Continuous-time impurity solvers

Philipp Werner

Theoretische Physik, ETH Zurich, 8093 Zürich, Switzerland

(Dated: May 2011)

I. QUANTUM IMPURITY MODELS

An quantum impurity model describes an atom or molecule embedded in some host or bath, with which it can exchange electrons. This exchange of electrons allows the impurity to make transitions between different quantum states, and leads to a non-trivial dynamics. Quantum impurity models play a prominent role in nano-science as representations of quantum dots or molecular conductors. They also serve as auxiliary problems, whose solution yields the “dynamical mean field” description of correlated lattice models.

The Hamiltonian of a quantum impurity model contains three terms,

$$H = H_{\text{loc}} + H_{\text{bath}} + H_{\text{mix}}.$$  \hfill (1)

$H_{\text{loc}}$ describes the impurity, characterized by a small number of degrees of freedom (typically spin and orbital degrees of freedom, which we denote by $a, b, \ldots$), $H_{\text{bath}}$ describes an infinite reservoir of free electrons, labeled by a continuum of quantum numbers $p$ and a discrete set of quantum numbers $\nu$ (e. g. spin). $H_{\text{mix}}$ describes the exchange of electrons between the impurity and the bath in terms of hybridization amplitudes $V_{p\nu}^{a\sigma}$. Explicitly, the three terms are

$$H_{\text{loc}} = \sum_{ab} E_{ab} d_a^\dagger d_b + \sum_{abcd} U_{abcd} d_a^\dagger d_b^\dagger d_c^\dagger d_d,$$  \hfill (2)

$$H_{\text{bath}} = \sum_{p,\nu} \epsilon_p a_p^{\dagger} a_{p,\nu},$$  \hfill (3)

$$H_{\text{mix}} = \sum_{p,a,\nu} (V_{p}^{a\sigma} d_a^\dagger a_{p,\nu} + \text{h.c.}).$$  \hfill (4)

We will concentrate in the following on the “one-orbital Anderson model” (AIM), a simplified representation of a magnetic impurity in a metallic host. In the AIM, the discrete quantum number labelling the impurity or bath state is the spin $\sigma$, so the Hilbert space of
FIG. 1: Left: Schematic representation of an AIM. Spin up and down electrons on the impurity (black dot) interact with an on-site energy $U$ and can hop to a continuum of non-interacting bath levels with energy $\epsilon_p$. The amplitudes for these transitions are given by the hybridization parameters $V_p^\ast$. Right: Chain representation of the AIM. All the hopping parameters can be chosen negative by a suitable gauge transformation.

the local problem $H_{\text{loc}} = H_0 + H_U$,

$$H_0 = -\mu(n_\uparrow + n_\downarrow),$$

$$H_U = Un_\uparrow n_\downarrow,$$

has dimension four, and the bath and mixing terms are given by

$$H_{\text{bath}} = \sum_{p,\sigma} \epsilon_p a_{p,\sigma}^\dagger a_{p,\sigma},$$

$$H_{\text{mix}} = \sum_{p,\sigma} (V_p^\sigma d^\sigma_{\sigma} a_{p,\sigma} + h.c.).$$

An illustration of the AIM is shown in the left hand panel of Fig. 1.

A. Chain representation

The AIM (5)-(8) can be mapped onto a semi-infinite chain, with the first site corresponding to the impurity. This mapping corresponds to a transformation of the operators $(d, a_{p_1}, a_{p_2}, \ldots)$ to new operators $(d, c_1, c_2, \ldots)$ such that $H_0 + H_{\text{bath}} + H_{\text{mix}}$ becomes tridiagonal.
In the chain representation, the impurity orbital remains unchanged, and the hopping term from the impurity to the first site of the chain is given by $V = (\sum_p |V_p|^2)^{1/2}$. The phase factors in this transformation can be chosen such that all the hopping terms are positive ($V > 0, t_i > 0, i = 1, 2, \ldots$).

### B. Action formulation

We may integrate out the bath degrees of freedom and express the partition function of the AIM as

$$Z = Tr Te^{-S}$$

with action $S = S_{\text{hyb}} + S_{\text{loc}}$ given by

$$S_{\text{hyb}} = \sum_{\sigma} \int_0^\beta d\tau d\tau' d_\sigma^\dagger(\tau)\Delta_\sigma(\tau - \tau')d_\sigma(\tau'),$$

$$S_{\text{loc}} = \int_0^\beta d\tau [-\mu(n_\uparrow(\tau) + n_\downarrow(\tau)) + Un_\uparrow(\tau)n_\downarrow(\tau)].$$

The hybridization function $\Delta_\sigma(\tau - \tau')$ in Eq. (11) represents the amplitude for hopping from the impurity into the bath at time $\tau'$ and back onto the impurity at time $\tau$. It is a function of the bath level energies and hybridization amplitudes, which is most conveniently expressed in frequency space ($i\omega_n = (2n + 1)\pi/\beta$):

$$\Delta_\sigma(i\omega_n) = \sum_p \frac{|V_p^\sigma|^2}{i\omega_n - \epsilon_p}.$$  

It is also sometimes useful to introduce the noninteracting bath Green’s function $G_0$ defined as

$$G_{0,\sigma}^{-1}(i\omega_n) = i\omega_n + \mu - \Delta_\sigma(i\omega_n).$$
Quantum impurity models are a key ingredient in the dynamical mean field (DMFT) formalism, which provides an approximate description of correlated lattice models. The success of DMFT has created a demand for powerful and flexible impurity solvers and triggered the development of the continuous-time solvers discussed in this chapter. We will thus briefly introduce the DMFT approximation, which maps an interacting lattice model, such as the one-band Hubbard model onto an effective single-site problem plus a self-consistency condition.

To appreciate the basic strategy, it is useful to briefly recall the static mean-field approximation of the classical Ising model, which is illustrated in the left hand panel of Fig. 2. Here, one focuses on a particular spin of the lattice, $S_0$, and replaces the remaining degrees of freedom by an effective external magnetic field $h_{\text{eff}} = zJm$ ($z$ is the coordination number and $m$ the magnetization per site). The lattice system

$$H_{\text{Ising}} = -J \sum_{\langle ij \rangle} S_i S_j$$

(15)
is thus mapped to the single site effective model

\[ H_{\text{eff}}^{\text{Ising}} = -h_{\text{eff}} S_0. \]

From this single-site model we can easily compute the magnetization

\[ m_{\text{eff}} = \tanh(\beta h_{\text{eff}}), \]

and identifying the magnetization \( m \) of the lattice problem with the magnetization \( m_{\text{eff}} \) of the single site effective model yields the self-consistency condition

\[ m \equiv m_{\text{eff}} = \tanh(\beta z J m). \]

We now turn to the Hubbard model,

\[ H_{\text{Hubbard}} = -\mu \sum n_{i,\sigma} + U \sum n_{i,\uparrow} n_{i,\downarrow} + t \sum_{(i,j)\sigma} a_{i,\sigma}^\dagger a_{j,\sigma} \]

which describes electrons hopping between nearest neighbor sites of some lattice with amplitude \( t \) and interacting on-site with energy \( U \). Pursuing a similar strategy as in the Ising case, we focus on one particular site (black in the right hand panels of Fig. 2) of the lattice and replace the remaining degrees of freedom of the model by a bath of non-interacting levels. The single-site effective problem thus becomes an AIM,

\[ H_{\text{imp}} = -\mu (n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow + \sum_{p,\sigma} (V_p^\sigma d_{p,\sigma}^\dagger a_{p,\sigma}^\dagger + h.c.) + \sum_{p,\sigma} \epsilon_p a_{p,\sigma}^\dagger a_{p,\sigma}. \]

Here, the \( d^\dagger \) create electrons on the “impurity”, \( n = d^\dagger d \) and the \( a_{p,\sigma}^\dagger \) create bath states labeled by a quantum number \( p \). The energy levels of the bath are \( \epsilon_p \). Processes where an electron hops from the black site into the lattice and after some excursion through the lattice returns to its original place (top right panel of Fig. 2) are represented in the single-site effective model by transitions from the impurity into the bath and back (bottom right panel of Fig. 2). The amplitudes for such transitions are given by the hybridization parameters \( V_p \) of the impurity model and the task will be to optimize the parameters \( \epsilon_p \) and \( V_p \) in such a way that the bath mimics the lattice environment.

More specifically, if \( G(k, i\omega_n) \) is the momentum dependent lattice Green function, we would like to determine bath parameters such that the impurity Green function \( G_{\text{imp}}(i\omega_n) \) reproduces the \textit{local} (momentum averaged) lattice Green function,

\[ \sum_k G(k, i\omega_n) \equiv G_{\text{imp}}(i\omega_n). \]
A. DMFT approximation

The solution to Eq. (21) is computed iteratively and these DMFT iterations involve as the essential approximation of the method a simplification of the momentum-dependence of the lattice self-energy. The self-energy describes the effect of interactions on the propagation of electrons. In the non-interacting model ($U = 0$) the lattice Green function is given by $G_{U=0}(k, \omega) = [i\omega_n + \mu - \epsilon_k]^{-1}$, with $\epsilon_k$ the Fourier transform of the hopping matrix, whereas the Green function of the interacting model is given by $G(k, \omega) = [i\omega_n + \mu - \epsilon_k - \Sigma(k, i\omega_n)]^{-1}$. Therefore $\Sigma(k, i\omega_n) = G_{U=0}^{-1}(k, i\omega_n) - G(k, i\omega_n)^{-1}$, and similarly the impurity self-energy is given by $\Sigma_{\text{imp}}(i\omega_n) = G_{\text{imp}, U=0}^{-1}(i\omega_n) - G_{\text{imp}}(i\omega_n)^{-1}$. The DMFT approximation amounts to identifying the lattice self-energy with the momentum-independent impurity self-energy,

$$\Sigma(k, i\omega_n) \approx \Sigma_{\text{imp}}(i\omega_n). \quad (22)$$

Using this approximation we can rewrite Eq. (21) as

$$\sum_k [i\omega_n + \mu - \epsilon_k - \Sigma_{\text{imp}}(i\omega_n)]^{-1} \equiv G_{\text{imp}}(i\omega_n). \quad (23)$$

Since both $G_{\text{imp}}(i\omega_n)$ and $\Sigma_{\text{imp}}(i\omega_n)$ depend on the impurity model parameters $\epsilon_p$ and $V_p$ we obtain a self-consistency condition for the impurity model.

B. DMFT self-consistency loop

Starting from an arbitrary initial bath Green function $G_0(i\omega_n)$ (for example the solution of the noninteracting problem), one iterates the following steps until convergence is reached:

1. Solve the impurity problem, i.e. compute the Green function $G_{\text{imp}}(i\omega_n)$ for the given “bath” $G_0(i\omega_n)$,

2. Extract the self-energy of the impurity model: $\Sigma_{\text{imp}}(i\omega_n) = G_0^{-1}(i\omega_n) - G_{\text{imp}}^{-1}(i\omega_n)$,

3. Identify the lattice self-energy with the impurity self-energy ($\Sigma(k, i\omega_n) = \Sigma_{\text{imp}}(i\omega_n)$) and compute the local lattice Green function $G_{\text{loc}}(i\omega_n) = \sum_k [i\omega_n + \mu - \Sigma_{\text{imp}}(i\omega_n)]^{-1}$,

4. Apply the DMFT self-consistency condition ($G_{\text{loc}}(i\omega_n) = G_{\text{imp}}(i\omega_n)$) and use this to define a new “bath” $G_{0,\text{new}}^{-1}(i\omega_n) = G_{\text{loc}}^{-1}(i\omega_n) + \Sigma_{\text{imp}}(i\omega_n)$. 

The computationally expensive step in this procedure is the solution of the impurity problem. Once the calculation has converged, the bath contains information about the topology of the lattice. The impurity, which exchanges electrons with the bath, will thus feel (at least to some extent) as if it were a site of the lattice. Obviously, not all the physics can be captured by a single-site impurity model. In particular spatial fluctuations, which become important in low-dimensional systems, are completely neglected. Dynamical mean field calculations become exact in the limit of infinite dimension or coordination number, in the non-interacting limit \((U = 0)\) and in the atomic limit \((t = 0)\).

C. Simulation of strongly correlated materials

The DMFT formalism can describe band-like behavior (quasi-particle peaks) and atomic-like behavior (Hubbard bands). It thus captures the competition between localization and delocalization which plays a crucial role in the physics of strongly correlated materials. In order to enable “ab-initio” simulations of real compounds, the dynamical mean field framework can be combined with density functional theory in the LDA approximation. The resulting formalism is called “LDA+DMFT”. The idea is to use the Kohn-Sham eigenvalues \(\epsilon_k^{KS}\) in the self-consistency equation (23) instead of the dispersion of some tight-binding model. However, by doing so one encounters a problem: while density functional theory in the LDA approximation does not take into account all the correlation effects it captures some of them. If we now explicitly describe the local interaction in the strongly correlated orbitals via some \(U\)-term in an effective impurity model, some interaction contributions appear twice and this “double counting” of interaction energy must be compensated by adding a double counting correction \(E_{DC}\) to the self-energy of the correlated orbitals. The self-consistency condition thus becomes

\[
\sum_k [i\omega_n + \mu - \epsilon_k^{KS} - \Sigma_{\text{imp}}(i\omega_n) - E_{DC}]^{-1} \equiv G_{\text{imp}}(i\omega_n). \tag{24}
\]

There is no clean and consistent solution to the double counting problem in LDA+DMFT. In practice, one uses formulas like \(E_{DC} = U \langle n \rangle\) with \(\langle n \rangle\) the average occupancy.

Most material simulations will involve several bands, so that the Kohn-Sham eigenvalues define a matrix \(H_k^{LDA}\) in Wannier orbital space. Only the \(d\)- or \(f\)-orbitals will be explicitly treated in the impurity calculation and yield a self-energy. Thus \(\Sigma_{\text{imp}}\) will be a matrix of
the same size as $H_k^{LDA}$, but the only non-zero elements will be in the block corresponding to the strongly correlated $d$- or $f$-orbitals. Similarly the double-counting correction will be a diagonal matrix with non-zero elements only for the correlated orbitals. In the multi-orbital case, one can use as double counting correction $E_{DC} = \langle U \rangle \langle n_{corr} \rangle$, with $\langle U \rangle$ the average of the interaction parameters of the (multiorbital) impurity problem and $\langle n_{corr} \rangle$ the average occupancy of the correlated orbitals. This orbital-independent shift assures that the crystal-field splittings in the LDA band structure are preserved by the double counting correction. The chemical potential $\mu$ is adjusted such that the correct total number of electrons in the correlated and uncorrelated orbitals is obtained.

III. CONTINUOUS-TIME IMPURITY SOLVERS - GENERAL RECIPE

Quantum impurity models are 0+1 dimensional quantum field theories and as such computationally much more tractable than interacting lattice models. By “solving the impurity model” we essentially mean computing the impurity Green function $(0 < \tau < \beta)$

$$G(\tau) = \langle Td(\tau)d^\dagger(0) \rangle = \frac{1}{Z} Tr \left[ e^{-(\beta-\tau)H} d e^{-\tau H} d^\dagger \right],$$

which $Z = Tr[e^{-\beta H}]$, the impurity model partition function, $\beta$ the inverse temperature, and $Tr = Tr_d Tr_a$ the trace over the impurity and bath states.

Hamiltonian based methods such as exact diagonalization or numerical RG explicitly treat a finite number of bath states, and are suitable for single orbital models. However, because the number of bath states must be increased proportional to the number of orbitals, the computational effort grows exponentially with system size, and requires severe truncations of the bath already for two orbitals. Monte Carlo methods have the advantage that the bath is integrated out and thus the (infinite) size of the bath Hilbert space does not affect the simulation. While restricted to finite temperature, Monte Carlo methods are thus the method of choice for the solution of large multi-orbital or cluster impurity problems.

We will discuss here two complementary continuous-time Monte Carlo techniques: (i) a weak-coupling approach, which scales favorably with system size and allows the efficient simulation of large impurity clusters, and (ii) a strong-coupling approach, which can handle impurity models with strong interactions. For simplicity, we will focus on the single-orbital AIM impurity model defined in Eqs. (5)-(8).
Continuous-time Monte Carlo algorithms are based on an expansion of the partition function into a series of “diagrams” and the stochastic sampling of (collections) of these diagrams. We represent the partition function as a sum (or, more precisely, integral) of configurations $c$ with weight $w_c$,

$$Z = \sum_c w_c,$$

and implement a random walk $c_1 \rightarrow c_2 \rightarrow c_3 \rightarrow \ldots$ in configuration space in such a way that each configuration can be reached from any other in a finite number of steps (ergodicity) and that detailed balance is satisfied,

$$|w_{c_1}|p(c_1 \rightarrow c_2) = |w_{c_2}|p(c_2 \rightarrow c_1).$$

(27)

This assures that each configuration is visited with a probability proportional to $|w_c|$ and one can thus obtain an estimate for the Green function from a finite number $N$ of measurements:

$$G = \frac{\sum_c w_c G_c}{\sum_c w_c} = \frac{\sum_c |w_c| \text{sign} G_c}{\sum_c |w_c| \text{sign} c} = \frac{\langle \text{sign} \cdot G \rangle_{MC}}{\langle \text{sign} \rangle_{MC}}.$$  

(28)

The first step in the derivation is to rewrite the partition function as a time ordered exponential using some interaction representation. We split the Hamiltonian into two parts, $H = H_1 + H_2$ and define the time dependent operators in the interaction picture as $O(\tau) = e^{\tau H_1} O e^{-\tau H_1}$. In a second step, the time ordered exponential is expanded into a power series,

$$Z = \text{Tr} \left[ e^{-\beta H_1} T e^{-\int_0^\beta d\tau H_2(\tau)} \right] = \sum_{n=0}^{\infty} \int_0^\beta d\tau_1 \ldots \int_0^{\tau_{n-1}} d\tau_n \text{Tr} \left[ e^{-(\beta-\tau_n)H_1}(-H_2)\ldots e^{-(\tau_2-\tau_1)H_1}(-H_2)e^{-\tau_1 H_1} \right],$$

(29)

which is a representation of the partition function of the form (26), namely the sum of all configurations $c = \{\tau_1, \ldots, \tau_n\}$, $n = 0, 1, \ldots, \tau_i \in [0, \beta)$ with weight

$$w_c = \text{Tr} \left[ e^{-(\beta-\tau_n)H_1}(-H_2)\ldots e^{-(\tau_2-\tau_1)H_1}(-H_2)e^{-\tau_1 H_1} \right] d\tau^n.$$  

(30)

The weak-coupling continuous-time Monte Carlo approach is based on an expansion of $Z$ in powers of the interaction $U$, and on an interaction representation in which the time evolution is determined by the quadratic part $H_0 + H_{\text{bath}} + H_{\text{mix}}$ of the Hamiltonian. The complementary “strong-coupling” approach is based on an expansion of $Z$ in powers of the impurity-bath hybridization $V$, and an interaction representation in which the time evolution is determined by the local part $H_0 + H_U + H_{\text{bath}}$ of the Hamiltonian.
IV. WEAK-COUPLING APPROACH

The weak-coupling continuous time impurity solver employs an expansion of the partition function in powers of $H_2 = H_U$. Equation (30) thus gives the weight of a configuration of $n$ interaction vertices. Since $H_1 = \mathbf{H} - H_2 = H_0 + H_{\text{bath}} + H_{\text{mix}}$ is quadratic, we can use Wick’s theorem to evaluate the trace. The result is a product of two determinants of $n \times n$ matrices (one for each spin), whose elements are bath Green functions $G_0$ evaluated at the time intervals defined by the vertex positions:

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

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

with $Z_0 = Tr[e^{-\beta H_1}]$ the partition function of the noninteracting model.

At this point, we encounter a problem. In the paramagnetic phase, where $G_{0,\uparrow} = G_{0,\downarrow}$, the product of determinants is positive, which means that for repulsive interaction ($U > 0$), odd perturbation orders yield negative weights. Except in the particle-hole symmetric case, where one can show that odd perturbation orders vanish, this will result in a severe sign problem. Fortunately, we can solve this sign problem by shifting the chemical potentials for up and down spins in an appropriate way. We rewrite the interaction term as

$$H_U = \frac{U}{2} \sum_{s,\sigma} (n_\sigma - \alpha_\sigma(s)) + \frac{U}{2} (n_\uparrow + n_\downarrow) - \frac{U}{4},$$

$$\alpha_\sigma(s) = 1/2 + \sigma s(1/2 + \delta).$$

Here $\delta$ is some constant and $s = \pm 1$ an Ising variable. The constant $-U/4$ in Eq. (33) is irrelevant, while the contribution $U(n_\uparrow + n_\downarrow)/2$ can be absorbed into the noninteracting Green function by shifting the chemical potential as $\mu \rightarrow \mu - U/2$. Explicitly, we redefine the bath Green function as $G_{0,\sigma}^{-1} = i\omega_n + \mu - \Delta_\sigma \rightarrow \tilde{G}_{0,\sigma}^{-1} = i\omega_n + \mu - U/2 - \Delta_\sigma$.

The introduction of an Ising variable $s_i$ at each vertex position $\tau_i$ enlarges the configuration space exponentially. A configuration $c$ now corresponds to a collection of Ising spin variables on the imaginary time interval: $c = \{(\tau_1, s_1), (\tau_2, s_2), \ldots, (\tau_n, s_n)\}$. The weight of
these configurations are

\[ \frac{w_c}{Z_0} = (-U d\tau/2)^n \prod_{\sigma} \det \tilde{M}_\sigma^{-1}, \]  

(35)

\[(\tilde{M}_\sigma^{-1})_{ij} = \tilde{G}_{0,\sigma}(\tau_i - \tau_j) - \alpha_\sigma(s_i)\delta_{ij}. \]  

(36)

The Ising variables are in fact not needed to cure the sign problem. They have been introduced to symmetrize the interaction term and prevent ergodicity problems.

A. Sampling procedure and detailed balance

For ergodicity it is sufficient to insert/remove spins with random orientation at random times, because this allows in principle to generate all possible configurations. Furthermore, the random walk in configuration space must satisfy the detailed balance condition (27). Splitting the probability to move from configuration \( c_i \) to configuration \( c_j \) into a probability to propose the move and a probability to accept it,

\[ p(c_i \rightarrow c_j) = p^{\text{prop}}(c_i \rightarrow c_j)p^{\text{acc}}(c_i \rightarrow c_j), \]  

(37)

we arrive at the condition

\[ \frac{p^{\text{acc}}(c_i \rightarrow c_j)}{p^{\text{acc}}(c_j \rightarrow c_i)} = \frac{p^{\text{prop}}(c_j \rightarrow c_i) |w(c_j)|}{p^{\text{prop}}(c_i \rightarrow c_j) |w(c_i)|}. \]  

(38)

There is some flexibility in choosing the proposal probabilities. A reasonable choice for the insertion/removal of a spin is the following (illustrated in Fig. 3):

- **Insertion**
  
  Pick a random time in \([0, \beta]\) and a random direction for the new spin:
  
  \[ p^{\text{prop}}(n \rightarrow n + 1) = (1/2)(d\tau/\beta), \]

- **Removal**
  
  Pick a random spin: \( p^{\text{prop}}(n + 1 \rightarrow n) = 1/(n + 1). \)

For this choice, the ratio of acceptance probabilities becomes

\[ \frac{p^{\text{acc}}(n \rightarrow n + 1)}{p^{\text{acc}}(n + 1 \rightarrow n)} = \frac{\beta U}{n + 1} \prod_{\sigma=1,1} \frac{|\det(M^{(n+1)}_\sigma)^{-1}|}{|\det(M^{(n)}_\sigma)^{-1}|}, \]  

(39)

and the random walk can thus be implemented for example on the basis of the Metropolis algorithm, *i.e.* the proposed move from \( n \) to \( n \pm 1 \) is accepted with probability \( \min[1, p^{\text{acc}}(n \rightarrow n \pm 1)/p^{\text{acc}}(n \pm 1 \rightarrow n)] \).
FIG. 3: Local update in the continuous-time auxiliary field method. The dashed line represents the imaginary time interval \([0, \beta]\). We increase the perturbation order by adding a spin with random orientation at a random time. The perturbation order is decreased by removing a randomly chosen spin.

B. Determinant ratios and fast matrix updates

From Eq. (39) it follows that each update requires the calculation of a ratio of two determinants. Computing the determinant of a matrix of size \((n \times n)\) is an \(O(n^3)\) operation. However, each insertion or removal of a spin merely changes one row and one column of the matrix \(M^{-1}\). We will now show that it is therefore possible to evaluate the ratio in Eq. (39) in a time \(O(n^2)\) (insertion) or \(O(1)\) (removal).

The objects which are stored and manipulated during the simulation are, besides the lists of the times \(\{\tau_i\}\) and spins \(\{s_i\}\), the matrices \(M_\sigma = (G_{0\sigma})^{-1}\). Inserting a spin adds a new row and column to \(M_\sigma^{-1}\). We define the blocks (omitting the \(\sigma\) index)

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

(40)

where \(Q, R, S\) denote \((n \times 1)\), \((1 \times n)\), and \((1 \times 1)\) matrices, respectively, which contain the contribution of the added spin. The determinant ratio needed for the acceptance/rejection probability is then given by

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

(41)

As we store \(M^{(n)}\), computing the acceptance/rejection probability of an insertion move is an \(O(n^2)\) operation. If the move is accepted, the new matrix \(M^{(n+1)}\) is computed out of
\(M^{(n)}, Q, R, \) and \(S,\) also in a time \(O(n^2)\):

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

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

\[
\tilde{R} = -\tilde{S}[RM^{(n)}],
\]

\[
\tilde{P} = N^{(n)} + [M^{(n)}Q]\tilde{S}[RM^{(n)}].
\]

It follows from Eq. (41) that the calculation of the determinant ratio for removing a spin is \(O(1)\), since it is just element \(\tilde{S}\), and from the above formulas we also immediately find the elements of the reduced matrix:

\[
M^{(n)} = \tilde{P} - \frac{[\tilde{Q}][\tilde{R}]}{\tilde{S}}.
\]

C. Measurement of the Green function

To compute the contribution of a configuration \(c\) to the Green function, \(G^c_\sigma(\tau)\), we insert in Eq. (??) a creation operator \(\dagger\) at time 0 and an annihilation operator \(d\) at time \(\tau\) and divide by \(w_c\). Wick’s theorem then leads to the expression

\[
G^c_\sigma(\tau) = G_{0\sigma}(i\omega_n) - \sum_k G_{0\sigma}(\tau - \tau_k) \sum_l [M_\sigma]_{kl} G_{0\sigma}(\tau_l).
\]

The impurity Green function is obtained as \(G(\tau) = \langle G^c_\sigma(\tau) \rangle_{MC}\).

It is possible to accumulate the Fourier components of the Green function directly. Using translational invariance of the Green functions one finds

\[
G^c_\sigma(i\omega_n) = G_{0\sigma}(i\omega_n) - G_{0\sigma}(i\omega_n) \sum_{k,l} \frac{1}{\beta} e^{i\omega_n(\tau_k - \tau_l)} [M_\sigma]_{kl} G_{0\sigma}(i\omega_n),
\]

so that \(G(i\omega_n) = G_0(i\omega_n) - \frac{1}{\beta} (G_0(i\omega_n))^2 \langle \sum_{k,l} e^{i\omega_n(\tau_k - \tau_l)} [M_\sigma]_{kl} \rangle_{MC}\). Note that because the bath Green function has the high-frequency behavior \(G_0(i\omega_n) \sim 1/i\omega_n\), the impurity Green function will inherit the correct high-frequency tail.

D. Generalization - multiorbital and cluster impurity problems

The generalization of the weak-coupling method to impurity clusters is straight forward. All we have to do is to add a site index to the interaction vertices (or auxiliary Ising spin
variables) and sample the vertices (spins) on a family of $n_{\text{sites}}$ imaginary time intervals. In principle, the weak-coupling solver can also be used to simulate lattice models, since the only difference to a multi-site impurity problem is the definition of the bath $G_0$. However, the $O(\beta^3)$ scaling is not competitive with the BSS algorithm.

General four fermion terms as in (2) are, at least in principle, also easily dealt with. One simply expands the partition function in powers of all the interaction terms $U^{abcd}$. The trace over the impurity and bath degrees of freedom then again yields a determinant of a matrix whose size is equal to the total perturbation order. To reduce the sign problem, it is advantageous to introduce auxiliary fields $\alpha$ and replace

\[
\sum_{abcd} U^{abcd} d^\dagger_a d^\dagger_b d_c d_d \rightarrow \sum_{abcd} U^{abcd} (d^\dagger_a d^\dagger_c - \alpha_{ac})(d^\dagger_b d_d - \alpha_{bd}),
\]

(49)

with an appropriate shift in the quadratic part of the Hamiltonian. However, in general, it will not be possible to completely eliminate the sign problem by a suitable choice of the parameters $\alpha$. Furthermore, since the number of interaction terms grows like $O(n_{\text{orbital}}^4)$ the computational cost rapidly escalates. In practice, the strong coupling approach discussed in the following section turns out to be a more suitable approach for single-site multi-orbital problems with complex interaction terms.

V. STRONG-COUPLING APPROACH - EXPANSION IN THE IMPURITY-BATH HYBRIDIZATION

A continuous-time Monte Carlo method, which is in many ways complementary to the weak-coupling approach, is based on an expansion of the partition function in powers of the impurity-bath hybridization $V$. Here, we decompose the Hamiltonian as $H_2 = H_{\text{mix}}$ and

\[
H_1 = H - H_2 = H_0 + H_U + H_{\text{bath}}.
\]

Since $H_2 \equiv H_2^d + H_2^d = \sum_{\sigma,p} V^\sigma_p d_{\sigma}^\dagger a_{p,\sigma} + \sum_{\sigma,y} V^\sigma_{y\sigma} d_{\sigma} a_{\sigma,y}^\dagger$

has two terms, corresponding to electrons hopping from the bath to the impurity and from the impurity back to the bath, only even perturbation orders contribute to Eq. (29). Furthermore, at perturbation order $2n$ only the $(2n)!/(n!)^2$ terms corresponding to $n$ creation operators $d^\dagger$ and $n$ annihilation operators $d$ will contribute. We can therefore write the
partition function as a sum over configurations \( c = \{\tau_1, \ldots, \tau_n; \tau'_1, \ldots, \tau'_{n'}\} \):

\[
Z = \sum_{n=0}^{\infty} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \int_0^\beta d\tau'_1 \cdots \int_0^\beta d\tau'_{n'} = \mathrm{Tr} \left[ e^{-\beta H_1} T H_2^d(\tau_n) H_2^d(\tau'_n) \cdots H_2^d(\tau_1) H_2^d(\tau'_1) \right].
\]

(50)

Since the time evolution of the AIM (given by \( H_1 \)) does not rotate the spin, there is an additional constraint, namely that the configuration contains an equal number of creation and annihilation operators for both for spin up and spin down. Taking this into account and writing out the expressions for \( H_2^d \) and \( H_2^d \) explicitly, we find

\[
Z = Z_{\text{bath}} \prod_{\sigma} \prod_{n_\sigma} \int_0^\beta d\tau_\sigma \cdots \int_0^\beta d\tau'_n \int_0^\beta d\tau'^\sigma \cdots \int_0^\beta d\tau'^{n'}_\sigma
\times \mathrm{Tr}_d \left[ e^{-\beta H_{\text{loc}}} T \int_\beta d\sigma (\tau_\sigma) d\sigma (\tau'_\sigma) \cdots d\sigma (\tau_{n_\sigma}) d\sigma (\tau'_{n_\sigma}) \right]
\times \frac{1}{Z_{\text{bath}}} \mathrm{Tr}_a \left[ e^{-\beta H_{\text{bath}}} T \int_\beta d\sigma (\tau_\sigma) d\sigma (\tau'_\sigma) \cdots d\sigma (\tau_{n_\sigma}) d\sigma (\tau'_{n_\sigma}) \right]
\times \frac{1}{Z_{\text{bath}}} \mathrm{Tr}_a \left[ e^{-\beta H_{\text{bath}}} T \sum_{\sigma} \sum_{n_\sigma} \sum_{p_1} \cdots \sum_{n_\sigma} \sum_{p_1} \cdots \sum_{n_\sigma} V_{\sigma p_1} V_{\sigma p_1'} \cdots V_{\sigma p_1} V_{\sigma p_1'{}^*} \right]
\times \frac{1}{Z_{\text{bath}}} \mathrm{Tr}_a \left[ e^{-\beta H_{\text{bath}}} T \sum_{\sigma} \sum_{n_\sigma} \sum_{p_1} \cdots \sum_{n_\sigma} \sum_{p_1} \cdots \sum_{n_\sigma} V_{\sigma p_1} V_{\sigma p_1'} \cdots V_{\sigma p_1} V_{\sigma p_1'{}^*} \right]
\times \frac{1}{Z_{\text{bath}}} \mathrm{Tr}_a \left[ e^{-\beta H_{\text{bath}}} T \sum_{\sigma} \sum_{n_\sigma} \sum_{p_1} \cdots \sum_{n_\sigma} \sum_{p_1} \cdots \sum_{n_\sigma} a_{\sigma p_1} (\tau_\sigma) a_{\sigma p_1'} (\tau'_\sigma) \cdots a_{\sigma p_1} (\tau_{n_\sigma}) a_{\sigma p_1'} (\tau'_{n_\sigma}) \right]
= \prod_{\sigma} \det M^{-1}_{\sigma}.
\]

(51)

where we have used the fact that \( H_1 \) does not mix the impurity and the bath to separate the \( d \) and \( a \) operators. \( Z_{\text{bath}} = \mathrm{Tr}_a e^{-\beta H_{\text{bath}}} \), and \( H_{\text{loc}} = H_0 + H_U \). Introducing the \( \beta \)-antiperiodic hybridization function (13), which in the time-domain reads

\[
\Delta_{\sigma}(\tau) = \sum_p \frac{|V_p|^2}{e^{-\beta p} + 1} \begin{cases} 
- e^{-\beta p \tau} & \tau > 0 \\
- e^{-\beta p (\beta + \tau)} & \tau < 0,
\end{cases}
\]

(52)

the trace over the bath states can be expressed as

\[
\frac{1}{Z_{\text{bath}}} \mathrm{Tr}_a \left[ e^{-\beta H_{\text{bath}}} T \sum_{\sigma} \sum_{n_\sigma} \sum_{p_1} \cdots \sum_{n_\sigma} \sum_{p_1} \cdots \sum_{n_\sigma} V_{\sigma p_1} V_{\sigma p_1'} \cdots V_{\sigma p_1} V_{\sigma p_1'{}^*} \right]
\times \frac{1}{Z_{\text{bath}}} \mathrm{Tr}_a \left[ e^{-\beta H_{\text{bath}}} T \sum_{\sigma} \sum_{n_\sigma} \sum_{p_1} \cdots \sum_{n_\sigma} \sum_{p_1} \cdots \sum_{n_\sigma} V_{\sigma p_1} V_{\sigma p_1'} \cdots V_{\sigma p_1} V_{\sigma p_1'{}^*} \right]
\times \frac{1}{Z_{\text{bath}}} \mathrm{Tr}_a \left[ e^{-\beta H_{\text{bath}}} T \sum_{\sigma} \sum_{n_\sigma} \sum_{p_1} \cdots \sum_{n_\sigma} \sum_{p_1} \cdots \sum_{n_\sigma} a_{\sigma p_1} (\tau_\sigma) a_{\sigma p_1'} (\tau'_\sigma) \cdots a_{\sigma p_1} (\tau_{n_\sigma}) a_{\sigma p_1'} (\tau'_{n_\sigma}) \right]
= \prod_{\sigma} \det M^{-1}_{\sigma}.
\]

(53)

where \( M^{-1}_{\sigma} \) is the \((n_\sigma \times n_\sigma)\) matrix with elements

\[
M^{-1}_{\sigma} (i, j) = \Delta_{\sigma}(\tau_{i}^{\sigma} - \tau_{j}^{\sigma}).
\]

(54)

In the hybridization expansion method, the configuration space consists of all sequences \( c = \{\tau_1^{\uparrow}, \ldots, \tau_n^{\uparrow}; \tau'_1^{\uparrow}, \ldots, \tau'_n^{\uparrow} \} \), of \( n^{\uparrow} \) creation and annihilation operators.
FIG. 4: Local update in the “segment” picture. The two segment configurations correspond to spin up and spin down. Each segment depicts a time interval in which an electron of the corresponding spin resides on the impurity (the end points are the locations of the operators $d^\dagger$ and $d$). We increase the perturbation order by adding a segment or anti-segment of random length for random spin. The perturbation order is decreased by removing a randomly chosen segment.

For spin up ($n_\uparrow = 0, 1, \ldots$), and $n_\downarrow$ creation and annihilation operators for spin down ($n_\downarrow = 0, 1, \ldots$). The weight of this configuration is

$$w_c = Z_{\text{bath}} \text{Tr}_d \left[ e^{-\beta H_{\text{loc}}} \prod_\sigma d_\sigma(\tau_{n_\sigma}) d^\dagger_\sigma(\tau_{n_\sigma}) \cdots d_\sigma(\tau_1) d^\dagger_\sigma(\tau_1) \right]$$

$$\times \prod_\sigma \det M^{-1}_\sigma(\tau_1, \ldots, \tau_{n_\sigma}, \tau'_1, \ldots, \tau'_{n_\sigma})(d\tau)^{2n_\sigma}. \quad (55)$$

The trace factor represents the contribution of the impurity, which fluctuates between different quantum states, as electrons hop in and out. The determinants resum all the bath evolutions which are compatible with the given sequence of transitions (see Section ??).

To evaluate the trace factor, one may use the eigenbasis of $H_{\text{loc}}$. In this basis, the time evolution operator $e^{-\tau H_{\text{loc}}}$ is diagonal while the operators $d_\sigma$ and $d^\dagger_\sigma$ will produce transitions between eigenstates with amplitude $\pm 1$.

Because the time evolution does not flip the spin, the creation and annihilation operators for given spin have to alternate. This allows us to separate the operators for spin up from those for spin down and to depict the time evolution by a collection of segments (each segment representing a time interval in which an electron of spin up or down resides on
the impurity). At each time, the eigenstate of the impurity follows immediately from the segment representation and we can easily compute the trace factor as

\[ \text{Tr} \left[ e^{-\beta H_{\text{loc}}} T \prod_{\sigma} d_\sigma(\tau_{n_\sigma}) d_\sigma^\dagger(\tau_{n_\sigma}^\prime) \cdots d_\sigma(\tau_1) d_\sigma^\dagger(\tau_1^\prime) \right] = s \exp \left[ \mu (l_1 + l_1^\prime) - U \delta l_{\text{overlap}} \right], \]  

with \( s \) a permutation sign, \( l_\sigma \) the total “length” of the segments for spin \( \sigma \) and \( \delta l_{\text{overlap}} \) the total length of the overlap between up and down segments. The lower panel of Fig. 4 shows a configuration with 3 segments for spin up and two segments for spin down; the time intervals where segments overlap, indicated by gray rectangles, correspond to a doubly occupied impurity and cost a repulsion energy \( U \).

### A. Sampling procedure and detailed balance

For ergodicity, it is sufficient to insert and remove pairs of creation and annihilation operators (segments or anti-segments) for spin up and down. One possible strategy for inserting a segment is the following: we pick a random time in \([0, \beta]\) for the creation operator. If it falls on an existing segment, the impurity is already occupied and the move is rejected. If it falls on an empty space, we compute \( l_{\text{max}} \), the length from this position to the next segment (in the direction of increasing \( \tau \)). If there are no segments, \( l_{\text{max}} = \beta \). The position of the new annihilation operator is then chosen randomly in this interval of length \( l_{\text{max}} \) (see Fig. 4). If we propose to remove a randomly chosen segment for this spin, then the proposal probabilities are

\[ p^{\text{prop}}(n_\sigma \to n_\sigma + 1) = \frac{d\tau}{\beta l_{\text{max}}}, \quad p^{\text{prop}}(n_\sigma + 1 \to n_\sigma) = \frac{1}{n_\sigma + 1}, \]  

and the ratio of acceptance probabilities therefore becomes

\[ \frac{p^{\text{acc}}(n_\sigma \to n_\sigma + 1)}{p^{\text{acc}}(n_\sigma + 1 \to n_\sigma)} = \frac{\beta l_{\text{max}}}{n_\sigma + 1} e^{\mu l_{\text{new}} - U \delta l_{\text{overlap}}} \frac{\det(M^{(n_\sigma + 1)}_{\sigma})^{-1}}{\det(M^{n_\sigma}_{\sigma})^{-1}}. \]  

Here, \( l_{\text{new}} \) is the length of the new segment, and \( \delta l_{\text{overlap}} \) the change in the overlap. Again, we compute the ratio of determinants using the fast update formulas discussed in Section IV B.
B. Measurement of the Green function

The strategy here is to create configurations which contribute to the Green function measurement by decoupling the bath from a given pair of creation and annihilation operators in \( c \). The idea is to write

\[
g(\tau) = \frac{1}{Z} \sum_c w_c \frac{w_c^{d(\tau)d(0)}}{w_c^{(\tau,0)}},
\]

where \( w_c^{d(\tau)d(0)} \) denotes the weight of configuration \( c \) with and additional operator \( d(0) \) and \( d(\tau) \) in the trace factor, and \( w_c^{(\tau,0)} \) the complete weight corresponding to the enlarged operator sequence (including enlarged hybridization determinants). Since the trace factors of both weights are identical,

\[
\frac{w_c^{d(\tau)d(0)}}{w_c^{(\tau,0)}} = \frac{\det M_c^{-1}}{\det (M_c^{(\tau,0)})^{-1}} = (M_c^{(\tau,0)})_{ji},
\]

with \( i \) and \( j \) denoting the row and column corresponding to the new operators \( d^\dagger \) and \( d \) in the enlarged \((M_c^{(\tau,0)})^{-1}\). Hence, the measurement formula for the Green function becomes

\[
G(\tau) = \frac{1}{Z} \sum_c w_c \sum_{i,j} \frac{1}{\beta} \Delta(\tau, \tau_i - \tau_j)(M_c)_{ji} = \left\langle \sum_{i,j} \frac{1}{\beta} \Delta(\tau, \tau_i - \tau_j)M_{ji} \right\rangle_{MC},
\]

with \( \Delta(\tau, \tau') = \delta(\tau - \tau') \) for \( \tau' > 0 \), and \( \Delta(\tau, \tau') = -\delta(\tau - \tau' - \beta) \) for \( \tau' < 0 \).

We may Fourier transform Eq. (61) to obtain a measurement formula for the Fourier coefficients of the Green function,

\[
G(i\omega_n) = \left\langle \sum_{i,j} \frac{1}{\beta} e^{i\omega_n(\tau_j - \tau_i)} M_{ji} \right\rangle_{MC}.
\]

Note that in contrast to the weak-coupling approach, where the Green function is measured as a \( O(1/(i\omega_n)^2) \) correction to the bath Green function, Eq. (62) does not automatically yield the correct high frequency tails. It is thus advantageous to accumulate the coefficients of an expansion of the Green function in Legendre polynomials.

C. Generalization - Matrix formalism

It is obvious from the derivation in Section V that the hybridization expansion formalism is applicable to general classes of impurity models. Because the trace factor in the weight
is computed exactly, $H_{\text{loc}}$ can contain essentially arbitrary interactions (e. g. spin-exchange terms in multi-orbital models), degrees of freedom (e. g. spins in Kondo-lattice models) or constraints (e. g. no double occupancy in the $t$-$J$ model).

For multi-orbital impurity models with density-density interaction, the segment formalism is still applicable: we have now a collection of segments for each flavor $\alpha$ (orbital, spin) and the trace factor can still be computed from the length of the segments (chemical potential contribution) and the overlaps between segments of different flavor (interaction terms).

If $H_{\text{loc}}$ is not diagonal in the occupation number basis defined by the $d_{\alpha}^\dagger$, the calculation of $\text{Tr}_d\left[e^{-\beta H_{\text{loc}}}T \prod_{\alpha} d_{\alpha}(\tau_{n_{\alpha}})d_{\alpha}^\dagger(\tau_{n_{\alpha}}')\ldots d_{\sigma}(\tau_{1}^\sigma)d_{\alpha}^\dagger(\tau_{1}^\alpha)\right]$ becomes more involved. We now have to compute the trace explicitly in some basis of $H_{\text{loc}}$ – for example the eigenbasis, in which the time evolution operators $e^{-H_{\text{loc}}\tau}$ become diagonal. The operators $d_{\alpha}$ and $d_{\alpha}^\dagger$ are expressed as matrices in this eigenbasis, and the evaluation of the trace factor thus involves the multiplication of matrices whose size is equal the size of the Hilbert space of $H_{\text{loc}}$. Since the dimension of the Hilbert space grows exponentially with the number of flavors, the calculation of the trace factor becomes the computational bottleneck of the simulation, and the matrix formalism is therefore restricted to a relatively small number of flavors (up to about 10).

An important point is the use of conserved quantum numbers (typically particle number for spin up and spin down, momentum, . . .). If the eigenstates of $H_{\text{loc}}$ are grouped according to these quantum numbers, the operator matrices will acquire a sparse block structure, because for example $d_{\uparrow,q}^\dagger$ will connect the states corresponding to quantum numbers $m = \{n_{\uparrow}, n_{\downarrow}, K\}$ to those corresponding to $m' = \{n_{\uparrow} + 1, n_{\downarrow}, K + q\}$ (if they exist). Checking the compatibility of the operator sequence with a given starting block furthermore allows one to find the (potentially) contributing quantum number sectors without any matrix multiplications. The evaluation of the trace is thus reduced to a block matrix multiplication of the form

$$\sum_{\text{contr.}m} \text{Tr}_m \left[\ldots (O)_{m''m'}(e^{-(\tau''-\tau')H_{\text{loc}}})_{m''m'}(O)_{m'm}(e^{-\tau H_{\text{loc}}})_{m}\right],$$

where $O$ is either a creation or annihilation operator, $m$ denotes the index of the matrix block, and the sum runs over those sectors which are compatible with the operator sequence.
VI. INFINITE-U LIMIT: KONDO MODEL

In the limit of very strong interaction, the half-filled AIM model cannot be simulated efficiently using the weak or strong coupling continuous-time Monte Carlo solvers. The weak-coupling approach is not suitable because the perturbation order becomes very large, while in the strong-coupling simulation, hybridization events correspond to transitions into doubly occupied or empty states with very high energy. While transitions into states with occupancy different from one can still be accepted, as long as the excursion is very short, and the strong-coupling code can in principle handle arbitrarily short “segments” or “anti-segments”, it is more appropriate and more efficient to project out the charge fluctuations and consider a low-energy effective model in which the singly occupied impurity (represented by a spin $S = 1/2$) exchanges spin with the bath. This projection is called “Schrieffer-Wolf” transformation and leads to the Kondo-Hamiltonian

$$H = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + JS \cdot \psi^\dagger c \bar{\sigma} \psi_c.$$

(64)

Here, $J$ is the exchange parameter of order $V^2 / U$ and $\psi^\dagger_c = (c_{0,\uparrow}^\dagger, c_{0,\downarrow}^\dagger)$, where $c_0$ is the first bath site in a chain representation of the impurity (see Fig. 5). To solve this model, we have to compute the Green function of the bath at site 0. The green function of the impurity is then given by the $T$-matrix of the bath, as can be shown using equations of motion. In the following sections we will discuss two complementary continuous-time solvers, a weak-coupling approach based on an expansion in powers of $J$ and a strong-coupling approach based on an expansion in powers of the hybridization between site 0 and the rest of the bath.

A. Weak-coupling approach

In the weak-coupling simulation, we fermionize the spin $S$ by introducing annihilation operators $f_\sigma$ and writing

$$S = \frac{1}{2} \psi^\dagger f \bar{\sigma} \psi_f,$$

(65)

with $\psi^\dagger_f = (f_{\uparrow}^\dagger, f_{\downarrow}^\dagger)$. The Hamiltonian (64) may then be written in the form

$$H = \sum_k \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + J \left[ S_z (c_{\uparrow}^\dagger c_{\uparrow} - c_{\downarrow}^\dagger c_{\downarrow}) + S^+ c_{\uparrow}^\dagger c_{\uparrow} + S^- c_{\downarrow}^\dagger c_{\downarrow} \right],$$

(66)
FIG. 5: Chain representation of the quantum impurity model in the Kondo limit. The impurity states are restricted to the singly occupied states $|\uparrow\rangle$ and $|\downarrow\rangle$. This spin-1/2 degree of freedom couples via $J$ to the spin $\vec{S} = \psi_0^\dagger \vec{\sigma} \psi_c$ on lattice site 0, represented in the figure by the first site of the chain.

With $S^+ = f_\uparrow^\dagger f_\uparrow$, $S^- = f_\downarrow^\dagger f_\downarrow$ and $S_z = \frac{1}{2}(f_\uparrow^\dagger f_\uparrow - f_\downarrow^\dagger f_\downarrow)$. Adding and subtracting a term $\frac{J}{2}(f_\uparrow^\dagger f_\uparrow + f_\downarrow^\dagger f_\downarrow)$ and using the constraint $f_\uparrow^\dagger f_\uparrow + f_\downarrow^\dagger f_\downarrow = 1$, we finally obtain

$$H = \sum_k \epsilon_k c_\uparrow^\dagger k c_\downarrow - \frac{J}{2} \sum_\sigma c_{0,\sigma}^\dagger c_{0,\sigma} + J \sum_{\sigma\sigma'} f_\uparrow^\dagger \sigma f_\downarrow^\dagger c_\sigma^\dagger c_\sigma. \tag{67}$$

We may now split the Hamiltonian into the exactly solved part $H_1 = \sum_k \epsilon_k c_\uparrow^\dagger k c_\downarrow - \frac{J}{2} \sum_\sigma c_{0,\sigma}^\dagger c_{0,\sigma}$ and expand the partition function into powers of $H_2 = J \sum_{\sigma\sigma'} f_\uparrow^\dagger \sigma f_\downarrow^\dagger c_\sigma^\dagger c_\sigma$. The trace over the fermionic degrees of freedom then yields the weight of the Monte Carlo configuration,

$$w = (-Jd\tau)^k Tr_f \left[ T f_\sigma^\dagger (\tau_1) f_\sigma^\dagger (\tau_1) \cdots f_\sigma^\dagger (\tau_k) f_\sigma^\dagger (\tau_k) \right]$$

$$\times \prod_\sigma \frac{1}{Z_c} Tr_c \left[ T c_\sigma^\dagger (\tau_1') c_\sigma (\tau_1') \cdots c_\sigma^\dagger (\tau_k') c_\sigma (\tau_k') \right] s, \tag{68}$$

with $0 < \tau_1 < \ldots < \tau_k < \beta$ the $H_2$-operator positions, $0 < \tau_1' < \ldots < \tau_k' < \beta$ the locations of the bath creation operators, $0 < \tau_1'' < \ldots < \tau_k'' < \beta$ the locations of the bath annihilation operators ($\sum_\sigma k_\sigma = k$), $s$ a permutation sign associated with the separation of the spin up and down operators and the grouping into pairs of creation/annihilation operators, and $Z_c$ the partition function for $H_1$.

While the trace over the $f$-states imposes a constraint on which type of operators can be inserted (either “diagonal operators” $c_\sigma^\dagger c_\sigma$ with $\sigma$ identical to the spin of the $f$-fermion, or pairs of spin flip operators $c_{\uparrow}^\dagger c_\downarrow$ or $c_{\downarrow}^\dagger c_\uparrow$), the trace over the $c$-states results in a product of determinants of two matrices $\det M_\uparrow \det M_\downarrow$. Due to the scattering term in Eq. (67), the elements of these matrices are given by noninteracting Green functions $\tilde{G}_{0,\sigma}$ which are
FIG. 6: Monte Carlo configuration corresponding to four off-diagonal and six diagonal operators. The upper two lines represent the time evolution of the $f$-states with $\sigma = \uparrow, \downarrow$ (i.e. of the orientation of the spin $S$). Full circles represent creation operators and empty circle annihilation operators. The sequence of $c_0$ creation and annihilation operators for spin up and down is shown on the lower two lines (full and empty squares). A diagonal operator $c_\sigma^\dagger(\tau)c_\sigma(\tau)$ can only be inserted if the spin $S$ is in state $\sigma$.

related to the bath Green functions $G_{0,\sigma}$ by

$$\tilde{G}_{0,\sigma}(i\omega_n) = \frac{G_{0,\sigma}(i\omega_n)}{1 + \frac{J_0^2}{2}G_{0,\sigma}(i\omega_n)}.$$  

(69)

Specifically, $(M_\sigma)_{ij} = \tilde{G}_{0,\sigma}(\tau_i'' - \tau_j)$.

A possible sequence of operators is shown in Fig. 6, where the upper two time lines represent the evolution of the spin, and the lower two time lines the sequence of bath creation and annihilation operators. Creation and annihilation operators are represented by full and empty squares, respectively. Half-full squares correspond to diagonal operators $c_\sigma^\dagger(\tau)c_\sigma(\tau)$, whose $\sigma$ must be identical to the spin represented by the $f$-lines.

The Monte Carlo sampling proceeds via insertion and removal of pairs of spin flips (vertical dashed lines in Fig. 6), and via insertion and removal of diagonal operators. The spin flip updates are analogous to the segment configuration updates discussed in Sec. V A. We can pick a random time for the first spin flip and define an interval $l_{\text{max}}$ up to the next operator (which may be a diagonal operator or a spin-flip event). The second spin flip is then chosen on a random point on this interval. The removal of a pair of adjacent spin-flips is only possible if there is no diagonal operator in between. The diagonal operators can be inserted and removed individually, but the insertion is only possible if their spin is compatible with
the state of the \( f \)-line.

The measurement of the bath Green’s function in the localized orbital 0 on the other hand, works as described in the weak-coupling Sec. IV C. This measurement amounts to the accumulation of the \( t \)-matrix

\[
\tilde{t}_\sigma(i\omega_n) = \left\langle -\frac{1}{\beta} \sum_{k,l} e^{i\omega_n(\tau_k - \tau_l)} [M_{\sigma}]_{kl} \right\rangle, \tag{70}
\]

where the tilde reminds us that this \( t \)-matrix is computed with respect to \( \tilde{G}_0 \), and is related to the Green function \( G \) and the true \( t \)-matrix by

\[
G_{\sigma}(i\omega_n) = \tilde{G}_{0,\sigma}(i\omega_n) + \tilde{G}_{0,\sigma}(i\omega_n)\tilde{t}_\sigma(i\omega_n)\tilde{G}_{0,\sigma}(i\omega_n) \nonumber \nonumber
\]

\[
= G_{0,\sigma}(i\omega_n) + G_{0,\sigma}(i\omega_n)t_\sigma(i\omega_n)G_{0,\sigma}(i\omega_n). \tag{71}
\]

Hence, the \( t \)-matrix of the bath is obtained from Eq. (70) as

\[
t_\sigma(i\omega_n) = \frac{-J}{2} \frac{\tilde{t}_\sigma(i\omega_n)}{1 + \frac{J}{2}G_{0,\sigma}(i\omega_n)(1 + \frac{1}{2}G_{0,\sigma}(i\omega_n))^2}. \tag{72}
\]

Using equations of motion, one can show that \( t_\sigma(i\omega_n) \) directly yields the impurity Green function.

**B. Strong-coupling approach**

The model (64) may also be simulated efficiently using the strong-coupling method discussed in Sec. V. In this approach, the local part of the Hamiltonian,

\[
H_{\text{loc}} = -\mu \sum_\sigma c_{0,\sigma}^\dagger c_{0,\sigma} + J\vec{S} \cdot \frac{1}{2} \psi_c^\dagger \vec{\sigma} \psi_c. \tag{73}
\]

is treated exactly and the partition function is expanded in powers of the hoppings from and to the localized orbital 0 of the \( c \)-electrons (parameter \( V \) in Fig. 5).

\( H_{\text{loc}} \) can be diagonalized in a basis labeled by the total number of electrons, the total spin and the \( z \)-component of the total spin. If the particle number is 0 or 2, then the spin state is determined by the state of the local moment, if the number is 1, the spin state is singlet (\( S \)) or triplet (\( T_{m_z} \)) with \( m_z = 1, 0 \) or \(-1 \). The eigenstates may thus be labeled as shown in Tab. I, where the first entry is the number of electrons and the second entry refers to the spin state. The singlet state is defined as \( S = \frac{1}{\sqrt{2}}(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) \), with the first entry
<table>
<thead>
<tr>
<th>Eigenstates</th>
<th>Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>(</td>
<td>1\rangle =</td>
</tr>
<tr>
<td>(</td>
<td>2\rangle =</td>
</tr>
<tr>
<td>(</td>
<td>3\rangle =</td>
</tr>
<tr>
<td>(</td>
<td>4\rangle =</td>
</tr>
<tr>
<td>(</td>
<td>5\rangle =</td>
</tr>
<tr>
<td>(</td>
<td>6\rangle =</td>
</tr>
<tr>
<td>(</td>
<td>7\rangle =</td>
</tr>
<tr>
<td>(</td>
<td>8\rangle =</td>
</tr>
</tbody>
</table>

TABLE I: Eigenstates and eigenenergies for the local part of the Kondo lattice hamiltonian. The first entry labels the number of electrons and the second entry the spin state: either impurity spin \(↑, ↓\) if the number of electrons is 0 or 2 or the total spin \(S\) (singlet) \(T_{m}\) (triplet with \(m_z = m\)) if \(n = 1\).

the conduction electron and the second entry the local moment spin direction. In this basis, the time evolution operator is diagonal, \(K(\tau)|n\rangle = \exp(-E_n\tau)|n\rangle\), with eigenenergies \(E_n\) listed in Tab. I. The creation operators for spin up and down become the sparse matrices

\[
c_{\uparrow} = \begin{pmatrix} 0 & 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \end{pmatrix}, \tag{74}
\]
The block structure corresponding to the conservation of the total number of electrons is indicated by horizontal and vertical lines. With these operators, the sampling then proceeds as described in Sec. V C and the measurement procedure for the bath Green function will be identical to that described in Sec. V B. The $t^{-1}$-matrix for the bath is finally extracted from

$$G_{\sigma}(i\omega_n) = G_{0,\sigma}(i\omega_n) + G_{0,\sigma}(i\omega_n)t_{\sigma}(i\omega_n)G_{0,\sigma}(i\omega_n),$$

with $G_{0,\sigma}(i\omega_n)$ defined in Eq. (14), and yields the impurity Green’s function.

While the weak-coupling approach is efficient in the regime of small $J$, the strong-coupling approach can easily capture the singlet-formation occurring at larger $J$. 

$$c_{\downarrow}^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}. \quad (75)$$