow} \quad {\mathbf{M}_\sigma}' = \mathbf{M}_\sigma + \mathbf{\Delta}^{\sigma\, m} \tag{18}$$

$$= \left(1 + \mathbf{\Delta}^{\sigma\, m} (\mathbf{M}_\sigma)^{-1}\right) \mathbf{M}_\sigma \tag{19}$$

$$\text{with} \qquad {\Delta_{ll'}^{\sigma}}^{m} = \delta_{ll'} \delta_{lm} \, 2\Delta\tau \; \lambda \; \sigma s_l \tag{20}$$

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Now: simple (and cheap!) formula for ratio of the determinants:

$$R^{\sigma\, m} := \frac{\det({\mathbf{M}_\sigma}')}{\det(\mathbf{M}_\sigma)} = \det\left(\mathbf{1} + \boldsymbol{\Delta}^{\sigma\, m}(\mathbf{M}_\sigma)^{-1}\right)$$

$$= 1 + 2\Delta\tau\, \lambda\, \sigma s_m\, (M_\sigma)^{-1}_{mm} \tag{21}$$

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The inversion of **M** is also elementary, one obtains:

$$(\mathbf{M}_\sigma{}')^{-1} = (\mathbf{M}_\sigma)^{-1} + \frac{1}{R^{\sigma\, m}}\, (\mathbf{M}_\sigma)^{-1} \boldsymbol{\Delta}^{\sigma\, m} (\mathbf{M}_\sigma)^{-1} \tag{22}$$

$\rightsquigarrow$ computational cost for each term: $\mathcal{O}(\Lambda^2)$.

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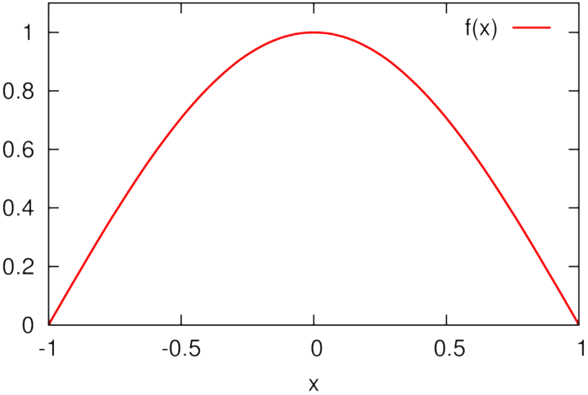
$\rightsquigarrow$ computational cost for each term: $\mathcal{O}(\Lambda^2)$. But: 2^Λ terms!

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

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



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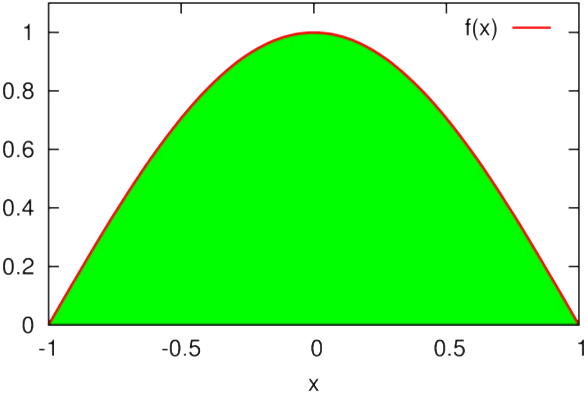

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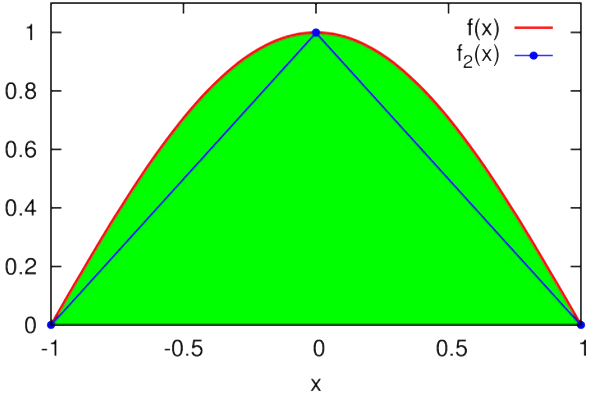

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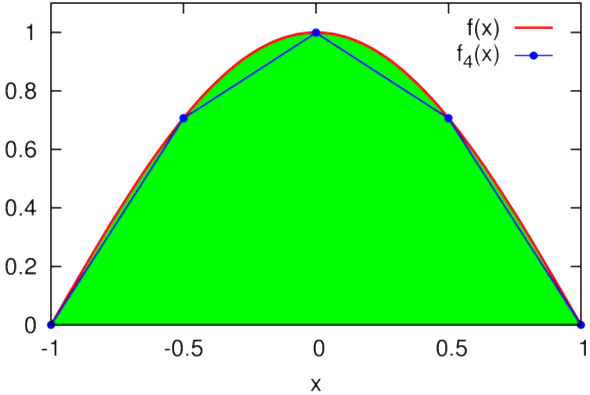

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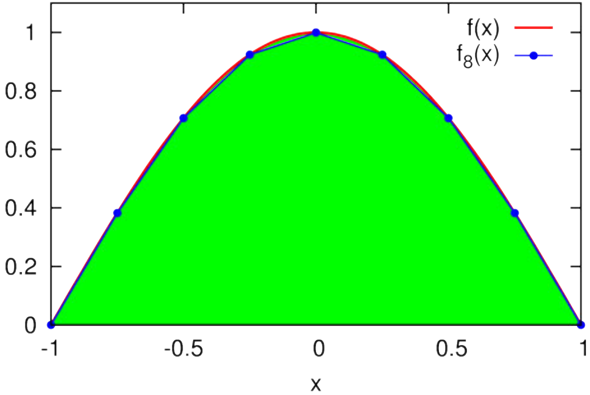

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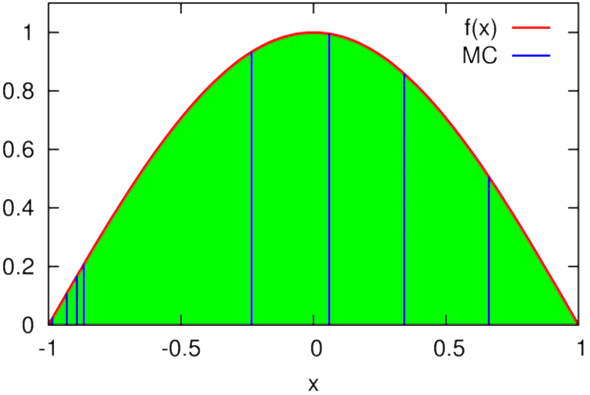

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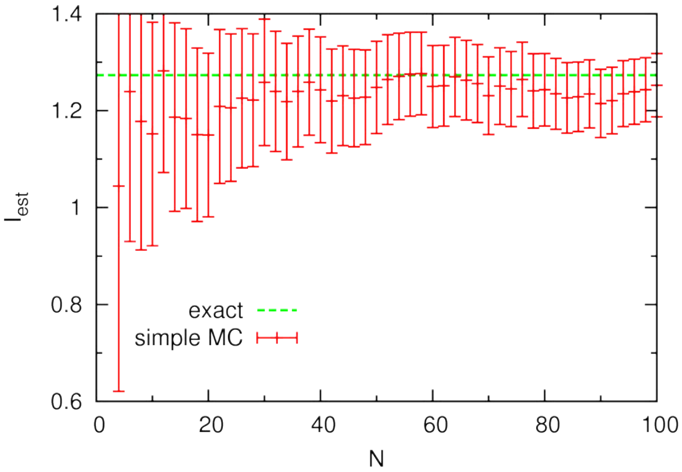
Numerical methods:

- discretization
- Monte Carlo

Convergence of results?



Non-deterministic MC results only meaningful within statistical error bars!

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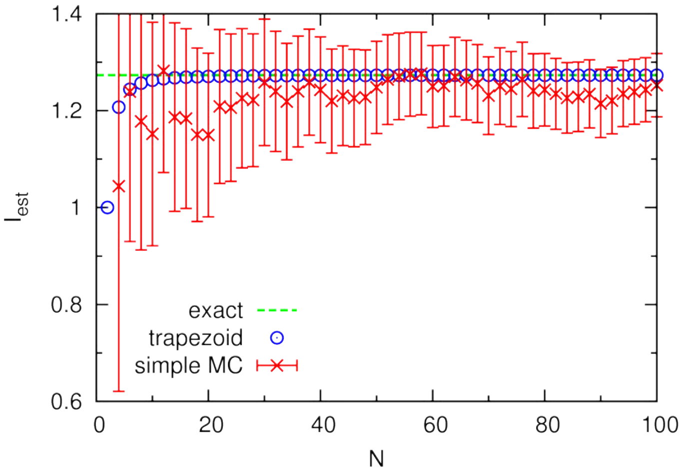

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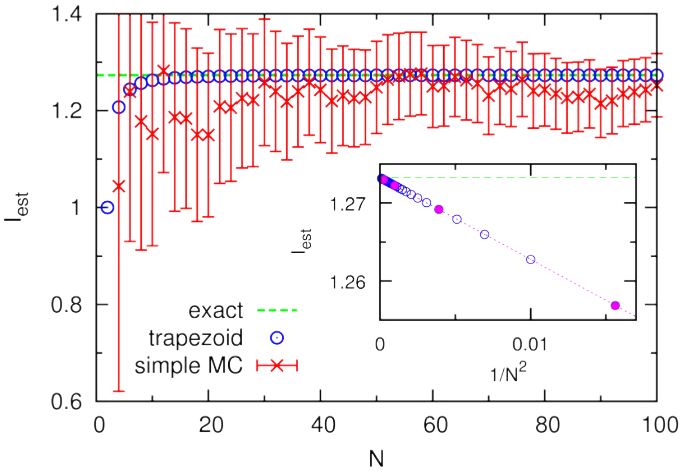

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Application of Monte Carlo in Statistical Physics

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

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.

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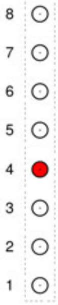

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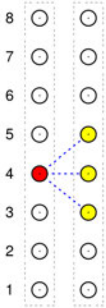

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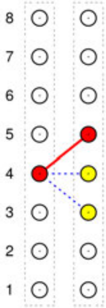

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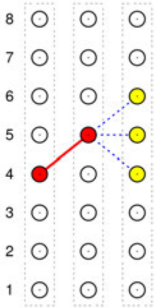

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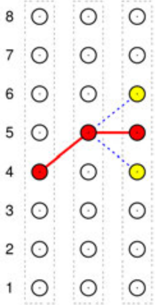

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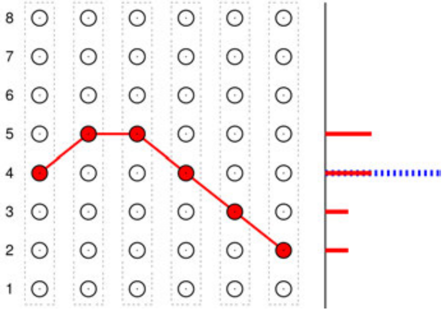

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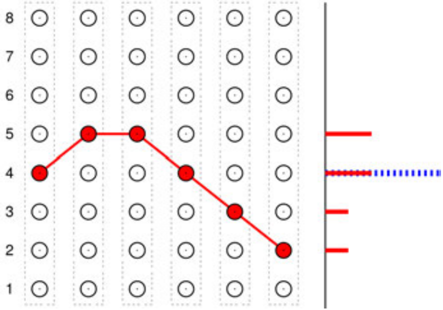

Ergodicity and detailed balance

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

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

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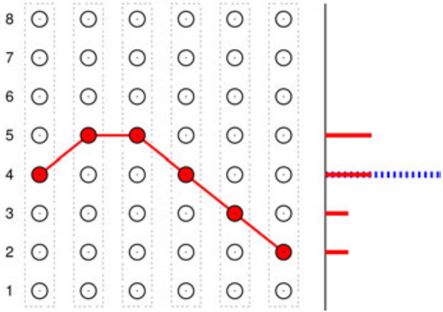

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Favorite choice: Metropolis rule

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

Monte Carlo importance sampling in Hirsch-Fye method

Sample configurations $\{s\}$ according to the (unnormalized) probability

$$P(\{s\}) = \left| \det \mathbf{M}_{\uparrow}^{\{s\}} \det \mathbf{M}_{\downarrow}^{\{s\}} \right|$$

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The Green function can then be calculated as an average $\langle \dots \rangle_s$:

$$G_{\sigma l l'} = \frac{1}{\tilde{\mathcal{Z}}} \left\langle \left(\mathbf{M}_{\sigma}^{\{s\}}\right)^{-1}_{ll'} \mathrm{sign}\left(\det \mathbf{M}_{\uparrow}^{\{s\}} \det \mathbf{M}_{\downarrow}^{\{s\}}\right) \right\rangle_s , \tag{29}$$

$$\tilde{\mathcal{Z}} = \left\langle \mathrm{sign}\left(\det \mathbf{M}_{\uparrow}^{\{s\}} \det \mathbf{M}_{\downarrow}^{\{s\}}\right) \right\rangle_s . \tag{30}$$

Note: $\tilde{\mathcal{Z}}$ deviates from full partition function by prefactor which cancels in (29)

MC with importance sampling $\not\rightarrow$ partition function, free energy, entropy!

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If the sign in (29) is constant (no sign problem) $\leadsto$ simplification:

$$G_{\sigma l l'} = \frac{1}{\tilde{\mathcal{Z}}} \left\langle \left(\mathbf{M}_{\sigma}^{\{s\}} \right)^{-1}_{ll'} \right\rangle_s , \qquad \tilde{\mathcal{Z}} = \langle 1 \rangle_s . \tag{31}$$

Recipe for practical HF-QMC calculations

(i) Choose starting HS-field configuration $\{s\}$ (uniform or from previous run)

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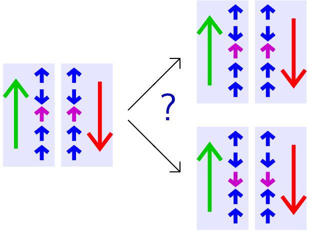

One sweep: attempt spin-flip for each auxiliary spin s_m $(1 \leq m \leq \Lambda)$

Metropolis acceptance probability:
$\min\{1, R^{\uparrow m} R^{\downarrow m}\}$, where

$$R^{\sigma\, m} = \frac{\det(\mathbf{M}_\sigma{}')}{\det(\mathbf{M}_\sigma)} = 1 + 2\Delta\tau\, \lambda\, \sigma s_m \left(M_\sigma\right)^{-1}_{mm}$$

Impact of HF-QMC parameters: number of sweeps, discretization $\Delta\tau$

- Statistical error:
  $(\Delta G)_{\text{statistical}} \propto 1/\sqrt{N_{\text{meas}}}$

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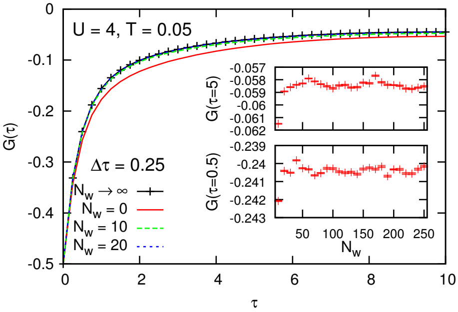

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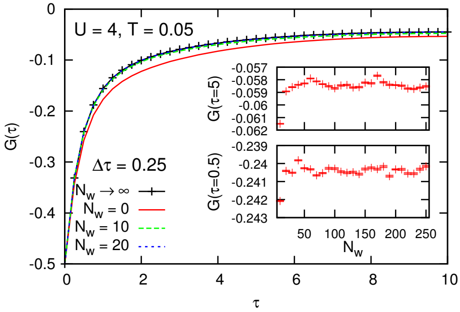
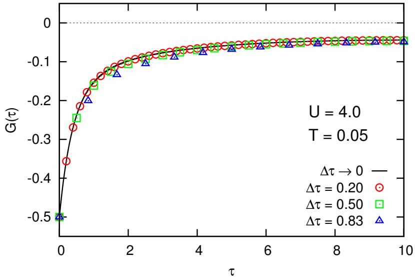
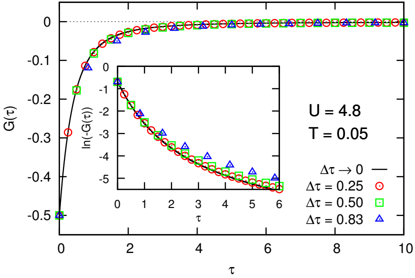
- **Discretization error:** $(\Delta G)_{\Delta\tau} \propto \Delta\tau^2$





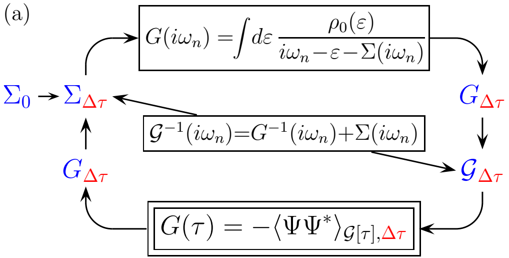


Achieving self-consistency using HF-QMC

Iterative solution of DMFT self-consistency equations

For each discretization $\Delta\tau$:

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



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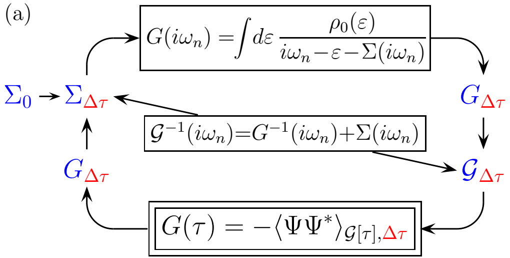
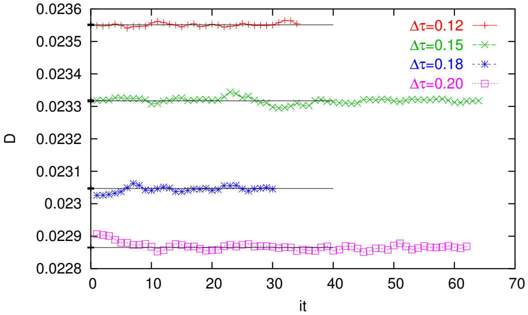


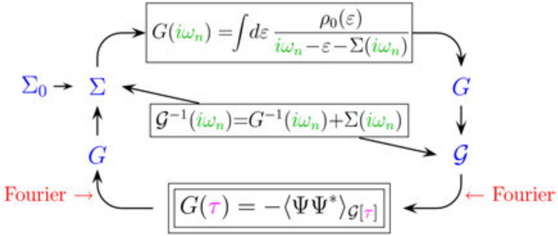


How many iterations?

Look at traces!

Special issue: Fourier transformations in DMFT-QMC cycle

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



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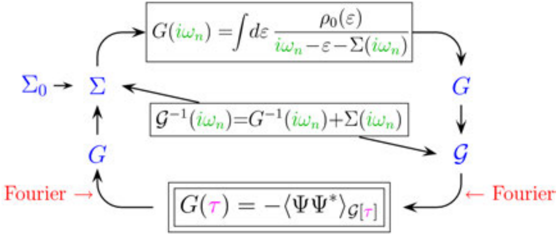
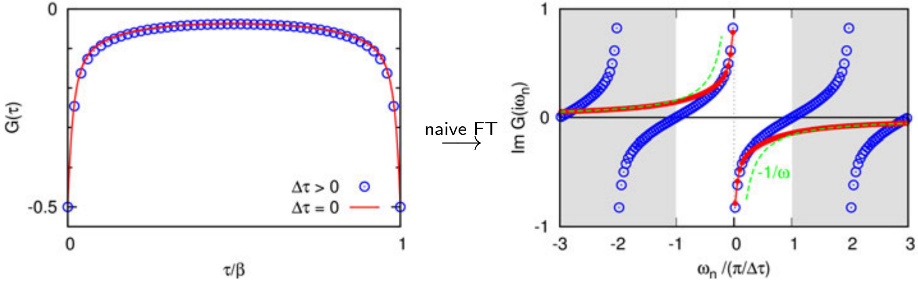


Naive discrete Fourier transformation ⇝ oscillations (instead of $G(\omega) \overset{\omega\to\infty}{\longrightarrow} 1/\omega$)



One 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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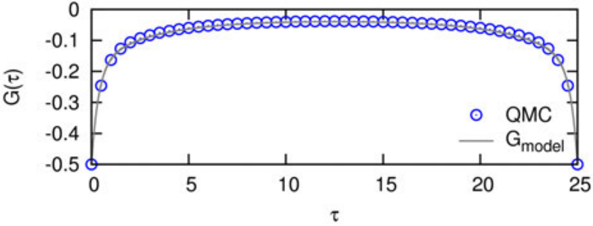

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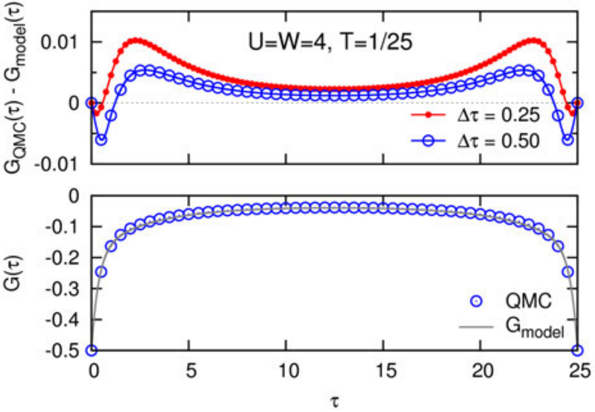

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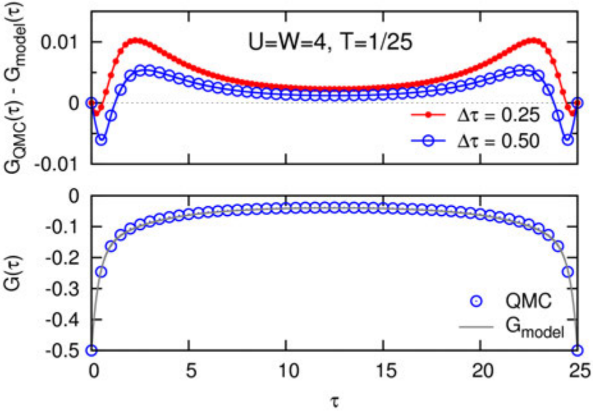

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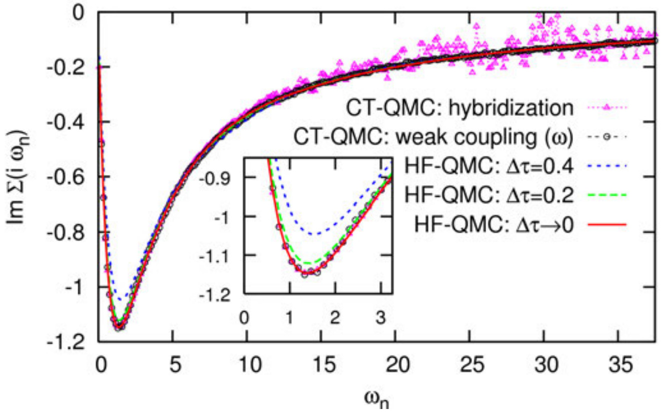
multi-band: more terms

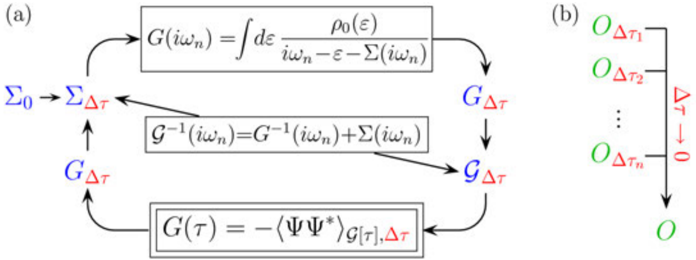
Sensitive test: high-frequency tails of self-energy



correct tails in HF-QMC for each $\Delta\tau$

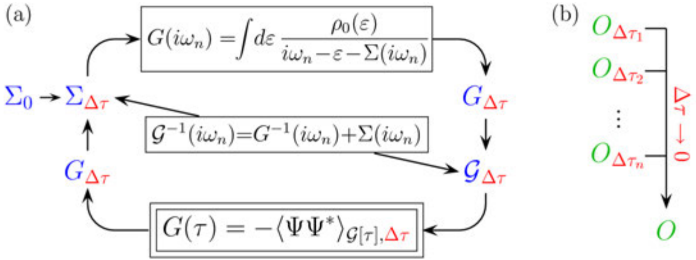
larger fluctuations in CT-QMC

Self-consistency cycle using conventional HF-QMC



Extrapolation

Self-consistency cycle using conventional HF-QMC



Extrapolation $\Delta\tau \to 0$ improves accuracy by orders of magnitude ($\sim$ same cost)

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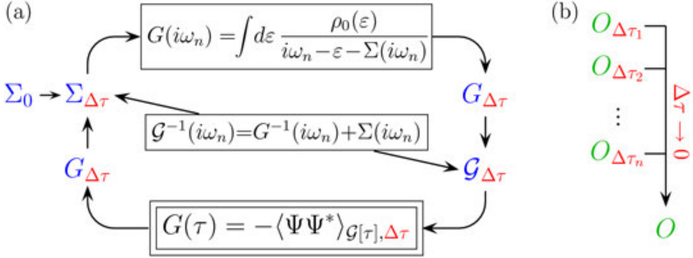

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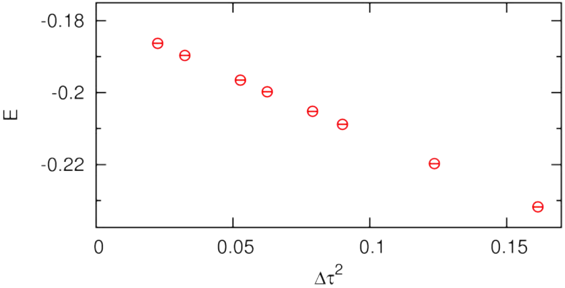
Example: energy E for $U = 4$, $T = 1/45$ (Bethe DOS)

[NB, PRB (2007)]



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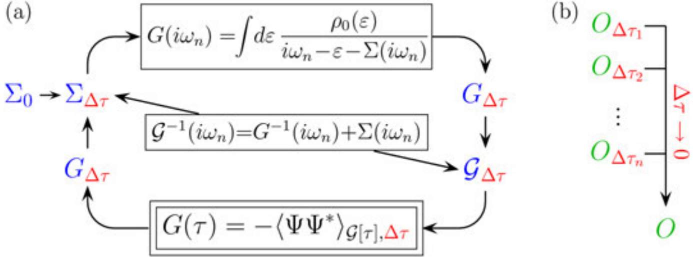

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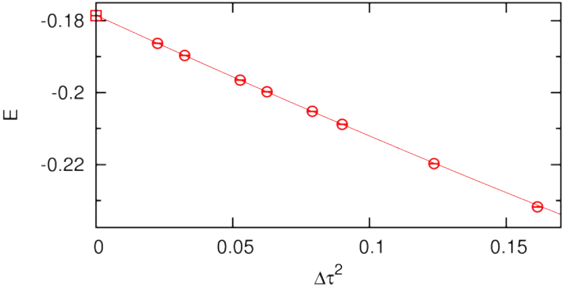
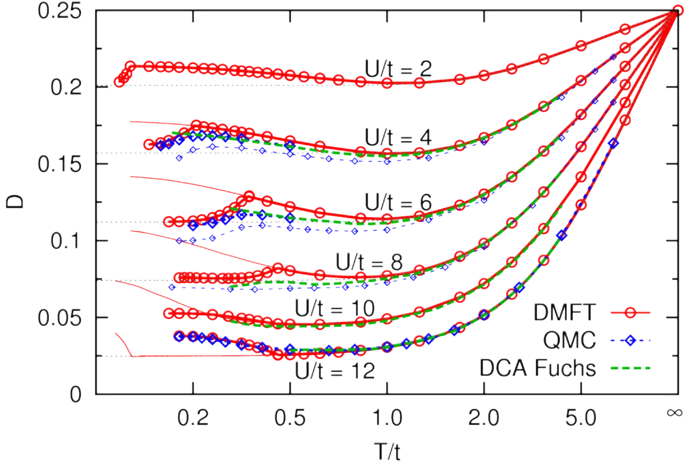


Recent developments

Verification: comparison of DMFT results ($d = 3$) with determinantal QMC

Extension: real-space DMFT for ultracold fermions on optical lattices

Comparison DMFT – direct QMC for the 3d cubic lattice ($n = 1$)



Excellent general agreement DMFT ↔ QMC, even at small U

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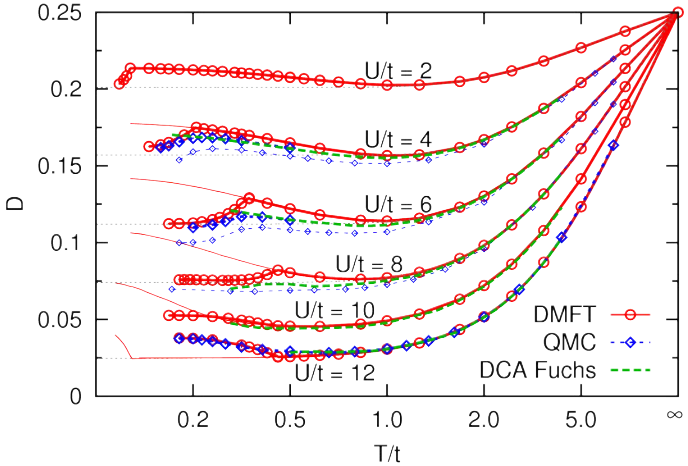

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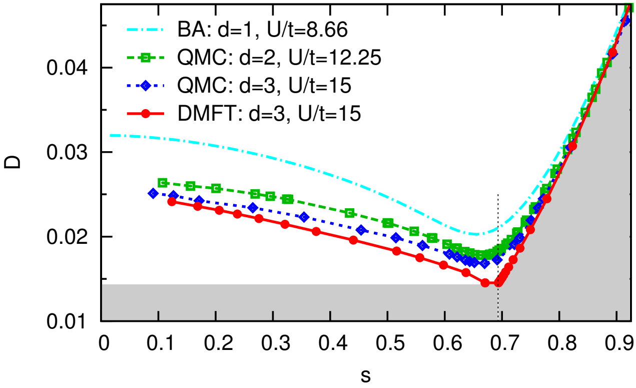
Typical QMC discretization errors (thin lines) larger than DMFT deviations!

Double occupancy as a universal measure of AF correlations + entropy



Minimum of $D(s)$ at $s \approx \log 2$ for all d!

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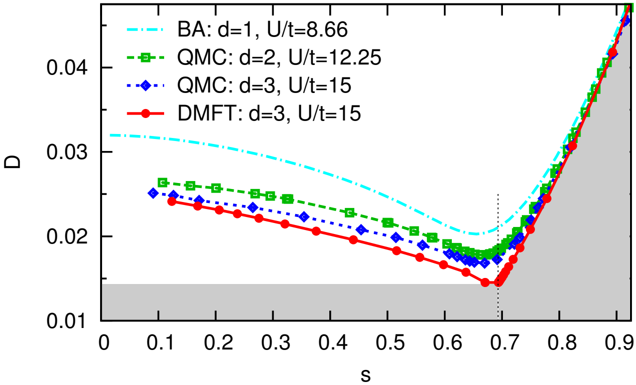
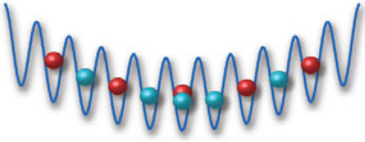


Minimum of $D(s)$ at $s \approx \log 2$ for all d!

No features seen at $d = 3$ Néel transition ($s_N \approx log(2)/2$)

Real-space DMFT: use local self-energy in inhomogeneous system

Include trapping potential, e.g.: $V_i = V r_i^2$



$$H = -\sum_{(ij),\sigma} t_{ij}\, c^\dagger_{i\sigma} c_{j\sigma} + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow} + \sum_{i,\sigma} V_i\, n_{i\sigma}$$

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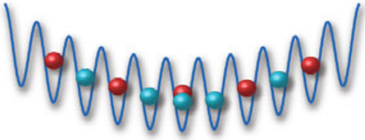

$\rightsquigarrow$ N single-site impurities, coupled by real-space lattice Dyson equation:

$$\left[G_\sigma(i\omega_n)\right]^{-1}_{ij} = \left(\mu_\sigma + i\omega_n\right)\delta_{ij} - t_{ij} - \left(V_i + \Sigma_{i\sigma}(i\omega_n)\right)\delta_{ij}$$

[M. Snoek, I. Titvinidze, C. Toke, K. Byczuk, and W. Hofstetter, NJP (2008); R. Helmes, T. A. Costi, and A. Rosch, PRL (2008)]

Note: impurity problems are site-parallel,
lattice Dyson equation is frequency-parallel

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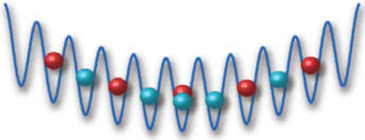

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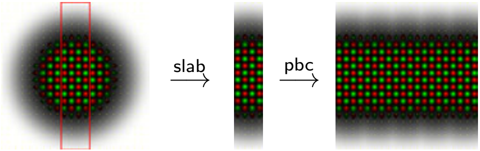
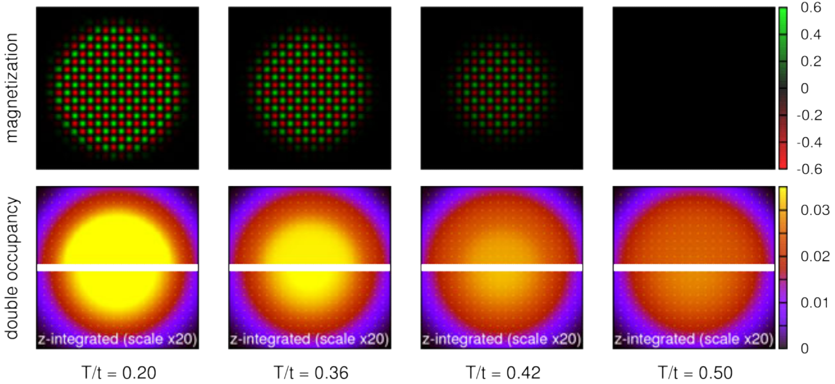
Here: HF-QMC (cost $\propto T^{-3}$)
"slab method" + pbc
$\sim$ exact for $\mathcal{O}(10^5)$ atoms



Results: RDMFT-QMC (cubic lattice, $V = 0.05t$, $U = W = 12t$)



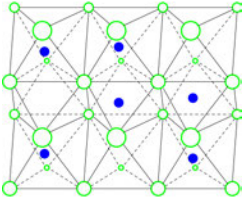
Proposal: enhanced double occupancy (i.e. interaction energy) as a signature of antiferromagnetic order at strong coupling
[Gorelik, Titvinidze, Hofstetter, Snoek, Blümer, PRL (2010)]

Tutorial: study Mott metal-insulator transition using HF-QMC

Elena Gorelik
Univ. Mainz

Daniel Rost
Univ. Mainz

Bandwidth control of metal-insulator transitions (example: V_2O_3)

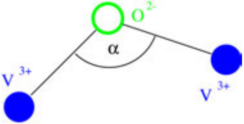


Corundum structure

Hydrostatic pressure or isovalent doping change

- lattice spacings
- bond angles

$\rightsquigarrow$ hopping amplitudes



$\alpha_{\mathbf{Cr}} < \alpha_{\mathbf{V}} < \alpha_{\mathbf{Ti}}$

Bond angles for V_2O_3 doped with Cr or Ti

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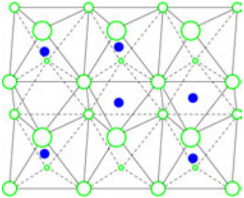

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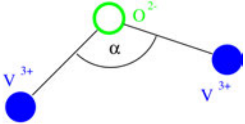

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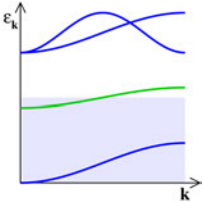
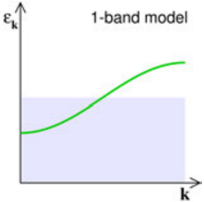
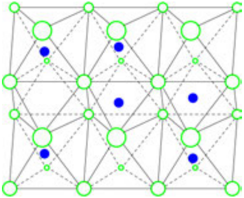
Breakdown of Bloch band description at paramagnetic Mott transition





Bloch states near Fermi energy

Bandwidth control of metal-insulator transitions (example: V_2O_3)



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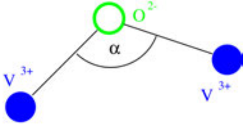

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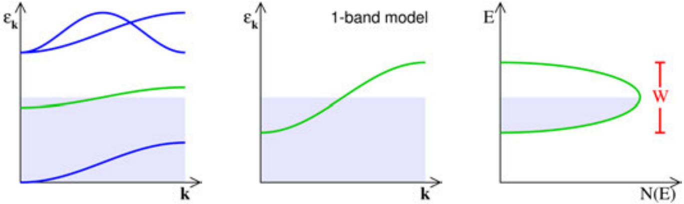

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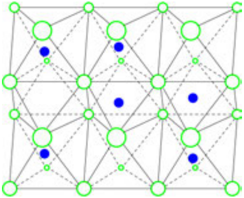

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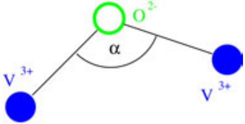

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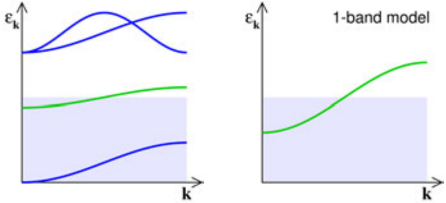

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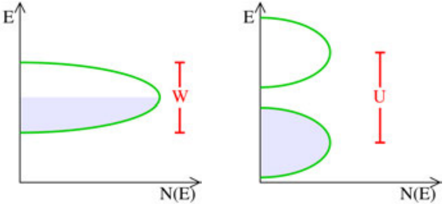
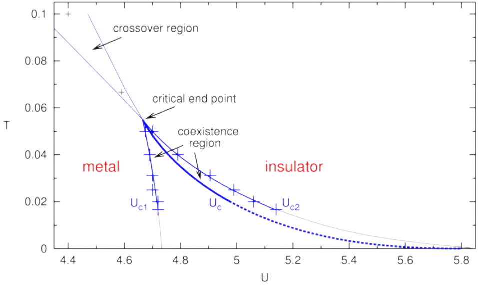


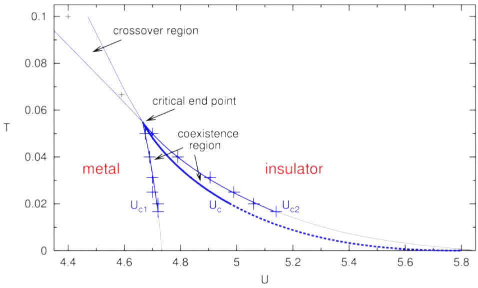
band-splitting by Coulomb correlations

Paramagnetic Mott transition at half filling within DMFT

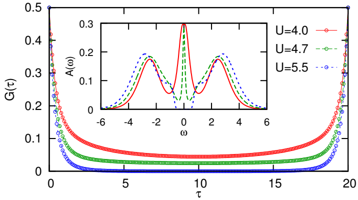


Phase diagram

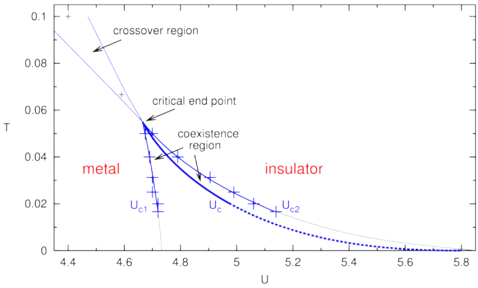
Paramagnetic Mott transition at half filling within DMFT

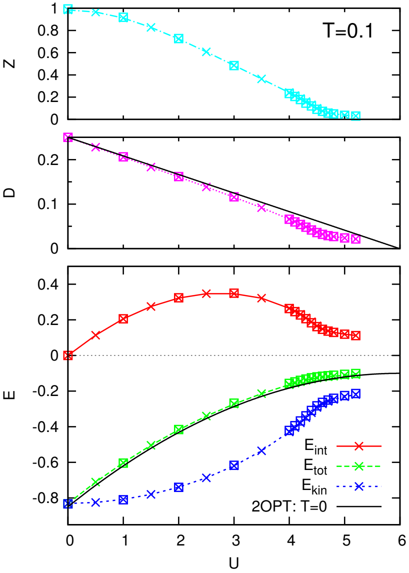


Phase diagram can be constructed from
(i) $G(\tau) \rightsquigarrow A(\omega)$;

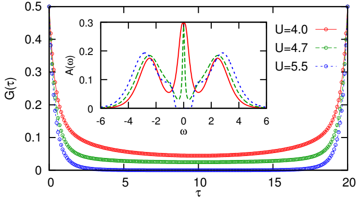


Paramagnetic Mott transition at half filling within DMFT





Phase diagram can be constructed from
(i) $G(\tau) \rightsquigarrow A(\omega)$; (ii) other observables



DMFT+HF-QMC Tutorial

- Task: Find and explore MIT
- Tools
- Background: Metal-Insulator Transition in the half-filled Hubbard model
- Manual for Mainz implementation of DMFT+HF-QMC
- Manual for Mainz implementation of Maximum Entropy method

[version of 2011/10/05]

Task: Find and explore MIT (Bethe lattice, paramagnetic case)

0. In your home directory create a symbolic link to the **bin** folder containing all the executables and scripts for this Tutorial:
   ln -s /home/bluemer/bin

1. Perform DMFT calculations for T = 0.04, fixed value of $\Delta\tau = 0.2$, and
   U = 3.5, 4, 4.5, 4.7, 4.8, 5, 5.5
   - in a series with increasing interaction values
   - in a series with decreasing interaction values

2. Extract observables:
   i. double occupancy D(U)
   ii. quasiparticle weight $Z(U) = (1 - Im\Sigma(\omega_1)/\omega_1)^{-1}$

3. Check convergency with D and/or Z

4. Compute spectra (using MaxEnt)

5. Explore the dependence of the results on the imaginary time discretization $\Delta\tau$:
   i. For one of the U values perform calculations for a set of $\Delta\tau$ values.
   ii. Plot double occupancy as a function of $\Delta\tau^2$
   iii. Perform $\Delta\tau \to 0$ extrapolation

Hint: you may use the provided scripts to create input files and extract observables.