6. Auxiliary field continuous time quantum Monte Carlo

The purpose of the auxiliary field continuous time quantum Monte Carlo method[1] is to calculate the full Greens function of the Anderson impurity model

$$H = -\mu \sum_{\sigma} n_{\sigma} + U n_{\uparrow} n_{\downarrow} + \sum_{k\sigma} t_{k\sigma} a^{\dagger}_{k\sigma} a_{k\sigma} + \sum_{k\sigma} V_{k\sigma} a^{\dagger}_{k\sigma} c_{k\sigma} + H.c. \quad (6.1)$$

Diagrammatic Monte Carlo

In order to evaluate the partition function, we write the Hamiltonian as $H = H_0 + V$ so that we have

$$e^{-\beta H} = e^{-\beta H_0} \exp\left\{ -T_{\tau} \int_0^{\beta} d\tau \hat{V}(\tau) \right\} \quad (6.2)$$

with $\hat{V}(\tau)$ in the interaction picture

$$\hat{V}(\tau) = e^{+\tau H_0} V e^{-\tau H_0} .$$

and the usual imaginary time ordering operatore T_{τ}. In Diagrammatic Monte-Carlo, the Feynman diagrams of the perturbation expansion are sampled by Monte Carlo. Then, the partition function is

$$Z = \mathrm{Tr}\left(e^{-\beta H}\right) = Z_0 \frac{\mathrm{Tr}\left(e^{-\beta H_0} \exp\left\{ -T_{\tau} \int_0^{\beta} d\tau \hat{V}(\tau) \right\}\right)}{\mathrm{Tr} e^{-\beta H_0}} \quad (6.3)$$

with $Z_0 = \mathrm{Tr} e^{-\beta H_0}$. Thus

$$\frac{Z}{Z_0} = \frac{1}{Z_0} \mathrm{Tr}\left(e^{-\beta H_0} \exp\left\{ -T_{\tau} \int_0^{\beta} d\tau \hat{V}(\tau) \right\}\right) = \left\langle \exp\left\{ -T_{\tau} \int_0^{\beta} d\tau \hat{V}(\tau) \right\} \right\rangle_0$$

[1] This chapter is based on a course given by Aaram J. Kim. The master thesis *Topological Phases of Interacting Fermions in Optical Lattices with Artificial Gauge Fields* by Michael Buchhold is used as a reference.

(6.4)

This expectation value will be calculated with quantum Monte Carlo. First, we write more explicitly

$$\exp\Big\{-T_\tau\int_0^\beta d\tau\hat{V}(\tau)\Big\} = \sum_{k=0}^{\infty}\frac{1}{k!}\int_0^\beta d\tau_k\ldots\int_0^\beta d\tau_1\big((-V(\tau_k)\big)\ldots\big((-V(\tau_1)\big)$$
$$= \sum_{k=0}^{\infty}\int_{\tau_{k-1}}^\beta d\tau_k\ldots\int_{\tau_1}^\beta d\tau_2\int_0^\beta d\tau_1\big((-V(\tau_k)\big)\ldots\big((-V(\tau_1)\big) \tag{6.5}$$

because if $S(\tau) = e^{+\tau H_0}e^{-\tau H}$, then

$$\partial_\tau S(\tau) = e^{+\tau H_0}(H_0 - H)e^{-\tau H} = e^{+\tau H_0}(-V)e^{-\tau H_0}S(\tau) = \big(-V(\tau)\big)S(\tau) \tag{6.6}$$

This is formally solved by integration:

$$S(\beta) = S(0) - \int_0^\beta d\tau V(\tau)S(\tau) \tag{6.7}$$

Iteration via

$$S(\tau) = S(0) - \int_0^\tau d\tau' V(\tau')S(\tau') \tag{6.8}$$

leads to the expression (6.5). Then

$$\frac{Z}{Z_0} = \Big\langle \exp\Big\{-T_\tau\int_0^\beta d\tau\hat{V}(\tau)\Big\}\Big\rangle_0$$
$$= \sum_k \frac{1}{k!}\int_0^\beta d\tau_k\ldots\int_0^\beta d\tau_1\Big\langle\big(-\hat{V}(\tau_k)\big)\ldots\big(-\hat{V}(\tau_1)\big)\Big\rangle_0$$
$$= \sum_x W(x) = \int dx W(x) \tag{6.9}$$

Here, we interpret $W(x)$ as a weight. In order to be able to interpret $W(x)$ as a probability, we assume it is positive.
In the continuous-time auxiliary field quantum Monte-Carlo algorithm, an auxilary field decomposition of the interaction part of the Anderson impurity model is used. In CT-AUX, the choice of interaction is

$$V = U\left(n_\uparrow n_\downarrow - \frac{n_\uparrow + n_\downarrow}{2}\right) - \frac{K}{\beta} \tag{6.10}$$

where the second term is a Hartree like term, and the third term is a control parameter for the expansion order. This means that the noninteracting Hamiltonian is modified as

$$H_0 = H - V \tag{6.11}$$

The choice of V yields the following values for empty, singly occupied and doubly ocupied impurity:

$$\begin{aligned} |0\rangle \quad & -\frac{K}{\beta} \\ |\uparrow\rangle \quad & -\frac{K}{\beta} - \frac{U}{2} \\ |\downarrow\rangle \quad & -\frac{K}{\beta} - \frac{U}{2} \\ |\uparrow\downarrow\rangle \quad & -\frac{K}{\beta} \end{aligned} \tag{6.12}$$

Now a Hubbard-Stratonovich transformation is applied to V:

$$V = U\left(n_\uparrow n_\downarrow - \frac{n_\uparrow + n_\downarrow}{2}\right) - \frac{K}{\beta} = -\frac{K}{2\beta}\sum_{s=\pm 1} e^{\gamma s(n_\uparrow - n_\downarrow)} \tag{6.13}$$

The identity can be checked by applying the last expression on the basis states in (6.12). For example, for $|0\rangle$, $n_\uparrow = n_\downarrow = 0$, and the expression yields $-\frac{K}{\beta}$. For $|\uparrow\rangle$,

$$n_\uparrow = 1, n_\downarrow = 0 \curvearrowright V = -\frac{K}{\beta}\cosh\gamma \curvearrowright \cosh\gamma = 1 + \frac{U\beta}{2K} \tag{6.14}$$

s represents an Ising type boson that was introduced, an auxiliary spin. Eventually there will be k auxiliary spins over which we sum:

$$\frac{Z}{Z_0} = \sum_{\{s_i\}}\left(+\frac{K}{2\beta}\right)^k \prod_\sigma \left\langle \left[e^{\gamma s_k \sigma n_\sigma(\tau_k)} \dots e^{\gamma s_1 \sigma n_\sigma(\tau_1)}\right]\right\rangle_0 \tag{6.15}$$

Here, σ is the physical spin, with numerical value $\sigma = +1$ for $\uparrow$ and $\sigma = -1$ for $\downarrow$. Then, for Monte Carlo sampling we identify

$$\frac{Z}{Z_0} = \sum_k \int d\tau_k \dots \int d\tau_1 \sum_{\{s_i\}} W(x) \tag{6.16}$$

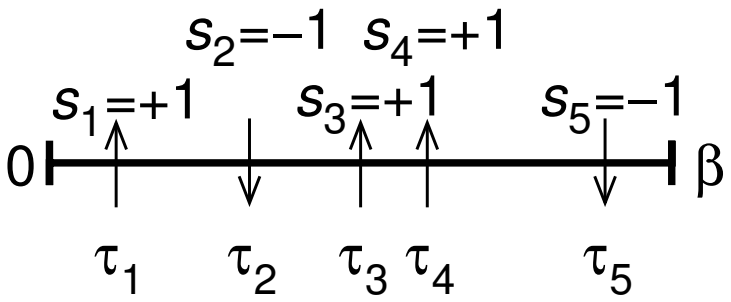

Figure 6.1: Example of a CT-AUX configuration at perturbation order 5.

The configuration space consists of perturbation order k, time indices τ and auxiliary spin indices s_i; there are k time points. The random walker needs to roam the entire configuration space. CT-AUX is a generalization of the discrete time quantum Monte Carlo algorithm (Hirsch-Fye).

Explicit calculation of the matrix

We now prepare to write the action in terms of Grassmann variables by rewriting the interaction

$$-V = \frac{K}{2\beta} \sum_{s=\pm 1} e^{\gamma s(n_\uparrow - n_\downarrow)} = \frac{K}{2\beta} \sum_{s=\pm 1} \prod_{\sigma} e^{\gamma s \sigma n_\sigma} \tag{6.17}$$

further. Taylor expansion of the exponential yields (because $n_\sigma^2 = n_\sigma$)

$$\begin{aligned} e^{\gamma s \sigma n_\sigma} &= 1 + \gamma s \sigma n_\sigma + \frac{1}{2!}(\gamma s \sigma)^2 n_\sigma + \dots \\ &= 1 + -n_\sigma + n_\sigma + \gamma s \sigma n_\sigma + \frac{1}{2!}(\gamma s \sigma)^2 n_\sigma + \dots \\ &= 1 - n_\sigma + e^{\gamma s \sigma} n_\sigma = 1 - \left(1 - e^{\gamma s \sigma}\right) n_\sigma \\ &= 1 - \left(1 - e^{\gamma s \sigma}\right)(1 - c_\sigma c_\sigma^\dagger) = 1 - \left[1 - e^{\gamma s \sigma} - c_\sigma c_\sigma^\dagger + e^{\gamma s \sigma} c_\sigma c_\sigma^\dagger\right] \\ &= e^{\gamma s \sigma} - (e^{\gamma s \sigma} - 1) c_\sigma c_\sigma^\dagger \\ &= e^{\gamma s \sigma}\left(1 - (1 - e^{-\gamma s \sigma}) c_\sigma c_\sigma^\dagger\right) \end{aligned} \tag{6.18}$$

where Fermion antiperiodicity $c_\sigma^\dagger c_\sigma = 1 - c_\sigma c_\sigma^\dagger$ was used. Thus, we have found that

$$-V = \frac{K}{2\beta} \sum_{s=\pm 1} e^{\gamma s(n_\uparrow - n_\downarrow)} = \frac{K}{2\beta} \sum_{s=\pm 1} \prod_{\sigma=\uparrow,\downarrow} \left[e^{\gamma s \sigma} - (e^{\gamma s \sigma} - 1) c_\sigma c_\sigma^\dagger\right] \tag{6.19}$$

Now we can go from Hamiltonian to action formalism, writing for the average of an operator A with respect to the noninteracting Hamiltonian

H_0

$$\langle A\rangle_0 = \frac{\mathrm{Tr}\left[Ae^{-\beta H_0}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \frac{\int \mathcal{D}[c^+c]Ae^{-S}}{\int \mathcal{D}[c^+c]e^{-S}} \tag{6.20}$$

While in the first expression, c, $c^\dagger$ are operators, in the second, c and c^+ are Grassmann variables. We now come back to the effective action of the previous chapter

$$S_{\mathrm{eff}} = \int d\tau d\tau' c^+(\tau)\mathcal{G}^{-1}(\tau-\tau')c(\tau) + \int d\tau V(\tau) \tag{6.21}$$

where the Weiss function $\mathcal{G}$ encodes the result of integrating out the bath degrees of freedom. We will use a number of identities for Grassmann variables:

$$\begin{aligned}
&\int \mathcal{D}[c^+c]e^{-\sum_{ij} c_i^+ S_{ij} c_j} = \det[S] \\
&\frac{\int \mathcal{D}[c^+c]c_x c_y^+ e^{-\sum_{ij} c_i^+ S_{ij} c_j}}{\int \mathcal{D}[c^+c]e^{-\sum_{ij} c_i^+ S_{ij} c_j}} = (S^{-1})_{xy} \\
&e^{-ac^+c} = 1 - ac^+c
\end{aligned} \tag{6.22}$$

We now introduce the matrix elements S_{ij} of the action with i, j indices for time, spin, lattice sites, etc., $i,j \in (0,...,M)$ where $M \to \infty$; as we have passed from continous imaginary time τ integrals to sums, the τ_i have to be infinitely dense. There are infinitely more times τ_i than the k times we have in a given configuration of perturbation order k. Thus

$$\mathcal{D}[c^+c]e^{-S} = \mathcal{D}[c^+c]e^{\sum_{ij} c_i^+ S_{ij} c_j} \text{ with } S_{ij} = (\mathcal{G}^{-1})_{ij}(\tau_i - \tau_j) \tag{6.23}$$

For the interaction, we introduce the matrices A and B with

$$\begin{aligned}
A_{ij} &= \begin{cases} \delta_{ij} e^{\gamma s_i \sigma_i} & \text{for } \tau_i \in \{\tau_1 \dots \tau_k\} \\ \delta_{ij} & \text{otherwise} \end{cases} \\
B_{ij} &= \begin{cases} \delta_{ij}\left(1 - e^{-\gamma s_i \sigma_i}\right) & \text{for } \tau_i \in \{\tau_1 \dots \tau_k\} \\ 0 & \text{otherwise} \end{cases}
\end{aligned} \tag{6.24}$$

The time mesh for the Feynman path integral now has the imaginary times τ_1 to τ_k as well as an infinite number of additional time indices τ_i. A has,

for perturbation order k, k exponentials on the diagonal for times τ_1, τ_2, $\ldots$, τ_k, and otherwise 1:

$$A = \begin{pmatrix} 1 & & & & \\ & e^{\gamma s_1 \sigma} & & & \\ & & 1 & & \\ & & & e^{\gamma s_2 \sigma} & \\ & & & & \cdots \end{pmatrix} \tag{6.25}$$

and consequently, B is

$$B = \begin{pmatrix} 0 & & & & \\ & 1 - e^{-\gamma s_1 \sigma} & & & \\ & & 0 & & \\ & & & 1 - e^{-\gamma s_2 \sigma} & \\ & & & & \cdots \end{pmatrix} \tag{6.26}$$

Then we can write the average of Eq. (6.9) as

$$\langle (-V) \ldots (-V) \rangle_0 = \frac{\left(\prod_\sigma \det A^\sigma \right) \int \mathcal{D}[c^+ c] e^{\sum_\sigma c^+_{i\sigma} B^\sigma_{ij} c_{j\sigma}} e^{\sum_\sigma c^+_{i\sigma} S^{\sigma 0}_{ij} c_{j\sigma}}}{\prod_\sigma \det S^\sigma} \tag{6.27}$$

The product over spin reflects the fact that the noninteracting part of the Hamiltonian H_0^σ contains only quadratic operators with index σ so that $H_0^\uparrow$ commutes with $H_0^\downarrow$ so that integration weights $W(x)$ are products of weights for the individual spin components $\sigma = \uparrow, \downarrow$. If we now rewrite the exponentials as

$$e^{\sum_\sigma c^+_{i\sigma} \left(S^\sigma - B^\sigma \right)^\sigma_{ij} c_{j\sigma}}$$

we find for the integral we need to compute

$$I = \frac{\prod_\sigma \det A^\sigma \det\left(S^\sigma - B^\sigma \right)}{\prod_\sigma \det S^\sigma} \tag{6.28}$$

Due to the M index, matrices A, S are infinite dimensional. The idea is now to use the zeros in the B matrix to make things finite-dimensional by reordering.

$$\det(S - B) = \det S \det(1 - B S^{-1}) \tag{6.29}$$

because $S-B=(1-BS^{-1})S$, and the determinant of a product splits into a product of determinants. We now exploit that at perturbation order k, only k entries in the B matrix are nonzero:

$$B=\begin{pmatrix} 0 & & & & & & & \\ & b_1 & & & & & & \\ & & 0 & & & & & \\ & & & \cdots & & & & \\ & & & & 0 & & & \\ & & & & & b_k & & \\ & & & & & & \cdots & \\ & & & & & & & 0 \end{pmatrix} \rightarrow \tilde{B}=\left(\begin{array}{ccc|c} b_1 & & & \\ & b_2 & & \\ & & \cdots & 0 \\ & & & b_k \\ \hline & 0 & & 0 \end{array}\right) \tag{6.30}$$

This rearrangement doesn't produce a sign as rows and columns are exchanged. In the same way, S^{-1} is rearranged into $\tilde{S}^{-1}$ only that this doesn't produce empty submatrices. Then

$$\left(\begin{array}{c|c} \tilde{B} & 0 \\ \hline 0 & 0 \end{array}\right)\left(\begin{array}{c|c} \tilde{S}^{-1} & x \\ \hline x & x \end{array}\right)=\left(\begin{array}{c|c} \tilde{B}\tilde{S}^{-1} & T \\ \hline 0 & 0 \end{array}\right) \tag{6.31}$$

and

$$1-BS^{-1}\rightarrow\left(\begin{array}{c|c} 1-\tilde{B}\tilde{S}^{-1} & T \\ \hline 0 & 1 \end{array}\right) \tag{6.32}$$

but in the determinant, only $1-\tilde{B}\tilde{S}^{-1}$ remains:

$$\det(1-BS^{-1})=\det(1-\tilde{B}\tilde{S}^{-1}) \tag{6.33}$$

In Eq. 6.28, $\det S^{\sigma}$ cancels with the denominator, so that we have

$$I=\prod_{\sigma}\det A^{\sigma}\det(1-\tilde{B}\tilde{S}^{-1})=\prod_{\sigma}\det\tilde{A}^{\sigma}\det(1-\tilde{B}\tilde{S}^{-1}) \tag{6.34}$$

because the rearranged $\tilde{A}^{\sigma}$ has only entries of 1 beyond the reduced space of dimension k. Now we arrive at the final expression

$$I=\prod_{\sigma}\det\big(\tilde{A}-\tilde{A}\tilde{B}\tilde{S}^{-1}\big)=\prod_{\sigma}\big(e^{\Gamma_{\sigma}}-(e^{\Gamma_{\sigma}}-1)\underline{\underline{G}}\big)\equiv\prod_{\sigma}\det N_{\sigma}^{-1} \tag{6.35}$$

where the $k\times k$ matrix $\underline{\underline{G}}$, with k numbering the time points, was introduced, and the entire matrix that needs to be manipulated is now called N_{σ}^{-1} matrix (N matrix). The notation for $\tilde{A}$ is

$$\tilde{A}\equiv e^{\Gamma_{\sigma}}\equiv\mathrm{diag}\big(e^{\gamma s_1\sigma},\ldots,e^{\gamma s_k\sigma}\big)$$

Later, the Weiss function $\mathcal{G}$ will be represented by a very large mesh with many more than k points; it will be interpolated linearly or by cubic methods from k points.

Insertion and removal

Now, we will assume that we know the N_σ^{-1} matrix at a given perturbation order k. To implement a random walk through configuration space, we need to either insert a time point or remove a time point, based on the Metropolis algorithm.

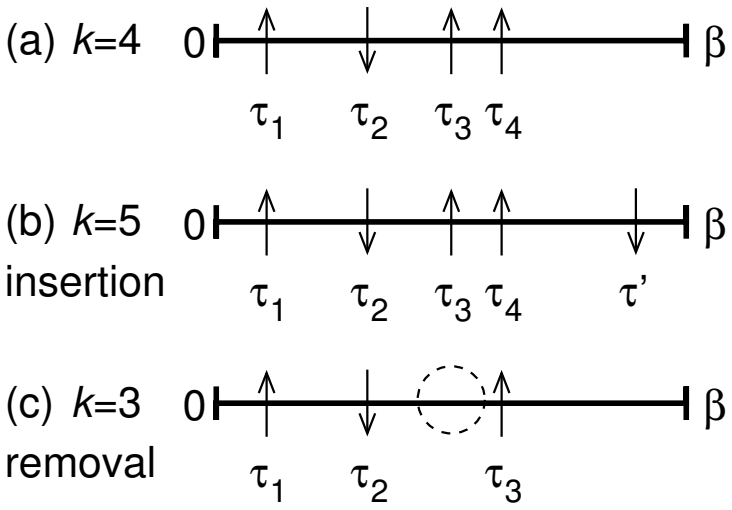

Figure 6.2: Schematic of insertion and removal updates to a configuration.

Insertion.- The decision to insert an auxiliary spin into the configuration is taken based on a uniform random number r in the range $[0, 1]$. If

$$r > \min\left(1, f\left|\frac{W_{k+1}}{W_k}\right|\right) \tag{6.36}$$

where f is factor explained later, the update is accepted, otherwise rejected. Thus, to take the decision, the ratio of weights needs to be calculated, specifically:

$$\begin{aligned}&\frac{\det\left(N^{(k+1)^{-1}}\right)}{\det\left(N^{(k)^{-1}}\right)}\\ &= \underbrace{\det\left(N^{(k)^{-1}}\right)}_{\left(\begin{array}{c|c} N^{(k)} & 0 \\ \hline 0 & 1 \end{array}\right)} \underbrace{\det\left(N^{(k+1)^{-1}}\right)}_{\left(\begin{array}{c|c} N^{(k)^{-1}} & Q \\ \hline R & S \end{array}\right)} = \det\left(\begin{array}{c|c} 1 & N^{(k)}Q \\ \hline R & S \end{array}\right) = S - RN^{(k)}Q\end{aligned} \tag{6.37}$$

This uses the fact that $\mathsf{N}^{(k)}$ and $\mathsf{N}^{(k)^{-1}}$ are inverses of each other, and matrices are multiplied using the properties of determinants. During the simulation $\mathsf{N}^{(k)}$ rather than $\mathsf{N}^{(k)^{-1}}$ is stored. For the enlarged matrix $\mathsf{N}^{(k)^{-1}}$ we have

$$\mathsf{N}^{(k+1)^{-1}} = \left(\begin{array}{c|c} \mathsf{N}^{(k)^{-1}} & \mathsf{Q} \\ \hline \mathsf{R} & \mathsf{S} \end{array}\right) \tag{6.38}$$

with $(k \times 1)$ vector Q, $(1 \times k)$ vector R and S defined by $(1 \leqslant l \leqslant n)$:

$$\begin{aligned} \mathsf{Q}_l &= -(e^{\gamma s_l \sigma} - 1)\mathcal{G}_{0\sigma}(\tau_l - \tau) \\ \mathsf{R}_l &= -(e^{\gamma s \sigma} - 1)\mathcal{G}_{0\sigma}(\tau - \tau_l) \\ \mathsf{S} &= e^{\gamma s \sigma} - (e^{\gamma s \sigma} - 1)\mathcal{G}_{0\sigma}(0^+) \end{aligned} \tag{6.39}$$

In case the insertion move is accepted, we now need the missing elements of the enlarged matrix $\mathsf{N}^{(k+1)}$, expressed in terms of the additional elements Q, R, S of $\mathsf{N}^{(k+1)^{-1}}$ which we know:

$$\mathsf{N}^{(k+1)}\left[\mathsf{N}^{(k+1)}\right]^{-1} = \mathbb{1} = \left(\begin{array}{c|c} \tilde{\mathsf{P}} & \tilde{\mathsf{Q}} \\ \hline \tilde{\mathsf{R}} & \tilde{\mathsf{S}} \end{array}\right) \left(\begin{array}{c|c} \mathsf{P} & \mathsf{Q} \\ \hline \mathsf{R} & \mathsf{S} \end{array}\right) \tag{6.40}$$

where we write P for $\mathsf{N}^{(k)^{-1}}$. This yields the equations

$$\begin{aligned} &\tilde{\mathsf{P}}\mathsf{P} + \tilde{\mathsf{Q}}\mathsf{R} = \mathbb{1} \\ &\tilde{\mathsf{P}}\mathsf{Q} + \tilde{\mathsf{Q}}\mathsf{S} = \vec{0} \\ &\tilde{\mathsf{R}}\mathsf{P} + \tilde{\mathsf{S}}\mathsf{R} = \vec{0}^{\mathsf{T}} \\ &\tilde{\mathsf{R}}\mathsf{Q} + \tilde{\mathsf{S}}\mathsf{S} = 1 \end{aligned} \tag{6.41}$$

which we have to solve for $\tilde{\mathsf{P}}(\mathsf{P}, \mathsf{Q}, \mathsf{R}, \mathsf{S})$ and so on. The third equation yields

$$\tilde{\mathsf{R}}\mathsf{P} = -\tilde{\mathsf{S}}\mathsf{R} \curvearrowright \tilde{\mathsf{R}} = -\tilde{\mathsf{S}}\mathsf{R}\mathsf{P}^{-1} \tag{6.42}$$

and inserting into the fourth equation

$$-\tilde{\mathsf{S}}\mathsf{R}\mathsf{P}^{-1}\mathsf{Q} + \tilde{\mathsf{S}}\mathsf{S} = 1 \curvearrowright \tilde{\mathsf{S}}\big(\mathsf{S} - \mathsf{R}\mathsf{P}^{-1}\mathsf{Q}\big) = 1 \curvearrowright \tilde{\mathsf{S}} = \frac{1}{\mathsf{S} - \mathsf{R}\mathsf{P}^{-1}\mathsf{Q}} \tag{6.43}$$

with $\mathsf{P}^{-1} = \mathsf{N}^{(k)}$. $\tilde{\mathsf{S}}$ is a number which we don't need to replace so that we have from the third equation

$$\tilde{\mathsf{R}} = -\tilde{\mathsf{S}}\mathsf{R}\mathsf{N}^{(k)}\,. \tag{6.44}$$

The second equation

$$\tilde{Q} = -\frac{\tilde{P}Q}{S} \tag{6.45}$$

is inserted into the first

$$\tilde{P}P - \frac{\tilde{P}QR}{S} = 1 \curvearrowright \tilde{P}\left(P - \frac{QR}{S}\right) = 1 \tag{6.46}$$

where Q is a column vector, R is a row vector. Now we use the Sherman-Morrison formula (for an invertible square matrix A, with $v^T A^{-1} u \neq 1$)

$$\left(A + uv^T\right)^{-1} = A^{-1} - \frac{A^{-1}uv^T A^{-1}}{1 - v^T A^{-1} u} \tag{6.47}$$

which allows a cheap update of the already known inverse of A if A is modified by the rank 1 matrix uv^T. Here, we have $u = -\frac{Q}{S}$, $v^T = R$ and

$$\begin{aligned}\tilde{P} &= \left(P - \frac{QR}{S}\right)^{-1} = P^{-1} - \frac{\left[P^{-1}\left(-\frac{Q}{S}\right)\right] \cdot \left[RP^{-1}\right]}{1 - RP^{-1}\left(-\frac{Q}{S}\right)} \\ &= N^{(k)} + \frac{\left[N^{(k)}Q\right] \cdot \left[RN^{(k)}\right]}{S - RN^{(k)}Q} = N^{(k)} + \tilde{S}\left[N^{(k)}Q\right] \cdot \left[RN^{(k)}\right]\end{aligned} \tag{6.48}$$

This is the most massive calculation in the update. Now we find for $\tilde{Q}$

$$\begin{aligned}\tilde{Q} &= -\frac{\tilde{P}Q}{S} = -\frac{N^{(k)}Q + \tilde{S}\left[N^{(k)}Q\right] \cdot \left[RN^{(k)}\right]Q}{S} \\ &- \frac{N^{(k)}Q}{S}\left(1 + \frac{RN^{(k)}Q}{S - RN^{(k)}Q}\right) = \frac{N^{(k)}Q}{S - RN^{(k)}Q} = -\tilde{S}N^{(k)}Q\end{aligned} \tag{6.49}$$

Removal.- The decision on insertion versus removal is taken with 50% probability. For the deletion of an auxiliary spin s at time τ from the matrix $N^{(k)}$, the situation is

$$\begin{aligned}&N^{(k+1)^{-1}} = \left(\begin{array}{c|c} N^{(k)^{-1}} & Q \\ \hline R & S \end{array}\right) \qquad N^{(k+1)} \left(\begin{array}{c|c} \tilde{P} & \tilde{Q} \\ \hline \tilde{R} & \tilde{S} \end{array}\right) \\ &\text{with } \tilde{S} = \left(S - RN^{(k)}Q\right)^{-1} \qquad \tilde{Q} = -\tilde{S}N^{(k)}Q \\ &\qquad \tilde{R} = -\tilde{S}RN^{(k)} \qquad \tilde{P} = N^{(k)} + \tilde{S}\left[N^{(k)}Q\right] \cdot \left[RN^{(k)}\right]\end{aligned} \tag{6.50}$$

The idea is now to use to solve the $\tilde{P}$ equation for $N^{(k)}$ using the expressions for $\tilde{Q}$ and $\tilde{R}$:

$$\tilde{P} = N^{(k)} + \frac{\tilde{Q}}{\tilde{S}}\tilde{S}\frac{\tilde{R}}{\tilde{S}} = N^{(k)} + \frac{\tilde{Q}\cdot\tilde{R}}{\tilde{S}}$$
$$\curvearrowright N^{(k)} = \tilde{P} - \frac{\tilde{Q}\cdot\tilde{R}}{\tilde{S}} \tag{6.51}$$

Monte Carlo procedure.- To summarize, we use the expansion of the partition function

$$Z = \sum_{k=0}^{\infty}\sum_{\{s_i\}}\int_0^\beta d\tau_k\int_0^\tau d\tau_1\left(\frac{K}{2\beta}\right)^k Z_k\big(\{s_i,\tau_i\}\big) \tag{6.52}$$

where

$$Z_k\big(\{s_i,\tau_i\}\big) = Z_0\prod_\sigma \det N_\sigma^{-1}\big(\{s_i,\tau_i\}\big) \tag{6.53}$$

For the specific formulation of the update, we need the condition of detailed balance

$$W(x)p(x\to x') = W(x')p(x'\to x) \tag{6.54}$$

Then in general, the Metropolis algorithm is to update, with a random number r, if

$$r < \min\left(1, \frac{W(x')}{W(x)}\right) \tag{6.55}$$

The detailed balance condition can be slightly modified by splitting the transition probability into proposal and acceptance probabilities:

$$p = p^{\text{proposal}}p^{\text{acceptance}} \tag{6.56}$$

For an insertion, the proposal probability is the probability p_1 of choosing a time τ from the interval $[1,\beta]$, $p_1 = \frac{d\tau}{\beta}$, times the probability $p_2 = \frac{1}{2}$ of choosing the auxiliary spin s from $\{-1,1\}$, *i.e.*

$$p^{\text{proposal}}(k\to k+1) = p_1p_2 = \frac{d\tau}{2\beta} \tag{6.57}$$

For deletion, the tuple (τ_i,s_i) must be chosen from the existing $k+1$ auxiliary spins, so that the proposal probability is

$$p^{\text{proposal}}(k+1\to k) = \frac{1}{n+1} \tag{6.58}$$

Then, the Metropolis update decision is modified to

$$r < \min\left(1, \frac{W(x')p^{\text{proposal}}(x' \to x)}{W(x)p^{\text{proposal}}(x \to x')}\right) \tag{6.59}$$

Detailed balance then yields for the acceptance probabilities

$$\frac{p^{\text{acceptance}}(k \to k+1)}{p^{\text{acceptance}}(k+1 \to k)} = \frac{2\beta}{(k+1)d\tau}\frac{W_{k+1}}{W_k} = \frac{K}{k+1}\prod_\sigma \frac{\det N_\sigma^{-1}(k+1)}{\det N_\sigma^{-1}(k)} \tag{6.60}$$

because

$$W_{k+1} = d\tau_1 \dots d\tau_k d\tau_{k+1}\left(\frac{K}{2\beta}\right)^{k+1}\det N_\sigma^{-1}(k+1)$$
$$W_k = d\tau_1 \dots d\tau_k\left(\frac{K}{2\beta}\right)^{k}\det N_\sigma^{-1}(k)$$

This means that

$$p^{\text{acceptance}}(k \to k+1) = \min\left\{1, \frac{K}{k+1}\prod_\sigma \frac{\det N_\sigma^{-1}(k+1)}{\det N_\sigma^{-1}(k)}\right\}$$
$$p^{\text{acceptance}}(k+1 \to k) = \min\left\{1, \frac{k+1}{K}\prod_\sigma \frac{\det N_\sigma^{-1}(k)}{\det N_\sigma^{-1}(k+1)}\right\} \tag{6.61}$$

Measurement of the Greens function

The Greens function, written for QMC without a minus sign, is

$$\begin{aligned} G_\sigma(\tau - \tau') &= \left\langle T_\tau c_\sigma(\tau) c_\sigma^\dagger(\tau')\right\rangle \\ &= \frac{\int \mathcal{D}[c^+c] c_{\sigma x} c^+_{\sigma y} e^{-\sum_{ij\sigma} c^+_{i\sigma}(S-B)_{ij}c_{\sigma j}}}{\int \mathcal{D}[c^+c] e^{-\sum_{ij\sigma} c^+_{i\sigma}(S-B)_{ij}c_{\sigma j}}} \\ &= \left[(S-B)^{-1}\right]_{xy} \end{aligned} \tag{6.62}$$

where x, y stand for arbitrary imaginary time indices. For the matrix inverse, we can write

$$\begin{aligned} (S-B)^{-1} &= \left[(1 - BS^{-1})S\right]^{-1} = S^{-1}(1-BS^{-1})^{-1} \\ &= S^{-1}(1-BS^{-1})^{-1}\left[(1-BS^{-1}) + BS^{-1}\right] \\ &= S^{-1} + S^{-1}(1-BS^{-1})^{-1}BS^{-1} \end{aligned} \tag{6.63}$$

Here we recapitulate the method of getting rid of the zero subspace: The matrices S, B are infinite dimensional but B has many zeros:

$$B = \left(\begin{array}{c|c} \tilde{B} & 0 \\ \hline 0 & 0 \end{array}\right) \qquad S^{-1} = \left(\begin{array}{c|c} \tilde{S}^{-1} & \dots \\ \hline \dots & \dots \end{array}\right) \quad \curvearrowright \quad BS^{-1} = \left(\begin{array}{c|c} \tilde{B}\tilde{S}^{-1} & T \\ \hline 0 & 0 \end{array}\right)$$
$$1 - BS^{-1} = \left(\begin{array}{c|c} 1 - \tilde{B}\tilde{S}^{-1} & T \\ \hline 1 & 0 \end{array}\right) \quad \curvearrowright \quad \left(1 - BS^{-1}\right)^{-1} = \left(\begin{array}{c|c} \left(1 - \tilde{B}\tilde{S}^{-1}\right)^{-1} & \dots \\ \hline 1 & 0 \end{array}\right)$$
$$\curvearrowright \quad \left(1 - BS^{-1}\right)^{-1} B = \left(\begin{array}{c|c} \left(1 - \tilde{B}\tilde{S}^{-1}\right)^{-1}\tilde{B} & 0 \\ \hline 0 & 0 \end{array}\right) \tag{6.64}$$

Now we go back to the definitions of the A, B and S matrices:

$$A = e^{\Gamma} \qquad B = 1 - e^{-\Gamma} \qquad S^{-1} = \mathcal{G}^0 \tag{6.65}$$

with the noninteracting Weiss function $\mathcal{G}^0$; thus S is invertible. Now we insert $\tilde{A}$:

$$\begin{aligned} \left(1 - BS^{-1}\right)^{-1} B &= \left(\begin{array}{c|c} \left(1 - \tilde{B}\tilde{S}^{-1}\right)^{-1}\tilde{A}^{-1}\tilde{A}\tilde{B} & 0 \\ \hline 0 & 0 \end{array}\right) = \left(\begin{array}{c|c} \left(\tilde{A} - \tilde{A}\tilde{B}\tilde{S}^{-1}\right)^{-1}\tilde{A}\tilde{B} & 0 \\ \hline 0 & 0 \end{array}\right) \\ &= \left(\begin{array}{c|c} N_\sigma\big(\{s_i, \tau_i\}\big)\left(e^{\Gamma_\sigma} - 1\right) & 0 \\ \hline 0 & 0 \end{array}\right) \equiv \left(\begin{array}{c|c} M & 0 \\ \hline 0 & 0 \end{array}\right) \end{aligned} \tag{6.66}$$

Then, coming back to the matrix inverse (6.63)

$$(S - B)^{-1} = \mathcal{G}^0 + \mathcal{G}^0 \left(\begin{array}{c|c} N_\sigma\big(\{s_i, \tau_i\}\big)\left(e^{\Gamma_\sigma} - 1\right) & 0 \\ \hline 0 & 0 \end{array}\right) \mathcal{G}^0 \tag{6.67}$$

This means that the full Greens function can be evaluated as

$$G_\sigma(\tau - \tau') = \mathcal{G}^0_\sigma(\tau - \tau') + \mathcal{G}^0_\sigma(\tau - \tau_i) M^\sigma_{ij} \mathcal{G}^0_\sigma(\tau_j - \tau') \tag{6.68}$$

where τ_i, τ_j are configuration time points. The $k \times k$ matrix M is

$$M^\sigma = N_\sigma\big(e^{\Gamma_\sigma} - 1\big) \tag{6.69}$$

The Weiss function $\mathcal{G}^0_\sigma$ does not depend on the configuration, but M does. Therefore, we only need to accumulate terms that depend on the configuration, in particular $M^\sigma_{ij}\mathcal{G}^0_\sigma(\tau_j - \tau')$. This is accumulated for many i, and only a vector needs to be stored. This also explains why the N_σ matrix is stored; it is needed for the Greens function. The matrix update cost is of order $\mathcal{O}(k^2)$ because only matrix vector multiplications are needed.