Guide for imaginary-time DMFT via Fishman-White

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Analytical background and context

We want to solve the Anderson impurity model given by the Hamiltonian:

$$\hat{H} = \hat{H}_{\text{imp}} + \sum_{k,\sigma} \epsilon_k \hat{c}^\dagger_{k,\sigma} \hat{c}_{k,\sigma} + \sum_{k,\sigma} \big(t_k \hat{d}^\dagger_\sigma \hat{c}_{k,\sigma} + h.c. \big), \tag{1}$$

with $\hat{H}_{\text{imp}} = \sum_\sigma \epsilon_{d,\sigma} \hat{d}^\dagger_\sigma \hat{d}_\sigma + U \hat{d}^\dagger_\uparrow \hat{d}_\uparrow \hat{d}^\dagger_\downarrow \hat{d}_\downarrow$.

The thermal expectation value of a local impurity-operator, $\langle \hat{O}_2(\tau) \hat{O}_1(0) \rangle_\beta$, can be expressed as a path integral over Grassmann variables of both the impurity and the bath fermions. After performing the Gaussian integral over the bath variables, the resulting path integral reads

$$\begin{aligned} \langle \hat{O}_2(\tau^*) \hat{O}_1(0) \rangle_\beta &= \frac{1}{Z} \int d(\bar{\eta}, \eta)\, \mathcal{O}_2[\bar{\eta}_{\sigma,\tau^*}, \eta_{\sigma,\tau^*}]\, \mathcal{O}_1[\bar{\eta}_{\sigma,0}, \eta_{\sigma,0}] \\ &\times \exp\Big[- \int_0^\beta d\tau \big(\sum_\sigma \bar{\eta}_{\sigma,\tau} \partial_\tau \eta_{\sigma,\tau} + \mathcal{H}_{\text{imp}}[\{\bar{\eta}_{\uparrow,\tau}, \bar{\eta}_{\downarrow,\tau}, \eta_{\uparrow,\tau}, \eta_{\downarrow,\tau}\}] \big) - \sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' \bar{\eta}_{\sigma,\tau} \Delta(\tau,\tau') \eta_{\sigma,\tau'} \Big], \end{aligned} \tag{2}$$

where Z is the partition sum that is computed by evaluating the path integral in Eq. (2) with the impurity operator set to identity. The effective action contains the time-local impurity action as well as the time-non-local function Δ, which is just the standard hybrization function of the impurity level.

Our goal is to compute this expectation value by rewriting Eq. (2) as an overlap of wavefunctions in the temporal domain. For this, we note that the textbook expression in Eq. (2) is defined as the limit $M \to \infty$ of a discrete-time expression, obtained by dividing the imaginary-time interval $[0, \beta]$ into M steps of size $\delta\tau = \beta/M$; we fix a sufficiently large M. The time τ^* coincides now with some point τ_n on the imaginary-time lattice.

Successive evolution of impurity and bath: $\hat{U} = \hat{U}_{\text{imp}} \cdot \hat{U}_{\text{hyb}}$

First, let us consider a trottzerization with successive evolution of bath and impurity. In this case, we can write the evolution operator as $\hat{U} = \hat{U}_{\text{imp}} \cdot \hat{U}_{\text{hyb}}$, where $\hat{U}_{\text{imp}} = \exp\big(- \delta\tau H_{\text{imp}} \big)$ and $\hat{U}_{\text{hyb}}$ encodes the bath evolution as well as the hopping between impurity and bath. Next, a number of formal manipulations of the path integral allow us to rewrite Eq. (2) in the form:

$$\boxed{\langle \hat{O}_2(\tau_n)\, \hat{O}_1(0) \rangle = \frac{1}{Z} \int d(\bar{\boldsymbol{\eta}}, \boldsymbol{\eta})\, \mathcal{I}[\{\boldsymbol{\eta}_\downarrow\}] e^{-\bar{\boldsymbol{\eta}}_\downarrow \boldsymbol{\eta}_\downarrow} \mathcal{D}_n^{\hat{O}_1, \hat{O}_2}[\bar{\boldsymbol{\eta}}_\downarrow, \boldsymbol{\eta}_\uparrow] e^{-\bar{\boldsymbol{\eta}}_\uparrow \boldsymbol{\eta}_\uparrow} \mathcal{I}[\{\bar{\boldsymbol{\eta}}_\uparrow\}] = \langle \mathcal{I}_\downarrow |\, \hat{D}_n^{\hat{O}_1, \hat{O}_2}\, | \mathcal{I}_\uparrow \rangle\,,} \tag{3}$$

where

$$\boldsymbol{\eta}_\sigma \equiv (\eta_{\sigma,0}, \eta_{\sigma,1/2}, \ldots, \eta_{\sigma,M-1/2}),\ \bar{\boldsymbol{\eta}}_\sigma \equiv (\bar{\eta}_{\sigma,M}, \bar{\eta}_{\sigma,1/2}, \ldots, \bar{\eta}_{\sigma,M-1/2}) \tag{4}$$

$$d(\bar{\boldsymbol{\eta}}, \boldsymbol{\eta}) \equiv \prod_\sigma d\bar{\eta}_{\sigma,M} d\eta_{\sigma,0}\, d\bar{\eta}_{\sigma,1/2}\, d\eta_{\sigma,1/2} \prod_{m=1}^{M-1} d\bar{\eta}_{\sigma,m}\, d\eta_{\sigma,m} d\bar{\eta}_{\sigma,m+1/2}\, d\eta_{\sigma,m+1/2}, \tag{5}$$

$$\begin{aligned} \mathcal{D}_n^{\hat{O}_1, \hat{O}_2}[\bar{\boldsymbol{\eta}}_\downarrow, \boldsymbol{\eta}_\uparrow] = \prod_{\substack{m=1 \\ m \neq n}}^{M-1} \exp\Big[- \Big(\eta_{\uparrow,m} \eta_{\uparrow,m-1/2} + \bar{\eta}_{\downarrow,m} \bar{\eta}_{\downarrow,m-1/2} + \delta\tau \mathcal{H}_{\text{imp}}[\{-\eta_{\uparrow,m}, \eta_{\uparrow,m-1/2}, \bar{\eta}_{\downarrow,m}, -\bar{\eta}_{\downarrow,m-1/2}\}] \Big) \Big] \\ \times \tilde{\mathcal{O}}_2[-\eta_{\uparrow,n}, \eta_{\uparrow,n-1/2}, \bar{\eta}_{\downarrow,n}, -\bar{\eta}_{\downarrow,n-1/2}]\, \tilde{\mathcal{O}}_1[\eta_{\uparrow,M}, \eta_{\uparrow,M-1/2}, -\bar{\eta}_{\downarrow,M}, -\bar{\eta}_{\downarrow,M-1/2}], \end{aligned} \tag{6}$$

where $\tilde{\mathcal{O}}_{1,2}$ are the combined kernels of the operator $\hat{O}_{1,2}$ and the evolution gate at the corresponding time, respectively.

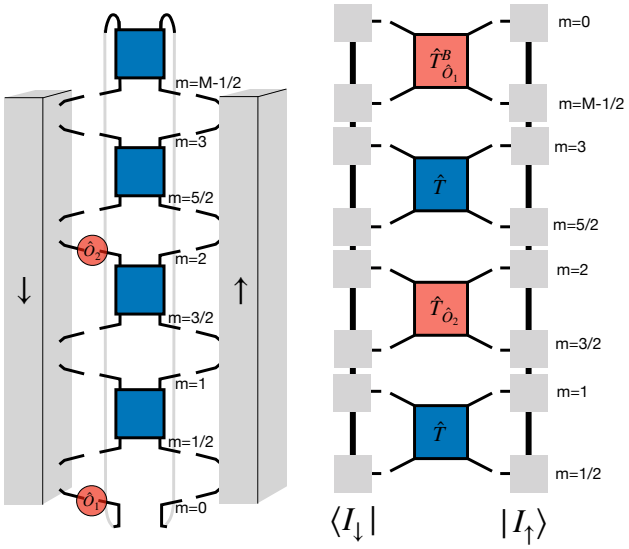

Figure 1: For successive evolution of bath and impurity: Illustration of $\langle \hat{O}_2(\tau_n)\hat{O}_1(0)\rangle_\beta$, here shown for a discretization into $M = 4$ intervals and $n = 2$. Left: The path integral expression, Eq. (2), where the hybridization part of the effective action is encoded in two influence "vectors", associated with the two spin species, respectively. These are correlated Gaussian fermionic wavefunctions in the imaginary-time lattice. Right: After performing analytical manipulations on the level of the path integral, the expectation value can be rewritten as an overlap. We compute this overlap as a standard tensor contraction between the influence vectors (transformed to MPS form) and the local impurity action (naturally a product operator).

Moreover, we have defined the imaginary-time influence functional:

$$\mathcal{I}[\{\boldsymbol{\eta}\}] \equiv \exp\Big[-(\delta\tau)^2 \sum_{m,n=0}^{M-1} \eta_{m+1/2}\Delta_{m,n}\eta_n + \sum_{m=0}^{M-1} \eta_{m+1/2}\eta_m\Big]. \tag{7}$$

As stated by the last equality in Eq. (3), the manipulated path integral can be directly read off as a sandwich between states and operator in the time domain. Indeed, note that the barred and non-barred variables have been suitably renamed to make this sandwich expression manifest. Our goal is to compactly represent such states and operator as MPSs and MPO, respectively, and hence to compute the sandwich via a standard tensor contraction. Notice that the normalization of $|I\rangle$ cancels out when dividing by Z, so we can tacitly assume the state to be normalized by $\sqrt{Z}$ and drop the denominator.

Determining the ingredients

The influence vector is uniquely determined by Eq. (7), and can be abstractly written in the form $\mathcal{I}[\{\boldsymbol{\eta}\}] = \exp\left(\boldsymbol{\eta}^T\mathcal{G}\boldsymbol{\eta}\right)$ where $\mathcal{G}$ is an antisymmetric matrix. The mapping from Grassman function to many-fermion wavefunction works by straightforward replacement of Grassman variables with corresponding creation operators on the vacuum. Thus, a Gaussian Grassmann function $\mathcal{I}[\{\boldsymbol{\eta}\}] = \exp\left(\boldsymbol{\eta}^T\mathcal{G}\boldsymbol{\eta}\right)$ can be straightforwardly associated with a Gaussian, BCS-type many-body wavefunction

$$|I\rangle = \exp\left(\boldsymbol{c}^{\dagger\,T}\mathcal{G}\boldsymbol{c}^\dagger\right)|\emptyset\rangle\,, \quad \boldsymbol{c}^\dagger = (c_0^\dagger, c_{1/2}^\dagger, c_1^\dagger, \ldots, c_{M-1/2}^\dagger). \tag{8}$$

Such a many-body wavefunction is entirely determined by its correlation matrix, which is the object we feed into the Fishman-White algorithm to construct a MPS form of $|I_\uparrow\rangle$. Note that because of our choice of conventions above, $\langle I_\downarrow|$ is represented by the transposed vector (no complex conjugation), hence literally the same MPS. Also note that the two sublattices (integer and half-integer indices) correspond to the barred and non-barred Grassman variables in the original path integral expression in Eq. (2), before the series of formal manipulations leading to Eq. (3). Number conservation in the original problem maps to a sublattice

symmetry in this formulation.

The final ingredient is the operator $\hat{D}_n^{\hat{O}_1,\hat{O}_2}$ which corresponds to the Grassmann kernel $\mathcal{D}_n^{\hat{O}_1,\hat{O}_2}$ in Eq. (6) and acts on the many-body Fock space in the temporal domain. Since the impurity action in Eq. (6) is local in time, the operator $\hat{D}_n^{\hat{O}_1,\hat{O}_2}$ is a product operator:

$$\hat{D}_n^{\hat{O}_1,\hat{O}_2} = \underbrace{\hat{T}\otimes\ldots\otimes\hat{T}}_{(n-1)\text{ times}}\otimes\hat{T}_{\hat{O}_2}\otimes\underbrace{\hat{T}\otimes\ldots\otimes\hat{T}}_{(M-n-1)\text{ times}}\otimes\hat{T}^B_{\hat{O}_1}. \tag{9}$$

With reference to Fig. 1, here each $\hat{T}$ is the "temporal-domain-version" of the impurity evolution operator $e^{-\delta\tau H_{\text{imp}}}$, acting between a "↑" two-fermion space (originally corresponding to the tensor product of input and output Hilbert spaces of the ↑ impurity fermion) and a "↓" two-fermion space (originally corresponding to the tensor product of input and output Hilbert spaces of the ↓ impurity fermion). $\hat{T}_{\hat{O}_2}$ is the "temporal-domain-version" of the impurity evolution operator including the observable operator $\hat{O}_2$. Finally, $\hat{T}^B_{\hat{O}_1}$ is the same for the observable $\hat{O}_1$ up to a slight modification to take into account the antiperiodic boundary conditions.

Derivation of the Local Impurity Kernels

Let us give this correspondence between a general operator $\hat{A}$ (e.g. the impurity evolution operator) and its "temporal-domain-version" $\hat{T}$ (explicit expression for SIAM below):

$$\hat{A} = \begin{pmatrix} |\emptyset\rangle \\ c_\uparrow^\dagger|\emptyset\rangle \\ c_\downarrow^\dagger|\emptyset\rangle \\ c_\downarrow^\dagger c_\uparrow^\dagger|\emptyset\rangle \end{pmatrix}^T \underbrace{\begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{pmatrix}}_{A} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset|c_\uparrow \\ \langle\emptyset|c_\downarrow \\ \langle\emptyset|c_\uparrow c_\downarrow \end{pmatrix}. \tag{10}$$

The Grassmann kernel of this operator can be written as:

$$\mathcal{A} = \begin{pmatrix} 1 \\ \bar{\eta}_\uparrow \\ \bar{\eta}_\downarrow \\ \bar{\eta}_\downarrow\bar{\eta}_\uparrow \end{pmatrix}^T \begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} 1 \\ \eta_\uparrow \\ \eta_\downarrow \\ \eta_\uparrow\eta_\downarrow \end{pmatrix} = \begin{pmatrix} 1 \\ \bar{\eta}_\downarrow \\ \eta_\downarrow \\ \bar{\eta}_\downarrow\eta_\downarrow \end{pmatrix}^T \begin{pmatrix} a_{00} & a_{10} & a_{01} & a_{11} \\ a_{20} & a_{30} & a_{21} & a_{31} \\ a_{02} & -a_{12} & -a_{03} & a_{13} \\ a_{22} & -a_{32} & -a_{23} & a_{33} \end{pmatrix} \begin{pmatrix} 1 \\ \bar{\eta}_\uparrow \\ \eta_\uparrow \\ \bar{\eta}_\uparrow\eta_\uparrow \end{pmatrix}, \tag{11}$$

where we just reordered the entries and kept track of the variable ordering which introduces some minus signs.

Next, we note that the variable substitutions needed for the overlap form of the path integral introduce minus signs to the outgoing up-fermions and to the ingoing down-fermions,

$$\bar{\eta}_\uparrow \to -\eta_m \tag{12}$$
$$\eta_\uparrow \to \eta_{m-1/2} \tag{13}$$
$$\bar{\eta}_\downarrow \to \bar{\eta}_m \tag{14}$$
$$\eta_\downarrow \to -\bar{\eta}_{m-1/2}. \tag{15}$$

Note that it is safe to drop the spin index since, after the substitution, all "barred" variables corresponding to spin down and all "non-barred" variables correspond to spin up. The previous role of the bars to indicate the in- or outgoing nature of the variable is now taken over by the indices $m-1/2$ and m, respectively.

Absorbing the signs from this substitution into the kernel yields:

$$\mathcal{A} \to \mathcal{A}_m = \begin{pmatrix} 1 \\ \bar{\eta}_m \\ \bar{\eta}_{m-1/2} \\ \bar{\eta}_m\bar{\eta}_{m-1/2} \end{pmatrix}^T \begin{pmatrix} a_{00} & -a_{10} & a_{01} & -a_{11} \\ a_{20} & -a_{30} & a_{21} & -a_{31} \\ -a_{02} & -a_{12} & a_{03} & a_{13} \\ -a_{22} & -a_{32} & a_{23} & a_{33} \end{pmatrix} \begin{pmatrix} 1 \\ \eta_m \\ \eta_{m-1/2} \\ \eta_m\eta_{m-1/2} \end{pmatrix}, \tag{16}$$

for the kernel connecting the in- and outgoing variables at time points $(m-1/2)$ and m, respectively.

Next, we must take care of the signs that are related to the global string of Grassmann variables.

Multiplying out the impurity kernels,

$$\mathcal{A}_M \cdot \mathcal{A}_{M-1} \cdot \ldots \cdot \mathcal{A}_{m=1}, \tag{17}$$

yields a sum of Grassmann monomials. For illustration, let's consider an explicit term as an example. Since the influence functional is even in Grassmann fermions, only terms with an even number of variables of each spin species are allowed in the impurity gates as well. Let's consider the allowed term:

$$\alpha \bar{\eta}_5 \bar{\eta}_{5-1/2} \eta_4 \, \bar{\eta}_{3-1/2} \, \eta_{3-1/2} \, \bar{\eta}_{2-1/2} \, \eta_2 \, \eta_{2-1/2} \, \bar{\eta}_1 \, \bar{\eta}_{1/2}. \tag{18}$$

This term is associated with *some* coefficient, α.
In order for us to represent the path integral as an overlap,

$$Z \propto \langle I | \, \hat{D}_n^{\hat{O}_1, \hat{O}_2} \, | I \rangle \, , \tag{19}$$

we need to convert each monomial as in Eq. (18) to an operator in the many-body basis. The ordering of the fermions in the many-body basis must be consistent with the fermion ordering in the state $|I\rangle$. Here, we choose the convention, that the fermions are arranged in ascending order, i.e. $|I\rangle$ consists of terms that are of the form:

$$|I\rangle \leftrightarrow c_i^\dagger c_j^\dagger \ldots c_k^\dagger \, |\emptyset\rangle \, , \tag{20}$$

with $i < j < k$. Importantly, we define $\langle I|$ with the variable ordering:

$$\langle I| \leftrightarrow \langle \emptyset| \, c_i c_j \ldots c_k, \tag{21}$$

with $i < j < k$ as before. Only in this way, the "bra", $\langle I| \, ,$ and "ket", $|I\rangle \, ,$ are represented by *exactly* the same MPS.

Our task is thus to bring each impurity monomial as the one in Eq. (18) into the order:

$$\bar{\eta}_l \, \bar{\eta}_m \, \bar{\eta}_n \eta_p \, \eta_q \, \eta_r, \text{ with } l > m > n \text{ and with } p > q > r. \tag{22}$$

The indices l, m, n are independent of the indices p, q, r.
In summary: The fermions in $|I\rangle$ are arranged in ascending order for each spin species individually, while the fermions in the impurity operator are arranged in descending order for each spin species individually.

Now, we derive the sign that is associated with rearranging the variables in a monomial as in Eq. (18). First, we successively bring all "barred" variables from each local gate to the leftmost position of the Grassmann string. We start with the variable $\bar{\eta}_{3-1/2}$

$$\alpha \underbrace{\bar{\eta}_5 \bar{\eta}_{5-1/2} \eta_4}_{*} \, \bar{\eta}_{3-1/2} \, \eta_{3-1/2} \, \bar{\eta}_{2-1/2} \, \eta_2 \, \eta_{2-1/2} \, \bar{\eta}_1 \, \bar{\eta}_{1/2} = -\alpha \, \bar{\eta}_{3-1/2} \, \bar{\eta}_5 \bar{\eta}_{5-1/2} \eta_4 \, \eta_{3-1/2} \, \bar{\eta}_{2-1/2} \, \eta_2 \, \eta_{2-1/2} \, \bar{\eta}_1 \, \bar{\eta}_{1/2}. \tag{23}$$

Note that we pick up a sign here since the term marked by a star is odd in Grassmann variables so any Grassmann variable (or any odd string of Grassmann variables) anticommutes with it. We call this **Rule 1**: Whenever we bring a single variable (or any odd string of Grassmann variables) to the very left of the global string, we must take into account the parity of the part of the string left from it.

Next, we move the variable $\bar{\eta}_{2-1/2}$ to the very left of the monomial:

$$-\alpha \underbrace{\bar{\eta}_{3-1/2} \, \bar{\eta}_5 \bar{\eta}_{5-1/2} \eta_4 \, \eta_{3-1/2}}_{*} \, \bar{\eta}_{2-1/2} \, \eta_2 \, \eta_{2-1/2} \, \bar{\eta}_1 \, \bar{\eta}_{1/2} = +\alpha \, \bar{\eta}_{2-1/2} \, \bar{\eta}_{3-1/2} \, \bar{\eta}_5 \bar{\eta}_{5-1/2} \eta_4 \, \eta_{3-1/2} \, \eta_2 \, \eta_{2-1/2} \, \bar{\eta}_1 \, \bar{\eta}_{1/2}. \tag{24}$$

By Rule 1, we pick up a minus sign again because the sub-string marked with a star contains an odd number of Grassmann variables.
We repeat the procedure one more time to bring the variable pair $\bar{\eta}_1\,\bar{\eta}_{1/2}$ to the left most position:

$$+\alpha\,\underbrace{\bar{\eta}_{2-1/2}\,\bar{\eta}_{3-1/2}\,\bar{\eta}_5\bar{\eta}_{5-1/2}\eta_4\,\eta_{3-1/2}\,\eta_2\,\eta_{2-1/2}}_{*}\,\bar{\eta}_1\,\bar{\eta}_{1/2} = +\alpha\,\bar{\eta}_1\,\bar{\eta}_{1/2}\,\bar{\eta}_{2-1/2}\,\bar{\eta}_{3-1/2}\,\bar{\eta}_5\bar{\eta}_{5-1/2}\eta_4\,\eta_{3-1/2}\,\eta_2\,\eta_{2-1/2}. \tag{25}$$

This time we don't pick up a sign as the term marked with a star is even in Grassmann variables, and anyways we commuted a *pair* of variables which commutes with everything.

We have achieved the first goal of separating the "barred" and "non-barred" variables.

Next, we need to order the "barred" and "non-barred" variables according to Eq. (22).

In fact, we notice that all "non-barred" variables are always automatically in the correct order due to the way we ordered the variables in Eq. (16). Hence, we need to only rearrange the "barred" variables.
We note that we can bring the "barred" string,

$$\bar{\eta}_1\,\bar{\eta}_{1/2}\,\bar{\eta}_{2-1/2}\,\bar{\eta}_{3-1/2}\,\bar{\eta}_5\bar{\eta}_{5-1/2}, \tag{26}$$

into the correct order by:

1. Reversing the ordering of variables that belong to the same local gate, e.g. $\bar{\eta}_5\bar{\eta}_{5-1/2} = -\bar{\eta}_{5-1/2}\bar{\eta}_5$. Here we pick up a minus sign for all terms where have two "barred" variables that correspond to the same local gate. We label this as **Rule 2.**
   Doing this for the two pairs $\bar{\eta}_1\,\bar{\eta}_{1/2}$ and $\bar{\eta}_5\bar{\eta}_{5-1/2}$ in our example leads to the "barred" part of the string:
   $$\bar{\eta}_1\,\bar{\eta}_{1/2}\,\bar{\eta}_{2-1/2}\,\bar{\eta}_{3-1/2}\,\bar{\eta}_5\bar{\eta}_{5-1/2} = (-1)^2\bar{\eta}_{1/2}\,\bar{\eta}_1\;\bar{\eta}_{2-1/2}\,\bar{\eta}_{3-1/2}\,\bar{\eta}_{5-1/2}\,\bar{\eta}_5. \tag{27}$$
2. Now, all there is left to do is reverse the entire "barred" string. We recall that only monomials with an even number of "barred" variables can contribute (because the Gaussian influence functional is even in Grassmann variables so all odd terms will vanish when computing the overlap). The global reversal of the "barred" string with n_{barred} variables comes thus with a minus sign if $mod_2(n_{\text{barred}}/2) = 1$ and with no sign if $mod_2(n_{\text{barred}}/2) = 0$.
   Since we do not want to keep track of the number of variables in every global term, we can use the trick of multiplying every "barred" variable with an imaginary factor i in each local gate. If $mod_2(n_{\text{barred}}/2) = 1$, i.e. $n_{\text{barred}} \in \{2, 6, 10, 14, ..\}$, the "barred" variables will thus combine to a factor of $i^{n_{\text{barred}}} = -1$ and if $mod_2(n_{\text{barred}}/2) = 0$, i.e. $n_{\text{barred}} \in \{4, 8, 12, ..\}$, we accumulate a factor $i^{n_{\text{barred}}} = +1$. This does precisely the job we want. We exploited that the IF is even in Grassmann variables in order to absorb the sign changing factors of imaginary i into the local gates. We call this **Rule 3**.

In our example, we have $n_{\text{barred}} = 6$ "barred" variables and thus pick up a factor of $i^6 = -1$.

Taken everything together, we hence arrive at the following sign for our example:

$$\alpha\bar{\eta}_5\bar{\eta}_{5-1/2}\eta_4\,\bar{\eta}_{3-1/2}\,\eta_{3-1/2}\,\bar{\eta}_{2-1/2}\,\eta_2\,\eta_{2-1/2}\,\bar{\eta}_1\,\bar{\eta}_{1/2} = -\alpha\,\bar{\eta}_5\,\bar{\eta}_{5-1/2}\,\bar{\eta}_{3-1/2}\,\bar{\eta}_{2-1/2}\,\bar{\eta}_1\,\bar{\eta}_{1/2}\eta_4\,\eta_{3-1/2}\,\eta_2\,\eta_{2-1/2}. \tag{28}$$

Note that this string is now in the order we specified in Eq. (22).
Importantly, we have now a precise set of rules that lets us determine the necessary sign changes in the *local* gates, such that the sign for each *global* string is generated correctly.

Let us first apply **Rule 1** to the local gates, Eq. (16), by defining a "string-variable" $\sigma = \pm 1$:

$$\mathcal{A}_m = \begin{pmatrix} 1 \\ \bar{\eta}_m \\ \bar{\eta}_{m-1/2} \\ \bar{\eta}_m\bar{\eta}_{m-1/2} \end{pmatrix}^T \begin{pmatrix} a_{00} & -a_{10} & a_{01} & -a_{11} \\ a_{20} & -a_{30} & a_{21} & -a_{31} \\ -a_{02} & -a_{12} & a_{03} & a_{13} \\ -a_{22} & -a_{32} & a_{23} & a_{33} \end{pmatrix} \begin{pmatrix} 1 \\ \eta_m \\ \eta_{m-1/2} \\ \eta_m\eta_{m-1/2} \end{pmatrix}$$
$$\xrightarrow{\text{Rule 1}} \begin{pmatrix} 1 \\ \bar{\eta}_m \\ \bar{\eta}_{m-1/2} \\ \bar{\eta}_m\bar{\eta}_{m-1/2} \end{pmatrix}^T \begin{pmatrix} a_{00} & -a_{10} & a_{01} & -a_{11} \\ \sigma a_{20} & -\sigma a_{30} & \sigma a_{21} & -\sigma a_{31} \\ -\sigma a_{02} & -\sigma a_{12} & \sigma a_{03} & \sigma a_{13} \\ -a_{22} & -a_{32} & a_{23} & a_{33} \end{pmatrix} \begin{pmatrix} 1 \\ \eta_m \\ \eta_{m-1/2} \\ \eta_m\eta_{m-1/2} \end{pmatrix}. \quad (29)$$

Here, $\sigma = 1$ if the string on the left of the gate at time m is even in Grassmanns and $\sigma = -1$ if it is odd in Grassmans. Since every gate in number-conserving models contains either only even Grassmann terms, e.g. as in the evolution gate $U = e^{-H_{\text{imp}}\delta\tau}$, or contains only odd terms, e.g. the operator $c_\uparrow^\dagger e^{-H_{\text{imp}}\delta\tau}$, the string-variable σ is always well defined for every local gate and just depends on where on the contour we insert odd operators.

Next, let's apply **Rule 2** and **Rule 3** to the gate from Eq. (29):

$$\mathcal{A}_m = \begin{pmatrix} 1 \\ \bar{\eta}_m \\ \bar{\eta}_{m-1/2} \\ \bar{\eta}_m\bar{\eta}_{m-1/2} \end{pmatrix}^T \begin{pmatrix} a_{00} & -a_{10} & a_{01} & -a_{11} \\ \sigma a_{20} & -\sigma a_{30} & \sigma a_{21} & -\sigma a_{31} \\ -\sigma a_{02} & -\sigma a_{12} & \sigma a_{03} & \sigma a_{13} \\ -a_{22} & -a_{32} & a_{23} & a_{33} \end{pmatrix} \begin{pmatrix} 1 \\ \eta_m \\ \eta_{m-1/2} \\ \eta_m\eta_{m-1/2} \end{pmatrix}$$
$$\xrightarrow{\text{Rule 2}} \begin{pmatrix} 1 \\ \bar{\eta}_m \\ \bar{\eta}_{m-1/2} \\ \bar{\eta}_m\bar{\eta}_{m-1/2} \end{pmatrix}^T \begin{pmatrix} a_{00} & -a_{10} & a_{01} & -a_{11} \\ \sigma a_{20} & -\sigma a_{30} & \sigma a_{21} & -\sigma a_{31} \\ -\sigma a_{02} & -\sigma a_{12} & \sigma a_{03} & \sigma a_{13} \\ +a_{22} & +a_{32} & -a_{23} & -a_{33} \end{pmatrix} \begin{pmatrix} 1 \\ \eta_m \\ \eta_{m-1/2} \\ \eta_m\eta_{m-1/2} \end{pmatrix}$$
$$\xrightarrow{\text{Rule 3}} \begin{pmatrix} 1 \\ \bar{\eta}_m \\ \bar{\eta}_{m-1/2} \\ \bar{\eta}_m\bar{\eta}_{m-1/2} \end{pmatrix}^T \begin{pmatrix} a_{00} & -a_{10} & a_{01} & -a_{11} \\ i\sigma a_{20} & -i\sigma a_{30} & i\sigma a_{21} & -i\sigma a_{31} \\ -i\sigma a_{02} & -i\sigma a_{12} & i\sigma a_{03} & i\sigma a_{13} \\ i^2 a_{22} & i^2 a_{32} & -i^2 a_{23} & -i^2 a_{33} \end{pmatrix} \begin{pmatrix} 1 \\ \eta_m \\ \eta_{m-1/2} \\ \eta_m\eta_{m-1/2} \end{pmatrix}$$
$$= \begin{pmatrix} 1 \\ \bar{\eta}_m \\ \bar{\eta}_{m-1/2} \\ \bar{\eta}_m\bar{\eta}_{m-1/2} \end{pmatrix}^T \begin{pmatrix} a_{00} & -a_{10} & a_{01} & -a_{11} \\ i\sigma a_{20} & -i\sigma a_{30} & i\sigma a_{21} & -i\sigma a_{31} \\ -i\sigma a_{02} & -i\sigma a_{12} & i\sigma a_{03} & i\sigma a_{13} \\ -a_{22} & -a_{32} & a_{23} & a_{33} \end{pmatrix} \begin{pmatrix} 1 \\ \eta_m \\ \eta_{m-1/2} \\ \eta_m\eta_{m-1/2} \end{pmatrix}. \quad (30)$$

This concludes the derivation. The main result for the construction of the gates from a conventional operator $\hat{A}$, Eq. (10), is thus:

$$\hat{A} = \begin{pmatrix} |\emptyset\rangle \\ c_\uparrow^\dagger |\emptyset\rangle \\ c_\downarrow^\dagger |\emptyset\rangle \\ c_\downarrow^\dagger c_\uparrow^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_\uparrow \\ \langle\emptyset| c_\downarrow \\ \langle\emptyset| c_\uparrow c_\downarrow \end{pmatrix}$$
$$\to \hat{T} = \begin{pmatrix} |\emptyset\rangle \\ c_m^\dagger |\emptyset\rangle \\ c_{m-1/2}^\dagger |\emptyset\rangle \\ c_m^\dagger c_{m-1/2}^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} a_{00} & -a_{10} & a_{01} & -a_{11} \\ i\sigma a_{20} & -i\sigma a_{30} & i\sigma a_{21} & -i\sigma a_{31} \\ -i\sigma a_{02} & -i\sigma a_{12} & i\sigma a_{03} & i\sigma a_{13} \\ -a_{22} & -a_{32} & a_{23} & a_{33} \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_m \\ \langle\emptyset| c_{m-1/2} \\ \langle\emptyset| c_m c_{m-1/2} \end{pmatrix} \quad (31)$$

We conclude this section by giving some explicit operators $\hat{A}$ (or more precisely, the coefficient A as

defined in Eq. (10)).

$$\hat{U}_{SIAM} = 1 + (e^{-\delta\tau\epsilon_\uparrow} - 1)n_\uparrow + (e^{-\delta\tau\epsilon_\downarrow} - 1)n_\downarrow + \Big[1 - e^{-\delta\tau\epsilon_\uparrow} - e^{-\delta\tau\epsilon_\downarrow} + e^{-\delta\tau(\epsilon_\uparrow+\epsilon_\downarrow+U)}\Big] n_\uparrow n_\downarrow \tag{32}$$

$$= |\emptyset\rangle\langle\emptyset| + e^{-\delta\tau\epsilon_\uparrow} c_\uparrow^\dagger |\emptyset\rangle\langle\emptyset| c_\uparrow + e^{-\delta\tau\epsilon_\downarrow} c_\downarrow^\dagger |\emptyset\rangle\langle\emptyset| c_\downarrow + e^{-\delta\tau(\epsilon_\uparrow+\epsilon_\downarrow+U)} c_\downarrow^\dagger c_\uparrow^\dagger |\emptyset\rangle\langle\emptyset| c_\uparrow c_\downarrow \tag{33}$$

$$\rightarrow A = \begin{pmatrix} 1 & 0 & 0 & e^{-\delta\tau\epsilon_\uparrow} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ e^{-\delta\tau\epsilon_\downarrow} & 0 & 0 & e^{-\delta(\epsilon_\uparrow+\epsilon_\downarrow+U)} \end{pmatrix}. \tag{34}$$

Applying e.g. the annihilation operator $c_\uparrow$ to this yields:

$$c_\uparrow \hat{U}_{SIAM} = e^{-\delta\tau\epsilon_\uparrow} |\emptyset\rangle\langle\emptyset| c_\uparrow - e^{-\delta(\epsilon_\uparrow+\epsilon_\downarrow+U)} c_\downarrow^\dagger |\emptyset\rangle\langle\emptyset| c_\uparrow c_\downarrow \tag{35}$$

$$\rightarrow A = \begin{pmatrix} 0 & e^{-\delta\tau\epsilon_\uparrow} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -e^{-\delta(\epsilon_\uparrow+\epsilon_\downarrow+U)} \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{36}$$

For the spin-hopping Hamiltonian, one has:

$$\hat{U}_{spinhop} = e^{-\delta\tau(tc_\uparrow^\dagger c_\downarrow + h.c.)} = 1 - \underbrace{\frac{2\tanh(\delta\tau t/2)}{1-\tanh^2(\delta\tau t/2)}}_{=\sinh(\delta\tau t)} (c_\uparrow^\dagger c_\downarrow + c_\downarrow^\dagger c_\uparrow) + \underbrace{\frac{\tanh(\delta\tau t/2)^2}{1-\tanh^2(\delta\tau t)}}_{=\sinh^2(\delta\tau t)} \Big[2(n_\uparrow + n_\downarrow) - 4n_\uparrow n_\downarrow\Big] \tag{37}$$

$$= 1 - \sinh(\delta\tau t)\Big(c_\uparrow^\dagger |\emptyset\rangle\langle\emptyset| c_\downarrow + c_\downarrow^\dagger |\emptyset\rangle\langle\emptyset| c_\uparrow\Big) \tag{38}$$

$$+ \underbrace{2\sinh^2(\delta\tau t/2) + 1)}_{=\cosh(\delta\tau t)} \Big(c_\uparrow^\dagger |\emptyset\rangle\langle\emptyset| c_\uparrow + c_\downarrow^\dagger |\emptyset\rangle\langle\emptyset| c_\downarrow\Big) \tag{39}$$

$$+ \underbrace{\Big(-4\sinh^2(\delta\tau t) + 1 + 4\sinh^2(\delta\tau t/2)\Big)}_{=1} c_\downarrow^\dagger c_\uparrow^\dagger |\emptyset\rangle\langle\emptyset| c_\uparrow c_\downarrow \tag{40}$$

$$\rightarrow A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cosh(\delta\tau t) & -\sinh(\delta\tau t) & 0 \\ 0 & -\sinh(\delta\tau t) & \cosh(\delta\tau t) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{41}$$

Again, one can now easily apply operators and evaluate the corresponding coefficients A. In order to obtain the impurity kernel, one simply applies Eq. (31) and directly obtains the result.

Recipe for the Anderson impurity model

The impurity evolution gate reads:

$$\hat{U} = \exp\Big(- \delta\tau(\epsilon_{d,\uparrow} n_\uparrow + \epsilon_{d,\downarrow} n_\downarrow) - \delta\tau U n_\uparrow n_\downarrow \Big).$$

This leads to the following effective fermionic operators in the temporal domain connecting times $(m-1/2, m)$:

$$\hat{T} = \begin{pmatrix} |\emptyset\rangle \\ c_m^\dagger |\emptyset\rangle \\ c_{m-1/2}^\dagger |\emptyset\rangle \\ c_m^\dagger c_{m-1/2}^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} 1 & 0 & 0 & -e^{-\delta\tau\epsilon_{d,\uparrow}} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -e^{-\delta\tau\epsilon_{d,\downarrow}} & 0 & 0 & e^{-\delta\tau(\epsilon_{d,\uparrow}+\epsilon_{d,\downarrow}+U)} \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_m \\ \langle\emptyset| c_{m-1/2} \\ \langle\emptyset| c_m c_{m-1/2} \end{pmatrix}. \tag{42}$$

The boundary operator reads:

$$\hat{T}^B = \begin{pmatrix} |\emptyset\rangle \\ c_m^\dagger |\emptyset\rangle \\ c_{m-1/2}^\dagger |\emptyset\rangle \\ c_m^\dagger c_{m-1/2}^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} 1 & 0 & 0 & e^{-\delta\tau\epsilon_{d,\uparrow}} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ e^{-\delta\tau\epsilon_{d,\downarrow}} & 0 & 0 & e^{-\delta\tau(\epsilon_{d,\uparrow}+\epsilon_{d,\downarrow}+U)} \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_m \\ \langle\emptyset| c_{m-1/2} \\ \langle\emptyset| c_m c_{m-1/2} \end{pmatrix}. \tag{43}$$

In the context of DMFT, we are usually interested in the propagator

$$G_\sigma(\tau_n) = \langle c_{\sigma,n} c_{\sigma,0}^\dagger \rangle_\beta. \tag{44}$$

For this, the effective temporal-domain operators for the observables, $\hat{O}_1 = c_\sigma^\dagger$, $\hat{O}_2 = c_\sigma$, read:

For $\sigma = \uparrow$:

$$\hat{T}_{c_{\uparrow,n}} = \begin{pmatrix} |\emptyset\rangle \\ c_m^\dagger |\emptyset\rangle \\ c_{m-1/2}^\dagger |\emptyset\rangle \\ c_m^\dagger c_{m-1/2}^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} 0 & 0 & e^{-\delta\tau\epsilon_{d,\uparrow}} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -e^{-\delta\tau(\epsilon_{d,\uparrow}+\epsilon_{d,\downarrow}+U)} & 0 \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_m \\ \langle\emptyset| c_{m-1/2} \\ \langle\emptyset| c_m c_{m-1/2} \end{pmatrix}, \tag{45}$$

$$\hat{T}_{c_{\uparrow,n-1/2}} = \begin{pmatrix} |\emptyset\rangle \\ c_m^\dagger |\emptyset\rangle \\ c_{m-1/2}^\dagger |\emptyset\rangle \\ c_m^\dagger c_{m-1/2}^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -e^{-\delta\tau\epsilon_{d,\downarrow}} & 0 \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_m \\ \langle\emptyset| c_{m-1/2} \\ \langle\emptyset| c_m c_{m-1/2} \end{pmatrix}, \tag{46}$$

$$\hat{T}^B_{c_{\uparrow,0}^\dagger} = \begin{pmatrix} |\emptyset\rangle \\ c_m^\dagger |\emptyset\rangle \\ c_{m-1/2}^\dagger |\emptyset\rangle \\ c_m^\dagger c_{m-1/2}^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & e^{-\delta\tau\epsilon_{d,\downarrow}} & 0 & 0 \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_m \\ \langle\emptyset| c_{m-1/2} \\ \langle\emptyset| c_m c_{m-1/2} \end{pmatrix} \tag{47}$$

$$\hat{T}^B_{(c_\uparrow c_\uparrow^\dagger),0} = \begin{pmatrix} |\emptyset\rangle \\ c_m^\dagger |\emptyset\rangle \\ c_{m-1/2}^\dagger |\emptyset\rangle \\ c_m^\dagger c_{m-1/2}^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ e^{-\delta\tau\epsilon_{d,\downarrow}} & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_m \\ \langle\emptyset| c_{m-1/2} \\ \langle\emptyset| c_m c_{m-1/2} \end{pmatrix}. \tag{48}$$

For $\sigma = \downarrow$:

$$\hat{T}_{c_{\downarrow,n}} = \begin{pmatrix} |\emptyset\rangle \\ c_m^\dagger |\emptyset\rangle \\ c_{m-1/2}^\dagger |\emptyset\rangle \\ c_m^\dagger c_{m-1/2}^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -e^{-\delta\tau\epsilon_{d,\downarrow}} & 0 & 0 & e^{-\delta\tau(\epsilon_{d,\uparrow}+\epsilon_{d,\downarrow}+U)} \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_m \\ \langle\emptyset| c_{m-1/2} \\ \langle\emptyset| c_m c_{m-1/2} \end{pmatrix}, \tag{49}$$

$$\hat{T}_{c_{\downarrow,n-1/2}} = \begin{pmatrix} |\emptyset\rangle \\ c_m^\dagger |\emptyset\rangle \\ c_{m-1/2}^\dagger |\emptyset\rangle \\ c_m^\dagger c_{m-1/2}^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & e^{-\delta\tau\epsilon_{d,\uparrow}} \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_m \\ \langle\emptyset| c_{m-1/2} \\ \langle\emptyset| c_m c_{m-1/2} \end{pmatrix}, \tag{50}$$

$$\hat{T}^B_{c^\dagger_{\downarrow,0}} = \begin{pmatrix} |\emptyset\rangle \\ c_m^\dagger |\emptyset\rangle \\ c_{m-1/2}^\dagger |\emptyset\rangle \\ c_m^\dagger c_{m-1/2}^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & -e^{-\delta\tau\epsilon_{d,\uparrow}} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_m \\ \langle\emptyset| c_{m-1/2} \\ \langle\emptyset| c_m c_{m-1/2} \end{pmatrix} \tag{51}$$

$$\hat{T}^B_{(c_\downarrow c^\dagger_\downarrow),0} = \begin{pmatrix} |\emptyset\rangle \\ c_m^\dagger |\emptyset\rangle \\ c_{m-1/2}^\dagger |\emptyset\rangle \\ c_m^\dagger c_{m-1/2}^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} 1 & 0 & 0 & e^{-\delta\tau\epsilon_{d,\uparrow}} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_m \\ \langle\emptyset| c_{m-1/2} \\ \langle\emptyset| c_m c_{m-1/2} \end{pmatrix}. \tag{52}$$

Constructing the hybridization function $\Delta_{m,n}$ from a spectral density $\Gamma(\omega)$
For a given spectral density $\Gamma(\omega) = 2\pi \sum_k t_k t_k^* \delta(\omega - \epsilon_k)$, the hybridization function $\Delta_{m,n}$ can be expressed in terms of the non-interacting bath Green's function through the relation:

$$\Delta_{m,n} = \int \frac{d\omega}{2\pi} \Gamma(\omega)\, g_{m,n}(\omega), \tag{53}$$

where

$$g_{m,n}(\omega) = -e^{-\omega(\tau_m - \tau_n)} \Big(\Theta(\tau_m - \tau_n) - \frac{1}{1 + e^{\beta\omega}} \Big). \tag{54}$$

For convenience, let us introduce the notation:

$$g^<_{m,n}(\omega) = e^{-\omega(\tau_m - \tau_n)} \frac{1}{1 + e^{\beta\omega}}, \tag{55}$$

$$g^>_{m,n}(\omega) = -e^{-\omega(\tau_m - \tau_n)} \frac{1}{1 + e^{-\beta\omega}}, \tag{56}$$

where $\tau_m = \delta\tau \cdot m$ and $\tau_n = \delta\tau \cdot n$.

Depending on the choice of discretization scheme, one obtains different prescriptions for the time-discrete hybridization function: In the above derivation, we have explicitly split the imaginary-time evolution operator as $\hat{U} = \hat{U}_{\text{imp}} \cdot \hat{U}_{\text{hyb}}$, with $\hat{U}_{\text{imp}} = \exp\big(-\delta\tau H_{\text{imp}}\big)$. We parametrize the hopping+bath evolution operator as $\hat{U}_{\text{hyb}} = e^{-\delta\tau(1-\alpha)H_{\text{bath}}} \cdot e^{-\delta\tau(H_{\text{hop}} + \alpha H_{\text{bath}})}$ with $\alpha \in [0,1]$, $H_{\text{bath}} = \sum_{k,\sigma} \epsilon_k \hat{c}^\dagger_{k,\sigma} \hat{c}_{k,\sigma}$ and $H_{\text{hop}} = \sum_{k,\sigma} \big(t_k \hat{d}^\dagger_\sigma \hat{c}_{k,\sigma} + h.c. \big)$.

With this, one obtains for the hybridization function:

$$\begin{pmatrix} \eta_m \\ \eta_{m+1/2} \end{pmatrix}^T \mathbf{\Delta}^{(\alpha)}_{m,n} \begin{pmatrix} \eta_n \\ \eta_{n+1/2} \end{pmatrix} = \int \frac{d\omega}{2\pi} \Gamma(\omega) \begin{cases} \begin{pmatrix} \eta_m \\ \eta_{m+1/2} \end{pmatrix}^T \begin{pmatrix} 0 & -g^<_{n,m+\alpha}(\omega) \\ g^>_{m,n+\alpha}(\omega) & 0 \end{pmatrix} \begin{pmatrix} \eta_n \\ \eta_{n+1/2} \end{pmatrix} & \text{for } m > n, \\ \begin{pmatrix} \eta_m \\ \eta_{m+1/2} \end{pmatrix}^T \begin{pmatrix} 0 & -g^<_{m,m+\alpha}(\omega) \\ g^<_{m,m+\alpha}(\omega) & 0 \end{pmatrix} \begin{pmatrix} \eta_n \\ \eta_{n+1/2} \end{pmatrix} & \text{for } m = n, \\ \begin{pmatrix} \eta_m \\ \eta_{m+1/2} \end{pmatrix}^T \begin{pmatrix} 0 & -g^>_{n,m+\alpha}(\omega) \\ g^<_{m,n+\alpha}(\omega) & 0 \end{pmatrix} \begin{pmatrix} \eta_n \\ \eta_{n+1/2} \end{pmatrix} & \text{for } m < n. \end{cases} \tag{57}$$

We note that the antiperiodic boundary conditions time translational invariance of the propagator lead to the relation:

$$g^<_{m,n}(\omega) = -g^>_{m+M,n}(\omega).$$

Defining the function $g_l(\omega) \equiv -e^{-\omega\tau_l} \frac{1}{1+e^{-\beta\omega}}$ for $l \geq 0$, we obtain

$$\begin{pmatrix} \eta_m \\ \eta_{m+1/2} \end{pmatrix}^T \mathbf{\Delta}^{(\alpha)}_{m,n} \begin{pmatrix} \eta_n \\ \eta_{n+1/2} \end{pmatrix} = \int \frac{d\omega}{2\pi} \Gamma(\omega) \begin{cases} \begin{pmatrix} \eta_m \\ \eta_{m+1/2} \end{pmatrix}^T \begin{pmatrix} 0 & g_{n+M-(m+\alpha)}(\omega) \\ g_{m-(n+\alpha)}(\omega) & 0 \end{pmatrix} \begin{pmatrix} \eta_n \\ \eta_{n+1/2} \end{pmatrix} & \text{for } m > n, \\ \begin{pmatrix} \eta_m \\ \eta_{m+1/2} \end{pmatrix}^T \begin{pmatrix} 0 & g_{M-\alpha}(\omega) \\ -g_{M-\alpha}(\omega) & 0 \end{pmatrix} \begin{pmatrix} \eta_n \\ \eta_{n+1/2} \end{pmatrix} & \text{for } m = n, \\ \begin{pmatrix} \eta_m \\ \eta_{m+1/2} \end{pmatrix}^T \begin{pmatrix} 0 & -g_{n-(m+\alpha)}(\omega) \\ -g_{m+M-(n+\alpha)}(\omega) & 0 \end{pmatrix} \begin{pmatrix} \eta_n \\ \eta_{n+1/2} \end{pmatrix} & \text{for } m < n. \end{cases} \tag{58}$$

On a technical note: If the function $\int \frac{d\omega}{2\pi}\Gamma(\omega)g_l(\omega)$ is stored in an array with M elements, given by,

$$g[i] = \int \frac{d\omega}{2\pi}\Gamma(\omega)g_{i+1-\alpha}(\omega), \quad i = 0, 1, \ldots, M-1,$$

the matrix $\mathbf{\Delta}^{(\alpha)}$ as the form:

$$\mathbf{\Delta}^{(\alpha)} = \begin{pmatrix} 0 & g[M-1] & 0 & -g[0] & 0 & -g[1] & \ldots & 0 & -g[M-2] \\ -g[M-1] & 0 & -g[M-2] & 0 & -g[M-3] & 0 & \ldots & -g[0] & 0 \\ 0 & g[M-2] & 0 & g[M-1] & 0 & -g[0] & \ldots & 0 & -g[M-3] \\ g[0] & 0 & -g[M-1] & 0 & -g[M-2] & 0 & \ldots & -g[1] & 0 \\ 0 & g[M-3] & 0 & g[M-2] & 0 & g[M-1] & \ldots & 0 & -g[M-4] \\ g[1] & 0 & g[0] & 0 & -g[M-1] & 0 & \ldots & -g[2] & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & g[0] & 0 & g[1] & 0 & g[2] & \ldots & 0 & g[M-1] \\ g[M-2] & 0 & g[M-3] & 0 & g[M-4] & 0 & \ldots & -g[M-1] & 0 \end{pmatrix}. \tag{59}$$

The influence functional from Eq. (7) can then be written as:

$$\mathcal{I}[\{\boldsymbol{\eta}\}] = \exp\left[\frac{1}{2}\sum_{m,n=0}^{M-1} \begin{pmatrix} \eta_m \\ \eta_{m+1/2} \end{pmatrix}^T \left(-(\delta\tau)^2 \mathbf{\Delta}^{(\alpha)}_{m,n} + \delta_{m,n} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \right) \begin{pmatrix} \eta_n \\ \eta_{n+1/2} \end{pmatrix}\right]. \tag{60}$$

Second order Trotter Decomposition

For a second-order Trotter-Suzuki decomposition, the impurity gate is further split into two parts. The observables are inserted between two successive half-steps of the impurity evolution which slightly alters the impurity gates. The MPS-MPO contraction of the impurity operator $\hat{D}_n^{\hat{O}_1,\hat{O}_2}$ with the IF-MPS remains unchanged, see Fig. 2 The second-order gates of the impurity take the following form:

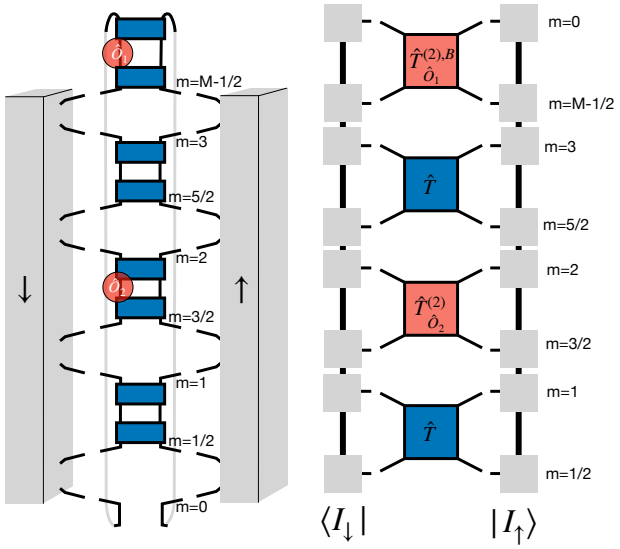

Figure 2: Second-order Trotter-Suzuki decomposition: The impurity gates are altered but the MPS-MPO contraction of the impurity operator $\hat{D}_n^{\hat{O}_1,\hat{O}_2}$ with the IF-MPS remains unchanged.

For $\sigma = \uparrow$:

$$\hat{T}^{(2)}_{c_{\uparrow,n}} = \begin{pmatrix} |\emptyset\rangle \\ c_m^\dagger |\emptyset\rangle \\ c_{m-1/2}^\dagger |\emptyset\rangle \\ c_m^\dagger c_{m-1/2}^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} 0 & 0 & e^{-\frac{\delta\tau}{2}\epsilon_{d,\uparrow}} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -e^{-\frac{\delta\tau}{2}(\epsilon_{d,\uparrow}+2\epsilon_{d,\downarrow}+U)} & 0 \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_m \\ \langle\emptyset| c_{m-1/2} \\ \langle\emptyset| c_m c_{m-1/2} \end{pmatrix}, \tag{61}$$

$$\hat{T}^{(2),B}_{c^\dagger_{\uparrow,0}} = \begin{pmatrix} |\emptyset\rangle \\ c_m^\dagger |\emptyset\rangle \\ c_{m-1/2}^\dagger |\emptyset\rangle \\ c_m^\dagger c_{m-1/2}^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} 0 & e^{-\frac{\delta\tau}{2}\epsilon_{d,\uparrow}} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & e^{-\frac{\delta\tau}{2}(\epsilon_{d,\uparrow}+2\epsilon_{d,\downarrow}+U)} & 0 & 0 \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_m \\ \langle\emptyset| c_{m-1/2} \\ \langle\emptyset| c_m c_{m-1/2} \end{pmatrix} \tag{62}$$

$$\hat{T}^{(2),B}_{(c_\uparrow c^\dagger_\uparrow),0} = \begin{pmatrix} |\emptyset\rangle \\ c_m^\dagger |\emptyset\rangle \\ c_{m-1/2}^\dagger |\emptyset\rangle \\ c_m^\dagger c_{m-1/2}^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ e^{-\delta\tau\epsilon_{d,\downarrow}} & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_m \\ \langle\emptyset| c_{m-1/2} \\ \langle\emptyset| c_m c_{m-1/2} \end{pmatrix}. \tag{63}$$

For $\sigma = \downarrow$:

$$\hat{T}^{(2)}_{c_{\downarrow,n}} = \begin{pmatrix} |\emptyset\rangle \\ c_m^\dagger |\emptyset\rangle \\ c_{m-1/2}^\dagger |\emptyset\rangle \\ c_m^\dagger c_{m-1/2}^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -e^{-\frac{\delta\tau}{2}\epsilon_{d,\downarrow}} & 0 & 0 & e^{-\frac{\delta\tau}{2}(2\epsilon_{d,\uparrow}+\epsilon_{d,\downarrow}+U)} \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_m \\ \langle\emptyset| c_{m-1/2} \\ \langle\emptyset| c_m c_{m-1/2} \end{pmatrix}, \tag{64}$$

$$\hat{T}^{(2),B}_{c^\dagger_{\downarrow,0}} = \begin{pmatrix} |\emptyset\rangle \\ c_m^\dagger |\emptyset\rangle \\ c_{m-1/2}^\dagger |\emptyset\rangle \\ c_m^\dagger c_{m-1/2}^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} 0 & 0 & 0 & 0 \\ -e^{-\frac{\delta\tau}{2}\epsilon_{d,\downarrow}} & 0 & 0 & -e^{-\frac{\delta\tau}{2}(2\epsilon_{d,\uparrow}+\epsilon_{d,\downarrow}+U)} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_m \\ \langle\emptyset| c_{m-1/2} \\ \langle\emptyset| c_m c_{m-1/2} \end{pmatrix} \tag{65}$$

$$\hat{T}^{(2),B}_{(c_\downarrow c^\dagger_\downarrow),0} = \begin{pmatrix} |\emptyset\rangle \\ c_m^\dagger |\emptyset\rangle \\ c_{m-1/2}^\dagger |\emptyset\rangle \\ c_m^\dagger c_{m-1/2}^\dagger |\emptyset\rangle \end{pmatrix}^T \begin{pmatrix} 1 & 0 & 0 & e^{-\delta\tau\epsilon_{d,\uparrow}} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \langle\emptyset| \\ \langle\emptyset| c_m \\ \langle\emptyset| c_{m-1/2} \\ \langle\emptyset| c_m c_{m-1/2} \end{pmatrix}. \tag{66}$$

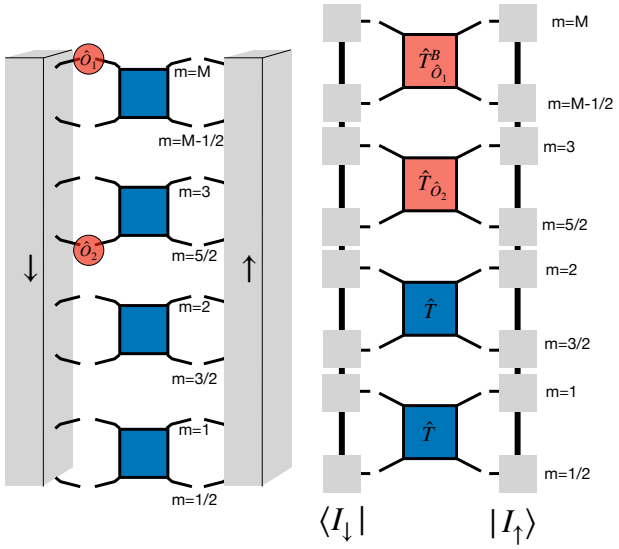

Figure 3: For simultaneous impurity-bath evolution: Illustration of $\langle \hat{O}_2(\tau_n)\hat{O}_1(0)\rangle_\beta$, here shown for a discretization into $M = 4$ intervals and $n = 2$. Left: The path integral expression, Eq. (75), where the blue impurity gates here are the same as the ones derived in the previous part and the IF is given by Eq. (76). Right: As opposed to the previous case, the conversion from IF to MPS does not require a reshuffling of legs. For the operator $\hat{T}_{\hat{O}_2}$ with $\hat{O}_2 = \hat{c}$, the gate $\hat{T}_{c_\sigma,n+1/2}$ from above should be used.

Simultaneous evolution of impurity and bath: $\hat{U} = \exp\big(-\delta\tau(H_{\mathbf{imp}} + H_{\mathbf{hop}} + H_{\mathbf{bath}})\big)$

Above, we have chosen to discretize the path integral in Eq. (2) in such a way that the local impurity evolution and the environment evolution are applied successively, $\hat{U} = \hat{U}_{\rm imp}\cdot\hat{U}_{\rm hyb}$. Another choice is to discretize Eq. (2) in a way that the evolution operator takes the form $\hat{U} = \exp\big(-\delta\tau H\big)$, where $H = H_{\rm imp}+H_{\rm hop}+H_{\rm bath}$ is the full Hamiltonian of impurity and environment. In this case, the IF is not expressed by an equation of the form of Eq. (60) as we derive in this section.

For the imaginary-time evolution operator $\hat{U} = \exp\big(-\delta\tau H\big)$, the thermal expectation value is written as:

$$\boxed{\langle \hat{O}_2(\tau_n)\,\hat{O}_1(0)\rangle = \frac{1}{Z}\int d(\boldsymbol{\eta}_\uparrow,\boldsymbol{\eta}_\downarrow)\, e^{S_{\rm hyb}[\boldsymbol{\eta}_\downarrow]}\mathcal{D}_n^{\hat{O}_1,\hat{O}_2}[\boldsymbol{\eta}_\downarrow,\boldsymbol{\eta}_\uparrow]e^{S_{\rm hyb}[\boldsymbol{\eta}_\uparrow]}} \tag{67}$$

where

$$\boldsymbol{\eta}_\sigma \equiv (\eta_{\sigma,1/2},\ldots,\eta_{\sigma,M}), \tag{68}$$

$$d(\boldsymbol{\eta}_\uparrow,\boldsymbol{\eta}_\downarrow) \equiv \prod_\sigma d\eta_{\sigma,M}\, d\eta_{\sigma,1/2} \prod_{m=1}^{M-1} d\eta_{\sigma,m}\, d\eta_{\sigma,m+1/2}, \tag{69}$$

$$\begin{aligned}\mathcal{D}_n^{\hat{O}_1,\hat{O}_2}[\boldsymbol{\eta}_\downarrow,\boldsymbol{\eta}_\uparrow] = &\prod_{\substack{m=1\\ m\neq n+1}}^{M-1} \exp\Big[-\Big(\eta_{\uparrow,m}\eta_{\uparrow,m-1/2}+\eta_{\downarrow,m}\eta_{\downarrow,m-1/2}+\delta\tau\mathcal{H}_{\rm imp}[\{-\eta_{\uparrow,m},\eta_{\uparrow,m-1/2},\eta_{\downarrow,m},-\eta_{\downarrow,m-1/2}\}]\Big)\Big]\\ &\times\tilde{\mathcal{O}}_2[-\eta_{\uparrow,n+1},\eta_{\uparrow,n+1/2},\eta_{\downarrow,n+1},-\eta_{\downarrow,n+1/2}]\,\tilde{\mathcal{O}}_1[\eta_{\uparrow,M},\eta_{\uparrow,M-1/2},-\eta_{\downarrow,M},-\eta_{\downarrow,M-1/2}]\end{aligned} \tag{70}$$

$$\begin{aligned}S_{\rm hyb}[\boldsymbol{\eta}_\sigma] = \sum_{\sigma=\uparrow,\downarrow}\Big((\delta\tau)^2\sum_{m=1}^{M-1}\sum_{n=1}^{M}\eta_{\sigma,m}\Delta^{(\alpha=1)}_{m,n}\eta_{\sigma,n-1/2} - (\delta\tau)^2\sum_{n=1}^{M}\eta_{\sigma,M}\Delta^{(\alpha=1)}_{M,n}\eta_{\sigma,n-1/2}\\ +\sum_{m=1}^{M-1}\eta_{\sigma,m}\eta_{\sigma,m+1/2}+\eta_{\sigma,M}\eta_{\sigma,1/2}\Big).\end{aligned} \tag{71}$$

Here, $\tilde{\mathcal{O}}_{1,2}$ are the combined kernels of the operator $\hat{O}_{1,2}$ and the evolution gate at the corresponding time, respectively. We made manipulations to the path integral in such a way that the sign convention in the impurity kernel $\mathcal{D}$ in Eq. (70) is unchanged with respect to Eq. (6). Note, however, that now the operator $\hat{O}_2$ is inserted *before* application of the impurity evolution gate, as opposed to the prescription with successive evolution of impurity and bath. Hence, the gate $\hat{T}_{\hat{O}_2}$ with $\hat{O}_2 = c$ here is $\hat{T}_{c_\sigma,n+1/2}$ from Eqs. (62,51), and not $\hat{T}_{c_\sigma,n}$ as before. [The latter gate corresponds to insertion of the operator c *after* application of the impurity evolution gate, and thus corresponds to insertion at half-time steps between impurity- and bath evolution in the successive-evolution case.]
The hybridization function $\Delta^{(\alpha=1)}$ in Eq. (71) corresponds to Eq. (58) for $\alpha = 1$. **Note that Eq. (67) does *not* have the form of an overlap.**

To obtain an equation that can interpreted as overlap, we introduce a more convenient notation and rewrite $S_{\rm hyb}$ as

$$S_{\rm hyb}[\boldsymbol{\eta}_\sigma] = \frac{1}{2}\sum_{m,n=1}^{M}\begin{pmatrix}\eta_{\sigma,m-1/2}\\ \eta_{\sigma,m}\end{pmatrix}^T \mathbf{A}_{m,n}\begin{pmatrix}\eta_{\sigma,n-1/2}\\ \eta_{\sigma,n}\end{pmatrix}, \tag{72}$$

where the matrix $\mathbf{A}$ has the following subblocks:

$$\mathbf{A}_{m,n} = \begin{cases}
\begin{pmatrix}\eta_{m-1/2}\\ \eta_m\end{pmatrix}^T\left[+(\delta\tau)^2\,\boldsymbol{\Delta}^{(\alpha=1)}_{m,n}+\begin{pmatrix}0 & -\delta_{m,n+1}\\ \delta_{m+1,n} & 0\end{pmatrix}\right]\begin{pmatrix}\eta_{n-1/2}\\ \eta_n\end{pmatrix} & \text{for } 1\le m,n<M\\
\begin{pmatrix}\eta_{m-1/2}\\ \eta_m\end{pmatrix}^T\left[-(\delta\tau)^2\,\boldsymbol{\Delta}^{(\alpha=1)}_{M,n}+\begin{pmatrix}0 & -\delta_{M-1,n}\\ 0 & 0\end{pmatrix}\right]\begin{pmatrix}\eta_{n-1/2}\\ \eta_n\end{pmatrix} & \text{for } m=M,\ 1<n<M\\
\begin{pmatrix}\eta_{m-1/2}\\ \eta_m\end{pmatrix}^T\left[-(\delta\tau)^2\,\boldsymbol{\Delta}^{(\alpha=1)}_{m,M}+\begin{pmatrix}0 & 0\\ \delta_{M-1,m} & 0\end{pmatrix}\right]\begin{pmatrix}\eta_{n-1/2}\\ \eta_n\end{pmatrix} & \text{for } 1<m<M,\ n=M\\
\begin{pmatrix}\eta_{m-1/2}\\ \eta_m\end{pmatrix}^T\left[-(\delta\tau)^2\,\boldsymbol{\Delta}^{(\alpha=1)}_{M,M}\right]\begin{pmatrix}\eta_{n-1/2}\\ \eta_n\end{pmatrix} & \text{for } m=n=M\\
\begin{pmatrix}\eta_{m-1/2}\\ \eta_m\end{pmatrix}^T\left[-(\delta\tau)^2\,\boldsymbol{\Delta}^{(\alpha=1)}_{1,M}+\begin{pmatrix}0 & -1\\ 0 & 0\end{pmatrix}\right]\begin{pmatrix}\eta_{n-1/2}\\ \eta_n\end{pmatrix} & \text{for } m=1,\ n=M\\
\begin{pmatrix}\eta_{m-1/2}\\ \eta_m\end{pmatrix}^T\left[-(\delta\tau)^2\,\boldsymbol{\Delta}^{(\alpha=1)}_{M,1}+\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}\right]\begin{pmatrix}\eta_{n-1/2}\\ \eta_n\end{pmatrix} & \text{for } m=M,\ n=1.
\end{cases} \tag{73}$$

Introducing a new set of impurity variables $\boldsymbol{\zeta}_\sigma$ (and thus doubling the degrees of freedom), we can rewrite

$$e^{S_{\rm hyb}[\boldsymbol{\eta}_\sigma]} = \frac{1}{pf(\mathbf{A}^{-1})}\int d\boldsymbol{\zeta}_\sigma \exp\Big[-\boldsymbol{\zeta}_\sigma^T\boldsymbol{\eta}_\sigma+\frac{1}{2}\boldsymbol{\zeta}_\sigma^T\mathbf{A}^{-1}\boldsymbol{\zeta}_\sigma\Big] = \frac{1}{pf(\mathbf{A}^{-1})}\int d\boldsymbol{\zeta}_\sigma \exp\Big[-\boldsymbol{\eta}_\sigma^T\boldsymbol{\zeta}_\sigma+\frac{1}{2}\boldsymbol{\zeta}_\sigma^T\mathbf{A}^{-1}\boldsymbol{\zeta}_\sigma\Big], \tag{74}$$

where the third term is is obtained from the second one by substituting $\begin{pmatrix}\zeta_{\sigma,m-1/2}\\ \zeta_{\sigma,m}\end{pmatrix} \to \begin{pmatrix}-\zeta_{\sigma,m-1/2}\\ -\zeta_{\sigma,m}\end{pmatrix}$, which flips the sign in the first term of the exponential and introduces a prefactor $(-1)^{2M} = 1$. By inserting this into Eq. (75), we obtain the expectation value in overlap form:

$$\boxed{\langle \hat{O}_2(\tau_n)\, \hat{O}_1(0)\rangle \propto \int d(\boldsymbol{\eta}_\uparrow, \boldsymbol{\eta}_\downarrow) \int d(\boldsymbol{\zeta}_\uparrow, \boldsymbol{\zeta}_\downarrow)\, \tilde{\mathcal{I}}[\boldsymbol{\zeta}_\downarrow]\, e^{-\boldsymbol{\eta}_\downarrow^T \boldsymbol{\zeta}_\downarrow}\, \mathcal{D}_n^{\hat{O}_1,\hat{O}_2}[\boldsymbol{\eta}_\downarrow, \boldsymbol{\eta}_\uparrow]\, e^{-\boldsymbol{\zeta}_\uparrow^T \boldsymbol{\eta}_\uparrow}\, \tilde{\mathcal{I}}[\boldsymbol{\zeta}_\uparrow],} \tag{75}$$

with

$$\tilde{\mathcal{I}}[\boldsymbol{\zeta}_\sigma] = \exp\Big[\frac{1}{2}\, \boldsymbol{\zeta}_\sigma^T \mathbf{A}^{-1} \boldsymbol{\zeta}_\sigma\Big], \tag{76}$$

At this point, Eq. (75) has the same form as Eq. (3) and we can therefore evaluate the overlap as usual.

Closing the DMFT loop

The DMFT loop follows the following steps (we omit the spin index in the equations below):

1. For a given hybridization function $\Delta_{m,n}$, either obtained from the previous iteration or computed from a spectral density $\Gamma(\omega)$, compute the interacting impurity Green's function $G_{\rm imp}(\tau_m)$, Eq. (44), for a finite number of discrete time-points τ_m as outlined above.

2. Perform a Fourier transform, $G_{\rm imp}(\tau_m) \to G_{\rm imp}(i\omega_n)$, where $\omega_n = \frac{(2n+1)\pi}{\beta}$ are fermionic Matsubara frequencies.

3. Extract the impurity self-energy, $\Sigma_{\rm imp}(i\omega_n) = G^{-1}_{0,\rm imp}(i\omega_n) - G^{-1}_{\rm imp}(i\omega_n)$, where $G^{-1}_{0,\rm imp}(i\omega_n) = i\omega_n - \epsilon_d + \mu - \Delta(i\omega_n)$ is the inverse non-interacting impurity Green's function (which could in principle also be obtained by computing $G_{\rm imp}$ with $U = 0$) and inverting the result.

4. Compute the *local lattice Green's function*, where we take as self-energy the impurity self-energy, $\Sigma_{\rm imp}$:

$$G_{ii}(i\omega_n) = \int dE \frac{D(E)}{i\omega_n - E + \mu - \Sigma_{\rm imp}(i\omega_n)}. \tag{77}$$

   Here, $D(E)$ is the density of states that is defined by the model that should be solved, e.g. Hubbard model in 2D. Hence, $D(E)$ is never updated.

5. From $G_{ii}(i\omega)$, compute an updated hybridization function, $\Delta(i\omega_n) = i\omega_n + \mu - G^{-1}_{ii}(i\omega_n) - \Sigma_{\rm imp}(i\omega_n)$.

6. Perform a Fourier transform $\Delta(i\omega_n) \to \Delta(\tau_m)$. Make sure, we have access to enough frequencies $i\omega_n$ to reach the tail. Inside the tail, apply an extrapolation procedure to avoid frequency-truncation effects in $\Delta(\tau_m)$ after the Fourier transform.

7. Use the components of the vector $\Delta[m] \equiv \Delta(\tau_m)$ with $(m = 0, 1, \ldots, M-1)$ to construct the next hybridization function $\Delta_{m,n}$. For this, use Eq. (78) which gives the correspondence between indices of the vector components $\Delta[m]$ and the entries of the matrix $\Delta_{m,n}$.

$$\mathbf{\Delta} = \begin{pmatrix} 0 & -\Delta[1] & 0 & -\Delta[2] & 0 & -\Delta[3] & \ldots & 0 & \Delta[0] \\ \Delta[1] & 0 & \Delta[0] & 0 & -\Delta[M-1] & 0 & \ldots & -\Delta[2] & 0 \\ 0 & -\Delta[0] & 0 & -\Delta[1] & 0 & -\Delta[2] & \ldots & 0 & -\Delta[M-1] \\ \Delta[2] & 0 & \Delta[1] & 0 & \Delta[0] & 0 & \ldots & -\Delta[3] & 0 \\ 0 & \Delta[M-1] & 0 & -\Delta[0] & 0 & -\Delta[1] & \ldots & 0 & -\Delta[M-2] \\ \Delta[3] & 0 & \Delta[2] & 0 & \Delta[1] & 0 & \ldots & -\Delta[4] & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \Delta[2] & 0 & \Delta[3] & 0 & \Delta[4] & \ldots & 0 & -\Delta[1] \\ -\Delta[0] & 0 & \Delta[M-1] & 0 & \Delta[M-2] & 0 & \ldots & \Delta[1] & 0 \end{pmatrix}. \tag{78}$$

Repeat steps 1–7 until convergence is reached.

Constructing the exact continuum-IF from a hybridization function $\Delta(i\omega_n)$
Our goal is to construct an IF, using only the hybridization function $\Delta(i\omega_n)$ is input. The scheme derived above becomes exact in the limit $\delta\tau \to 0$. In order to obtain an IF with only a small number of external legs, while still encoding the continuous-time dynamics, we had to construct the IF on a very fine time grid [where $(\delta\tau)^{-1}$ is much smaller than all energy scales of the system] and numerically integrate out most of the legs in order to reduce the IF to only a few open legs.

Here, we generalize the above approach to a scheme which allows us to directly construct the continuous-time IF by analytically taking into account all possible quantum mechanical trajectories between the external legs of the IF.

The input is the hybridization function $\Delta(i\omega_n)$, which we obtain either explicitly from a given spectral density or as the result of a DMFT cycle. In the former case, it is given by :

$$\Delta(i\omega_n) = \int \frac{d\epsilon}{2\pi}\, \Gamma(\epsilon) \frac{1}{i\omega_n - \epsilon + \mu}, \tag{79}$$

where $\Gamma(\epsilon) = 2\pi \sum_k t_k t_k^* \, \delta(\epsilon - \epsilon_k)$ is the spectral density as usual.
This allows us to determine the non-interacting impurity Green's function,

$$G^0(i\omega_n) = \frac{1}{i\omega_n - \epsilon_d - \Delta(i\omega_n)}. \tag{80}$$

We stress that we explicitly included the impurity onsite-potential ϵ_d in Eq. (80), which corresponds to absorbing the non-interacting part of the impurity into the IF. **If we keep this part on the impurity (as above), it should be set to zero in Eq. (80)**.
The main quantity determining the components of the continuous-time IF is the non-interacting impurity Green's function in imaginary time, either obtained by the Fourier transform of Eq. (80),

$$G^0(\tau) = \frac{1}{\beta} \sum_n e^{-i\omega_n \tau}\, G^0(i\omega_n), \tag{81}$$

or by solving the Volterra integro-differential equation,

$$\partial_\tau G^0(\tau) = -\epsilon_d G^0(\tau) - \int_0^\tau d\tau' \Delta(\tau - \tau') G^0(\tau'). \tag{82}$$

We want to write the IF in the form: $\mathcal{I} = \exp\big(\sum_{m,n} \bar{\eta}_{m+1/2} A_{m,n} \eta_n\big)$. The components $A_{m,0}$ can be written as multipoint correlation functions in the non-interacting continuous-time problem, which have the form:

$$A_{m,0} = \int d\big(\bar{\eta}_\tau, \eta_\tau\big) \exp\Big[- \int_0^\beta d\tau\, \bar{\eta}_\tau \partial_\tau \eta_\tau - \int_0^\beta d\tau \int_0^\beta d\tau'\, \bar{\eta}_\tau \Delta(\tau - \tau')\, \eta_{\tau'} \Big] \eta_M \bar{\eta}_{M-(m+1)} \prod_{\substack{l=1 \\ l \neq M-(m+1)}}^{M-1} \eta_l \bar{\eta}_l. \tag{83}$$

Using Wick's theorem, one can rewrite $A_{m,0}$ as product of $G^0(\tau)$. For this, we define the matrix:

$$\boldsymbol{G}^0 \equiv \begin{pmatrix} G^0(0) & G^0(\delta\tau) & G^0(2\delta\tau) & \dots & G^0(\beta) \\ G^0(-\delta\tau) & G^0(0) & G^0(\delta\tau) & \dots & G(\beta - \delta\tau) \\ G^0(-2\delta\tau) & G^0(-\delta\tau) & G^0(0) & \dots & G(\beta - 2\delta\tau) \\ \vdots & \vdots & \vdots & \ddots & \\ G^0(-\beta) & G^0(-\beta + \delta\tau) & G^0(-\beta + 2\delta\tau) & \dots & G^0(0) \end{pmatrix}. \tag{84}$$

The components $A_{m,0}$ for $m < M$ are then given by:

$$A_{m,0} = Z \cdot \det\left[\boldsymbol{G}^0\big|_{[0,1,\ldots,(\text{no } m+1),\ldots,M-1],[m+1,1,\ldots,(\text{no } m+1),\ldots,M-1]}\right] \tag{85}$$

For $m = M$, we have:

$$A_{m,0} = -Z \cdot \det\left[\boldsymbol{G}^0\big|_{[0,1,\ldots,M-1],[M,1,\ldots,M-1]}\right]. \tag{86}$$

The (sign-adjusted) partition sum is given by

$$Z = -1/\det\left[\boldsymbol{G}^0\big|_{[0,\ldots,M-1],[0,\ldots,M-1]}\right],$$

where we defined the minus sign to cancel the minus sign included in the definition of G^0. Note that $G^0(\tau) = -G^0(\tau + \beta)$, such that we can always evaluate the Green's function with a time argument in the range $\tau \in [0, \beta]$.
Furthermore, note that with the above equation, we can construct all elements $A_{m,n}$ as $A_{m,n} = -A_{n+M,m}$, such that from $A_{m,0}$, we can compute all elements of the IF.

Constructing the continuous-time IF for an explicit discrete bath

Starting from the Hamiltonian: $H_{\rm hyb} = H_0 + H_{\rm hop} + H_{\rm bath}$ with

$$H_0 = \epsilon_d d^\dagger d, \tag{87}$$

$$H_{\rm hop} = \sum_k \big(t_k d^\dagger c_k + h.c.\big), \tag{88}$$

$$H_{\rm bath} = \sum_k \epsilon_k c_k^\dagger c_k, \tag{89}$$

the imaginary-time evolution operator for a time step $\delta\tau$ is given by $U(\delta\tau) = e^{-\delta\tau H_{\rm hyb}}$, to which a Grassmann kernel can be associated that formally reads:

$$\langle\bar\eta,\bar{\boldsymbol\xi}|U(\tau)|\eta,\boldsymbol\xi\rangle = \exp\Big[\exp\big(-\tau\begin{pmatrix}\bar\eta\\ \bar{\boldsymbol\xi}\end{pmatrix}^T\begin{pmatrix}\epsilon_d & (\vec{\boldsymbol t})^T\\ \vec{\boldsymbol t}^* & \mathrm{diag}(\epsilon_k)\end{pmatrix}\begin{pmatrix}\eta\\ \boldsymbol\xi\end{pmatrix}\big)\Big] \tag{90}$$

$$= \exp\Big[\begin{pmatrix}\bar\eta\\ \bar{\boldsymbol\xi}\end{pmatrix}^T\begin{pmatrix}G^0(\tau) & \big(\vec G^{\rm hop}(\tau)\big)^T\\ \big(\vec G^{\rm hop}(\tau)\big)^* & \boldsymbol G^{\rm bath}(\tau)\end{pmatrix}\begin{pmatrix}\eta\\ \boldsymbol\xi\end{pmatrix}\Big]. \tag{91}$$

The eom's for the propagators in the exponent read (suppressing time arguments in the notation):

$$\partial_\tau\begin{pmatrix}G^0 & \big(\vec G^{\rm hop}\big)^T\\ \big(\vec G^{\rm hop}\big)^* & \boldsymbol G^{\rm bath}\end{pmatrix} = -\begin{pmatrix}\epsilon_d & (\vec{\boldsymbol t})^T\\ \vec{\boldsymbol t}^* & \mathrm{diag}(\epsilon_k)\end{pmatrix}\cdot\begin{pmatrix}G^0 & \big(\vec G^{\rm hop}\big)^T\\ \big(\vec G^{\rm hop}\big)^* & \boldsymbol G^{\rm bath}\end{pmatrix} \tag{92}$$

$$= -\begin{pmatrix}\epsilon_d G^0 + (\vec{\boldsymbol t})^T\big(\vec G^{\rm hop}\big)^* & \epsilon_d\big(\vec G^{\rm hop}\big)^T + (\vec{\boldsymbol t})^T\boldsymbol G^{\rm bath}\\ \vec{\boldsymbol t}^* G^0 + \mathrm{diag}(\epsilon_k)\big(\vec G^{\rm hop}\big)^* & \vec{\boldsymbol t}^*\big(\vec G^{\rm hop}\big)^T + \mathrm{diag}(\epsilon_k)\boldsymbol G^{\rm bath}.\end{pmatrix} \tag{93}$$

From the entry in the bottom left we obtain:

$$G_k^{\rm hop}(i\omega_n)^* = \frac{t_k^* G^0(i\omega_n)}{i\omega_n - \epsilon_k} \tag{94}$$

Inserting this into the top left component, we obtain a closed differential equation for G^0:

$$\partial_\tau G^0(\tau) = -\epsilon_d G^0(\tau) - \int_0^\tau d\tau' \underbrace{\Big(-\sum_k |t_k|^2 \frac{e^{-(\tau-\tau')\epsilon_k}}{1+e^{-\beta\epsilon_k}}\Big)}_{=\Delta(\tau-\tau')} G^0(\tau'), \tag{95}$$

with the boundary condition $G^0(0) = 1$.

Alternatively, G^0 can be obtained by performing the Fourier transform of the function:

$$G^0(i\omega_n) = \Big(i\omega_n - \epsilon_d - \Delta(i\omega)\Big)^{-1}, \quad \Delta(i\omega_n) = \sum_k \frac{|t_k|^2}{i\omega_n - \epsilon_k}. \tag{96}$$

In physical terms, $G^0(\tau)$ describes the non-interacting impurity propagator with local onsite-energy ϵ that propagates across a time interval τ in presence of the bath (no trotterization present here), whose effect is described by the hybridization function $\Delta(\tau-\tau')$. Setting $\Delta(\tau-\tau')$ to zero, one obtains the free imaginary-time propagator of a single mode at energy ϵ_d : $G^0(i\omega_n) = (i\omega_n - \epsilon_d)^{-1}$.

Having obtained $G^0(i\omega_n)$, we can now determine (imposing the boundary condition $((G_k^{\rm hop}(0))^* = 0$):

$$(G_k^{\rm hop}(\tau))^* = t_k^* \int_0^\tau d\tau' \Big(-\frac{e^{-(\tau-\tau')\epsilon_k}}{1+e^{-\beta\epsilon_k}}\Big) G^0(\tau'). \tag{97}$$

Hence:

$$G_k^{\rm hop}(\tau) = t_k \int_0^\tau d\tau' \Big(-\frac{e^{-(\tau-\tau')\epsilon_k}}{1+e^{-\beta\epsilon_k}}\Big) G^0(\tau'). \tag{98}$$

Finally, the "bath only" component reads:

$$G^{\rm bath}_{k,k'}(\tau) = -\frac{e^{-\tau\epsilon_k}}{1+e^{-\beta\epsilon_k}}\delta_{k,k'} - t^*_k t_{k'}\int_0^\tau d\tau'\, G^0(\tau-\tau')\cdot\frac{e^{\beta\epsilon_k}e^{-\epsilon_k\tau'}n_{\rm F}(\epsilon_k) - e^{\beta\epsilon_{k'}}e^{-\epsilon_{k'}\tau'}n_{\rm F}(\epsilon_{k'})}{\epsilon_k-\epsilon_{k'}}. \tag{99}$$

The component of the IF connecting the two variables $\bar\eta_m$ and η_n is given by:
$\underline{m > n:}$

$$A_{m,n} = \det\Big(\mathbb{1} + (\boldsymbol{G}^{\rm bath}(\delta\tau))^M\Big)\sum_{k,k'} G^{\rm hop}_k(\delta\tau)\Big[\Big(\boldsymbol{G}^{\rm bath}(\delta\tau)\Big)^{-(m-n-1)}\Big]_{k,k'}(G^{\rm hop}_{k'}(\delta\tau))^*. \tag{100}$$

$\underline{m \le n:}$

$$A_{m,n} = \delta_{m,n}G^0(\delta\tau) - \det\Big(\mathbb{1} + (\boldsymbol{G}^{\rm bath}(\delta\tau))^M\Big)\sum_{k,k'} G^{\rm hop}_k(\delta\tau)\Big[\Big(\boldsymbol{G}^{\rm bath}(\delta\tau)\Big)^{-(M-n+m-1)}\Big]_{k,k'}(G^{\rm hop}_{k'}(\delta\tau))^*. \tag{101}$$

The corresponding IF reads simply: $\mathcal{I} = \exp\big(\sum_{m,n}\bar\eta_m A_{m,n}\eta_n\big)$.