Appendix

A Hybrid Monte Carlo algorithm

In Chapter 2 we described how to implement the Metropolis algorithm to update a scalar field configuration $[\Phi]$ in order to achieve configurations distributed according to $p \propto \exp(-S[\Phi])$, where $S[\Phi]$ is the discretized Euclidean action. To update the configuration from $[\Phi]$ to $[\Phi']$ with this algorithm, one performs local updates $\Phi_x \to \Phi'_x$ which are accepted based on the ratio

$$\frac{p[\Phi']}{p[\Phi]} = e^{-\Delta S[\Phi,\Phi']}, \tag{A.1}$$

where

$$\Delta S = S[\Phi'] - S[\Phi]. \tag{A.2}$$

Now, when we consider gauge fields interacting with fermions, the partition function is given by

$$Z = \int \mathcal{D}[U]\,\mathcal{D}[\overline{\psi},\psi]\,e^{-S[\psi,\overline{\psi},U]} = \int \mathcal{D}[U]\,\mathcal{D}[\overline{\psi},\psi]\,e^{-S_F[\psi,\overline{\psi},U]}e^{-S_G[U]}, \tag{A.3}$$

where ψ and $\overline{\psi}$ are Grassmann fields and where U denotes the link variables. If we use eq. (2.50) and the first line of eqs. (2.98), we can rewrite the partition function as

$$Z = \int \mathcal{D}[U]\,e^{-S_G[U]}\det D[U], \tag{A.4}$$

where $D[U]$ is a discretization of the Dirac operator. Thus, the probability of a configuration $[U]$ is

$$p[U] = \frac{1}{Z}e^{-S_G[U]}\det D[U]. \tag{A.5}$$

We observe that in order to update the link variables, we will have to compute the ratio $\det D[U']/\det D[U]$, which is computationally expensive . Therefore, algorithms that perform local updates are not very efficient when one deals with fermions and gauge fields, since one has to consider complete configurations to calculate determinants.

Several algorithms that update entire configurations in one step have been introduced. For fermions interacting with gauge fields, the most efficient is the Hybrid Monte Carlo (HMC) algorithm [1], which introduces auxiliary momenta π, distributed according to $p[\pi] \propto \exp(-\pi^2/2)$, conjugated to the link variables U. By solving the Hamilton equations we can evolve (π, U) to (π', U') for N steps along a trajectory in the phase space. This is known as molecular dynamics evolution. After these N steps, one performs a *Langevin step*[1], that is, the momenta are generated again and the molecular dynamics evolution is repeated. We describe the HMC procedure for a scalar field. The steps are the same for

[1] This comes from another algorithm, known as Langevin algorithm (see for instance ref. [2]). Mixing this step with molecular dynamics is the reason of the "hybrid" name.

the implementation in QED; however, it involves a more subtle treatment of the fermion fields and the link variables, which is reviewed in refs. [3–5].

Let us suppose a scalar field configuration $[\Phi]$ with Euclidean action $S[\Phi]$. By introducing the conjugate momenta

$$\pi_x = \frac{\partial \mathcal{L}}{\partial \dot{\Phi}_x}, \tag{A.6}$$

the Hamiltonian is given by

$$H[\Phi, \pi] = \frac{1}{2}\pi^2 + S[\Phi], \tag{A.7}$$

where $\pi^2 = \sum_x \pi_x^2$ and where x runs over all the lattice sites. The momentum configuration is generated with a Gaussian distribution

$$p[\pi] \propto e^{-\frac{1}{2}\pi^2} \tag{A.8}$$

and $[\Phi]$ with a cold or hot start. From eq. (2.42), we know that expectation value of an observable A is given by

$$\langle A \rangle = \frac{\int \mathcal{D}[\Phi] e^{-S[\Phi]} A[\Phi]}{\int \mathcal{D}[\Phi] e^{-S[\Phi]}}, \quad \mathcal{D}[\Phi] = \prod_x \Phi_x. \tag{A.9}$$

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

$$\langle A \rangle = \frac{\int \mathcal{D}[\Phi]\mathcal{D}[\pi] e^{-\frac{1}{2}\pi^2} e^{-S[\Phi]} A[\Phi]}{\int \mathcal{D}[\Phi]\mathcal{D}[\pi] e^{-\frac{1}{2}\pi^2} e^{-S[\Phi]}}, \qquad \mathcal{D}[\pi] = \prod_x \pi_x. \tag{A.10}$$

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

$$\frac{d\Phi_x}{d\tau} = \frac{\partial H}{\partial \pi_x} = \pi_x, \quad \frac{d\pi_x}{d\tau} = -\frac{\partial H}{\partial \Phi_x} = -\frac{\partial S}{\partial \Phi_x}. \tag{A.11}$$

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

$$\frac{W([\Phi] \to [\Phi'])}{W([\Phi'] \to [\Phi])} = \frac{p[\Phi']}{p[\Phi]} = \frac{e^{-S[\Phi']}}{e^{-S[\Phi]}}, \quad p[\Phi] \propto e^{-S[\Phi]} \tag{A.12}$$

has to be fulfilled. We will show that the condition is satisfied when the transitions 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.11) are deterministic, there is a transformation rule

$$f(\pi, \Phi) = (\pi', \Phi') \tag{A.13}$$

that maps $(\pi, \Phi) \to (\pi', \Phi')$ and reversibility means that

$$f(\pi, \Phi) = (\pi', \Phi') \Leftrightarrow f(-\pi', \phi') = (-\pi, \phi). \tag{A.14}$$

Both conditions can be achieved numerically by solving eqs. (A.11), for instance 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.11) 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 $(\pi, \Phi) \to (\pi', \Phi')$ when $\Delta H \leq 0$, or if $\Delta H > 0$, accept it with probability $\exp(-\Delta H)$.

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

$$\begin{aligned} &\Phi_x\left[(i-1)\Delta\tau\right] && \longrightarrow && \Phi_x(i\Delta\tau), \\ &\pi_x\left[(i-1)\Delta\tau\right] && \to \pi_x\left[(i-\tfrac{1}{2})\Delta\tau\right] \to && \pi_x(i\Delta\tau), \quad i = 1, \ldots N. \end{aligned} \tag{A.15}$$

The equations for updating the values are

$$\begin{aligned} \Phi_x(i\Delta\tau) &= \Phi_x\left[(i-1)\Delta\tau\right] + \Delta\tau \frac{d\Phi_x}{d\tau}\bigg|_{\tau=(i-1/2)\Delta\tau}, \\ \pi_x\left[\left(i-\frac{1}{2}\right)\Delta\tau\right] &= \pi_x\left[(i-1)\Delta\tau\right] + \frac{\Delta\tau}{2}\frac{d\pi_x}{d\tau}\bigg|_{\tau=(i-1)\Delta\tau}, \\ \pi_x(i\Delta\tau) &= \pi_x\left[\left(i-\frac{1}{2}\right)\Delta\tau\right] + \frac{\Delta\tau}{2}\frac{d\pi_x}{d\tau}\bigg|_{\tau=i\Delta\tau}. \end{aligned} \tag{A.16}$$

We can substitute the derivatives by using eqs. (A.11) and combine eqs. (A.16) to obtain

$$\begin{aligned} \Phi_x(i\Delta\tau) &= \Phi_x\left[(i-1)\Delta\tau\right] + \Delta\tau\, \pi_x\left[(i-1)\Delta\tau\right] - \frac{\Delta\tau^2}{2}\frac{\partial S}{\partial \Phi_x}\bigg|_{\Phi_x[(i-1)\Delta\tau]}, \\ \pi_x(i\Delta\tau) &= \pi_x\left[(i-1)\Delta\tau\right] - \frac{\Delta\tau}{2}\left[\frac{\partial S}{\partial \Phi_x}\bigg|_{\Phi_x[(i-1)\Delta\tau]} + \frac{\partial S}{\partial \Phi_x}\bigg|_{\Phi_x(i\Delta\tau)}\right]. \end{aligned} \tag{A.17}$$

Let us verify 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 of derivatives of eqs. (A.17) yields

$$J = \det \begin{pmatrix} 1 - \frac{\Delta\tau^2}{2}\frac{\partial}{\partial \Phi_x[(i-1)\Delta\tau]}\frac{\partial S}{\partial \Phi_x}\Big|_{\Phi_x[(i-1)\Delta\tau]} & \Delta\tau \\ -\frac{\Delta\tau}{2}\frac{\partial}{\partial \Phi_x[(i-1)\Delta\tau]}\frac{\partial S}{\partial \Phi_x}\Big|_{\Phi_x[(i-1)\Delta\tau]} & 1 \end{pmatrix} = 1. \tag{A.18}$$

Thus, the measure does not change in any 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.17) for $i = 1, \ldots, N$, we conclude that the measure does not change after N steps, *i.e.* $\mathcal{D}[\Phi]\mathcal{D}[\pi] = \mathcal{D}[\Phi']\mathcal{D}[\pi']$.

To show the reversibility we identify eqs. (A.17) as the transformation rule f that we mentioned in eq. (A.13). To check eq. (A.14) we interchange

$$\Phi_x\left[(i-1)\Delta\tau\right] \leftrightarrow \Phi_x\left(i\Delta\tau\right), \quad \pi_x\left[(i-1)\Delta\tau\right] \leftrightarrow -\pi_x(i\Delta\tau) \tag{A.19}$$

on the right-hand side of eqs. (A.17)

$$\Phi_x(i\Delta\tau) - \Delta\tau\, \pi_x(i\Delta\tau) - \tfrac{\Delta\tau^2}{2}\frac{\partial S}{\partial \Phi_x}\Big|_{\Phi_x(i\Delta\tau)}$$

$$= \Phi_x(i\Delta\tau) - \Delta\tau\, \pi_x[(i-1)\Delta\tau] + \tfrac{\Delta\tau^2}{2}\left[\frac{\partial S}{\partial \Phi_x}\bigg|_{\Phi_x[(i-1)\Delta\tau]} + \frac{\partial S}{\partial \Phi_x}\bigg|_{\Phi_x(i\Delta\tau)}\right] - \frac{\Delta\tau^2}{2}\frac{\partial S}{\partial \Phi_x}\bigg|_{\Phi_x(i\Delta\tau)}$$

$$= \Phi_x(i\Delta\tau) - \Delta\tau\,\pi_x[(i-1)\Delta\tau] + \tfrac{\Delta\tau^2}{2}\frac{\partial S}{\partial\Phi_x}\Big|_{\Phi_x[(i-1)\Delta\tau]}$$

$$= \Phi_x[(i-1)\Delta\tau] - \pi_x(i\Delta\tau) - \tfrac{\Delta\tau}{2}\left[\frac{\partial S}{\partial\Phi_x}\Big|_{\Phi_x[(i-1)\Delta\tau]} + \frac{\partial S}{\partial\Phi_x}\Big|_{\Phi_x(i\Delta\tau)}\right]$$

$$= \text{-}\ \pi_x[(i-1)\Delta\tau]. \tag{A.20}$$

Therefore eq. (A.14) is established.

Now, we still have to 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.11) 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 accepting the change with probability $W_M = \min(1, \exp(-\Delta H))$.

These three steps are repeated the required number of times and together they conform a sweep. It is important to mention that for each new sweep, the momentum configuration has to be generated again.

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

$$W(\Phi'|\Phi) = \int \mathcal{D}[\pi]\mathcal{D}[\pi']\, W_M(\pi',\Phi'|\pi,\Phi) W_R(\pi',\Phi'|\pi,\Phi) e^{-\pi^2/2}, \tag{A.21}$$

where we introduced the simplified notation $W(A|B)$, which means "the probability to move from B to A" (here we deviate from the notation in eq. (A.12)). W_R stands for the probability to evolve the system from (π',Φ') to (π,Φ), which satisfies reversibility $W_R(\pi',\Phi'|\pi,\Phi) = W_R(-\pi,\Phi|-\pi',\Phi')$. 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

$$\begin{aligned} W_M(\pi',\Phi'|\pi,\Phi) &= \min(1,\exp(-\Delta H)) = \exp(-\Delta H)\min(\exp(\Delta H),1) \\ &= \exp(-\Delta H) W_M(\pi,\Phi|\pi',\Phi'). \end{aligned} \tag{A.22}$$

Since H does not depend on the sign of π, we obtain the relation

$$W_M(\pi',\Phi'|\pi,\Phi) = \exp(-\Delta H) W_M(-\pi,\Phi|-\pi',\Phi'). \tag{A.23}$$

Then

$$\begin{aligned} W(\Phi'|\Phi) &= \int \mathcal{D}[\pi]\mathcal{D}[\pi']\, W_M(\pi',\Phi'|\pi,\Phi) W_R(\pi',\Phi'|\pi,\Phi) e^{-\pi^2/2} \\ &= \int \mathcal{D}[\pi]\mathcal{D}[\pi']\, e^{-\Delta H} W_M(-\pi,\Phi|-\pi',\Phi') W_R(-\pi,\Phi|-\pi',\Phi') e^{-\pi^2/2} \\ &= \int \mathcal{D}[\pi]\mathcal{D}[\pi']\, W_M(-\pi,\Phi|-\pi',\Phi') W_R(-\pi,\Phi|-\pi',\Phi') e^{-S[\Phi']+S[\Phi]-\pi'^2/2}. \end{aligned} \tag{A.24}$$

Under sign flip $\pi \to -\pi$, $\pi' \to -\pi'$ the measure does not change, 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

$$\frac{W(\Phi'|\Phi)}{W(\Phi|\Phi')} = \frac{e^{-S[\Phi']}}{e^{-S[\Phi]}} = \frac{p[\Phi']}{p[\Phi]}, \tag{A.25}$$

i.e. detailed balance is satisfied.

B Second order numerical integral

In Chapter 3 we have to evaluate several integrals of the form

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

to solve the equations obtained by Hosotani. In order to do so, we construct a numerical integral 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 approximate the second derivative as

$$f_i'' \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}. \tag{B.2}$$

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

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

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

$$I \approx \sum_{i=1}^{\frac{N-1}{2}} 2\Delta x f_{2i} + \frac{\Delta x^3}{3} f_{2i}''. \tag{B.4}$$

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

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

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

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

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, because we do not have any more points to the left of the grid. Thus, we use the following discretization for the derivatives (see e.g. ref. [6]), which only relies on forward steps

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

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

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

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

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

We test the result with the following definite integrals

$$\int_{-1/\sqrt{2}}^{1/\sqrt{2}} xe^{-x^2}\,dx = 0, \quad \int_0^{\pi} e^x \cos(x)\,dx = -\frac{1}{2}(1+e^{\pi}). \tag{B.10}$$

In figure 2 we show the numerical value of these integrals as a function of the number of points, N, on the lattice. We also compare the result of eq. (B.9) with a calculation of the integrals by using midpoint Riemann sums. In figure 2 (a) we observe that the Riemann sum converges faster and that the numerical integral computed with eq. (B.9) oscillates around the right value for small N. In figure 2, (b) eq. (B.9) converges faster.

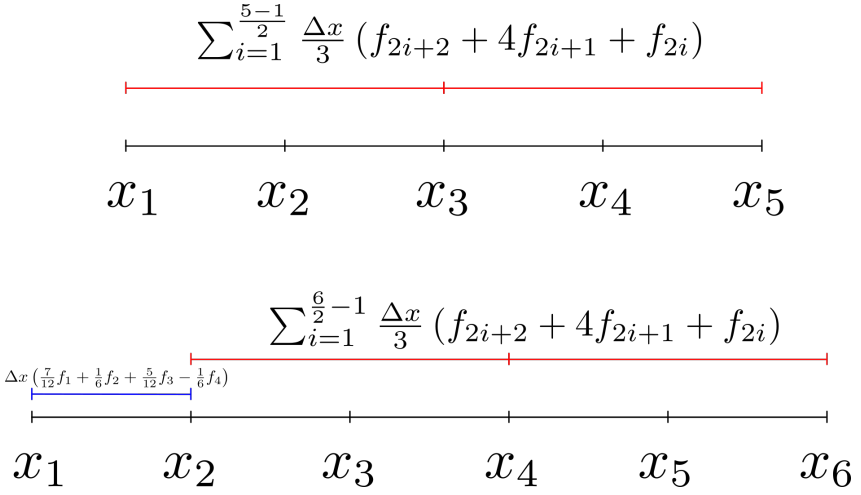
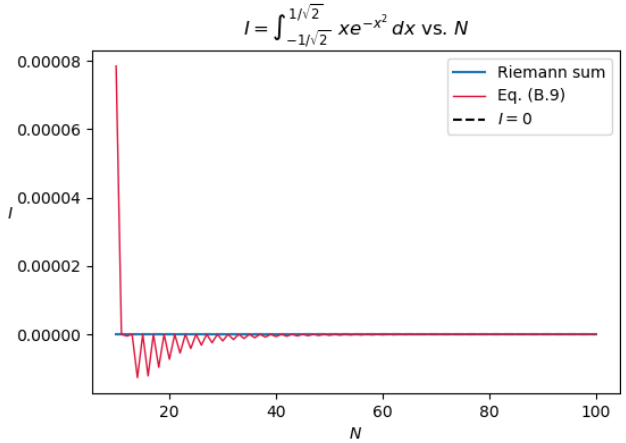
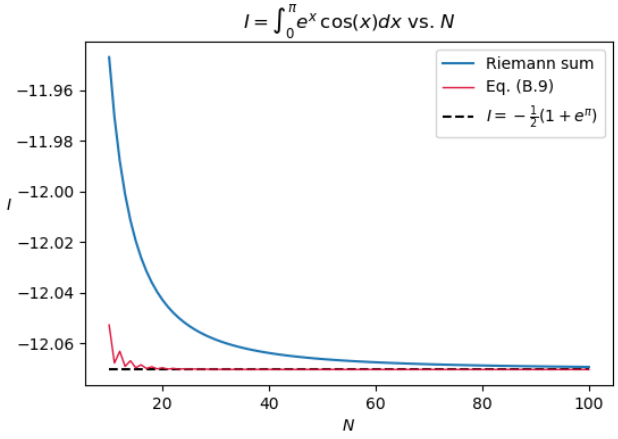


Figure 1: In the upper image we show a lattice with an odd number of points, where we see that by integrating only in the even sites from $x_{2i} - \Delta x$ to $x_{2i} + \Delta x$, we can compute the numerical integral. In the lower image we show the case of a lattice with even N. There, we can compute 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, we have to use eqs. (B.7) to calculate the contribution from the blue region, which is given by eq. (B.8).



(a) $\int_{-1/\sqrt{2}}^{1/\sqrt{2}} xe^{-x^2}\,dx$ as a function of the number of points used to evaluate the integral.



(b) $\int_0^\pi e^x \cos(x)\, dx$ as a function of the number of points used to evaluate the integral.

Figure 2: Test of the convergence of the numerical integral with the examples of eq. (B.10). We compare the results of the numerical integral presented in this section with the results obtained with Riemann sums.

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 autocorrelations. It is also useful to determine the error of a fit parameter. For instance, an error to the energy gap given by the correlation function (eq. (2.44)) can be obtained by fitting a cosh function to several data subsets and by estimating σ_J, using the resultant parameter of each fit as a measurement.

Let us suppose that we have N measurements of a variable x. We describe the calculation of σ_J 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 $N/M \in \mathbb{N}$.
- 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

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

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

$$\langle x \rangle_m = \frac{1}{N-1} \sum_{m' \neq m}^{N} x_{m'} \quad \Longrightarrow \quad \langle x \rangle_m - \langle x \rangle = \frac{1}{N-1} \left(\langle x \rangle - x_m \right). \tag{C.2}$$

Then

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

However, it is not the idea to take $M = N$, but to work with $M \ll N$. In general, σ_J changes for a different number of blocks M and it tends to be larger than the standard error. Therefore, normally one calculates the right-hand side of eq. (C.1) for several M and chooses the error as the largest value of the σ_J that were computed.

D Autocorrelation time

The autocorrelation time is a quantitative measure of the autocorrelation between the Markov chain configurations. It depends on a specific observable X. To define it, we make use of the correlation function

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

where $t = |i - j|$, $i, j = 1, \ldots, N$, 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. 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 (see e.g. ref. [7]), the statistical error σ_X is related to the 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, different from the jackknife error. Another interpretation of eq. (D.5) is that it tells us that we are using an effective sample of $N/(2\tau_{\text{int}})$ measurements. If $\tau_{\text{int}} = 1/2$, the effective sample is N, which indicates a perfect decorrelation. This is motivated by the fact that with decorrelated data the uncertainty is simply the standard error $\sqrt{\text{Var}/N}$. Deeper discussions of the autocorrelation time can be found in refs. [7–9].

Bibliography

[1] S. Duane, A. D. Kennedy, B. J. Pendleton, and D. Roweth. Hybrid Monte Carlo. *Phys. Lett. B*, 195:216–222, 1987.

[2] H. J. Rothe. *Lattice gauge theories: An Introduction*, volume 43. World Scientific, 1992.

[3] C. Gattringer and C. B. Lang. *Quantum Chromodynamics on the Lattice*. Springer, 2010.

[4] T. R. Haar. *Optimisations to Hybrid Monte Carlo for Lattice QCD*. PhD thesis, Adelaide U., 2019.

[5] A. Sternbeck. Simulations with (hybrid) monte carlo algorithms. *Helmholtz International Summer School, JINR Dubna*, 2014.

[6] B. Fornberg. Generation of finite difference formulas on arbitrarily spaced grids. *Math. Comp.*, 51:699–699, 1988.

[7] A. Sokal. *Monte Carlo Methods in Statistical Mechanics: Foundations and New Algorithms*, pages 131–192. Springer, 1997.

[8] F. Niedermayer. Cluster algorithms. *Lect. Notes Phys.*, 501:36, 1998.

[9] B. A. Berg. *Markov Chain Monte Carlo Simulations and Their Statistical Analysis*. World Scientific, 2004.