

Note on the continuous-time quantum Monte Carlo (CT-QMC) simulation method

– Application to the Anderson model –

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1 The CT-QMC method

The Anderson model is given by the Hamiltonian

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}\sigma} + \varepsilon_f \sum_{\sigma} f_{\sigma}^+ f_{\sigma} + U n_{f,\uparrow} n_{f,\downarrow} + \sum_{\mathbf{k}\sigma} [V_{\mathbf{k}} c_{\mathbf{k},\sigma}^+ f_{\sigma} + V_{\mathbf{k}}^* f_{\sigma}^+ c_{\mathbf{k},\sigma}]. \quad (1)$$

The physical properties of the Anderson model are discussed in Appendix A.

We separate the Hamiltonian into an unperturbed part \mathcal{H}_0 and a perturbation \mathcal{H}_1 as $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$.

Thus, the partition function is given by

$$\mathcal{Z} = \text{Tr} \left[e^{-\beta \mathcal{H}_0} T_{\tau} e^{-\int_0^{\beta} d\tau \mathcal{H}_1(\tau)} \right] = \text{Tr} \left[e^{-\beta \mathcal{H}_0} T_{\tau} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left(-\int_0^{\beta} d\tau \mathcal{H}_1(\tau) \right)^n \right], \quad (2)$$

where $\mathcal{H}_1(\tau)$ is given in the interaction picture as $\mathcal{H}_1(\tau) = e^{\tau \mathcal{H}_0} \mathcal{H}_1 e^{-\tau \mathcal{H}_0}$. The CT-QMC simulation samples the infinite sum of multiple integrals in eq. (2) stochastically.

Two basically different methods exist in CT-QMC. Namely,

- * *weak-coupling method*: we make expansion in eq. (2) in the Coulomb interaction [1];
- * *hybridization method*: we make expansion in eq. (2) in the hybridization term¹ [2], [3].

In the following we discuss the details of the hybridization method.

2 Hybridization method

2.1 Partition function

Following the example of the Anderson model given by the Hamiltonian (1), we take

$$\mathcal{H}_1 = \sum_{\mathbf{k}\sigma} [V_{\mathbf{k}} c_{\mathbf{k},\sigma}^+ f_{\sigma} + V_{\mathbf{k}}^* f_{\sigma}^+ c_{\mathbf{k},\sigma}] \equiv h_1 + h_1^* \quad (3)$$

in the partition function

$$\mathcal{Z} = \text{Tr}_c \text{Tr}_f \left[e^{-\beta \mathcal{H}_0} T_{\tau} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left(-\int_0^{\beta} d\tau \mathcal{H}_1(\tau) \right)^n \right]. \quad (4)$$

¹We note that this method is further developed for the case of Kondo and Coqblin-Schrieffer models, where the expansion is in the Kondo coupling J [6].

Only terms with the same power give contribution to the trace:

$$\begin{aligned} \frac{(-1)^n}{n!} \left(- \int_0^\beta d\tau \mathcal{H}_1(\tau) \right)^n &= \frac{(-1)^{2q}}{q!} c(2q, q) \left(- \int_0^\beta d\tau h_1(\tau) \right)^q \left(- \int_0^\beta d\tau h_1^*(\tau) \right)^q \\ &= \frac{1}{(q!)^2} \left(- \int_0^\beta d\tau h_1(\tau) \right)^q \left(- \int_0^\beta d\tau h_1^*(\tau) \right)^q \equiv \mathcal{Z}_q, \end{aligned} \quad (5)$$

where $c(k, q) = k!/(q!(k - q)!)$. Thus, the partition function has the form

$$\mathcal{Z} = \text{Tr}_c \text{Tr}_f \left[e^{-\beta \mathcal{H}_0} T_\tau \sum_{q=0}^{\infty} \mathcal{Z}_q \right]. \quad (6)$$

The detailed form of \mathcal{Z}_q is given as

$$\begin{aligned} \mathcal{Z}_q &= \frac{1}{(q!)^2} \int \mathcal{D}[\tilde{q}] \int \mathcal{D}[\tilde{q}]' V_{\mathbf{k}_1 \sigma_1} \dots V_{\mathbf{k}_q \sigma_q} V_{\mathbf{k}_1 \sigma_1}^* \dots V_{\mathbf{k}_q \sigma_q}^* \times \\ &\times c_{\mathbf{k}_1, \sigma_1}^+(\tau_1) c_{\mathbf{k}'_1, \sigma'_1}(\tau'_1) \dots c_{\mathbf{k}_q, \sigma_q}^+(\tau_q) c_{\mathbf{k}'_q, \sigma'_q}(\tau'_q) f_{\sigma_1}(\tau_1) f_{\sigma'_1}^+(\tau'_1) \dots f_{\sigma_q}(\tau_q) f_{\sigma'_q}^+(\tau'_q) \\ &= \frac{1}{(q!)^2} \int_0^\beta d\tau_1 \dots \int_0^\beta d\tau_{q_\alpha} \int_0^\beta d\tau'_1 \dots \int_0^\beta d\tau'_{q_\alpha} \sum_{\mathbf{k}_1 \dots \mathbf{k}_{q_\alpha}} \sum_{\mathbf{k}'_1 \dots \mathbf{k}'_{q_\alpha}} V_{\mathbf{k}_1 \sigma_1} \dots V_{\mathbf{k}_{q_\alpha} \sigma_{q_\alpha}} V_{\mathbf{k}_1 \sigma_1}^* \dots V_{\mathbf{k}_{q_\alpha} \sigma_{q_\alpha}}^* \times \\ &\times \left\{ \prod_{\alpha} c_{\mathbf{k}_1, \alpha}^+(\tau_1) c_{\mathbf{k}'_1, \alpha}(\tau'_1) \dots c_{\mathbf{k}_{q_\alpha}, \alpha}^+(\tau_{q_\alpha}) c_{\mathbf{k}'_{q_\alpha}, \alpha}(\tau'_{q_\alpha}) \right\} \left\{ \prod_{\alpha} f_{\alpha}(\tau_1) f_{\alpha}^+(\tau'_1) \dots f_{\alpha}(\tau_{q_\alpha}) f_{\alpha}^+(\tau'_{q_\alpha}) \right\}, \end{aligned} \quad (7)$$

where we introduced the notation

$$\int \mathcal{D}[\tilde{q}] \equiv \int_0^\beta d\tau_1 \dots \int_0^\beta d\tau_q \sum_{\mathbf{k}_1 \dots \mathbf{k}_q} \sum_{\sigma_1 \dots \sigma_q}. \quad (8)$$

For the simplicity we take $V_{\mathbf{k}_1 \sigma_1} = V_{\mathbf{k}_2 \sigma_2} = \dots = V_{\mathbf{k}_q \sigma_q} = V_{\mathbf{k}_1 \sigma_1}^* = V_{\mathbf{k}_2 \sigma_2}^* = \dots = V_{\mathbf{k}_q \sigma_q}^* = V$ in the following.

$$\begin{aligned} \frac{\mathcal{Z}}{\mathcal{Z}_c \mathcal{Z}_f} &= \frac{1}{\mathcal{Z}_c \mathcal{Z}_f} \sum_{q=0}^{\infty} \text{Tr}_c \text{Tr}_f \left[e^{-\beta \mathcal{H}_c} e^{-\beta \mathcal{H}_f} T_\tau \mathcal{Z}_q \right] \\ &= \sum_{q=0}^{\infty} \frac{1}{(q!)^2} \int \mathcal{D}[\tilde{q}] \int \mathcal{D}[\tilde{q}]' (V^2)^q \langle T_\tau c_{\mathbf{k}_1}^+(\tau_1) c_{\mathbf{k}'_1}(\tau'_1) \dots c_{\mathbf{k}_q}^+(\tau_q) c_{\mathbf{k}'_q}(\tau'_q) \rangle_c \times \\ &\times \langle T_\tau f_{\sigma_1}(\tau_1) f_{\sigma'_1}^+(\tau'_1) \dots f_{\sigma_q}(\tau_q) f_{\sigma'_q}^+(\tau'_q) \rangle_f \\ &= \sum_{\{q_\alpha\}} \frac{1}{(q!)^2} \left(\frac{q!}{\prod_{\alpha} (q_\alpha!)} \right)^2 \int_0^\beta d\tau_1 \dots \int_0^\beta d\tau_{q_\alpha} \int_0^\beta d\tau'_1 \dots \int_0^\beta d\tau'_{q_\alpha} \sum_{\mathbf{k}_1 \dots \mathbf{k}_{q_\alpha}} \sum_{\mathbf{k}'_1 \dots \mathbf{k}'_{q_\alpha}} (V^2)^{q_\alpha} \times \\ &\times \left\langle T_\tau \left\{ \prod_{\alpha} c_{\mathbf{k}_1, \alpha}^+(\tau_1) c_{\mathbf{k}'_1, \alpha}(\tau'_1) \dots c_{\mathbf{k}_{q_\alpha}, \alpha}^+(\tau_{q_\alpha}) c_{\mathbf{k}'_{q_\alpha}, \alpha}(\tau'_{q_\alpha}) \right\} \right\rangle_c \left\langle T_\tau \left\{ \prod_{\alpha} f_{\alpha}(\tau_1) f_{\alpha}^+(\tau'_1) \dots f_{\alpha}(\tau_{q_\alpha}) f_{\alpha}^+(\tau'_{q_\alpha}) \right\} \right\rangle_f, \end{aligned} \quad (9)$$

where $\langle \dots \rangle_{c(f)} = \text{Tr}_{c(f)} \left(e^{-\beta \mathcal{H}_{c(f)}} \dots \right) / \mathcal{Z}_{c(f)}$. In the last part of eq. (9) we summed for the state number ' q_α ' by the change $\sum_q \rightarrow \sum_{\{q_\alpha\}} q! / \prod_{\alpha} (q_\alpha!)$, where $\sum_{\alpha} q_\alpha = q$.

We can perform the trace calculation over the conduction electron operators by using Wick's theorem:

$$\begin{aligned}
& \sum_{\mathbf{k}_1 \dots \mathbf{k}_{q_\alpha}} \sum_{\mathbf{k}'_1 \dots \mathbf{k}'_{q_\alpha}} (V^2)^{q_\alpha} \left\langle T_\tau \left\{ \prod_{\alpha} c_{\mathbf{k}_1, \alpha}^+(\tau_1) c_{\mathbf{k}'_1, \alpha}(\tau'_1) \dots c_{\mathbf{k}_{q_\alpha}, \alpha}^+(\tau_{q_\alpha}) c_{\mathbf{k}'_{q_\alpha}, \alpha}(\tau'_{q_\alpha}) \right\} \right\rangle_c \\
&= \sum_{\mathbf{k}_1 \dots \mathbf{k}_{q_\alpha}} \sum_{\mathbf{k}'_1 \dots \mathbf{k}'_{q_\alpha}} (V^2)^{q_\alpha} \sum_{\{c\}} \text{sign}(c) \left\langle T_\tau \left\{ \prod_{\alpha} c_{\mathbf{k}_1}^+(\tau_1) c_{\mathbf{k}'_1}(\tau'_1) \dots \langle T_\tau c_{\mathbf{k}_{q_\alpha}}^+(\tau_{q_\alpha}) c_{\mathbf{k}'_{q_\alpha}}(\tau'_{q_\alpha}) \right\rangle \right\} \right\rangle_c = \prod_{\alpha} (\det \hat{\Delta}_{\alpha}^{(q_\alpha)}), \tag{10}
\end{aligned}$$

where $\{c\}$ means the all possible connections, and matrix $\hat{\Delta}_{\alpha}^{(q_\alpha)}$ has the form

$$\hat{\Delta}_{\alpha}^{(q_\alpha)} = V^2 \begin{pmatrix} g_{\alpha}(\tau'_1 - \tau_1) & g_{\alpha}(\tau'_2 - \tau_1) & \cdot & g_{\alpha}(\tau'_{q_\alpha} - \tau_1) \\ g_{\alpha}(\tau'_1 - \tau_2) & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ g_{\alpha}(\tau'_1 - \tau_{q_\alpha}) & \cdot & \cdot & g_{\alpha}(\tau'_{q_\alpha} - \tau_{q_\alpha}) \end{pmatrix}, \tag{11}$$

where

$$g_{\alpha}(\tau' - \tau) = \sum_{\mathbf{k}} g_{\alpha, \mathbf{k}}(\tau' - \tau) = -\langle T_\tau c_{\mathbf{k}, \alpha}(\tau') c_{\mathbf{k}, \alpha}(\tau)^+ \rangle_c \tag{12}$$

is the bare conduction electron Green's function.

The sequence of τ -integrals in the last part of eq. (9) is arbitrary. By time-ordering the arguments we obtain

$$\int_0^\beta d\tau_1 \dots \int_0^\beta d\tau_{q_\alpha} = (q_\alpha!) \int^{\text{ordered}} d\tau_1 \dots \int^{\text{ordered}} d\tau_{q_\alpha} \equiv (q_\alpha!) \int^{\text{ordered}} \mathcal{D}[\tau], \tag{13}$$

where $\beta > \tau_1 > \tau_2 > \dots > \tau_{q_\alpha} \geq 0$. Thus, we obtain the partition function as

$$\begin{aligned}
\frac{\mathcal{Z}}{\mathcal{Z}_c \mathcal{Z}_f} &= \sum_{\{q_\alpha\}} \int^{\text{ordered}} \mathcal{D}[\tau] \int^{\text{ordered}} \mathcal{D}[\tau'] \prod_{\alpha} (\det \hat{\Delta}_{\alpha}^{(q_\alpha)}) \left\langle T_\tau \left\{ \prod_{\alpha} f_{\alpha}(\tau_1) f_{\alpha}^+(\tau'_1) \dots f_{\alpha}(\tau_{q_\alpha}) f_{\alpha}^+(\tau'_{q_\alpha}) \right\} \right\rangle_f \\
&\equiv \int \mathcal{D}[q] W[q], \tag{14}
\end{aligned}$$

where

$$W[q] = \prod_{\alpha} (\det \hat{\Delta}_{\alpha}^{(q_\alpha)}) \left\langle T_\tau \left\{ \prod_{\alpha} f_{\alpha}(\tau_1) f_{\alpha}^+(\tau'_1) \dots f_{\alpha}(\tau_{q_\alpha}) f_{\alpha}^+(\tau'_{q_\alpha}) \right\} \right\rangle_f, \tag{15}$$

$$\int \mathcal{D}[q] = \sum_{\{q_\alpha\}} \int^{\text{ordered}} \mathcal{D}[\tau] \int^{\text{ordered}} \mathcal{D}[\tau']. \tag{16}$$

2.2 Metropolis algorithm

The average of quantity \mathcal{O} is given by

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[q] W[q] \mathcal{O}(q), \quad (17)$$

where the partition function has the form $\mathcal{Z} = \int \mathcal{D}[q] W[q]$. In Monte Carlo simulation we evaluate the average given by eq. (17) stochastically. It is not possible to consider all the configurations q . Instead, we choose a set $\{q\}$ where the configurations q are generated by the weight $\widetilde{W}[q]$. In this case the average is reweighted as

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}[q] W[q] / \widetilde{W}[q] \mathcal{O}(q)}{\int \mathcal{D}[q] W[q] / \widetilde{W}[q]}. \quad (18)$$

The simplest case when we generate the configurations randomly. However, the sampling is more efficient when we generate the configurations with the weight they contribute to the partition function, namely when $\widetilde{W}[q] = W[q]$. This method is called *importance sampling*. The importance sampling method can be achieved when we assure the

- * *ergodicity*: each configuration can be reached during the generates of configurations;
- * *detailed balance condition*: $W_{xy}/W_{yx} = W[y]/W[x]$, where W_{xy} is the transition probability from configuration x to configuration y , and $W[x]$ is the weight of the configuration x .

The detailed balance condition can be realized by the *Metropolis algorithm*. In this algorithm we divide W_{xy} into a proposal part and an acceptance part as

$$W_{xy} = W_{\text{prop}}(x \rightarrow y) W_{\text{acc}}(x \rightarrow y). \quad (19)$$

We can find that

$$W_{\text{acc}}(x \rightarrow y) = \min \left(1, \frac{W[y] W_{\text{prop}}(y \rightarrow x)}{W[x] W_{\text{prop}}(x \rightarrow y)} \right). \quad (20)$$

When we generate a new configuration y from the configuration x , we accept this new configuration y by the acceptance rate $W_{\text{acc}}(x \rightarrow y)$. Namely, we choose a random number r from the interval $[0, 1]$, and accept the new configuration if $r < W_{\text{acc}}$. The average in the Monte Carlo simulation is obtained as a simple arithmetic average

$$\langle \mathcal{O} \rangle_{\text{MC}} = \frac{1}{N} \sum_{q_1, \dots, q_N} \mathcal{O}(q_k), \quad (21)$$

since $\widetilde{W}[q] = W[q]$ in eq. (18).

2.3 Segment picture

In the case of the Anderson model the configuration is a set of the imaginary times: $\{\tau_1, \tau'_1, \dots, \tau_k, \tau'_k\}$. The f -operators f and f^+ should occur in alternating order, otherwise the expectation value in eq. (14) is zero. This statement is held also for models where the Hamiltonian has only density-density interaction terms (no exchange terms), i.e., it is diagonal in component indices. In this case the configuration can be represented by segment picture. The two possible configurations are shown in Fig. 1. There are two components for the f -electron operators, namely $\sigma = \uparrow, \downarrow$. These two

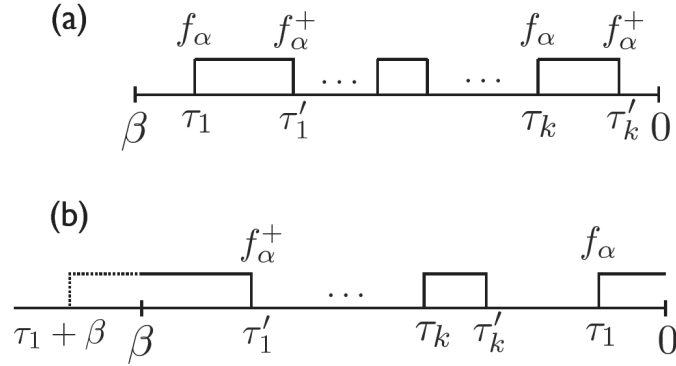


Figure 1: Segment representation of a k th-order configuration. The lines correspond to occupied f -electron state (particle number 1), while the empty spaces to particle number 0.

components lead to two independent channels in the segment picture as it is shown in Fig. 2.

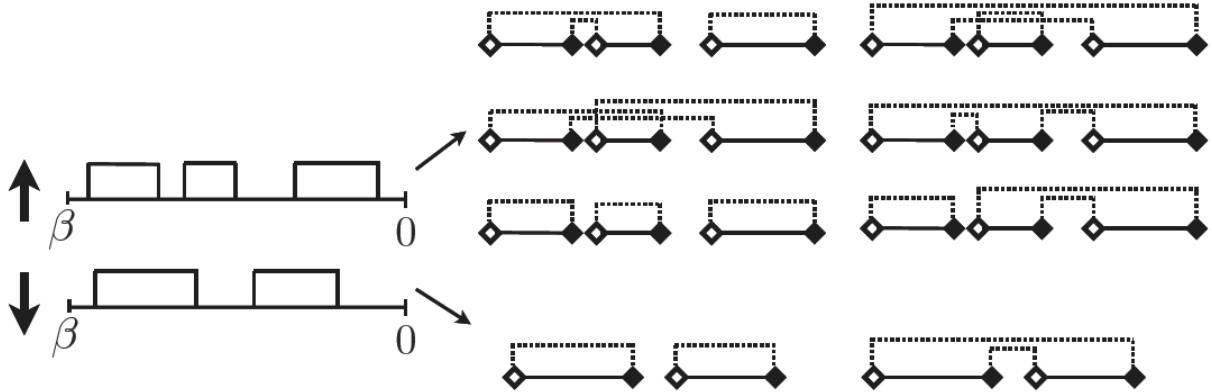


Figure 2: The two spin indices leads to two independent channels in the segment picture. The right part of the figure shows all possible connections of operators $c^+(f)$ and $c(f^+)$, where the weighted contributions of the diagrams are summed up into the determinant of matrix $\Delta_\alpha^{(k)}$ with $k = \uparrow, \downarrow$. Open and filled diamonds correspond to operators $c^+(f)$ and $c(f^+)$, respectively, while the dashed lines mean the hybridization lines $V^2 g_\alpha (\tau'_j - \tau_i)$.

There are two basic operations when we generate a new configuration: addition or removal a segment. When we add a new segment to a k th-order configuration, first we add the operator $f^+(\tau')$ by choosing τ' from the interval $(\beta, 0]$. If $f^+(\tau')$ is on an existing segment, we reject the new configuration. If the operator $f^+(\tau')$ is located between the operators $f^+(\tau'_l)$ and $f(\tau_{l+1})$, we put the operator $f(\tau)$ somewhere in the interval $[0, l_{\max}]$, where $l_{\max} = \text{mod}(\tau'_l + \beta - \tau', \beta)$. The transition probability of this process is given by

$$W_{\text{prop}}(k \rightarrow k+1) = \frac{1}{\beta l_{\max}}. \quad (22)$$

When we remove a segment from a $k+1$ th-order configuration, we obtain the transition probability as

$$W_{\text{prop}}(k+1 \rightarrow k) = \frac{1}{k+1} \quad (23)$$

since we have $k+1$ choice to remove one segment. The acceptance rate given by eq. (20) becomes for the Anderson model as

$$W_{\text{acc}}(k \rightarrow k+1) = \min\left(1, \frac{W[k+1] \beta l_{\max}}{W[k] (k+1)}\right). \quad (24)$$

First, let us consider the case of $U = 0$, when it is enough to consider only one channel. In this case we can write

$$\frac{W[k+1]}{W[k]} = \frac{\det \hat{\Delta}^{(k+1)} \langle T_\tau f(\tau_1) f^+(\tau'_1) \dots f(\tau_{k+1}) f^+(\tau'_{k+1}) \rangle_f}{\det \hat{\Delta}^{(k)} \langle T_\tau f(\tau_1) f^+(\tau'_1) \dots f(\tau_k) f^+(\tau'_k) \rangle_f}, \quad (25)$$

expectation value in eq. (25) can be evaluated as

$$\langle \mathcal{O}_1(\tau_1) \dots \mathcal{O}_{2k}(\tau_{2k}) \rangle = \text{Tr} \left(e^{-\mathcal{H}_f(\beta-\tau_1)} \mathcal{O}_1(\tau_1) e^{-\mathcal{H}_f(\tau_1-\tau_2)} \dots \mathcal{O}_{2k}(\tau_{2k}) e^{-\mathcal{H}_f(\tau_{2k})} \right), \quad (26)$$

where

$$\mathcal{H}_f = \varepsilon_f \sum_{\sigma} f_{\sigma}^+ f_{\sigma}, \quad (27)$$

and operators \mathcal{O}_k denote the f -operators f or f^+ . The trace is evaluated as $\text{Tr}_f = \sum_{n=0,1} \langle n | \dots | n \rangle$.

$$\begin{aligned} & \langle T_\tau f(\tau_1) f^+(\tau'_1) \dots f(\tau_k) f^+(\tau'_k) \rangle_f \\ &= \sum_{n=0,1} \langle n | e^{-\mathcal{H}_f(\beta-\tau_1)} \mathcal{O}_1(\tau_1) | n \rangle \langle n | e^{-\mathcal{H}_f(\tau_1-\tau_2)} \mathcal{O}_2(\tau_2) | n \rangle \langle n | \dots e^{-\mathcal{H}_f(\tau_{2k-1}-\tau_{2k})} \mathcal{O}_{2k}(\tau_{2k}) e^{-\mathcal{H}_f(\tau_{2k})} | n \rangle \\ &= e^{-E_0(\beta-\tau_1)} \langle n^{(0)} | \mathcal{O}_1(\tau_1) | n^{(1)} \rangle e^{-E_1(\tau_1-\tau_2)} \langle n^{(1)} | \mathcal{O}_2(\tau_2) | n^{(2)} \rangle \dots \langle n^{(2k-1)} | \mathcal{O}_{2k}(\tau_{2k}) | n^{(2k)} \rangle e^{-E_{2k}(\tau_{2k})} \end{aligned} \quad (28)$$

The non-zero matrix elements in eq. (28) are when $\langle n^{(l-1)} | \mathcal{O}_l(\tau_l) | n^{(l)} \rangle$ is $\langle 0 | f | 1 \rangle$ or $\langle 1 | f^+ | 0 \rangle$ with the energy eigenvalue $E_{l-1} = 0$ and $E_{l-1} = \varepsilon_f$, respectively. The first and last operators are $\mathcal{O}_1 = f$

and $\mathcal{O}_{2k} = f^+$ which gives that $E_0 = E_{2k} = 0$, and the operators have the sequence $ff^+ff^+\dots ff^+$. Thus, expression (28) becomes

$$\left\langle T_\tau f(\tau_1)f^+(\tau'_1)\dots f(\tau_k)f^+(\tau'_k) \right\rangle_f = e^{-\varepsilon_f(\tau_1-\tau'_1)}e^{-\varepsilon_f(\tau_2-\tau'_2)}\dots e^{-\varepsilon_f(\tau_k-\tau'_k)} = e^{-\varepsilon_f \sum_q l_q}, \quad (29)$$

where $l_q = \tau_q - \tau'_q$ is the length of the q th segment.

When we consider also the Coulomb interaction term ($U \neq 0$), then the trace over the f states becomes

$$\left\langle T_\tau \left\{ \prod_{\alpha=\sigma,\bar{\sigma}} f_\alpha(\tau_1)f_\alpha^+(\tau'_1)\dots f_\alpha(\tau_{q_\alpha})f_\alpha^+(\tau'_{q_\alpha}) \right\} \right\rangle_f = e^{-\varepsilon_f \sum_q l_q} e^{-U l_{\text{ov}}}, \quad (30)$$

where l_{ov} is the overlap between the two channels σ and $\bar{\sigma}$ since the Coulomb interaction acts when we have $|\uparrow\rangle$ and $|\downarrow\rangle$ f -electron states at the same imaginary time. Thus, eq. (24) becomes

$$W_{\text{acc}}(k \rightarrow k+1) = \min \left(1, \text{sign}(\tau - \tau') \frac{\beta l_{\text{max}}}{k+1} \frac{\det \hat{\Delta}^{(k+1)}}{\det \hat{\Delta}^{(k)}} e^{-\varepsilon_f \tilde{l}} e^{-U \Delta l_{\text{ov}}} \right), \quad (31)$$

where \tilde{l} is the length of the newly inserted segment, and Δl_{ov} means the change in the overlap between the two channels. The term $\text{sign}(\tau - \tau')$ is inserted because a minus sign comes in case (b) of Fig. 1 when we rearrange the f -operators into the same sequence as it is in case (a).

The acceptance rate for the process $k \rightarrow k-1$ can be obtained by similar consideration as

$$W_{\text{acc}}(k \rightarrow k-1) = \min \left(1, \text{sign}(\tau - \tau') \frac{k}{\beta l_{\text{max}}} \frac{\det \hat{\Delta}^{(k-1)}}{\det \hat{\Delta}^{(k)}} e^{\varepsilon_f \tilde{l}} e^{U \Delta l_{\text{ov}}} \right). \quad (32)$$

There are a further operation besides the segment addition and removal that we use in the simulation. This is the shift operation when we shift one of the τ s or τ' s, which makes the sampling more efficient. The acceptance rate of the shift operation is given as

$$W_{\text{acc}}(k \rightarrow k)^{(\text{shift})} = \min \left(1, (\tau - \tau') \frac{k}{\beta l_{\text{max}}} \frac{\det \tilde{\hat{\Delta}}^{(k)}}{\det \hat{\Delta}^{(k)}} e^{-\varepsilon_f(\tilde{l}-l)} e^{-U \Delta l_{\text{ov}}} \right), \quad (33)$$

where l and \tilde{l} are the lengths of the segment before and after the shift operation, respectively.

The determinant ratios in eqs. (31), (32), and (33), and also the matrix inverse $\hat{M} = (\hat{\Delta})^{-1}$ which will be important in the calculation of the f -electron Green's function can be calculated by using fast-update formulas. The derivation is given in Appendix B.

The probability distribution of the random walk in the configuration space according to the acceptance rates $W_{\text{acc}}(k \rightarrow k+1)$ and $W_{\text{acc}}(k \rightarrow k-1)$ is shown in Fig. 3.

We note that special attention is necessary when all the segments are absent in one of the channels. In this case the trace calculation over the f states is modified as follows. First we discuss the case

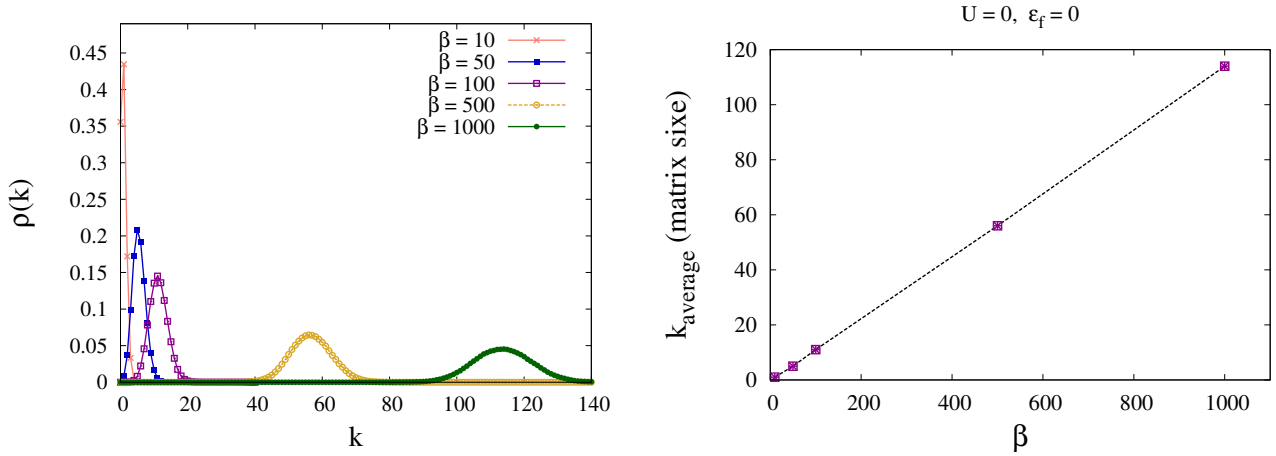


Figure 3: *Left*: Probability distribution ρ of the random walk in the configuration space as a function of the expansion order (k) at temperatures $\beta = 10, 50, 100, 500, 1000$. *Right*: The position of the maximum probability as a function of the inverse temperature. The parameter values are $U = 0$, $V^2 = 0.1$, $\epsilon_f = 0$.

of segment addition. We note the number of segments in channel A by k_A , and write the acceptance rate as

$$W_{\text{acc}}(k \rightarrow k+1) = \min \left(1, \text{sign}(\tau - \tau') \frac{\beta l_{\text{max}} \det \hat{\Delta}^{(k+1)}}{k+1 \det \hat{\Delta}^{(k)}} Q \right), \quad (34)$$

where

$$Q = \frac{\text{Tr}_f \left(e^{-\beta \mathcal{H}_f} f(\tau_1) f^+(\tau'_1) \dots f(\tau_{k+1}) f^+(\tau'_{k+1}) \right)}{\text{Tr}_f \left(e^{-\beta \mathcal{H}_f} f(\tau_1) f^+(\tau'_1) \dots f(\tau_k) f^+(\tau'_k) \right)}. \quad (35)$$

We have to distinguish the following cases:

- $k_\sigma = 0, k_{\bar{\sigma}} \neq 0$

The empty channel σ gives the contributions

$$\begin{aligned} \langle 0n_{\bar{\sigma}} | \dots | 0n_{\bar{\sigma}} \rangle &\rightarrow 1 \\ \langle 1n_{\bar{\sigma}} | \dots | 1n_{\bar{\sigma}} \rangle &\rightarrow e^{-\beta \epsilon_f}, \end{aligned}$$

where in the last term the empty configuration is taken as the full segment (= filled from β to 0) since the empty and full configurations are degenerate. The notation \dots means $e^{-\beta \mathcal{H}_f} f f^+ \dots f f^+$, which should be rewritten as in eq. (26). Combining these results with the other channel $\bar{\sigma}$, we obtain before the segment addition

$$\langle 01 | \dots | 01 \rangle \rightarrow 0$$

$$\begin{aligned}
\langle 11|\dots|11\rangle &\rightarrow 0 \\
\langle 00|\dots|00\rangle &\rightarrow e^{-l_{\bar{\sigma}}\varepsilon_f} \\
\langle 10|\dots|10\rangle &\rightarrow e^{-l_{\bar{\sigma}}\varepsilon_f} e^{-\beta\varepsilon_f} e^{-l_{\bar{\sigma}}U}.
\end{aligned}$$

Adding a new segment with length l_{σ} to the channel σ , we obtain

$$\begin{aligned}
\langle 01|\dots|01\rangle &\rightarrow 0 \\
\langle 11|\dots|11\rangle &\rightarrow 0 \\
\langle 00|\dots|00\rangle &\rightarrow e^{-l_{\sigma}\varepsilon_f} e^{-l_{\bar{\sigma}}\varepsilon_f} e^{-l_{\sigma}U} \\
\langle 10|\dots|10\rangle &\rightarrow 0.
\end{aligned}$$

Thus,

$$Q = \frac{e^{-l_{\sigma}\varepsilon_f} e^{-l_{\bar{\sigma}}\varepsilon_f} e^{-l_{\sigma}U}}{e^{-l_{\bar{\sigma}}\varepsilon_f} + e^{-l_{\bar{\sigma}}\varepsilon_f} e^{-\beta\varepsilon_f} e^{-l_{\bar{\sigma}}U}} = \frac{e^{-l_{\sigma}\varepsilon_f} e^{-l_{\sigma}U}}{1 + e^{-\beta\varepsilon_f} e^{-l_{\bar{\sigma}}U}}. \quad (36)$$

- $k_{\sigma} = 0, k_{\bar{\sigma}} = 0$

Before the segment addition we obtain

$$\begin{aligned}
\langle 01|\dots|01\rangle &\rightarrow e^{-\beta\varepsilon_f} \\
\langle 11|\dots|11\rangle &\rightarrow e^{-\beta\varepsilon_f} e^{-\beta\varepsilon_f} e^{-\beta U} \\
\langle 00|\dots|00\rangle &\rightarrow 1 \\
\langle 10|\dots|10\rangle &\rightarrow e^{-\beta\varepsilon_f},
\end{aligned}$$

and after adding a new segment with length l_{σ} to the channel σ :

$$\begin{aligned}
\langle 01|\dots|01\rangle &\rightarrow e^{-l_{\sigma}\varepsilon_f} e^{-\beta\varepsilon_f} e^{-l_{\sigma}U} \\
\langle 11|\dots|11\rangle &\rightarrow 0 \\
\langle 00|\dots|00\rangle &\rightarrow e^{-l_{\sigma}\varepsilon_f} \\
\langle 10|\dots|10\rangle &\rightarrow 0.
\end{aligned}$$

Thus, we obtain

$$Q = \frac{e^{-l_{\sigma}\varepsilon_f} (1 + e^{-\beta\varepsilon_f} e^{-l_{\sigma}U})}{1 + 2e^{-\beta\varepsilon_f} + e^{-\beta(2\varepsilon_f + U)}}. \quad (37)$$

- $k_{\sigma} \neq 0, k_{\bar{\sigma}} = 0$

Before the segment addition we obtain

$$\begin{aligned}
\langle 01|\dots|01\rangle &\rightarrow e^{-l_\sigma \varepsilon_f} e^{-\beta \varepsilon_f} e^{-l_\sigma U} \\
\langle 11|\dots|11\rangle &\rightarrow 0 \\
\langle 00|\dots|00\rangle &\rightarrow e^{-l_\sigma \varepsilon_f} \\
\langle 10|\dots|10\rangle &\rightarrow 0,
\end{aligned}$$

and after adding a new segment with length l_σ to the channel σ :

$$\begin{aligned}
\langle 01|\dots|01\rangle &\rightarrow e^{-(l_\sigma+l_{\bar{\sigma}})\varepsilon_f} e^{-\beta \varepsilon_f} e^{-(l_\sigma+l_{\bar{\sigma}})U} \\
\langle 11|\dots|11\rangle &\rightarrow 0 \\
\langle 00|\dots|00\rangle &\rightarrow e^{-(l_\sigma+l_{\bar{\sigma}})\varepsilon_f} \\
\langle 10|\dots|10\rangle &\rightarrow 0.
\end{aligned}$$

Thus, we obtain

$$Q = \frac{e^{-\tilde{l}_\sigma \varepsilon_f} (1 + e^{-\beta \varepsilon_f} e^{-(l_\sigma + \tilde{l}_\sigma)U})}{1 + e^{-\beta \varepsilon_f} e^{-l_\sigma U}}. \quad (38)$$

- $k_\sigma \neq 0, k_{\bar{\sigma}} \neq 0$

We already discussed this case and the result is given in eq. (31).

In the case of segment removal, the acceptance rate is given by

$$W_{\text{acc}}(k \rightarrow k-1) = \min \left(1, \text{sign}(\tau - \tau') \frac{k}{\beta l_{\text{max}}} \frac{\det \hat{\Delta}^{(k-1)}}{\det \hat{\Delta}^{(k)}} Q' \right), \quad (39)$$

where $Q' = Q^{-1}$.

In the case of the shift operation we have to distinguish the case

- $k_\sigma \neq 0, k_{\bar{\sigma}} = 0$

Before the segment addition we obtain

$$\begin{aligned}
\langle 01|\dots|01\rangle &\rightarrow e^{-l_\sigma \varepsilon_f} e^{-\beta \varepsilon_f} e^{-l_\sigma U} \\
\langle 11|\dots|11\rangle &\rightarrow 0 \\
\langle 00|\dots|00\rangle &\rightarrow e^{-l_\sigma \varepsilon_f} \\
\langle 10|\dots|10\rangle &\rightarrow 0,
\end{aligned}$$

and after adding a new segment with length l_σ to the channel σ :

$$\begin{aligned}\langle 01|\dots|01\rangle &\rightarrow e^{-\bar{l}_\sigma \varepsilon_f} e^{-\beta \varepsilon_f} e^{-\bar{l}_\sigma U} \\ \langle 11|\dots|11\rangle &\rightarrow 0 \\ \langle 00|\dots|00\rangle &\rightarrow e^{-\bar{l}_\sigma \varepsilon_f} \\ \langle 10|\dots|10\rangle &\rightarrow 0.\end{aligned}$$

Thus, we obtain

$$Q = \frac{e^{-(\bar{l}_\sigma - l_\sigma) \varepsilon_f} (1 + e^{-\beta \varepsilon_f} e^{-\bar{l}_\sigma U})}{1 + e^{-\beta \varepsilon_f} e^{-l_\sigma U}}. \quad (40)$$

2.4 Measuring the f -electron Green's function

The f -electron Green's function is given by

$$G_f(\tau' - \tau) = -\langle T_\tau f(\tau') f(\tau)^+ \rangle. \quad (41)$$

In order to measure this Green's function, we need a configuration where operators $f(\tau')$ and $f(\tau)^+$ are unconnected. In the hybridization method it is achieved by removing one of the hybridization lines.

We consider a k th-order partition function configuration, which weight is given by

$$p_Z = \langle T_\tau f(\tau_1) f^+(\tau'_1) \dots f(\tau_k) f^+(\tau'_k) \rangle_f \det \hat{\Delta}^{(k)}. \quad (42)$$

We remove the hybridization line $V^2 g_\alpha(\tau'_i - \tau_j)$, and then we can write the weight of the "Green's function configuration" as

$$\begin{aligned}p_G &= \langle T_\tau f(\tau_j) f(\tau'_i)^+ f(\tau_1) f^+(\tau'_1) \dots f(\tau_{k-1}) f^+(\tau'_{k-1}) \rangle_f \det \hat{\Delta}^{(k-1)} \\ &= (-1)^{i+j} \langle T_\tau f(\tau_1) f^+(\tau'_1) \dots f(\tau_k) f^+(\tau'_k) \rangle_f \det \hat{\Delta}^{(k-1)}.\end{aligned} \quad (43)$$

The contribution to the Green's function at $\tau = \tau'_i - \tau_j$ is given by

$$\frac{p_G}{p_Z} = \frac{(-1)^{i+j} \det \hat{\Delta}_{\neq ij}^{(k-1)}}{\det \hat{\Delta}^{(k)}}, \quad (44)$$

where notation $\hat{\Delta}_{\neq ij}^{(k-1)}$ means that line i and column j are removed from the matrix $\hat{\Delta}^{(k)}$. Using the matrix identity

$$(-1)^{i+j} \det \hat{\Delta}_{\neq ij}^{(k-1)} = \det \hat{\Delta}^{(k)} \left(\hat{\Delta}^{(k)} \right)_{ji}^{-1}, \quad (45)$$

we obtain the f -electron Green's function as ²

$$G_f(\tau) = \left\langle \frac{1}{\beta} \sum_{ij}^k \left(\hat{\Delta}^{(k)} \right)_{ji}^{-1} \delta(\tau, \tau'_i - \tau_j) \right\rangle_{\text{MC}} = \left\langle \frac{1}{\beta} \sum_{ij}^k \hat{M}_{ji}^{(k)} \delta(\tau, \tau'_i - \tau_j) \right\rangle_{\text{MC}}. \quad (46)$$

2.5 Correlation functions

Before discussing the correlation functions, we consider the density operator $n = f^+ f$. In CT-QMC we obtain the density operator as

$$\langle n \rangle = \frac{1}{\beta} \int_0^\beta d\tau' n(\tau') = \frac{1}{\beta} \sum_i (\tau_i - \tau'_i), \quad (47)$$

which is nothing else than the total length of the segments.

Now we discuss the density-density correlation function:

$$\begin{aligned} \chi(\tau) &= \langle n(\tau) n(0) \rangle = \langle T_\tau n(\tau) n(0) \rangle = \langle T_\tau f^+(\tau) f(\tau) f^+(0) f(0) \rangle = -\langle T_\tau f^+(\tau) f^+(0) f(\tau) f(0) \rangle \\ &= -\langle T_\tau f^+(\tau) f(0) \rangle \langle T_\tau f^+(0) f(\tau) \rangle + \langle T_\tau f^+(\tau) f(\tau) \rangle \langle T_\tau f^+(0) f(0) \rangle \\ &= -\langle T_\tau f(0) f^+(\tau) \rangle \langle T_\tau f(\tau) f^+(0) \rangle + \langle n \rangle^2 = (-G_f(-\tau))(-G_f(\tau)) + \langle n \rangle^2 = G_f(\tau)^2 + \langle n \rangle^2 \end{aligned} \quad (48)$$

We introduce $\tilde{\chi}(\tau) \equiv \chi(\tau) - \langle n \rangle^2$.

In CT-QMC we can evaluate $\langle n(\tau) n(0) \rangle$ as

$$\langle n(\tau) n(0) \rangle = \frac{1}{\beta} \int_0^\beta d\tau' n(\tau + \tau') n(\tau') = \left\langle \frac{1}{\beta} \int_0^\beta d\tau' \frac{\langle T_\tau n(\tau + \tau') n(\tau') f f^+ \dots f f^+ \rangle_f}{\langle T_\tau f f^+ \dots f f^+ \rangle_f} \right\rangle_{\text{MC}}. \quad (49)$$

This ratio is evaluated in CT-QMC as the overlap between a configuration and its shift by τ as it is shown in Fig. 4.

In the limits of $\tau = 0$ and $\tau = \beta$ we obtain

$$\tilde{\chi}(0) = \tilde{\chi}(\beta) = \langle n^2 \rangle - \langle n \rangle^2 = \langle n \rangle - \langle n \rangle^2 = 1/2 - (1/2)^2 = (1/2)^2. \quad (50)$$

The result for the f -electron Green's function $G_f(\tau)$ and the density-density correlation function $\tilde{\chi}(\tau)$ obtained by CT-QMC is shown in Fig. 5.

²Another derivation of this formula is: $G_f(\tau'_i - \tau_j) = -\int D \det \hat{\Delta}_{\neq ij}^{(k-1)} \langle T_\tau f(\tau_j) f(\tau'_i)^+ f(\tau_1) f^+(\tau'_1) \dots f(\tau_{k-1}) f^+(\tau'_{k-1}) \rangle_f = -\int D (-1)^{i+j} \det \hat{\Delta}^{(k)} \left(\hat{\Delta}^{(k)} \right)_{ji}^{-1} \langle T_\tau f(\tau_j) f(\tau'_i)^+ f(\tau_1) f^+(\tau'_1) \dots f(\tau_{k-1}) f^+(\tau'_{k-1}) \rangle_f = -\int D \det \hat{\Delta}^{(k)} \left(\hat{\Delta}^{(k)} \right)_{ji}^{-1} \langle T_\tau f(\tau_1) f^+(\tau'_1) \dots f(\tau_k) f^+(\tau'_k) \rangle_f = -\left\langle \left(\hat{\Delta}^{(k)} \right)_{ji}^{-1} \right\rangle = -\left\langle \hat{M}_{ji}^{(k)} \right\rangle$

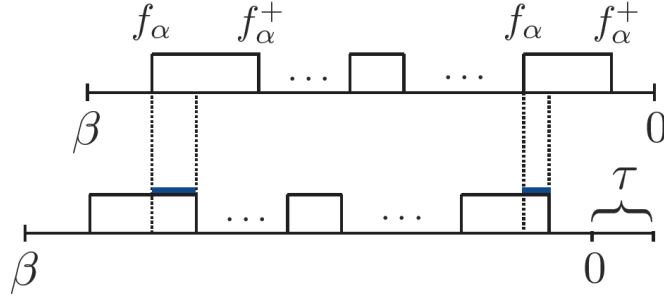


Figure 4: Calculation of the susceptibility $\langle n(\tau)n(0) \rangle$ in CT-QMC as the calculation of overlap between a configuration and its shift by τ .

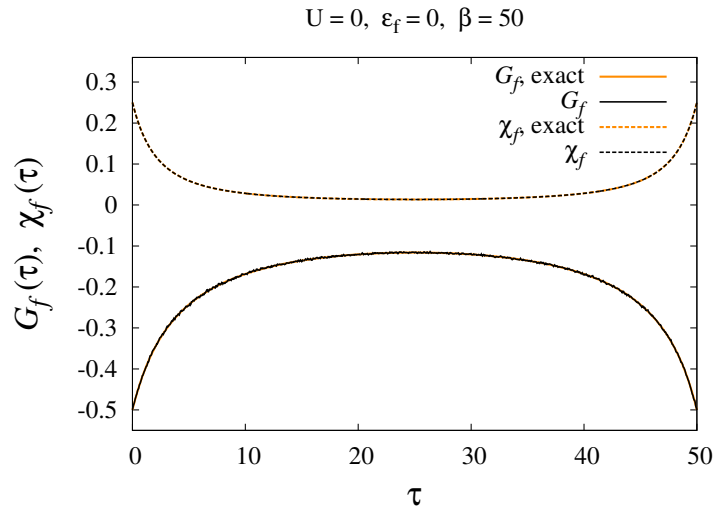


Figure 5: Imaginary-time dependence of the f -electron Green's function $G_f(\tau)$ and the density-density correlation function $\tilde{\chi}(\tau)$. The parameter values are $U = 0$, $\beta = 50$, $V^2 = 0.1$, $\varepsilon_f = 0$. The exact results are also shown by orange color.

2.6 Spectral function

The spectral function (density of states) as a function of the real frequency is given by

$$\rho(\omega) = -\frac{1}{\pi} \text{Im}[G(\omega + i\delta)]. \quad (51)$$

The spectral function in the case of the symmetric Anderson model for different temperatures and Coulomb interactions is shown in Fig. 6.

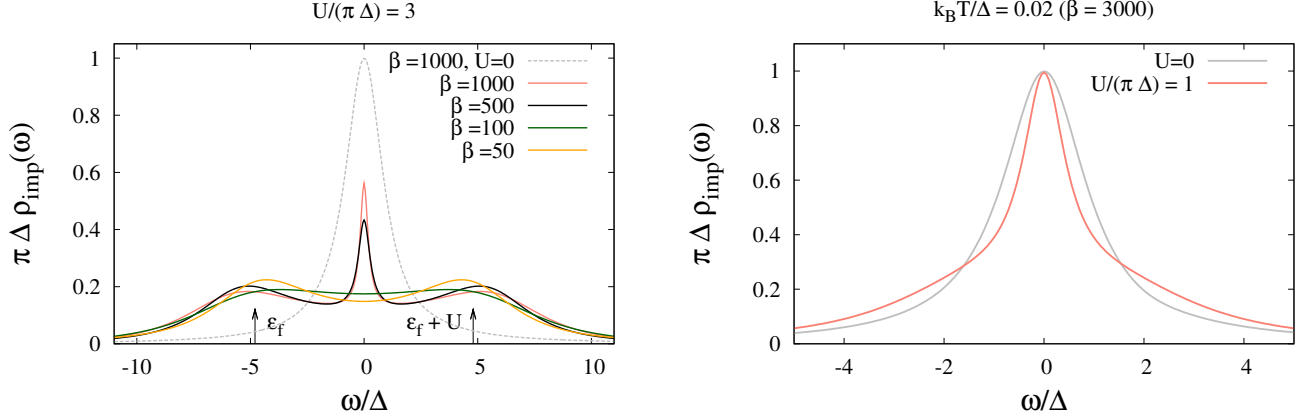


Figure 6: Impurity density of states as a function of frequency in the case of the symmetric Anderson model for $U/(\pi\Delta) = 3$ with temperatures $\beta = 50, 100, 500, 1000$ (*upper panel*) and for $\beta = 3000$ with Coulomb interactions $U/(\pi\Delta) = 1$ and $U = 0$ (*bottom panel*). The parameter values are $V^2 = 0.01$, $D = 1$, ($\Delta = 0.0156$).

3 Dynamical mean field theory (DMFT)

In general, it is very difficult to solve lattice fermion problems. Thus, we need to use some approximation. A commonly used method is the dynamical mean field theory (DMFT), which approximate the original lattice problem by an effective impurity problem plus a self-consistency condition (see Fig. 7), where the effective impurity problem can be solved efficiently by the CT-QMC impurity solver. In infinite dimension the diagonal elements of the Green's function are much larger than the off-diagonal elements ($G_{ii}(\tau) \gg G_{ij}(\tau)$). Thus, the self-energy becomes local ($\Sigma(\mathbf{k}, \tau) \rightarrow \Sigma(\tau)$), which leads to that DMFT is exact in $d = \infty$. First, we discuss the formulation for the f -electrons. Formulation for the f -electrons:

In the effective impurity picture the site is embedded into an effective medium described by the cavity Green's function \mathcal{G} , which incorporates the effect of interaction U at the surrounding sites. Thus, the Green's function is given by

$$G_f(z)^{-1} = \mathcal{G}_f(z)^{-1} - \Sigma_f(z). \quad (52)$$

The self-consistency condition means that the Green's function $G_f(z)$ is the same as the site-diagonal part of the Green's function of the original lattice problem, which is the case in infinite dimension. Namely,

$$G_f(z) = \overline{G_f(\mathbf{k}, z)} = \int d\varepsilon \rho(\varepsilon) \left(z - \varepsilon_f - \Sigma_f(z) - \frac{V^2}{z - \varepsilon} \right)^{-1}. \quad (53)$$

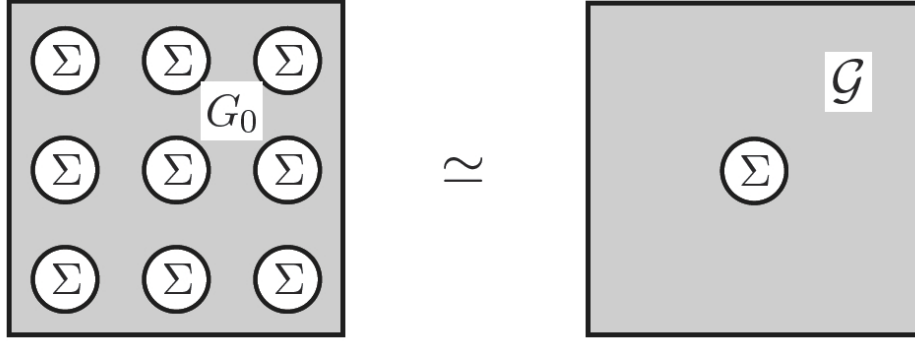


Figure 7: *Left side* shows the original lattice problem, which is approximated by an effective impurity problem in DMFT shown in the *right side*.

We use iteration to perform the DMFT procedure. First, we start with a trial cavity Green's function $\mathcal{G}_f(z)$ and use the CT-QMC solver to obtain the Green's function $G_f(z)$. Using eq. (52) we obtain the self-energy $\Sigma_f(z)$, what we use in eq. (53) to obtain a further approximate for the Green's function $G_f(z)$. Then we calculate the cavity Green's function from equation $\mathcal{G}_f(z)^{-1} = G_f(z)^{-1} + \Sigma_f(z)$, what we use in the next step of the iteration. We continue this procedure until a convergent result is obtained for $G_f(z)$.

Right part of Fig. 8 shows the self-energy

$$\Sigma_f(z) = \mathcal{G}_f(z)^{-1} - G_f(z)^{-1}, \quad (54)$$

which is very noisy for large frequencies because the inversion of $G_f(z)$ in eq. (54) amplifies the statistical errors. Thus, we may have problem in DMFT that we can cross over if we reformulate the DMFT procedure for the conduction electrons. We can do it as far as the f -level has no dispersion, i.e. it is sharp.

Formulation for the conduction electrons:

First we derive a relation between the f -electron Green's function and the conduction electron Green's function:

$$\begin{aligned} G_f(z) &= \frac{1}{z - \varepsilon_f - \Sigma_f(z) - \frac{V^2}{z - \varepsilon_{\mathbf{k}}}} = \frac{1}{z - \varepsilon_f - \Sigma_f(z)} \left[\frac{z - \varepsilon_{\mathbf{k}} - \frac{V^2}{z - \varepsilon_f - \Sigma_f(z)} + \frac{V^2}{z - \varepsilon_f - \Sigma_f(z)}}{z - \varepsilon_{\mathbf{k}} - \frac{V^2}{z - \varepsilon_f - \Sigma_f(z)}} \right] \\ &= \frac{1}{z - \varepsilon_f - \Sigma_f(z)} + \frac{V^2}{(z - \varepsilon_f - \Sigma_f(z))^2} \left[\frac{1}{z - \varepsilon_{\mathbf{k}} - \frac{V^2}{z - \varepsilon_f - \Sigma_f(z)}} \right] \\ &= \frac{1}{z - \varepsilon_f - \Sigma_f(z)} + \frac{V^2}{(z - \varepsilon_f - \Sigma_f(z))^2} G_c(z) \equiv \left(\Sigma_c(z) + \Sigma_c(z)^2 G_c(z) \right) \frac{1}{V^2}, \quad (55) \end{aligned}$$

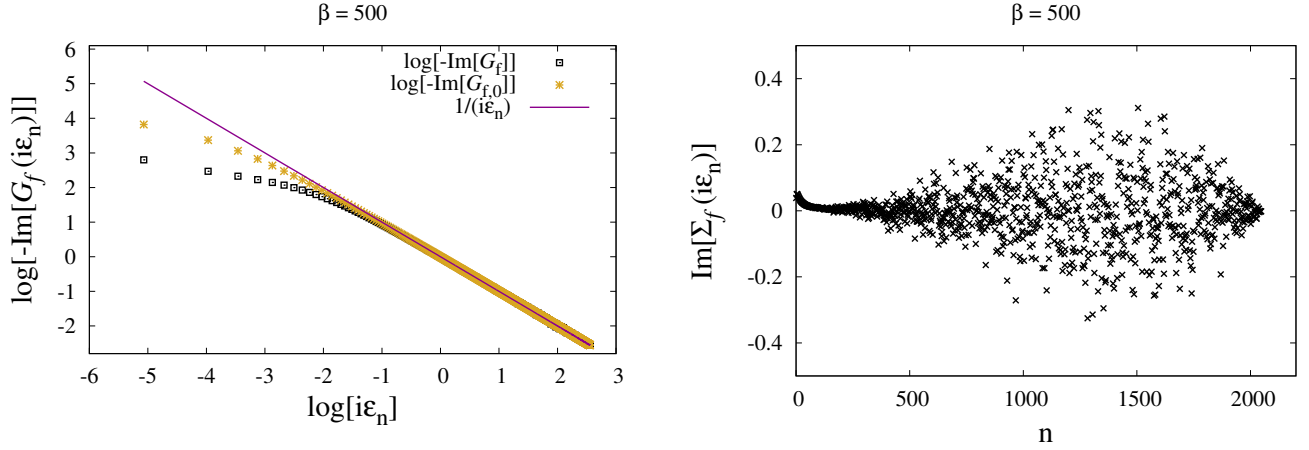


Figure 8: *Left*: Log-log plot of the imaginary part of the interacting and non-interacting ($U=0$) f -electron Green's functions as a function of the Matsubara frequencies $i\varepsilon_n = i(2n - 1)\pi\beta$. *Right*: Imaginary part of the f -electron Matsubara self-energy $\Sigma_f(i\varepsilon_n)$ as a function of n . The parameter values are $U/(\pi\Delta) = 3$, $\epsilon_f = -0.075$, $\beta = 500$, $V^2 = 0.01$, $D = 1$, ($\Delta = 0.0156$).

where we defined Σ_c as

$$\Sigma_c(z) \equiv \frac{V^2}{z - \varepsilon_f - \Sigma_f(z)}. \quad (56)$$

Thus, we have the relation

$$V^2 G_f(z) = t = \Sigma_c + \Sigma_c^2 G_c, \quad (57)$$

where t is the t-matrix. We define the conduction electron cavity Green's function as

$$\mathcal{G}_f(z) = \frac{1}{z - \varepsilon_f - V^2 \mathcal{G}_c(z)}. \quad (58)$$

Thus, eq. (56) can be rewritten as

$$\Sigma_c \equiv \frac{V^2}{z - \varepsilon_f - \Sigma_f} = \frac{V^2}{\mathcal{G}_f^{-1} + V^2 \mathcal{G}_c - \mathcal{G}_f^{-1} + G_f^{-1}} = \frac{V^2 G_f}{1 + V^2 G_f \mathcal{G}_c} = \frac{t}{1 + t \mathcal{G}_c} \quad (59)$$

From eqs. (57) and (59) we have

$$\Sigma_c = \frac{\Sigma_c + \Sigma_c^2 G_c}{1 + t \mathcal{G}_c} \longrightarrow 1 + t \mathcal{G}_c = 1 + \Sigma_c G_c \longrightarrow t \mathcal{G}_c = \frac{t}{1 + t \mathcal{G}_c} G_c \longrightarrow G_c = \mathcal{G}_c + \mathcal{G}_c t \mathcal{G}_c. \quad (60)$$

From eq. (59) we write

$$t = \frac{1}{\Sigma_c^{-1} - \mathcal{G}_c}, \quad (61)$$

and using this relation in eq. (60), we have

$$G_c = \mathcal{G}_c + \mathcal{G}_c \frac{1}{\Sigma_c^{-1} - \mathcal{G}_c} \mathcal{G}_c = \mathcal{G}_c + \frac{\mathcal{G}_c}{\mathcal{G}_c^{-1} \Sigma_c^{-1} - 1} \longrightarrow \Sigma_c = \mathcal{G}_c^{-1} - G_c^{-1} \quad (62)$$

as we expect. In the formulation for the conduction electrons the self-consistency condition is the following

$$G_c(z) = \overline{G_c(\mathbf{k}, z)} = \int d\varepsilon \rho(\varepsilon) (z - \varepsilon - \Sigma_c(z))^{-1}. \quad (63)$$

We perform the iteration as follows. We start with a trial conduction electron cavity Green's function \mathcal{G}_c , and obtain the f -electron Green's function G_f by applying the CT-QMC impurity solver. Then, we use the t -matrix $t = V^2 G_f$ in eq. (59), and obtain Σ_c . With this self-energy we calculate the site-diagonal conduction electron Green's function G_c using eq. (63), which gives the new trial cavity Green's function through the relation $\mathcal{G}_c^{-1} = G_c^{-1} + \Sigma_c$. Then, we start the iteration again until a convergent result is obtained for $G_f(z)$.

In order to use the CT-QMC for solving the DMFT problem of the periodic Anderson model, we assume semi-circle density of states for the conduction electrons, which is the exact result for Bethe lattice in $d = \infty$:

$$\rho_0(\omega) = \frac{2}{\pi D^2} \sqrt{D^2 - \omega^2}. \quad (64)$$

The DMFT results for the Anderson lattice with $U = 0$ using the CT-QMC solver together with the analytic results (see Appendix A) are shown in Fig. 9. We can see that the hybridization gap is reproduced.

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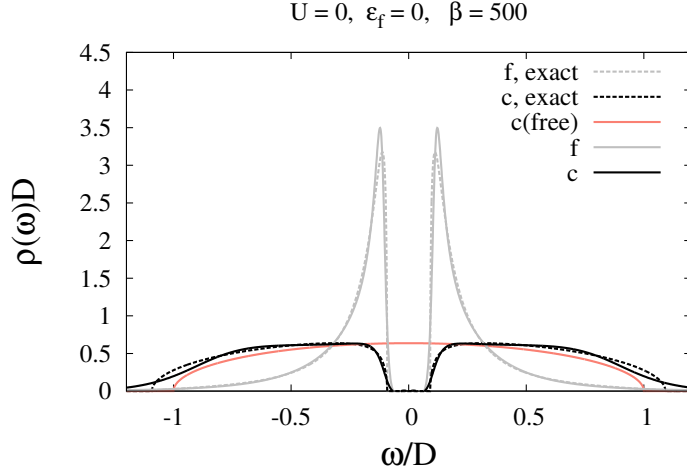


Figure 9: Conduction electron and f -electron density of states as a function of frequency in the case of the Anderson lattice with parameters $U = 0$, $\epsilon_f = 0$, $V^2 = 0.1$, $D = 1$, ($\beta = 500$). The *black dashed*, *gray dashed*, and *pink solid* lines show the analytic results for $\rho_c(\omega)$, $\rho_f(\omega)$, and $\rho_0(\omega)$, respectively, given by eqs. (A.83), (A.84), and (64).

A The Anderson model

A.1 Single-impurity Anderson model

One of the simplest models to deal with an impurity embedded into the sea of conduction electrons is the Anderson model, which is described by the Hamiltonian

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}\sigma} + \epsilon_f \sum_{\sigma} f_{\sigma}^+ f_{\sigma} + U n_{f,\uparrow} n_{f,\downarrow} + \sum_{\mathbf{k}\sigma} [V_{\mathbf{k}} c_{\mathbf{k},\sigma}^+ f_{\sigma} + V_{\mathbf{k}}^* f_{\sigma}^+ c_{\mathbf{k},\sigma}]. \quad (\text{A.65})$$

In the atomic limit ($V = 0$) the possible configurations for the f -electrons are the empty, singly or doubly occupied states:

$$\begin{aligned} |f^2\rangle &: E(f^2) = 2\epsilon_f + U \\ |f^0\rangle &: E(f^0) = 0 \\ |f^1 \uparrow\rangle, |f^1 \downarrow\rangle &: E(f^1) = \epsilon_f. \end{aligned}$$

For example, when the conditions

$$\begin{aligned} E(f^2) - E(f^1) &= \epsilon_f + U > 0 \\ E(f^0) - E(f^1) &= -\epsilon_f > 0 \end{aligned}$$

are satisfied, the ground state is the singly occupied state which possesses magnetic moment. In the following we consider this case.

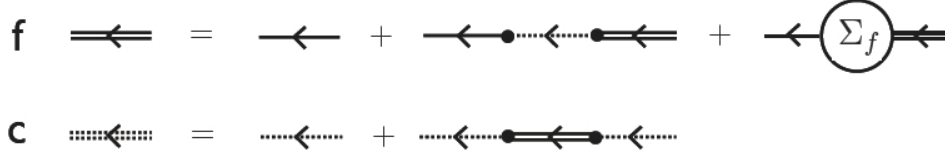


Figure 10: Diagrammatic representation of the f and conduction electron Green's functions for the single-impurity Anderson model.

When we allow coupling between the f and conduction electrons, the sharp f -state broadens due to the hybridization. Using the resolvent form of the Green's function $(z - \mathcal{H})\hat{G}(z) = \hat{1}$, we can write the Green's function matrix of the single-impurity Anderson model as

$$\hat{G}(z) = \begin{pmatrix} z - \varepsilon_{\mathbf{k}} & \cdot & \cdot & -V_{\mathbf{k}}^* \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & z - \varepsilon_{\mathbf{k}'} & -V_{\mathbf{k}'}^* \\ -V_{\mathbf{k}} & \cdot & -V_{\mathbf{k}'} & z - \varepsilon_f - \Sigma_f(z) \end{pmatrix}^{-1} = \begin{pmatrix} \hat{G}_c(z) & \hat{G}_{cf}(z)^* \\ \hat{G}_{cf}(z) & \hat{G}_f(z) \end{pmatrix}, \quad (\text{A.66})$$

where we find that

$$G_f(z) = \langle f | \hat{G}(z) | f \rangle = \left(z - \varepsilon_f - \Sigma_f(z) - \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{z - \varepsilon_{\mathbf{k}}} \right)^{-1}; \quad (\text{A.67})$$

$$G_c(z, \mathbf{k}, \mathbf{k}') = \langle \mathbf{k} | \hat{G}(z) | \mathbf{k}' \rangle = g(z, \mathbf{k}) \delta_{\mathbf{k}, \mathbf{k}'} + g(z, \mathbf{k}) V_{\mathbf{k}}^* G_f(z) V_{\mathbf{k}'} g(z, \mathbf{k}'), \quad (\text{A.68})$$

where $g(z, \mathbf{k})$ is the bare conduction electron Green's function with the form $g(z, \mathbf{k}) = (z - \varepsilon_{\mathbf{k}})^{-1}$, and the effect of the Coulomb interaction is inserted into Σ_f . The corresponding diagrams are shown in Fig. 10.

In the further discussion we distinguish two cases, i.e., the cases of small and large Coulomb interaction.

Small Coulomb interaction ($U < \pi\Delta$)

In this case we regard U as perturbation. We write the Green's function as

$$G_f(z) = (z - \varepsilon_f - \Sigma_f(z) - \Sigma_V)^{-1}, \quad (\text{A.69})$$

where $\Sigma_V = \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 / (z - \varepsilon_{\mathbf{k}})$ is the contribution from the hybridization. The Hartree approximation for the f -electron self-energy shown in Fig. 11 gives that ε_f is shifted as $\varepsilon_f \rightarrow E_f = \varepsilon_f + U n_{f,-\sigma}$. We used the constant density of states for the conduction electrons:

$$\begin{aligned} \rho_0(\omega) &= \frac{1}{2D} \quad \text{for } -D < \omega < D; \\ \rho_0(\omega) &= 0 \quad \text{otherwise,} \end{aligned} \quad (\text{A.70})$$

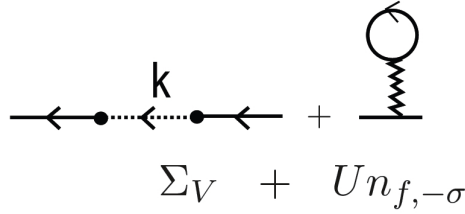


Figure 11: Hartree approximation for the self-energy Σ_f in the case of the single-impurity Anderson model.

and evaluate Σ_V for real frequencies as

$$\Sigma_V(\omega + i\delta) = \sum_{\mathbf{k}} \frac{V^2}{\omega + i\delta - \varepsilon_{\mathbf{k}}} = \mathcal{P} \sum_{\mathbf{k}} \frac{V^2}{\omega - \varepsilon_{\mathbf{k}}} - i\pi V^2 \sum_{\mathbf{k}} \delta(\omega - \varepsilon_{\mathbf{k}}) = V^2 \rho_0 \ln \left| \frac{D + \omega}{D - \omega} \right| - i\Delta, \quad (\text{A.71})$$

where we introduced $\Delta \equiv \pi V^2 \rho_0$. When the bandwidth $2D$ is large the real part of Σ_V is much smaller than the imaginary part. Thus, we can approximate

$$\Sigma_V(\omega + i\delta) \approx -i\Delta. \quad (\text{A.72})$$

The impurity density of states is obtained as

$$\rho_f(\omega) = -\frac{1}{\pi} \text{Im} G_f(\omega + i\delta) = -\frac{1}{\pi} \text{Im}(\omega - E_f + i\Delta)^{-1} = \frac{\Delta}{(\omega - E_f)^2 + \Delta^2}, \quad (\text{A.73})$$

which has Lorentzian form centered around E_f .

Large Coulomb interaction ($U \gg \pi\Delta$)

In the atomic limit the impurity Green's function has the form

$$G_f(\omega) = \frac{1 - \langle n_{f,-\sigma} \rangle}{\omega - \varepsilon_f} + \frac{\langle n_{f,-\sigma} \rangle}{\omega - \varepsilon_f - U}. \quad (\text{A.74})$$

Thus, when the Coulomb interaction is large, the single peak in the impurity density of states splits into two peaks centered around ε_f and $\varepsilon_f + U$ which correspond to the excitation energies on adding an electron to the system in the atomic limit.

We consider the symmetric case: $\varepsilon_f = -U/2$, when $\langle n_{f,\sigma} \rangle = 1/2$ for all temperatures. There is no any singularities when we increase the Coulomb interaction from small values towards large values. This means that there is one-to-one correspondence with the excitations of the non-interacting case $U = 0$ and that we have a local Fermi-liquid. We expand Σ_f in powers of $(\omega - \varepsilon_f)$ in eq. (A.69), and obtain

$$\begin{aligned} G_f(\omega) &= (\omega - \varepsilon_f + i\Delta - \Sigma_f(\omega))^{-1} \approx \left[\omega - \varepsilon_f - \text{Re}[\Sigma(\varepsilon_f)] + i\Delta - (\omega - \varepsilon_f) \frac{\partial \text{Re}[\Sigma(\varepsilon_f)]}{\partial \omega} - i\mathcal{O}(\omega^2) \right]^{-1} \\ &= \frac{z}{\omega - \varepsilon_f - z(\varepsilon_f - \varepsilon_F + \text{Re}[\Sigma(\varepsilon_f)]) + iz\Delta - i\mathcal{O}(\omega^2)} = \frac{z}{\omega - \varepsilon_f - \tilde{\varepsilon}_f + i\tilde{\Delta}}, \end{aligned} \quad (\text{A.75})$$

where we used that $\text{Im}[\Sigma_f(\omega)] = 0$ at $\omega = \varepsilon_f$, and $z = 1/(1 - \partial\text{Re}[\Sigma(\varepsilon_f)]/\partial\omega)$ is called wavefunction renormalization. The Green's function $G_f(\omega)$ looks like as the $U = 0$ Green's function. In the symmetric case we obtain at low energies:

$$G_f(\omega) = \frac{z}{\omega + iz\Delta - i\mathcal{O}(\omega^2)}, \quad (\text{A.76})$$

which gives that the impurity density of states possesses a peak around $\omega \sim 0$ which is called Kondo resonance, whose height does not depend on the interaction U :

$$\rho_f(\omega \sim 0) = -\frac{1}{\pi} \text{Im} [G_f(\omega + i\delta)]_{\omega=0} = \frac{1}{\pi\Delta}. \quad (\text{A.77})$$

This peak exists for low temperatures, and disappears when $T > 4T_K$, where T_K is the Kondo temperature. The weight of the Kondo resonance sharpens as U increases due to the renormalization $\Delta \rightarrow z\Delta$ in eq. (A.76). These behaviors can be seen in Fig. 6.

A.2 Periodic Anderson model

The periodic Anderson lattice is described by the Hamiltonian

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \varepsilon_f \sum_{i\sigma} f_{i\sigma}^{\dagger} f_{i\sigma} + \sum_i U n_{i f, \uparrow} n_{i f, \downarrow} + V \sum_{i\sigma} [c_{i\sigma}^{\dagger} f_{i\sigma} + f_{i\sigma}^{\dagger} c_{i\sigma}]. \quad (\text{A.78})$$

We can diagonalizing the Hamiltonian (A.78) in the non-interacting case ($U = 0$):

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} (c_{\mathbf{k}\sigma}^{\dagger}, f_{\mathbf{k}\sigma}^{\dagger}) \begin{pmatrix} \varepsilon_{\mathbf{k}} & V \\ V & \varepsilon_f \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\sigma} \\ f_{\mathbf{k}\sigma} \end{pmatrix} = \sum_{\mathbf{k}\sigma} (a_{\mathbf{k}\sigma}^{\dagger}, b_{\mathbf{k}\sigma}^{\dagger}) \begin{pmatrix} E_{k+} & 0 \\ 0 & E_{k-} \end{pmatrix} \begin{pmatrix} a_{\mathbf{k}\sigma} \\ b_{\mathbf{k}\sigma} \end{pmatrix}, \quad (\text{A.79})$$

where

$$E_{k\pm} = \frac{\varepsilon_{\mathbf{k}} + \varepsilon_f}{2} \pm \sqrt{\left(\frac{\varepsilon_{\mathbf{k}} - \varepsilon_f}{2}\right)^2 + V^2}. \quad (\text{A.80})$$

Thus, the hybridization of the f -electron and the conduction electron bands leads to the appearance of two bands, which are separated by a hybridization gap δ ($\delta \sim 2V^2/D$ if $D \gg V, \varepsilon_f$).

The f -electron and conduction electron Green's functions and density of states are obtained as

$$G_c(\mathbf{k}, z) = \left(z - \varepsilon_{\mathbf{k}} - \frac{V^2}{z - \varepsilon_f} \right)^{-1}; \quad (\text{A.81})$$

$$G_f(\mathbf{k}, z) = \left(z - \varepsilon_f - \frac{V^2}{z - \varepsilon_{\mathbf{k}}} \right)^{-1} = \frac{1}{z - \varepsilon_f} + \frac{V^2}{(z - \varepsilon_f)^2} G_c(\mathbf{k}, z); \quad (\text{A.82})$$

$$\rho_c(\omega) = -\frac{1}{\pi} \frac{1}{N} \text{Im} \left[\sum_{\mathbf{k}} G_c(\mathbf{k}, \omega + i\delta) \right] = \rho_0 \left(\omega - \frac{V^2}{\omega - \varepsilon_f} \right); \quad (\text{A.83})$$

$$\rho_f(\omega) = -\frac{1}{\pi} \frac{1}{N} \text{Im} \left[\sum_{\mathbf{k}} G_f(\mathbf{k}, \omega + i\delta) \right] = \frac{V^2}{(\omega - \varepsilon_f)^2} \rho_0 \left(\omega - \frac{V^2}{\omega - \varepsilon_f} \right) \quad (\text{A.84})$$

for $U = 0$.

B Fast-update formulas

The fast-update formulas are the generalization of the Sherman-Morrison formula, which gives a recipe for the case when we know the inverse of a matrix \hat{A} , and we want to calculate the inverse of another matrix which only slightly differs from the matrix \hat{A} . Namely,

$$\begin{aligned} \hat{A} &\longrightarrow \hat{A}^{-1} \\ \hat{A} + \underline{u} \otimes \underline{v} &\longrightarrow (\hat{A} + \underline{u} \otimes \underline{v})^{-1} = \hat{A}^{-1} - \frac{(\hat{A}^{-1} \cdot \underline{u}) \otimes (\underline{v} \cdot \hat{A}^{-1})}{1 + \lambda}, \end{aligned} \quad (\text{B.85})$$

where

$$\lambda = \underline{v} \cdot \hat{A}^{-1} \cdot \underline{u}. \quad (\text{B.86})$$

With this method we can calculate the inverse of a matrix with N^2 operations instead of N^3 operations, where N is the matrix size.

In each Monte Carlo step we calculate and store the matrix $\hat{M}^{(k)} = (\hat{\Delta}^{(k)})^{-1}$, where $(\hat{\Delta}^{(k)})_{ij} = V^2 g(\tau'_j - \tau_i)$. We discuss separately the following cases:

- shift operation I: $f^+(\tau'_n) \rightarrow f^+(\tilde{\tau}'_n)$

We change the j th column of $\hat{\Delta}^{(k)}$ as $\Delta_{nj}^{(k)} \rightarrow \bar{\Delta}_{nj}$ where $n = 1, 2, \dots, k$. Thus,

$$\underline{u}: u_n = \bar{\Delta}_{nj} - \Delta_{nj}^{(k)}, \quad (\text{B.87})$$

$$\underline{v}: v_n = 1 \text{ if } n = j, \quad v_n = 0 \text{ otherwise} \quad (\text{B.88})$$

in the formula (B.85). Furthermore,

$$\lambda = \sum_l (\Delta^{-1})_{jl} (\bar{\Delta}_{lj} - \Delta_{lj}^{(k)}) = \sum_l (\Delta^{-1})_{jl} \bar{\Delta}_{lj} - 1 = \sum_l M_{jl}^{(k)} \bar{\Delta}_{lj} - 1 \equiv \lambda_I - 1 \quad (\text{B.89})$$

in the formula (B.86). Using the formula (B.85) we obtain

$$\begin{aligned} M_{nm} &= (\Delta^{-1})_{nm} - \frac{1}{(1 + \lambda)} \left(\sum_l (\Delta^{-1})_{nl} (\bar{\Delta}_{lj} - \Delta_{lj}^{(k)}) \right) (\Delta^{-1})_{jm} \\ &= M_{nm}^{(k)} - \frac{1}{\lambda_I} \left(\sum_l M_{nl}^{(k)} \bar{\Delta}_{lj} - 0 \right) M_{jm}^{(k)} \quad \text{when } n \neq j, \end{aligned} \quad (\text{B.90})$$

$$\begin{aligned} M_{jm} &= (\Delta^{-1})_{jm} - \frac{1}{(1 + \lambda)} \left(\sum_l (\Delta^{-1})_{jl} (\bar{\Delta}_{lj} - \Delta_{lj}^{(k)}) \right) (\Delta^{-1})_{jm} \\ &= M_{jm}^{(k)} - \frac{1}{\lambda_I} \left(\sum_l M_{jl}^{(k)} \bar{\Delta}_{lj} - 1 \right) M_{jm}^{(k)} = M_{jm}^{(k)} - \frac{1}{\lambda_I} (\lambda_I - 1) M_{jm}^{(k)} = M_{jm}^{(k)} \frac{1}{\lambda_I} \end{aligned} \quad (\text{B.91})$$

- shift operation II: $f(\tau_n) \rightarrow f(\tilde{\tau}_n)$

We change the i th row of $\hat{\Delta}^{(k)}$ as $\Delta_{in}^{(k)} \rightarrow \bar{\Delta}_{in}$ where $n = 1, 2, \dots, k$. Thus,

$$\underline{u} : u_n = 1 \text{ if } n = i, \quad u_n = 0 \text{ otherwise,} \quad (\text{B.92})$$

$$\underline{v} : v_n = \bar{\Delta}_{in} - \Delta_{in}^{(k)} \quad (\text{B.93})$$

in the formula (B.85). Furthermore,

$$\lambda = \sum_l (\bar{\Delta}_{il} - \Delta_{il}^{(k)}) (\Delta^{-1})_{li} = \sum_l \bar{\Delta}_{il} (\Delta^{-1})_{li} - 1 = \sum_l \bar{\Delta}_{il} M_{li}^{(k)} - 1 \equiv \lambda_{II} - 1 \quad (\text{B.94})$$

in the formula (B.86). Using the formula (B.85) we obtain

$$\begin{aligned} M_{nm} &= (\Delta^{-1})_{nm} - \frac{1}{(1+\lambda)} (\Delta^{-1})_{ni} \left(\sum_l (\bar{\Delta}_{il} - \Delta_{il}^{(k)}) (\Delta^{-1})_{lm} \right) \\ &= M_{nm}^{(k)} - \frac{1}{\lambda_{II}} M_{ni}^{(k)} \left(\sum_l \bar{\Delta}_{il} M_{lm}^{(k)} - 0 \right) \quad \text{when } m \neq i, \end{aligned} \quad (\text{B.95})$$

$$\begin{aligned} M_{ni} &= (\Delta^{-1})_{ni} - \frac{1}{(1+\lambda)} (\Delta^{-1})_{ni} \left(\sum_l (\bar{\Delta}_{il} - \Delta_{il}^{(k)}) (\Delta^{-1})_{li} \right) \\ &= M_{ni}^{(k)} - \frac{1}{\lambda_{II}} M_{ni}^{(k)} \left(\sum_l \bar{\Delta}_{il} M_{li}^{(k)} - 1 \right) = M_{ni}^{(k)} - \frac{1}{\lambda_{II}} M_{ni}^{(k)} (\lambda_{II} - 1) = M_{ni}^{(k)} \frac{1}{\lambda_{II}} \end{aligned} \quad (\text{B.96})$$

- segment addition ($k \rightarrow k+1$)

We add i th row and j th column to the matrix $\hat{\Delta}^{(k)}$ as

$$\hat{\Delta}^{(k)} = \begin{pmatrix} \cdot & \cdot & 0 & \cdot \\ \cdot & \cdot & 0 & \cdot \\ 0 & 0 & 1 & 0 \\ \cdot & \cdot & 0 & \cdot \end{pmatrix}, \quad (\text{B.97})$$

which operation does not change the determinant of $\hat{\Delta}^{(k)}$. Then, we add a new row i and column j to $\hat{\Delta}^{(k)}$ and obtain $\hat{\Delta}_{+ij}^{(k+1)}$ by adding the new elements $\bar{\Delta}_{i1}, \bar{\Delta}_{i2}, \dots, \bar{\Delta}_{ik+1}$ and $\bar{\Delta}_{1j}, \bar{\Delta}_{2j}, \dots, \bar{\Delta}_{k+1j}$.

We consider this operation in two separate steps.

step 1: We change the j th column of $\hat{\Delta}^{(k)}$ as $\Delta_{nj}^{(k)} \rightarrow \bar{\Delta}_{nj}$ with $n = 1, 2, \dots, k+1$ similarly to shift operation I, and obtain the matrix $\hat{\delta}_{+ij}^{(k+1)}$. Thus,

$$\underline{u} : u_n = \bar{\Delta}_{nj} - \Delta_{nj}^{(k)}, \quad (\text{B.98})$$

$$\underline{v} : v_n = 1 \text{ if } n = j, \quad v_n = 0 \text{ otherwise} \quad (\text{B.99})$$

in the formula (B.85). Parameter λ in formula (B.86) becomes

$$\lambda = \sum_l (\Delta^{-1})_{jl} (\bar{\Delta}_{lj} - \Delta_{lj}^{(k)}) = (\Delta^{-1})_{ji} (\bar{\Delta}_{ij} - \Delta_{ij}^{(k)}) = \bar{\Delta}_{ij} - 1 \equiv \lambda_I - 1. \quad (\text{B.100})$$

For later convenience we introduce the row vector \underline{R} and column vector \underline{L} as

$$R_t = \sum_{l=1}^k \bar{\Delta}_{il} M_{lt}^{(k)} \quad (\text{B.101})$$

$$L_s = \sum_{l=1}^k M_{sl}^{(k)} \bar{\Delta}_{lj}. \quad (\text{B.102})$$

Using expressions (B.90) and (B.91) we obtain

$$M_{nm} = M_{nm}^{(k)} \quad \text{when } n \neq j \text{ and } m \neq i; \quad (\text{B.103})$$

$$M_{ni} = -\frac{1}{\lambda_I} \sum_l M_{nl}^{(k)} \bar{\Delta}_{lj} = -\frac{1}{\lambda_I} L_n \quad \text{when } n \neq j; \quad (\text{B.104})$$

$$M_{ji} = \frac{1}{\lambda_I}. \quad (\text{B.105})$$

step 2: Now we change the i th row of $\hat{\delta}_{+ij}^{(k+1)}$ as $\Delta_{in}^{(k)} \rightarrow \bar{\Delta}_{in}$ where $n = 1, 2, \dots, k$, and obtain the matrix $\hat{\Delta}_{+ij}^{(k+1)}$. Thus,

$$\underline{u}: \quad u_n = 1 \text{ if } n = i, \quad u_n = 0 \text{ otherwise,} \quad (\text{B.106})$$

$$\underline{v}: \quad v_n = \bar{\Delta}_{in} - \Delta_{in}^{(k)} \quad (\text{B.107})$$

in the formula (B.85). Parameter λ in formula (B.86) becomes

$$\begin{aligned} \lambda &= \sum_l (\bar{\Delta}_{il} - \Delta_{il}^{(k)}) ((\hat{\delta}_{+ij}^{(k+1)})^{-1})_{li} = -\frac{1}{\lambda_I} \sum_{l'} (\bar{\Delta}_{il} - \Delta_{il}^{(k)}) M_{l'l}^k \bar{\Delta}_{l'j} = -\frac{1}{\lambda_I} \sum_{l'} \bar{\Delta}_{il} M_{l'l}^k \bar{\Delta}_{l'j} \\ &\equiv \lambda_{II} - 1, \end{aligned} \quad (\text{B.108})$$

where we used eq. (B.104). Using expressions (B.95) and (B.96) together with the expressions (B.103), (B.104), and (B.105), we obtain

$$\begin{aligned} M_{nm} &= M_{nm}^{(k)} - \frac{1}{\lambda_{II}} \left(-\frac{1}{\lambda_I} \sum_l M_{nl}^{(k)} \bar{\Delta}_{lj} \right) \left(\sum_l \bar{\Delta}_{il} M_{lm}^{(k)} \right) = M_{nm}^{(k)} + \frac{1}{\lambda_{II}} \frac{1}{\lambda_I} L_n R_m \\ &\quad \text{when } n \neq j \text{ and } m \neq i; \end{aligned} \quad (\text{B.109})$$

$$M_{ni} = -\frac{1}{\lambda_I} L_n - \frac{1}{\lambda_{II}} \left(-\frac{1}{\lambda_I} L_n \right) (\lambda_{II} - 1) = -\frac{1}{\lambda_I} \frac{1}{\lambda_{II}} L_n \quad \text{when } n \neq j; \quad (\text{B.110})$$

$$\begin{aligned} M_{jm} &= 0 - \frac{1}{\lambda_{II}} ((\hat{\delta}_{+ij}^{(k+1)})^{-1})_{ji} \left(\sum_l (\bar{\Delta}_{il} - \Delta_{il}^{(k)}) ((\hat{\delta}_{+ij}^{(k+1)})^{-1})_{lm} \right) = -\frac{1}{\lambda_{II}} \frac{1}{\lambda_I} R_m \\ &\quad \text{when } m \neq i; \end{aligned} \quad (\text{B.111})$$

$$\begin{aligned} M_{ji} &= \frac{1}{\lambda_I} - \frac{1}{\lambda_{II}} ((\hat{\delta}_{+ij}^{(k+1)})^{-1})_{ji} \left(\sum_l (\bar{\Delta}_{il} - \Delta_{il}^{(k)}) ((\hat{\delta}_{+ij}^{(k+1)})^{-1})_{li} \right) = \frac{1}{\lambda_I} - \frac{1}{\lambda_{II}} \frac{1}{\lambda_I} (\lambda_{II} - 1) \\ &= \frac{1}{\lambda_I} \frac{1}{\lambda_{II}}. \end{aligned} \quad (\text{B.112})$$

Thus, we obtained the inverse of the new matrix as

$$\hat{M}^{k+1} = \left(\begin{array}{c|c|c} \hat{M}' & -\underline{L}^{(i)}/\lambda_+ & \hat{M}' \\ \hline -\underline{R}^{(j)}/\lambda_+ & 1/\lambda_+ & -\underline{R}^{(j)}/\lambda_+ \\ \hline \hat{M}' & -\underline{L}^{(i)}/\lambda_+ & \hat{M}' \end{array} \right), \quad (\text{B.113})$$

where $M'_{ts} = M_{ts}^{(k)} + L_t^{(i)} R_s^{(j)}/\lambda_+$, and we introduced the notation

$$\lambda_I \lambda_{II} = \bar{\Delta}_{ij} - \sum_{st} \bar{\Delta}_{sj} M_{ts}^{(k)} \bar{\Delta}_{it} \equiv \lambda_+. \quad (\text{B.114})$$

We can also obtain the determinant ratio as

$$\frac{\det \hat{\Delta}_{+ij}^{(k+1)}}{\det \hat{\Delta}^{(k)}} = (-1)^{i+j} \frac{1}{M_{ji}^{(k+1)}} = (-1)^{i+j} \lambda_+, \quad (\text{B.115})$$

where we used the relation

$$\det \hat{\Delta}^{(k)} M_{ji}^{(k)} = (-1)^{i+j} \det \hat{\Delta}_{\neq ij}^{(k-1)} \longrightarrow \det \hat{\Delta}_{+ij}^{(k+1)} M_{ji}^{(k+1)} = (-1)^{i+j} \det \hat{\Delta}^{(k)}. \quad (\text{B.116})$$

- segment removal ($k \rightarrow k-1$)

We erase the i th row and j th column from $\hat{\Delta}^{(k)}$ and obtain $\hat{\Delta}_{\neq ij}^{(k-1)}$. The inverse of matrix $\hat{M}^{(k-1)}$ is given by

$$M_{st}^{(k-1)} = M_{st}^{(k)} - \frac{M_{si}^{(k)} M_{jt}^{(k)}}{\lambda_-}, \quad (\text{B.117})$$

where $\lambda_- = M_{ji}^{(k)}$.

The determinant ratio is obtained in this case as

$$\frac{\det \hat{\Delta}_{\neq ij}^{(k-1)}}{\det \hat{\Delta}^{(k)}} = \frac{1}{(-1)^{i+j}} M_{ji}^{(k)} = \frac{1}{(-1)^{i+j}} \lambda_- = (-1)^{i+j} \lambda_-. \quad (\text{B.118})$$

C Padé approximation

In CT-QMC we obtain the Green's function as a function of imaginary time τ . Thus, we have to perform Fourier transform (FT) to obtain the Green's function in the Matsubara representation

$$G(i\varepsilon_n) = \int_0^\beta d\tau e^{i\varepsilon_n \tau} G(\tau), \quad (\text{C.119})$$

and then make analytic continuation to obtain the Green's function along the real frequency axis

$$G(i\varepsilon_n) \rightarrow G(\omega + i\delta). \quad (\text{C.120})$$

To perform analytic continuation, we use the Padé approximation. The problem is the following. We know the values of a complex function C at N complex points z_i : $C(z_1) = u_1, C(z_2) = u_2 \dots C(z_N) = u_N$, and we want to obtain C at real points. The Padé approximant is expressed as a rational function

$$C_N(z) = \frac{A_N(z)}{B_N(z)}, \quad (\text{C.121})$$

where $A_N(z)$ and $B_N(z)$ are polynomials of z of order $(N-1)/2$ and $(N-1)/2$ when N is odd, and $(N-2)/2$ and $N/2$ when N is even [8]. We express $C_N(z)$ as continued fraction:

$$C_N(z) = \frac{a_1}{1+} \frac{a_2(z-z_1)}{1+} \dots \frac{a_N(z-z_{N-1})}{1+} = \frac{a_1}{1 + \frac{a_2(z-z_1)}{1+\dots}}, \quad (\text{C.122})$$

where the coefficients a_i are determined that $C_N(z_n) = u_n$ by the recursion formulas

$$a_i = g_i(z_i), \quad g_1(z_i) = u_i, \quad g_k(z) = \frac{g_{k-1}(z_{k-1}) - g_{k-1}(z)}{(z - z_{k-1})g_{k-1}(z)}. \quad (\text{C.123})$$

Then, $C_N(z)$ at arbitrary z is evaluated as

$$C_N(z) = \frac{A_N(z)}{B_N(z)}, \quad (\text{C.124})$$

where

$$A_{n+1}(z) = A_n(z) + (z - z_n)a_{n+1}A_{n-1}(z) \quad (\text{C.125})$$

$$B_{n+1}(z) = B_n(z) + (z - z_n)a_{n+1}B_{n-1}(z) \quad (\text{C.126})$$

with $A_0 = 0, A_1 = a_1, B_0 = B_1 = 0$.