Chapter 2

Lattice formulation

Quantum Chromodynamics (QCD) is the established theory of the strong interaction. Its high energy regime can be managed through perturbation theory, since the quarks and gluons are asymptotically free. This means that the strong coupling α_s becomes small at high energies. It is known that

$$\alpha_s(q) \propto \frac{1}{\ln\left(\frac{q}{\Lambda_{\mathrm{QCD}}}\right)},$$

where q is the transfer momentum and Λ_{QCD} is the intrinsic energy scale of QCD. This enables one to perform expansions in powers of the coupling constant, when the energy is much larger than Λ_{QCD}. However, the low energy regime of QCD cannot be treated by perturbation theory, because the coupling becomes large. A non-perturbative approach to investigate this regime are lattice simulations. The main idea of this method is based on discretizing the space-time, on a four dimensional lattice. By means of the path integral and Monte Carlo simulations it is possible to generate field configurations that allow us to calculate relevant physical quantities. The first step to implement this procedure is a transition to *Euclidean time*, which is a rotation of the time coordinate to the imaginary axis. Some important properties of the Euclidean formulation will be discussed in the next section.

2.1 Path integral and Euclidean space-time

Let us begin by discussing the path integral for quantum mechanics in one dimension, the generalization to higher dimensions is straightforward. The starting point is the Green's function or time propagator $\hat{U}(t, t_0)$ of the Schrödinger equation, which must satisfy

$$\left(\hat{H} - i\hbar\frac{\partial}{\partial t}\right)\hat{U}(t, t_0) = -i\hbar\hat{\mathbb{I}}\delta(t - t_0), \tag{2.1}$$

where $\hat{\mathbb{I}}$ is the identity operator and $\hat{H}$ the Hamilton operator. If $\hat{H}$ does not depend explicitly on time, the solution to eq. (2.1) reads

$$\hat{U}(t, t_0) = \theta(t - t_0)e^{-\frac{i}{\hbar}\hat{H}(t - t_0)}, \tag{2.2}$$

where θ is the Heaviside function. We assume $t > t_0$, hence $\theta = 1$. The propagator allows us to find the temporal evolution of a known state at t_0 by using

$$|\psi(t)\rangle = \hat{U}(t, t_0)|\psi(t_0)\rangle. \tag{2.3}$$

The idea now is finding an expression for the propagator. Let us consider a complete orthonormal set of position eigenstates $\{|x\rangle\}$, thus we define

$$U(x, t; x_0, t_0) = \langle x| \hat{U}(t, t_0) |x_0\rangle. \tag{2.4}$$

We will take $N - 1$ different intermediate times

$$t_0 < t_1 < ... < t_{N-1} < t. \tag{2.5}$$

Two consecutive times will be separated by an equidistant length $\epsilon = \frac{t-t_0}{N}$, i.e. $t_{j+1} - t_j = \epsilon$. We can write the propagator in the form

$$\begin{aligned}
U(x, t; x_0, t_0) &= \langle x| e^{-\frac{i}{\hbar}\hat{H}(t-t_0)} |x_0\rangle \\
&= \langle x| e^{-\frac{i}{\hbar}\hat{H}(t-t_{N-1})} e^{-\frac{i}{\hbar}\hat{H}(t_{N-1}-t_{N-2})} \cdots e^{-\frac{i}{\hbar}\hat{H}(t_2-t_1)} e^{-\frac{i}{\hbar}\hat{H}(t_1-t_0)} |x_0\rangle \\
&= \langle x| e^{-\frac{i}{\hbar}\epsilon\hat{H}} \cdots e^{-\frac{i}{\hbar}\epsilon\hat{H}} |x_0\rangle \\
&= \langle x| \left(e^{-\frac{i}{\hbar}\epsilon\hat{H}} \right)^N |x_0\rangle.
\end{aligned} \tag{2.6}$$

Since $\{|x\rangle\}$ is complete, we apply the operator

$$\int dx\, |x\rangle \langle x| = \hat{\mathbb{1}} \tag{2.7}$$

$N - 1$ times, once at each intermediate time $t_1, \ldots, t_{N-1}$,

$$\begin{aligned}
U(x, t; x_0, t_0) &= \int dx_1 \int dx_2 \cdots \int dx_{N-1} \langle x| e^{-\frac{i}{\hbar}\epsilon\hat{H}} |x_{N-1}\rangle \cdots \langle x_2| e^{-\frac{i}{\hbar}\epsilon\hat{H}} |x_1\rangle \\
&\quad \times \langle x_1| e^{-\frac{i}{\hbar}\epsilon\hat{H}} |x_0\rangle \\
&= \int dx_1 \int dx_2 \cdots \int dx_{N-1} \prod_{j=0}^{N-1} \langle x_{j+1}| e^{-\frac{i}{\hbar}\epsilon\hat{H}} |x_j\rangle,
\end{aligned} \tag{2.8}$$

where $x_N \equiv x$. We assume the Hamilton operator to have the standard form

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}, \tag{2.9}$$

where $\hat{p}$ is the momentum operator with a complete orthonormal basis $\{|p\rangle\}$ and $\hat{V}$ is a potential term that only depends on the position operator $\hat{x}$. Now we use Trotter's formula[1], which states that for two bounded or semi-bounded (from below) operators $\hat{A}$ and $\hat{B}$ the following relation is satisfied

$$e^{\hat{A}+\hat{B}} = \lim_{n\to\infty} \left(e^{\hat{A}/n} e^{\hat{B}/n} \right)^n. \tag{2.10}$$

Since this is often the case of $\hat{p}^2$ and $\hat{V}$, we rewrite

$$\left(e^{-\frac{i}{\hbar}\epsilon\hat{H}} \right)^N = \lim_{N\to\infty} \left(e^{-\frac{i\epsilon\hat{p}^2}{2m\hbar}} e^{-\frac{i}{\hbar}\epsilon\hat{V}} \right)^N, \tag{2.11}$$

and conclude

$$U(x, t; x_0, t_0) = \lim_{N\to\infty} \int dx_1 \int dx_2 \cdots \int dx_N \prod_{j=0}^{N-1} \langle x_{j+1}| e^{-\frac{i\epsilon\hat{p}^2}{2m\hbar}} e^{-\frac{i}{\hbar}\epsilon\hat{V}} |x_j\rangle. \tag{2.12}$$

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[1]See section 2.3.1 of ref. [1] for a proof.

In order to simplify this expression we apply

$$\int dp \, |p\rangle \, \langle p| = \hat{\mathbb{1}} \tag{2.13}$$

to the matrix element

$$\langle x_{j+1}| \, e^{-\frac{i\epsilon \hat{p}^2}{2m\hbar}} e^{-\frac{i}{\hbar}\epsilon \hat{V}} \, |x_j\rangle = \int dp \, \langle x_{j+1}| \, e^{-\frac{i\epsilon \hat{p}^2}{2m\hbar}} \, |p\rangle \, \langle p| \, e^{-\frac{i}{\hbar}\epsilon \hat{V}} \, |x_j\rangle . \tag{2.14}$$

Since $\hat{V}$ only depends on $\hat{x}$, we obtain

$$e^{-\frac{i}{\hbar}\epsilon \hat{V}} \, |x_j\rangle = e^{-\frac{i}{\hbar}\epsilon V(x_j)} \, |x_j\rangle . \tag{2.15}$$

From

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} = \langle x|p\rangle^* \tag{2.16}$$

we have

$$
\begin{aligned}
\langle x_{j+1}| \, e^{-\frac{i\epsilon \hat{p}^2}{2m\hbar}} e^{-\frac{i}{\hbar}\epsilon \hat{V}} \, |x_j\rangle &= \int dp \, e^{-\frac{i\epsilon p^2}{2m\hbar}} e^{-\frac{i}{\hbar}\epsilon V(x_j)} \, \langle x_{j+1}|p\rangle \, \langle p|x_j\rangle \\
&= \frac{1}{2\pi\hbar} \int dp \, e^{-\frac{i\epsilon p^2}{2m\hbar}} e^{-\frac{i}{\hbar}\epsilon V(x_j)} e^{\frac{i}{\hbar}p(x_{j+1}-x_j)} .
\end{aligned} \tag{2.17}
$$

This is a Gaussian integral of the form

$$\int dx \, e^{-ax^2+bx} = \sqrt{\frac{\pi}{a}} e^{b^2/4a}, \quad \mathrm{Re}(a) \geq 0. \tag{2.18}$$

The case $\mathrm{Re}(a) = 0$ is non-trivial, but it can be shown by using Cauchy's integral theorem. Identifying $a = i\epsilon/(2m\hbar)$ and $b = i(x_{j+1} - x_j)/\hbar$, the result for the integral in eq. (2.17) reads

$$e^{-\frac{i}{\hbar}\epsilon V(x_j)} \sqrt{\frac{m}{2\pi i\hbar\epsilon}} e^{im\epsilon(x_{j+1}-x_j)^2/2\epsilon^2\hbar}. \tag{2.19}$$

Substituting this result in eq. (2.12) yields

$$
\begin{aligned}
U(x,t;x_0,t_0) &= \lim_{N\to\infty} \int dx_1 \int dx_2 \cdots \int dx_{N-1} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2} \\
&\quad \times \exp\left(\frac{i\epsilon}{\hbar} \sum_{j=0}^{N-1} \left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\epsilon}\right)^2 - V(x_j)\right]\right) .
\end{aligned} \tag{2.20}
$$

This expression is known as the path integral. It can be interpreted as a sum over all the possible trajectories that a non-relativistic particle can travel when moving from x_0 to x, because there is an integral over all positions at each intermediate time step t_j[2], see figure 2.1. In the continuum limit $N \to \infty \leftrightarrow \epsilon \to 0$, the argument of the exponential is the continuous time action

$$S[x] = \int dt \, \left(\frac{1}{2}m\dot{x}^2 - V\right) = \lim_{\epsilon\to 0} \sum_{j=0}^{N-1} \epsilon \left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\epsilon}\right)^2 - V(x_j)\right] . \tag{2.21}$$

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[2]In field theory this interpretation is not right and one can question whether the name *path integral* is appropriate. For that reason, *functional integral* is used as well. Still, we will refer to it as path integral.
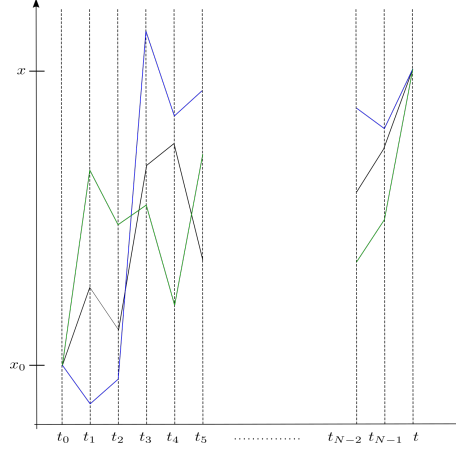
Figure 2.1: The path integral can be interpreted as a coherent sum over all possible paths from x_0 to x.

For this reason, the propagator can also be written as

$$U(x,t;x_0,t_0) = \int \mathcal{D}[x]e^{\frac{i}{\hbar}S[x]}, \quad \mathcal{D}[x] = \lim_{\epsilon \to 0} dx_1 dx_2 \cdots dx_{N-1} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2}. \tag{2.22}$$

Further details about the path integral can be found in refs. [1, 2].

If we consider t as a purely imaginary parameter, we can perform the change of variable $it \to \tau$, where τ is known as *Euclidean time*. It follows that $d\tau^2 = (idt)^2 = -dt^2$. Thus, under this transformation all the terms of the interval ds^2 have the same sign, in contrast with Minkowski space-time. This change of coordinate transforms $\dot{x}(t) = ix'(\tau)$ and $dt = -id\tau$. As a result the action turns into

$$S[x] = \int dt \left(\frac{1}{2}m\dot{x}^2 - V\right) = i\int d\tau \left(\frac{1}{2}mx'^2 + V\right) = iS_E[x], \tag{2.23}$$

where we define the *Euclidean action* as

$$\begin{aligned} S_E[x] &= \int d\tau \left(\frac{1}{2}mx'^2 + V\right) \\ &= \lim_{a \to 0} \sum_{j=1}^{N-1} a \left[\frac{m}{2}\left(\frac{x_{j+1} - x_j}{a}\right)^2 + V(x_j)\right], \end{aligned} \tag{2.24}$$

where $a = i\epsilon$. By taking periodic boundary conditions $x_0 = x_N = x$, fixing $t_0 = 0$ (for convenience) and assuming that the system evolves during a Euclidean time $\tau_{\max} = Na$, we define the *Euclidean path integral* as

$$Z = \int dx \langle x|\hat{U}(\tau_{\max}, 0)|x\rangle = \int \mathcal{D}[x]e^{-S_E[x]/\hbar}, \quad \mathcal{D}[x] = \lim_{a \to 0} dx_1 dx_2 \cdots dx_N \left(\frac{m}{2\pi\hbar a}\right)^{N/2}$$

$$\hat{U}(\tau_{\max}, 0) = e^{-\tau_{\max}\hat{H}/\hbar}. \tag{2.25}$$

Note that there is an extra dx_N in $\mathcal{D}[x]$ that involves one more integration. This gives a link with statistical mechanics, where the partition function is given by

$$Z = \text{tr}\left[e^{-\beta\hat{H}}\right], \quad \beta = \frac{1}{k_B T}, \tag{2.26}$$

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where T denotes temperature. In the case of the path integral, the factor β is

$$\beta = \frac{1}{\hbar}\tau_{\max}, \tag{2.27}$$

Thus, we see that the Euclidean path integral is mathematically equivalent to the partition function in statistical mechanics. This equivalence enables us to interpret

$$p[x] = \frac{1}{Z}e^{-S_E[x]/\hbar} \tag{2.28}$$

as the probability of the path $[x]$. A first calculation with this interpretation can be done if we consider the eigenstates $|n\rangle$ of $\hat{H}$

$$
\begin{aligned}
\int dx \, \langle x| \hat{U}(\tau_{\max}, 0) |x\rangle &= \mathrm{tr}\left[e^{-\beta\hat{H}}\right] \\
&= \mathrm{tr}\left[e^{-\frac{\tau_{\max}}{\hbar}\hat{H}}\right] \\
&= \sum_n \langle n| e^{-\frac{\tau_{\max}}{\hbar}\hat{H}} |n\rangle \\
&= \sum_n e^{-\frac{\tau_{\max}}{\hbar}E_n}.
\end{aligned}
\tag{2.29}
$$

As $\tau_{\max}$ grows, only the exponential with the ground state energy E_0 (which we suppose non-degenerate) in its argument persists

$$\int dx \, \langle x| \hat{U}(\tau_{\max}, 0) |x\rangle \rightarrow e^{-\tau_{\max}E_0/\hbar}, \quad \text{for large } \tau_{\max}. \tag{2.30}$$

Therefore, it is possible to calculate the ground state energy through the decay of Z at large Euclidean time. Another consequence of the interpretation of the Euclidean path integral as a partition function is that one can calculate *thermal expectation values* using $\exp(-S_E[x]/\hbar)$ as a weight factor. For example, let us suppose an operator $\hat{A}$ that depends on the position operator $\hat{x}$, then its expectation value is

$$\langle \hat{A}(\hat{x}(\tau))\rangle = \frac{1}{Z}\mathrm{tr}\left[\hat{A}(\hat{x}(\tau))e^{-\beta\hat{H}}\right] = \frac{1}{Z}\int \mathcal{D}[x]A(x(\tau))e^{-S_E[x]/\hbar}, \tag{2.31}$$

where Z is given by eq. (2.25). We obtain the correlation of two operators $\hat{A}(\hat{x})$ and $\hat{B}(\hat{x})$ as well

$$
\begin{aligned}
\langle \hat{A}(\hat{x}(\tau))\hat{B}(\hat{x}(0))\rangle &= \frac{1}{Z}\int \mathcal{D}[x]A(x(\tau))B(x(0))e^{-S_E[x]/\hbar} \\
&= \frac{1}{Z}\mathrm{tr}\left[\hat{A}(\hat{x}(\tau))\hat{B}(\hat{x}(0))e^{-\beta\hat{H}}\right] \\
&= \frac{1}{Z}\mathrm{tr}\left[e^{\tau\hat{H}/\hbar}\hat{A}(\hat{x}(0))e^{-\tau\hat{H}/\hbar}\hat{B}(\hat{x}(0))e^{-\beta\hat{H}}\right] \\
&= \frac{1}{Z}\sum_n \langle n| e^{\tau\hat{H}/\hbar}\hat{A}(\hat{x}(0))e^{-\tau\hat{H}/\hbar}\hat{B}(\hat{x}(0))e^{-\beta\hat{H}} |n\rangle \\
&= \frac{1}{Z}\sum_{n,m} \langle n| e^{\tau\hat{H}/\hbar}\hat{A}(\hat{x}(0))e^{-\tau\hat{H}/\hbar} |m\rangle \langle m| \hat{B}(\hat{x}(0))e^{-\beta\hat{H}} |n\rangle \\
&= \frac{1}{Z}\sum_{n,m} \langle n| \hat{A}(\hat{x}(0)) |m\rangle \, e^{\tau(E_n-E_m)/\hbar} \langle m| \hat{B}(\hat{x}(0)) |n\rangle \, e^{-\beta E_n} \\
&= \frac{1}{Z}\sum_{n,m} \langle n| \hat{A}(\hat{x}(0)) |m\rangle \langle m| \hat{B}(\hat{x}(0)) |n\rangle \, e^{-\tau E_m/\hbar}e^{-(\tau_{\max}-\tau)E_n/\hbar}. \tag{2.32}
\end{aligned}
$$

From the second to the third line we made use of the fact that a time dependent operator can be written in Euclidean time according to the Heisenberg picture

$$\hat{O}(\tau) = e^{\tau \hat{H}/\hbar} \hat{O}(0) e^{-\tau \hat{H}/\hbar}. \tag{2.33}$$

In the other lines we have made use of the following properties

$$\sum_m |m\rangle \langle m| = \hat{\mathbb{1}}, \quad e^{\alpha \hat{H}} |m\rangle = e^{\alpha E_m} |m\rangle, \quad \langle m| e^{\alpha \hat{H}} = e^{\alpha E_m} \langle m|, \tag{2.34}$$

where α is a constant. In addition, we assume the eigenenergies to be non-degenerate. If we use eq. (2.29) for Z we can rewrite eq. (2.32) as

$$\langle \hat{A}(\hat{x}(\tau)) \hat{B}(\hat{x}(0)) \rangle = e^{\tau_{\max} E_0/\hbar} \frac{\sum_{n,m} \langle n| \hat{A}(\hat{x}(0)) |m\rangle \langle m| \hat{B}(\hat{x}(0)) |n\rangle e^{-\tau E_m/\hbar} e^{-(\tau_{\max}-\tau)E_n/\hbar}}{1 + e^{-\tau_{\max}(E_1-E_0)/\hbar} + e^{-\tau_{\max}(E_2-E_1)/\hbar} + \cdots}. \tag{2.35}$$

We have factorized $e^{-\tau_{\max} E_0/\hbar}$ from the partition function. Then

$$\langle \hat{A}(\hat{x}(\tau)) \hat{B}(\hat{x}(0)) \rangle = \frac{\sum_{n,m} \langle n| \hat{A}(\hat{x}(0)) |m\rangle \langle m| \hat{B}(\hat{x}(0)) |n\rangle e^{-\tau(E_m-E_0)/\hbar} e^{-(\tau_{\max}-\tau)(E_n-E_0)/\hbar}}{1 + e^{-\tau_{\max}(E_1-E_0)/\hbar} + e^{-\tau_{\max}(E_2-E_1)/\hbar} + \cdots}. \tag{2.36}$$

From this expression we see that if $\tau_{\max} \to \infty$ only those terms where $E_n = E_0$ will persist, giving as a result

$$\lim_{\tau_{\max} \to \infty} \langle \hat{A}(\hat{x}(\tau)) \hat{B}(\hat{x}(0)) \rangle = \sum_m \langle 0| \hat{A}(\hat{x}(0)) |m\rangle \langle m| \hat{B}(\hat{x}(0)) |0\rangle e^{-\tau(E_m-E_0)/\hbar}. \tag{2.37}$$

If now we take $\hat{A} = \hat{B}$ the correlator is

$$\begin{aligned} \lim_{\tau_{\max} \to \infty} \langle \hat{A}(\hat{x}(\tau)) \hat{A}(\hat{x}(0)) \rangle &= |\langle 0| \hat{A} |0\rangle|^2 + |\langle 1| \hat{A} |0\rangle|^2 e^{-\tau(E_1-E_0)/\hbar} \\ &+ \sum_{m=2} |\langle m| \hat{A}(\hat{x}(0)) |0\rangle|^2 e^{-\tau(E_m-E_0)/\hbar}. \end{aligned} \tag{2.38}$$

As τ becomes large, only the first two terms contribute, therefore

$$\lim_{\tau_{\max} \to \infty} \langle \hat{A}(\hat{x}(\tau)) \hat{A}(\hat{x}(0)) \rangle - |\langle 0| \hat{A} |0\rangle|^2 = |\langle 1| \hat{A} |0\rangle|^2 e^{-\tau(E_1-E_0)/\hbar}, \quad \tau \text{ large.} \tag{2.39}$$

We see that this quantity decays exponentially in the Euclidean time. This decay depends directly on the energy gap $E_1 - E_0$, in that manner, this gap can be obtained by calculating the correlation $\langle \hat{A}(\hat{x}(\tau)) \hat{A}(\hat{x}(0)) \rangle$. This is relevant because $E_1 - E_0$ is related to the mass of a particle in field theory.

All these concepts can be described in bosonic fields by promoting the paths to field configurations

$$\begin{aligned} x_i &\leftrightarrow \Phi(\vec{x}, t), \\ \prod_i dx_i &\leftrightarrow \prod_x d\Phi_x = \mathcal{D}[\Phi], \\ S_E[x] &\leftrightarrow S_E[\Phi(x)], \end{aligned} \tag{2.40}$$

where $S_E[\Phi(x)] = \int d^4x \left[\frac{1}{2}\partial_\mu \Phi(x) \partial_\mu \Phi(x) + \frac{m^2}{2}\Phi(x)^2\right]$. From now on let us set $\hbar = 1$. In this case, the partition function and the probability of a configuration $[\Phi]$ are

$$Z = \int \mathcal{D}[\Phi] e^{-S_E[\Phi]}, \quad p[\Phi] = \frac{1}{Z} e^{-S_E[\Phi]}. \tag{2.41}$$

The expectation values are calculated through

$$\langle \hat{A}(\tau) \rangle = \frac{1}{Z} \int \mathcal{D}[\Phi] e^{-S_E[\Phi]} \hat{A}[\Phi], \tag{2.42}$$

and the exponential decay of eq. (2.39) now occurs between the sites of the field configuration

$$\langle \Phi_x \Phi_y \rangle - \langle \Phi_x \rangle \langle \Phi_y \rangle \propto \exp\left(-\frac{|x-y|}{\xi} \right), \quad \text{for infinite volume.} \tag{2.43}$$

ξ is known as the *correlation length*, it is the inverse of the energy gap $E_1 - E_0$ and it sets the scale of the system. In actual simulations an infinite volume is impossible, so instead one fixes a volume $(aL)^d$ with d the dimension of the system. By imposing periodic boundary conditions, the relation in eq. (2.43) is modified to

$$\langle \Phi_x \Phi_y \rangle - \langle \Phi_x \rangle \langle \Phi_y \rangle \propto \cosh\left(\frac{|x-y| - La/2}{\xi} \right). \tag{2.44}$$

In general, one can compute *n-point functions*

$$\langle \hat{\Phi}(x_1) \cdots \hat{\Phi}(x_n) \rangle = \frac{1}{Z} \int \mathcal{D}[\Phi] \Phi(x_1) \cdots \Phi(x_n) e^{-S_E[\Phi]}. \tag{2.45}$$

When one deals with fermion fields the path integral formulation is different, since they obey anticommutation rules. In order to define the path integral for fermions one has to treat the components of the spinor fields as *Grassmann numbers*, which are anticonmmuting variables. We will give a brief summary of the most important formulas to handle this numbers.

Let us define the Grassmann numbers η_i, $i = 1, 2, \ldots, N$ as a set of variables that satisfy the relation

$$\{\eta_i, \eta_j\} = 0. \tag{2.46}$$

This implies that $\eta_i^2 = 0$ and therefore any function that depends on these numbers can be written as

$$f(\eta) = f + \sum_i f_i \eta_i + \sum_{i,j} f_{ij} \eta_i \eta_j + \sum_{i,j,k} f_{ijk} \eta_i \eta_j \eta_k, \tag{2.47}$$

where f, f_i, f_{ij} and f_{ijk} are complex numbers in general. The differentiation rules are

$$\frac{\partial \eta_i}{\partial \eta_j} = \delta_{ij}, \quad \frac{\partial(\eta_i \eta_j)}{\partial \eta_i} = \eta_j, \quad \frac{\partial(\eta_j \eta_i)}{\partial \eta_i} = -\eta_j, \quad i \neq j, \tag{2.48}$$

while the integration rules are

$$\int d\eta_i \, \eta_j = \delta_{ij}, \quad \int d\eta_i d\eta_j \, \eta_i \eta_j = -1, \quad i \neq j. \tag{2.49}$$

In this formalism, the spinor fields $\overline{\psi}$ and ψ are independent fields of N Grassmann components. The following relation can be proved for any arbitrary matrix M of dimension $N \times N$

$$\int \mathcal{D}[\overline{\psi}, \psi] \exp(-\overline{\psi} M \psi) = \det M,$$

$$\mathcal{D}[\overline{\psi}, \psi] = \prod_i d\overline{\psi}_i \, d\psi_i. \tag{2.50}$$

If M is also invertible, then

$$\int \mathcal{D}[\overline{\psi}, \psi] \, \psi_x \overline{\psi}_y \exp(-\overline{\psi} M \psi) = (M)^{-1}_{xy} \det M. \tag{2.51}$$

The partition function is defined as the integral in eq. (2.50), but regarding M as a discretization of the Dirac operator. Further details about the Euclidan path integral and the Grassmann numbers can be found in refs. [3–5].

2.2 Concept of a lattice simulation

The idea of a lattice simulation is to generate field configurations $[\Phi]$, distributed according to the probability distribution in eq. (2.41). One can numerically compute n-point functions of the field configurations and obtain various observables, given by exponential decays, using expressions like eq. (2.44).

In order to obtain configurations with the desired probability distribution, one must rely on Monte Carlo algorithms. These algorithms create *Markov chains*, which are sequences of configurations where each new configuration is generated by considering only the previous one

$$[\Phi_1] \to [\Phi_2] \to [\Phi_3] \to \cdots \tag{2.52}$$

The Markov chains have to be *ergodic*, that is, if one has two arbitrary configurations $[\Phi]$ and $[\Phi']$, then the algorithm has to be able to move from $[\Phi]$ to $[\Phi']$ in a finite number of updates. They also have to satisfy the *detailed balance* condition, which will be explained below.

There are several algorithms to perform the configuration updates. Perhaps the simplest one to explain is the *Metropolis algorithm*, which we describe as a recipe for a scalar field.

1. First of all, one has to create an initial $[\Phi]$. This can be done, for instance, by assigning the same value to all the elements $\Phi_x \in [\Phi]$ (*cold start*) or by the assignation of random values to each site (*hot start*).

2. Then one has to update the configuration. To do so one chooses a site x with the corresponding value Φ_x and calculates $\Phi_x + \epsilon$, with ϵ randomly selected in the interval $(-\epsilon_0, \epsilon_0)$, $\epsilon_0 > 0$. One has the freedom to set ϵ_0, normally it is the same for all the sites x.

3. Now, one considers the transition probability

   $$\frac{W([\Phi] \to [\Phi'])}{W([\Phi'] \to [\Phi])} = \frac{p[\Phi']}{p[\Phi]} = e^{-\Delta S_E[\Phi, \Phi']}, \ \ \Delta S_E[\Phi, \Phi'] = S_E[\Phi'] - S_E[\Phi], \tag{2.53}$$

   where $W([A] \to [B])$ is the probability of moving from $[A]$ to $[B]$. The configurations $[\Phi]$ and $[\Phi']$ only differ at the site x, where $\Phi'_x = \Phi_x + \epsilon$. Based on eq. (2.53), the Metropolis algorithm implements detailed balance as follows: if $\Delta S_E[\Phi, \Phi'] \leq 0$, the new configuration is $[\Phi']$, otherwise, the algorithm accepts the update $[\Phi] \to [\Phi']$ with a probability $\exp(-\Delta S_E[\Phi, \Phi'])$.

4. The first three steps are repeated for all x on the lattice. When the whole configuration has been updated we say that a *sweep* was performed. It can be proved (see e.g. ref. [6]) that this algorithm generates configurations with the required probability.

Before measuring any type of quantity with the configurations generated through Monte Carlo algorithms, one has to perform a large number of sweeps until they have the correct

distribution; this process is called *thermalization*. When the thermalization has been achieved, one can start to measure different observables numerically. For example, let us suppose that one wants to know the value of the field Φ at the site x of the lattice. The first step to do is thermalization, after that one can use "well-behaved"[3] configurations to measure $\langle \Phi_x \rangle$. Between each configuration that is used for measurements, one has to apply several sweeps, because each measurement has to be decorrelated (statistically independent) from the others.

2.3   QED in the continuum and on the lattice

In this section we review relevant features of the discretization of the action in Quantum Electrodynamics S_{QED}. First, let us discuss some properties of its continuum action.

The first step to build S_{QED} refers to the action of the one flavor free fermion field

$$S_F[\psi, \overline{\psi}] = \int d^4x \, \overline{\psi}(x) \left(i\gamma^\mu \partial_\mu - m \right) \psi(x). \tag{2.54}$$

This equation is written in Minkowski space-time and in units of $\hbar = c = 1$, later we will rewrite everything in Euclidean space. This action is invariant under global unitary transformations

$$\psi(x) \rightarrow \psi'(x) = \Omega \psi(x), \quad \overline{\psi}(x) \rightarrow \overline{\psi}'(x) = \overline{\psi}(x)\Omega^{-1}, \tag{2.55}$$

because the derivative does not act in Ω. However, if one promotes the global transformation to a local one, *i.e.* $\Omega \rightarrow \Omega(x)$, then S_F is not invariant anymore. In order to preserve the invariance one promotes the derivative ∂_μ to a covariant derivative D_μ that obeys

$$D'_\mu \psi'(x) = \Omega(x) D_\mu \psi(x), \tag{2.56}$$

where $\Omega(x) = e^{i\alpha(x)} \in \text{U}(1)$. This is satisfied by

$$D_\mu = \partial_\mu + igA_\mu(x), \tag{2.57}$$

where g is the coupling constant and $A_\mu(x)$ is a four vector potential or *gauge field*, that transforms as

$$A_\mu(x) \rightarrow A'_\mu(x) = A_\mu(x) - \frac{1}{g}\partial_\mu \alpha(x). \tag{2.58}$$

It can be checked that these expressions fulfill eq. (2.56),

$$
\begin{aligned}
D'_\mu \psi' &= \left(\partial_\mu + igA'_\mu \right) \Omega(x)\psi(x) \\
&= i\partial_\mu \alpha \, e^{i\alpha}\psi + e^{i\alpha}\partial_\mu \psi + igA_\mu e^{i\alpha}\psi - i\partial_\mu \alpha \, e^{i\alpha}\psi \\
&= \Omega D_\mu \psi.
\end{aligned}
\tag{2.59}
$$

To finish constructing the QED action, we add the term

$$S_G[A] = -\frac{1}{4} \int d^4x \, F_{\mu\nu} F^{\mu\nu}, \tag{2.60}$$

where $F_{\mu\nu}$ is the field strength tensor given by $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$. This tensor is invariant under the transformation in eq. (2.58). Therefore the complete QED action is

$$S_{\text{QED}}[\psi, \overline{\psi}, A] = -\frac{1}{4} \int d^4x \, F_{\mu\nu} F^{\mu\nu} + \int d^4x \, \overline{\psi}(i\gamma^\mu D_\mu - m)\psi. \tag{2.61}$$

---

[3]By "well-behaved" we mean that the configurations have the proper probability distribution.

To transform the action to Euclidean space we have to replace $x^0 \to -ix_4$, thus the integration measure now is $dx_1 dx_2 dx_3(-idx_4) = -id^4 x$. The index 4 is to mark the difference between Euclidean and real time. As a consequence of this change of coordinate, the time derivative and A^0 transform as well

$$\partial^0 \to i\partial_4, \quad A^0 \to iA_4. \tag{2.62}$$

The change of A^0 is because it has to behave as the derivative, due to eq. (2.58). We also introduce the Euclidean gamma matrices, whose relation with the Minkowski gamma matrices is

$$\gamma_4^E = \gamma^0, \quad \gamma_j^E = -i\gamma^j, \quad \gamma_5^E = \gamma_1^E \gamma_2^E \gamma_3^E \gamma_4^E. \tag{2.63}$$

These matrices satisfy $\{\gamma_\mu^E, \gamma_\nu^E\} = 2\delta_{\mu\nu}\mathbb{I}$, $\mu, \nu = 1, 2, 3, 4$. Then, S_F becomes

$$
\begin{aligned}
S_F[\psi, \overline{\psi}, A] &= -i \int d^4 x \, \overline{\psi} \left(i\gamma^0 D_0 + i\gamma^j D_j - m \right) \psi \\
&= -i \int d^4 x \, \overline{\psi} \left(i\gamma_4^E iD_4 - \gamma_j^E D_j - m \right) \psi \\
&= iS_F^E[\psi, \overline{\psi}, A],
\end{aligned}
\tag{2.64}
$$

where $S_F^E[\psi, \overline{\psi}, A]$ is defined by

$$S_F^E[\psi, \overline{\psi}, A] = \int d^4 x \, \overline{\psi} \left(\gamma_\mu^E D_\mu + m \right) \psi. \tag{2.65}$$

On the other hand, the pure gauge term transforms as

$$S_G[A] = iS_G^E[A], \quad S_G^E[A] = \frac{1}{4} \int d^4 x \, F_{\mu\nu} F_{\mu\nu}. \tag{2.66}$$

Therefore, the action is (see ref. [5] for further details)

$$S_{\text{QED}} = iS_{\text{QED}}^E, \quad S_{\text{QED}}^E = \frac{1}{4} \int d^4 x \, F_{\mu\nu} F_{\mu\nu} + \int d^4 x \, \overline{\psi} \left(\gamma_\mu^E D_\mu + m \right) \psi. \tag{2.67}$$

We proceed to discretize S_{QED}^E by taking into account two important properties:

1. In the continuum limit, the discretization has to yield eq. (2.67).

2. The discretization of the fields has to preserve the gauge invariance, in analogy to the continuum.

Let us consider a four dimensional hypercubic lattice

$$L = \{\vec{n} = (n_1, n_2, n_3, n_4)| \, n_\mu = 0, 1, \ldots, N_\mu - 1; \mu = 1, 2, 3, 4\}, \tag{2.68}$$

where $\vec{n}$ labels a point in the Euclidean space. We will assume that the points are separated by a distance a, named lattice constant. The fermion fields are only defined at the sites labeled by $\vec{n}$: $\overline{\psi}(\vec{n})$, $\psi(\vec{n})$. Now, we begin in the same way as in the continuum, that is, by considering the Euclidean action of a free fermion field, eq. (2.65). A first discretization can be obtained by replacing the continuum derivative by a discrete one,

$$\partial_\mu \psi(x) \to \frac{\psi(\vec{n} + \hat{\mu}) - \psi(\vec{n} - \hat{\mu})}{2a}, \quad \text{(central finite differences)}, \tag{2.69}$$

where $\vec{n} \pm \hat{\mu}$ are the nearest neighbors of the site $\vec{n}$ in the μ-direction. This leads to the following discrete version of S_F^E

$$S_F^E[\overline{\psi}, \psi] = a^4 \sum_{\vec{n} \in L} \overline{\psi}(\vec{n}) \left(\sum_{\mu=1}^{4} \gamma_\mu^E \frac{\psi(\vec{n} + \hat{\mu}) - \psi(\vec{n} - \hat{\mu})}{2a} + m\psi(\vec{n}) \right). \tag{2.70}$$
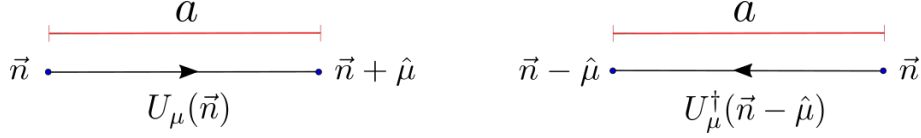
Figure 2.2: The link variables connect nearest neighbors lattice sites: $U_\mu(\vec{n})$ connects $\vec{n}$ with $\vec{n} + \hat{\mu}$, while $U_\mu^\dagger(\vec{n} - \hat{\mu})$ connects $\vec{n}$ with $\vec{n} - \hat{\mu}$.

We would like this action to remain invariant under local transformations $\Omega(\vec{n}) \in \mathrm{U}(1)$,

$$\psi'(\vec{n}) = \Omega(\vec{n})\psi(\vec{n}), \;\; \overline{\psi}(\vec{n}) = \overline{\psi}'(\vec{n})\Omega^{-1}(\vec{n}). \tag{2.71}$$

The mass term in eq. (2.70) does indeed remain invariant, since the transformations $\Omega(\vec{n})$ and $\Omega^{-1}(\vec{n})$ cancel. The discretized derivative, however, does not remain invariant

$$\overline{\psi}'(\vec{n})\psi'(\vec{n} + \hat{\mu}) = \overline{\psi}(\vec{n})\Omega^{-1}(\vec{n})\Omega(\vec{n} + \hat{\mu})\psi(\vec{n} + \hat{\mu}) \neq \overline{\psi}(\vec{n})\psi(\vec{n} + \hat{\mu}). \tag{2.72}$$

The last expression shows that eq. (2.70) is not a proper discretization if we want to preserve local invariance. This forces us to introduce a gauge field in order to preserve the local symmetry, as in the continuum. We introduce a field $U_\mu(\vec{n})$ that transforms as

$$U_\mu \to U_\mu'(\vec{n}) = \Omega(\vec{n})U_\mu(\vec{n})\Omega^{-1}(\vec{n} + \hat{\mu}). \tag{2.73}$$

That way, the product $\psi(\vec{n})U_\mu(\vec{n})\psi(\vec{n} + \hat{\mu})$ is locally U(1) invariant

$$\begin{aligned}
\psi'(\vec{n})U_\mu'(\vec{n})\psi'(\vec{n} + \hat{\mu}) &= \overline{\psi}(\vec{n})\Omega^{-1}(\vec{n})\Omega(\vec{n})U_\mu(\vec{n})\Omega^{-1}(\vec{n} + \hat{\mu})\Omega(\vec{n} + \hat{\mu})\psi(\vec{n} + \hat{\mu}) \\
&= \psi(\vec{n})U_\mu(\vec{n})\psi(\vec{n} + \hat{\mu}).
\end{aligned} \tag{2.74}$$

In order to preserve the symmetry of the term $\overline{\psi}(\vec{n})\psi(\vec{n} - \hat{\mu})$, we multiply by $U_\mu^\dagger(\vec{n} - \hat{\mu})$, because its transformation rule is

$$\begin{aligned}
U_\mu^{\dagger\prime}(\vec{n} - \hat{\mu}) &= \left[\Omega(\vec{n} - \hat{\mu})U_\mu(\vec{n} - \hat{\mu})\Omega^{-1}(\vec{n})\right]^\dagger \\
&= \Omega(\vec{n})U_\mu^\dagger(\vec{n} - \hat{\mu})\Omega^{-1}(\vec{n} - \hat{\mu}).
\end{aligned}$$

This implies that

$$\begin{aligned}
\overline{\psi}'(\vec{n})U_\mu^{\dagger\prime}(\vec{n} - \hat{\mu})\psi'(\vec{n} - \hat{\mu}) &= \overline{\psi}(\vec{n})\Omega(\vec{n})^{-1}\Omega(\vec{n})U_\mu^\dagger(\vec{n} - \hat{\mu})\Omega(\vec{n} - \hat{\mu})^{-1}\Omega(\vec{n} - \hat{\mu})\psi(\vec{n} - \hat{\mu}) \\
&= \overline{\psi}(\vec{n})U_\mu^\dagger(\vec{n} - \hat{\mu})\psi(\vec{n} - \hat{\mu}).
\end{aligned} \tag{2.75}$$

The field $U_\mu(\vec{n})$ provides a link between the site $\vec{n}$ and the sites $\vec{n} + \hat{\mu}$, for that reason it is known as *link variable*. A schematic representation of these links is shown in figure 2.2.

With the link variables one can discretize the action S_F^E in a gauge invariant way

$$S_F^E[\overline{\psi}, \psi, U] = a^4 \sum_{\vec{n} \in L} \overline{\psi}(\vec{n}) \left(\sum_{\mu=1}^4 \gamma_\mu^E \frac{U_\mu(\vec{n})\psi(\vec{n} + \hat{\mu}) - U_\mu^\dagger(\vec{n} - \hat{\mu})\psi(\vec{n} - \hat{\mu})}{2a} + m\psi(\vec{n}) \right). \tag{2.76}$$

Up to this point we have not given an explicit representation for the link variables. In order to do that we are going to revise the analogue of these variables in the continuum. Let us suppose that we want to preserve gauge invariance of the product $\overline{\psi}(x)\psi(y)$, which usually transforms as

$$\overline{\psi}'(x)\psi'(y) = \overline{\psi}(x)\Omega^{-1}(x)\Omega(y)\psi(y) \neq \overline{\psi}(x)\psi(y), \quad \text{for } x \neq y. \tag{2.77}$$

To maintain the symmetry one uses the so-called *paralell transporter* or *Schwinger line integral*

$$U(x, y) = e^{ig \int_{\mathcal{C}} A_\mu dx^\mu}, \tag{2.78}$$

where $A_\mu(x)$ is the gauge field, g the gauge coupling constant and $\mathcal{C}$ is a curve connecting x and y. The important property of this term is that it transforms under U(1) as

$$U(x, y) \to U'(x, y) = \Omega(x)U(x, y)\Omega^{-1}(y), \tag{2.79}$$

then

$$
\begin{aligned}
\overline{\psi}'(x)U'(x, y)\psi'(y) &= \overline{\psi}(x)\Omega^{-1}(x)\Omega(x)U(x, y)\Omega^{-1}(y)\Omega(y)\psi(y) \\
&= \overline{\psi}(x)U(x, y)\psi(y).
\end{aligned}
\tag{2.80}
$$

Let us consider $|\epsilon_\mu| \ll 1$, thus

$$U(x, x + \epsilon_\mu) \approx e^{ig\epsilon_\mu A_\mu(x)}, \tag{2.81}$$

where we have approximated the line integral by the product of $A_\mu(x)$ with $(x + \epsilon_\mu) - x$. This suggests the following expression for the link variables

$$U_\mu(\vec{n}) = e^{igaA_\mu(\vec{n})}. \tag{2.82}$$

In order to verify that this expression is appropriate, we need to check that in the limit $a \to 0$, the continuum action is recovered. As we will see, eq. (2.82) does this right. By expanding the link variables we obtain

$$U_\mu(\vec{n}) = 1 + igaA_\mu(\vec{n}) + \mathcal{O}(a^2),$$
$$U_\mu^\dagger(\vec{n} - \hat{\mu}) = 1 - igaA_\mu(\vec{n} - \hat{\mu}) + \mathcal{O}(a^2). \tag{2.83}$$

Substituting in eq. (2.76) yields

$$
\begin{aligned}
S_F^E &= a^4 \sum_{\vec{n} \in L} \overline{\psi}(\vec{n}) \Bigg(\sum_{\mu=1}^{4} \gamma_\mu^E \frac{(1 + igaA_\mu(\vec{n}))\psi(\vec{n} + \hat{\mu}) - (1 - igaA_\mu(\vec{n} - \hat{\mu}))\psi(\vec{n} - \hat{\mu})}{2a} \\
&\quad + m\psi(\vec{n}) + \mathcal{O}(a) \Bigg) \\
&= a^4 \sum_{\vec{n} \in L} \overline{\psi}(\vec{n}) \Bigg(\sum_{\mu=1}^{4} \gamma_\mu^E \frac{\psi(\vec{n} + \hat{\mu}) - \psi(\vec{n} - \hat{\mu})}{2a} \\
&\quad + \frac{ig}{2}\left(A_\mu(\vec{n})\psi(\vec{n} + \hat{\mu}) + A_\mu(\vec{n} - \hat{\mu})\psi(\vec{n} - \hat{\mu}) \right) + m\psi(\vec{n}) + \mathcal{O}(a) \Bigg).
\end{aligned}
\tag{2.84}
$$

The first term in the parentheses is a discrete version of $\gamma_\mu^E \partial_\mu \psi(x)$, while in the second term we will take $\psi(\vec{n} \pm \hat{\mu})A_\mu(\vec{n} - \hat{\mu}) = \psi(\vec{n})A_\mu(\vec{n}) + \mathcal{O}(a)$ because the sites are separated by a distance a. Then, eq. (2.84) reduces to

$$S_F^E = a^4 \sum_{\vec{n} \in L} \overline{\psi}(\vec{n}) \Bigg(\sum_{\mu=1}^{4} \gamma_\mu^E \frac{\psi(\vec{n} + \hat{\mu}) - \psi(\vec{n} - \hat{\mu})}{2a} + igA_\mu(\vec{n})\psi(\vec{n}) + m\psi(\vec{n}) + \mathcal{O}(a) \Bigg). \tag{2.85}$$

When $a \to 0$ we obtain

$$
\begin{aligned}
S_F^E &= \int d^4x \, \overline{\psi}(x) \left[\gamma_\mu^E (\partial_\mu + igA_\mu(x)) + m \right] \psi(x) \\
&= \int d^4x \, \overline{\psi}(x)(\gamma_\mu^E D_\mu + m)\psi(x).
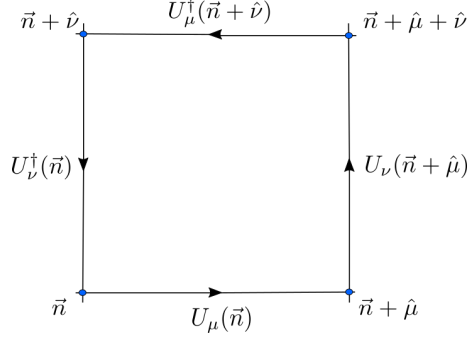\end{aligned}
\tag{2.86}
$$

Figure 2.3: Schematic representation of the plaquette variable $U_{\mu\nu}$. It links the points $\vec{n}$, $\vec{n} + \hat{\mu}$, $\vec{n} + \hat{\mu} + \hat{\nu}$ and $\vec{n} + \hat{\nu}$ on the lattice by using the link variables.

Therefore, the discretization in eq. (2.76) of S_F^E satisfies the two conditions that we mentioned at the beginning. However, this expression is not completely right for a non-trivial reason that we will revise in the next section[4].

For now let us continue with the discretization of the pure gauge term

$$S_G^E = \frac{1}{4} \int d^4x \, F_{\mu\nu} F_{\mu\nu}. \tag{2.87}$$

Again we have to make sure that the expression we use is gauge invariant and that in the limit $a \to 0$ eq. (2.87) is recovered. For this purpose, we define a *plaquette variable*

$$U_{\mu\nu}(\vec{n}) \equiv U_{\mu}(\vec{n}) U_{\nu}(\vec{n} + \hat{\mu}) U_{\mu}^{\dagger}(\vec{n} + \hat{\nu}) U_{\nu}^{\dagger}(\vec{n}), \tag{2.88}$$

where $\hat{\mu}$ and $\hat{\nu}$ denote different directions. From eq. (2.82) we see that the link variables are group elements of U(1) and as a result $U_{\mu\nu} \in$ U(1) as well. Geometrically, the plaquette $U_{\mu\nu}(\vec{n})$ connects the sites $\vec{n}$, $\vec{n} + \hat{\mu}$, $\vec{n} + \hat{\mu} + \hat{\nu}$ and $\vec{n} + \hat{\nu}$ (see figure 2.3). Besides, by using the following transformation rules

$$
\begin{aligned}
U_{\mu}'(\vec{n}) &= \Omega(\vec{n}) U_{\mu}(\vec{n}) \Omega^{-1}(\vec{n} + \hat{\mu}), \\
U_{\nu}'(\vec{n} + \hat{\mu}) &= \Omega(\vec{n} + \hat{\mu}) U_{\nu}(\vec{n} + \hat{\mu}) \Omega^{-1}(\vec{n} + \hat{\mu} + \hat{\nu}), \\
U_{\mu}^{\dagger\prime}(\vec{n} + \hat{\nu}) &= \Omega(\vec{n} + \hat{\mu} + \hat{\nu}) U_{\mu}^{\dagger}(\vec{n} + \hat{\nu}) \Omega^{-1}(\vec{n} + \hat{\nu}) \\
U_{\nu}^{\dagger\prime}(\vec{n}) &= \Omega(\vec{n} + \hat{\nu}) U_{\nu}^{\dagger}(\vec{n}) \Omega^{-1}(\vec{n}),
\end{aligned}
\tag{2.89}
$$

we can see that the plaquette transforms as

$$U_{\mu\nu}'(\vec{n}) = \Omega(\vec{n}) U_{\mu\nu}(\vec{n}) \Omega^{-1}(\vec{n}). \tag{2.90}$$

Since $\Omega(\vec{n})$ and $U_{\mu\nu}(\vec{n})$ belong to U(1), which is an Abelian group (*i.e.* its elements commute), we conclude that

$$U_{\mu\nu}'(\vec{n}) = U_{\mu\nu}(\vec{n}). \tag{2.91}$$

Hence, the plaquettes are gauge invariant when the transformation group is U(1). Having said this, we define the *Wilson gauge action* in U(1) as

$$S_G^E[U] = \frac{1}{g^2} \sum_{\vec{n} \in L} \sum_{\mu < \nu} \left[1 - \frac{1}{2} \left(U_{\mu\nu}(\vec{n}) + U_{\mu\nu}^{\dagger}(\vec{n}) \right) \right]. \tag{2.92}$$

---

[4]Equation (2.76) is known as the *naive fermion action*.

13

Let us revise that this action coincides with eq. (2.87) in the limit $a \to 0$. We can substitute eq. (2.82) in the definition of the plaquette

$$U_{\mu\nu}(\vec{n}) = e^{igaA_\mu(\vec{n})}e^{igaA_\nu(\vec{n}+\hat{\mu})}e^{-igaA_\mu(\vec{n}+\hat{\nu})}e^{-igaA_\nu(\vec{n})}. \tag{2.93}$$

The exponents can be rearranged

$$
\begin{aligned}
U_{\mu\nu}(\vec{n}) &= e^{iga^2\left(\frac{A_\nu(\vec{n}+\hat{\mu})-A_\nu(\vec{n})}{a} - \frac{A_\mu(\vec{n}+\hat{\nu})-A_\mu(\vec{n})}{a}\right)} \\
&= e^{iga^2(\partial_\mu A_\nu(\vec{n})-\partial_\nu A_\mu(\vec{n})+\mathcal{O}(a))} \\
&= e^{iga^2(F_{\mu\nu}(\vec{n})+\mathcal{O}(a))}.
\end{aligned} \tag{2.94}
$$

Then

$$
\begin{aligned}
U_{\mu\nu}(\vec{n}) + U_{\mu\nu}^\dagger(\vec{n}) &= 2 - g^2 a^4 (F_{\mu\nu}(\vec{n}) + \mathcal{O}(a))^2 + g^4 a^8 (F_{\mu\nu} + \mathcal{O}(a))^4 + \cdots \\
&= 2 - g^2 a^4 F_{\mu\nu}(\vec{n})F_{\mu\nu}(\vec{n}) + \mathcal{O}(a^5)
\end{aligned} \tag{2.95}
$$

Substituting in eq. (2.92) yields

$$
\begin{aligned}
S_G^E[U] &= \frac{1}{g^2}\sum_{\vec{n}\in L}\sum_{\mu<\nu}\frac{g^2 a^4}{2}F_{\mu\nu}(\vec{n})F_{\mu\nu}(\vec{n}) + \mathcal{O}(a^5) \\
&= \frac{1}{4}a^4 \sum_{\vec{n}\in L}\sum_{\mu,\nu}F_{\mu\nu}(\vec{n})F_{\mu\nu}(\vec{n}) + \mathcal{O}(a^5).
\end{aligned} \tag{2.96}
$$

The factor of 2 comes from the fact that on the right-hand side $F_{\mu\nu}$ is antisymmetric and that the sum extends over all possible values of μ and ν, not only those where $\mu < \nu$. When $a \to 0$ the Wilson action converges to the continuum action (2.87). Finally, the complete naive discretization of the Euclidean QED action takes the form

$$
\begin{aligned}
S_{\text{QED}}^E[\psi,\overline{\psi},U] &= a^4 \sum_{\vec{n}\in L}\overline{\psi}(\vec{n})\left(\sum_{\mu=1}^{4}\gamma_\mu^E \frac{U_\mu(\vec{n})\psi(\vec{n}+\hat{\mu}) - U_\mu^\dagger(\vec{n}-\hat{\mu})\psi(\vec{n}-\hat{\mu})}{2a} + m\psi(\vec{n})\right) \\
&+ \frac{1}{g^2}\sum_{\vec{n}\in L}\sum_{\mu<\nu}\left[1 - \frac{1}{2}\left(U_{\mu\nu}(\vec{n}) + U_{\mu\nu}^\dagger(\vec{n})\right)\right].
\end{aligned} \tag{2.97}
$$

2.4 Wilson fermions

As we mentioned in the last section, the discretization of the fermion action given in eq. (2.76) is not fully right. To see why, let us rewrite it as follows

$$S_F^E[\psi,\overline{\psi},U] = a^4 \sum_{\vec{n},\vec{m}\in L}\overline{\psi}(\vec{n})D(\vec{n},\vec{m})\psi(\vec{m}),$$

$$D(\vec{n},\vec{m}) = \sum_{\mu=1}^{4}\gamma_\mu^E\frac{U_\mu(\vec{n})\delta_{\vec{n}+\hat{\mu},\vec{m}} - U_\mu^\dagger(\vec{n}-\hat{\mu})\delta_{\vec{n}-\hat{\mu},\vec{m}}}{2a} + m\delta_{\vec{n},\vec{m}}, \tag{2.98}$$

where $D(\vec{n},\vec{m})$ is the Dirac operator. Let us suppose for the moment that we are working in the chiral limit, *i.e.* $m = 0$ and that there are no gauge fields. We will compute the inverse of the Dirac operator $D^{-1}(\vec{n},\vec{m})$. To do so we use the Fourier transform, defined for an arbitrary function $f(\vec{n})$ as

$$\tilde{f}(\vec{p}) = \frac{1}{\sqrt{|L|}}\sum_{\vec{n}\in L}f(\vec{n})e^{-i\vec{p}\cdot\vec{n}a}, \qquad |L| \equiv N_1 N_2 N_3 N_4. \tag{2.99}$$

The inverse transformation is

$$\tilde{f}(\vec{n}) = \frac{1}{\sqrt{|L|}} \sum_{\vec{p} \in \tilde{L}} \tilde{f}(\vec{p}) e^{i\vec{p} \cdot \vec{n} a},$$

$$\tilde{L} = \left\{ \vec{p} = (p_1, p_2, p_3, p_4) | \, p_\mu = \frac{2\pi}{a N_\mu} k_\mu, \; k_\mu = -\frac{N_\mu}{2} + 1, -\frac{N_\mu}{2} + 2, \ldots, \frac{N_\mu}{2} \right\}. \qquad (2.100)$$

Then, if one transforms the fermion fields the Dirac operator takes the form

$$\begin{aligned}
\tilde{D}(\vec{p}, \vec{q}) &= \frac{1}{|L|} \sum_{\vec{n}, \vec{m} \in L} e^{-i\vec{p} \cdot \vec{n} a} D(\vec{n}, \vec{m}) e^{i\vec{q} \cdot \vec{m} a} \\
&= \frac{1}{|L|} \sum_{\vec{n} \in L} e^{-i(\vec{p} - \vec{q}) \cdot \vec{n} a} \sum_{\mu=1}^{4} \gamma_\mu^E \left(\frac{e^{i\vec{q} \cdot \hat{\mu} a} - e^{-i\vec{q} \cdot \hat{\mu} a}}{2a} \right) \\
&= \frac{1}{|L|} \sum_{\vec{n} \in L} e^{i(\vec{p} - \vec{q}) \cdot \vec{n} a} \sum_{\mu=1}^{4} \left(\gamma_\mu^E \frac{i}{a} \sin(q_\mu a) \right).
\end{aligned} \qquad (2.101)$$

The first sum can be expressed as

$$\frac{1}{|L|} \sum_{\vec{n} \in L} e^{i(\vec{p} - \vec{q}) \cdot \vec{n} a} = \prod_{\nu=1}^{4} \frac{1}{N_\nu} \sum_{n_\nu = 0}^{N_\nu - 1} e^{i(p_\nu - q_\nu) n_\nu a}, \qquad (2.102)$$

where $p_\nu = 2\pi k_\nu / (a N_\nu)$ and $q_\nu = 2\pi k_\nu' / (a N_\nu)$. When $k_\nu = k_\nu'$ the product is equal to one. Now let us analyze its value when $k_\nu \neq k_\nu'$,

$$\begin{aligned}
\frac{1}{N_\nu} \sum_{n_\nu = 0}^{N_\nu - 1} e^{i(p_\nu - q_\nu) n_\nu a} &= \frac{1}{N_\nu} \sum_{n_\nu = 0}^{N_\nu - 1} \left(e^{i(p_\nu - q_\nu) a} \right)^{n_\nu} \\
&= \frac{1}{N_\nu} \frac{1 - e^{i(p_\nu - q_\nu) N_\nu a}}{1 - e^{i(p_\nu - q_\mu) a}} \\
&= \frac{1}{N_\nu} \frac{1 - e^{i 2\pi (k_\nu - k_\nu')}}{1 - e^{i 2\pi (k_\nu - k_\nu')/N_\nu}}.
\end{aligned} \qquad (2.103)$$

Since $k_\nu - k_\nu' \in \mathbb{Z}$, the numerator vanishes. Hence

$$\frac{1}{|L|} \sum_{\vec{n} \in L} e^{i(\vec{p} - \vec{q}) \cdot \vec{n} a} = \delta_{p_1, q_1} \delta_{p_2, q_2} \delta_{p_3, q_3} \delta_{p_4, q_4} = \delta_{\vec{p}, \vec{q}}. \qquad (2.104)$$

Substituting in eq. (2.101) yields

$$\tilde{D}(\vec{p}, \vec{q}) = \delta_{\vec{p}, \vec{q}} \tilde{D}(\vec{p}), \quad \tilde{D}(\vec{p}) = \frac{i}{a} \sum_{\mu=1}^{4} \left(\gamma_\mu^E \sin(p_\mu a) \right). \qquad (2.105)$$

In order to calculate $D^{-1}(\vec{n}, \vec{m})$ we use the inverse transformation

$$D^{-1}(\vec{n}, \vec{m}) = \frac{1}{|L|} \sum_{\vec{p} \in \tilde{L}} \tilde{D}^{-1}(\vec{p}) e^{i\vec{p} \cdot (\vec{n} - \vec{m}) a}. \qquad (2.106)$$

To find $\tilde{D}^{-1}(\vec{p})$ we multiply

$$-\tilde{D}(\vec{p}) \tilde{D}(\vec{p}) = \frac{1}{a^2} \left[\sum_{\mu=1}^{4} \left(\gamma_\mu^E \right)^2 \sin^2(p_\mu a) + \sum_{\mu \neq \nu} \gamma_\mu^E \gamma_\nu^E \sin(p_\mu a) \sin(p_\nu a) \right]. \qquad (2.107)$$

Since $\{\gamma_\mu^E, \gamma_\nu^E\} = 2\delta_{\mu\nu}\mathbb{I}$, the product reduces to

$$-\tilde{D}(\vec{p})\tilde{D}(\vec{p}) = \frac{1}{a^2}\sum_{\mu=1}^{4}\sin^2(p_\mu a), \tag{2.108}$$

thus

$$\tilde{D}^{-1}(\vec{p}) = \frac{\frac{-i}{a}\sum_\mu \gamma_\mu^E \sin(p_\mu a)}{\frac{1}{a^2}\sum_\mu \sin^2(p_\mu a)}. \tag{2.109}$$

As a consequence of the Fourier transform, the momentum components are in $(-\pi/a, \pi/a]$ (first Brillouin zone). When $a \to 0$ one obtains the propagator in the continuum

$$\tilde{D}^{-1}(\vec{p}) = \frac{-i\sum_\mu \gamma_\mu^E p_\mu}{p^2}. \tag{2.110}$$

We see that in the continuum there is only one pole at $\vec{p} = (0,0,0,0)$; this is correct since the poles of the propagator represent particles and we are dealing with just one. On the other hand, the discrete version has poles at $\vec{p} = (0,0,0,0)$ and whenever a component of $\vec{p}$ is equal to π/a. Thus the discrete version has 16 poles, with 15 of them being unphysical[5]. This is known as the *fermion doubling* problem and shows that the naive discretization that we gave in the last section is wrong, even though it is gauge invariant and converges to the right expression in the continuum limit. A way of solving this issue was proposed by Kenneth Wilson [7]: the idea is modifying the Dirac operator by adding a term that eliminates the unwanted particles, but that vanishes when $a \to 0$. The term he adds is called the Wilson term and it is a discretization of the Laplace operator multiplied by $-a/2$

$$W = -\frac{a}{2}\sum_{\mu=1}^{4}\frac{\delta_{\vec{n}+\hat{\mu},\vec{m}} - 2\delta_{\vec{n},\vec{m}} + \delta_{\vec{n}-\hat{\mu},\vec{m}}}{a^2}. \tag{2.111}$$

The sum is just a discrete version of $\partial_\mu\partial_\mu$, so the full term convergences to zero when $a \to 0$. In the case with gauge fields, to preserve the gauge invariance we have to insert the link variables

$$W = -\frac{a}{2}\sum_{\mu=1}^{4}\frac{U_\mu(\vec{n})\delta_{\vec{n}+\hat{\mu},\vec{m}} - 2\delta_{\vec{n},\vec{m}} + U_\mu^\dagger(\vec{n}-\hat{\mu})\delta_{\vec{n}-\hat{\mu},\vec{m}}}{a^2}. \tag{2.112}$$

Adding this term to the Dirac operator yields

$$D_{\mathrm{W}} = \left(m - \frac{4}{a}\right)\delta_{\vec{n},\vec{m}} - \frac{1}{2a}\sum_{\mu=1}^{4}\left[(1 - \gamma_\mu^E)U_\mu(\vec{n})\delta_{\vec{n}+\hat{\mu},\vec{m}} + (1 - \gamma_\mu^E)U_\mu^\dagger(\vec{n}-\hat{\mu})\delta_{\vec{n}-\hat{\mu},\vec{m}}\right]. \tag{2.113}$$

This version of the Dirac operator eliminates the fermion doublers. The fermions simulated with this formulation are known as *Wilson fermions* and they were implemented in a Hybrid Monte Carlo (HMC) algorithm to obtain results with the Schwinger model (see Appendix A for a discussion of this algorithm with a scalar field). Unfortunately, there is one problem with this formulation: it breaks chiral symmetry explicitly, even when $m = 0$. This can be seen if one substitutes the chiral transformations

$$\overline{\psi}(\vec{n}) \to \overline{\psi}\,'(\vec{n}) = \overline{\psi}(\vec{n})e^{i\alpha\gamma_5}, \ \ \psi(\vec{n}) \to \psi'(\vec{n}) = e^{i\alpha\gamma_5}\psi(\vec{n}), \ \ \alpha \in \mathbb{R} \tag{2.114}$$

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[5]In d dimensions $2^d - 1$ unwanted fermions appear.

and revises W when multiplied by the fermion fields

$$\overline{\psi}{}'(\vec{n})W\psi'(\vec{m}) = \overline{\psi}(\vec{n})We^{i\alpha\gamma_5^E}e^{i\alpha\gamma_5^E}\psi(\vec{m}) \neq \overline{\psi}(\vec{n})W\psi(\vec{m}). \qquad (2.115)$$

Still, it is feasible to work with Wilson fermions up to an additive renormalization of the fermion mass. The expectation values can be calculated through

$$\langle \hat{A} \rangle = \frac{1}{Z} \int \mathcal{D}[\overline{\psi},\psi]\mathcal{D}[U]e^{-S_{\text{QED}}^E[\psi,\overline{\psi},U]}A[\psi,\overline{\psi},U],$$

$$Z = \int \mathcal{D}[\overline{\psi},\psi]\mathcal{D}[U]e^{-S_{\text{QED}}^E[\psi,\overline{\psi},U]},$$

$$\mathcal{D}[U] = \prod_{\vec{n}\in L}\prod_{\mu=1}^{4} dU_\mu(\vec{n}) \quad \text{(Haar measure)}. \qquad (2.116)$$

There are more ways of discretizing $D(\vec{n},\vec{m})$ that deal with the doubling problem and they introduce other kind of fermions, such as *staggered fermions, Ginsparg-Wilson fermions*, etc. A review of those formulations can be found in refs. [4, 8], however they will not be used in this work.

2.5 QCD on the lattice

To finish this chapter, we make an extension of the ideas of the discretization of the QED action to QCD, which is a non-Abelian gauge theory. We begin by considering the Euclidean action

$$\int d^4x\,\overline{\psi}(\gamma_\mu^E D_\mu + m)\psi + \frac{1}{4}\int d^4x\,\text{tr}\left[G_{\mu\nu}(x)G_{\mu\nu}(x)\right], \qquad (2.117)$$

where $G_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + ig[A_\mu, A_\nu]$ is the gluon field strength tensor and $A_\mu(x) \in \text{SU}(3)$. In order to assure invariance under local SU(3) transformations, the covariant derivative must satisfy

$$D_\mu'\psi'(x) = \Omega(x)D_\mu\psi(x), \qquad (2.118)$$

which is accomplished if A_μ transforms as

$$A_\mu(x) \to A_\mu'(x) = \Omega(x)A_\mu(x)\Omega^{-1}(x) - \frac{i}{g}\Omega(x)\partial_\mu\Omega^{-1}(x). \qquad (2.119)$$

We verify this by substitution

$$\begin{aligned}
D_\mu'\psi' &= \left(\partial_\mu + igA_\mu'\right)\Omega(x)\psi(x) \\
&= \partial_\mu\Omega\psi + \Omega\partial_\mu\psi + ig\Omega A_\mu\psi + \Omega\partial_\mu\Omega^{-1}\Omega\psi \\
&= \partial_\mu\Omega\psi + \Omega\partial_\mu\psi + ig\Omega A_\mu\psi + \Omega\partial_\mu(\Omega^{-1}\Omega)\psi - \Omega\Omega^{-1}\partial_\mu\Omega\psi \\
&= \Omega(\partial_\mu\psi + igA_\mu\psi) \\
&= \Omega D_\mu\psi.
\end{aligned} \qquad (2.120)$$

The discretization of the Dirac operator is the same as in QED, *i.e.* the discretization without the fermion doublers corresponds to eq. (2.113). The link variables definition is the same as in eq. (2.82). Also, the plaquette variables are defined as in eq. (2.88), but in this case one has to preserve the order of the operations because the link variables are matrices. Even though these definitions are the same, the construction of the gauge action

is different, since the plaquettes are not gauge invariant due to the non-commutativity of the link variables. Still, we can construct a gauge invariant Wilson action using the trace operator as follows

$$S_G^E[U] = \frac{3}{g^2} \sum_{\vec{n} \in L} \sum_{\mu < \nu} \left(1 - \frac{1}{3} \text{Re tr} \left[U_{\mu\nu}(\vec{n}) \right] \right), \quad U_{\mu\nu} \in \text{SU}(3). \tag{2.121}$$

Let us revise that this action will converge to the correct expression in the continuum. First we simplify the plaquettes expression

$$U_{\mu\nu}(\vec{n}) = e^{igaA_\mu(\vec{n})} e^{igaA_\nu(\vec{n}+\hat{\mu})} e^{-igaA_\mu(\vec{n}+\hat{\nu})} e^{-igaA_\nu(\vec{n})}, \tag{2.122}$$

by using the Baker-Campbell-Hausdorff formula, which states that for two matrices A and B

$$e^{aA} e^{aB} = e^{aA + aB + \frac{a^2}{2}[A,B] + \mathcal{O}(a^3)}. \tag{2.123}$$

If we apply the formula to (2.122) we obtain

$$U_{\mu\nu}(\vec{n}) = \exp\left(iga \left(A_\mu(\vec{n}) + A_\nu(\vec{n}+\hat{\mu}) - A_\mu(\vec{n}+\hat{\nu}) - A_\nu(\vec{n}) \right) - \frac{g^2 a^2}{2} [A_\mu(\vec{n}), A_\nu(\vec{n}+\hat{\mu})] \right.$$

$$+ \frac{g^2 a^2}{2} [A_\mu(\vec{n}), A_\mu(\vec{n}+\hat{\nu})] + \frac{g^2 a^2}{2} [A_\nu(\vec{n}+\hat{\mu}), A_\mu(\vec{n}+\hat{\nu})] + \frac{g^2 a^2}{2} [A_\mu(\vec{n}), A_\nu(\vec{n})]$$

$$\left. + \frac{g^2 a^2}{2} [A_\nu(\vec{n}+\hat{\mu}), A_\nu(\vec{n})] - \frac{g^2 a^2}{2} [A_\mu(\vec{n}+\hat{\nu}), A_\nu(\vec{n})] + \mathcal{O}(a^3) \right). \tag{2.124}$$

Now, if we use a Taylor expansion for the field

$$A_\nu(\vec{n}+\hat{\mu}) = A_\nu(\vec{n}) + a\, \partial_\mu A_\nu(\vec{n}) + \mathcal{O}(a^2), \tag{2.125}$$

we reduce eq. (2.124) to

$$\begin{aligned} U_{\mu\nu}(\vec{n}) &= e^{iga^2(\partial_\mu A_\nu(\vec{n}) - \partial_\nu A_\mu(\vec{n}) + ig[A_\mu(\vec{n}), A_\nu(\vec{n})]) + \mathcal{O}(a^3)} \\ &= e^{iga^2(G_{\mu\nu}(\vec{n}) + \mathcal{O}(a))}. \end{aligned} \tag{2.126}$$

Then

$$\text{Re tr}[U_{\mu\nu}(\vec{n})] = \text{tr} \left[\mathbb{I} - \frac{a^4 g^2}{2} G_{\mu\nu}(\vec{n}) G_{\mu\nu}(\vec{n}) \right] + \mathcal{O}(a^5). \tag{2.127}$$

Substituting in eq. (2.121) yields

$$\begin{aligned} S_G^E[U] &= \frac{3}{g^2} \sum_{\vec{n} \in L} \sum_{\mu < \nu} \left(\frac{a^4 g^2}{6} \text{tr} \left[G_{\mu\nu}(\vec{n}) G_{\mu\nu}(\vec{n}) \right] \right) + \mathcal{O}(a^5) \\ &= \frac{a^4}{4} \sum_{\vec{n} \in L} \sum_{\mu, \nu} \left(\text{tr} \left[G_{\mu\nu}(\vec{n}) G_{\mu\nu}(\vec{n}) \right] \right) + \mathcal{O}(a^5). \end{aligned} \tag{2.128}$$

In the limit $a \to 0$, we obtain the gauge action

$$S_G^E = \frac{1}{4} \int d^4x \, \text{tr} \left[G_{\mu\nu}(x) G_{\mu\nu}(x) \right]. \tag{2.129}$$

A deeper insight of lattice QCD can be revised in refs. [4, 5].

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