Quantum Monte Carlo impurity solvers

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Monte Carlo impurity solvers

History

- Different types of solvers for different applications

based on Hubbard-Stratonovich
mainly for lattice problems

based on weak-coupling expansion

weak-coupling CT-QMC (2005)
Rubtsov, Lichtenstein, ...

BSS algorithm (1981)
Blankenbecler, Scalapino, Sugar

DMFT

noneq. DMFT

pnictides

inchworm algorithm (2015)
Cohen, Gull, Millis, Reichman

Hirsch-Fye algorithm (1986)
Hirsch, Fye

based on Hubbard-Stratonovich
mainly for impurity problems

strong-coupling CT-QMC (2006)
Werner, Troyer, Millis ...

based on hybridization expansion

based on resummed propagators
mainly for real-time simulations

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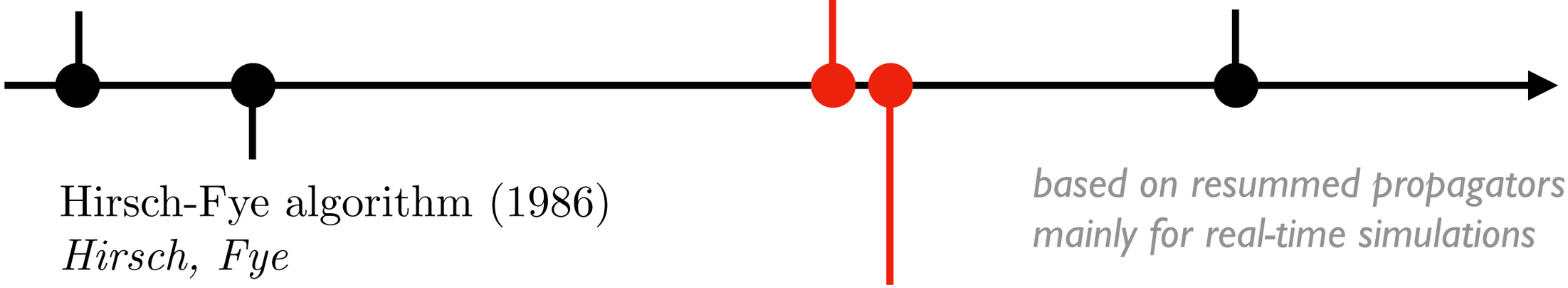

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based on Hubbard-Stratonovich
mainly for impurity problems

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based on hybridization expansion

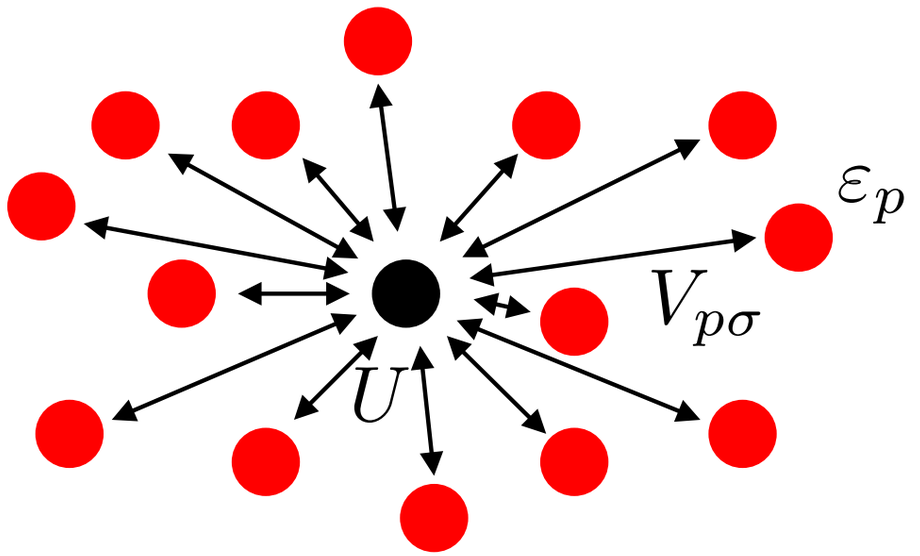
Quantum impurity models

Hamiltonian formulation $Z = \mathrm{Tr}_d \mathrm{Tr}_c \left[e^{-\beta H} \right]$

- Single-orbital Anderson impurity model

$$H = H_{\mathrm{loc}} + H_{\mathrm{bath}} + H_{\mathrm{mix}}$$

correlated impurity — *noninteracting electron bath* — *hybridization (mixing) term*



$$\begin{aligned} H_{\mathrm{loc}} &= H_\mu + H_U \\ H_\mu &= -\mu(n_\uparrow + n_\downarrow) \\ H_U &= U n_\uparrow n_\downarrow \end{aligned}$$

$$H_{\mathrm{bath}} = \sum_{p\sigma} \varepsilon_p c^\dagger_{p\sigma} c_{p\sigma}$$

$$H_{\mathrm{mix}} = \sum_{p\sigma} \left[V_{p\sigma} d^\dagger_\sigma c_{p\sigma} + V^*_{p\sigma} c^\dagger_{p\sigma} d_\sigma \right]$$

Quantum impurity models

Action formulation $Z = \mathrm{Tr}_d\left[\mathcal{T} e^{-S}\right]$

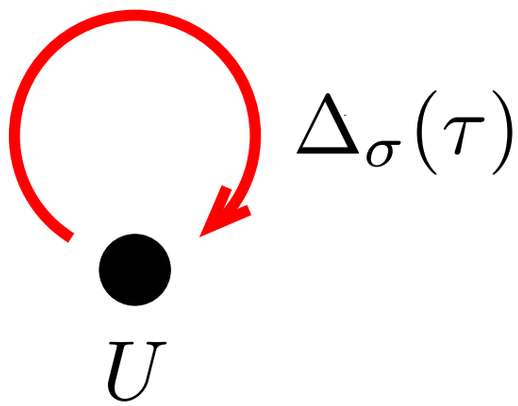
- Single-orbital Anderson impurity model

$$S = S_{\mathrm{loc}} + S_{\mathrm{mix}}$$

correlated impurity

hybridization (mixing) term

noninteracting bath is integrated out and replaced by the hybridization function



$$S_{\mathrm{mix}} = \sum_\sigma \int_0^\beta d\tau d\tau' d_\sigma^\dagger(\tau') \Delta^\sigma(\tau' - \tau) d_\sigma(\tau)$$

$$S_{\mathrm{loc}} = \int_0^\beta d\tau \Big[-\mu(n_\uparrow(\tau) + n_\downarrow(\tau)) + U n_\uparrow(\tau) n_\downarrow(\tau) \Big]$$

definition of hybridization function

$$\Delta^\sigma(i\omega_n) = \sum_p \frac{|V_{p\sigma}|^2}{i\omega_n - \varepsilon_p} \quad \overset{\mathrm{FT}}{\Longrightarrow} \quad \Delta^\sigma(\tau' - \tau)$$

relation to noninteracting impurity Green's function

$$[\mathcal{G}_0^\sigma]^{-1}(i\omega_n) = i\omega_n + \mu - \Delta^\sigma(i\omega_n)$$

Continuous-time QMC

General formalism

- Main objective: calculate the impurity Green's function

$$G(\tau) = -\langle \mathcal{T} d(\tau) d^\dagger(0) \rangle$$

- Strategy:

$$Z = \sum_C w_C$$

express partition sum as a sum over configurations

$$C_1 \to C_2 \to C_3 \to \cdots$$

implement a random walk such that ergodicity and detailed balance are satisfied

all configurations accessible in a finite number of steps

assures that configurations are visited with a probability proportional to their weight

Continuous-time QMC

General formalism

- Main objective: calculate the impurity Green's function

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- Strategy:

$$Z = \sum_C w_C \qquad C_1 \to C_2 \to C_3 \to \cdots$$

express partition sum as a sum over configurations

implement a random walk such that ergodicity and detailed balance are satisfied

$$G = \sum_C \frac{w_C G_C}{Z} = \frac{\sum_C |w_C| \mathrm{sign}_C G_C}{\sum_C |w_C| \mathrm{sign}_C} \approx \frac{\sum_{i=1}^M \mathrm{sign}_{C_i} G_{C_i}}{\sum_{i=1}^M \mathrm{sign}_{C_i}}$$

$$\equiv \frac{\langle \mathrm{sign} \cdot G \rangle_{\mathrm{MC}}}{\langle \mathrm{sign} \rangle_{\mathrm{MC}}}$$

Continuous-time QMC

General formalism

- CT-QMC configurations and weights

(i) split impurity Hamiltonian into two parts

$$H = H_1 + H_2$$

(ii) switch to an interaction representation where the time evolution is given by H_1

$$O(\tau) = e^{\tau H_1} O e^{-\tau H_1} \qquad Z = \mathbf{Tr}\left[e^{-\beta H_1} \mathcal{T} e^{-\int_0^\beta d\tau H_2(\tau)}\right]$$

(iii) expand time ordered exponential into a power series

$$Z = \sum_{n=0}^{\infty} \int_0^\beta d\tau_1 \cdots \int_{\tau_{n-1}}^\beta d\tau_n \mathbf{Tr}\left[e^{-(\beta-\tau_n)H_1}(-H_2) \cdots e^{-(\tau_2-\tau_1)H_1}(-H_2)e^{-\tau_1 H_1}\right]$$

Continuous-time QMC

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$$\Longrightarrow \quad Z = \sum_C w_C$$

representation of the partition sum as a sum over configurations

Continuous-time QMC

General formalism

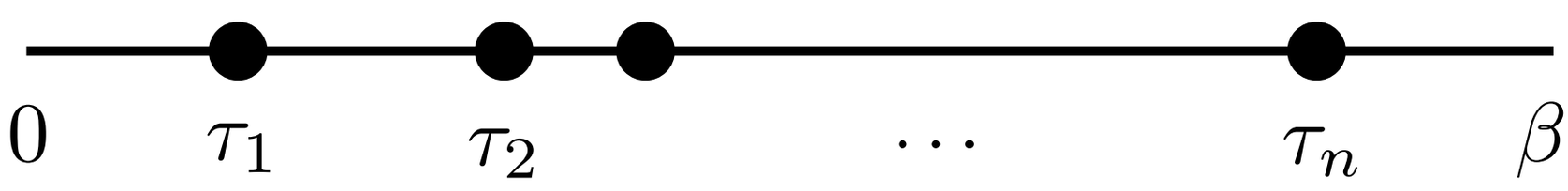
- CT-QMC configurations and weights

configurations are collections of time-points on the imaginary-time interval

$$C = \{\tau_1, \ldots, \tau_n\}, n = 0, 1, \ldots$$

with weight

$$w_C = \mathbf{Tr}\left[e^{-(\beta-\tau_n)H_1}(-H_2)\cdots e^{-(\tau_2-\tau_1)H_1}(-H_2)e^{-\tau_1 H_1}\right](d\tau)^n$$



Questions about the general formalism?

Weak-coupling CT-QMC

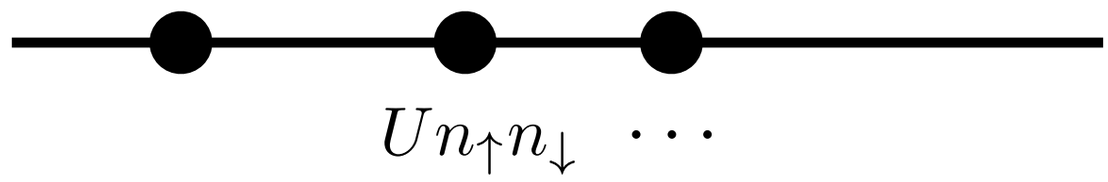
PRB 72, 035122 (05)

Formalism

- Configurations and weights

$$H_2 = H_U$$

points represent interaction vertices



$$H_1 = H - H_2 = H_\mu + H_{\rm bath} + H_{\rm mix}$$

$$\frac{w_C}{Z_0} = (-U d\tau)^n \frac{1}{Z_0} \mathbf{Tr}\left[e^{-(\beta-\tau_n)H_1} n_\uparrow n_\downarrow \cdots e^{-(\tau_2-\tau_1)H_1} n_\uparrow n_\downarrow e^{-\tau_1 H_1}\right]$$

$$= (-U d\tau)^n \prod_\sigma \det M_\sigma^{-1}$$

H_1 quadratic in the fermionic operators

$$[M_\sigma^{-1}]_{ij} = \mathcal{G}_0^\sigma(\tau_i - \tau_j)$$

$$\mathcal{G}_0^\sigma(\tau) = -\mathbf{Tr}[e^{-\beta H_1}\mathcal{T} d(\tau) d^\dagger(0)]/Z_0$$

$$Z_0 = \mathbf{Tr}[e^{-\beta H_1}]$$

Weak-coupling CT-QMC

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H_1 quadratic in the fermionic operators

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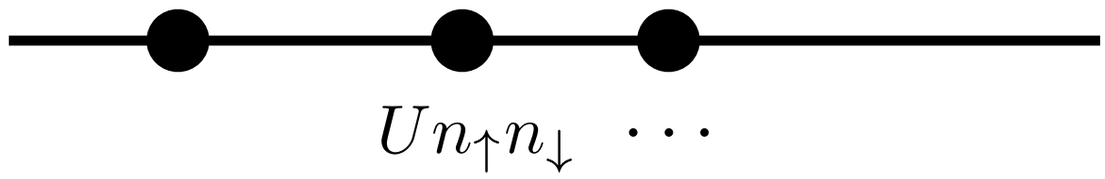

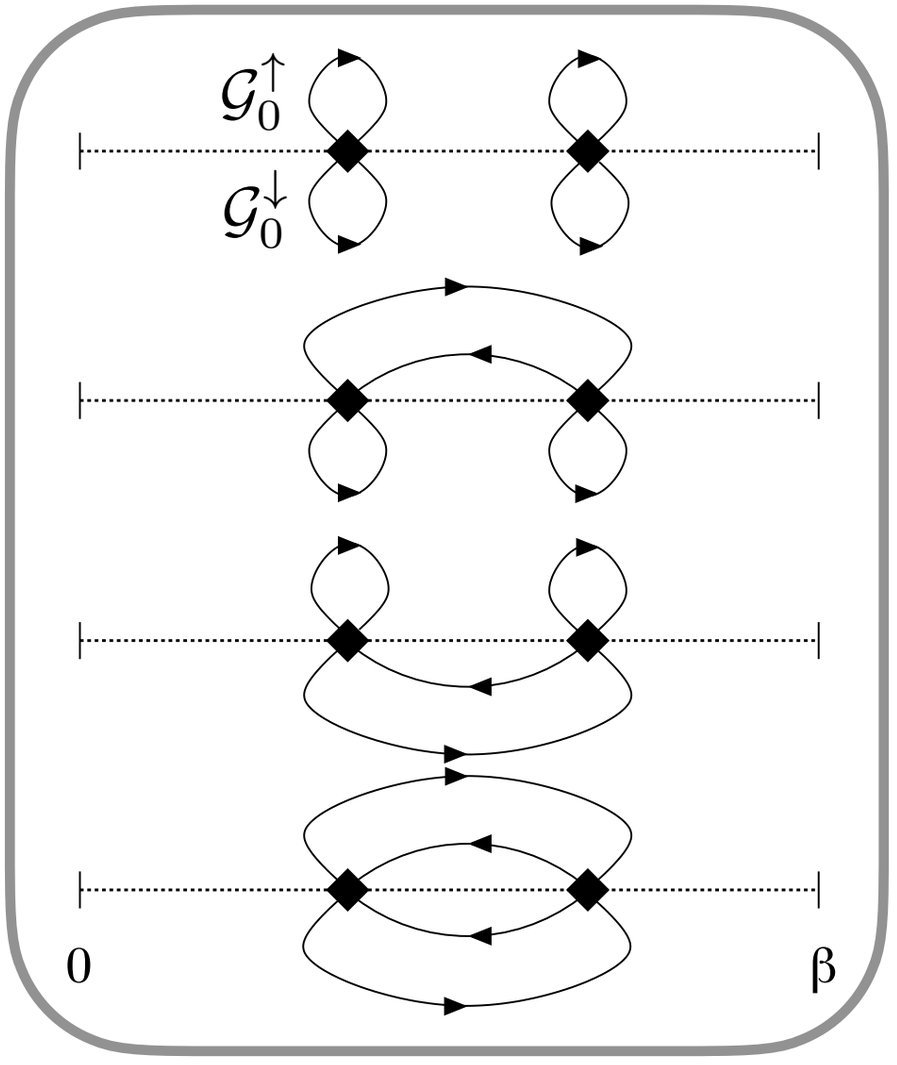

Weak-coupling CT-QMC

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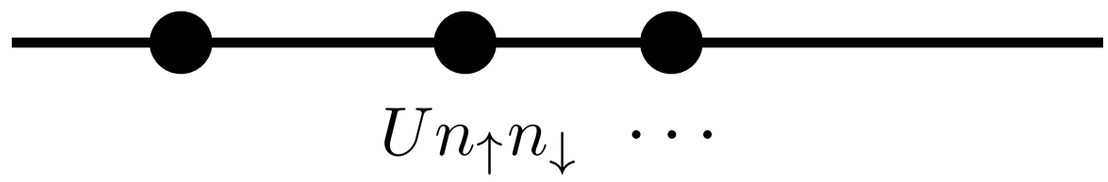


$$H_1 = H - H_2 = H_\mu + H_{\rm bath} + H_{\rm mix}$$

$$\frac{w_C}{Z_0} = (-U d\tau)^n \frac{1}{Z_0} \mathbf{Tr}\left[e^{-(\beta-\tau_n)H_1} n_\uparrow n_\downarrow \cdots e^{-(\tau_2-\tau_1)H_1} n_\uparrow n_\downarrow e^{-\tau_1 H_1}\right]$$

$$= (-U d\tau)^n \prod_\sigma \det M_\sigma^{-1}$$

sign problem for repulsive U?

Weak-coupling CT-QMC

Formalism

- Avoid sign problem by shifting chemical potential for spin-up/down

$$H_U = \frac{U}{2}\sum_s \prod_\sigma (n_\sigma - \alpha_\sigma(s)) + \frac{U}{2}(n_\uparrow + n_\downarrow) + U\left[\left(\frac{1}{2}+\delta\right)^2 - \frac{1}{4}\right]$$

absorb this term into a shift of chemical potential

absorb this term into a shift of chemical potential

irrelevant constant

$$[\mathcal{G}_0^\sigma]^{-1} = i\omega_n + \mu - \Delta^\sigma$$

$$\rightarrow [\tilde{\mathcal{G}}_0^\sigma]^{-1} = i\omega_n + \mu - \tfrac{1}{2}U - \Delta^\sigma$$

$$\alpha_\sigma(s) = \frac{1}{2} + \sigma s\left(\frac{1}{2}+\delta\right)$$

Ising variable

constant

Weak-coupling CT-QMC

Formalism

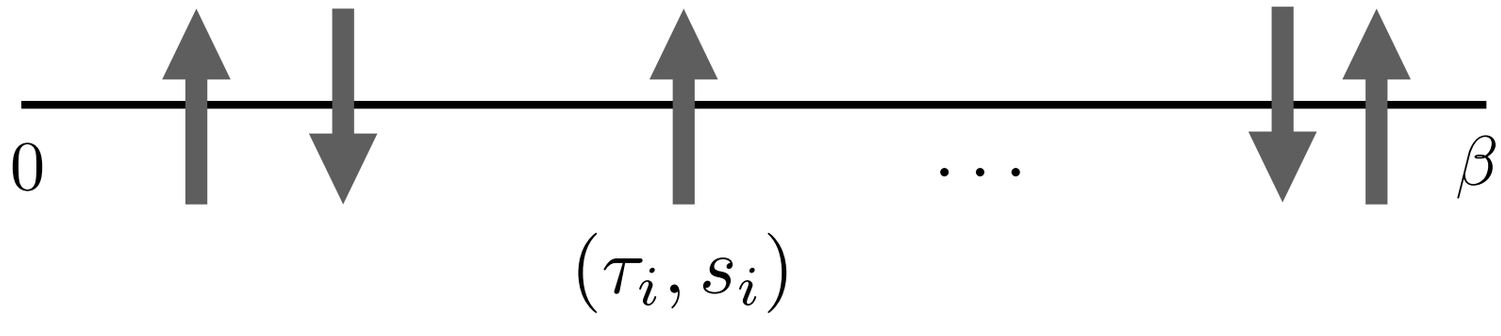
- Configurations in the expanded sampling space

$$C = \{(\tau_1, s_1), (\tau_2, s_2), \ldots, (\tau_n, s_n)\}$$

$$w_C = \tilde{Z}_0(-U d\tau/2)^n \prod_\sigma \det \tilde{M}_\sigma^{-1}$$

why does this solve the sign problem?

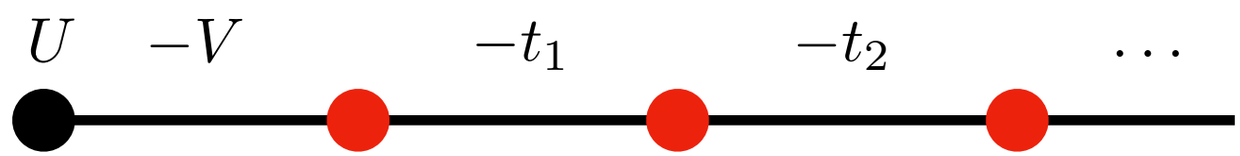
$$[\tilde{M}_\sigma^{-1}]_{ij} = \tilde{\mathcal{G}}_0^\sigma(\tau_i - \tau_j) - \alpha_\sigma(s_i)\delta_{ij}$$



Weak-coupling CT-QMC

Formalism

- Absence of sign problem



By mapping the impurity problem to a chain one can show that the weights can be expressed as

$$w_C = \mathrm{Tr}\left[e^{-(\beta-\tau_n)\tilde{H}_0} A(s_n) e^{-(\tau_n-\tau_{n-1})\tilde{H}_0} A(s_{n-1}) \ldots\right]$$

with time evolution operators represented by matrices with only positive elements

Also the matrix

$$A(s) = (-U d\tau/2)\left[n_\uparrow - 1/2 - s(1/2+\delta)\right]\left[n_\downarrow - 1/2 + s(1/2+\delta)\right]$$

has only non-negative elements for $U, \delta \geq 0$

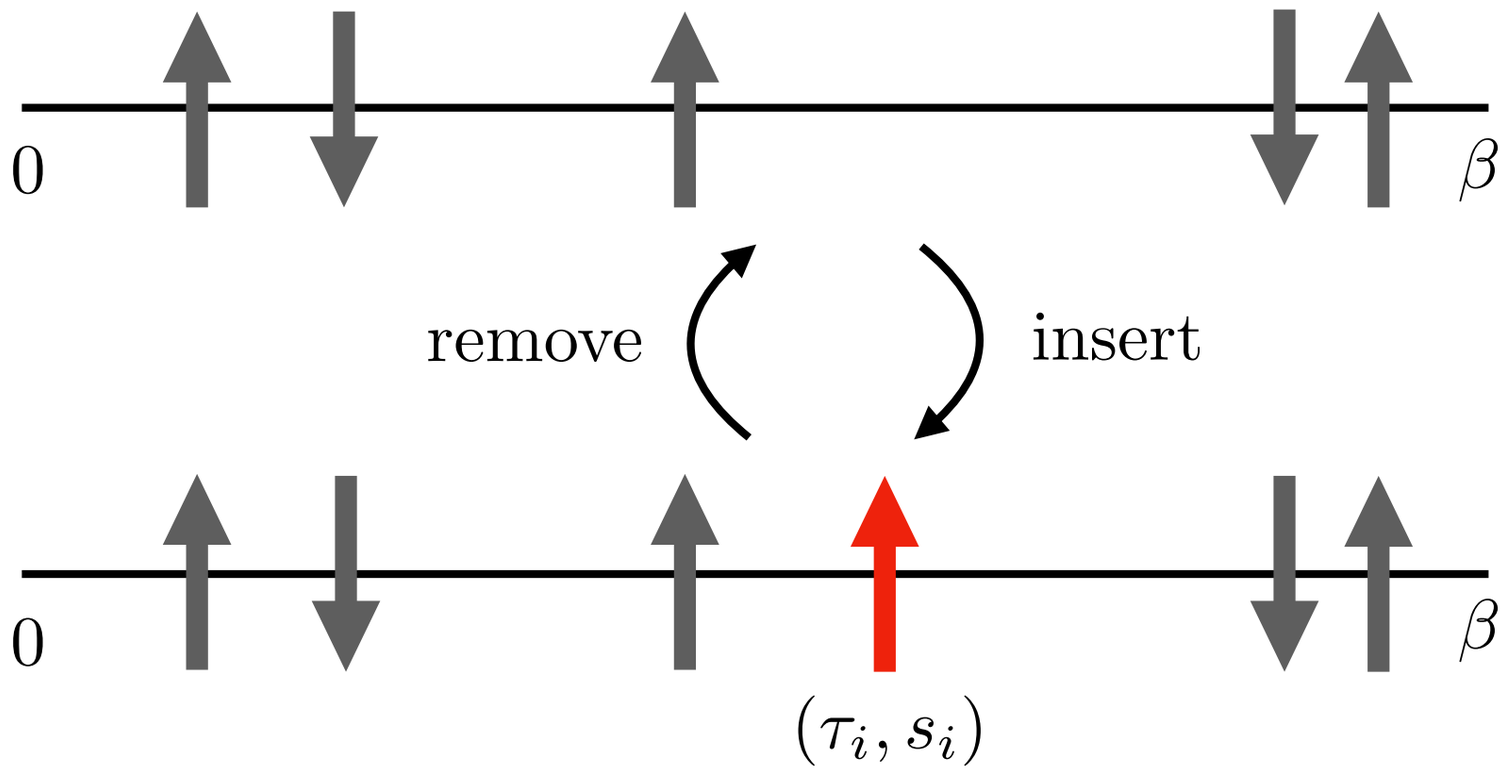
$$s = 1: \underbrace{(-U d\tau/2)}_{\leq 0} \underbrace{(n_\uparrow - 1 - \delta)}_{\leq 0} \underbrace{(n_\downarrow + \delta)}_{\geq 0}$$

$$s = -1: \underbrace{(-U d\tau/2)}_{\leq 0} \underbrace{(n_\uparrow + \delta)}_{\geq 0} \underbrace{(n_\downarrow - 1 - \delta)}_{\leq 0}$$

Weak-coupling CT-QMC

Monte Carlo updates

- Insertion and removal of spins



Weak-coupling CT-QMC

Monte Carlo updates

- Insertion and removal of spins

ergodicity: *insert spins with random orientation at random times, and remove randomly selected spins*

detailed balance:

$$w(C)p(C \to C') = w(C')p(C' \to C)$$

$$p(C \to C') = p^{\text{prop}}(C \to C')p^{\text{acc}}(C \to C')$$

split transition probability into proposal / acceptance probability

Metropolis-Hastings algorithm:

$$p^{\text{acc}}(C \to C') = \min[1, \mathcal{R}(C \to C')]$$

$$\mathcal{R}(C \to C') = \frac{w(C')p^{\text{prop}}(C' \to C)}{w(C)p^{\text{prop}}(C \to C')}$$

Weak-coupling CT-QMC

Monte Carlo updates

- Insertion and removal of spins

insertion: *insert spins with random orientation at random times*

$$p^{\text{prop}}(n \to n+1) = \tfrac{1}{2}(d\tau/\beta)$$

removal: *pick a random spin*

$$p^{\text{prop}}(n+1 \to n) = 1/(n+1)$$

Metropolis-Hastings algorithm

$$p^{\text{acc}}(n \to n+1) = \min[1, \mathcal{R}_{\text{insert}}(n \to n+1)]$$

$$\mathcal{R}_{\text{insert}}(n \to n+1) = \frac{-\beta U}{n+1} \prod_{\sigma} \frac{\det[\tilde{M}_{\sigma}^{(n+1)}]^{-1}}{\det[\tilde{M}_{\sigma}^{(n)}]^{-1}}$$

acceptance probability for removal follows from

$$\mathcal{R}_{\text{remove}}(n+1 \to n) = 1/\mathcal{R}_{\text{insert}}(n \to n+1)$$

Weak-coupling CT-QMC

Monte Carlo updates

- Determinant ratios and fast matrix updates

acceptance probability requires calculation of determinant ratios: *do updates scale* $\mathcal{O}(n^3)$*?*

can be evaluated more efficiently, since we only change one row/column of the matrix

note: in the program, *we store and manipulate the matrix* $M_\sigma = [\mathcal{G}_0^\sigma]^{-1}$ *not* $M_\sigma^{-1} = [\mathcal{G}_0^\sigma]$

insertion: assume that we insert the new row/column at the border of the matrix

$$M^{(n+1)} = \begin{pmatrix} \tilde{P} & \tilde{Q} \\ \tilde{R} & \tilde{S} \end{pmatrix} \quad \Longleftarrow \quad [M^{(n+1)}]^{-1} = \begin{pmatrix} [M^{(n)}]^{-1} & Q \\ R & S \end{pmatrix}$$

needed *easy to compute*

Weak-coupling CT-QMC

Monte Carlo updates

- Determinant ratios and fast matrix updates

using the expression for the determinant ratio of a block matrix and the block inversion of a matrix one finds

$$\frac{\det[M^{(n+1)}]^{-1}}{\det[M^{(n)}]^{-1}} = \det(S - RM^{(n)}Q) = S - RM^{(n)}Q$$

needed for the acceptance probability

$$\begin{aligned}
\tilde{S} &= (S - [R]\,[M^{(n)}\,Q])^{-1} \\
\tilde{Q} &= -[M^{(n)}Q]\,\tilde{S} \\
\tilde{R} &= -\tilde{S}\,[R\,M^{(n)}] \\
\tilde{P} &= M^{(n)} + [M^{(n)}Q]\,\tilde{S}\,[RM^{(n)}]
\end{aligned}$$

needed for the updated matrix $M^{(n+1)}$

all operations are $\mathcal{O}(n^2)$

Weak-coupling CT-QMC

Monte Carlo updates

- Determinant ratios and fast matrix updates

in the case of the removal update:

$$\frac{\det[M^{(n)}]^{-1}}{\det[M^{(n+1)}]^{-1}} = \tilde{S} \qquad \mathcal{O}(1)$$

$$M^{(n)} = \tilde{P} - [\tilde{Q}][\tilde{R}]/\tilde{S} \qquad \mathcal{O}(n^2)$$

Weak-coupling CT-QMC

Measurement of the Green's function $G = \sum_C w_C G_C / Z$

- Use Wick's theorem and the formula for determinant ratios

insert creation / annihilation operators

d_σ $\qquad$ $d^\dagger_\sigma$ $\quad \Rightarrow \quad w_C^{d_\sigma d^\dagger_\sigma}$

$$w_C = \mathrm{Tr}\left[e^{-(\beta-\tau_n)H_1}(-H_2)\cdots e^{-(\tau_2-\tau_1)H_1}(-H_2)e^{-\tau_1 H_1}\right](d\tau)^n$$

contribution to the Green's function $G^\sigma_C = w_C^{d_\sigma d^\dagger_\sigma}/w_C$

$$G^\sigma_C(\tau) \;\; = \;\; \mathcal{G}^\sigma_0(\tau) - \sum_k \mathcal{G}^\sigma_0(\tau-\tau_k)\sum_l [M_\sigma]_{kl}\mathcal{G}^\sigma_0(\tau_l)$$

after Fourier transformation, we get the measurement formula

$$G^\sigma(i\omega_n) = \mathcal{G}^\sigma_0(i\omega_n) - \frac{1}{\beta}(\mathcal{G}^\sigma_0(i\omega_n))^2 \left\langle \sum_{kl} e^{i\omega_n(\tau_k-\tau_l)}[M_\sigma]_{kl} \right\rangle_{\mathrm{MC}}$$

this formula automatically produces the correct high-frequency tail $\sim 1/(i\omega_n)$

Questions about weak-coupling CT-QMC?

Hybridization expansion CT-QMC *PRL 97, 076405 (06)*

Formalism

- Configurations and weights

$$H_2 = H_{\mathrm{mix}}$$

$$H_1 = H - H_2 = H_\mu + H_U + H_{\mathrm{bath}} \equiv H_{\mathrm{loc}} + H_{\mathrm{bath}}$$

$$H_2 \equiv H_2^{d^\dagger} + H_2^d = \sum_{p\sigma} V_{p\sigma} d_\sigma^\dagger c_{p\sigma} + \sum_{p\sigma} V_{p\sigma}^* c_{p\sigma}^\dagger d_\sigma$$

only even expansion orders (same number of creation/annihilation operators) contribute

$$Z = \sum_{n=0}^{\infty} \int_0^\beta d\tau_1 \cdots \int_{\tau_{n-1}}^\beta d\tau_n \int_0^\beta d\tau_1' \cdots \int_{\tau_{n-1}'}^\beta d\tau_n' \times \mathrm{Tr}\left[e^{-\beta H_1} \mathcal{T} H_2^d(\tau_n) H_2^{d^\dagger}(\tau_n') \cdots H_2^d(\tau_1) H_2^{d^\dagger}(\tau_1') \right]$$

$$C = \{\tau_1, \ldots, \tau_n; \tau_1', \ldots, \tau_n'\}$$

configurations are collections of time-points for creation and annihilation operators

Hybridization expansion CT-QMC

Formalism

- Configurations and weights

if H_1 *conserves spin:* *same number of creation and annihilation operators for each spin*

insert explicit expressions for hybridization operators and *separate impurity from bath operators*

$$
\begin{aligned}
Z &= Z_{\mathrm{bath}} \sum_{\{n_\sigma\}} \prod_\sigma \int_0^\beta d\tau_1^\sigma \cdots \int_{\tau_{n_\sigma-1}^\sigma}^\beta d\tau_{n_\sigma}^\sigma \int_0^\beta d\tau_1'^\sigma \cdots \int_{\tau_{n_\sigma-1}'^\sigma}^\beta d\tau_{n_\sigma}'^\sigma \\
&\times \mathrm{Tr}_d \left[e^{-\beta H_{\mathrm{loc}}} \mathcal{T} \prod_\sigma d_\sigma(\tau_{n_\sigma}^\sigma) d_\sigma^\dagger(\tau_{n_\sigma}'^\sigma) \ldots d_\sigma(\tau_1^\sigma) d_\sigma^\dagger(\tau_1'^\sigma) \right] \\
&\times \frac{1}{Z_{\mathrm{bath}}} \mathrm{Tr}_c \Big[e^{-\beta H_{\mathrm{bath}}} \mathcal{T} \prod_\sigma \sum_{p_1 \ldots p_{n_\sigma}} \sum_{p_1' \ldots p_{n_\sigma}'} V_{p_1\sigma}^* V_{p_1'\sigma} \cdots V_{p_{n_\sigma}\sigma}^* V_{p_{n_\sigma}'\sigma} \\
&\qquad c_{p_{n_\sigma}\sigma}^\dagger(\tau_{n_\sigma}^\sigma) c_{p_{n_\sigma}'\sigma}(\tau_{n_\sigma}'^\sigma) \ldots c_{p_1\sigma}^\dagger(\tau_1^\sigma) c_{p_1'\sigma}(\tau_1'^\sigma) \Big]
\end{aligned}
$$

Hybridization expansion CT-QMC

Formalism

- Configurations and weights

the trace over the bath states can be simplified by introducing the hybridization function

$$\Delta^\sigma(\tau) = \sum_p \frac{|V_{p\sigma}|^2}{e^{\varepsilon_p \beta} + 1} \begin{cases} -e^{-\varepsilon_p(\tau-\beta)} & 0 < \tau < \beta \\ e^{-\varepsilon_p \tau} & -\beta < \tau < 0 \end{cases}$$

$$\frac{1}{Z_{\text{bath}}} \text{Tr}_c \left[e^{-\beta H_{\text{bath}}} \mathcal{T} \prod_\sigma \sum_{p_1 \dots p_{n_\sigma}} \sum_{p'_1 \dots p'_{n_\sigma}} V^*_{p_1\sigma} V_{p'_1\sigma} \cdots V^*_{p_{n_\sigma}\sigma} V_{p'_{n_\sigma}\sigma} \right.$$

$$\left. c^\dagger_{p_{n_\sigma}\sigma}(\tau^\sigma_{n_\sigma}) c_{p'_{n_\sigma}\sigma}(\tau^\sigma_{n_\sigma}) \dots c^\dagger_{p_1\sigma}(\tau^\sigma_1) c_{p'_1\sigma}(\tau'^\sigma_1) \right] = \prod_\sigma \det M^{-1}_\sigma$$

Wick theorem for the (noninteracting) bath

$$[M^{-1}_\sigma]_{ij} = \Delta^\sigma(\tau'^\sigma_i - \tau^\sigma_j)$$

matrix elements are given by hybridization functions

Hybridization expansion CT-QMC

Formalism

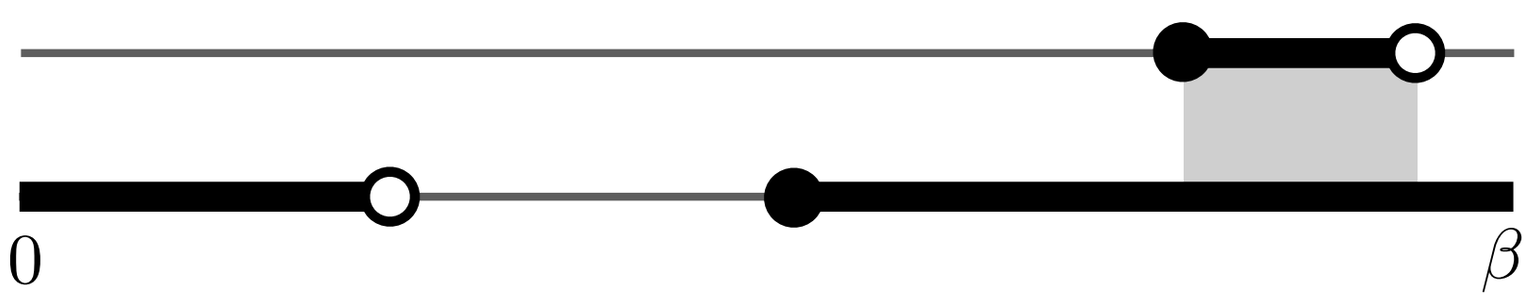
- Configurations and weights

$$C = \{\tau_1^{\uparrow}, \ldots, \tau_{n_\uparrow}^{\uparrow}; \tau_1'^{\uparrow}, \ldots, \tau_{n_\uparrow}'^{\uparrow} | \tau_1^{\downarrow}, \ldots, \tau_{n_\downarrow}^{\downarrow}; \tau_1'^{\downarrow}, \ldots, \tau_{n_\downarrow}'^{\downarrow}\}$$

$$w_C = Z_{\mathrm{bath}} \mathrm{Tr}_d \left[e^{-\beta H_{\mathrm{loc}}} \mathcal{T} \prod_\sigma d_\sigma(\tau_{n_\sigma}^\sigma) d_\sigma^\dagger(\tau_{n_\sigma}'^\sigma) \cdots d_\sigma(\tau_1^\sigma) d_\sigma^\dagger(\tau_1'^\sigma) \right]$$

$$\times \prod_\sigma \det M_\sigma^{-1} (d\tau)^{2n_\sigma}$$

density-density interaction: can represent the local weight using "segment configurations"



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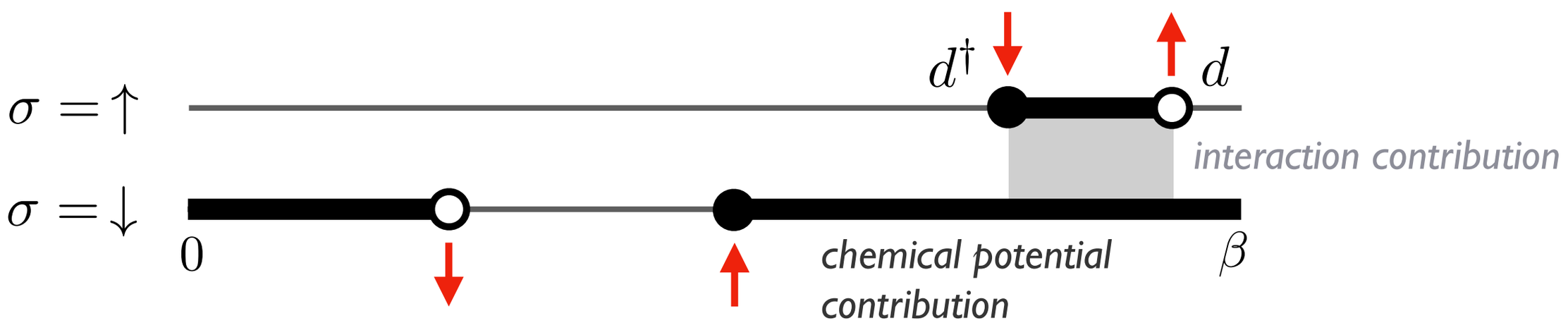
- Configurations and weights

$$C = \{\tau_1^{\uparrow}, \ldots, \tau_{n_\uparrow}^{\uparrow}; \tau_1'^{\uparrow}, \ldots, \tau_{n_\uparrow}'^{\uparrow} | \tau_1^{\downarrow}, \ldots, \tau_{n_\downarrow}^{\downarrow}; \tau_1'^{\downarrow}, \ldots, \tau_{n_\downarrow}'^{\downarrow}\}$$

$$w_C = Z_{\mathrm{bath}} \mathrm{Tr}_d \left[e^{-\beta H_{\mathrm{loc}}} \mathcal{T} \prod_\sigma d_\sigma(\tau_{n_\sigma}^\sigma) d_\sigma^\dagger(\tau_{n_\sigma}'^\sigma) \cdots d_\sigma(\tau_1^\sigma) d_\sigma^\dagger(\tau_1'^\sigma) \right]$$

$$\times \prod_\sigma \det M_\sigma^{-1} (d\tau)^{2n_\sigma}$$

density-density interaction: can represent the local weight using "segment configurations"



Hybridization expansion CT-QMC

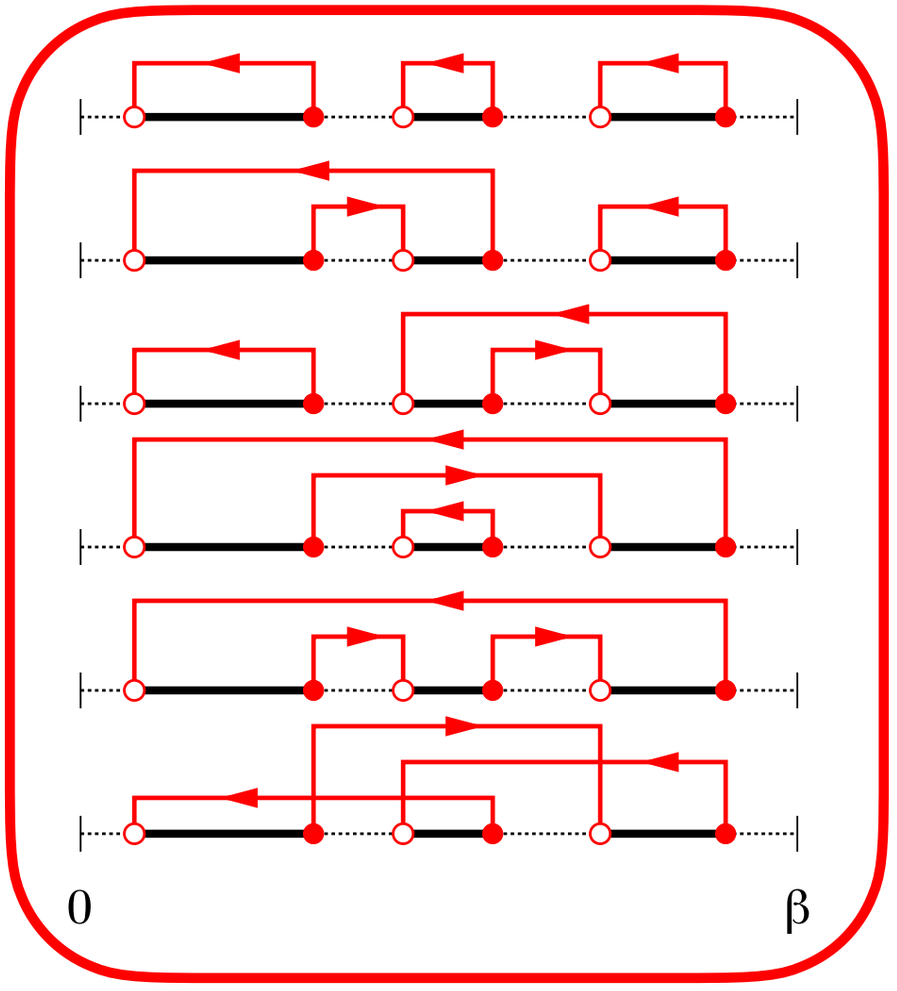
Formalism

- Configurations and weights

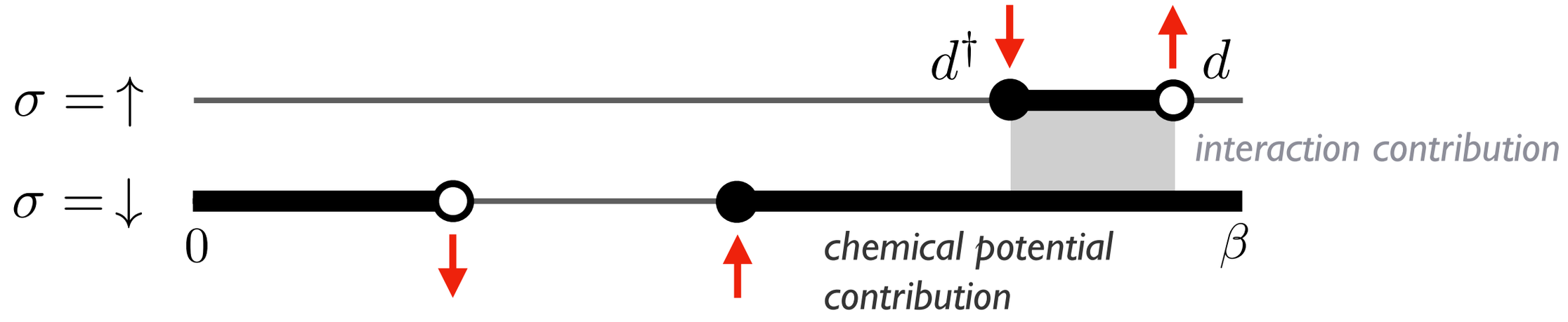
$$C = \{\tau_1^{\uparrow}, \ldots, \tau_{n_\uparrow}^{\uparrow}; \tau_1'^{\uparrow}, \ldots, \tau_{n_\uparrow}'^{\uparrow} | \tau_1^{\downarrow}, \ldots, \tau_{n_\downarrow}^{\downarrow};$$

$$w_C = Z_{\mathrm{bath}} \mathrm{Tr}_d \left[e^{-\beta H_{\mathrm{loc}}} \mathcal{T} \prod_\sigma d_\sigma(\tau_{n_\sigma}^\sigma) d_\sigma^\dagger \right.$$

$$\times \prod_\sigma \det M_\sigma^{-1} (d\tau)^{2n_\sigma}$$



density-density interaction: can represent the local weight using "segment configurations"



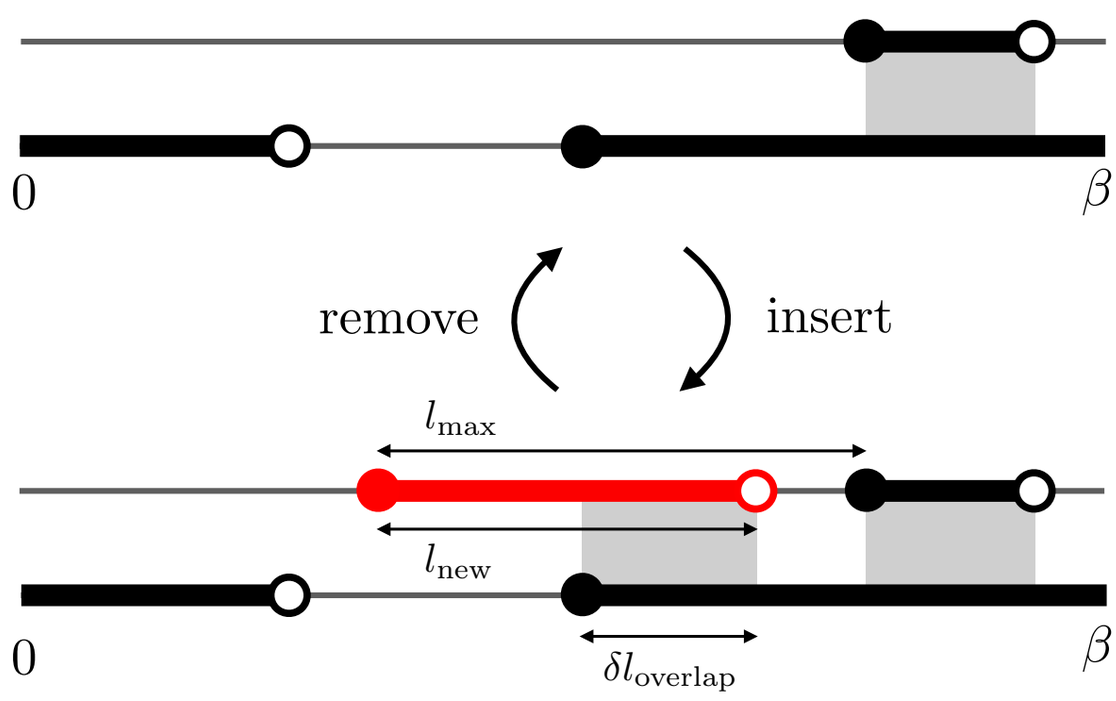
Hybridization expansion CT-QMC

Monte Carlo updates

- Local updates in the segment formalism

$$\mathrm{Tr}_d\left[e^{-\beta H_{\mathrm{loc}}}\mathcal{T}\prod_\sigma d_\sigma(\tau^\sigma_{n_\sigma})d^\dagger_\sigma(\tau'^\sigma_{n_\sigma})\cdots d_\sigma(\tau^\sigma_1)d^\dagger_\sigma(\tau'^\sigma_1)\right]$$

$$= \mathcal{S}\exp\left[\mu(l_\uparrow + l_\downarrow) - U l_{\mathrm{overlap}}\right]$$



ergodicity: enough to insert/remove random segments for spin up and down

Hybridization expansion CT-QMC

Monte Carlo updates

- Detailed balance

insertion:

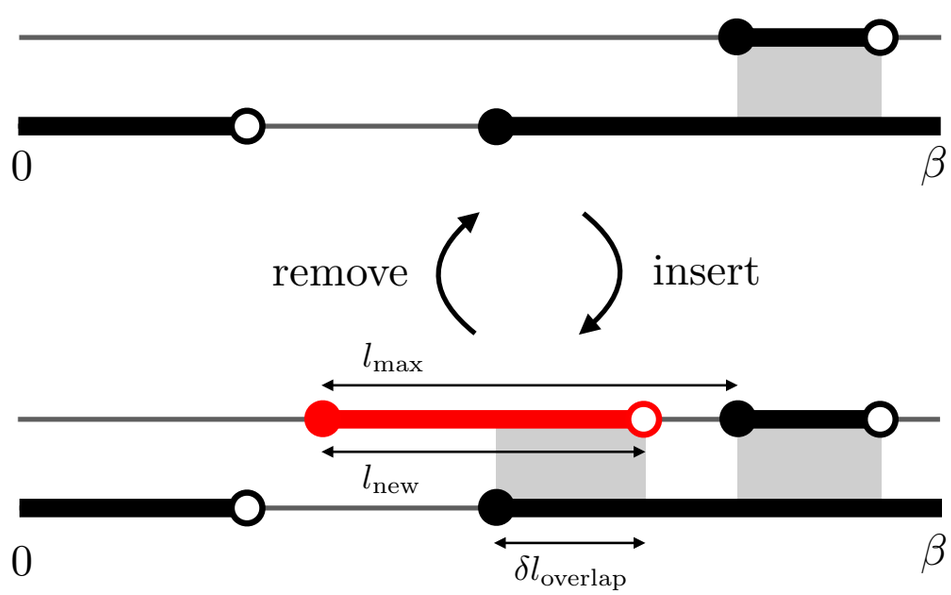
(i) chose random time for creation operator
if it falls on a segment: reject move
otherwise: calculate distance to the next operator

(ii) choose annihilation operator randomly in the corresponding interval

removal:

randomly pick a segment

$$p^{\text{prop}}(n_\sigma \to n_\sigma + 1) = \frac{d\tau}{\beta}\frac{d\tau}{l_{\max}} \qquad p^{\text{prop}}(n_\sigma + 1 \to n_\sigma) = \frac{1}{n_\sigma + 1}$$



Hybridization expansion CT-QMC

Monte Carlo updates

- Detailed balance

acceptance probability for the insertion of a segment

$$p^{\mathrm{acc}}(n_\sigma \to n_\sigma + 1) = \mathbf{min}[1, \mathcal{R}_{\mathrm{insert}}(n_\sigma \to n_\sigma + 1)]$$

$$\mathcal{R}_{\mathrm{insert}}(n_\sigma \to n_\sigma + 1) = \frac{\beta l_{\mathrm{max}}}{n_\sigma + 1} e^{\mu l_{\mathrm{new}} - U \delta l_{\mathrm{overlap}}} \frac{\det\left[M_\sigma^{(n_\sigma+1)}\right]^{-1}}{\det\left[M_\sigma^{(n_\sigma)}\right]^{-1}}$$

acceptance probability for removal obtained from

$$\mathcal{R}_{\mathrm{remove}}(n_\sigma + 1 \to n_\sigma) = 1/\mathcal{R}_{\mathrm{insert}}(n_\sigma \to n_\sigma + 1)$$

Hybridization expansion CT-QMC

Measurement of the Green's function

- Cannot use Wick's theorem

weight of configuration with additional creation and annihilation operators in Tr

$$G(\tau) = -\frac{1}{Z}\sum_C w_C^{d(\tau)d^\dagger(0)} = -\frac{1}{Z}\sum_C w_C^{(\tau,0)}\,\frac{w_C^{d(\tau)d^\dagger(0)}}{w_C^{(\tau,0)}}$$

complete weight of configuration with additional creation and annihilation operators (including enlarged determinant)

identical trace factors in both weights

$$\frac{w_C^{d(\tau)d^\dagger(0)}}{w_C^{(\tau,0)}} = \frac{(-1)^{i+j}\det\left[M_C\right]^{-1}}{\det\left[M_C^{(\tau,0)}\right]^{-1}} = \left[M_C^{(\tau,0)}\right]_{ji}$$

i and j are the row/column corresponding to the extra creation/annihilation operator

Hybridization expansion CT-QMC

Measurement of the Green's function

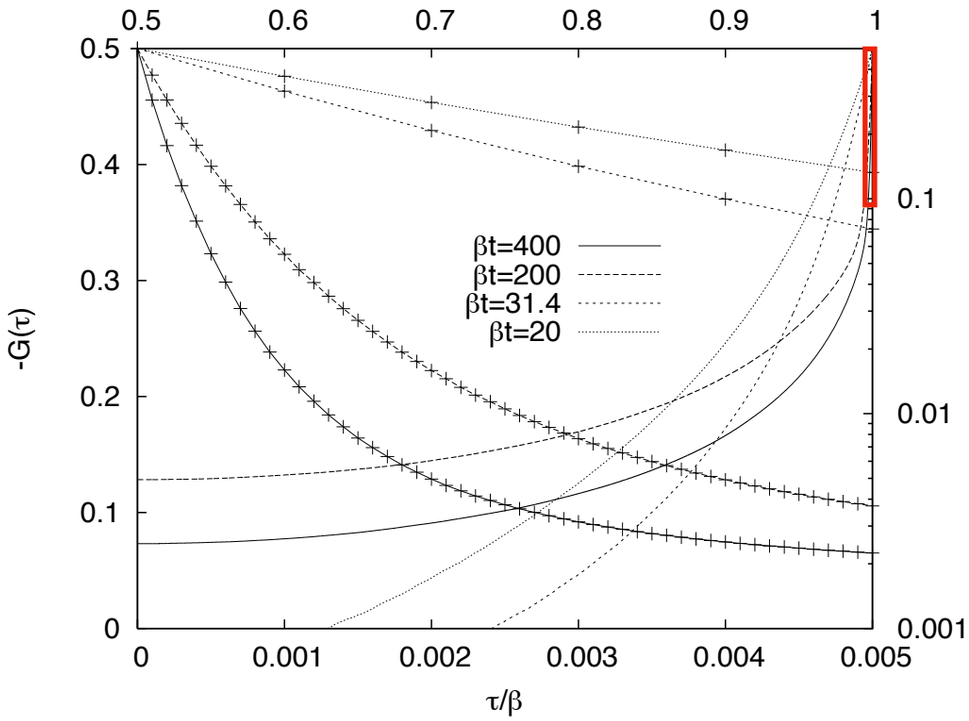
- Cannot use Wick's theorem

with this, the measurement formula becomes

$$G(\tau) = \left\langle -\sum_{ij} \frac{1}{\beta} \delta(\tau, \tau_i - \tau'_j) M_{ij} \right\rangle_{\mathrm{MC}}$$

or in frequency space

$$G(i\omega_n) = \left\langle -\sum_{ij} \frac{1}{\beta} e^{i\omega_n(\tau_i - \tau'_j)} M_{ij} \right\rangle_{\mathrm{MC}}$$

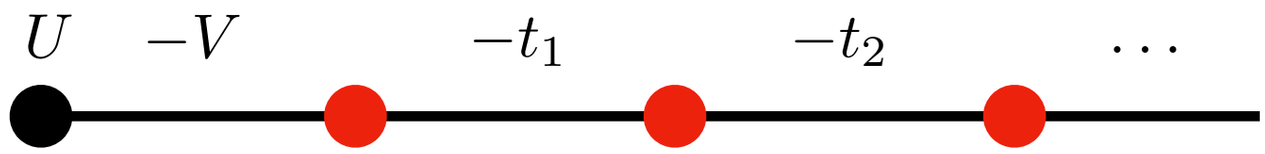


note that this formula does not guarantee the correct high-frequency behavior $\sim 1/(i\omega_n)$
(need improved estimators)

Hybridization expansion CT-QMC

Absence of sign problem

- Use again the chain basis:



$$-H^{d^\dagger}_{\rm mix} = V c_0^\dagger c_1, \; -H^{d}_{\rm mix} = V c_1^\dagger c_0 \; (c_0 \equiv d)$$

$$w_C = \mathrm{Tr}\left[e^{-(\beta-\tau_n)(H_{\rm loc}+H_{\rm bath})} (-H^{d^\dagger}_{\rm mix}) \dots (-H^{d}_{\rm mix}) e^{-(\tau_2-\tau_1)(H_{\rm loc}+H_{\rm bath})} \right] (d\tau)^{2n}$$

$V > 0$: *mixing terms are positive*

$H_{\rm loc}$ *has only diagonal elements*

can choose chain basis such that $H_{\rm bath}$ *has only negative off-diagonal elements*

$$e^{-\tau(H_{\rm loc}+H_{\rm bath})} = \lim_{N\to\infty} \left(1 - \frac{\tau}{N} \left[H_{\rm loc} + H_{\rm bath} \right] \right)^N$$ *also positive*

Hybridization expansion CT-QMC

General impurity models

- Matrix formalism

if $H_{\rm loc}$ is not diagonal in the occupation number basis, the calculation of the trace becomes costly

$$\mathrm{Tr}_d \left[e^{-\beta H_{\rm loc}} \mathcal{T} \prod_\alpha d_\alpha(\tau^\alpha_{n_\alpha}) d^\dagger_\alpha(\tau'^\alpha_{n_\alpha}) \cdots d_\alpha(\tau^\alpha_1) d^\dagger_\alpha(\tau'^\alpha_1) \right]$$

in the matrix formalism, we use the eigenbasis of the time evolution operator $e^{-H_{\rm loc}\tau}$

in this basis, the creation/annihilation operators $d^\dagger_\alpha$, d_α *are however non-diagonal*

important: use of conserved quantum numbers, such as particle number or spin

example: $d^\dagger_\uparrow(\tau_4) d^\dagger_\uparrow(\tau_3) d_\uparrow(\tau_2) d_\uparrow(\tau_1)$ **(with** $\tau_1 < \tau_2 < \tau_3 < \tau_4$**)**

$$\{n_\uparrow = 1; n_\downarrow\} \underset{d_\uparrow}{\rightarrow} \{n_\uparrow = 0; n_\downarrow\} \underset{d_\uparrow}{\rightarrow} \emptyset$$

Hybridization expansion CT-QMC

General impurity models

- Matrix formalism

having identified the contributing blocks, the trace reduces to block-matrix multiplications

$$\sum_{\text{contributing}} \mathrm{Tr}_m \left[\cdots [O]_{m''m'} [e^{-(\tau'-\tau)H_{\text{loc}}}]_{m'} [O]_{m'm} [e^{-\tau H_{\text{loc}}}]_m \right]$$

matrix blocks are dense and largest block grows exponentially with number of sites / orbitals

two types of truncation

1. Restriction of the trace $\sum_{\text{contributing } m} \mathrm{Tr}_m[\ldots]$ to those quantum number sectors or states which give the dominant contribution

2. Reduction of the size of the operator blocks $[O]_{m'm''}$ by eliminating high-energy states

CT-QMC

Scaling of the algorithms

- Average perturbation order

weak-coupling approach: related to the potential energy

$$H_1 = H_\mu + \tfrac{1}{2}U(n_\uparrow + n_\downarrow) + H_{\rm bath} + H_{\rm mix}$$

$$H_2 = U n_\uparrow n_\downarrow - \tfrac{1}{2}U(n_\uparrow + n_\downarrow)$$

$$\langle -H_2 \rangle = \frac{1}{\beta}\int_0^\beta d\tau \langle -H_2(\tau)\rangle =$$

$$\frac{1}{\beta}\frac{1}{Z}\sum_{n=0}^{\infty}\frac{n+1}{(n+1)!}\int_0^\beta d\tau \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n$$

$$\times \mathbf{Tr}\left[e^{-\beta H_1}\mathcal{T}(-H_2(\tau))(-H_2(\tau_n))\cdots(-H_2(\tau_1))\right]$$

$$= \frac{1}{\beta}\frac{1}{Z}\sum_C n_C w_C = \frac{1}{\beta}\langle n\rangle$$

CT-QMC

Scaling of the algorithms

- Average perturbation order

weak-coupling approach: related to the potential energy

$$\langle n \rangle_{\text{weak-coupling}} = -\beta E_{\text{pot}} + \tfrac{1}{2}\beta U \langle n_\uparrow + n_\downarrow \rangle \sim \beta U$$

CT-QMC

Scaling of the algorithms

- Average perturbation order

weak-coupling approach: *related to the potential energy*

$$\langle n \rangle_{\text{weak-coupling}} = -\beta E_{\text{pot}} + \tfrac{1}{2}\beta U \langle n_\uparrow + n_\downarrow \rangle \sim \beta U$$

strong-coupling approach: *related to the kinetic energy*

$$E_{\text{kin}} = \sum_\sigma \int_0^\beta d\tau G_\sigma(\tau)\Delta^\sigma(-\tau)$$

$$E_{\text{kin}} = \sum_\sigma \int_0^\beta d\tau \left\langle -\sum_{ij} \frac{1}{\beta}\delta(\tau, \tau_i - \tau'_j)[M_\sigma]_{ij} \right\rangle_{\text{MC}} \Delta^\sigma(-\tau)$$

$$= -\sum_\sigma \left\langle \frac{1}{\beta} \sum_{ij} [M_\sigma]_{ij} \Delta^\sigma(\tau'_j - \tau_i) \right\rangle_{\text{MC}}$$

CT-QMC

Scaling of the algorithms

- Average perturbation order

weak-coupling approach: *related to the potential energy*

$$\langle n \rangle_{\text{weak-coupling}} = -\beta E_{\text{pot}} + \tfrac{1}{2}\beta U \langle n_\uparrow + n_\downarrow \rangle \sim \beta U$$

strong-coupling approach: *related to the kinetic energy*

$$E_{\text{kin}} = -\sum_\sigma \left\langle \frac{1}{\beta} \sum_{ij} [M_\sigma]_{ij} \Delta^\sigma(\tau'_j - \tau_i) \right\rangle_{\text{MC}}$$

$$[M_\sigma]_{ij} = (-1)^{i+j} \det M_\sigma^{-1}[j,i] / \det M_\sigma^{-1}$$

hybridization matrix with row j and column i removed

$$\sum_j (-1)^{i+j} \det M_\sigma^{-1}[j,i] \Delta^\sigma(\tau'_j - \tau_i) = \det M_\sigma^{-1}$$

expansion of determinant along column i

CT-QMC

Scaling of the algorithms

- Average perturbation order

weak-coupling approach: *related to the potential energy*

$$\langle n \rangle_{\text{weak-coupling}} = -\beta E_{\text{pot}} + \tfrac{1}{2}\beta U \langle n_\uparrow + n_\downarrow \rangle \sim \beta U$$

strong-coupling approach: *related to the kinetic energy*

$$E_{\text{kin}} = -\sum_\sigma \left\langle \frac{1}{\beta} \sum_{ij} [M_\sigma]_{ij} \Delta^\sigma(\tau'_j - \tau_i) \right\rangle_{\text{MC}}$$

$$= -\sum_\sigma \left\langle \frac{1}{\beta} \sum_i \frac{\det M_\sigma^{-1}}{\det M_\sigma^{-1}} \right\rangle_{\text{MC}} = -\frac{1}{\beta} \sum_\sigma \langle n_\sigma \rangle$$

CT-QMC

Scaling of the algorithms

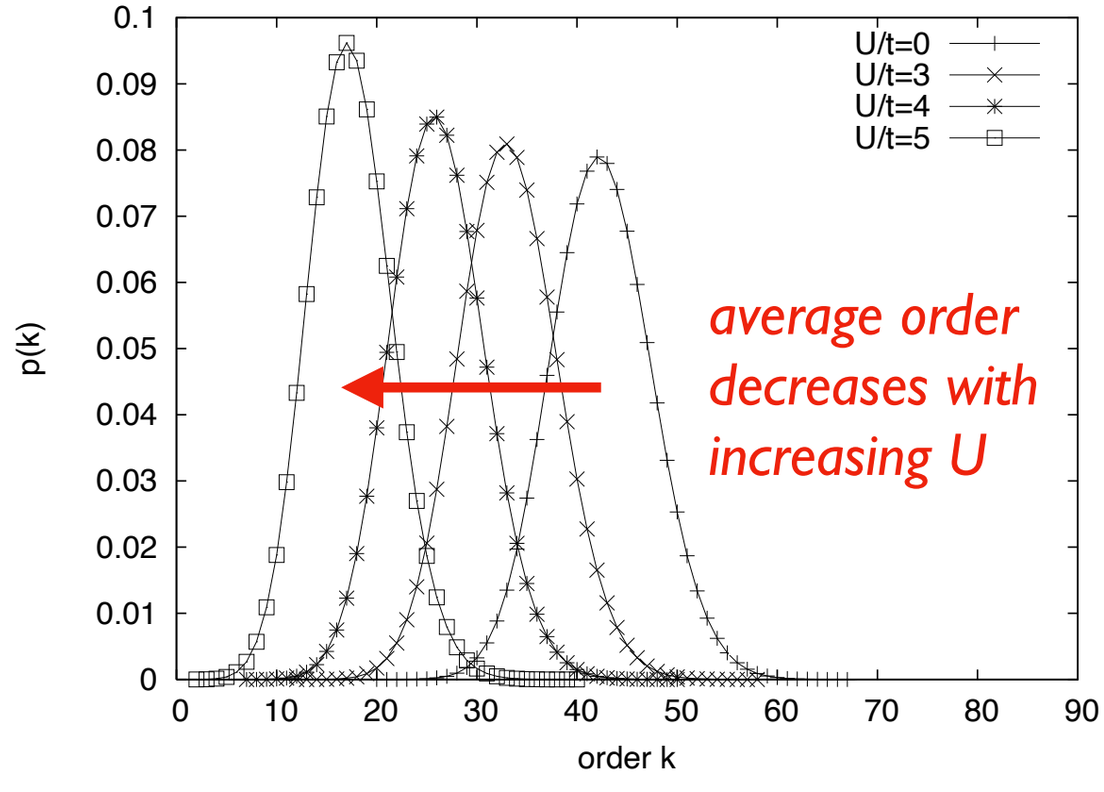
- Average perturbation order

weak-coupling approach: *related to the potential energy*

$$\langle n \rangle_{\text{weak-coupling}} = -\beta E_{\text{pot}} + \tfrac{1}{2}\beta U \langle n_\uparrow + n_\downarrow \rangle \sim \beta U$$

strong-coupling approach: *related to the kinetic energy*

$$\langle n \rangle_{\text{hybridization-expansion}} = -\beta E_{\text{kin}}$$



CT-QMC

Scaling of the algorithms

- Average perturbation order

weak-coupling approach: *related to the potential energy*

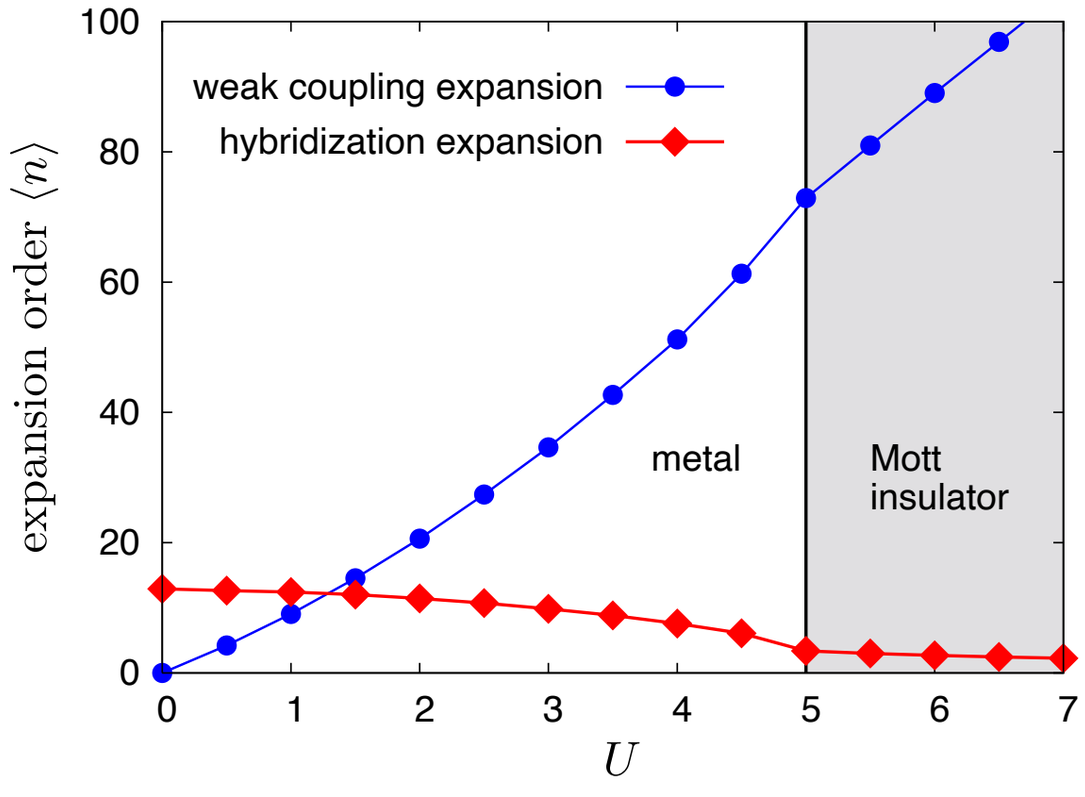
$$\langle n \rangle_{\text{weak-coupling}} = -\beta E_{\text{pot}} + \tfrac{1}{2}\beta U \langle n_\uparrow + n_\downarrow \rangle \sim \beta U$$

strong-coupling approach: *related to the kinetic energy*

$$\langle n \rangle_{\text{hybridization-expansion}} = -\beta E_{\text{kin}}$$

computational effort scales as

$$\mathcal{O}(\langle n \rangle^3)$$



CT-QMC

Scaling of the algorithms

- Average perturbation order

weak-coupling approach: *related to the potential energy*

$$\langle n \rangle_{\text{weak-coupling}} = -\beta E_{\text{pot}} + \tfrac{1}{2}\beta U \langle n_\uparrow + n_\downarrow \rangle \sim \beta U$$

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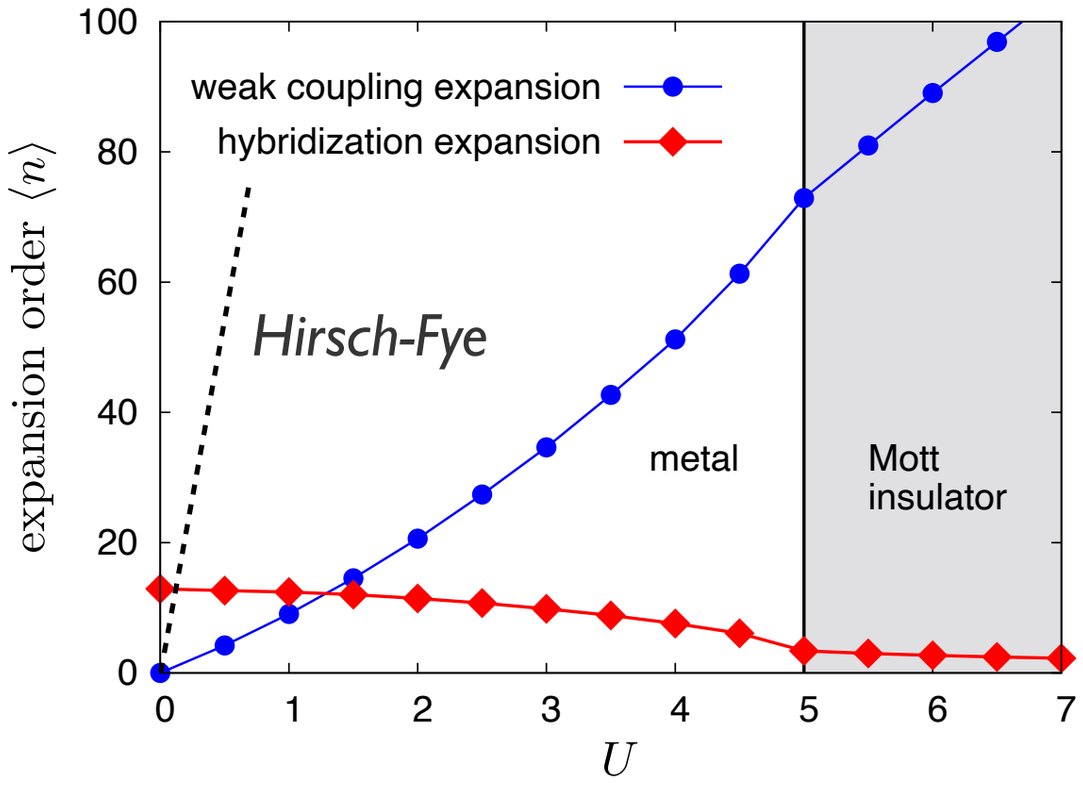
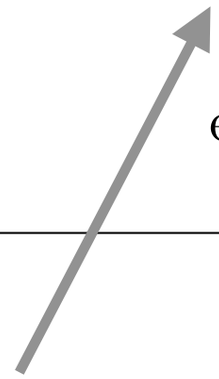


CT-QMC

Scaling of the algorithms

- Summary and main applications

Solver	Scaling		Use
Weak-coupling	β^3	L^3	Impurity clusters with density-density interaction
Hybridization expansion (segment formalism)	β^3	L	Single-site multi-orbital models with density-density interaction
Hybridization expansion (matrix/Krylov formalism)	β	$\exp(L)$	Single-site multi-orbital models with general U_{ijkl}



if calculation of determinant ratios dominates overlap calculation

Questions about strong-coupling CT-QMC?

Electron-boson systems

PRL 99, 146404 (07)

Local phonons

- Anderson-Holstein model

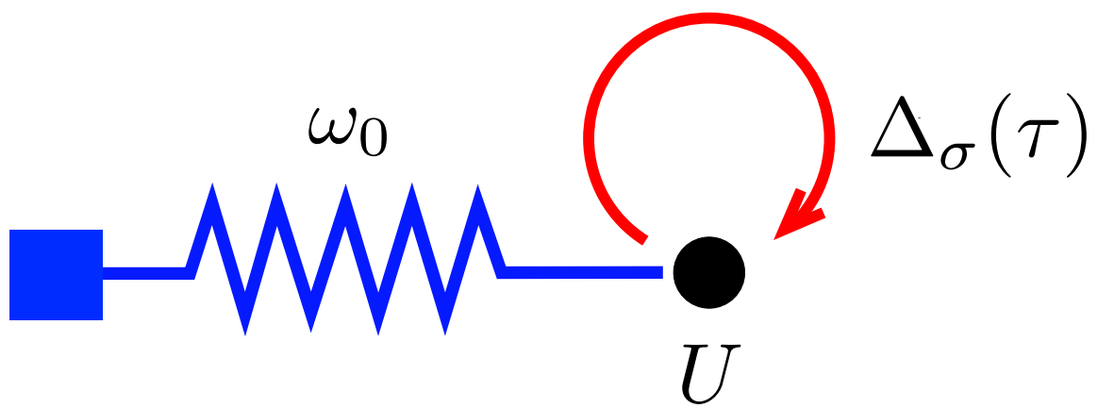
$$H = H_{\rm loc} + H_{\rm mix} + H_{\rm bath}$$

phonon coupling ↓ ↓ *phonon frequency*

$$H_{\rm loc} = -\mu(n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow + g(n_\uparrow + n_\downarrow - 1)(b^\dagger + b) + \omega_0 b^\dagger b$$

written with the phonon position / momentum operators $X = (b^\dagger + b)/\sqrt{2}, P = i(b^\dagger - b)/\sqrt{2}$

$$H_{\rm loc} = -\mu(n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow + \sqrt{2} g(n_\uparrow + n_\downarrow - 1) X + \frac{\omega_0}{2}\left(X^2 + P^2\right)$$



Electron-boson systems

Local phonons

- Anderson-Holstein model

$$H = H_{\mathrm{loc}} + H_{\mathrm{mix}} + H_{\mathrm{bath}}$$

phonon coupling ↓ ↓ *phonon frequency*

$$H_{\mathrm{loc}} = -\mu(n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow + g(n_\uparrow + n_\downarrow - 1)(b^\dagger + b) + \omega_0 b^\dagger b$$

written with the phonon position / momentum operators $X = (b^\dagger + b)/\sqrt{2}, P = i(b^\dagger - b)/\sqrt{2}$

$$H_{\mathrm{loc}} = -\mu(n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow + \sqrt{2} g(n_\uparrow + n_\downarrow - 1)X + \frac{\omega_0}{2}\left(X^2 + P^2\right)$$

after expansion in hybridization

$$w(\{O_i(\tau_i)\}) = \mathrm{Tr}_d \mathrm{Tr}_b \left[e^{-\beta H_{\mathrm{loc}}} \mathcal{T} O_{2n}(\tau_{2n}) \dots O_1(\tau_1)\right] d\tau_1 \dots d\tau_{2n}$$

$$\times \prod_\sigma (\det M_\sigma^{-1}) s_\sigma$$

Electron-boson systems

Local phonons

- Calculation of the local trace $\mathrm{Tr}_d \mathrm{Tr}_b[\ldots]$

Lang-Firsov transformation *decouples electrons and phonons in* H_{loc}

$$\tilde{H}_{\mathrm{loc}} = e^{iPX_0} H_{\mathrm{loc}} e^{-iPX_0} \qquad X_0 = (\sqrt{2}g/\omega_0)(n_\uparrow + n_\downarrow - 1)$$

$$\tilde{H}_{\mathrm{loc}} = -\tilde{\mu}(\tilde{n}_\uparrow + \tilde{n}_\downarrow) + \tilde{U}\tilde{n}_\uparrow\tilde{n}_\downarrow + \frac{\omega_0}{2}(X^2 + P^2) \qquad \begin{aligned} \tilde{\mu} &= \mu - g^2/\omega_0 \\ \tilde{U} &= U - 2g^2/\omega_0 \end{aligned}$$

electron creation and annihilation operators get dressed ("polaron operators")

$$\begin{aligned} \tilde{d}^\dagger_\sigma &= e^{iPX_0} d^\dagger_\sigma e^{-iPX_0} = e^{\frac{g}{\omega_0}(b^\dagger - b)} d^\dagger_\sigma \\ \tilde{d}_\sigma &= e^{iPX_0} d_\sigma e^{-iPX_0} = e^{-\frac{g}{\omega_0}(b^\dagger - b)} d_\sigma \end{aligned}$$

Electron-boson systems

Local phonons

- Calculation of the local trace $\mathrm{Tr}_d \mathrm{Tr}_b[\ldots]$

separate electron and phonon operators: expectation value becomes the product of a term with only electron operators (analogous to the Anderson impurity model) and a phonon term

$$w(\{O_i(\tau_i)\}) = w_b(\{O_i(\tau_i)\})\tilde{w}_{\mathrm{AIM}}(\{O_i(\tau_i)\})$$

$$w_b(\{O_i(\tau_i)\}) = \left\langle e^{s_{2n}A(\tau_{2n})} e^{s_{2n-1}A(\tau_{2n-1})} \cdots e^{s_1 A(\tau_1)} \right\rangle_b$$

s_i is +1 (-1) if the ith electron operator operator is a creation (annihilation) operator

$$A(\tau) = \frac{g}{\omega_0}(e^{\omega_0 \tau} b^\dagger - e^{-\omega_0 \tau} b)$$

$$e^{\tau\omega_0 b^\dagger b} b^\dagger e^{-\tau\omega_0 b^\dagger b} = e^{\omega_0 \tau} b^\dagger$$

$$e^{\tau\omega_0 b^\dagger b} b^\dagger e^{-\tau\omega_0 b^\dagger b} = e^{-\omega_0 \tau} b$$

use the formula $e^{X+Y} = e^X e^Y e^{-\frac{1}{2}[X,Y]}$

$$e^{sA(\tau)} = e^{-\frac{g^2}{2\omega_0^2}} e^{s\frac{g}{\omega_0} e^{\omega_0 \tau} b^\dagger} e^{-s\frac{g}{\omega_0} e^{-\omega_0 \tau} b}$$

Electron-boson systems

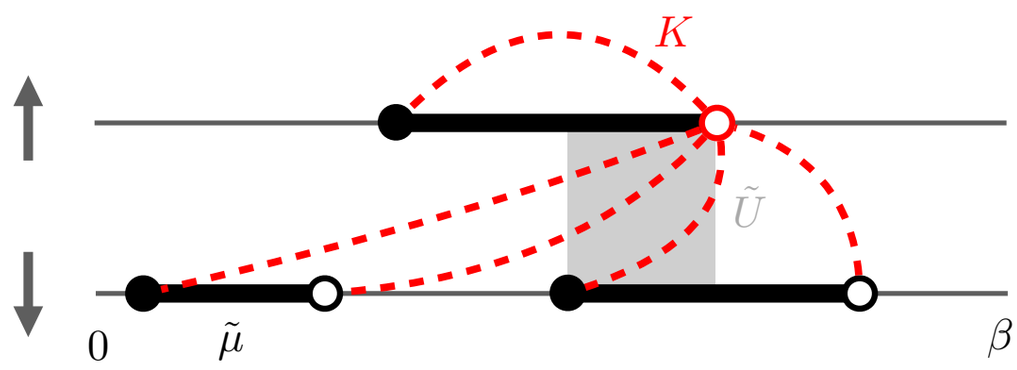
Local phonons

- Calculation of the local trace $\mathrm{Tr}_d \mathrm{Tr}_b[\ldots]$

with this disentangling and the formula $\langle e^{ub^\dagger} e^{vb} \rangle_b = e^{uv/(e^{\beta\omega_0}-1)}$ *we obtain*

$$w_b(\{O_i(\tau_i)\}) = \exp\left[-\frac{g^2/\omega_0^2}{e^{\beta\omega_0}-1} \left(n\left(e^{\beta\omega_0}+1\right) + \sum_{2n\geq i>j\geq 1} s_i s_j \left\{ e^{\omega_0(\beta-(\tau_i-\tau_j))} + e^{\omega_0(\tau_i-\tau_j)} \right\} \right) \right]$$

this phonon contribution corresponds to an interaction K between all pairs of operators



in addition, we have a shift of the interaction and chemical potential

Electron-boson systems

Local phonons

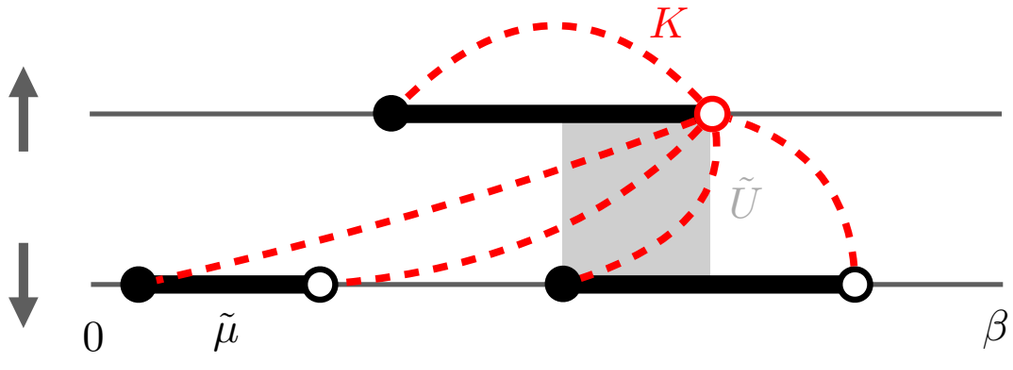
- Summary: Trace over the electron and phonon states

$$w(\{O_i(\tau_i)\}) = w_b(\{O_i(\tau_i)\})\tilde{w}_{\mathrm{AIM}}(\{O_i(\tau_i)\})$$

phonon factor corresponds to the additional "interaction" between creation/annihilation operators

$$K(\tau) = -\frac{g^2}{\omega_0^2}\frac{\cosh(\omega_0(\tau-\beta/2)) - \cosh(\omega_0\beta/2)}{\sinh(\omega_0\beta/2)}$$

representation of a segment diagram

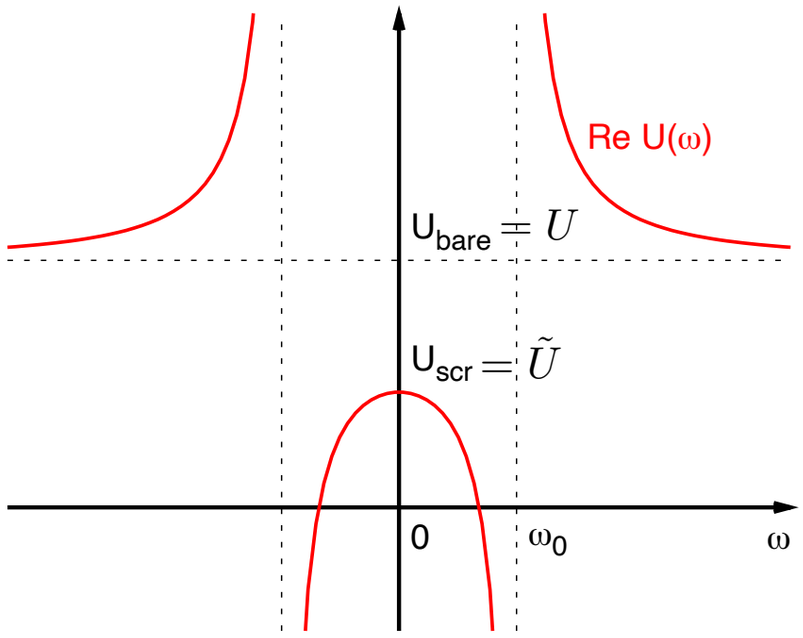


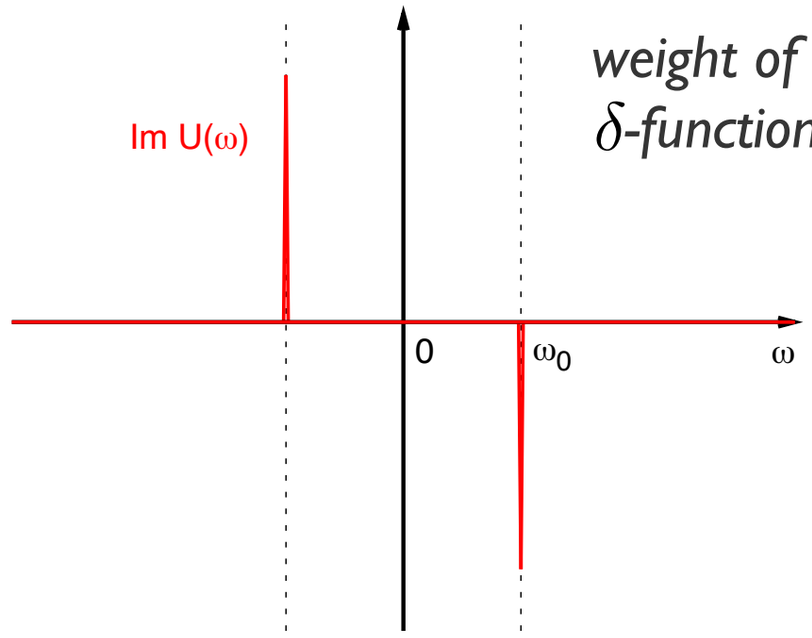
$$\begin{aligned}\tilde{\mu} &= \mu - g^2/\omega_0 \\ \tilde{U} &= U - 2g^2/\omega_0\end{aligned}$$

Electron-boson systems

Frequency-dependent interaction

- Holstein phonon corresponds to a frequency dependent $U(\omega)$





weight of the δ-functions is $\mp g^2\pi$

coupling strength to the bosonic mode with frequency ω

$$g_\omega^2 = -\mathrm{Im}U(\omega)/\pi$$

each boson contributes an "interaction"

$$K(\tau_i-\tau_j) = -\frac{g_\omega^2}{\omega^2}\frac{\cosh(\omega(\beta/2-(\tau_i-\tau_j))-\cosh(\beta\omega/2)}{\sinh(\beta\omega/2)}$$

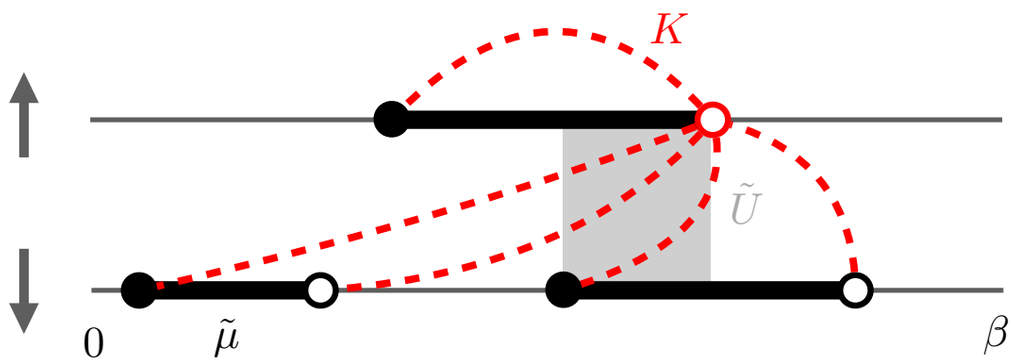
Electron-boson systems

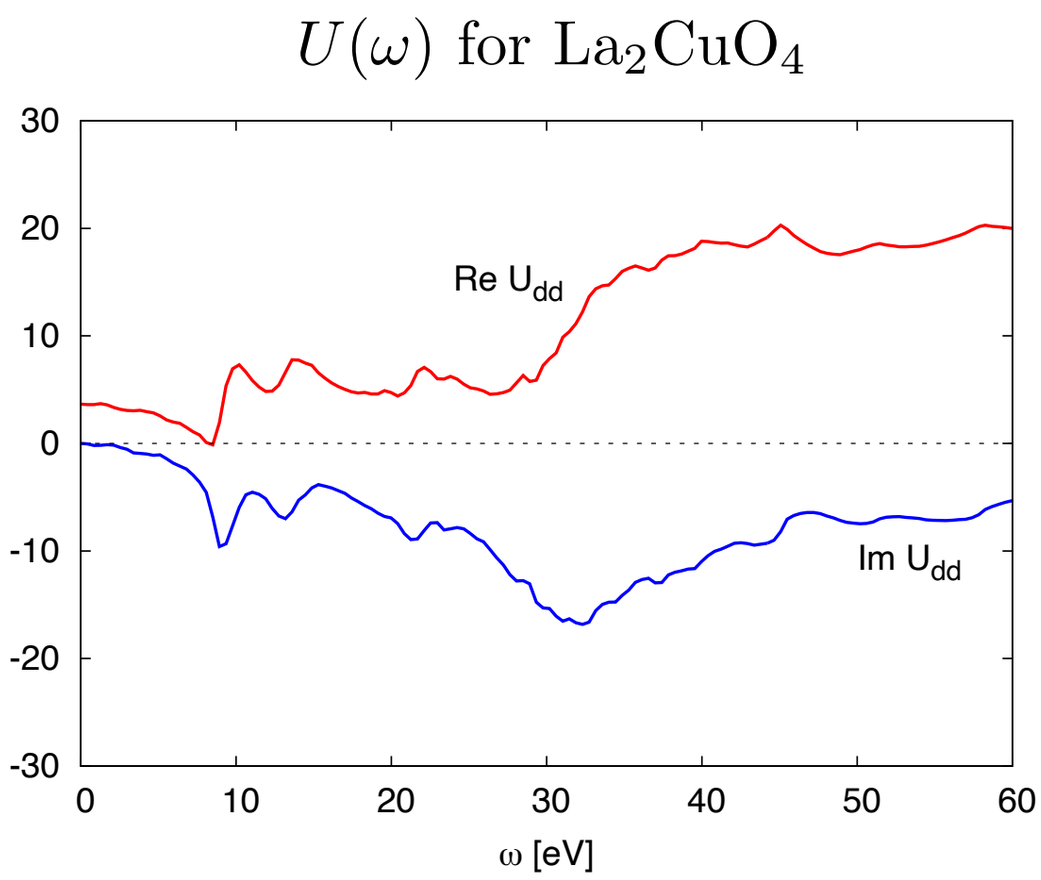
Frequency-dependent interaction

- General frequency dependent $U(\omega)$

$$K(\tau) = \int_0^\infty d\omega \frac{\mathrm{Im}U(\omega)}{\pi\omega^2} \frac{\cosh(\omega(\beta/2-\tau)) - \cosh(\beta\omega/2)}{\sinh(\beta\omega/2)}$$

$$\begin{aligned} \tilde{\mu} &= \mu + \int_0^\infty d\omega \frac{\mathrm{Im}U(\omega)}{\pi\omega} \\ \tilde{U} &= U + 2\int_0^\infty d\omega \frac{\mathrm{Im}U(\omega)}{\pi\omega} = U_{\mathrm{scr}} \end{aligned}$$





Questions about electron-boson systems?