Special session: Methods for correlated materials

Nils Blümer (chair)

Mats Granath:	*Distributional ED, a real-frequency impurity solver*
Daniel C. Rost:	*Quasi-CT impurity solver linear in β*
Martin Ganahl:	*Efficient impurity solver using Matrix Product States*
Georg Rohringer:	*1-particle irreducible functional approach (DMFT+X)*
Ciro Taranto:	*From ∞ to d dimensions: DMFT + functional RG*

real-frequency (vs. analytic continuation), scaling of effort, beyond DMFT

Nils Blümer (chair): *Introduction to DMFT*

Mats Granath: *Distributional ED, a real-frequency impurity solver*

Daniel C. Rost: *Quasi-CT impurity solver linear in β*

Martin Ganahl: *Efficient impurity solver using Matrix Product States*

Georg Rohringer: *1-particle irreducible functional approach (DMFT+X)*

Ciro Taranto: *From ∞ to d dimensions: DMFT + functional RG*

real-frequency (vs. analytic continuation), scaling of effort, beyond DMFT

Essential steps in the DMFT development

1989 Metzner/Vollhardt: $d \to \infty$ nontrivial for fermions if $t = t^*/\sqrt{2d}$
Gutzwiller approximation exact

Müller-Hartmann: local self-energy: $\Sigma(\mathbf{q}, \omega) \to \Sigma(\omega)$

Brandt/Mielsch: exact solution of Falicov-Kimball model for $d = \infty$

Essential steps in the DMFT development

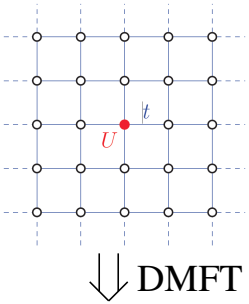
1989 Metzner/Vollhardt: $d \to \infty$ nontrivial for fermions if $t = t^*/\sqrt{2d}$
Gutzwiller approximation exact

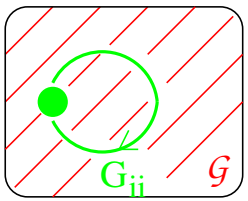
Müller-Hartmann: local self-energy: $\Sigma(\mathbf{q}, \omega) \to \Sigma(\omega)$

Brandt/Mielsch: exact solution of Falicov-Kimball model for $d = \infty$

1992 Georges/Kotliar: mapping to Anderson impurity model

Jarrell: HF-QMC $\rightsquigarrow$ antiferromagnetism, Mott-Hubbard behavior





Essential steps in the DMFT development

1989 Metzner/Vollhardt: $d \to \infty$ nontrivial for fermions if $t = t^*/\sqrt{2d}$
Gutzwiller approximation exact

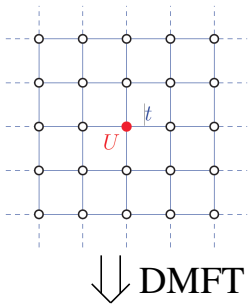
Müller-Hartmann: local self-energy: $\Sigma(\mathbf{q}, \omega) \to \Sigma(\omega)$

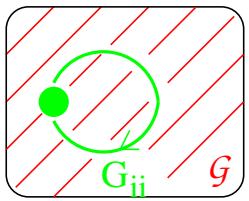
Brandt/Mielsch: exact solution of Falicov-Kimball model for $d = \infty$

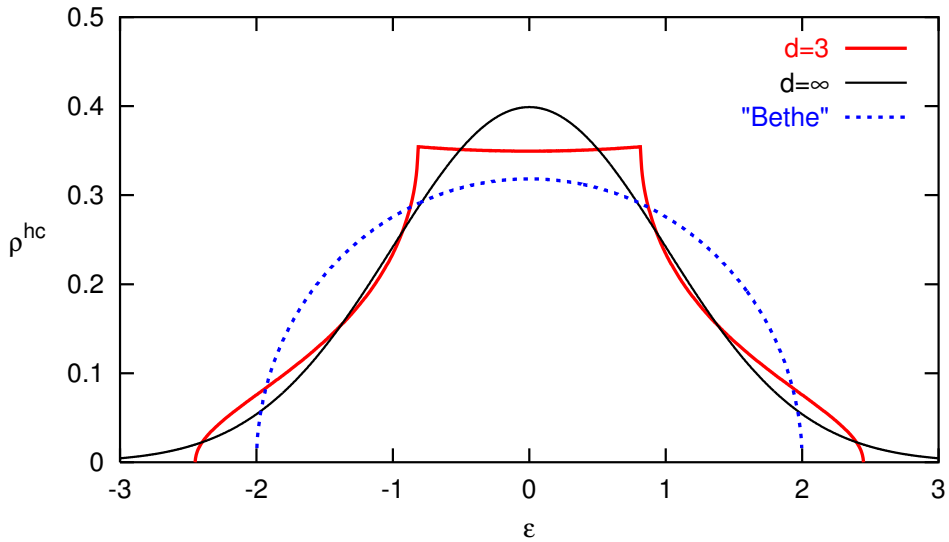
1992 Georges/Kotliar: mapping to Anderson impurity model

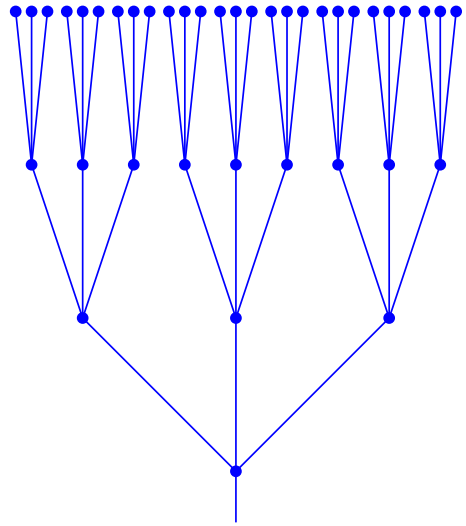
Jarrell: HF-QMC $\rightsquigarrow$ antiferromagnetism, Mott-Hubbard behavior

1993 Georges et al., Kotliar et al.: Bethe lattice (IPT/QMC) $\rightsquigarrow$ MIT



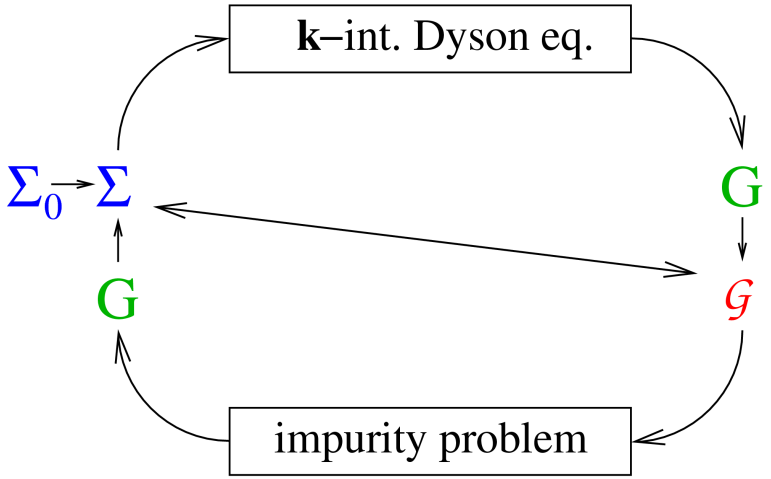






Iterative solution of DMFT self-consistency equations

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

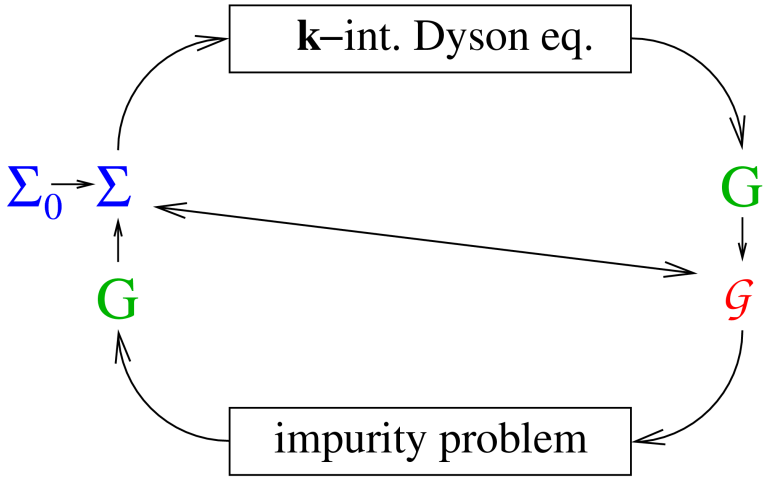


$\longleftarrow$ DOS / t_{ij}^{ν} / $\epsilon_{\nu\mathbf{k}}$

$\longleftarrow$ interactions

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} / $\epsilon_{\nu\mathbf{k}}$

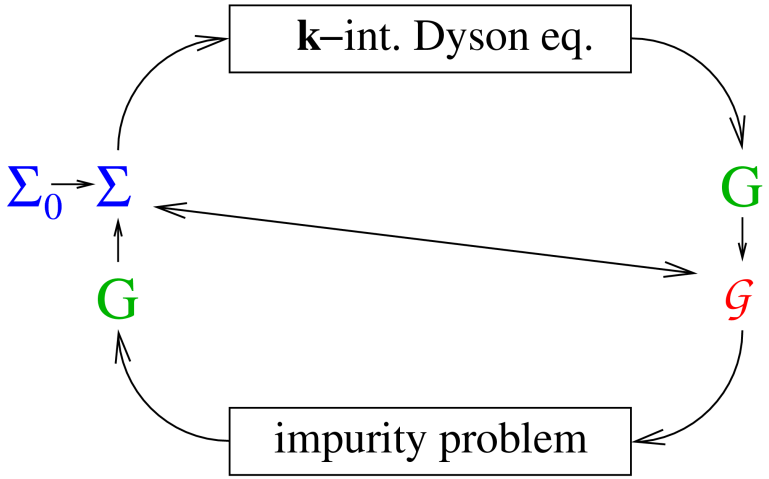
$\longleftarrow$ interactions

Impurity solver:

- Iterative perturbation theory (IPT), FLEX
- Non-crossing approximation (NCA) $\rightsquigarrow$ OCA
- Hirsch-Fye quantum Monte-Carlo (HF-QMC)
- Continuous-time quantum Monte-Carlo (CT-QMC)

Iterative solution of DMFT self-consistency equations

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

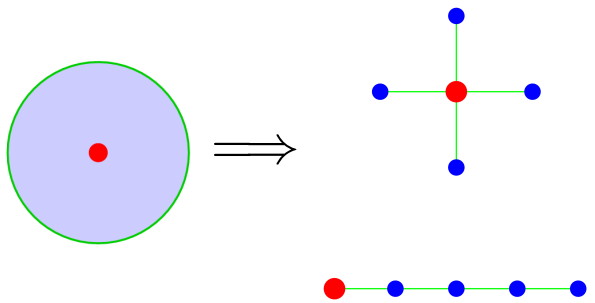


$\longleftarrow$ DOS / t_{ij}^{ν} / $\epsilon_{\nu\mathbf{k}}$

$\longleftarrow$ interactions

Impurity solver:

- Iterative perturbation theory (IPT), FLEX
- Non-crossing approximation (NCA) $\rightsquigarrow$ OCA
- 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 $1/T$)



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

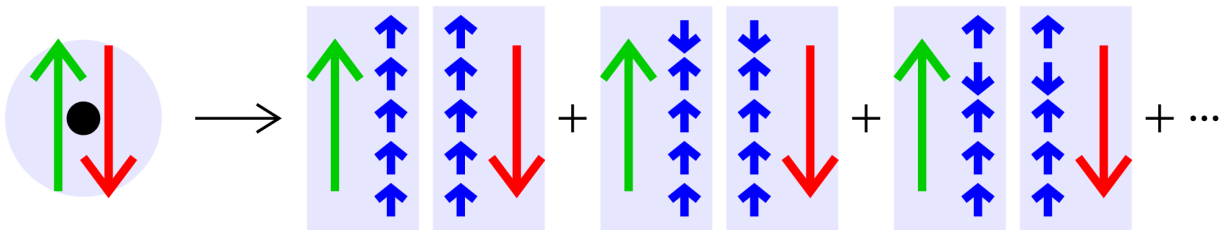
(i) Imaginary-time discretization $\beta = \Lambda\,\Delta\tau$

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

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

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

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



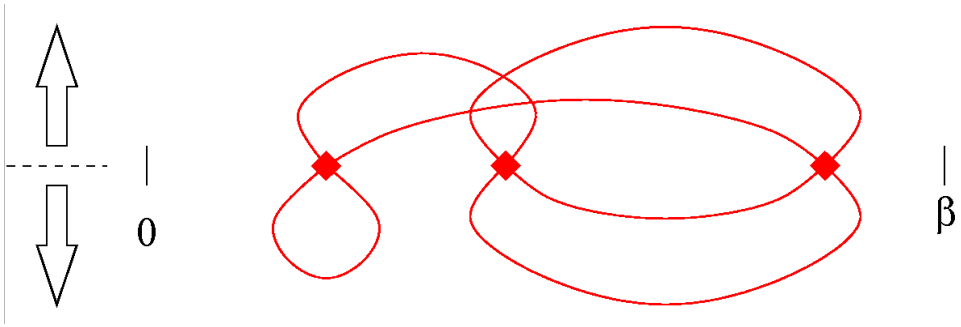
Wick theorem:

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

Alternative: continuous-time QMC algorithms

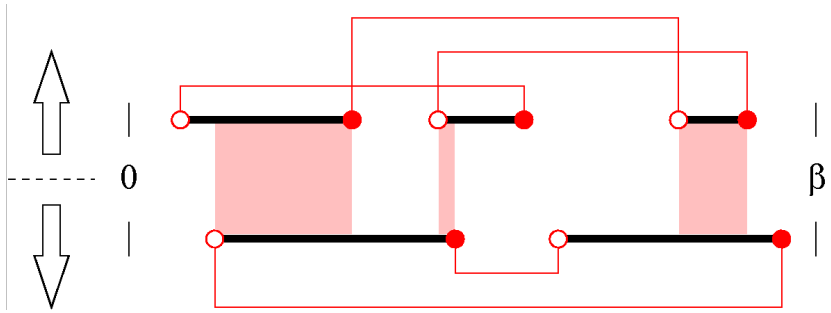
1. weak-coupling expansion

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



2. hybridization expansion

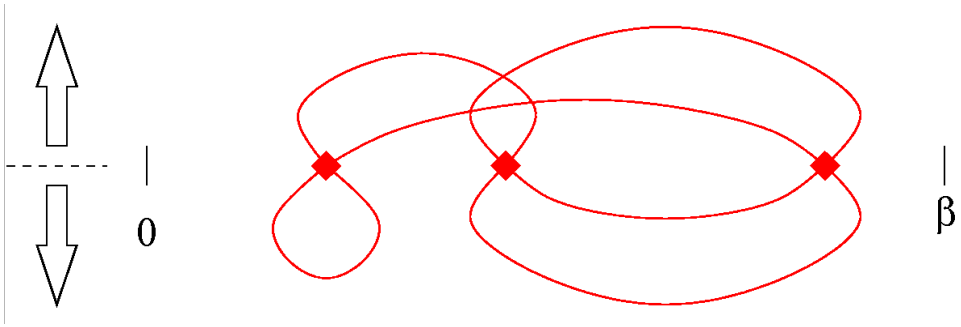
[Werner et al., PRL (2006)]



Alternative: continuous-time QMC algorithms

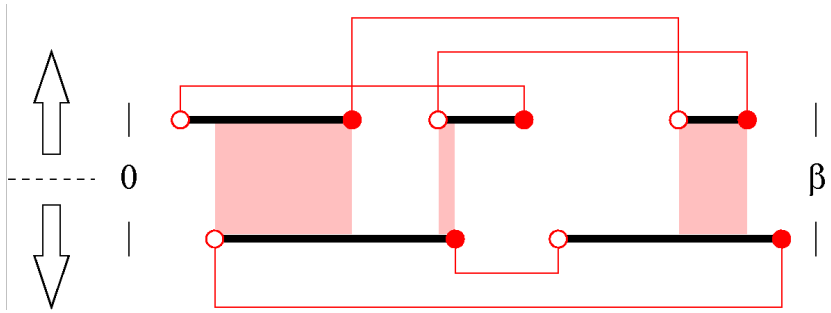
1. weak-coupling expansion

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



2. hybridization expansion

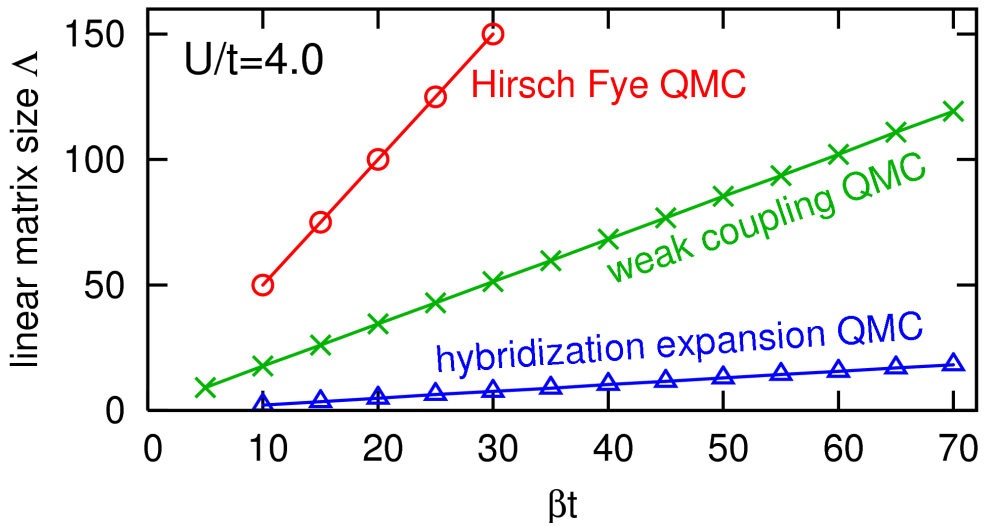
[Werner et al., PRL (2006)]



CT-QMC: smaller matrices

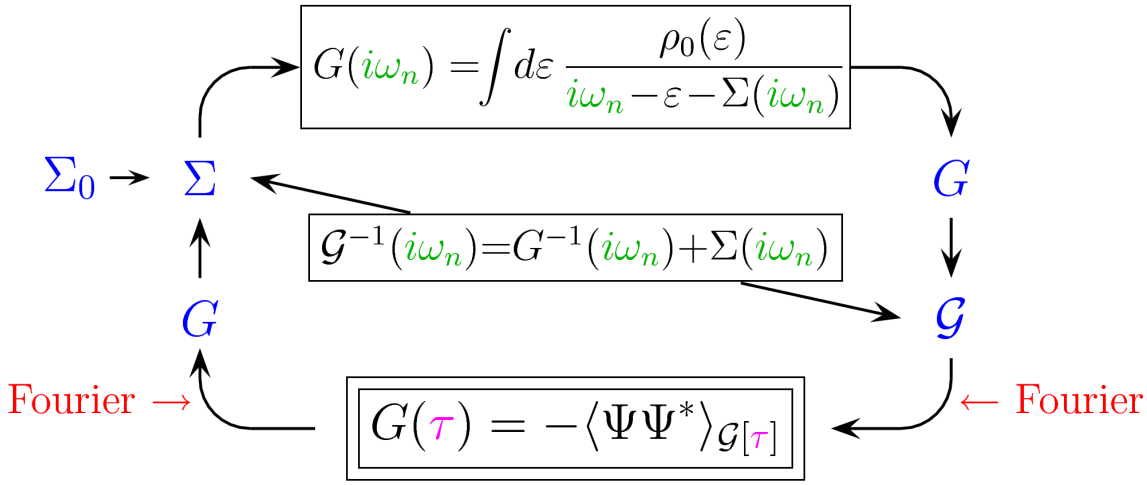
All QMC methods: effort $\propto \Lambda^3$

But: prefactor important!



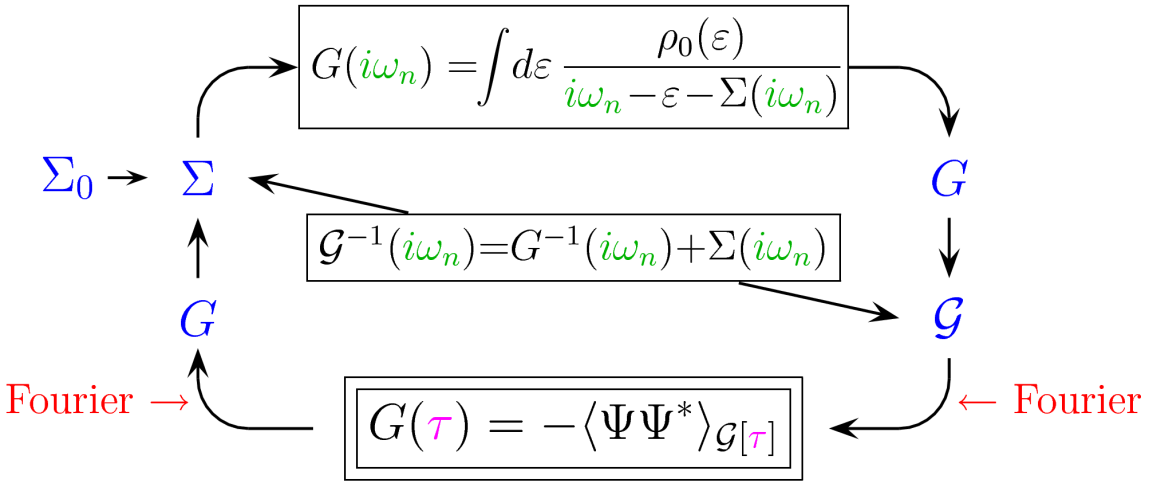
Consequences of imaginary-time formulation (HF-QMC, CT-QMC)

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

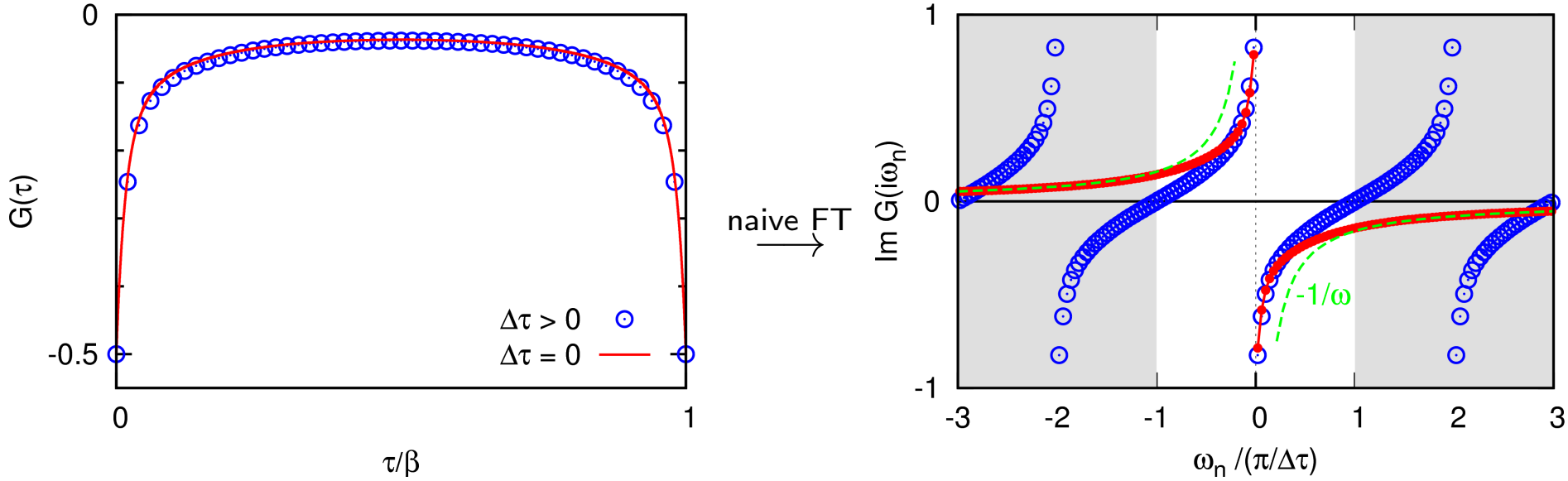


Consequences of imaginary-time formulation (HF-QMC, CT-QMC)

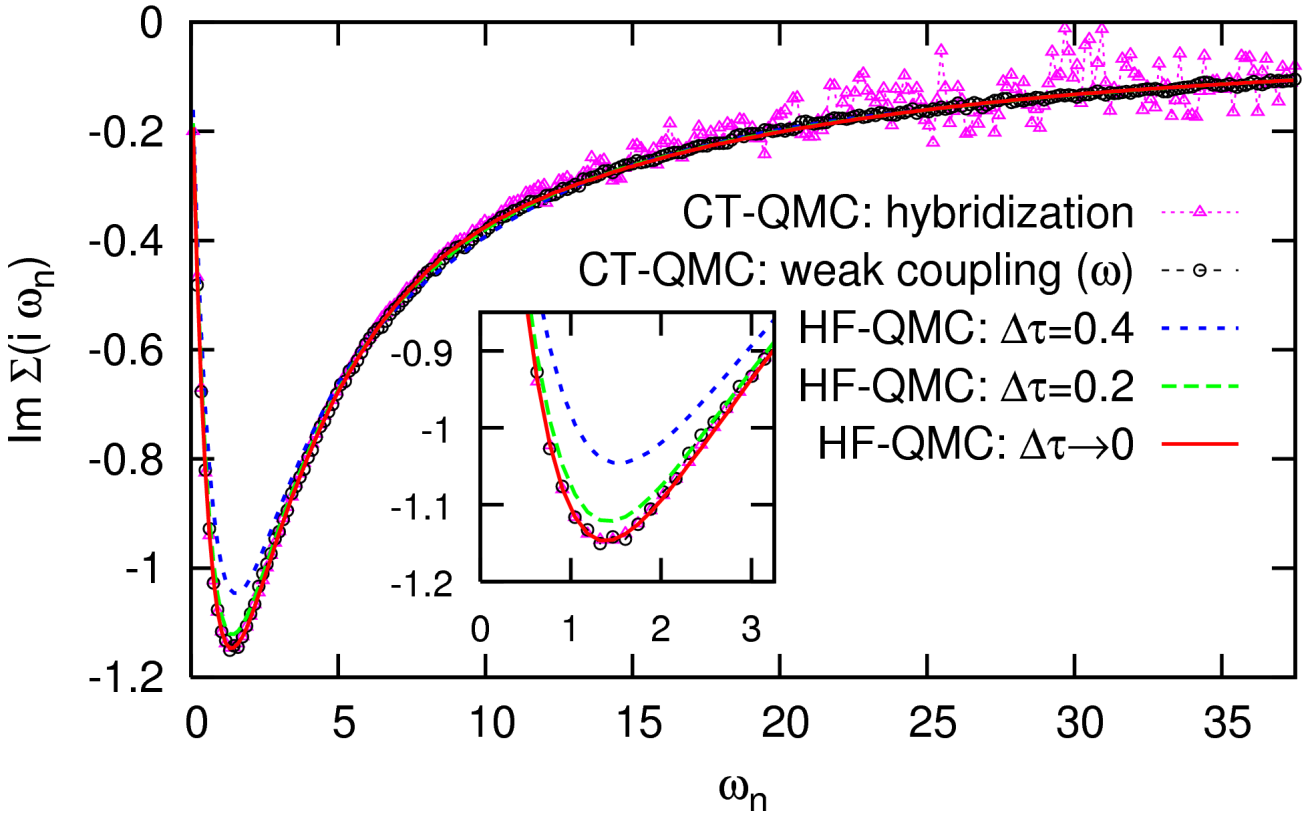
Iterative solution of DMFT equations (for imaginary-time impurity solver)



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



Sensitive test: high-frequency tails of self-energy



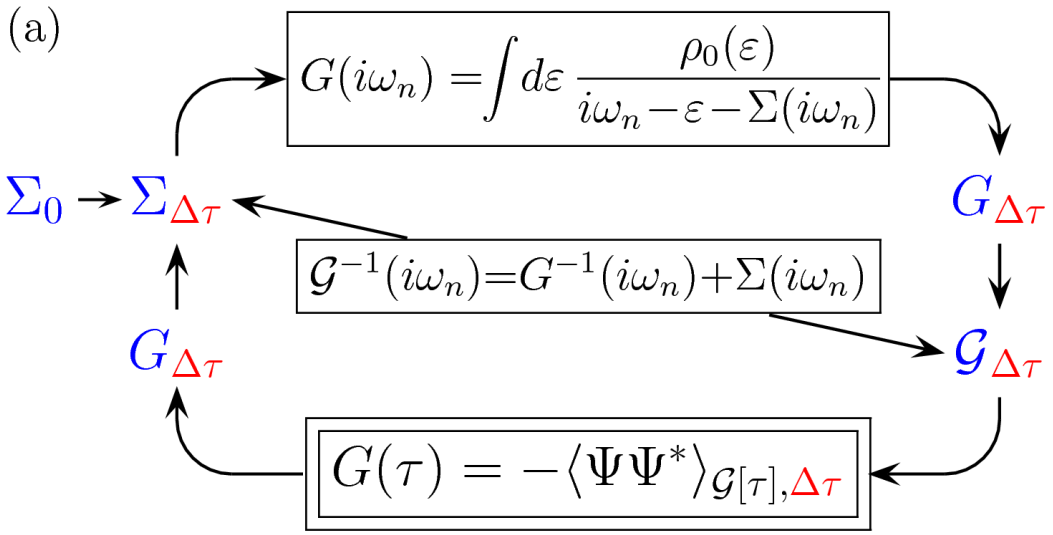
correct tails in HF-QMC for each $\Delta\tau$

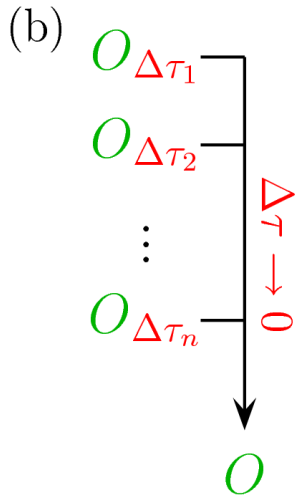
larger fluctuations in CT-QMC

Better: orthogonal polynomials
[Boehnke et al. (2011)]

Extrapolation

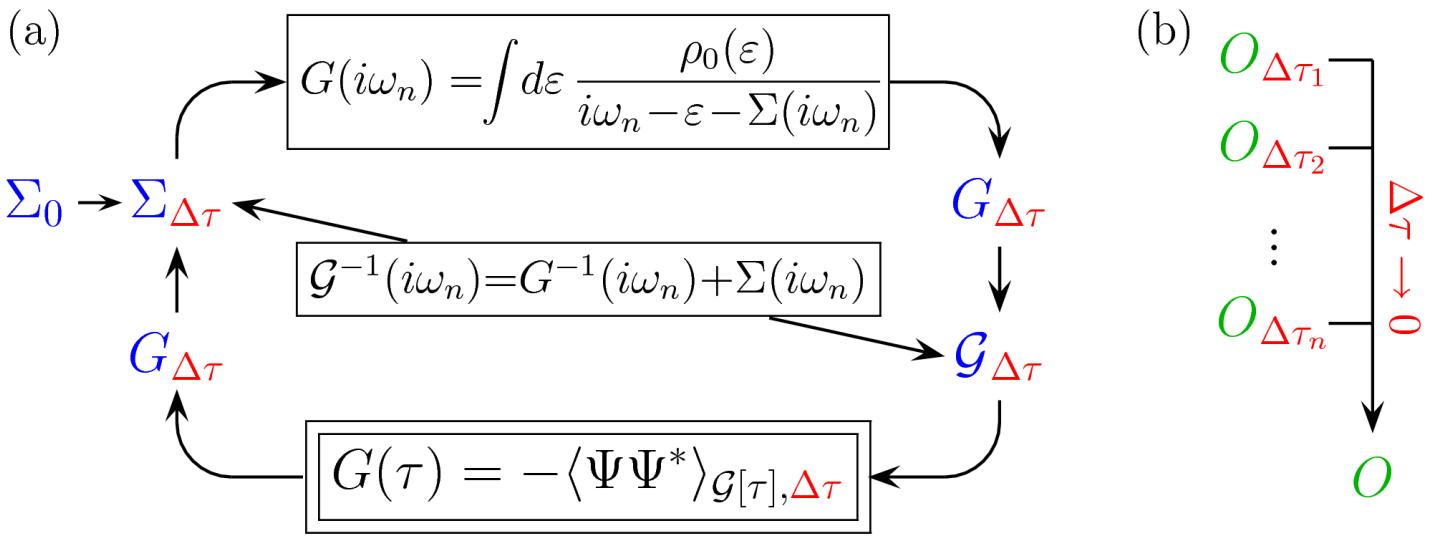
Self-consistency cycle using conventional HF-QMC





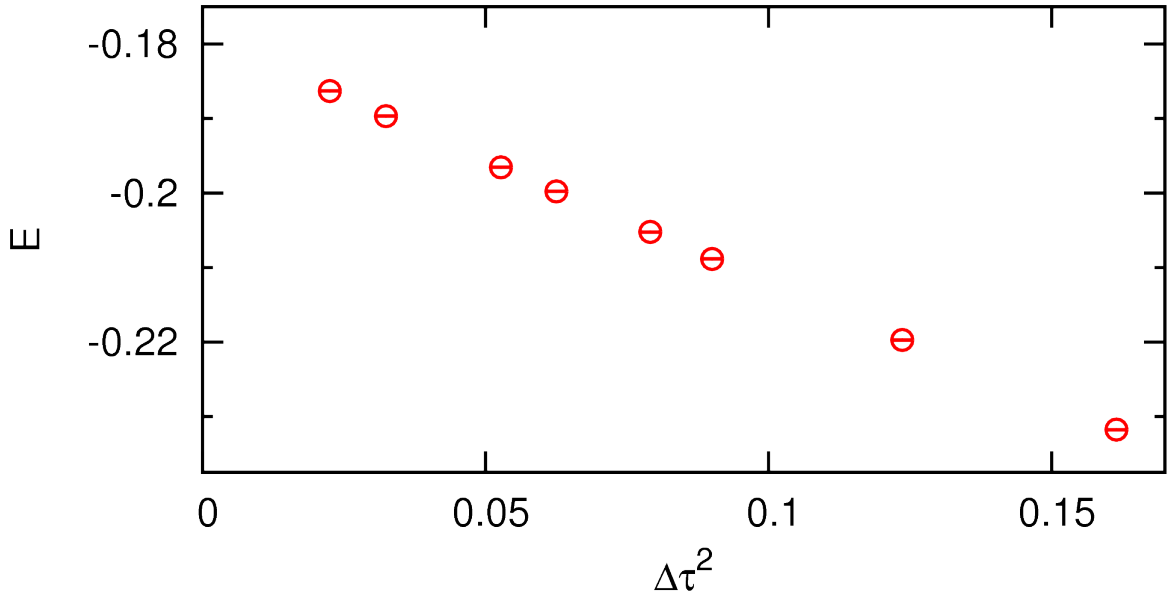
Extrapolation

Self-consistency cycle using conventional HF-QMC



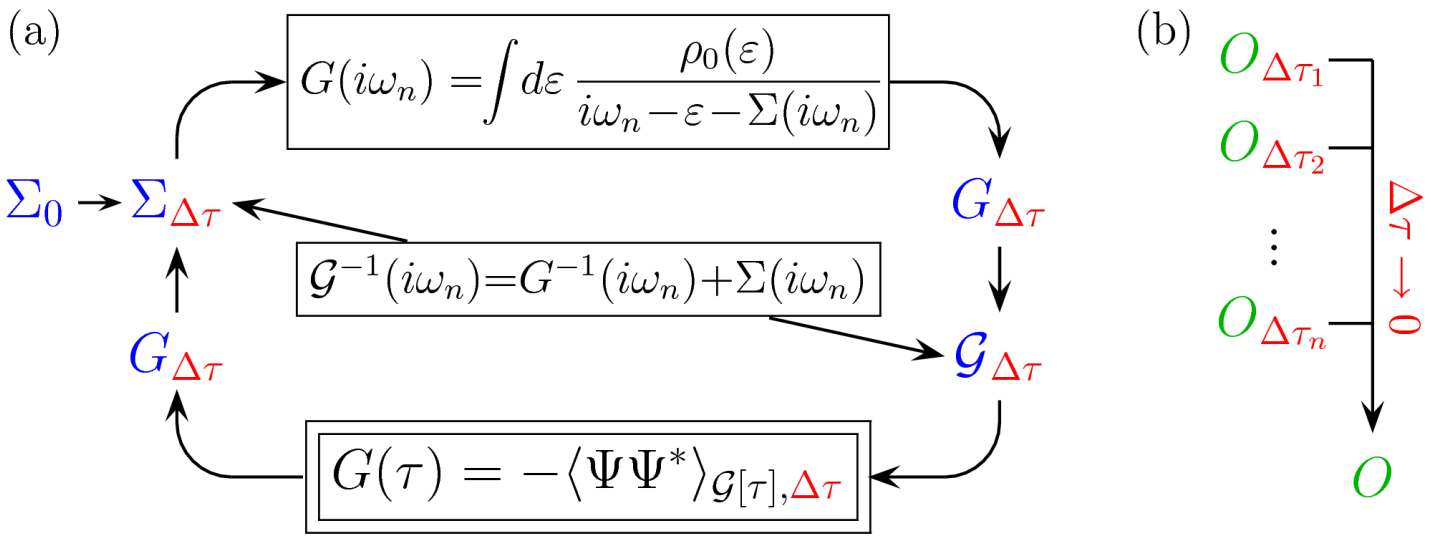
Extrapolation $\Delta\tau \to 0$ improves accuracy by orders of magnitude ($\sim$ same cost)

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



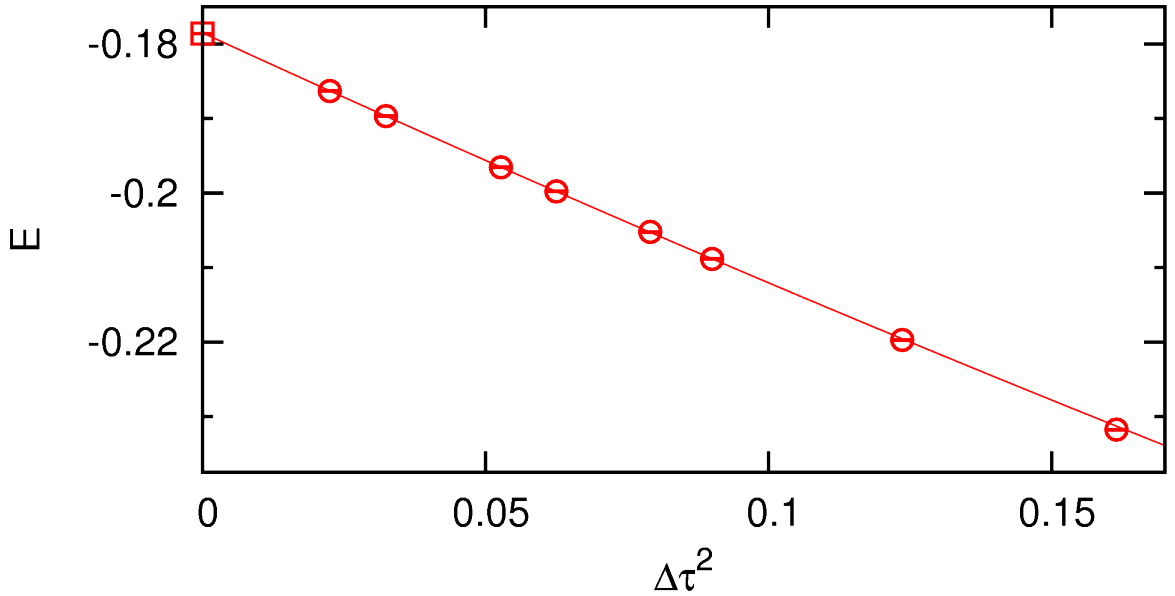
Extrapolation

Self-consistency cycle using conventional HF-QMC



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

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



Nils Blümer (chair)

Mats Granath: *Distributional ED, a real-frequency impurity solver*

Daniel C. Rost: *Quasi-CT impurity solver linear in β*

Martin Ganahl: *Efficient impurity solver using Matrix Product States*

Georg Rohringer: *1-particle irreducible functional approach (DMFT+X)*

Ciro Taranto: *From ∞ to d dimensions: DMFT + functional RG*

real-frequency (vs. analytic continuation), scaling of effort, beyond DMFT