

Chapter 2

Monte Carlo Methods

No way to compute the path integral of lattice QCD analytically is known. Even on a finite lattice it amounts of solving the very-high-dimensional integral of Eq. (1.85). The integral receives large contributions only from a miniscule fraction of the space of integration variables, which suggests one way to estimate the path integral is through importance sampling using Markov chain Monte Carlo. In this chapter we introduce the basic concepts of a Markov chain. We then focus on the simulations of the path integral for gauge fields only. The fermions fields cannot be directly simulated due their anti-commuting nature and require special treatment, which is the subject of Chap. 3.

2.1 Markov Chain Monte Carlo

In general, a probability space $(\Omega, \sigma(\Omega), F_\Pi)$ is given by a non-empty space Ω , a sigma-algebra $\sigma(\Omega)$ of Ω a probability measure F_Π , which might be given by a probability density $dF_\Pi = \Pi(x)dx$ (see Sect. A.3). In QCD, we set the non-empty space Ω as $\Omega = (SU(N))^n$ (with n defining the dimension of the system), and consider the probability density Π given by

$$\Pi(U) = \frac{e^{-S(U)}}{Z} \quad \text{with} \quad Z = \int_{\Omega} e^{-S(U)} dU, \quad (2.1)$$

defined via an action S acting on $U \in \Omega$. We require S to be real. The task will be to compute the expectation of an operator $\hat{O}$ acting on U :

$$E(\hat{O}) = \int_{\Omega} O(U) \Pi(U) dU. \quad (2.2)$$

The basic idea of Markov chain Monte Carlo schemes in QCD is to approximate such expectation values $E(\hat{O})$ by Monte Carlo integration: $E(\hat{O}) \approx \frac{1}{n} \sum_{i=1}^n O(U_i)$, where the sequence of U -field configurations $\{U_1, U_2, \dots, U_n\}$ has been drawn at

random from $\Pi(U)$. If this sequence is generated by a Markov chain that is ergodic and satisfies the detailed balance condition it will converge to the unique fixed point distribution given by the density $\Pi(U)$.

To proceed, we have to recall three concepts from stochastic analysis, for simplicity here in discrete setting: (a) Markov chain, (b) detailed balance condition and (c) ergodicity:

- (a) A *Markov chain* is given by a sequence of random variables $X_1, X_2, \dots$ with the Markov property

$$P(X_{n+1} = y | X_n = x, X_i = x_i, i = 1, \dots, n-1) = P(X_{n+1} = y | X_n = x)$$

for conditional probabilities $P(A|B) = P(A \cap B)/P(B)$, *i.e.*, the probability of moving to the next state $X_{n+1} = y$ depends only on the present state $X_n = x$, but not on previous states.

Hence the transition probability from x to y can be described by a transition function $T(y, z)$, which fulfills the property

$$\sum_y T(x, y) = 1. \quad (2.3)$$

- (b) The detailed balance condition links the transition function and the fixed point distribution:

$$\Pi(x)T(x, y) = \Pi(y)T(y, x). \quad (2.4)$$

In the non-discrete setting, as given in Sect. 2.3 for the Hybrid Monte Carlo scheme, the transition function has to be generalised to a transition kernel.

- (c) The Markov process is ergodic, if for any pair of states x and y there is a finite number n of applications of the transition function such that $T^n(x, y) > 0$. Moreover the property $T(x, x) > 0$ called aperiodicity has to hold in order to avoid that the Markov chain gets trapped in cycles.

In order to give insight into the behaviour of a Markov process, let us examine the simplest possible example acting on a system with just two allowed states, $\{\chi_1, \chi_2\}$. The system evolves in a discrete time variable t and is in state ψ_t at time t . The dynamics of this Markov process can be encoded in a 2×2 matrix T , containing the transition probabilities $T_{ij} = P(\psi_{t+1} = \chi_i | \psi_t = \chi_j)$ and it is easy to see that the Markov property tells us

$$P(\psi_{t+k} = \chi_i | \psi_t = \chi_j) = [T^k]_{ij}. \quad (2.5)$$

Suppose the Markov matrix can be expressed as

$$T = \begin{pmatrix} 1-p & q \\ p & 1-q \end{pmatrix} \text{ with } 0 \leq p, q \leq 1, \quad (2.6)$$

then the detailed balance condition gives us the fixed-point probability $\underline{\pi}$ as

$$T\underline{\pi} = \underline{\pi} \quad \text{with} \quad \underline{\pi} = \frac{1}{p+q} \begin{pmatrix} q \\ p \end{pmatrix}. \quad (2.7)$$

The other eigenvalue of T is $\lambda = 1 - p - q$ with $|\lambda| < 1$. So we can write a general expression for T^k using the decomposition $T = SDS^{-1}$ which gives

$$T^k = \frac{1}{p+q} \begin{pmatrix} p & q \\ p & q \end{pmatrix} + \frac{\lambda^k}{p+q} \begin{pmatrix} q & -q \\ -p & p \end{pmatrix}. \quad (2.8)$$

The first term in this expression is the projection operator onto the fixed point and the second gives the rate of approach to this steady state, since $\lim_{k \rightarrow \infty} \lambda^k = 0$. We see that the memory of the chain falls exponentially as the Markov time-separation grows; states along the chain are correlated exponentially. Writing $\lambda^k = \exp(-k \ln \lambda)$, defines the *exponential autocorrelation time* $\tau = -1/\ln(1 - p - q)$ for this system. The difference between Markov chain algorithms lie in the value of the second largest eigenvalue λ , $|\lambda| < 1$ which determines the rate of approach to the steady state. The better algorithm has the smaller λ .

2.2 Sampling Yang–Mills Gauge Fields

We will consider in this section local Monte Carlo updates of the gauge links. The terms of the gauge action in Eq. (1.70) which contain a particular link $U_\mu(x)$ are

$$S[U_\mu(x)] = -\frac{\beta}{N} \text{Re tr} \left(U_\mu(x) \Sigma_\mu^\dagger(x) \right), \quad (2.9)$$

where

$$\Sigma_\mu(x) = \sum_{v \neq \mu} \left[U_v(x) U_\mu(x + a\hat{v}) U_v(x + a\hat{\mu})^{-1} + U_v(x - a\hat{v})^{-1} U_\mu(x - a\hat{v}) U_v(x - a\hat{v} + a\hat{\mu}) \right] \quad (2.10)$$

is the sum of the $2(d-1)$ so-called “staples”. The lattice can be divided into a checkerboard ordering of even and odd points. A point is even (odd) if the sum of its integer coordinates is even (odd). Since the staples contain links of the same direction μ as the link $U_\mu(x)$ we want to update located at nearest-neighbour points

of x , we can update the links of a given direction μ on all the even (or odd) sites independently. From here on we drop the argument (x, μ) of the gauge link to be updated.

We remark that Eq. (2.9) holds also for improved gauge actions like Eq. (1.137). The staples Σ contains more terms than in Eq. (2.10) originating from the 1×2 rectangles. Even/odd ordering of the lattice points is not enough to parallelize the update in this case.

2.2.1 Random Numbers and the Rejection Method

We assume that the reader is familiar with the generation of samples $W_1, W_2, \dots$ for a pseudorandom variable W which is uniformly distributed in the interval $[0, 1]$. For the algorithms which we will describe below it is crucial to have excellent random number generators, e.g. we mention the program RANLUX [1]. The density function for this variable is $f_W(w) = 1$. Typically one needs to generate samples $X_1, X_2, \dots$ of a variable $x \in [a, b]$ with a given density $f_X(x)$. The conservation of probability yields the relation

$$W = \int_0^W dw f_W(w) = \int_a^X dx f_X(x) = y(X) \quad (2.11)$$

By inverting the function y one finds the desired sample $X = y^{-1}(W)$. One example is the generation of a random variable $X \geq 0$ with an exponential density $f_X(x) = \exp(-x)$. A sample is obtained by setting $X_1 = -\ln(1 - W_1)$. Another example are normal (or Gaussian) distributed variables with density $f_X(x) = \exp(-x^2)/\sqrt{\pi}$. In the Box–Muller algorithm, two independent samples X_1 and X_2 are generated simultaneously according to

$$X_1 = \sqrt{-\ln(1 - W_2)} \cos(2\pi W_1), \quad X_2 = \sqrt{-\ln(1 - W_2)} \sin(2\pi W_1). \quad (2.12)$$

This result can be derived by setting in Eq. (2.11) $x_1 = \rho \cos(\phi)$, $x_2 = \rho \sin(\phi)$.

If the function $y(X)$ in Eq. (2.11) cannot be analytically inverted, an alternative is provided by the rejection method. One generates a trial sample X_1 from a trial density $h_{\text{trial}}(x)$. Then a uniform random number W_1 is drawn and the trial X_1 is accepted if

$$W_1 \leq \rho(X_1) = A \frac{f_X(X_1)}{h_{\text{trial}}(X_1)}, \quad (2.13)$$

where the factor A ensures $\rho(x) \leq 1$. Otherwise the trial X_1 is rejected and this step is repeated until a new trial is accepted. The average acceptance is given by $\int dx h_{\text{trial}}(x) \rho(x) = A$. One can show, by summing a geometric series which represents all possibilities to generate X , that the desired density function f_X is obtained.

2.2.2 Heatbath Algorithms

Heatbath algorithms visit each gauge link $U = U_\mu(x)$ on the lattice in turn and draw a new, independent value for the link from the distribution

$$dP(U) \propto \exp(-S[U]) dU, \quad (2.14)$$

where dP/dU is the density $\exp(-S[U])$ and $S[U]$ is defined in Eq. (2.9). We discuss in detail how this can be implemented for the gauge groups $U(1)$, $SU(2)$ and $SU(3)$.

Gauge group $U(1)$. We parameterise a $U(1)$ link variable by $U = \exp(i\phi)$ with an angle $\phi \in [-\pi, \pi]$. If we write the sum of staples in Eq. (2.10) as $\Sigma = s \exp(i\psi)$, Eq. (2.9) becomes

$$S[U] = -\beta s \cos(\phi - \psi). \quad (2.15)$$

The heatbath algorithm produces a new link variable $U = \exp(i\phi)$ by generating an angle Φ whose density function is (cf. Eq. (2.15))

$$f_\Phi(\phi) = N_q^{-1} e^{b \cos(\phi)}, \quad (2.16)$$

where the normalisation factor is

$$N_q = 2\pi I_0(b). \quad (2.17)$$

I_0 is the modified Bessel function. Then for the new link we set

$$\phi = \Phi + \psi. \quad (2.18)$$

Equation (2.16) is called the von Mises distribution. The procedure is described in [2, 3] and consists of a trial density with the rejection method described above,

$$h_{\text{trial}}(\phi) = \frac{N_t^{-1}}{1 - \alpha \cos(\phi)}, \quad N_t = 2\pi(1 - \alpha^2)^{-1/2}, \quad (2.19)$$

which has a free parameter α .

1. draw a uniform random number $W_1 \in [0, 1]$ and compute a trial $\Phi(W_1)$ from

$$\tan(\Phi/2) = \left(\frac{1 - \alpha}{1 + \alpha} \right)^{1/2} \tan(\pi(W_1 - \frac{1}{2})) \quad (2.20)$$

2. draw a second uniform random number $W_2 \in [0, 1]$ and accept the trial if

$$W_2 \leq \rho(\Phi) = A \frac{f_\Phi(\Phi)}{h_{\text{trial}}(\Phi)}. \quad (2.21)$$

If rejected go back to step 1. and repeat until the trial is accepted. The acceptance A can be computed analytically through $A = \min_{-\pi \leq \varphi \leq \pi} \frac{h_{\text{trial}}(\varphi)}{f_{\phi}(\varphi)}$. The optimal value α_{opt} for the parameter α , which maximizes the acceptance A is

$$\alpha_{\text{opt}} = \frac{2b}{1 + \sqrt{1 + 4b^2}} \quad (2.22)$$

and results in

$$\rho(\varphi) = \mu(\varphi) e^{1-\mu(\varphi)} \quad (2.23)$$

with $\mu(\varphi) = \frac{1}{2} \left(1 + \sqrt{1 + 4b^2} \right) - b \cos(\varphi)$. The maximal acceptance is

$$A(\alpha_{\text{opt}}) = I_0(b) \cosh(\beta) e^{-\sinh^2 \beta}, \quad (2.24)$$

where we introduced $2b = \sinh 2\beta$ in terms of which $\alpha_{\text{opt}} = \tanh \beta$. We remark that this procedure works both for positive and negative b .

Gauge group $SU(2)$. We represent a $SU(2)$ matrix using Eq. (1.62). This representation is also valid for any complex 2×2 matrix W which can be written as $W = w_0 + iw_j \sigma_j$, where now w_μ are complex numbers. For any two such matrices W and W' we have $\text{tr}(WW') = 2(w_0 w'_0 - w_j w'_j)$. We define a new $SU(2)$ variable $V = U \hat{\Sigma}^\dagger$ with $\hat{\Sigma} = \Sigma / \sqrt{\det(\Sigma)} \in SU(2)$. Then Eq. (2.14) becomes

$$dP(V) = dP(U) \propto \exp\left[\frac{\rho}{2} \text{tr}(V)\right] dV, \quad (2.25)$$

where $\rho = \beta \sqrt{\det(\Sigma)}$ and we used the invariance property of the Haar measure. The algorithm we describe here is based on Refs. [4, 5]. Using Eq. (1.62) for V , Eq. (2.25) becomes

$$dP(V) \propto \sqrt{1 - a_0^2} \exp(\rho a_0) da_0 d^3 n \delta(n^2 - 1), \quad (2.26)$$

where $a_j = n_j \sqrt{1 - a_0^2}$, $j = 1, 2, 3$. Once a_μ have been generated from the distribution Eq. (2.26), the new link variable is

$$U' = V \hat{\Sigma}. \quad (2.27)$$

In order to generate $a_0 \in [-1, 1]$, we perform a change of variable

$$y = \rho (1 - a_0). \quad (2.28)$$

The probability density of y follows from Eq. (2.26) and is given by

$$f_Y(y) \propto \sqrt{2 - \frac{y}{\rho}} \sqrt{y} \exp(-y). \quad (2.29)$$

It is realised by first generating a number Y with the trial density

$$h_{\text{trial}}(y) = \frac{2}{\sqrt{\pi}} \sqrt{y} \exp(-y), \quad (2.30)$$

and then correcting for the omitted factor $\sqrt{2 - \frac{y}{\rho}}$ by the rejection method. A random number W_3 is generated and Y is accepted if $2W_3^2 \leq 2 - \frac{Y}{\rho}$. The rejection rate is small in the limit when β is large (because ρ is large), which improves the original method in Ref. [6]. For the generation of Y we present the method of Ref. [7], which is a slight variation of that of Ref. [4]. First we generate a pseudorandom variable $A \geq 0$ with density

$$f_A(a) = \frac{2}{\sqrt{\pi}} \exp(-a^2) \quad (2.31)$$

and a second variable $B \geq 0$ with density

$$f_B(b) = \exp(-b). \quad (2.32)$$

Then

$$Y = A^2 + B \quad (2.33)$$

has the desired density Eq. (2.30). The generation of A and B can be done as described in Sect. 2.2.1. Notice that in Eq. (2.12) the angle 2π has to be replaced by $\pi/2$ so $A \geq 0$. Four uniform random numbers give two values of the trial Y . The last step is the generation of points n uniformly distributed on the unit sphere S^2 in three dimensions. This can be done by setting

$$n_1 = 1 - 2W_4, \quad n_2 = \sqrt{1 - n_1^2} \cos(2\pi W_5), \quad n_3 = \sqrt{1 - n_1^2} \sin(2\pi W_5), \quad (2.34)$$

with the help of two uniform random numbers W_4 and W_5 .

Gauge group $SU(3)$. $SU(N)$ gauge links can be updated [8] by applying sequential updates in $SU(2)$ subgroups embedded in $SU(N)$. Here this is described for $SU(3)$ following [9]. Consider three $SU(2)$ subgroups of $SU(3)$ parameterised by the matrices

$$A_{1,2} = \begin{pmatrix} a_{11} & a_{12} & 0 \\ a_{21} & a_{22} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad A_{2,3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & a_{11} & a_{12} \\ 0 & a_{21} & a_{22} \end{pmatrix}, \quad A_{1,3} = \begin{pmatrix} a_{11} & 0 & a_{12} \\ 0 & 1 & 0 \\ a_{21} & 0 & a_{22} \end{pmatrix}, \quad (2.35)$$

where $a \in SU(2)$. The Cabibbo–Marinari heatbath algorithm is a sequence of updates in the subgroups defined in Eq. (2.35). A minimal set consists of two of the

subgroups but all three subgroups can be taken. In each step the current gauge link U is multiplied by a matrix $A = A_{i,j}$ from Eq. (2.35). Equation (2.9) becomes $S[AU] = s[a] + \text{terms independent of } a$, where

$$s[a] = -\frac{\beta}{3} \text{Re tr}(AW), \quad W = U \Sigma^\dagger. \quad (2.36)$$

We denote by w the complex 2×2 submatrix of W , whose elements W_{ij} corresponds to the $SU(2)$ subgroup of A in Eq. (2.35). Using the quaternionic representations for a and w gives,

$$s[a] = -\frac{\beta}{3} \text{Re tr}(aw) = -\frac{\beta}{6} \text{tr}(av^\dagger), \quad (2.37)$$

where $v = 2\text{Re} w_0 I - i \sum_{k=1}^3 2\text{Re } w_k \sigma_k$. From here we follow the $SU(2)$ heatbath described above to generate a matrix a . The $SU(3)$ link is updated according to

$$U' = A U, \quad (2.38)$$

and then the next $SU(2)$ subgroup in the sequence is considered. In Ref [8] it is shown this procedure defines a Monte–Carlo heatbath algorithm for $SU(3)$.

2.2.3 Overrelaxation Algorithms

The heatbath algorithms described in Sect. 2.2.2 suffer from critical slowing down, becoming less efficient as the lattice spacing is decreased. Acceleration is achieved using a different type of algorithm called overrelaxation. It proposes changing link U to U' such that the action in Eq. (2.9) is preserved $S[U] = S[U']$ *i.e.* the change is microcanonical, the measure is preserved $dU = dU'$ and the change is reversible, *i.e.* applying the update to U' gives back U . Such a change is always accepted. Since it is not ergodic, the overrelaxation algorithm has to be used in combination with an ergodic algorithm like the heatbath. This combination is called a hybrid overrelaxation algorithm. A change of all links of the lattice is called a sweep. Usually one separates two heatbath sweeps by $L/(2a)$ overrelaxation sweeps to propagate the changes over a lattice of linear size L .

The $U(1)$ transformation (cf. Eq. (2.15))

$$\phi' = 2\psi - \phi \quad (2.39)$$

defines a overrelaxation update for gauge group $U(1)$.

The $SU(2)$ transformation (cf. Eq. (2.9))

$$U' = \hat{\Sigma} U^\dagger \hat{\Sigma} = -U + \text{tr}(U \hat{\Sigma}^\dagger) \hat{\Sigma} \quad (2.40)$$

defines an overrelaxation update for gauge group $SU(2)$.

For gauge group $SU(3)$ it is possible to make overrelaxation updates with respect to the various $SU(2)$ subgroups of the form $U \rightarrow U' = A U$, where $A = A_{ij}$ is one of the matrices in Eq. (2.35) [10, 11]. The action Eq. (2.37) is preserved, i.e. the property $\text{tr } v^\dagger = \text{tr } (av^\dagger)$ holds if

$$a = \frac{2}{\text{tr } (vv^\dagger)} v^2 = -I + 2 \frac{2v_0}{\text{tr } (vv^\dagger)} v \quad \text{with} \quad v_0 = \frac{1}{2} \text{tr } v. \quad (2.41)$$

Since $av^\dagger = v$, performing the same update on U' one has $a' = a^\dagger$ and the link changes to $U'' = A^\dagger U' = U$, i.e. the update is an involution. As a consequence the Jacobian of the update has unit modulus and the integration measure is preserved.

2.3 Hybrid Monte Carlo

Hybrid Monte Carlo (HMC) uses an augmented Markov chain that constructs samples of pairs of links $U \in SU(N)$ and momenta $P \in \hat{\mathcal{S}} = \mathfrak{su}(N)$ according to the probability distribution F_v with probability density $v(U, P)$ given by

$$v(U, P) = \underbrace{\frac{(2\pi)^{N/2}}{Z_H} \exp(-S(U))}_{\Pi(U)} \underbrace{\frac{1}{(2\pi)^{N/2}} \exp(-\langle P, P \rangle / 2)}_{\varphi(P)} = \frac{1}{Z_H} \exp(-H(U, P)), \quad (2.42)$$

with $Z_H = \int_{\Omega \times \hat{\mathcal{S}}} v(U, P) d(U, P)$ and $H(U, P) = \langle P, P \rangle / 2 + S(U)$ where $\langle P, P \rangle = \sum_{x, \mu} \langle P_{x, \mu}, P_{x, \mu} \rangle$, cf. Eq. (A.4). The transition from one configuration (U_0, P_0) to the next consists of a proposal step

$$(U_0, P_0) \rightarrow g(U_0, P_0), \quad (2.43)$$

with a mapping $g : \Omega \times \hat{\mathcal{S}} \rightarrow \Omega \times \hat{\mathcal{S}}$ which is for the moment arbitrary, followed by an acceptance step: $g(U_0, P_0)$ is accepted with probability

$$\alpha((U_0, P_0), g(U_0, P_0)) = \min \left(1, \frac{v(g(U_0, P_0))}{v(U_0, P_0)} \right) = \min \left(1, e^{-(H(g(U_0, P_0)) - H(U_0, P_0))} \right), \quad (2.44)$$

otherwise the old configuration (U_0, P_0) is kept as the next entry in the chain. In the following we show that the detailed balance equation holds, iff this mapping g is both time-reversible, i.e.,

$$P \cdot g(P \cdot g(U_0, P_0)^\top) = (U_0, P_0)^\top \quad \text{for } P = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (2.45)$$

and volume preserving:

$$\left| \det \left(\frac{\partial g(U_0, P_0)}{\partial (U_0, P_0)} \right) \right| = 1. \quad (2.46)$$

2.3.1 Detailed Balance Condition

The transition kernel $K((U_0, P_0), (\Omega' \times \hat{\Omega}'))$ describes the probability of drawing the sample following (U_0, P_0) from the subset $(\Omega' \times \hat{\Omega}') \subset (\Omega \times \hat{\Omega})$, i.e.,

$$K((U_0, P_0), (\Omega' \times \hat{\Omega}')) = P((U^*, P^*) \in (\Omega' \times \hat{\Omega}') | (U_0, P_0)), \quad (2.47)$$

where (U^*, P^*) is the next element in the Markov chain defined by the proposal and acceptance step. The transition kernel for HMC is given by

$$K((U_0, P_0), (\Omega' \times \hat{\Omega}')) = \alpha((U_0, P_0), g(U_0, P_0)) \delta_{g(U_0, P_0)}(\Omega' \times \hat{\Omega}') + (1 - \alpha((U_0, P_0), g(U_0, P_0))) \delta_{(U_0, P_0)}(\Omega' \times \hat{\Omega}'). \quad (2.48)$$

As we are only interested in the transition of the links, we can define a restricted transition kernel

$$K_L(U_0, \Omega') = P(U_0^* \in \Omega' | U_0) = \int_{\hat{\Omega}} K((U_0, P), (\Omega' \times \hat{\Omega})) \varphi(P) dP. \quad (2.49)$$

Now we have to check whether the detailed balance condition holds for K_L with respect to the static distribution $\Pi(U)$, i.e.,

$$\int_A K_L(U, B) \Pi(U) dU = \int_B K_L(U, A) \Pi(U) dU \quad (2.50)$$

holds for all $A, B \in \sigma(\Omega)$. With $\delta_{(U, P)}(B \times \hat{\Omega}) = \delta_U(B)$, the left-hand side of (2.50) becomes

$$\begin{aligned} & \int_A \int_{\hat{\Omega}} \min \left(1, \frac{v(g(U, P))}{v(U, P)} \right) \delta_{g(U, P)}(B \times \hat{\Omega}) \varphi(P) \Pi(U) dP dU \\ & + \int_{A \cap B} \int_{\hat{\Omega}} \left(1 - \min \left(1, \frac{v(g(U, P))}{v(U, P)} \right) \right) \varphi(P) \Pi(U) dP dU. \end{aligned}$$

Correspondingly, the right-hand side reads

$$\int_B \int_{\hat{\Omega}} \min \left(1, \frac{v(g(U, P))}{v(U, P)} \right) \delta_{g(U, P)}(A \times \hat{\Omega}) \varphi(P) \Pi(U) dP dU + \\ \int_{B \cap A} \int_{\hat{\Omega}} \left(1 - \min \left(1, \frac{v(g(U, P))}{v(U, P)} \right) \right) \varphi(P) \Pi(U) dP dU.$$

As the last terms on both sides coincide, it remains to show

$$\int_A \int_{\hat{\Omega}} \min (v(U, P), v(g(U, P))) \delta_{g(U, P)}(B \times \hat{\Omega}) d(P, U) \\ = \int_B \int_{\hat{\Omega}} \min (v(U, P), v(g(U, P))) \delta_{g(U, P)}(A \times \hat{\Omega}) d(P, U).$$

With $\delta_{g(U, P)}(B \times \hat{\Omega}) = \delta_{(U, P)}(g^{-1}(B \times \hat{\Omega}))$ this is equivalent to

$$\underbrace{\int_{(A \times \hat{\Omega}) \cap g^{-1}(B \times \hat{\Omega})} \min (v(U, P), v(g(U, P))) d(P, U)}_{F_1} \\ = \underbrace{\int_{(B \times \hat{\Omega}) \cap g^{-1}(A \times \hat{\Omega})} \min (v(U, P), v(g(U, P))) d(P, U)}_{F_2}$$

As $\varphi(P) = \varphi(-P)$, $v(U, P) = v(U, -P)$, and the time reversibility of g leads to

$$v(g(U, P)) = v(g^{-1}(U, -P)). \quad (2.51)$$

Integration by substitution now yields

$$F_1 = \int_{g^{-1}(B \times \hat{\Omega})} \min (v(U, P), v(g(U, P))) \delta_{(U, P)}(A \times \hat{\Omega}) d(P, U) \\ = \int_{B \times \hat{\Omega}} \min (v(g^{-1}(U, P)), v(U, P)) \delta_{g^{-1}(U, P)}(A \times \hat{\Omega}) \cdot \left| \det \frac{dg^{-1}(U, P)}{d(U, P)} \right| d(P, U) \\ = \int_{B \times \hat{\Omega}} \min (v(g(U, -P)), v(U, -P)) \delta_{g^{-1}(U, P)}(A \times \hat{\Omega}) \cdot \left| \det \frac{dg^{-1}(U, P)}{d(U, P)} \right| d(P, U) \\ = \int_{B \times \hat{\Omega}} \min (v(g(U, -P)), v(U, -P)) \delta_{g(U, -P)}(A \times \hat{\Omega}) \cdot \left| \det \frac{dg^{-1}(U, P)}{d(U, P)} \right| d(P, U),$$

where we have used in the last step that $\delta_{g^{-1}(U, P)}(A \times \hat{\Omega}) = \delta_{g(U, -P)}(A \times \hat{\Omega})$. With $\delta_{g(U, P)}(A \times \hat{\Omega}) = \delta_{(U, P)}(g^{-1}(A \times \hat{\Omega}))$, we finally have

$$F_1 = \int_{(B \times \hat{\Omega}) \cap g^{-1}(A \times \hat{\Omega})} \min (v(g(U, P)), v(U, P)) \left| \det \frac{dg^{-1}(U, P)}{d(U, P)} \right| d(P, U) = F_2.$$

Hence $F_1 = F_2$, iff the mapping g is time-reversible and volume-preserving.

As a conclusion we can state that the kernel K_L fulfills the detailed balance condition, iff the mapping $g : \Omega \times \hat{\Omega} \rightarrow \Omega \times \hat{\Omega}$ is time-reversible and volume preserving. This can be achieved if we define g to be the Hamiltonian flow $(U(T), P(T)) = g(U_0, P_0)$ at some arbitrary time point T according to the Hamiltonian $H(U, P) = \langle P, P \rangle / 2 + S(U)$, if started from the initial value (U_0, P_0) . Note that we do not have to compute the flow exactly, any numerical approximation is feasible, provided it is both time-reversible and volume preserving. We will come back to this point in Sect. 2.5.

2.3.2 Hamilton's Equation of Motion

There are several ways to derive Hamilton's equation of motion. A first, physically intuitive way can be found in many textbooks. The time derivative of $U_\mu(x)$ is derived via an infinitesimal rotation on the group manifold:

$$\dot{U}_\mu(x) = P_\mu(x) U_\mu(x). \quad (2.52)$$

The remaining equation for $\dot{P}_\mu(x)$ is then obtained from the fact that the total time derivative of the Hamiltonian is zero, and $\dot{H}(U, P)$ is solved for $\dot{P}_\mu(x)$. For details we refer to Chap. 7.2.3 in [12]. Alternatively, $\dot{P}_\mu(x)$ can be computed via

$$\dot{P}_\mu(x) = -\partial_{x,\mu} H(U, P) = -\partial_{x,\mu} S(U), \quad (2.53)$$

where the link differential operator acting on $S(U)$ and is defined in Eq. (A.6). We will use the Wilson action defined in Eq. (1.70),

$$S(U) = S_w(U) = \frac{\beta}{2N} \sum_x \sum_{\mu, \nu} \text{Re tr} [1 - P_{\mu, \nu}(x)], \quad (2.54)$$

for $U \in SU(N)$, as an example for this approach, where the sum runs over all oriented plaquettes $P_{\mu, \nu}(x)$. In the following we will need to collect all the terms in the action that depends on a specific link variable $U_\mu(x)$:

$$S(U) = -\frac{\beta}{N} \text{Re tr} (U_\mu(x) \Sigma_\mu^\dagger(x)) + \text{terms independent of } U_\mu(x),$$

where $\Sigma_\mu(x)$ is the sum of staples defined in Eq. (2.10). Computing now the link derivative of the Wilson action, one gets its Lie-algebra components

$$\begin{aligned}
\partial_{x,\mu}^i S(U) &= -\frac{\beta}{N} \text{Re tr} \left\{ T^i U_\mu(x) \Sigma_\mu^\dagger(x) \right\} + \sum_{(y,\nu) \neq (x,\mu)} 0 \\
&= -\frac{\beta}{N} \text{Re tr} \left\{ T^i U_\mu(x) \Sigma_\mu^\dagger(x) \right\}.
\end{aligned} \tag{2.55}$$

Finally we obtain

$$\partial_{x,\mu} S(U) = -\frac{\beta}{2N} Z_\mu(x), \tag{2.56}$$

in terms of the Lie-algebra-valued field

$$Z_\mu(x) = -\{U_\mu(x) \Sigma_\mu^\dagger(x)\}_{TA}. \tag{2.57}$$

Here we have used the notation

$$W_{TA} = \frac{W - W^\dagger}{2} - \frac{\text{tr}(W - W^\dagger)}{2N},$$

for the traceless, antihermitian part of a matrix W . Equation (2.56) follows from the identity

$$-2T^i \text{Re tr} \left\{ T^i U_\mu(x) \Sigma_\mu^\dagger(x) \right\} = \left\{ U_\mu(x) \Sigma_\mu^\dagger(x) \right\}_{TA}, \tag{2.58}$$

which can be proved by computing the components of W_{TA} in the Lie algebra. These components are given by $-2\text{tr}(W_{TA} T^i)$.

A second approach generalizes the case of classical Hamiltonian mechanics to Lattice QCD. In classical Hamiltonian mechanics, the symplectic structure of the phase space (q, p) is defined by the closed 2-form $\omega = dq \wedge dp$. Correspondingly, the equations of motion for a Hamiltonian function $H(p, q) = T(p) + U(q)$ are

$$\dot{q} = \{H, q\} = \hat{H}q, \tag{2.59}$$

$$\dot{p} = \{H, p\} = \hat{H}p, \quad (i = 1, \dots, n) \tag{2.60}$$

where the Poisson brackets are defined via the closed 2-form by

$$\{A, B\} = -\omega(\hat{A}, \hat{B}) = \left(\frac{\partial A}{\partial q} \frac{\partial A}{\partial p} \right) J \left(\frac{\partial B}{\partial q} \right) = \frac{\partial A}{\partial p} \frac{\partial B}{\partial q} - \frac{\partial A}{\partial q} \frac{\partial B}{\partial p}, \tag{2.61}$$

with

$$J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix} \tag{2.62}$$

and the Hamiltonian vector field $\hat{A}$ for the 0-form A is given by

$$\frac{\partial A}{\partial p} \frac{\partial}{\partial q} - \frac{\partial A}{\partial q} \frac{\partial}{\partial p}. \quad (2.63)$$

This gives the well-known equations of motion

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = J \begin{pmatrix} \frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial p} \end{pmatrix} = \begin{pmatrix} \frac{\partial H}{\partial p} \\ -\frac{\partial H}{\partial q} \end{pmatrix}. \quad (2.64)$$

As Ω is a Lie group and $\hat{\Omega}$ the corresponding Lie-algebra, we can write $P \in \hat{\Omega}$ as $P = p^i T_i$ with T_i generators of the representation of P in $\hat{\Omega}$. These generators are linked to the group variables U via the right-hand invariant vector field defined by e_i : $e_i U = -T_i U$. We can now define Hamilton's equations governing the Hamiltonian flow (U, P) :

$$\begin{aligned} \dot{U} &= \{H, U\} = \hat{H}U, \\ \dot{P} &= \{H, P\} = \hat{H}P, \end{aligned} \quad (2.65)$$

where now the Lie brackets are defined via the closed 2-form $\omega = -dp$ defining the symplectic structure of the phase space (U, P) . For this 2-form, the vector field $\hat{H}$ associated to the Hamiltonian 0-form $H = p^i p_i / 2 + S(U)$ turns out to be

$$\hat{H} = p_i e_i - e_i(S) \frac{\partial}{\partial p_i}, \quad (2.66)$$

which gives

$$\begin{aligned} \dot{U} &= \hat{H}U = p^i e_i(U) = -p_i T_i U = -PU, \\ \dot{P} &= \hat{H}P = -e_i(S) \frac{\partial P}{\partial p_i} = -e_i(S) T_i. \end{aligned} \quad (2.67)$$

Depending on the action S , the force $e_i(S) T_i$ can be computed further: for the pure gauge part $S = -(\beta/N) S_G$ with $S_G = \text{Re tr}(\Sigma^\dagger U)$ see Eq. (2.9), we get

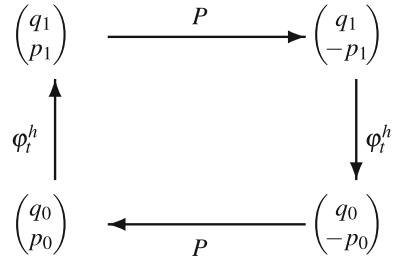
$$e_i(S_G) T_i = \text{Re tr}(\Sigma^\dagger e_i(U)) T^i = -\text{Re tr}(\Sigma^\dagger T_i U) T^i = -\text{Re tr}(U \Sigma^\dagger T_i) T^i,$$

which is equivalent to the result already obtained in (2.56).

2.4 Symplectic Integration Schemes

As seen in Sect. 2.3, any time-reversible and volume-preserving numerical approximation scheme is suitable to establish the detailed balance condition. Before discussing the non-Abelian case of Lattice QCD, we will briefly recapitulate the

Fig. 2.1 Time-reversibility of a numerical flow φ_t^h : applying the transformations φ_t^h , P , φ_t^h and finally P to the initial value (q_0, p_0) yields the initial value again



concepts of time-reversibility and symplecticity of numerical schemes applied to Hamiltonian initial-value problems (ODE-IVP)

$$\dot{y} = J^{-1} \nabla H(y), \quad y(t_0) = y_0, \quad (2.68)$$

with $y = (q, p)^\top, f : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}^{2n}$ at least continuously differentiable.

Consider a numerical scheme defined by $\varphi_t^h(y_0)$ applied to the ODE-IVP, which constructs a numerical approximation at time $t_0 + h$, starting at the exact solution y_0 at time t_0 . $\varphi_t^h(y_0)$ is said to be

- *symplectic*, if the numerical scheme defines a symplectic transformation, i.e. if

$$\left(\frac{\partial \varphi_t^h}{\partial y_0} \right)^\top J \left(\frac{\partial \varphi_t^h}{\partial y_0} \right) = J \quad (2.69)$$

with the matrix J defined in (2.62).

- *time reversible*, if (see Fig. 2.1)

$$P \cdot \varphi_t^h(P \cdot \varphi_t^h(y_0)) = y_0 \quad \text{for } P = \begin{pmatrix} I_n & 0 \\ 0 & -I_n \end{pmatrix}, \quad (2.70)$$

which is equivalent to $P\varphi_t^h = \varphi_t^{-h}P$ for symmetric schemes $\varphi_t^h\varphi_t^{-h} = I$.

A consequence of symplecticity is volume preservation:

$$\left| \det \left(\frac{\partial \varphi_t^h}{\partial y_0} \right) \right| = 1, \quad (2.71)$$

which implies that symplecticity is a sufficient condition for volume-preservation.

Due to the symmetry of the scheme, the most simple symplectic and symmetric numerical method has at least order two, i.e., the difference between exact solution and numerical approximation at time T after n steps of step size h ($T = nh$) is of order $\mathcal{O}(h^2)$ when h is sufficiently small. It is given by the Störmer-Verlet method (or Leap-Frog scheme), which can be written as an explicit scheme for separable

Hamiltonians $H(q, p) = V(p) + U(q)$. One step, starting from initial values (q_0, p_0) , to obtain numerical approximations (q_1, p_1) at time $t_0 + h$ reads

$$\begin{aligned} p_{1/2} &= p_0 - \frac{h}{2} U_q(q_0), \\ q_1 &= q_0 + h V_p(p_{1/2}), \\ p_1 &= p_{1/2} - \frac{h}{2} U_q(q_1), \end{aligned} \quad (2.72)$$

with short-hands U_q and V_p for $\partial U / \partial q$ and $\partial V / \partial p$, respectively. Symplecticity of the scheme follows directly from the fact that is defined by the composition of three symplectic mappings

$$\begin{aligned} (q_0, p_0) &\rightarrow p_{h/2}(q_0, p_0) = (q_0, p_{1/2}), \\ (q_0, p_{1/2}) &\rightarrow q_h(q_0, p_{1/2}) = (q_1, p_{1/2}), \\ (q_1, p_{1/2}) &\rightarrow p_{h/2}(q_1, p_{1/2}) = (q_1, p_1), \end{aligned} \quad (2.73)$$

so-called p - and q -updates with step sizes $h/2$, h and $h/2$, resp., which enables us to rewrite the leap-frog scheme as

$$p_{h/2} \circ q_h \circ p_{h/2}(q_0, p_0). \quad (2.74)$$

Symmetry follows directly by changing the sign of h and replacing (q_0, p_0) by (q_1, p_1) . Time reversibility is then given for symmetrical Jacobians V_p which fulfill $V_p(p) = -V_p(-p)$.

An easy way to derive symplectic and time-reversible higher-order schemes $\tilde{\varphi}_t^h$ is based on the composition of m symplectic and time-reversible basic schemes φ_t^h :

$$\tilde{\varphi}_t^h = \varphi_t^{\gamma_1 h} \circ \varphi_t^{\gamma_2 h} \circ \dots \circ \varphi_t^{\gamma_m h}. \quad (2.75)$$

Besides the time-reversibility of the underlying basic schemes φ_t^h , the coefficients have to be symmetric too to get an overall time-reversible system:

$$\gamma_{m-k+1} = \gamma_k \quad \text{for } k = 1, 2, \dots, m. \quad (2.76)$$

It can easily be shown that the composition scheme has order $p + 1$ (with the underlying scheme having order p), if the following two conditions hold for the free parameters $\gamma_1, \dots, \gamma_m$:

$$\sum_{j=1}^m \gamma_j = 1, \quad \sum_{j=1}^m \gamma_j^p = 0. \quad (2.77)$$

Symplecticity and time-reversibility of the composition scheme follow directly from symplecticity and time-reversibility of the underlying scheme.

This approach allows us to construct symplectic and time-reversible schemes of any arbitrary (even) high order. We start with the Störmer-Verlet scheme φ_t^h and define

$$\tilde{\varphi}_t^h = \varphi_t^{\gamma_1 h} \circ \varphi_t^{\gamma_2 h} \circ \varphi_t^{\gamma_3 h} \quad (2.78)$$

with

$$\gamma_1 = \gamma_3 = \frac{1}{2 - 2^{\frac{1}{3}}}, \gamma_2 = 1 - 2\gamma_1. \quad (2.79)$$

These coefficients fulfill both conditions above, which gives at least order 3 for the composition scheme $\tilde{\varphi}_t^h$. As the order of symmetric methods is even, we get order 4 for $\tilde{\varphi}_t^h$. We can now repeat this process by just replacing φ_t^h by $\tilde{\varphi}_t^h$, and we get schemes of order 6, 8, etc.

Another idea is to use splitting schemes to treat different parts of the right-hand side independently, i.e., the different parts of the right-hand side are updated one after the other, while freezing the remaining part. In other words: for the momenta, we solve

$$\dot{q} = 0, \quad \dot{p} = -\nabla_q U(q),$$

and for the coordinates

$$\dot{q} = \nabla_p V(p), \quad \dot{p} = 0.$$

In general, this approach yields schemes of order one. If the splitting is symmetric, one gets methods of at least order two. An important class of splitting schemes is given by Omelyan et al. [13] and force-gradient schemes [14]. Omelyan schemes are based on a symmetric five-stage scheme (updating the sequence U, P, U, P and U), introducing a free parameter λ in the step size of the P -updates. Though the scheme is only of second order, the parameter λ can be used to minimize the leading error term. This gives, for example, the optimal five stage method

$$p_{\lambda h} \circ q_{h/2} \circ p_{(1-2\lambda)h} \circ q_{h/2} \circ p_{\lambda h}(q_0, p_0) \quad \text{with} \\ \lambda = \frac{1}{2} - \frac{(2\sqrt{326} + 36)^{1/3}}{12} + \frac{1}{6(2\sqrt{326} + 36)^{1/3}} \quad (2.80)$$

with the p - and q -updates defined above, cf. Eq. (2.74). The idea of force-gradient schemes is to add an additional update of a higher-order term, the so-called force-gradient term, which introduces additional parameters ξ and χ , and to use the freedom in the additional parameters to increase the accuracy. To obtain order four, only five stages are needed, yielding the family of force-gradient schemes

$$\tilde{p}_{\lambda h, \xi h^3} \circ q_{h/2} \circ \tilde{p}_{(1-2\lambda)h, \chi h^3} \circ q_{h/2} \circ \tilde{p}_{\lambda h, \xi h^3}(q_0, p_0) \quad (2.81)$$

with the force gradient updates $\tilde{p}_{\alpha h, \beta h^3}$ being defined by the mapping

$$\begin{pmatrix} q_0 \\ p_0 \end{pmatrix} \rightarrow \begin{pmatrix} q_0 \\ p_0 - \alpha h U_q(q_0) + \beta h^3 \nabla_q |V_q(q_0)|^2 \end{pmatrix} \quad (2.82)$$

One possible choice of parameters to obtain fourth order is $\lambda = 1/6$, $\xi = 0$, $\chi = 1/72$. Both schemes can be linked to the idea of nested integration (or multirate integration in the mathematical literature) described in Sect. 3.4.2.

In Lattice QCD, where the links $U \in \Omega = SU(N)$ and momenta $P \in \hat{\Omega} = \mathfrak{su}(N)$ we have to deal with more structure compared to the Abelian case where both q and $p \in \mathbb{R}^n$. To preserve the non-Abelian structure, the leap-frog scheme for one step with step size h from (U^0, P^0) to (U^1, P^1) , defined by a sequence of P , U and P updates with step sizes $h/2$, h and $h/2$, has to be rewritten as

$$\begin{aligned} P^{1/2} &= P^0 - \frac{h}{2} \partial_{x,\mu} S(U^0), \\ U^1 &= e^{hP^{1/2}} \cdot U^0, \\ P^1 &= P^{1/2} - \frac{h}{2} \partial_{x,\mu} S(U^1). \end{aligned} \quad (2.83)$$

This follows from defining an U -update $U^0 \rightarrow U_1$ with step size h and initial values (U^0, P^0) by $U_h(U^0, P^0) = e^{hP^0} \cdot U^0$ to preserve the multiplicative structure of the Lie group $SU(N)$ according to the Lie-group differential equation (2.52). The P -update $P^0 \rightarrow P_1$ with step size h and initial values (U^0, P^0) can be defined in the usual way as $P_h(U^0, P^0) = P^0 - h \partial_{x,\mu} S(U^0)$ due to the additive structure of the Lie algebra $\mathfrak{su}(N)$. This defines completely the non-Abelian setting, as all schemes can be described as a sequence of U and P updates with different step sizes and coefficients. An alternative approach to preserve the non-Abelian structure of links and momenta based on Runge-Kutta schemes is discussed in [15].

2.5 Summary and Further Reading

In this chapter the conditions for a Markov chain Monte Carlo algorithm are formulated. The focus is on algorithms to simulate the path integral of a pure gauge theory. Heatbath and overrelaxation algorithms for gauge groups $U(1)$, $SU(2)$ and $SU(3)$ are described in detail. An alternative algorithm is the Hybrid Monte Carlo based on Hamilton's equations of motion. The detailed balance condition is proved and two derivations of the equations of motion are presented. These equations are solved by numerical integration schemes. Detailed balance requires that the integration schemes are time-reversible and volume preserving. The construction of such schemes is discussed in detail, first for the Abelian and then for the case of non Abelian Lie groups.

The theory of Markov chains is reviewed by M. Lüscher in Ref. [16]. The formulation of Hamilton's equations of motion on Lie groups is discussed in detail by A. D. Kennedy et al. in Ref. [17]. We mention that the search for other algorithms for gauge theories to improve critical slowing down is an active field, see e.g. [18–20].

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