Appendix

A Hybrid Monte Carlo algorithm

The Hybrid Monte Carlo (HMC) [1] is an algorithm that updates the field configurations of a Markov Chain by introducing auxiliary momentums $\pi_\mu(\vec{n})$ conjugated to the link variables $U_\mu(\vec{n})$. This enable us to change the configuration $(\pi, U) \to (\pi', U')$ along a direction τ in the phase space. We describe the HMC procedure for a scalar field. The steps are the same for the implementation in QED; however, it involves a more subtle treatment of the fermion fields and the link variables, which can be revised in refs. [2, 3, 4].

Let us suppose a scalar field Φ with Euclidean action $S[\Phi]$. By introducing the conjugate momentum π, the Hamiltonian is given by

$$H[\Phi, \pi] = \frac{1}{2}\pi^2 + S[\Phi]. \tag{A.1}$$

On the lattice, $[\Phi]$ represents the field configuration and $\pi^2 = \sum_x \pi_x^2$, where x runs over all the lattice sites. The momentum configuration is generated with a distribution

$$p[\pi] \propto e^{-\frac{1}{2}\pi^2} \tag{A.2}$$

and $[\Phi]$ with a cold or hot start. From eq. (2.42), we know that expectation value of an operator $\hat{A}$ can be calculated through

$$\langle \hat{A} \rangle = \frac{\int \mathcal{D}[\Phi] e^{-S[\Phi]} \hat{A}[\Phi]}{\int \mathcal{D}[\Phi] e^{-S[\Phi]}}, \quad \mathcal{D}[\Phi] = \prod_x \Phi_x. \tag{A.3}$$

We can insert the momentum to this expression without modifying its final outcome

$$\langle \hat{A} \rangle = \frac{\int \mathcal{D}[\Phi]\mathcal{D}[\pi] e^{-\frac{1}{2}\pi^2} e^{-S[\Phi]} \hat{A}[\Phi]}{\int \mathcal{D}[\Phi]\mathcal{D}[\pi] e^{-\frac{1}{2}\pi^2} e^{-S[\Phi]}}, \qquad \mathcal{D}[\pi] = \prod_x \pi_x. \tag{A.4}$$

Now, we can evolve Φ_x and π_x along a trajectory τ with the Hamilton equations

$$\frac{d\Phi_x}{d\tau} = \frac{\partial H}{\partial \pi_x} = \pi_x, \quad \frac{d\pi_x}{d\tau} = -\frac{\partial H}{\partial \Phi_x} = -\frac{\partial S}{\partial \Phi_x}. \tag{A.5}$$

After $N\Delta\tau$ steps, the system arrives to a new configuration (π', ϕ'). As we mention in Chapter 2, the detailed balance condition

$$\frac{W([\Phi] \to [\Phi'])}{W([\Phi'] \to [\Phi])} = \frac{p[\Phi']}{p[\Phi]}, \quad p[\Phi] \propto e^{-S[\Phi]} \tag{A.6}$$

has to be fulfilled. We will prove that the condition is satisfied when the configurations are reversible, *i.e.* if we can go from (π, Φ) to (π', Φ') with the same probability as from $(-\pi', \Phi')$ to $(-\pi, \Phi)$, and when the measure does not change $\mathcal{D}[\Phi]\mathcal{D}[\pi] = \mathcal{D}[\Phi']\mathcal{D}[\pi']$.

Since eqs. (A.5) are deterministic, there is a transformation rule $f(\pi,\Phi)=(\pi',\Phi')$ and reversibility means that $f(\pi,\Phi)=(\pi',\Phi') \Leftrightarrow f(-\pi',\phi')=(-\pi,\phi)$. Both conditions can be achieved numerically by solving eqs. (A.5) with the so-called *leapfrog integrator*, which we describe below.

The Hamiltonian is a constant of motion and the configurations are constrained to $H=H[\Phi,\pi]$; so, in principle, (π',Φ') could be used as the new configuration of the Markov chain. However, eqs. (A.5) cannot be solved exactly, thus $H[\Phi,\pi]\neq H[\Phi',\pi']$. A way to correct this defect is to apply a Metropolis step, *i.e.* to calculate $\Delta H=H[\Phi',\pi']-H[\Phi,\pi]$ and only accept the change $(\pi,\Phi)\to(\pi',\Phi')$ with probability $\exp(-\Delta H)$.

The leapfrog integrator updates the values of Φ_x and π_x in a trajectory of length $N\Delta\tau$, $N\in\mathbb{Z}$, by evolving the value of Φ_x in N steps of size $\Delta\tau$ and evolving π_x in N steps conformed by two intermediate steps of length $\Delta\tau/2$

$$\begin{array}{lcll} \Phi_x\left[(i-1)\Delta\tau\right] & \longrightarrow & \Phi_x(i\Delta\tau), & \\ \pi_x\left[(i-1)\Delta\tau\right] & \to \pi_x\left[(i-\frac{1}{2})\Delta\tau\right] \to & \pi_x(i\Delta\tau), & i=1,\dots N. \end{array} \tag{A.7}$$

The equations for updating the values are

$$\begin{aligned} \Phi_x(i\Delta\tau) &= \Phi_x\left[(i-1)\Delta\tau\right]+\Delta\tau\left.\frac{d\Phi_x}{d\tau}\right|_{\tau=(i-1/2)\Delta\tau}, \\ \pi_x\left[\left(i-\frac{1}{2}\right)\Delta\tau\right] &= \pi_x\left[(i-1)\Delta\tau\right]+\frac{\Delta\tau}{2}\left.\frac{d\pi_x}{d\tau}\right|_{\tau=(i-1)\Delta\tau}, \\ \pi_x(i\Delta\tau) &= \pi_x\left[\left(i-\frac{1}{2}\right)\Delta\tau\right]+\frac{\Delta\tau}{2}\left.\frac{d\pi_x}{d\tau}\right|_{\tau=i\Delta\tau}. \end{aligned} \tag{A.8}$$

We can substitute the derivatives by using eqs. (A.5) and combine eqs. (A.8) to obtain

$$\begin{aligned} \Phi_x(i\Delta\tau) &= \Phi_x\left[(i-1)\Delta\tau\right]+\Delta\tau\,\pi_x\left[(i-1)\Delta\tau\right]-\frac{\Delta\tau^2}{2}\left.\frac{\partial S}{\partial\Phi_x}\right|_{\Phi_x[(i-1)\Delta\tau]}, \\ \pi_x(i\Delta\tau) &= \pi_x\left[(i-1)\Delta\tau\right]-\frac{\Delta\tau}{2}\left[\left.\frac{\partial S}{\partial\Phi_x}\right|_{\Phi_x[(i-1)\Delta\tau]}+\left.\frac{\partial S}{\partial\Phi_x}\right|_{\Phi_x(i\Delta\tau)}\right]. \end{aligned} \tag{A.9}$$

Let us revise that the Jacobian of the transformation $(\Phi_x[(i-1)\Delta\tau],\pi_x[(i-1)\Delta\tau])\to(\Phi_x(i\Delta\tau),\pi_x(i\Delta\tau))$ is equal to one. A computation of the matrix derivative of eqs. (A.9) yields

$$J=\det\begin{pmatrix} 1-\frac{\Delta\tau^2}{2}\left.\frac{\partial}{\partial\Phi_x[(i-1)\Delta\tau]}\frac{\partial S}{\partial\Phi_x}\right|_{\Phi_x[(i-1)\Delta\tau]} & \Delta\tau \\ -\frac{\Delta\tau}{2}\left.\frac{\partial}{\partial\Phi_x[(i-1)\Delta\tau]}\frac{\partial S}{\partial\Phi_x}\right|_{\Phi_x[(i-1)\Delta\tau]} & 1 \end{pmatrix}=1. \tag{A.10}$$

Thus, the measure does not change in each integration step $i-1\to i$. Since the Jacobian of the transformation from $\tau=0$ to $\tau=N\Delta\tau$ is the multiplication of all the Jacobians of eqs. (A.9) for $i=1,\dots,N$, we conclude that the measure does not change after N steps, *i.e.* $\mathcal{D}[\Phi]\mathcal{D}[\pi]=\mathcal{D}[\Phi']\mathcal{D}[\pi']$.

On the other hand, to show the reversibility we identify eqs. (A.9) as the transformation rule f that we mentioned above. Thus, to check that $f(\pi,\Phi)=(\pi,\Phi)\Leftrightarrow f(-\pi',\phi')=(-\pi,\phi)$ we interchange

$$\Phi_x\left[(i-1)\Delta\tau\right]\leftrightarrow\Phi_x\left(i\Delta\tau\right),\quad \pi_x\left[(i-1)\Delta\tau\right]\leftrightarrow-\pi_x(i\Delta\tau) \tag{A.11}$$

in the right hand side of eqs. (A.9)

$$\begin{aligned}
\Phi_x(i\Delta\tau) - \Delta\tau\,\pi_x(i\Delta\tau) - \frac{\Delta\tau^2}{2}\frac{\partial S}{\partial\Phi_x}\Big|_{\Phi_x(i\Delta\tau)} &= \Phi_x(i\Delta\tau) - \Delta\tau\,\pi_x[(i-1)\Delta\tau] \\
&+ \frac{\Delta\tau^2}{2}\left[\frac{\partial S}{\partial\Phi_x}\Big|_{\Phi_x[(i-1)\Delta\tau]} + \frac{\partial S}{\partial\Phi_x}\Big|_{\Phi_x(i\Delta\tau)}\right] \\
&- \frac{\Delta\tau^2}{2}\frac{\partial S}{\partial\Phi_x}\Big|_{\Phi_x(i\Delta\tau)} \\
&= \Phi_x(i\Delta\tau) - \Delta\tau\,\pi_x[(i-1)\Delta\tau] \\
&+ \frac{\Delta\tau^2}{2}\frac{\partial S}{\partial\Phi_x}\Big|_{\Phi_x[(i-1)\Delta\tau]} \\
&= \Phi_x[(i-1)\Delta\tau] \\
-\pi_x(i\Delta\tau) - \frac{\Delta\tau}{2}\left[\frac{\partial S}{\partial\Phi_x}\Big|_{\Phi_x[(i-1)\Delta\tau]} + \frac{\partial S}{\partial\Phi_x}\Big|_{\Phi_x(i\Delta\tau)}\right] &= -\pi_x[(i-1)\Delta\tau]. \qquad \text{(A.12)}
\end{aligned}$$

Therefore $f(\pi,\Phi) = (\pi,\Phi) \Leftrightarrow f(-\pi',\phi') = (-\pi,\phi)$ and reversibility is established. Now, we must show that the HMC algorithm obeys detailed balance. But first, let us summarize the algorithm steps as a recipe

1. We generate an auxiliary momentum configuration $[\pi]$ distributed according to $p[\pi] \propto \exp(-\sum_x \pi_x^2/2)$.
2. Then, we solve the Hamilton equations (A.5) by using the leapfrog integrator in order to evolve the system from $(\pi,\phi) \to (\pi',\phi')$.
3. If $\Delta H = H[\pi',\phi'] - H[\pi,\phi] \leq 0$ the configuration is updated, otherwise the update $(\pi,\phi) \to (\pi',\phi')$ is accepted only with probability $\exp(-\Delta H)$. This is equivalent to accept the change with probability $W_M = \min(1, \exp(-\Delta H))$.

These three steps are repeated the required number of types and each one of them conforms a sweep. It is important to mention that for each new sweep, the momentum configurations have to be generated again.

To show detailed balance, we begin with the transition probability to move from $[\Phi]$ to $[\Phi']$

$$W(\Phi'|\Phi) = \int \mathcal{D}[\pi]\mathcal{D}[\pi']\, W_M(\pi',\Phi'|\pi,\Phi) W_R(\pi',\Phi'|\pi,\Phi) e^{-\pi^2/2}, \qquad \text{(A.13)}$$

where we introduced the simplified notation $W(A|B)$, which means "the probability to move from B to A" (compare for instance with the notation in eq. (A.6)); where W_R stands for the probability of to evolve the system from $(\pi,\Phi') \to (\pi,\Phi)$, which satisfy reversibility $W_R(\pi',\Phi'|\pi,\Phi) = W_R(-\pi,\Phi|-\pi',\Phi')$ and where W_M is the probability to accept the update (step 3 of the recipe). We can rewrite $W_M(\pi',\Phi'|\pi,\Phi)$ as follows

$$\begin{aligned}
W_M(\pi',\Phi'|\pi,\Phi) &= \min(1,\exp(-\Delta H)) = \exp(-\Delta H)\min(\exp(\Delta H),1) \\
&= \exp(-\Delta H) W_M(\pi,\Phi|\pi',\Phi'). \qquad \text{(A.14)}
\end{aligned}$$

Since H depends on π^2, we have that

$$W_M(\pi',\Phi'|\pi,\Phi) = \exp(-\Delta H) W_M(-\pi,\Phi|-\pi',\Phi'). \qquad \text{(A.15)}$$

Then

$$W(\Phi'|\Phi) = \int \mathcal{D}[\pi]\mathcal{D}[\pi']\, W_M(\pi', \Phi'|\pi, \Phi) W_R(\pi', \Phi'|\pi, \Phi) e^{-\pi^2/2}$$
$$= \int \mathcal{D}[\pi]\mathcal{D}[\pi']\, e^{-\Delta H} W_M(-\pi, \Phi| - \pi', \Phi') W_R(-\pi, \Phi| - \pi', \Phi') e^{-\pi^2/2}$$
$$= \int \mathcal{D}[\pi]\mathcal{D}[\pi']\, W_M(-\pi, \Phi| - \pi', \Phi') W_R(-\pi, \Phi| - \pi', \Phi') e^{-S[\Phi']+S[\Phi]-\pi'^2/2}. \quad \text{(A.16)}$$

If we change variables $\pi \to -\pi$, $\pi' \to -\pi'$ the measure does not modify, therefore

$$\begin{aligned} W(\Phi'|\Phi) &= \int \mathcal{D}[\pi]\mathcal{D}[\pi']\, W_M(\pi, \Phi|\pi', \Phi') W_R(\pi, \Phi|\pi', \Phi') e^{-S[\Phi']+S[\Phi]-\pi'^2/2} \\ &= W(\Phi|\Phi') e^{-S[\Phi']+S[\Phi]}. \end{aligned}$$

Hence

$$\frac{W(\Phi'|\Phi)}{W(\Phi|\Phi')} = \frac{e^{-S[\Phi']}}{e^{-S[\Phi]}} = \frac{p[\Phi']}{p[\Phi]}, \quad \text{(A.17)}$$

i.e. detailed balance is satisfied.

B Second order numerical integrator

We wish to evaluate

$$I = \int_a^b f(x)dx \quad \text{(B.1)}$$

numerically. In order to do it, we construct a numerical integrator up to second order. Let us consider a lattice of N points separated by a length Δx, with the condition $f(x_1) = f(a)$, $f(x_N) = f(b)$. For the interior points of the lattice, we can express the second derivative as

$$f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}. \quad \text{(B.2)}$$

where we denote $f_i \equiv f(x_i)$. If N is an odd number, then (B.1) can be written, up to second order, by using a Taylor series

$$I = \sum_{i=1}^{\frac{N-1}{2}} \int_{x_{2i}-\Delta x}^{x_{2i}+\Delta x} \left[f_{2i} + f_{2i}'(x - x_{2i}) + f_{2i}'' \frac{(x - x_{2i})^2}{2} \right] dx, \quad \text{(B.3)}$$

where we are only integrating on the even sites. Simplifying eq. (B.3) yields

$$I = \sum_{i=1}^{\frac{N-1}{2}} 2\Delta x f_{2i} + \frac{\Delta x^3}{3} f_{2i}''. \quad \text{(B.4)}$$

If we substitute eq. (B.2) we obtain an expression that allows us to evaluate eq. (B.1) when N is odd

$$I = \sum_{i=1}^{\frac{N-1}{2}} \frac{\Delta x}{3} \left(f_{2i+1} + 4f_{2i} + f_{2i-1} \right). \quad \text{(B.5)}$$

On the other hand, if N is an even number, we can use the following version of eq. (B.5)

$$I = \sum_{i=1}^{\frac{N}{2}-1} \frac{\Delta x}{3} \left(f_{2i+2} + 4f_{2i+1} + f_{2i} \right). \quad \text{(B.6)}$$

However, we still need to integrate from the site x_1 to x_2 (see figure 1 for a graphical depiction). In this case, eq. (B.2) is not valid for the derivatives. Thus, we use the following discretization for the derivatives (see e.g. ref. [5])

$$f_1' = \frac{-3f_1 + 4f_2 - f_3}{2\Delta x}, \quad f_1'' = \frac{2f_1 - 5f_2 + 4f_3 - f_4}{\Delta x^2}. \tag{B.7}$$

Then, the contribution of the interval $[x_1, x_1 + \Delta x]$ to the integral is

$$\begin{aligned} \int_{x_1}^{x_1+\Delta x} \left[f_1 + f_1'(x - x_1) + f_1'' \frac{(x - x_1)^2}{2} \right] &= f_1 \Delta x + \frac{f_1'}{2}\Delta x^2 + \frac{f_1''}{6}\Delta x^3 \\ &= \Delta x \left(\frac{7}{12} f_1 + \frac{1}{6} f_2 + \frac{5}{12} f_3 - \frac{1}{6} f_4 \right). \end{aligned} \tag{B.8}$$

Therefore, the general result for the second order numerical integral reads

$$I = \begin{cases} \sum_{i=1}^{\frac{N-1}{2}} \frac{\Delta x}{3} \left(f_{2i+1} + 4 f_{2i} + f_{2i-1} \right) & \text{for odd } N \\ \sum_{i=1}^{\frac{N}{2}-1} \frac{\Delta x}{3} \left(f_{2i+2} + 4 f_{2i+1} + f_{2i} \right) \Delta x \left(\frac{7}{12} f_1 + \frac{1}{6} f_2 + \frac{5}{12} f_3 - \frac{1}{6} f_4 \right) & \text{for even } N. \end{cases} \tag{B.9}$$

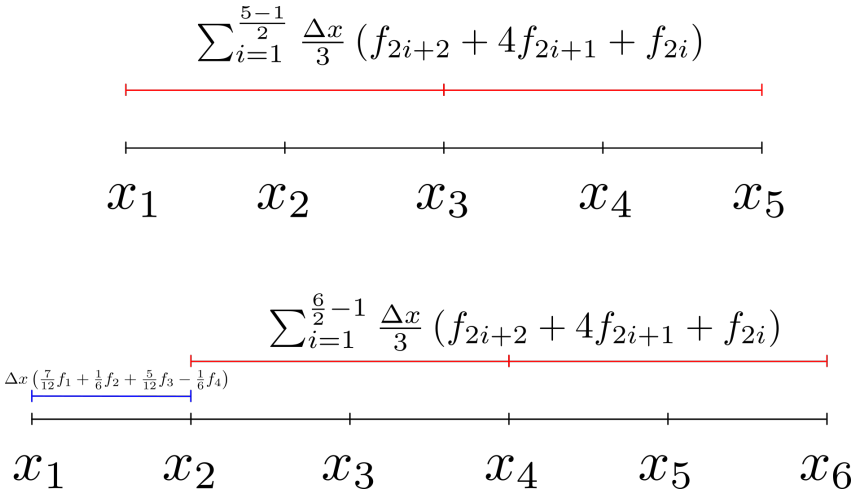

Figure 1: In the upper image we show a lattice with an odd number of points, where we can see that by integrating only in the even sites from $x_{2i} - \Delta x$ to $x_{2i} + \Delta x$, we can compute the numerical integral. In the lower image we show the case of a lattice with even N. There, we can compute the integral from x_2 up to the last site (x_6 in the figure); however, the contribution from x_1 to x_2 would be missing if we only use eq. (B.6). For that reason, one has to use eqs. (B.7) to calculate the contribution from the blue region, which is given by eq. (B.8).

C Jackknife error

The Jackknife error, σ_J, is a special kind of error that allows us to compute the uncertainty of a set of measurements by taking into account possible correlations between them. Let us suppose that we have N measurements of a variable x, we describe σ_J construction as a recipe:

- We calculate the average $\langle x \rangle$ of the N measurements.
- We divide the N measurements in M blocks. M should preferably be a number that satisfies $N/M \in \mathbb{Z}$.

- For each block $m = 1 \dots M$, we consider the set of the N measurements without the block m and calculate its average $\langle x \rangle_m$.
- The Jackknife error is defined as follows

$$\sigma_J = \sqrt{\frac{M-1}{M} \sum_{m=1}^{M} (\langle x \rangle_m - \langle x \rangle)^2}. \tag{C.1}$$

An important remark is that when $M = N$, σ_J coincides with the standard error, since for that case we have

$$\langle x \rangle_m = \frac{1}{N-1} \sum_{m' \neq m}^{N} x_m \Rightarrow \langle x \rangle_m - \langle x \rangle = \frac{1}{N-1} \langle x \rangle - x_m. \tag{C.2}$$

Then

$$\sigma_J = \sqrt{\frac{N-1}{N(N-1)^2} \sum_{m=1}^{N} (x_m - \langle x \rangle)^2} = \sqrt{\frac{1}{N(N-1)} \sum_{m=1}^{N} (x_m - \langle x \rangle)^2}. \tag{C.3}$$

In general, σ_J changes for a different number of blocks M. Due to that, normally one chooses the biggest σ_J for all possible M. Otherwise, the number of blocks has to be specified.

D Autocorrelation time

The autocorrelation time is a quantitative measurement of the correlation between the Monte Carlo configurations. It depends on a specific observable X, the lattice parameters and the algorithm that was used. To define it, we make use of the autocorrelation function

$$C_X(t) = \langle X_i X_{i+t} \rangle - \langle X_i \rangle \langle X_{i+t} \rangle, \tag{D.1}$$

where $t = |i - j|$, $i, j = 1, \dots N$, with N the number of measurements of X. For large t, the following behavior is known

$$C_X(t) \propto e^{-t/\tau_{\text{exp}}}, \tag{D.2}$$

where we refer to τ_{exp} as the *exponential autocorrelation time*. τ_{exp} can be obtained by measuring $C_X(t)$ for large t and fitting eq. (D.2). A small τ_{exp} means that the configurations are well decorrelated from each other. When that is not the case, it is recommendable to increment the number of sweeps between each configuration that is used to take measurements.

There is another autocorrelation time that can be defined, known as the *integrated autocorrelation time*

$$\tau_{\text{int}} = \frac{1}{2} + \sum_{t=1}^{N} \frac{C_X(t)}{C_X(0)}. \tag{D.3}$$

It can be proved that for large N, the statistical error σ_X is related to the decorrolated variance

$$\text{Var} = \langle X - \langle X \rangle^2 \rangle \tag{D.4}$$

by

$$\sigma_X^2 = 2\tau_{\text{int}} \frac{\text{Var}}{N}. \tag{D.5}$$

Thus, τ_{int} provides a way of finding an error that takes into account correlations between measurements. However, one can use the Jackknife error to do that; so instead it is possible to calculate τ_{int} with (D.5) by substituting $\sigma_J = \sigma_X$. One would expect that this result for τ_{int} coincides with eq. (D.3). Another utility of eq. (D.5) is that it tells us that we are using an effective sample of $N/(2\tau_{\text{int}})$ measurements. This is motivated by the fact that with decorrolated data the error is $\sqrt{\text{Var}/N}$. A deeper discussion about the autocorrelation time can be found in refs. [6, 7].

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