Quantum Monte Carlo impurity solvers

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Monte Carlo impurity solvers



Different types of solvers for different applications



Monte Carlo impurity solvers

History

Different types of solvers for different applications



Quantum impurity models

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

Single-orbital Anderson impurity model



correlated impurity

noninteracting electron bath

hybridization (mixing) term



$$\begin{aligned} H_{\text{loc}} &= H_{\mu} + H_{U} & H_{\text{bath}} &= \sum_{p\sigma} \varepsilon_{p} c_{p\sigma}^{\dagger} c_{p\sigma} \\ H_{\mu} &= -\mu (n_{\uparrow} + n_{\downarrow}) \\ H_{U} &= U n_{\uparrow} n_{\downarrow} & H_{\text{mix}} &= \sum_{p\sigma} \left[V_{p\sigma} d_{\sigma}^{\dagger} c_{p\sigma} + V_{p\sigma}^{*} c_{p\sigma}^{\dagger} d_{\sigma} \right] \end{aligned}$$

Quantum impurity models

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

Single-orbital Anderson impurity model



definition of hybridization function

relation to noninteracting impurity Green's function

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

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

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



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

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

$$G = \sum_{C} \frac{w_{C}G_{C}}{Z} = \frac{\sum_{C} |w_{C}| \operatorname{sign}_{C}G_{C}}{\sum_{C} |w_{C}| \operatorname{sign}_{C}} \approx \frac{\sum_{i=1}^{M} \operatorname{sign}_{C_{i}}G_{C_{i}}}{\sum_{i=1}^{M} \operatorname{sign}_{C_{i}}}$$
$$\equiv \frac{\langle \operatorname{sign} \cdot G \rangle_{\mathrm{MC}}}{\langle \operatorname{sign} \rangle_{\mathrm{MC}}}$$

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

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

(iii) expand time ordered exponential into a power series

$$Z = \sum_{n=0}^{\infty} \int_{0}^{\beta} d\tau_{1} \cdots \int_{\tau_{n-1}}^{\beta} d\tau_{n} \operatorname{Tr} \left[e^{-(\beta - \tau_{n})H_{1}} (-H_{2}) \cdots e^{-(\tau_{2} - \tau_{1})H_{1}} (-H_{2}) e^{-\tau_{1}H_{1}} \right]$$

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$$\implies Z = \sum_{C} w_{C}$$

representation of the partition sum as a sum over configurations

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

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



Questions about the general formalism?

PRB 72, 035122 (05)

Formalism

fermionic operators

Configurations and weights points represent interaction vertices $H_2 = H_U$ $Un_{\uparrow}n_{\downarrow}$... $H_1 = H - H_2 = H_{\mu} + H_{\text{bath}} + H_{\text{mix}}$ $\frac{w_C}{Z_0} = \left(-Ud\tau\right)^n \frac{1}{Z_0} \operatorname{Tr} \left[e^{-(\beta - \tau_n)H_1} n_{\uparrow} n_{\downarrow} \cdots e^{-(\tau_2 - \tau_1)H_1} n_{\uparrow} n_{\downarrow} e^{-\tau_1 H_1} \right]$ $= (-Ud\tau)^n \prod_{\sigma} \det M_{\sigma}^{-1}$ $[M_{\sigma}^{-1}]_{ii} = \mathcal{G}_0^{\sigma}(\tau_i - \tau_i)$ H_1 quadratic in the

 $[M_{\sigma}]_{ij} = \mathcal{G}_0(\tau_i - \tau_j)$ $\mathcal{G}_0^{\sigma}(\tau) = -\mathrm{Tr}[e^{-\beta H_1}\mathcal{T}d(\tau)d^{\dagger}(0)]/Z_0$ $Z_0 = \mathrm{Tr}[e^{-\beta H_1}]$

PRB 72, 035122 (05)

Formalism

- Configurations and weights
 - $H_2 = H_U$

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

$$\frac{w_C}{Z_0} = (-Ud\tau)^n \frac{1}{Z_0} \operatorname{Tr} \left[e^{-(\beta - \tau_n)H_1} n_{\uparrow} n_{\downarrow} \right]$$
$$= (-Ud\tau)^n \prod_{\sigma} \det M_{\sigma}^{-1} \bullet$$

 H_1 quadratic in the fermionic operators



points represent interaction vertices

Formalism

Configurations and weights points represent interaction vertices $H_2 = H_U$ $Un_{\uparrow}n_{\downarrow}$... $H_1 = H - H_2 = H_{\mu} + H_{\text{bath}} + H_{\text{mix}}$ $\frac{w_C}{Z_0} = \left(-Ud\tau\right)^n \frac{1}{Z_0} \operatorname{Tr} \left[e^{-(\beta - \tau_n)H_1} n_{\uparrow} n_{\downarrow} \cdots e^{-(\tau_2 - \tau_1)H_1} n_{\uparrow} n_{\downarrow} e^{-\tau_1 H_1} \right]$ $= (-Ud\tau)^n \prod \det M_{\sigma}^{-1}$

sign problem for repulsive U?

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

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

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



Formalism

Configurations in the expanded sampling space

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

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

why does this solve the sign problem?

$$[\tilde{M}_{\sigma}^{-1}]_{ij} = \tilde{\mathcal{G}}_{0}^{\sigma}(\tau_{i} - \tau_{j}) - \alpha_{\sigma}(s_{i})\delta_{ij}$$



Formalism

Absence of sign problem



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

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

with time evolution operators represented by matrices with only positive elements

Also the matrix

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

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

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

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

Monte Carlo updates

Insertion and removal of spins



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:

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

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

Monte Carlo updates

Insertion and removal of spins

insertion: insert spins with random orientation at random times

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

removal: pick a random spin

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

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

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

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

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

needed

easy to compute

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

$$\tilde{S} = (S - [R] [M^{(n)} Q])^{-1}$$

$$\tilde{Q} = -[M^{(n)} Q] \tilde{S}$$

$$\tilde{R} = -\tilde{S} [R M^{(n)}]$$

$$\tilde{P} = M^{(n)} + [M^{(n)} Q] \tilde{S} [R M^{(n)}]$$

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

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

Monte Carlo updates

Determinant ratios and fast matrix updates

in the case of the removal update:

$$\frac{\det[M^{(n)}]^{-1}}{\det[M^{(n+1)}]^{-1}} = \tilde{S} \qquad \mathcal{O}(1)$$
$$M^{(n)} = \tilde{P} - [\tilde{Q}][\tilde{R}]/\tilde{S} \qquad \mathcal{O}(n^2)$$

Measurement of the Green's function $G = \sum_{C} w_{C}G_{C}/Z$

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

contribution to the Green's function $G_C^{\sigma} = w_C^{d_{\sigma}d_{\sigma}^{\dagger}}/w_C$

$$G_C^{\sigma}(\tau) = \mathcal{G}_0^{\sigma}(\tau) - \sum_k \mathcal{G}_0^{\sigma}(\tau - \tau_k) \sum_l [M_{\sigma}]_{kl} \mathcal{G}_0^{\sigma}(\tau_l)$$

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

$$H_{2} = H_{\text{mix}}$$

$$H_{1} = H - H_{2} = H_{\mu} + H_{U} + H_{\text{bath}} \equiv H_{\text{loc}} + H_{\text{bath}}$$

$$H_{2} \equiv H_{2}^{d^{\dagger}} + H_{2}^{d} = \sum_{p\sigma} V_{p\sigma} d_{\sigma}^{\dagger} c_{p\sigma} + \sum_{p\sigma} V_{p\sigma}^{*} c_{p\sigma}^{\dagger} d_{\sigma}$$
only even expansion orders (same number of creation/annihilation operators) contribute
$$Z = \sum_{n=0}^{\infty} \int_{0}^{\beta} d\tau_{1} \cdots \int_{\tau_{n-1}}^{\beta} d\tau_{n} \int_{0}^{\beta} d\tau_{1}^{\prime} \cdots \int_{\tau_{n-1}^{\prime}}^{\beta} d\tau_{n}^{\prime}$$

$$\times \text{Tr} \left[e^{-\beta H_{1}} \mathcal{T} H_{2}^{d}(\tau_{n}) H_{2}^{d^{\dagger}}(\tau_{n}^{\prime}) \cdots H_{2}^{d}(\tau_{1}) H_{2}^{d^{\dagger}}(\tau_{1}^{\prime}) \right]$$

 $C = \{\tau_1, \ldots, \tau_n; \tau'_1, \ldots, \tau'_n\}$

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

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

$$Z = Z_{\text{bath}} \sum_{\{n_{\sigma}\}} \prod_{\sigma} \int_{0}^{\beta} d\tau_{1}^{\sigma} \cdots \int_{\tau_{n_{\sigma}-1}}^{\beta} d\tau_{n_{\sigma}}^{\sigma} \int_{0}^{\beta} d\tau_{1}^{\prime\sigma} \dots \int_{\tau_{n_{\sigma}-1}^{\prime\sigma}}^{\beta} d\tau_{n_{\sigma}}^{\prime\sigma}$$

$$\times \operatorname{Tr}_{d} \left[e^{-\beta H_{\text{loc}}} \mathcal{T} \prod_{\sigma} d_{\sigma}(\tau_{n_{\sigma}}^{\sigma}) d_{\sigma}^{\dagger}(\tau_{n_{\sigma}}^{\prime\sigma}) \dots d_{\sigma}(\tau_{1}^{\sigma}) d_{\sigma}^{\dagger}(\tau_{1}^{\prime\sigma}) \right]$$

$$\times \frac{1}{Z_{\text{bath}}} \operatorname{Tr}_{c} \left[e^{-\beta H_{\text{bath}}} \mathcal{T} \prod_{\sigma} \sum_{p_{1} \dots p_{n_{\sigma}}} \sum_{p_{1}' \dots p_{n_{\sigma}}'} V_{p_{1}\sigma}^{*} V_{p_{1}'\sigma} \cdots V_{p_{n_{\sigma}}\sigma}^{*} V_{p_{n_{\sigma}}\sigma} V_{p_{n_{\sigma}}\sigma}^{\dagger} \right]$$

Formalism

Configurations and weights

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

$$\begin{split} \Delta^{\sigma}(\tau) &= \sum_{p} \frac{|V_{p\sigma}|^{2}}{e^{\varepsilon_{p}\beta} + 1} \begin{cases} -e^{-\varepsilon_{p}(\tau-\beta)} & 0 < \tau < \beta \\ e^{-\varepsilon_{p}\tau} & -\beta < \tau < 0 \end{cases} \\ \\ \frac{1}{Z_{\text{bath}}} \text{Tr}_{c} \Big[e^{-\beta H_{\text{bath}}} \mathcal{T} \prod_{\sigma} \sum_{p_{1} \dots p_{n_{\sigma}}} \sum_{p_{1}' \dots p_{n_{\sigma}}'} V_{p_{1}\sigma}^{*} V_{p_{1}'\sigma} \cdots V_{p_{n_{\sigma}}\sigma}^{*} V_{p_{n_{\sigma}}'\sigma} \\ \\ c^{\dagger}_{p_{n_{\sigma}}\sigma}(\tau_{n_{\sigma}}^{\sigma}) c_{p_{n_{\sigma}}'\sigma}(\tau_{n_{\sigma}}^{\prime\sigma}) \dots c^{\dagger}_{p_{1}\sigma}(\tau_{1}^{\sigma}) c_{p_{1}'\sigma}(\tau_{1}^{\prime\sigma}) \Big] = \prod_{\sigma} \det M_{\sigma}^{-1} \\ \uparrow \sigma \\ \begin{bmatrix} M_{\sigma}^{-1} \end{bmatrix}_{ij} = \Delta^{\sigma}(\tau_{i}^{\prime\sigma} - \tau_{j}^{\sigma}) & \text{matrix elements are given by} \\ \text{by it for the given for the (noninteracting) bath} \\ \end{bmatrix} \end{split}$$

matrix elements are given by hybridization functions

(noninteracting) bath

Formalism

Configurations and weights

$$C = \{\tau_1^{\uparrow}, \dots, \tau_{n_{\uparrow}}^{\uparrow}; \tau_1^{\prime\uparrow}, \dots, \tau_{n_{\uparrow}}^{\prime\uparrow} | \tau_1^{\downarrow}, \dots, \tau_{n_{\downarrow}}^{\downarrow}; \tau_1^{\prime\downarrow}, \dots, \tau_{n_{\downarrow}}^{\prime\downarrow} \}$$
$$w_C = Z_{\text{bath}} \operatorname{Tr}_d \left[e^{-\beta H_{\text{loc}}} \mathcal{T} \prod_{\sigma} d_{\sigma}(\tau_{n_{\sigma}}^{\sigma}) d_{\sigma}^{\dagger}(\tau_{n_{\sigma}}^{\prime\sigma}) \cdots d_{\sigma}(\tau_1^{\sigma}) d_{\sigma}^{\dagger}(\tau_1^{\prime\sigma}) \right]$$
$$\times \prod_{\sigma} \det M_{\sigma}^{-1} (d\tau)^{2n_{\sigma}}$$

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



Formalism

Configurations and weights

$$C = \{\tau_1^{\uparrow}, \dots, \tau_{n_{\uparrow}}^{\uparrow}; \tau_1^{\prime\uparrow}, \dots, \tau_{n_{\uparrow}}^{\prime\uparrow} | \tau_1^{\downarrow}, \dots, \tau_{n_{\downarrow}}^{\downarrow}; \tau_1^{\prime\downarrow}, \dots, \tau_{n_{\downarrow}}^{\prime\downarrow}\}$$

$$w_{C} = Z_{\text{bath}} \operatorname{Tr}_{d} \left[e^{-\beta H_{\text{loc}}} \mathcal{T} \prod_{\sigma} d_{\sigma}(\tau_{n_{\sigma}}^{\sigma}) d_{\sigma}^{\dagger}(\tau_{n_{\sigma}}^{\prime\sigma}) \cdots d_{\sigma}(\tau_{1}^{\sigma}) d_{\sigma}^{\dagger}(\tau_{1}^{\prime\sigma}) \right] \\ \times \prod_{\sigma} \det M_{\sigma}^{-1} (d\tau)^{2n_{\sigma}}$$

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



Formalism

Configurations and weights

$$C = \{\tau_1^{\uparrow}, \dots, \tau_{n_{\uparrow}}^{\uparrow}; \tau_1^{\prime\uparrow}, \dots, \tau_{n_{\uparrow}}^{\prime\uparrow} | \tau_1^{\downarrow}, \dots, \tau_{n_{\downarrow}}^{\downarrow};$$

$$w_{C} = Z_{\text{bath}} \operatorname{Tr}_{d} \left[e^{-\beta H_{\text{loc}}} \mathcal{T} \prod_{\sigma} d_{\sigma}(\tau_{n_{\sigma}}^{\sigma}) d_{\sigma}^{\dagger} \right]$$
$$\times \prod_{\sigma} \det M_{\sigma}^{-1} (d\tau)^{2n_{\sigma}}$$

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



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Monte Carlo updates

Local updates in the segment formalism



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

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

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

Monte Carlo updates

Detailed balance

acceptance probability for the insertion of a segment

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

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

acceptance probability for removal obtained from

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

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

Measurement of the Green's function

Cannot use Wick's theorem

with this, the measurement formula becomes



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

Absence of sign problem
Use again the chain basis:



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

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

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

General impurity models

Matrix formalism

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

$$\operatorname{Tr}_{d}\left[e^{-\beta H_{\operatorname{loc}}}\mathcal{T}\prod_{\alpha}d_{\alpha}(\tau_{n_{\alpha}}^{\alpha})d_{\alpha}^{\dagger}(\tau_{n_{\alpha}}^{\prime\alpha})\cdots d_{\alpha}(\tau_{1}^{\alpha})d_{\alpha}^{\dagger}(\tau_{1}^{\prime\alpha})\right]$$

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

in this basis, the creation/annihilation operators d^{\dagger}_{lpha} , d_{lpha} are however non-diagonal

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

example:
$$d^{\dagger}_{\uparrow}(\tau_4)d^{\dagger}_{\uparrow}(\tau_3)d_{\uparrow}(\tau_2)d_{\uparrow}(\tau_1) \text{ (with } \tau_1 < \tau_2 < \tau_3 < \tau_4)$$

 $\{n_{\uparrow} = 1; n_{\downarrow}\} \xrightarrow[d_{\uparrow}]{} \{n_{\uparrow} = 0; n_{\downarrow}\} \xrightarrow[d_{\uparrow}]{} \emptyset$

General impurity models

Matrix formalism

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

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

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

two types of truncation

- 1. Restriction of the trace $\sum_{\text{contributing } m} \text{Tr}_m[\dots]$ 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

$$H_1 = H_{\mu} + \frac{1}{2}U(n_{\uparrow} + n_{\downarrow}) + H_{\text{bath}} + H_{\text{mix}}$$
$$H_2 = Un_{\uparrow}n_{\downarrow} - \frac{1}{2}U(n_{\uparrow} + n_{\downarrow})$$

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

$$\frac{1}{\beta} \frac{1}{Z} \sum_{n=0}^\infty \frac{n+1}{(n+1)!} \int_0^\beta d\tau \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \\ \times \operatorname{Tr} \left[e^{-\beta H_1} \mathcal{T}(-H_2(\tau))(-H_2(\tau_n)) \cdots (-H_2(\tau_1)) \right] \\ = \frac{1}{\beta} \frac{1}{Z} \sum_C n_C w_C = \frac{1}{\beta} \langle n \rangle$$

CT-QMC

Scaling of the algorithms

Average perturbation order

weak-coupling approach: related to the potential energy

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

The set of the set of

strong-coupling approach: related to the kinetic energy

tes (Fuchs et al.³, 2011), at least in parameter regimes where $E_{kin} = \sum_{i=1}^{n} \frac{1}{2} \frac{1}$ of states of bandwidth 4 and temperature T = 1/30e The 30e/30 or e different for each data⁴ point? (Figure adapted from the fourth of U

age perturbation order for the weak-coupling and strong signspiscies of the static new prophy of the set of the the second and temperature of second second and the ball of the second s istion Eledys FEEs is ter a light store high sets connel to be defined a considering set of the store is a c t al., 2011), at least in parameter regimes where there is em. The strong-coupling approach, on the other hand, is olver or the study of (single-site) multi-orbital problems with teractions. Such problems typically have to be solved velationality of the transfer of the solved ition metal impurities (Surer et al

rtieglar tor the study of (single site) multirorbit 30 problems rectifienterfections.dStuckpopre>bleig&reypicplexd have (tGubleesc e DMFT studies of strongly correlated materials, or in real of transition metal impurities (Surer et al., 2012). age perturbation order for the weak-coupling and strong Eather the set of the s tion problem. Proverting to complete lapping to achi-our the other ha of barrely idth frand temperature 1/302 The bathis problem of the site of the study of single-site multi-orbital problem for each data point. (Figure adapted from (Gull et al., indglocal interactions Such problems pupically stars with deens ite DMFT studies of strongly correlated interation or in re snofxfrænsistion met a i Mplurifies (Seinerlætiæl.m20ti2)rbital mo Fralis2011), at least in parameter regimes wilg den streitstera = $\sum_{n=1}^{n} \sum_{j=1}^{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{j=1}^{n} \sum_{i=1}^{n} \sum_$ em. Tha enstin itionstept size Apulation of the segment algorithm. We assume

$\begin{array}{ccc} \mathsf{CT}\ \mathcal{O}^3\mathsf{MC} & L^3 & \text{Impurity clusters with density-} \\ \text{density interaction} \end{array}$

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 Average perturbation orde with density-density interaction

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$\begin{array}{ccc} \mathsf{CT} \mathcal{O}^3 \mathsf{MC} & L^3 & \text{Impurity clusters with density-} \\ \text{density interaction} \end{array}$

ion Scaling of the algorithms Single site multi-orbital models
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CT-QMC L^3 Impurity clusters with densitydensity interaction

ion Scaling of the algorithms Single site multi-orbital models • Average perturbation ordewith density-density interaction

weak coupling approach plated to the Single esite multi-orbital models ion with general $U_{ijkl_{T}}$ alism)

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40

20

0

0

2

3

metal

4

U

5

Mott insulator

6

7

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

CT-QMC

Scaling of the algorithms

• Summary and main applications

Solver	Scaling	Use
Weak-coupling	eta^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)	$\beta \qquad \exp(L)$	Single-site multi-orbital models with general U_{ijkl}
	if calculation of determind ratios dominates overlap calculation	Int

Questions about strong-coupling CT-QMC?

Local phonons

Anderson-Holstein model

$$\begin{split} H &= H_{\rm loc} + H_{\rm mix} + H_{\rm bath} & \text{phonon coupling} & \text{phonon frequency} \\ \bigstar & & \bigstar \\ H_{\rm loc} &= -\mu(n_{\uparrow} + n_{\downarrow}) + Un_{\uparrow}n_{\downarrow} + g(n_{\uparrow} + n_{\downarrow} - 1)(b^{\dagger} + b) + \omega_0 b^{\dagger} b \end{split}$$

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

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



Electron-boson systems

Local phonons

Anderson-Holstein model

$$\begin{split} H &= H_{\rm loc} + H_{\rm mix} + H_{\rm bath} & \text{phonon coupling} & \text{phonon frequency} \\ \bigstar & & \bigstar \\ H_{\rm loc} &= -\mu(n_{\uparrow} + n_{\downarrow}) + Un_{\uparrow}n_{\downarrow} + g(n_{\uparrow} + n_{\downarrow} - 1)(b^{\dagger} + b) + \omega_0 b^{\dagger} b \end{split}$$

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after expansion in hybridization

$$w(\{O_i(\tau_i)\}) = \operatorname{Tr}_d \operatorname{Tr}_b \left[e^{-\beta H_{\operatorname{loc}}} \mathcal{T}O_{2n}(\tau_{2n}) \dots O_1(\tau_1) \right] d\tau_1 \dots d\tau_{2n}$$
$$\times \prod_{\sigma} \left(\det M_{\sigma}^{-1} \right) s_{\sigma}$$



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

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

$$\widetilde{d}_{\sigma}^{\dagger} = e^{iPX_{0}}d_{\sigma}^{\dagger}e^{-iPX_{0}} = e^{\frac{g}{\omega_{0}}(b^{\dagger}-b)}d_{\sigma}^{\dagger}
\widetilde{d}_{\sigma} = e^{iPX_{0}}d_{\sigma}e^{-iPX_{0}} = e^{-\frac{g}{\omega_{0}}(b^{\dagger}-b)}d_{\sigma}$$

Electron-boson systems

Local phonons

• Calculation of the local trace $Tr_d Tr_b[...]$

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

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

$$w_b(\{O_i(\tau_i)\}) = \langle e^{s_{2n}A(\tau_{2n})}e^{s_{2n-1}A(\tau_{2n-1})}\cdots e^{s_1A(\tau_1)}\rangle_b$$

 s_i is +1 (-1) if the *i*th electron operator operator is a creation (annihilation) operator

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

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 $Tr_d Tr_b[...]$

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

$$w_{b}(\{O_{i}(\tau_{i})\}) = \exp\left[-\frac{g^{2}/\omega_{0}^{2}}{e^{\beta\omega_{0}}-1}\left(n\left(e^{\beta\omega_{0}}+1\right)\right) + \sum_{2n\geq i>j\geq 1}s_{i}s_{j}\left\{e^{\omega_{0}(\beta-(\tau_{i}-\tau_{j}))}+e^{\omega_{0}(\tau_{i}-\tau_{j})}\right\}\right)\right]$$

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

Retarded interaction-corresponding Soy hettelstein-Hubbard model with on-site interac-

- U_{bare} , bosonic frequency ω_0 and electron-boson coupling g. The difference between bare ened interaction is $\lambda = 2g^2/\omega_0$.
 - Summary: Trace over the electron and phonon states

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

e the DMFT approximation simplifies the problem considerably, by mapping the phonon factor corresponds to the additional "interaction" between creation/annihilation operators -Hubbard lattice model onto an auxiliary single-site impurity model, this effective $g^2 \cosh(\omega_0(\tau - \beta/2)) - \cosh(\omega_0\beta/2)$ s still a Komplicated interacting many-body system. The electron-boson coupling ω_0^2 es additional energy scales, besides the bandwidth and Kondo scale of the Anderurity models in the effective coupling strength ω_0 and the effective coupling strength ω_0 . (In the high-frequency limit, the Holstein-Hubbard model simplifies to the I model with interaction $U_{\rm scr} = U - \lambda$. Even in the DMFT $\tilde{\mu}_{\rm ap}$ proximated, $\omega_{\rm scr}^2/\omega_{\rm ap}$ I in nce of long-range order, the Holstein Hubbard model features a rich phase glidgiam tallic, Mott insulating and bipolaronic insulating phases (Sec. III B 4) [77–81]. Anagnetic, charge-ordered, superconducting and supersolid phases can also be found

model, namely the boson frequency ω_{ex} and the effective coupling strength model with interaction $U_{scr} = U - \lambda$. Even in the DMFT dependence of the propagate of the second sec (In the high-frequency limit the Helstein-Hubbard model simplifies to the new distance of long-range order, the Holstein-Hubbard model features a vick phase magraking is del with interaction $U_{\text{scr}} = U - \lambda$.) Even in the DMFT approximation eraph inproaches for salic, Mott insulating and bipolaronic insulating phases (Sec. III B 4) [77-81]. Anof long range order dependent in the brinch model features a rich where the present charge techniques can agnetic, charge-ordered, superconducting and supersolid phases can also be found bosonic modes (or arbitrary reta bosonic modes) (An-f symmetry breaking is allowed. In the following, we will discuss sinfluctions, or correlated tic, charge-ordered, superconducting and supersolid phases can also be found improvemented by the Holstein-Hubbard impurity provemented by the Holstein-Hubb nmetry breaking is allowed. In the following, we will discuss efficient function $f_{A} = \beta_{A}^{2} = \beta_{A} = \beta_{A}$ is the techniques can be generalized to models with a coupling to a continuum of rical approaches for solving the Holstein-Hubbard impurity problem, and also nodes (or arbitrary retarded interactions). In fact, in the context of DMFT based *ab* ese techniques can be generalized to models with a coupling to a continuum of nulations of correlated materials, the numerical challenge of treating dynamically es (or arbitrary retarded interactions). In fact, in the context of DMFT based ab interactions has been a major bottleneck which has hampered the implementations of correlated materials, the numerical challenge of treating dynamically dvanced LDA+DMFT or GW+DMFT schemes for many years. The techniques ractionschassne seengen majes botte lenge kvitte hiehe have hampered the implementa-

nced $LD \underline{A}^2 + DMET \underline{M} U \underline{G} \underline{M} + \underline{P} MFT$ schemes for many years. The techniques

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

 \bullet General frequency dependent $U(\omega)$

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



Questions about electron-boson systems?