# Chapter 9

# Quantum Monte Carlo for fermions

In this final chapter we will discuss an algorithm for the simulation of fermions by quantum Monte Carlo (QMC). The world line representations employed previously for fermions and spins are not suitable for fermions since they will give a horrible sign problem: any exchange of fermions during the propagation from imaginary time 0 to $\beta$ will give a minus sign in the action.[1] One thus uses a different representation, where the sign problem is not as severe and absent at least for non-interacting fermions. In this chapter we will give an introduction to modern continuous time quantum Monte Carlo (CT-QMC) methods for fermions.

The specific model we will consider here is the Hubbard model with Hamiltonian

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} \left( c_{i,\sigma}^{\dagger} c_{j,\sigma} + c_{j,\sigma}^{\dagger} c_{i,\sigma} \right) + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}, \tag{9.1}$$

where $c_{i,\sigma}^{\dagger}$ creates a fermion on site $i$ with spin $\sigma$ and $n_{i,\sigma} = c_{i,\sigma}^{\dagger} c_{i,\sigma}$. This chapter closely follows a recent review[2] and we refer the interested student to this review for details on how to simulate other models.

## 9.1 Diagrammatic Monte Carlo

### 9.1.1 QMC as sampling of time-dependent perturbation expansions

As already mentioned in Sec. 7.2.2, the world line representation used for spins is just a time-dependent perturbation expansion of the operator $\exp(-\beta H)$. Continuous time QMC methods (CT-QMC) methods stochastically sample time-dependent perturbation theory. One splits the Hamiltonian $H = H_a + H_b$ into two parts, writes the partition function $Z = \text{Tr} e^{-\beta H}$ in the interaction representation with respect to $H_a$ and expands

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[1]The exception are purely one-dimensional systems where fermions cannot exchange.

[2]E. Gull, *et al.*, Rev. Mod. Phys. **83**, 349 (2011)

in powers of $H_b$, thus ($T_\tau$ is the time ordering operator)

$$Z = \text{Tr } T_\tau e^{-\beta H_a} \exp\left[-\int_0^\beta d\tau H_b(\tau)\right] \tag{9.2}$$

$$= \sum_k (-1)^k \int_0^\beta d\tau_1 \ldots \int_{\tau_{k-1}}^\beta d\tau_k \text{Tr}\left[e^{-\beta H_a} H_b(\tau_k) H_b(\tau_{k-1}) \ldots H_b(\tau_1)\right],$$

where $H_b(\tau) = \exp(+\tau H_a) H_b \exp(-\tau H_a)$ is $H_b$ in the interaction representation. Note that the usual factor $1/k!$ is absorbed by the time ordering.

The trace evaluates to a number and diagrammatic Monte Carlo methods enable a sampling over all orders $k$, all topologies of the paths/diagrams and all times $\tau_1, \cdots, \tau_k$ in the same calculation. Because the method is formulated in continuous time from the beginning, time discretization errors do not arise and therefore do not have to be controlled. Provided the spectrum of the perturbation term is bounded from above the contributions of very large orders are exponentially suppressed by the factor $\frac{1}{k!}$ originating from the expansion of an exponential. Thus the sampling process does not run off to infinite order and no truncation of the diagram order is needed. For bosons one chooses the interaction as the unperturbed term $H_a$ and the hopping as the perturbation $H_b$. For spins one chooses the Ising coupling ($J_z$) and the magnetic field as $H_a$ and the off-diagonal exchange ($J_{xy}$) as perturbation $H_b$. One then sees that the continuous time weight (7.21) is just our equation (9.2).

For fermions we will follow the opposite approach and treat the hopping term and chemical potential

$$H_a = -t \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} \left(c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma}\right) - \mu \sum_{i,\sigma} n_{i,\sigma} \tag{9.3}$$

as the unperturbed Hamiltonian and the interaction

$$H_b = U \sum_i n_{i,\uparrow} n_{i,\downarrow} \tag{9.4}$$

as the perturbation. The expansion of the partition function in powers of $U$ then reads

$$Z/Z_0 = 1 + \frac{(-U)}{1!} \sum_{\vec{r}_1} \int_0^\beta d\tau_1 \langle n_{\vec{r}_1,\uparrow}(\tau_1) n_{\vec{r}_1,\downarrow}(\tau_1) \rangle_0 \tag{9.5}$$

$$+ \frac{(-U)^2}{2!} \sum_{\vec{r}_1,\vec{r}_2} \iint_0^\beta d\tau_1 d\tau_2 \langle n_{\vec{r}_1,\uparrow}(\tau_1) n_{\vec{r}_1,\downarrow}(\tau_1) n_{\vec{r}_2,\uparrow}(\tau_2) n_{\vec{r}_2,\downarrow}(\tau_2) \rangle_0 + \cdots,$$

where the notation $\langle \ldots \rangle_0 = \frac{1}{Z_0}\text{Tr}(e^{-\beta H_a}[\ldots])$ denotes an average in the non-interacting ensemble with quadratic action $S_0$ and $Z_0 = Tre^{-\beta H_a}$. Employing Wick's theorem we may express the expectation value in terms of determinants of the non-interacting Green's function

$$\mathcal{G}^0(\vec{r}_i - \vec{r}_j, \tau_i - \tau_j) = -\langle T c_{\vec{r}_i}(\tau_i) c_{\vec{r}_j}^\dagger(\tau_j) \rangle_0 \tag{9.6}$$

and obtain

$$\langle n_{\vec{r}_1,\uparrow}(\tau_1) n_{\vec{r}_1,\downarrow}(\tau_1) n_{\vec{r}_2,\uparrow}(\tau_2) n_{\vec{r}_2,\downarrow}(\tau_2) \cdots n_{\vec{r}_k,\uparrow}(\tau_k) n_{\vec{r}_k,\downarrow}(\tau_k) \rangle_0 = \det \mathbf{D}_k^\uparrow \det \mathbf{D}_k^\downarrow, \tag{9.7}$$

where the matrix elements of the $k \times k$ matrices $\mathbf{D}_k^\sigma$ are given by

$$(\mathbf{D}_k^\sigma)_{ij} = \mathcal{G}_\sigma^0(\vec{r}_i - \vec{r}_j, \tau_i - \tau_j). \tag{9.8}$$

Summing the contractions into a determinant instead of sampling them individually avoids a sign problem coming from the fermionic exchange .

We thus arrive at the following series for the partition function:

$$Z/Z_0 = \sum_{k=0}^{\infty} \frac{(-U)^k}{k!} \sum_{\vec{r}_1,\dots,\vec{r}_k} \int_0^\beta d\tau_1 \dots d\tau_k \left( \prod_\sigma \det \mathbf{D}_k^\sigma \right). \tag{9.9}$$

### 9.1.2 The non-interacting Green's function

To calculate the weights we still need to obtain the Green's function $\mathcal{G}^0(\vec{r}, \tau)$ of the non-interacting problem. This Green's function is best calculated by Fourier-transformation, as we had done in Sec. 6.5.1 and in the homework exercises for the tight binding model. After Fourier-transformation the non-interacting model becomes

$$H = \sum_{\vec{k},\sigma} \left( \epsilon_{\vec{k}} - \mu \right) n_{\vec{k},\sigma}. \tag{9.10}$$

To calculate Green's functions we have to Fourier transform also in time. Since the Green's function is an anti-periodic function in time (the minus sign coming from permutation of fermion operators), the Fourier transform needs half-integer frequencies, the so-called Matsubara frequencies $\omega_n = \frac{2\pi}{\beta}(n + 1/2)$. With these, the Green's function as a function of momentum and frequency is

$$\mathcal{G}^0(\vec{k}, \omega_n) = \frac{1}{i\omega_n - (\epsilon_{\vec{k}} - \mu)} \tag{9.11}$$

The Green's function $\mathcal{G}^0(\vec{r}, \tau)$ is obtained by Fourier transformation in space and imaginary time

$$\mathcal{G}^0(\vec{r}, \tau) = \frac{V}{(2\pi)^d} \int d\vec{k} \frac{1}{\beta} \sum_n \frac{\exp(i\vec{k}\vec{r} - i\omega_n\tau)}{i\omega_n - (\epsilon_{\vec{k}} - \mu)}. \tag{9.12}$$

Instead of performing an expensive Fourier transform for every update, $\mathcal{G}^0(\vec{r}, \tau)$ is best tabulated on an imaginary-time mesh, and then interpolated to the time $\tau$ required in a simulation.

## 9.2 Sign problem

Two "sign problems" may potentially occur in this expansion: an "intrinsic" sign problem arising from fermion exchange because the determinants might become negative and an "interaction" sign problem, arising for $U > 0$ from the $(-U)^k$ factor.

For attractive fermions, $U < 0$, and the second sign problem is absent. The determinants might have a sign problem, but in the absence of a magnetic field the Green's function for up and down fermions is the same. The two determinants are the same

and the weight is a square of a determinant, which is always positive. In the presence of a magnetic field we will, however, get a sign problem.

For repulsive fermions, which is the usual case in electronic problems, we can avoid the sign problem by doing a particle-hole transformation on one of the spin species and introduce new operators:

$$
\begin{aligned}
\tilde{c}_{i,\uparrow} &= c_{i,\uparrow} \\
\tilde{c}_{i,\uparrow}^{\dagger} &= c_{i,\uparrow}^{\dagger} \\
\tilde{c}_{i,\downarrow} &= c_{i,\downarrow}^{\dagger} \\
\tilde{c}_{i,\downarrow}^{\dagger} &= c_{i,\downarrow}^{\dagger}
\end{aligned}
\tag{9.13}
$$

As a consequence we have for the densities

$$
\begin{aligned}
\tilde{n}_{i,\uparrow} &= n_{i,\uparrow} \\
\tilde{n}_{i,\downarrow} &= 1 - n_{i,\downarrow}.
\end{aligned}
\tag{9.14}
$$

This transformation does not change the hopping term but it changes the sign of the interaction term, and thus removes the sign problem due to the interaction:

$$
U n_{i,\uparrow} n_{i,\downarrow} = U \tilde{n}_{i,\uparrow} (1 - \tilde{n}_{i,\downarrow}) = -U \tilde{n}_{i,\uparrow} \tilde{n}_{i,\downarrow} + U \tilde{n}_{i,\downarrow}.
\tag{9.15}
$$

The second term on the right hand side of above equation is just a shift in the chemical potentials of the down fermions. Let us thus look in more detail at the chemical potentials, considering both the chemical potential $-\mu(n_{i,\uparrow} + n_{i,\downarrow})$ and the magnetic field $-\frac{h}{2}(n_{i,\uparrow} - n_{i,\downarrow})$. We find that after the transformation the chemical potential for up-fermions

$$
\mu_{\uparrow} = \tilde{\mu}_{\uparrow} = \mu + h/2
\tag{9.16}
$$

is unchanged, but that for down-fermions $\mu_{\downarrow} = \mu - h/2$ changes sign and acquires the above shift:

$$
\tilde{\mu}_{\downarrow} = -\mu_{\downarrow} - U = -\mu + h/2 - U
\tag{9.17}
$$

It is now non-trivial to make the two determinants equal. The Green's functions agree only if the chemical potentials are the same: $\tilde{\mu}_{\uparrow} = \tilde{\mu}_{\downarrow}$, which implies $\mu = -U/2$, or equivalently the same densities $\tilde{n}_{i,\uparrow} = \tilde{n}_{i,\downarrow}$. Expressed in the original densities this means $n_{i,\uparrow} = 1 - n_{i,\downarrow}$ or $n_{i,\uparrow} + n_{i,\downarrow} = 1$. At this special density of half band filling we will thus have no sign problem,but the sign problem will reappear immediately when we change the filling.

## 9.3   Monte Carlo updates

The partition function Eq. (9.2) may be expressed as a sum of integrals originating from a diagrammatic expansion:

$$
Z = \sum_{k=0}^{\infty} \sum_{\vec{r}_1,\ldots,\vec{r}_k} \int_0^{\beta} d\tau_1 \ldots \int_{\tau_{k-1}}^{\beta} d\tau_k w(k, \vec{r}_1, \tau_1, \ldots, \vec{r}_k, \tau_k),
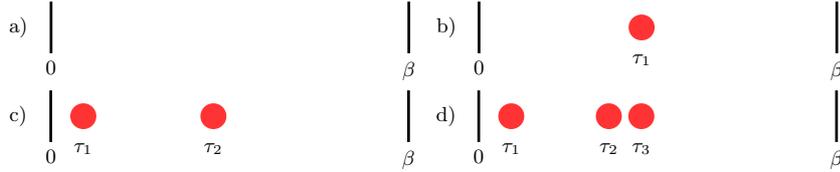\tag{9.18}
$$

Figure 9.1: Diagrammatic representation of configurations for a simplified model with only a single site. Shown are examples with orders $k = 0, 1, 2, 3$ and vertices (represented by dots) at times $\tau_1, \ldots, \tau_3$.
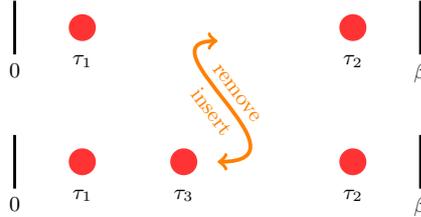


Figure 9.2: An insertion update (top to bottom) inserting a vertex at time $\tau_3$ and the corresponding removal update (bottom to top), removing the vertex at time $\tau_3$.

The individual configurations are of the form

$$\mathbf{x} \equiv (k, \vec{c}) \equiv (k, (\vec{r}_1, \tau_1, \ldots, \vec{r}_k, \tau_k)). \tag{9.19}$$

A configuration has a weight

$$w(k, \vec{r}_1, \tau_1, \ldots, \vec{r}_k, \tau_k) d\tau_1 \cdots d\tau_k, \tag{9.20}$$

which we will assume to be non-negative for now. In the following we will always assume time-ordering $\tau_1 \leq \tau_2 \leq \ldots \leq \tau_k$ and visualize the configurations using a diagrammatic representation as in Fig. 9.1.

Although these weights are well-defined probability densities they involve infinitesimals $d\tau$, which one might worry could cause difficulties with proposal and acceptance probabilities in the random walk in configuration space, but as we will show below this is not the case.

There are two types of Monte Carlo updates: (i) updates that increase the order $k$ by inserting an additional vertex at a position $\vec{r}$ and time $\tau$ and (ii) updates that decrease the order $k$ by removing a vertex $\tau_j$. These insertion and removal updates are necessary to satisfy the ergodicity requirement and are already sufficient: we can reach any configuration from another one by removing all the existing vertices and then inserting new ones.

In the following we will focus on the insertion and removal updates, illustrated in Fig. 9.2. For the insertion let us start from a configuration $(k, \vec{c}) = (k, \vec{r}_1, \tau_1, \ldots, \vec{r}_k, \tau_k)$ of order $k$. We propose to insert a new vertex at a time $\tau$ uniformly chosen in the interval $[0, \beta)$, to obtain a new time-ordered configuration $(k + 1, \vec{c}') = (k + 1, \vec{r}_1, \tau_1, \ldots, \vec{r}, \tau, \ldots, \vec{r}_k, \tau_k) \equiv (k + 1, \vec{r}'_1, \tau'_1, \ldots, \vec{r}'_{k+1}, \tau'_{k+1})$. The proposal rate for this

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insertion is given by the probability density

$$W^{\text{prop}}_{(k,\vec{c}),(k+1,\vec{c}')} = \frac{1}{N_s}\frac{d\tau}{\beta}, \tag{9.21}$$

where $N_s$ is the number of sites.

The reverse move is the removal of a randomly chosen vertex. The probability of removing a particular vertex to go back from $(k+1,\vec{c}')$ to $(k,\vec{c})$ is just one over the number of available vertices:

$$W^{\text{prop}}_{(k+1,\vec{c}'),(k,\vec{c})} = \frac{1}{k+1}. \tag{9.22}$$

To obtain the acceptance rates we first calculate the acceptance ratio

$$R_{(k,\vec{c}),(k+1,\vec{c}')} = \frac{p((k+1,\vec{c}'))}{p((k,\vec{c}))}\frac{W^{\text{prop}}_{(k+1,\vec{c}'),(k,\vec{c})}}{W^{\text{prop}}_{(k,\vec{c}),(k+1,\vec{c}')}} \tag{9.23}$$

$$= \frac{w(k+1,\vec{c}')d\tau_1'\cdots d\tau_{k+1}'}{w(k,\vec{c})d\tau_1\cdots d\tau_k}\frac{1/(k+1)}{d\tau/N_s\beta} = \frac{w(k+1,\vec{c}')}{w(k,\vec{c})}\frac{N_s\beta}{k+1}.$$

Observe that all infinitesimals cancel: the additional infinitesimal in the weight $p((k+1,\vec{c}'))$ is canceled by the infinitesimal of the proposal rate for insertions.

Equation (9.23) implies that the acceptance rates $W^{\text{acc}}$ are well defined finite numbers given by

$$W^{\text{acc}}_{(k,\vec{c}),(k+1,\vec{c}')} = \min\left[1, R_{(k,\vec{c}),(k+1,\vec{c}')}\right], \tag{9.24}$$

$$W^{\text{acc}}_{(k+1,\vec{c}'),(k,\vec{c})} = \min\left[1, 1/R_{(k,\vec{c}),(k+1,\vec{c}')}\right]. \tag{9.25}$$

Plugging in the explicit form of the weights we get

$$R = \frac{N_s\beta U}{(k+1)}\prod_\sigma\frac{\det \mathbf{D}^\sigma_{k+1}}{\det \mathbf{D}^\sigma_k}. \tag{9.26}$$

The complexity for this is naïvely $\mathcal{O}(k^3)$, but fast update formulas exist that reduce the complexity to $\mathcal{O}(k^2)$. Since $k \sim N_s\beta$ and we need to update each vertex on average once per sweep, the complexity is still $\mathcal{O}((N_s\beta)^3)$, much worse than the almost linear scaling for bosons and spins. However this difference is small compared to the additional $\mathcal{O}(\exp(N_s\beta))$ factor in case of a sign problem.