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

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Outline

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


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

[Blümer, Gorelik, Comp. Phys. Comm. (2011); Gorelik, Blümer, JLTP (2011)]

Tutorial: study Mott metal-insulator transition using HF-QMC
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[1105.3356]

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[Gorelik, Titvinidze, Hofstetter, Snoek, Blümer, PRL (2010)]
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Tutorial: study Mott metal-insulator transition using HF-QMC
Hubbard model (arbitrary hopping, 1 band)

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

\[
= \sum_{k,\sigma} \varepsilon_k \hat{n}_{k\sigma} + U \sum_i \hat{D}_i; \quad \hat{D}_i = \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}
\]
Introduction: Hubbard model and DMFT self-consistency

Hubbard model (arbitrary hopping, 1 band)

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\[ = \sum_{k, \sigma} \varepsilon_k \hat{n}_{k\sigma} + U \sum_{i} \hat{D}_i; \quad \hat{D}_i = \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \]

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


+ non-perturbative \( \rightsquigarrow \) valid at MIT

+ in thermodynamic limit

+/- exact for coordination \( Z \rightarrow \infty \)

(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)

\[ \Sigma_0 \rightarrow \Sigma \rightarrow G \rightarrow \Sigma \rightarrow G \]

\[ \text{impurity problem} \]

\[ \leftarrow \text{DOS} / t_{ij}^\nu / \epsilon_{\nu k} \]

\[ \leftarrow \text{interactions} \]
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Impurity solver:
- Iterative perturbation theory (IPT; not controlled)
- Hirsch-Fye quantum Monte-Carlo (HF-QMC)

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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 $\psi$, $\psi^*$):

$$G_\sigma(\tau) = -\frac{1}{Z} \int \mathcal{D}[\psi, \psi^*] \langle \psi_\sigma(\tau) \psi^*_\sigma(0) \rangle \exp \left[ A_0 - U \int_0^\beta d\tau' \psi_\downarrow^* \psi_\uparrow \psi_\downarrow^* \psi_\downarrow \right] \approx \hat{c}_\sigma \hat{c}_\sigma^\dagger \Rightarrow \hat{n}_\uparrow \hat{n}_\downarrow$$
Auxiliary-field QMC algorithm [Hirsch, Fye (1986)]

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

(ii) Trotter decoupling $e^{-\beta(\hat{T} + \hat{V})} \approx e^{-\Delta \tau \hat{T}} e^{-\Delta \tau \hat{V}}$
**Auxiliary-field QMC algorithm [Hirsch, Fye (1986)]**

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$$\approx \hat{c}_\sigma \hat{c}_\sigma^\dagger$$

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

$$\hat{n}_\uparrow \hat{n}_\downarrow = \frac{1}{2} \left[ \hat{n}_\uparrow + \hat{n}_\downarrow - (\hat{n}_\uparrow - \hat{n}_\downarrow)^2 \right] \quad \sim \quad e^{-\Delta \tau U \hat{n}_\uparrow \hat{n}_\downarrow} = e^{-\Delta \tau U/2} e^{\Delta \tau U(\hat{n}_\uparrow - \hat{n}_\downarrow)^2/2}$$
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(iii) Hubbard-Stratonovich transform

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

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

Wick theorem:

$$G = \frac{\sum M \text{det}\{M\}}{\sum \text{det}\{M\}}$$
Action $A_0 = U \int_0^\beta d\tau' \psi^*_\uparrow \psi^*_\downarrow \psi^*_\downarrow \psi^*_\uparrow$ in discretized form:

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

Matrix $G_{\sigma}$ consists of elements $G_{\sigma ll'} \equiv G_{\sigma}(l\Delta \tau - l'\Delta \tau)$; $\psi_{\sigma l} \equiv \psi_{\sigma}(l\Delta \tau)$. 

Hirsch-Fye QMC: some more details (1/3) . . .
Action $A_0 - U \int_0^\beta d\tau' \psi^*_\uparrow \psi^*_\downarrow \psi^*_\downarrow \psi^*_\uparrow$ in discretized form:

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Matrix $G_\sigma$ consists of elements $G_{\sigma ll'} \equiv G_{\sigma} (l \Delta \tau - l' \Delta \tau)$; $\psi_{\sigma l} \equiv \psi_{\sigma} (l \Delta \tau)$.

The Trotter decomposition yields to lowest order

$$\exp (A^\Lambda[\psi, \psi^*, G, U]) = \prod_{l=0}^{\Lambda-1} \left[ \exp \left( (\Delta \tau)^2 \sum_{\sigma} \sum_{l'=0}^{\Lambda-1} \psi^*_\sigma l (G^{-1}_\sigma)_{l'l'} \psi_{\sigma l'} \right) \right. \times \left. \exp \left( -\Delta \tau \ U \psi^*_\uparrow l \psi^*_\downarrow l \psi^*_\downarrow l \psi^*_\uparrow l \right) \right].$$  \hspace{1cm} (12)
Hubbard-Stratonovich transformation (+ Trotter again) yields

\[ G_{\sigma l_1 l_2} = \frac{1}{Z} \sum_{\{s\}} \int \mathcal{D}[\psi] \mathcal{D}[\psi^*] \psi^*_\sigma l_1 \psi^*_\sigma l_2 \exp \left( \sum_{\sigma, l, l'} \psi^*_\sigma l M_{\sigma l l'}^{s_i} \psi_{\sigma l'} \right), \]  \hspace{1cm} (14)

With

\[ M_{\sigma l l'}^{s_i} = (\Delta \tau)^2 (G_{\sigma}^{-1})_{l l'} - \lambda \sigma \delta_{l l'} s_l \]
Hirsch-Fye QMC: some more details (2/3) . . .

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with* \( M^s_{\sigma l l'} = (\Delta \tau)^2 (G^{-1}_\sigma)_{l l'} - \lambda \sigma \delta_{l l'} s_l \)

Apply Wick’s theorem \( \leadsto \)

\[ G_{\sigma l l'} = \frac{1}{Z} \sum_{\{s\}} (M^s_\sigma)_{l l'}^{-1} \det M^s_\uparrow \det M^s_\downarrow, \]

\[ Z = \sum_{\{s\}} \det M^s_\uparrow \det M^s_\downarrow. \]
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(14)

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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Apply Wick’s theorem \( \leadsto \)

\[ G_{\sigma ll'} = \frac{1}{Z} \sum_{\{s\}} (M^{\{s\}}_\sigma)_{ll'}^{-1} \det M^{\{s\}}_\uparrow \det M^{\{s\}}_\downarrow, \]  

(16)

\[ Z = \sum_{\{s\}} \det M^{\{s\}}_\uparrow \det M^{\{s\}}_\downarrow. \]  

(17)

Computational cost of naive computation of each term:

matrix inverse: \( \mathcal{O}(\Lambda^3) \)  
determinants worse than \( \mathcal{O}(\Lambda^4) \)
Gray code (or MC): *flip single spin* between subsequent configuration:

\[
\begin{align*}
M_{\sigma} \xrightarrow{s_m \rightarrow -s_m} M'_{\sigma} &= M_{\sigma} + \Delta^{\sigma \cdot m} \\
&= (1 + \Delta^{\sigma \cdot m} (M_{\sigma})^{-1}) M_{\sigma} \\
\text{with} \\
\Delta^{\sigma \cdot m}_{ll'} &= \delta_{ll'} \delta_{lm} 2\Delta \tau \lambda \sigma s_l
\end{align*}
\]
Hirsch-Fye QMC: fast update scheme

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

\[ M_\sigma^{s_m \rightarrow -s_m} M_\sigma' = M_\sigma + \Delta^{\sigma m} \]
\[ = (1 + \Delta^{\sigma m}(M_\sigma)^{-1}) M_\sigma \]

with \[ \Delta^{\sigma l'm}_{ll'} = \delta_{ll'} \delta_{lm} 2\Delta \tau \lambda \sigma s_l \] (18)

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

\[
R^{\sigma m} := \frac{\det(M_\sigma')}{\det(M_\sigma)} = \det(1 + \Delta^{\sigma m}(M_\sigma)^{-1})
\]
\[ = 1 + 2\Delta \tau \lambda \sigma s_m (M_\sigma)^{-1}_{mm} \]

(19)
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The inversion of \( M \) is also elementary, one obtains:

\[ (M'_\sigma)^{-1} = (M_\sigma)^{-1} + \frac{1}{R^{\sigma m}} (M_\sigma)^{-1} \Delta^{\sigma m}(M_\sigma)^{-1} \]  
\[ \sim \text{computational cost for each term: } \mathcal{O}(\Lambda^2). \]
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\begin{align*}
M_\sigma \xrightarrow{s_m \rightarrow -s_m} M_\sigma' &= M_\sigma + \Delta_\sigma^m \\
&= (1 + \Delta_\sigma^m (M_\sigma)^{-1}) M_\sigma
\end{align*}
\]

with \( \Delta_\|_l^m = \delta_\|_l \delta_l m \, 2\Delta \tau \nu \sigma s_l \) \hfill (18)

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\[
(M_\sigma')^{-1} = (M_\sigma)^{-1} + \frac{1}{R_\sigma^m} (M_\sigma)^{-1} \Delta_\sigma^m (M_\sigma)^{-1}
\]

\( \sim \) computational cost for each term: \( \mathcal{O}(\Lambda^2) \). \hfill But: \( 2^\Lambda \) terms!
General task: evaluation of (high-dimensional) sums/integrals

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

\[ I = \int_{a}^{b} f(x) \, dx = ? \]
Monte Carlo methods: principles and classical simulations

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Convergence of results?

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Application of Monte Carlo in Statistical Physics

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

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

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**Importance Sampling MC:** Probability distribution given by Boltzmann weights \( p_i \). **Problem:** Normalization \( 1/Z \) unknown.
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Solution: approach target probability distribution by random walk (e.g.: 8 states)
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Ergodicity and detailed balance

\[ p_i \ P \{ i \rightarrow j \} = p_j \ P \{ j \rightarrow i \} \]

\[ \Rightarrow \ P\ [\text{state } i \ \text{after update } N] \xrightarrow{N \to \infty} p_i \]
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Favorite choice: **Metropolis rule**

\[ P\{i \rightarrow j\} = \min\left\{ \frac{p_j}{p_i}, 1 \right\} , \quad \frac{p_j}{p_i} = e^{\Delta E/(k_B T)} \]
Monte Carlo importance sampling in Hirsch-Fye method

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

\[ P(\{s\}) = \left| \det M^{\uparrow} \det M^{\downarrow} \right| \]
Monte Carlo importance sampling in Hirsch-Fye method

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

\[
P(\{s\}) = \left| \det M_\uparrow^{\{s\}} \det M_\downarrow^{\{s\}} \right| \tag{28}
\]

The Green function can then be calculated as an average \( \langle \ldots \rangle_s \):

\[
G_{\sigma ll'} = \frac{1}{\tilde{Z}} \left\langle \left( M_\sigma^{\{s\}} \right)^{-1} \operatorname{sign} \left( \det M_\uparrow^{\{s\}} \det M_\downarrow^{\{s\}} \right) \right\rangle_s , \tag{29}
\]

\[
\tilde{Z} = \left\langle \operatorname{sign} \left( \det M_\uparrow^{\{s\}} \det M_\downarrow^{\{s\}} \right) \right\rangle_s . \tag{30}
\]

Note: \( \tilde{Z} \) 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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(28)

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

\[ G_{\sigma ll'} = \frac{1}{\tilde{\mathcal{Z}}} \left\langle \left( M_{\sigma}^{\{s\}} \right)_{ll'}^{-1} \text{sign} \left( \det M_{\uparrow}^{\{s\}} \det M_{\downarrow}^{\{s\}} \right) \right\rangle_s, \]  
(29)

\[ \tilde{\mathcal{Z}} = \left\langle \text{sign} \left( \det M_{\uparrow}^{\{s\}} \det M_{\downarrow}^{\{s\}} \right) \right\rangle_s. \]  
(30)

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

MC with importance sampling \(\not\sim\) partition function, free energy, entropy!

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

\[ G_{\sigma ll'} = \frac{1}{\tilde{\mathcal{Z}}} \left\langle \left( M_{\sigma}^{\{s\}} \right)_{ll'}^{-1} \right\rangle_s, \quad \tilde{\mathcal{Z}} = \left\langle 1 \right\rangle_s. \]  
(31)
Recipe for practical HF-QMC calculations

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

(ii) Compute initial Green function matrix \( M^{-1} \) (determinant not needed)
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(iii) Thermalization of Markov chain by \( N_{\text{warm}} \) warm-up sweeps
(iv) Perform \( N_{\text{meas}} \) measurement sweeps
   (accumulate sum of intermediate Green functions \( M^{-1} \) and observables)
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\(\rightsquigarrow\) Green function, other observables (double occupancy, susceptibilities, \ldots)
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    \( \rightsquigarrow \) Green function, other observables (double occupancy, susceptibilities, \ldots )

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

Metropolis acceptance probability:
\[
\text{min}\{1, R^{\uparrow m} R^{\downarrow m}\}, \quad \text{where}
\]
\[
R^{\sigma m} = \frac{\det(M^{\sigma'})}{\det(M_\sigma)} = 1 + 2\Delta \tau \lambda \sigma s_m (M_\sigma)^{-1}_{mm}
\]
Impact of HF-QMC parameters: number of sweeps, discretization $\Delta \tau$

- **Statistical error:**
  \[
  (\Delta G)_{\text{statistical}} \propto \frac{1}{\sqrt{N_{\text{meas}}}}
  \]
Impact of HF-QMC parameters: number of sweeps, discretization $\Delta \tau$

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  \[(\Delta G)_{\text{statistical}} \propto 1/\sqrt{N_{\text{meas}}}\]

- **Thermalization error:** $N_{\text{warm}}$ “large enough” (e.g. $N_{\text{warm}} = N_{\text{meas}}/100$)
Impact of HF-QMC parameters: number of sweeps, discretization $\Delta \tau$

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- **Thermalization error:** $N_{\text{warm}}$ “large enough” (e.g. $N_{\text{warm}} = N_{\text{meas}}/100$)

- **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)

\[ G(i\omega_n) = \int d\varepsilon \frac{\rho_0(\varepsilon)}{i\omega_n - \varepsilon - \Sigma(i\omega_n)} \]

\[ G^{-1}(i\omega_n) = G^{-1}(i\omega_n) + \Sigma(i\omega_n) \]

\[ G(\tau) = -\langle \Psi \Psi^* \rangle_{g[\tau], \Delta \tau} \]
Iterative solution of DMFT self-consistency equations

For each discretization $\Delta \tau$:

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2. Solve single impurity Anderson model (SIAM)

\[
G(\tau) = -\langle \Psi \Psi^* \rangle G[\tau], \Delta \tau
\]

\[
\Sigma_0 \rightarrow \Sigma_{\Delta \tau}
\]

\[
G^{-1}(i\omega_n) = G^{-1}(i\omega_n) + \Sigma(i\omega_n)
\]

\[
G(\tau) = \int d\varepsilon \frac{\rho_0(\varepsilon)}{i\omega_n - \varepsilon - \Sigma(i\omega_n)}
\]

How many iterations?

Look at traces!
Iterative solution of DMFT equations
(for imaginary-time impurity solver)
Special issue: Fourier transformations in DMFT-QMC cycle

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

Naive discrete Fourier transformation $\rightsquigarrow$ oscillations (instead of $G(\omega) \xrightarrow{\omega \to \infty} 1/\omega$)
One solution: interpolate $G_{QMC}(\tau)$, e.g., by cubic splines [Jarrell, Krauth, Gull, ...]

But: $\frac{d^2 G(\tau)}{d\tau^2}$ maximal for $\tau \to 0, \beta \sim$ natural boundary conditions inappropriate
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- adjust boundary cond. [Oudovenko]
- spline-fit only
difference w.r.t. reference problem:
  - IPT [Jarrell]
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But: \( \frac{d^2 G(\tau)}{d\tau^2} \) maximal for \( \tau \to 0, \beta \sim \text{natural boundary conditions inappropriate} \)

- adjust boundary cond. [Oudovenko]
- spline-fit only difference w.r.t. reference problem:
  - IPT [Jarrell]
  - high-frequency expansion for \( \Sigma(\omega) \) [Knecht, NB]

\[
\Sigma_\sigma(\omega) = U\left(\langle \hat{n}_{-\sigma} \rangle - \frac{1}{2}\right) \omega^0 + U^2 \langle \hat{n}_{-\sigma} \rangle \left(1 - \langle \hat{n}_{-\sigma} \rangle\right) \omega^{-1} + O(\omega^{-2})
\]
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- adjust boundary cond. [Oudovenko]
- spline-fit only difference w.r.t. reference problem:
  - IPT [Jarrell]
  - high-frequency expansion for $\Sigma(\omega)$ [Knecht, NB]

\[
\Sigma_{\sigma}(\omega) = U\left(\langle \hat{n}_{-\sigma} \rangle - \frac{1}{2}\right) \omega^0 + U^2 \langle \hat{n}_{-\sigma} \rangle \left(1 - \langle \hat{n}_{-\sigma} \rangle \right) \omega^{-1} + O(\omega^{-2})
\]

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
Extrapolation

Self-consistency cycle using conventional HF-QMC

\[ G(i\omega_n) = \int d\varepsilon \frac{\rho_0(\varepsilon)}{i\omega_n - \varepsilon - \Sigma(i\omega_n)} \]

\[ G^{-1}(i\omega_n) = G^{-1}(i\omega_n) + \Sigma(i\omega_n) \]

\[ G(\tau) = -\langle \Psi \Psi^* \rangle_{g[\tau],\Delta \tau} \]
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Extrapolation $\Delta \tau \to 0$ improves accuracy by orders of magnitude ($\sim$ same cost)
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Example: energy $E$ for $U = 4$, $T = 1/45$ (Bethe DOS) [NB, PRB (2007)]
Extrapolation

Self-consistency cycle using conventional HF-QMC

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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 $\leftrightarrow$ QMC, even at small $U$
Comparison DMFT – direct QMC for the 3d cubic lattice ($n = 1$)

Excellent general agreement DMFT ↔ QMC, even at small $U$

Typical QMC discretization errors (thin lines) larger than DMFT deviations!
Double occupancy as a universal measure of AF correlations + entropy

![Graph showing double occupancy as a function of s for different dimensions and models.]

Minimum of $D(s)$ at $s \approx \log 2$ for all $d$!
Double occupancy as a universal measure of AF correlations + entropy

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.: \( V_i = V r_i^2 \)

\[ H = - \sum_{(ij),\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow} + \sum_{i,\sigma} V_i n_{i\sigma} \]
Real-space DMFT: use local self-energy in inhomogeneous system

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\]

\( \sim N \) single-site impurities, coupled by real-space lattice Dyson equation:

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


Note: impurity problems are site-parallel,
lattice Dyson equation is frequency-parallel
Real-space DMFT: use local self-energy in inhomogeneous system

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\end{bmatrix}^{-1}_{ij} = 
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Here: HF-QMC (cost $\propto T^{-3}$)

"slab method" + pbc

$\sim$ exact for $O(10^5)$ atoms

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"slab method" + pbc

$\sim$ exact for $O(10^5)$ 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

[Goerlik, Titvinidze, Hofstetter, Snoek, Blümer, PRL (2010)]
Tutorial: study Mott metal-insulator transition using HF-QMC

Elena Gorelik
Univ. Mainz

Daniel Rost
Univ. Mainz
Physics of the Mott transition

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

Hydrostatic pressure or isovalent doping change
- lattice spacings
- bond angles

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

Bond angles for $V_2O_3$ doped with Cr or Ti
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$\sim\sim$ hopping amplitudes

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

Bond angles for $V_2O_3$ doped with Cr or Ti

Breakdown of Bloch band description at paramagnetic Mott transition

Bloch states near Fermi energy
Physics of the Mott transition

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Bloch states near Fermi energy

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) $G(\tau) \sim A(\omega)$;
Paramagnetic Mott transition at half filling within DMFT

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