

Chapter 2

Lattice formulation

QCD is the theory that studies the strong interaction, its high energy level can be managed through perturbation theory, since it is known that phenomenologically the quarks show asymptotic freedom, that is, the strong coupling α_s becomes smaller at high energies. Using perturbation theory to leading order it is found that

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

where q is the transfer momentum and Λ_{QCD} sets the energy scale of the system. This allows to perform expansions in powers of the coupling constant when the energy is much larger than Λ_{QCD} . However, the low energy level of QCD can not be treated through perturbation theory, because the coupling becomes large [1]. A non perturbative approach to investigate this regime are lattice simulations. The main idea of such tool is based on discretizing the space-time, usually in a fourth dimensional lattice, that way the fields are only defined on each lattice site. By means of the path integral and Monte Carlo simulations it is possible to generate field configurations that allow to calculate relevant physical quantities. The first step to describe this procedure is by analyzing the path integral in *Euclidean time*, which is a rotation of the time coordinate to the imaginary axis. Some important properties under this change of coordinate arise in the interpretation of the path integral and they will be the subject of this chapter's first 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 three dimensions is direct. The starting point is the Green's function or time propagator $\hat{U}(t, t_0)$ of the Schrödinger equation, which must satisfy

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

$\hat{\mathbb{I}}$ is the identity operator and \hat{H} the Hamiltonian of the system. If \hat{H} does not depend explicitly in time, then the solution to (2.1) is

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

where θ is the Heaviside function, we will take $t > t_0$, then $\theta = 1$. The solution can be checked by substitution. The propagator allows to find the temporal evolution of a known

state at t_0 using the following expression:

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

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

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

Now, we will take $N - 1$ different intermediate times such that

$$t_0 < t_1 < \dots < t_{N-1} < t. \quad (2.5)$$

Two consecutive times will be separated by an equidistant length $\epsilon = \frac{t-t_0}{N}$, i.e. $t_{j+1} - t_j = \epsilon$. Due to the fact that \hat{H} commutes with itself, we can write

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

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

$$\int dx |x\rangle \langle x| = \hat{\mathbb{I}} \quad (2.7)$$

$N - 1$ times, one per each intermediate time, giving

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

where $x_N \equiv x$. We suppose that the Hamiltonian has the following expression:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V} \quad (2.9)$$

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} . In virtue of the Trotter's formula¹, which says that for two operators A and B the following is satisfied:

$$e^{A+B} = \lim_{n \rightarrow \infty} \left(e^{A/n} e^{B/n} \right)^n, \quad (2.10)$$

we can rewrite

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

¹See section 2.3.1 of [2] for a proof

Then

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

In order to simplify the expression we apply the projection operator in momentum space

$$\int dp |p\rangle \langle p| = \hat{\mathbb{I}} \quad (2.13)$$

to the integrand:

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

Since \hat{V} only depends on \hat{x} , then

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

Besides

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

It follows that

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

This is a Gaussian integral of the form

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

Identifying $a = i\epsilon/2m\hbar$ and $b = i(x_{j+1} - x_j)/\hbar$ the result for the integral in (2.17) is

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

Substituting this result in (2.12) gives

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

This expression is known as the path integral and it can be interpreted as sum over all the possible trajectories that a particle can travel when going from x_0 to x , because there is an integral over all positions at each intermediate time step t_j (see figure 2.1). Let us note that in the continuum limit $N \rightarrow \infty \leftrightarrow \epsilon \rightarrow 0$, the argument of the exponential is the action of the system

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

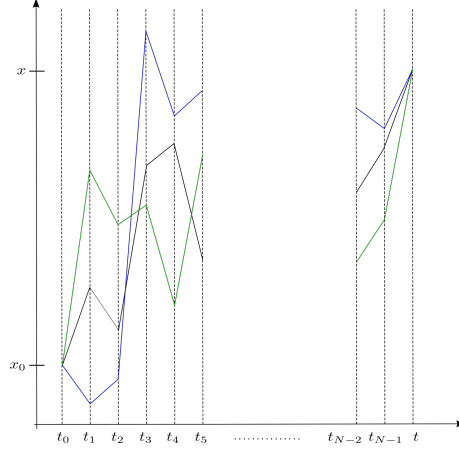


Figure 2.1: The path integral can be interpreted as a sum over all possible paths from x_0 to x .

For this reason, the propagator can also be written as

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

Further details about the path integral can be found in [2] and [3].

Now we will discuss the Euclidean time. Let us suppose that t is a complex parameter, furthermore, let us suppose that it is purely imaginary, that way we can perform the change of variable $it \rightarrow \tau$, where τ is real. Even though we are thinking of t as an imaginary parameter and τ as real one, τ is called imaginary or Euclidean time [4]. From the definition of τ it follows that $d\tau^2 = (idt)^2 = -dt^2$, thus, in Euclidean time 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 $dt = -i d\tau$ and as a result the action is turned into

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

where we define the *Euclidean action* as

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

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

$$\begin{aligned} Z &= \int dx \langle x | \hat{U}(T, 0) | x \rangle = \int \mathcal{D}[x] e^{-S_E[x]/\hbar}, \quad \mathcal{D}[x] = \lim_{a \rightarrow 0} dx_1 dx_2 \cdots dx_N \left(\frac{m}{2\pi \hbar a} \right)^{N/2} \\ \hat{U}(T, 0) &= e^{-T\hat{H}/\hbar}. \end{aligned} \quad (2.25)$$

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

$$Z = \text{tr} \left[e^{-\beta \hat{H}} \right], \quad \beta = \frac{1}{k_B \Theta}, \quad \text{here } \Theta \text{ denotes temperature.} \quad (2.26)$$

In the case of the path integral, the factor β would be

$$\beta = \frac{1}{\hbar} T. \quad (2.27)$$

Thus, we can see that the Euclidean path integral is mathematically equivalent to the partition function from statistical mechanics. This equivalence allows to interpret

$$p[x] = \frac{1}{Z} e^{-S_E[x]} \quad (2.28)$$

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

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

as T grows larger, only the exponential with the ground state (which we suppose non degenerate and which we will denote as E_0) in its argument will survive

$$\int dx \langle x | \hat{U}(T, 0) | x \rangle \rightarrow e^{-TE_0/\hbar}, \text{ for large } T. \quad (2.30)$$

Therefore, it is possible to calculate the ground state through Z . 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

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

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

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

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

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

In the other rows we have made use of the following properties:

$$\sum_m |m\rangle \langle m| = \hat{\mathbb{I}}, \quad e^{\alpha \hat{H}} |m\rangle = e^{\alpha E_m} |m\rangle, \quad \langle m| e^{\alpha \hat{H}} = e^{\alpha E_m} \langle m|, \quad \alpha \text{ a constant.} \quad (2.34)$$

If we use (2.29) for Z we can rewrite (2.32) as

$$\langle \hat{A}(\hat{x}(\tau)) \hat{B}(\hat{x}(0)) \rangle = e^{TE_0/\hbar} \frac{\sum_{n,m} \langle n| \hat{A}(\hat{x}(0)) |m\rangle \langle m| \hat{B}(\hat{x}(0)) |n\rangle e^{-\tau E_m/\hbar} e^{-(T-\tau)E_n/\hbar}}{1 + e^{-T(E_1-E_0)/\hbar} + e^{-T(E_2-E_1)/\hbar}}. \quad (2.35)$$

We have factorized $e^{-TE_0/\hbar}$ from the partition function. Let us note that

$$\begin{aligned} -\tau E_m - TE_n + \tau E_n + TE_0 &= -\tau E_m + \tau E_0 - TE_n + TE_0 + \tau E_n - \tau E_0 \\ &= -\tau(E_m - E_0) - (T - \tau)(E_n - E_0), \end{aligned} \quad (2.36)$$

then

$$\langle \hat{A}(\hat{x}(\tau)) \hat{B}(\hat{x}(0)) \rangle = \frac{\sum_{n,m} \langle n| \hat{A}(\hat{x}(0)) |m\rangle \langle m| \hat{B}(\hat{x}(0)) |n\rangle e^{-\tau(E_m-E_0)/\hbar} e^{-(T-\tau)(E_n-E_0)/\hbar}}{1 + e^{-T(E_1-E_0)/\hbar} + e^{-T(E_2-E_1)/\hbar}}. \quad (2.37)$$

From this expression we can see that if $T \rightarrow \infty$ only those terms where $E_n = E_0$ will survive, giving as a result

$$\lim_{T \rightarrow \infty} \langle \hat{A}(\hat{x}(\tau)) \hat{B}(\hat{x}(0)) \rangle = \sum_m \langle 0| \hat{A}(\hat{x}(0)) |m\rangle \langle m| \hat{B}(\hat{x}(0)) |0\rangle e^{-\tau(E_m-E_0)}. \quad (2.38)$$

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

$$\begin{aligned} \lim_{T \rightarrow \infty} \langle \hat{A}(\hat{x}(\tau)) \hat{A}(\hat{x}(0)) \rangle &= |\langle 0| \hat{A} |0\rangle|^2 + |\langle 1| \hat{A} |0\rangle|^2 e^{-\tau(E_1-E_0)} \\ &+ \sum_{m=2} |\langle m| \hat{A}(\hat{x}(0)) |0\rangle|^2 e^{-\tau(E_m-E_0)}. \end{aligned} \quad (2.39)$$

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

$$\lim_{T \rightarrow \infty} \langle \hat{A}(\hat{x}(\tau)) \hat{A}(\hat{x}(0)) \rangle - |\langle 0| \hat{A} |0\rangle|^2 = |\langle 1| \hat{A} |0\rangle|^2 e^{-\tau(E_1-E_0)}, \quad \tau \rightarrow \infty. \quad (2.40)$$

This equation shows that the left hand side quantity decays exponentially. Such 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 and in lattice simulations it is calculated with eq. (2.40), [5], [6].

All these concepts can be described in bosonic fields by promoting the configuration of positions to a field configuration, that is

$$\begin{aligned} x_i &\leftrightarrow \Phi(\vec{x}, t), \\ \prod_i dx_i &\leftrightarrow \prod_x d\Phi_x = \mathcal{D}[\Phi], \\ S_E[x] &\leftrightarrow S_E[\Phi(x)], \end{aligned} \quad (2.41)$$

where $S_E[\Phi(x)] = \int dx^4 \left[\frac{1}{2} \partial_\mu \Phi(x) \partial_\mu \Phi(x) + \frac{m^2}{2} \Phi(x)^2 \right]$. In such case, the partition function and the probability of a configuration $[\Phi]$ are

$$Z = \int \mathcal{D}[\Phi] e^{-S_E[\Phi]}, \quad p[\Phi] = \frac{1}{Z} e^{-S_E[\Phi]}. \quad (2.42)$$

The expectation values are calculated through

$$\langle \hat{A}(\tau) \rangle = \frac{1}{Z} \int \mathcal{D}[\Phi] e^{-S_E[\Phi]} \hat{A}[\Phi], \quad (2.43)$$

and the exponential decay of eq. (2.40) now occurs between the sites of the field configuration:

$$\langle \Phi_x \Phi_y \rangle - \langle \Phi_x \rangle \langle \Phi_y \rangle \propto \exp\left(-\frac{|x-y|}{\xi}\right), \text{ for infinite volume.} \quad (2.44)$$

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

$$\langle \Phi_x \Phi_y \rangle - \langle \Phi_x \rangle \langle \Phi_y \rangle \propto \cosh\left(\frac{|x-y| - La/2}{\xi}\right). \quad (2.45)$$

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

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

$$\{\eta_i, \eta_j\} = 0. \quad (2.46)$$

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

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

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

$$\frac{\partial \eta_i}{\partial \eta_i} = 1, \quad \frac{\partial(\eta_i \eta_j)}{\partial \eta_i} = \eta_j, \quad \frac{\partial(\eta_j \eta_i)}{\partial \eta_i} = -\eta_j, \quad i \neq j, \quad (2.48)$$

while the integration rules are

$$\int d\eta_j = 0, \quad \int d\eta_i \eta_i = 1, \quad \int d\eta_i d\eta_j \eta_i \eta_j = -1, \quad i \neq j. \quad (2.49)$$

Now, if we consider the spinor fields $\bar{\psi}$ and ψ as independent fields of dimension N and we treat their components as Grassmann numbers, the following relation can be proofed for an arbitrary matrix M of dimension $N \times N$:

$$\begin{aligned} \int \mathcal{D}[\bar{\psi}] \mathcal{D}[\psi] \exp(-\bar{\psi} M \psi) &= \det M, \\ \mathcal{D}[\bar{\psi}] &= \prod_i d\bar{\psi}_i, \quad \mathcal{D}[\psi] = \prod_i d\psi_i \end{aligned} \quad (2.50)$$

If M is also invertible, then

$$\int \mathcal{D}\bar{\psi} \mathcal{D}\psi \psi_x \bar{\psi}_y = (M)_{xy}^{-1} \det M. \quad (2.51)$$

The partition function, and therefore the Euclidean path integral, is defined as the integral in eq. (2.50) but regarding M as a discretization of the Dirac operator. Further details about the Grassmann numbers and derivation of these equations can be found in [5], [6], [7].

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 $p[\Phi]$ given in eq. (2.42), then one can calculate correlation functions of the field configuration and obtain different quantities, like the mass of particles ($m = 1/\xi$) using the expression in eq. (2.45), or the ground state energy.

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

$$[\Phi_1] \rightarrow [\Phi_2] \rightarrow [\Phi_3] \rightarrow \dots \quad (2.52)$$

The Markov chains have to be *ergodic* so they can be useful, that is, if one has two different arbitrary configurations $[\Phi]$ and $[\Phi']$, then one has to be able to go from $[\Phi]$ to $[\Phi']$ in a finite number of updates of the algorithm. There are many algorithms to perform the configuration updates, perhaps the simplest one to explain is the *Metropolis algorithm*. We will do it as a recipe.

1. First of all, one has to give an initial $[\Phi]$, this can be done by assigning the same value to all the elements $\Phi_x \in [\Phi]$ (*cold start*) or by the assignation of random numbers to each site (*hot start*).
2. Then one has to update the configuration, to do that one chooses a site x with the corresponding value Φ_x and calculates $\Phi_x + \epsilon$ (one has the freedom of selecting ϵ , normally it is the same for all the sites x).
3. Based on the transition probability given by the condition of *Detailed balance*:

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

where $[\Phi']$ is the same configuration as $[\Phi]$ but with the change $\Phi_x \rightarrow \Phi_x + \epsilon$, the value of the configuration on the site x is updated to $\Phi_x + \epsilon$. This means the following: if $\Delta S_E[\Phi, \Phi'] < 0$, we update the value Φ_x on x by $\Phi_x + \epsilon$, otherwise, a random number r between 0 and 1 is generated. In such case, Φ_x is substituted by $\Phi_x + \epsilon$ only if $W([\Phi] \rightarrow [\Phi']) > r$

4. Finally, the last three steps have to be repeated for all x on the lattice. When the whole configuration has been updated we say that a *sweep* was performed. It can be proofed (see e.g. [8]) that this algorithm generates configurations with the required probability and that it is ergodic.

Before determining any type of quantity with the configurations generated through Monte Carlo algorithms, one has to perform several sweeps until they have the correct distribution, this process is called *thermalization*. When the thermalization has been

achieved, one can start to *measure* different values numerically. For example, let us suppose that one wants to know the value of the field Φ on the site x of the lattice, the first thing to do is thermalizing the configurations, after that one can use a “well-behaved”² configuration to measure the value of Φ_x ; however, using only one configuration does not provide a reliable result, thus one generates many configurations and averages the value of Φ_x for all the different “well-behaved” $[\Phi]$ that were generated. Between each of the configurations that are being used to measure Φ_x , one has to apply several sweeps, because each measurement has to be decorrelated from the others.

2.3 Lattice formulation of QED

In this section we will give relevant features about the discretization of the action in quantum electrodynamics, but first let us review some properties of this action in the continuum that are important before discretizing it.

The first step to build the QED action is by considering the action of the free fermion field

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

This equation is written in Minkowski space-time and in units of $\hbar = c = 1$, latter we will rewrite everything in Euclidean space-time. Let us note that this action is invariant under global transformations of the U(1) group

$$\begin{aligned} \psi(x) &\rightarrow \psi'(x) = \Omega \psi(x), \quad \bar{\psi}(x) \rightarrow \bar{\psi}'(x) = \bar{\psi}(x) \Omega^{-1} \\ \Omega &= e^{i\alpha}, \quad \alpha \in \mathbb{R}, \end{aligned} \quad (2.55)$$

because the derivative does not act over 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 must change the derivative ∂_μ by a covariant derivative D_μ that obeys

$$D'_\mu \psi'(x) = \Omega(x) D_\mu \psi(x). \quad (2.56)$$

The following expression for D_μ satisfies this

$$D_\mu = \partial_\mu + ig A_\mu(x), \quad (2.57)$$

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

$$A_\mu \rightarrow A'_\mu(x) = \Omega(x) A_\mu(x) \Omega^{-1}(x) - \frac{i}{g} \Omega(x) \partial_\mu \Omega^{-1}(x) \quad (2.58)$$

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

$$\begin{aligned} D'_\mu \psi' &= (\partial_\mu + ig A'_\mu) \Omega(x) \psi(x) \\ &= \partial_\mu \Omega \psi + \Omega \partial_\mu \psi + ig \Omega A_\mu \psi + \Omega \partial_\mu \Omega^{-1} \Omega \psi \\ &= \partial_\mu \Omega \psi + \Omega \partial_\mu \psi + ig \Omega A_\mu \psi + \Omega \partial_\mu (\Omega^{-1} \Omega) \psi - \Omega \Omega^{-1} \partial_\mu \Omega \psi \\ &= \Omega (\partial_\mu \psi + ig A_\mu \psi) \\ &= \Omega D_\mu \psi. \end{aligned} \quad (2.59)$$

²By well-behaved we mean that the configurations have the proper probability distribution.

For the case of QED we know that $\Omega(x) = e^{i\alpha(x)} \in U(1)$, thus the transformation rule for A_μ is

$$A_\mu(x) \rightarrow A'_\mu(x) = A_\mu(x) - \frac{1}{g} \partial_\mu \alpha(x), \quad (2.60)$$

nevertheless, equations (2.57) and (2.58) hold for other transformation groups that satisfy $\Omega^\dagger = \Omega^{-1}$, for example, the SU(3) group which is associated with QCD. To finish constructing the QED action the following term is added:

$$S_G[A] = -\frac{1}{4} \int d^4x F_{\mu\nu} F^{\mu\nu}, \quad (2.61)$$

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 (2.60). Therefore the complete QED action is

$$S_{\text{QED}}[\psi, \bar{\psi}, A] = -\frac{1}{4} \int d^4x F_{\mu\nu} F^{\mu\nu} + \int d^4x \bar{\psi} (i\gamma^\mu D_\mu - m) \psi. \quad (2.62)$$

To transform the action to Euclidean time we have to interchange $x^0 \rightarrow -ix^4$. The index 4 is to remark the difference between Euclidean and normal time. As a consequence of this change of coordinate, the time derivative and A_0 transform as well:

$$\partial_0 \rightarrow i\partial_4, \quad A_0 \rightarrow iA_4. \quad (2.63)$$

The change of A_0 is because we are thinking of A_μ as the derivative of a field $A_\mu = \partial_\mu \gamma(x)$, so it transforms in the same way as ∂_0 . We also introduce the *Euclidean* gamma matrices, whose relation with the Minkowski gamma matrices is

$$\gamma_4^E = \gamma^0, \quad \gamma_j^E = -i\gamma^j, \quad \gamma_5^E = \gamma_1^E \gamma_2^E \gamma_3^E \gamma_4^E. \quad (2.64)$$

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

$$\begin{aligned} S_F[\psi, \bar{\psi}, A] &= -i \int d^4x \bar{\psi} (i\gamma^0 D_0 + i\gamma^j D_j - m) \psi \\ &= -i \int d^4x \bar{\psi} (i\gamma_4^E iD_4 - \gamma_j^E D_j - m) \psi \\ &= iS_F^E, \end{aligned} \quad (2.65)$$

where $S_E^F[\psi, \bar{\psi}, A]$ is defined by

$$S_E^F[\psi, \bar{\psi}, A] = \int d^4x \bar{\psi} (\gamma_\mu^E D_\mu + m) \psi. \quad (2.66)$$

On the other hand, the gauge term transforms as

$$S_G[A] = \frac{i}{4} \int d^4x F_{\mu\nu} F_{\mu\nu}. \quad (2.67)$$

Therefore, the action is [7]

$$S_{\text{QED}} = iS_E, \quad S_E = \frac{1}{4} \int d^4x F_{\mu\nu} F_{\mu\nu} + \int d^4x \bar{\psi} (\gamma_\mu^E D_\mu + m) \psi. \quad (2.68)$$

We proceed to discretize (2.68) by taking into account two important things:

1. In the continuum limit, the discretization has to yield (2.68).
2. The discretization of the fields has to preserve the invariance under $U(1)$ transformations, in the same way the continuum case does.

Having said this, let us consider a four dimensional lattice

$$L = \{\vec{n} = (n_1, n_2, n_3, n_4) | n_1, n_2, n_3 = 0, 1, \dots, N-1; n_4 = 0, 1, \dots, N_T-1\}, \quad (2.69)$$

here \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 on the sites labeled by \vec{n} : $\bar{\psi}(\vec{n})$, $\psi(\vec{n})$. Now, we begin in the same way we did in the continuum case, that is, by regarding the Euclidean action of a free fermion field (eq. (2.66)). A first discretization can be obtained by interchanging the continuum derivative by a discrete one:

$$\partial_\mu \psi(x) \rightarrow \frac{\psi(\vec{n} + \hat{\mu}) - \psi(\vec{n} - \hat{\mu})}{2a}, \quad (\text{central finite differences}), \quad (2.70)$$

where $\hat{\mu}$ denotes a vector of length a in one of the four possible directions. This would lead to the following discrete version of S_F^E

$$S_F^E[\bar{\psi}, \psi] = a^4 \sum_{\vec{n} \in L} \bar{\psi}(\vec{n}) \left(\sum_{\mu=1}^4 \gamma_\mu^E \frac{\psi(\vec{n} + \hat{\mu}) - \psi(\vec{n} - \hat{\mu})}{2a} + m\psi(\vec{n}) \right). \quad (2.71)$$

We would like that this action remained invariant under local gauge transformations $\Omega(\vec{n}) \in U(1)$ that transform the fields as

$$\psi(\vec{n})' = \Omega(\vec{n})\psi(\vec{n}), \quad \bar{\psi}(\vec{n}) = \bar{\psi}'(\vec{n})\Omega^{-1}(\vec{n}). \quad (2.72)$$

The second term in (2.71) does indeed remain invariant, since the transformations $\Omega(\vec{n})$ and $\Omega(\vec{n})^{-1}$ cancel; nevertheless, the discretized derivative does not remain invariant, we can check for example the term $\bar{\psi}(\vec{n})\psi(\vec{n} + \hat{\mu})$

$$\bar{\psi}(\vec{n})'\psi(\vec{n} + \hat{\mu})' = \bar{\psi}(\vec{n})\Omega^{-1}(\vec{n})\Omega(\vec{n} + \hat{\mu})\psi(\vec{n} + \hat{\mu}) \neq \bar{\psi}(\vec{n})\psi(\vec{n} + \hat{\mu}). \quad (2.73)$$

This tells us that equation (2.71) is not a proper discretization if we want to preserve $U(1)$ invariance³. This forces to introduce external fields in order to preserve the local symmetry, as in the continuum situation. We introduce a field $U_\mu(\vec{n})$, where μ denotes one of the four possible directions, that transforms as

$$U_\mu \rightarrow U'_\mu(\vec{n}) = \Omega(\vec{n})U_\mu(\vec{n})\Omega^{-1}(\vec{n} + \hat{\mu}). \quad (2.74)$$

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

$$\begin{aligned} \psi(\vec{n})'U_\mu(\vec{n})'\psi(\vec{n} + \hat{\mu})' &= \bar{\psi}(\vec{n})\Omega^{-1}(\vec{n})\Omega(\vec{n})U_\mu(\vec{n})\Omega^{-1}(\vec{n} + \hat{\mu})\Omega(\vec{n} + \hat{\mu})\psi(\vec{n} + \hat{\mu}) \\ &= \bar{\psi}(\vec{n})U_\mu(\vec{n})\psi(\vec{n} + \hat{\mu}). \end{aligned} \quad (2.75)$$

If one wants to preserve the symmetry with the term $\bar{\psi}(\vec{n})\psi(\vec{n} - \hat{\mu})$, then we multiply by $U_\mu^\dagger(\vec{n} - \hat{\mu})$, because its transformation rule is

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

³There are cases where the discretization of the derivative given in (2.70) works well, for example the scalar field theory, however, that is not the case of the theories that involve gauge transformations.



Figure 2.2: The link variables connect points on the lattice, $U_\mu(\vec{n})$ connects \vec{n} with $\vec{n} + \hat{\mu}$, while $U_\mu^\dagger(\vec{n} - \hat{\mu})$ connects \vec{n} with $\vec{n} - \hat{\mu}$.

This implies that

$$\begin{aligned} \bar{\psi}(\vec{n})' U_\mu^\dagger(\vec{n} - \hat{\mu})' \psi(\vec{n} - \hat{\mu})' &= \bar{\psi}(\vec{n}) \Omega(\vec{n})^{-1} \Omega(\vec{n}) U_\mu^\dagger(\vec{n} - \hat{\mu}) \Omega(\vec{n} - \hat{\mu})^{-1} \Omega(\vec{n} - \hat{\mu}) \psi(\vec{n} - \hat{\mu}) \\ &= \bar{\psi}(\vec{n}) U_\mu^\dagger(\vec{n} - \hat{\mu}) \psi(\vec{n} - \hat{\mu}). \end{aligned} \quad (2.76)$$

Let us note that the fields $U_\mu(\vec{n})$ provide a link between the site \vec{n} and the sites $\vec{n} + \hat{\mu}$, for that reason they are known as *link variables*, 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 the correct way

$$S_F^E[\bar{\psi}, \psi, U] = a^4 \sum_{\vec{n} \in L} \bar{\psi}(\vec{n}) \left(\sum_{\mu=1}^4 \gamma_\mu^E \frac{U_\mu(\vec{n}) \psi(\vec{n} + \hat{\mu}) - U_\mu^\dagger(\vec{n} - \hat{\mu}) \psi(\vec{n} - \hat{\mu})}{2a} + m \psi(\vec{n}) \right), \quad (2.77)$$

this expression is U(1) invariant. Up this point we have not given an explicit representation for the link variables, in order to do that we are going to revise the analogous of this variables in the continuum. Let us suppose that we want to preserve gauge invariance of the product $\bar{\psi}(x)\psi(y)$, which usually transforms as

$$\bar{\psi}'(x)\psi(y) = \bar{\psi}(x)\Omega^{-1}(x)\Omega(y)\psi(y) \neq \bar{\psi}(x)\psi(y). \quad (2.78)$$

However, to maintain the symmetry one uses the so-called *gauge transporter* or *Schwinger line integral*

$$U(x, y) = e^{ig \int_{\mathcal{C}} A_\mu dx^\mu}, \quad (2.79)$$

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 object is that it transforms under U(1) as [6],[7]

$$U(x, y) \rightarrow U'(x, y) = \Omega(x)U(x, y)\Omega^{-1}(y), \quad (2.80)$$

then

$$\begin{aligned} \bar{\psi}'(x)U'(x, y)\psi'(y) &= \bar{\psi}(x)\Omega^{-1}(x)\Omega(x)U(x, y)\Omega^{-1}(y)\Omega(y)\psi(y) \\ &= \bar{\psi}(x)U(x, y)\psi(y). \end{aligned} \quad (2.81)$$

Let us consider $\epsilon_\mu \ll 1$, allowing us to write

$$U(x, x + \epsilon_\mu) \approx e^{ig\epsilon_\mu A_\mu}, \quad (2.82)$$

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

$$U_\mu(\vec{n}) = e^{igaA_\mu(\vec{n})}. \quad (2.83)$$

How do we know that this proposal is right? Until now we have checked that the discrete action is invariant under U(1) transformations, but we need to verify that in the limit

$a \rightarrow 0$, the continuum action is recovered. As we will see now, eq. (2.83) does this right. In the limit $a \rightarrow 0$ we can approximate

$$\begin{aligned} U_\mu(\vec{n}) &\approx 1 + ig a A_\mu(\vec{n}), \\ U_\mu^\dagger(\vec{n} - \hat{\mu}) &\approx 1 - ig a A_\mu(\vec{n} - \hat{\mu}). \end{aligned} \quad (2.84)$$

Substituting in equation (2.77)

$$\begin{aligned} S_F^E &\approx a^4 \sum_{\vec{n} \in L} \bar{\psi}(\vec{n}) \left(\sum_{\mu=1}^4 \gamma_\mu^E \frac{(1 + ig a A_\mu(\vec{n}))\psi(\vec{n} + \hat{\mu}) - (1 - ig a A_\mu(\vec{n} - \hat{\mu}))\psi(\vec{n} - \hat{\mu})}{2a} \right. \\ &\quad \left. + m\psi(\vec{n}) \right) \\ &= a^4 \sum_{\vec{n} \in L} \bar{\psi}(\vec{n}) \left(\sum_{\mu=1}^4 \gamma_\mu^E \frac{\psi(\vec{n} + \hat{\mu}) - \psi(\vec{n} - \hat{\mu})}{2a} \right. \\ &\quad \left. + \frac{ig}{2} (A_\mu(\vec{n})\psi(\vec{n} + \hat{\mu}) + A_\mu(\vec{n} - \hat{\mu})\psi(\vec{n} - \hat{\mu})) + m\psi(\vec{n}) \right). \end{aligned} \quad (2.85)$$

The first term in the parenthesis is a discrete version of $\partial_\mu(x)$ and we will approximate $\psi(\vec{n} \pm \hat{\mu}) \approx \psi(\vec{n})$ and $A_\mu(\vec{n} - \hat{\mu}) \approx A_\mu(\vec{n})$ in the second term, because $|\hat{\mu}| = a$. This yields

$$S_F^E \approx a^4 \sum_{\vec{n} \in L} \bar{\psi}(\vec{n}) \left(\sum_{\mu=1}^4 \gamma_\mu^E \frac{\psi(\vec{n} + \hat{\mu}) - \psi(\vec{n} - \hat{\mu})}{2a} + ig A_\mu(\vec{n}) + m\psi(\vec{n}) \right). \quad (2.86)$$

When $a \rightarrow 0$ one obtains

$$\begin{aligned} S_F^E &= \int d^4x \bar{\psi}(x) [\gamma_\mu^E (\partial_\mu + ig A_\mu(x)) + m] \psi(x) \\ &= \int d^4x \bar{\psi}(x) (\gamma_\mu^E \mathcal{D}_\mu + m) \psi(x). \end{aligned} \quad (2.87)$$

Therefore, the discretization (2.77) of the second term in (2.68) satisfies the two conditions that we mentioned at the beginning, nevertheless, this expression is not completely right for a non trivial reason that we will revise in the next section⁴, for now let us continue with the discretization of the gauge term

$$S_G^E = \frac{1}{4} \int d^4x F_{\mu\nu} F_{\mu\nu} \quad (2.88)$$

in (2.68). Again we have to make sure that the expression we use is gauge invariant and that in the limit $a \rightarrow 0$ we recover (2.88). To do that, we define a *plaquette variable* as

$$U_{\mu\nu}(\vec{n}) \equiv U_\mu(\vec{n}) U_\nu(\vec{n} + \hat{\mu}) U_\mu^\dagger(\vec{n} + \hat{\nu}) U_\nu^\dagger(\vec{n}), \quad (2.89)$$

where $\hat{\mu}$ and $\hat{\nu}$ denote direction, $|\hat{\mu}| = |\hat{\nu}| = a$. Let us note from (2.83) that the link variables are members of $U(1)$ and as a result $U_{\mu\nu} \in U(1)$ as well. Geometrically, the plaquette $U_{\mu\nu}$ connects the points \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

⁴Eq (2.77) is known as the *naive fermion action*.

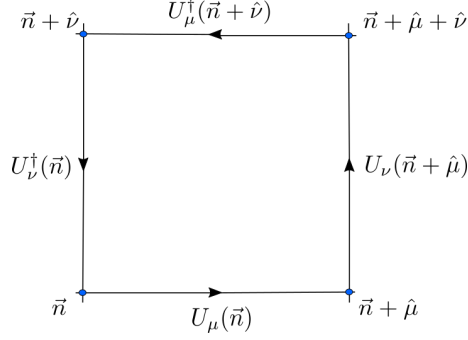


Figure 2.3: Schematic representation of the plaquette variable $U_{\mu\nu}$. It links the points \vec{n} , $\vec{n} + \hat{\mu}$, $\vec{n} + \hat{\mu} + \hat{\nu}$ and $\vec{n} + \hat{\nu}$ on the lattice by using the link variables.

$$\begin{aligned}
 U'_{\mu}(\vec{n}) &= \Omega(\vec{n})U_{\mu}(\vec{n})\Omega^{-1}(\vec{n} + \hat{\mu}), \quad U'_{\nu}(\vec{n} + \hat{\mu}) = \Omega(\vec{n} + \hat{\mu})U_{\nu}(\vec{n} + \hat{\mu})\Omega^{-1}(\vec{n} + \hat{\mu} + \hat{\nu}) \\
 U'_{\mu}^{\dagger}(\vec{n} + \hat{\nu}) &= \Omega(\vec{n} + \hat{\mu} + \hat{\nu})U_{\mu}^{\dagger}(\vec{n} + \hat{\nu})\Omega^{-1}(\vec{n} + \hat{\nu}), \quad U'_{\nu}^{\dagger}(\vec{n}) = \Omega(\vec{n} + \hat{\nu})U_{\nu}^{\dagger}(\vec{n})\Omega^{-1}(\vec{n}),
 \end{aligned} \tag{2.90}$$

it can be seen that the plaquette transforms as

$$U'_{\mu\nu}(\vec{n}) = \Omega(\vec{n})U_{\mu\nu}(\vec{n})\Omega^{-1}(\vec{n}). \tag{2.91}$$

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 can conclude that

$$U'_{\mu\nu}(\vec{n}) = U_{\mu\nu}(\vec{n}). \tag{2.92}$$

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

$$S_G^E[U] = \frac{1}{g^2} \sum_{\vec{n} \in L} \sum_{\mu < \nu} \left[1 - \frac{1}{2} \left(U_{\mu\nu}(\vec{n}) + U_{\mu\nu}^{\dagger}(\vec{n}) \right) \right]. \tag{2.93}$$

Let us revise that this action becomes (2.88) when $a \rightarrow 0$. We can substitute eq. (2.83) in the definition of the plaquette

$$U_{\mu\nu}(\vec{n}) = e^{igaA_{\mu}(\vec{n})} e^{igaA_{\nu}(\vec{n} + \hat{\mu})} e^{-igaA_{\mu}(\vec{n} + \hat{\nu})} e^{-igaA_{\nu}(\vec{n})}. \tag{2.94}$$

The exponents can be rearranged

$$U_{\mu\nu}(\vec{n}) = e^{iga^2 \left(\frac{A_{\nu}(\vec{n} + \hat{\mu}) - A_{\nu}(\vec{n})}{a} - \frac{A_{\mu}(\vec{n} + \hat{\nu}) - A_{\mu}(\vec{n})}{a} \right)}, \tag{2.95}$$

when $a \ll 1$ this is approximately

$$U_{\mu\nu} \approx e^{iga^2(\partial_{\mu}A_{\nu}(\vec{n}) - \partial_{\nu}A_{\mu}(\vec{n}))} = e^{iga^2F_{\mu\nu}}. \tag{2.96}$$

Then

$$U_{\mu\nu}(\vec{n}) + U_{\mu\nu}^{\dagger}(\vec{n}) \approx e^{iga^2F_{\mu\nu}} + e^{-iga^2F_{\mu\nu}} = 2 \cos(ga^2F_{\mu\nu}) \tag{2.97}$$

$$\approx 2 - g^2a^4F_{\mu\nu}F_{\mu\nu}. \tag{2.98}$$

Substituting in (2.93) yields

$$S_G^E[U] \approx \frac{1}{g^2} \sum_{\vec{n} \in L} \sum_{\mu < \nu} \frac{g^2 a^4}{2} F_{\mu\nu} F_{\mu\nu} = \frac{1}{4} a^4 \sum_{\vec{n} \in L} \sum_{\mu, \nu} F_{\mu\nu} F_{\mu\nu}. \quad (2.99)$$

The factor of 2 comes from the fact that in the right hand side of the equation $F_{\mu\nu}$ is antisymmetric and that the sum extends over all possible values of μ and ν , not only those where $\mu < \nu$. When $a \rightarrow 0$ the Wilson action converges to (2.88). Finally, the complete naive discretization of the QED action given in (2.68) is

$$\begin{aligned} S_{\text{QED}}^E[\psi, \bar{\psi}, U] &= a^4 \sum_{\vec{n} \in L} \bar{\psi}(\vec{n}) \left(\sum_{\mu=1}^4 \gamma_\mu^E \frac{U_\mu(\vec{n}) \psi(\vec{n} + \hat{\mu}) - U_\mu^\dagger(\vec{n} - \hat{\mu}) \psi(\vec{n} - \hat{\mu})}{2a} + m \psi(\vec{n}) \right) \\ &+ \frac{1}{g^2} \sum_{\vec{n} \in L} \sum_{\mu < \nu} \left[1 - \frac{1}{2} (U_{\mu\nu}(\vec{n}) + U_{\mu\nu}^\dagger(\vec{n})) \right]. \end{aligned} \quad (2.100)$$

To finish this section, let us make some brief remarks about how this discretization can be taken to QCD. Some of the definitions and relations given here hold when the transformation group is $SU(3)$. For example, the definition of the link variables and the plaquettes is the same; however, in such case the components of the gauge field A_μ are matrices and they do not commute in general, so one has to be careful to preserve the order of the operations that define the plaquette variables. Another consequence of the non-commutativity is that the plaquette will not be gauge invariant, even so, one can still construct a gauge invariant Wilson action using the trace operator as follows

$$S_G^E[U] = \frac{6}{g^2} \sum_{\vec{n} \in L} \sum_{\mu < \nu} \left(1 - \frac{1}{6} \text{Re tr} [U_{\mu\nu}(\vec{n})] \right), \quad U_{\mu\nu} \in SU(3). \quad (2.101)$$

This action will converge to the correct expression in the continuum

$$S_G^E = \frac{1}{4} \int d^4x G_{\mu\nu}^a(x) G_{\mu\nu}^a(x), \quad (2.102)$$

where $G_{\mu\nu}^a(x)$ is the gluon field strength tensor, a denotes the eight gluons. A deeper insight of Lattice QCD can be revised in [6], [7] and [9].

2.4 Wilson fermions

As we mentioned in the last section, the discretization of the fermion action given in (2.77) is not fully right. To see why, let us rewrite (2.77) as follows

$$\begin{aligned} S_F^E[\psi, \bar{\psi}, U] &= a^4 \sum_{\vec{n}, \vec{m} \in L} \bar{\psi}(\vec{n}) D(\vec{n}, \vec{m}) \psi(\vec{m}), \\ D(\vec{n}, \vec{m}) &= \sum_{\mu=1}^4 \gamma_\mu^E \frac{U_\mu(\vec{n}) \delta_{\vec{n}+\hat{\mu}, \vec{m}} - U_\mu^\dagger(\vec{n} - \hat{\mu}) \delta_{\vec{n}-\hat{\mu}, \vec{m}}}{2a} + m \delta_{\vec{n}, \vec{m}}. \end{aligned} \quad (2.103)$$

$D(\vec{n}, \vec{m})$ is the Dirac operator. Let us suppose for a moment that we are working at the chiral limit, *i.e.* $m = 0$, if one computes the discrete Fourier transform $\tilde{D}(p)$ of the Dirac operator and then its inverse $\tilde{D}^{-1}(p)$, one arrives at (see[6] for details)

$$\tilde{D}^{-1}(p) = \frac{\frac{-i}{a} \sum_\mu \gamma_\mu^E \sin(p_\mu a)}{\frac{1}{a^2} \sum_\mu \sin(p_\mu a)^2}. \quad (2.104)$$

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

$$\tilde{D}^{-1}(p) = \frac{-i \sum_{\mu} \gamma_{\mu}^E p_{\mu}}{p^2}. \quad (2.105)$$

We can see that in the continuum there is only one pole at $p = (0, 0, 0, 0)$, this is correct since the poles of the propagator represent particles and we are dealing with just one; nevertheless, the discrete version has poles at $p = (0, 0, 0, 0)$ and whenever a component of p is equal to π/a , thus the discrete version has 16 poles, with 15 of them being unphysical⁵. This is known as the *fermion doubling* problem and shows that the naive discretization 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 [10], the idea is modifying the Dirac operator by adding a term that eliminates the unwanted particles, but that vanishes when $a \rightarrow 0$. The term he adds is called the Wilson term and is a discretization of the Laplace operator multiplied by $-a/2$

$$D_{\text{Wilson}} = -\frac{a}{2} \sum_{\mu=1}^4 \frac{\delta_{\vec{n}+\hat{\mu}, \vec{m}} - 2\delta_{\vec{n}, \vec{m}} + \delta_{\vec{n}-\hat{\mu}, \vec{m}}}{a^2}. \quad (2.106)$$

Since the sum is just a discrete version of $\partial_{\mu}\partial_{\mu}$, it goes to zero when $a \rightarrow 0$. To preserve the gauge invariance we have to put the link variables

$$D_{\text{Wilson}} = -\frac{a}{2} \sum_{\mu=1}^4 \frac{U_{\mu}(\vec{n})\delta_{\vec{n}+\hat{\mu}, \vec{m}} - 2\delta_{\vec{n}, \vec{m}} + U_{\mu}^{\dagger}(\vec{n} - \hat{\mu})\delta_{\vec{n}-\hat{\mu}, \vec{m}}}{a^2}. \quad (2.107)$$

Adding this term to the naive version of the Dirac operator gives

$$D(\vec{n}, \vec{m}) = \left(m - \frac{4}{a}\right) \delta_{\vec{n}, \vec{m}} - \frac{1}{2a} \sum_{\mu=1}^4 \left[(1 - \gamma_{\mu}^E) U_{\mu}(\vec{n}) \delta_{\vec{n}+\hat{\mu}, \vec{m}} + (1 - \gamma_{\mu}^E) U_{\mu}^{\dagger}(\vec{n} - \hat{\mu}) \delta_{\vec{n}-\hat{\mu}, \vec{m}} \right]. \quad (2.108)$$

This version of $D(\vec{n}, \vec{m})$ eliminates the doubling problem. 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. 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

$$\bar{\psi}(\vec{n}) \rightarrow \bar{\psi}'(\vec{n}) = \bar{\psi}(\vec{n}) e^{i\alpha\gamma_5}, \quad \psi(\vec{n}) \rightarrow \psi'(\vec{n}) = e^{i\alpha\gamma_5} \psi(\vec{n}), \quad \alpha \in \mathbb{R} \quad (2.109)$$

and analyzes the term $4/a\delta_{\vec{n}, \vec{m}}$ when inserted in the action

$$\bar{\psi}'(\vec{n}) \frac{4}{a} \psi'(\vec{m}) = \bar{\psi}(\vec{n}) \frac{4}{a} \delta_{\vec{n}, \vec{m}} e^{i\alpha\gamma_5^E} e^{i\alpha\gamma_5^E} \psi(\vec{m}) \neq \bar{\psi}(\vec{n}) \frac{4}{a} \psi(\vec{m}). \quad (2.110)$$

Still, one can work with Wilson fermions and then renormalize the outcome. The expectation values can be calculated through

$$\begin{aligned} \langle \hat{A} \rangle &= \frac{1}{Z} \int \mathcal{D}[\psi] \mathcal{D}[\bar{\psi}] \mathcal{D}[U] e^{-S_{\text{QED}}^E[\psi, \bar{\psi}, U]} A[\psi, \bar{\psi}, U], \\ Z &= \int \mathcal{D}[\psi] \mathcal{D}[\bar{\psi}] \mathcal{D}[U] e^{-S_{\text{QED}}^E[\psi, \bar{\psi}, U]}, \\ \mathcal{D}[U] &= \prod_{\vec{n} \in L} \prod_{\mu=1}^4 dU_{\mu}(\vec{n}). \end{aligned} \quad (2.111)$$

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

There are more ways of discretizing $D(\vec{n}, \vec{m})$ that deal with the doubling problem and they introduce other kinds of fermions, such as *staggered fermions*, *chiral fermions*, etc. A detailed explanation of those formulations can be found in [7], however they will not be used in this work.

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