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Applications of the Wilson Flow in Lattice Gauge Theory

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a.a. 2011/2012

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Chapter 1

Introduction

The Standard Model of particle physics is the theory in which strong, weak and electromagnetic interactions are currently described. Its and action are invariant under the gauge group:

$$G = SU(3)_c \times SU(2)_L \times U(1)_Y \tag{1.1}$$

The quantum numbers are called color for $SU(3)$, weak isospin for $SU(2)$ and weak hypercharge for $U(1)$.

In particular, quantum chromodynamics (QCD) is the currently accepted theory to describe strong interactions. Three requests lie at the basis of QCD:

- gauge symmetry, QCD is a local gauge theory with the color gauge group $SU(3)_c$;
- matter content of the theory;
- renormalizability, the theory should be renormalizable.

The matter components are the quarks, which are described by spinor fields in the fundamental representation carrying three color indexes and appearing in six flavors (up, down, charm, strange, top and bottom). Since SU(3) is non-Abelian the vector bosons that mediate the interactions, the gluons, can self-interact; furthermore this property provides that the theory is asymptotically free.

QCD was formulated over the years after a series of theoretical and experimental advances, with the aim to describe the properties of the vast number of new particles discovered in the 1950s and 1960s and to explain the observed properties of the strong interaction; in particular any viable theoretical model was required to have two features: asymptotic freedom and confinement, which manifested themselves respectively at high and low energies.

The classification of the observed hadrons in multiplets reflecting underlying symmetries was one of the first steps toward the formulation of the hypothesis that hadrons are composed of more elementary constituents, called quarks [1, 2].

Asymptotic freedom was formulated in the contest of deep inelastic scattering experiments, where the phenomenon of Bjorken scaling was observed. Scaling refers to an important simplifying feature of a large class of dimensionless physical quantities in elementary particles, in particular the cross section is determined not by the absolute energy of an experiment but by dimensionless kinematic quantities, such as the scattering angle or the ratio of the energy to momentum transfer. Since increasing energy implies potentially improved spatial resolution, scaling implies independence of the absolute resolution scale, and hence strongly suggest that experimentally observed strongly interacting particles (hadrons) behave as collections of point-like constituents when probed at sufficient high energies. Feynman's parton model [3, 4, 5] where the proton was assumed to consist of point-like constituents called partons, gave an explanation to the observed experimental phenomenon of scaling. Later partons were identified with quarks.

In 1973 Fritzsch, Gell-Mann and Leutwyler [6] proposed QCD as the non-Abelian gauge theory built from the SU(3) gauge group associated with the color symmetry.

In the same year, it was shown by Gross and Wilczek [7] and Politzer [8] that non-Abelian gauge theory exhibits asymptotic freedom.

The insertion of quantum corrections leads to divergences in the evaluation of physical observables; these can be eliminated via renormalizing the theory by adding counterterms in the Lagrangian in a proper way. The consequence of the renormalization of a quantum field theory is that the coupling constant that appears in the Lagrangian becomes a running coupling. The so-called β-function quantifies the dependence of the coupling on the energy scale. Through the perturbative study of the β-function it was shown that at very high energies (or equivalently at small distances) the coupling becomes small, so that the quarks behave as free particles. In this regime it is expected that perturbative methods furnish reliable predictions for physical observables, and Bjorken scaling is explained.

On the other hand, quarks have never been detected in isolation, but only as constituents of hadrons. From the theoretical point of view, this should correspond to the fact that all physical states are singlets with respect to the color group. In order to check whether this feature is contained in QCD, one can not apply perturbative methods, since the coupling is expected to be large at scales corresponding to the size of hadrons. It is however widely believed that this behavior is a consequence of quantum chromodynamics, although up to now no analytical proof exists.

One of the strongest evidence for this to be true comes from lattice field theory. In 1974 Wilson proposed [9] a formulation of a gauge field theory on a discretized Euclidean space-time. In this framework, by using a strong coupling expansion it was possible to demonstrate that at sufficiently strong couplings, pure SU(3) lattice gauge theory exhibits color confinement. Since then lattice field theory has been widely studied and became a powerful tool to investigate properties of strong interactions and today a rich set of numerical results support the model description that in the limit of large distances, the energy needed to separate a pair of quark-antiquark grows proportionally to the separation.

In the first chapter we present the QCD action and its euclidean version, we then review the transformation symmetries constituting the chiral group and their consequences on the QCD action and its massless version. After having derived the classical currents and their conservation laws, we obtain their quantum version known as Ward–Takahashi identities. We analyze the consequences of the spontaneous breaking of the chiral symmetry as the appearance of Goldstone bosons (the pions), and then we review the consequences of the fact that u, d and s quarks have masses which can be assumed to be small with respect to the

Λ_{QCD} scale rendering the chiral symmetry only an approximate one. We conclude our reasoning deriving the Gell-Mann–Oakes–Renner relation (GMOR). Then we analyze the so-called $U(1)_A$ problem and the origin of the mass of the η' meson. To do so we review the anomalous version of the Ward–Takahashi identity for the axial current and we derive the Witten–Veneziano formula, introducing quantities of interest as the topological charge Q and the topological susceptibility χ. An alternative solution of the $U(1)_A$ problem, known as dilute instanton gas, is then presented.

In the second chapter we review lattice gauge field theory and its recent advancements which have led to the possibility to describe a discretized version of the QCD on the lattice which possess chiral invariance.

In the third chapter we obtain the lattice version of the Ward–Takahashi identities and we justify the origin of the anomaly on the lattice, thus we write the lattice version of the aforementioned quantities Q and χ. In particular, we discuss in further details the consequences of the discretization of the topological charge and we introduce the main technical tool that we have used for its computation on the lattice: the Wilson flow.

In the fourth chapter we review the parameters of our simulation run, we present the results we have obtained and we discuss their consequences on the $U(1)_A$ problem, for which a solution is indicated.

1.1 Euclidean Action

The action we are interested to study is given by:

$$S = S_G + S_F = -\frac{1}{4}\int d^4x F_{\mu\nu}F^{\mu\nu} + \int d^4x \bar{\psi}(i\not{D} - M)\psi \tag{1.2}$$

which is a gauge field action whom gauge group is $SU(3)$; M is a $N_f \times N_f$ matrix real diagonal matrix containing the quark masses. The field strenght tensor is:

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + ig[A_\mu, A_\nu]$$

and the Dirac operator is

$$\not{D} = \gamma^\mu \partial_\mu - ig\gamma^\mu A^a_\mu T^a$$

where a summation over $\mu = 0, \ldots, 3$ and over $a = 1, \ldots, 8$ is intended.

The term

$$S_G = -\frac{1}{4}\int d^4x F_{\mu\nu}F^{\mu\nu}$$

is usually referred to as the *pure gauge* part of them action, while the term

$$S_F = \int d^4x \bar{\psi}(i\not{D} - M)\psi$$

is referred to as the *fermionic* part of the action.

We will Wick-rotate the temporal axis and write the above action in an Euclidean spacetime, this is performed making the following substitution:

$$x^0 \to -i(x^{\mathrm{E}})^4 \tag{1.3}$$

we will thus adopt the following conventions:

$$\begin{aligned} ix^0 &= (x^{\mathrm{E}})^4 & \partial_0 &= i\frac{\partial}{\partial (x^{\mathrm{E}})^4} = i\partial_4^{\mathrm{E}} \\ \gamma^0 &= (\gamma^{\mathrm{E}})^4 & \gamma^i &= i(\gamma^{\mathrm{E}})^i \\ A_0 &= iA_4^{\mathrm{E}} \end{aligned} \tag{1.4}$$

the γ_5 matrix is given by:

$$\gamma_5 = \gamma^4\gamma^1\gamma^2\gamma^3 \tag{1.5}$$

Then the action transforms in the following way:

$$S \to iS^{\mathrm{E}} \tag{1.6}$$

where we have:

$$S^{\mathrm{E}} = S_G^{\mathrm{E}} + S_F^{\mathrm{E}} \tag{1.7}$$

with:

$$S_G^{\mathrm{E}} = \frac{1}{4}\int d^4x F_{\mu\nu}F_{\mu\nu} \tag{1.8}$$

and

$$S_F^{\mathrm{E}} = \int d^4x \bar{\psi}(D + M)\psi \tag{1.9}$$

where $D = \gamma_\mu D_\mu$ and a summation over $\mu = 1, \ldots, 4$ is intended.

In the following we shall drop any superscript reminding us of the Euclidean spacetime.

1.2 Classical Conservation Laws

In the following we review some of the invariances of the action (1.9). Then, using Noether theorem, we derive the classical currents and their conservation laws.

1.2.1 The Chiral Group

The massless action $\tilde{S}_F$ is invariant under the group of global symmetries:

$$G = U(N_f)_L \times U(N_f)_R \tag{1.10}$$

where N_f is the number of quark flavors, the group G in (1.10) is also called the *chiral group*.

The fermion field ψ can be decomposed in its *chiral components*, i.e. left- and right-handed parts, where the following relation holds:

$$\psi = \psi_R + \psi_L \tag{1.11}$$

the left ψ_L and right ψ_R components of ψ can be obtained through the action of two projectors, $P_{L,R}$, defined as follows:

$$P_{L,R} = \frac{1}{2}(1 \mp \gamma_5) \tag{1.12}$$

which satisfy the following properties:

$$(P_{L,R})^2 = P_{L,R}, \qquad P_L P_R = P_R P_L = 0 \qquad P_L + P_R = \mathbb{1} \tag{1.13}$$

The chiral components of the fermion and anti-fermion fields ψ_R, ψ_L, $\bar{\psi}_R$, $\bar{\psi}_R$ are obtained as:

$$\psi_R = P_R \psi \qquad \psi_L = P_L \psi \tag{1.14}$$

and

$$\bar{\psi}_R = \bar{\psi} P_L \qquad \bar{\psi}_L = \bar{\psi} P_R \tag{1.15}$$

where we have assigned to the left-handed (right-handed) component of the field the chirality eigenvalue -1 $(+1)$, i.e.:

$$\gamma_5 \psi_{L,R} = \mp \psi_{L,R} \tag{1.16}$$

The Lagrangian can be decomposed into separated left- and right-handed parts:

$$\mathcal{L} \equiv \mathcal{L}^L + \mathcal{L}^R := \bar{\psi}_L \not{D} \psi_L + \bar{\psi}_R \not{D} \psi_R \tag{1.17}$$

and the mass term would be given by:

$$(\bar{\psi}_L M \psi_R + \bar{\psi}_R M \psi_L) \tag{1.18}$$

The symmetry group (1.10) can also be decomposed as the product:

$$G_{\tilde{S}_F} = SU(N_f)_L \times SU(N_f)_R \times U(1)_V \times U(1)_A \tag{1.19}$$

where the subscript V stands for *vector* and the subscript A stands for *axial*[1]. The notation used in eq. (1.19) stresses that the massless action is invariant under four possible symmetries:

- a non-abelian symmetry on the left components of the fields $SU(N_f)_L$;
- a non-abelian symmetry on the right components of the fields $SU(N_f)_R$;
- a vector abelian symmetry $U(1)_V$;
- an axial abelian symmetry $U(1)_A$;

Non-abelian symmetry transformations are also called *non-singlet* transformations whereas abelian symmetry transformation are called *singlet* transformations.

When the fully quantized theory is considered one finds that the fermion measure is not invariant under the axial symmetries, expressed by the $U(1)_A$ group. It is found that it is explicitly broken by a non-invariance of the fermion integration measure, this phenomenon is called axial anomaly. Thus, the remaining symmetry is:

$$SU(N_f)_L \times SU(N_f)_R \times U(1)_V \tag{1.20}$$

Combining transformations in the group $SU(N_f)_L \times SU(N_f)_R$ the subgroup $SU(N_f)_V$ of vector non-abelian rotations can also be obtained; the remaining generators are called the axial generators.

[1] The name "vector" and "axial" transformations comes from the fact that the related Noether currents are vector or axial currents respectively.

Reinserting a degenerate quark mass in the action breaks the symmetry $SU(N_f)_L \times SU(N_f)_R$ explicitly to its subgroup $SU(N_f)_V$ thus we remain with the symmetry:

$$SU(N_f)_V \times U(1)_V \qquad (M = 0) \tag{1.21}$$

If non-degenerate masses are allowed the symmetry is further reduced to:

$$U(1)_V \times U(1)_V \times \cdots \times U(1)_V \qquad N_f \text{ factors} \tag{1.22}$$

1.2.2 Symmetry Transformations

We will focus on the following Lagrangian:

$$\mathcal{L} = \bar{\psi} \not{D} \psi + \bar{\psi} M \psi \tag{1.23}$$

Left- and Right-Handed Transformations

In the massless case we can see now explicitly that the Lagrangian is invariant under separated transformations on the chirality components. Let $H = L, R$ we can define the following:

$$\begin{aligned} \psi_H &\to \psi'_H = g_H^{-1} \psi_H \\ \bar{\psi}_H &\to \bar{\psi}'_H = \bar{\psi}_H g_H \end{aligned} \tag{1.24}$$

where $g_H \in U(N_f)_H$ and can be written as:

$$g_H = e^{\Lambda_H} \tag{1.25}$$

The infinitesimal version of these transformations is:

$$\begin{aligned} \delta\psi_H &= -\Lambda_H \psi_H \\ \delta\bar{\psi}_H &= \Lambda_H \bar{\psi}_H \end{aligned} \tag{1.26}$$

We can define the vector and axial transformations setting:

$$\begin{aligned} \alpha &:= \frac{1}{2}(\Lambda_L + \Lambda_R) \qquad \text{(vector transformation)} \\ \beta &:= \frac{1}{2}(\Lambda_R - \Lambda_L) \qquad \text{(axial transformation)} \end{aligned} \tag{1.27}$$

Conversely, from vector and axial transformations we can recover the left- and right-handed transformations with:

$$\begin{aligned} \Lambda_L &= \frac{1}{2}(\beta - \alpha) \\ \Lambda_R &= \frac{1}{2}(\alpha + \beta) \end{aligned} \tag{1.28}$$

Vector Non-Abelian Transformations

If we allow for degenerate masses $M = \mathrm{diag}(m, m, \ldots, m)$, the Lagrangian (1.23) remains invariant under the transformations of the vector symmetry group $SU(N)_V$:

$$\begin{aligned} \psi &\to \psi' = g^{-1} \psi \\ \bar{\psi} &\to \bar{\psi}' = \bar{\psi} g \end{aligned} \tag{1.29}$$

where g is an element of the gauge group $SU(N)$ and therefore can be written as:

$$g(x) = e^{\alpha} \tag{1.30}$$

with $\alpha(x) = \alpha^a T^a$. We have chosen the T^a matrices to be anti-hermitian so that:

$$\alpha^\dagger = -\alpha \tag{1.31}$$

The infinitesimal version of the transformations in eq. (1.29) is:

$$\begin{aligned} \delta\psi &= -\alpha\psi \\ \delta\bar{\psi} &= \bar{\psi}\alpha \end{aligned} \tag{1.32}$$

Chiral Non-Abelian Transformations

We now consider the axial transformations:

$$\begin{aligned} \psi \to \psi' &= e^{\beta\gamma_5}\psi \\ \bar{\psi} \to \bar{\psi}' &= \bar{\psi}e^{\beta\gamma_5} \end{aligned} \tag{1.33}$$

where

$$\beta = \beta^a T^a \tag{1.34}$$

These transformations leave the Lagrangian (1.23) invariant only if $M = 0$. Their infinitesimal form is:

$$\begin{aligned} \delta\psi &= \beta\gamma_5\psi \\ \delta\bar{\psi} &= \bar{\psi}\beta\gamma_5 \end{aligned} \tag{1.35}$$

Vector Abelian Transformations

The above Lagrangian (1.23) remains invariant also under the local vector symmetry $U(1)_V$[2]:

$$\begin{aligned} \psi \to \psi' &= e^{i\alpha^0}\psi \\ \bar{\psi} \to \bar{\psi}' &= \bar{\psi}e^{-i\alpha^0} \end{aligned} \tag{1.36}$$

The infinitesimal version of the transformations (1.36) is:

$$\begin{aligned} \delta\psi &= i\alpha^0\psi \\ \delta\bar{\psi} &= -i\alpha^0\bar{\psi} \end{aligned} \tag{1.37}$$

Chiral Abelian Transformations

For the axial symmetry $U(1)_A$ we have:

$$\begin{aligned} \psi \to \psi' &= e^{i\beta^0\gamma_5}\psi \\ \bar{\psi} \to \bar{\psi}' &= \bar{\psi}e^{i\beta^0\gamma_5} \end{aligned} \tag{1.38}$$

The infinitesimal version of the transformations (1.38) is:

$$\begin{aligned} \delta\psi &= i\beta^0\gamma_5\psi \\ \delta\bar{\psi} &= \bar{\psi}i\beta^0\gamma_5 \end{aligned} \tag{1.39}$$

[2]The choice of the superscript 0 is customary

Currents and Classical Conservation Laws

We derive now the currents and the classical conservation law descending from the aforementioned symmetries, starting with:

$$\int d^4x\bar{\psi}(\gamma_\mu D_\mu + M)\psi \tag{1.40}$$

We can write a generic infinitesimal transformation as:

$$\psi \to \psi' = (\mathbb{1} + i\varepsilon(x)\lambda)\,\psi(x) \tag{1.41}$$
$$\bar{\psi} \to \bar{\psi}' = \bar{\psi}(x)\left(\mathbb{1} + i\varepsilon(x)\hat{\lambda}\right) \tag{1.42}$$

where we will assign to λ and $\hat{\lambda}$ different values.

The action transforms as:

$$S_F = S_F[\psi, \bar{\psi}] \to S'_F = S_F[\psi', \bar{\psi}'] = \int d^4x\bar{\psi}'(\not{D} + M)\psi' \tag{1.43}$$

and to order $\mathcal{O}(\varepsilon)$ the change in S_F is given by:

$$\begin{aligned}\delta S = i\int d^4x\bar{\psi}\Big(&\varepsilon\hat{\lambda}\gamma_\mu\partial_\mu + \gamma_\mu\lambda\partial_\mu\varepsilon + \\ &+ ig\varepsilon A_\mu(\hat{\lambda}\gamma_\mu + \gamma_\mu\lambda) + \varepsilon(\hat{\lambda}M + M\lambda)\Big)\end{aligned} \tag{1.44}$$

Choosing λ to be one of $\mathbb{1}, \gamma_5, T^a, \gamma_5 T^a$ and $\hat{\lambda}$ to be $-\mathbb{1}, -T^a, \gamma_5, \gamma_5 T^a$ respectively we have that the term

$$(\hat{\lambda}\gamma_\mu + \gamma_\mu\lambda) = 0 \tag{1.45}$$

vanishes.

We can finally write:

$$\begin{aligned}\delta S_F &= i\int d^4x\left((\partial_\mu\varepsilon(x))\bar{\psi}\gamma_\mu\lambda\psi + \varepsilon(x)\bar{\psi}\left(\hat{\lambda}M + M\lambda\right)\psi\right) = \\ &= i\int d^4x\varepsilon(x)\left(-\partial_\mu(\bar{\psi}\gamma_\mu\lambda\psi) + \bar{\psi}(\hat{\lambda}M + M\lambda)\psi\right)\end{aligned} \tag{1.46}$$

in the last step we applied an integration by parts since boundary terms do not contribute.

If we request the change of the action δS_F to vanish for every $\varepsilon(x)$ from eq. (1.46) we conclude:

$$\partial_\mu(\bar{\psi}\gamma_\mu\lambda\psi) = \bar{\psi}(\hat{\lambda}M + M\lambda)\psi \tag{1.47}$$

We can now obtain various identities for the aforementioned values of λ, $\hat{\lambda}$:

- $\lambda = \mathbb{1}$, $\hat{\lambda} = -\mathbb{1}$

$$\partial_\mu(\bar{\psi}\gamma_\mu\psi) = 0 \tag{1.48}$$

- $\lambda = T^a$, $\hat{\lambda} = -T^a$

$$\partial_\mu(\bar{\psi}\gamma_\mu T^a\psi) = \bar{\psi}[M, T^a]\psi \tag{1.49}$$

- $\lambda = \gamma_5$, $\hat{\lambda} = \gamma_5$

$$\partial_\mu(\bar{\psi}\gamma_\mu\gamma_5\psi) = 2\bar{\psi}M\gamma_5\psi \tag{1.50}$$

- $\lambda = \gamma_5 T^a$, $\hat{\lambda} = \gamma_5 T^a$

$$\partial_\mu(\bar{\psi}\gamma_\mu\gamma_5 T^a\psi) = \bar{\psi}\{M, T^a\}\gamma_5\psi \tag{1.51}$$

Now it is possible to define several currents:

$$j_\mu = \bar{\psi}\gamma_\mu\psi \quad \text{(vector abelian)} \tag{1.52}$$
$$j_\mu^a = \bar{\psi}\gamma_\mu T^a\psi \quad \text{(vector non-abelian)} \tag{1.53}$$
$$j_\mu^5 = \bar{\psi}\gamma_\mu\gamma_5\psi \quad \text{(axial abelian)} \tag{1.54}$$
$$j_\mu^{5a} = \bar{\psi}\gamma_\mu\gamma_5 T^a\psi \quad \text{(axial non-abelian)} \tag{1.55}$$

and we can finally write:

$$\partial_\mu j_\mu = 0 \tag{1.56}$$
$$\partial_\mu j_\mu^a = \bar{\psi}[M, T^a]\psi \tag{1.57}$$
$$\partial_\mu j_\mu^5 = 2\bar{\psi}M\gamma_5\psi \tag{1.58}$$
$$\partial_\mu j_\mu^{5a} = \bar{\psi}\{M, T^a\}\gamma_5\psi \tag{1.59}$$

In the case of degenerate quark masses, i.e. for:

$$M = m \cdot \mathbb{1} \tag{1.60}$$

we have:

$$\partial_\mu j_\mu^a = 0 \tag{1.61}$$
$$\partial_\mu j_\mu^5 = 2m\bar{\psi}\gamma_5\psi = 2mP \tag{1.62}$$
$$\partial_\mu j_\mu^{5a} = 2m\bar{\psi}\gamma_5 T^a\psi = 2mP^a \tag{1.63}$$

In the next section we will discuss the quantum version of the conservation laws (1.56)–(1.59).

1.3 Ward Identities and GMOR

1.3.1 Ward Identities

The fact that from a given field theory we can derive a classical conservation relation for a current does not assure that the current is indeed conserved in QFT. We need to derive for these conservation relations their quantum version known as Ward–Takahashi identities, i.e. we need to check if the classical conservation laws still holds when inserted in correlators. There are cases, known as anomalies, where a classical current conservation law does not hold at the quantum level. In the following we derive the Ward identities related to the currents defined above, in the next section we will state the anomalous version of the chiral current.

In the path integral formalism, the expression for the partition function is:

$$\begin{aligned} Z = & \int \mathcal{D}A\mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-S} = \\ = & \int \mathcal{D}A'\mathcal{D}\bar{\psi}'\mathcal{D}\psi' e^{-S'} \end{aligned} \tag{1.64}$$

If the action S is invariant

$$S' \equiv S[\psi', \bar{\psi}'] = S[\psi, \bar{\psi}] \tag{1.65}$$

under a given transformation, Ward identities can be obtained.

In particular we are interested in how the expectation value of generic operators, function of the fields, vary if we perform a symmetry transformation.

The expectation value of the operator $\mathcal{O}[\psi, \bar{\psi}]$ is given by:

$$\langle \mathcal{O}[\psi, \bar{\psi}] \rangle = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-S[\psi,\bar{\psi}]}\mathcal{O}[\psi, \bar{\psi}] \tag{1.66}$$

If we perform the following generic symmetry transformation:

$$\begin{aligned} \psi \to \psi' &= g(x)\psi(x) \approx \psi + \delta\psi \\ \bar{\psi} \to \bar{\psi}' &= \bar{\psi}(x)\tilde{g}(x) \approx \bar{\psi} + \delta\bar{\psi} \end{aligned} \tag{1.67}$$

such that the action, to the first order, transforms as:

$$S[\psi, \bar{\psi}] \to S[\psi', \bar{\psi}'] + \delta S[\psi', \bar{\psi}'] \tag{1.68}$$

and the operator $\mathcal{O}[\psi, \bar{\psi}]$ as:

$$\mathcal{O}[\psi, \bar{\psi}] \to \mathcal{O}[\psi', \bar{\psi}'] + \delta O[\psi', \bar{\psi}'] \tag{1.69}$$

Thus the expectation value using the transformed fields $\bar{\psi}'$, ψ' transforms as:

$$\langle \mathcal{O}[\psi, \bar{\psi}] \rangle = \int \mathcal{D}A'\mathcal{D}\bar{\psi}'\mathcal{D}\psi' e^{-(S[\psi',\bar{\psi}']+\delta S[\psi',\bar{\psi}'])} \left\{ \mathcal{O}[\psi', \bar{\psi}'] + \delta\mathcal{O}[\psi', \bar{\psi}'] \right\} \tag{1.70}$$

In writing eq. (1.70) we are making an implicit assumption, that the integration measure is invariant under the transformation (1.67), formally:

$$\int \mathcal{D}A'\mathcal{D}\bar{\psi}'\mathcal{D}\psi' \to \int \mathcal{D}A'\mathcal{D}\bar{\psi}'\mathcal{D}\psi' \tag{1.71}$$

This assumption will be proven wrong in the case of anomalous Ward identities.

Expanding the above expression using infinitesimal transformations we arrive at the following relation:

$$\langle \mathcal{O}[\psi, \bar{\psi}] \rangle = \langle \mathcal{O}[\psi', \bar{\psi}'] \rangle - \langle \delta S_F[\psi', \bar{\psi}']\mathcal{O}[\psi', \bar{\psi}'] \rangle + \langle \delta\mathcal{O}[\psi', \bar{\psi}'] \rangle \tag{1.72}$$

we should not be able to distinguish the transformed case (ψ',$\bar{\psi}'$ fields) from the non-transformed case, since these transformations are purely mathematical, thus the following equality must hold:

$$\langle \mathcal{O}[\psi, \bar{\psi}] \rangle = \langle \mathcal{O}[\psi', \bar{\psi}'] \rangle \tag{1.73}$$

then we arrive to the following identity:

$$\langle \delta S_F[\psi', \bar{\psi}']\mathcal{O}[\psi', \bar{\psi}'] \rangle = \langle \delta\mathcal{O}[\psi', \bar{\psi}'] \rangle \tag{1.74}$$

which expresses a family of relations known as *Ward–Takahashi identities.*

1.3.2 Gell-Mann–Oakes–Renner Relation

If we specialize eq. (1.74), for non-singlet chiral rotations with $\mathcal{O}[\psi, \bar{\psi}] = P^a$, we can write:

$$\langle i \left(\partial_\mu j^{5b}_\mu - \bar{\psi}\{M, T^b\}\gamma_5 \psi \right) P^a \rangle = \langle \frac{\delta P^a}{\delta \alpha^b(x)} \rangle \tag{1.75}$$

the variation of $P^a[\psi, \bar{\psi}]$ is:

$$\begin{aligned} \delta_{\alpha^b(x)} P^a(y) &= \frac{\delta[(P')^a - P^a](y)}{\delta\alpha^b(x)} \\ &= \frac{\delta[\bar{\psi}'(y)\gamma_5 T^a \psi'(y) - \bar{\psi}(y)\gamma_5 T^a \psi(y)]}{\delta\alpha^b(x)} = \\ &= \frac{\delta[(\bar{\psi} + \delta\bar{\psi})\gamma_5 T^a (\psi + \delta\psi) - \bar{\psi}\gamma_5 T^a \psi]}{\delta\alpha^b(x)} = \\ &= -\frac{\delta[i\alpha^a(y)\bar{\psi}\gamma_5^2\{T^a, T^a\}\psi]}{\delta\alpha^b(x)} = \\ &= -\frac{i\delta(x-y)}{N_f}\bar{\psi}\psi\delta^{ab} \end{aligned} \tag{1.76}$$

For simplicity, we will suppose the case of degenerate masses $M = m \cdot \mathbb{1}$, so we can write:

$$\langle 2m \left(\partial_\mu j^{5a}_\mu - P^a \right) P^a \rangle = -\frac{\delta^{(4)}(x)}{N_f} \langle \bar{\psi}\psi \rangle \tag{1.77}$$

the quantity on the r.h.s of the equation is also known as the *chiral condensate*, in the chiral limit it is defined as:

$$\Sigma = \lim_{m \to 0} -\frac{\langle \bar{\psi}\psi \rangle}{N_f}. \tag{1.78}$$

We can integrate eq. (1.77) and applying the Gauss theorem to the total divergence of the current we get:

$$2m \int d^4x \langle P^a(x) P^a(0) \rangle = -\frac{1}{N_f} \langle \bar{\psi}\psi \rangle \tag{1.79}$$

Inserting a 1-particle completeness over pion states we can write

$$2m \int d^4x \int \frac{d^3p}{(2\pi)^3} \frac{1}{2p^0} \frac{\langle 0|P^a(x)|p, \pi^b\rangle\langle \pi^b, p|P^a(0)|0\rangle}{p^2 + M_\pi^2} = -\frac{1}{N_f}\langle \bar{\psi}\psi \rangle \tag{1.80}$$

Where we made use of the completeness relation:

$$(\mathbb{1})_{\text{1-particle}} = \sum_{\pi^a} \int \frac{d^3p}{(2\pi)^3} \frac{1}{2p^0} |p, \pi^a\rangle\langle \pi^a, p| \tag{1.81}$$

where the single particle states are normalized as:

$$\langle \pi^a, p | q, \pi^b \rangle = \delta^{ab} 2p^0 (2\pi)^3 \delta(\vec{p} - \vec{q}) \tag{1.82}$$

and with $p^0 = \sqrt{|\vec{p}|^2 + M_\pi^2}$

By assuming that the condesate is not null in the chiral limit ($m \to 0$) eq. (1.80) we are led to the conclusion that the integral on the l.h.s. must have a pole in $p = 0$, thus we obtain to the following equality:

$$\lim_{m\to 0} \frac{2m}{M_\pi^2} |\langle 0|P^a|\pi^a\rangle|^2 = \lim_{m\to 0} -\frac{1}{N_f}\langle\bar\psi\psi\rangle \tag{1.83}$$

Requesting $x \neq 0$ for the case case of the chiral non-abelian current (1.63) we obtain:

$$\langle \partial_\mu j_\mu^{5a}(x) P^a(0)\rangle = 2m\langle P^a(x)P^a(0)\rangle \tag{1.84}$$

Integrating the previous equation over the space we obtain:

$$\int d^3x \langle \partial_\mu j_\mu^{5a}(x) P^a(0)\rangle = 2m \int d^3x \langle P^a(x)P^a(0)\rangle \tag{1.85}$$

Applying the Gauss theorem to the space components of the integral we arrive to:

$$\partial_0 \int d^3x \langle j_0^{5a}(x) P^a(0)\rangle = 2m \int d^3x \langle P^a(x)P^a(0)\rangle \tag{1.86}$$

where the matrix element of $j_\mu^5(x)$ between the vacuum and an on-shell pions is normalized according to:

$$\langle 0|j_\mu^5(x)|\pi^b(p)\rangle = -ip_\mu F_\pi \delta^{ab} e^{-ipx} \tag{1.87}$$

and F_π is a constant with the dimension of (mass)^1, known as the *pion decay constant*[3] Using eq. (1.87) in eq. (1.86) we obtain:

$$M_\pi |\langle 0|j_0^{5a}(0)|\pi\rangle||\langle\pi|P^a(0)|0\rangle| = 2m|\langle 0|P^a(0)|\pi\rangle|^2 \tag{1.88}$$

thus

$$M_\pi |\langle 0|\partial_0 j_0^{5a}(0)|\pi\rangle| = 2m|\langle\pi|P^a(0)|\pi\rangle| \tag{1.89}$$

and

$$M_\pi^2 F_\pi = 2m|\langle\pi|P^a(0)|\pi\rangle|. \tag{1.90}$$

We obtain the following relation for P^a:

$$|\langle 0|P^a(0)|\pi\rangle| = \frac{M_\pi^2 F_\pi}{2m} \tag{1.91}$$

and finally we can write:

$$\lim_{m\to 0} \frac{2m}{M_\pi} \frac{M_\pi^4 F_\pi}{4m^2} = \lim_{m\to 0} -\frac{1}{N_f}\langle\bar\psi\psi\rangle \tag{1.92}$$

We arrive at the following formula:

$$M_\pi^2 = \frac{2m\Sigma}{F^2} + \mathcal{O}(m^2) \tag{1.93}$$

where we used the definition of the condensate Σ given in eq. (1.78), and we omitted higher order corrections in m. We also defined

$$\lim_{m\to 0} F_\pi = F \tag{1.94}$$

[3]The value of F_π can be determined from the π^+ decay through the weak interactions and one can find that $F_\pi = 92.4$ MeV

In case of non-degenerate masses we would have obtained:

$$M_\pi^2 = \frac{\Sigma}{F^2}(m_u + m_d) + \mathcal{O}\left(m_{u,d}^2\right) \tag{1.95}$$

also known as *Gell-Mann–Oakes–Renner relation* [10] or GMOR. The GMOR relation (1.93) clarifies the meaning of the following claims:

- the pions (and, in case of three light flavors, the kaons and the η meson) are, in the chiral limit, i.e. when $m_u, m_d, m_s = 0$, the Goldstone boson of the spontaneously broken chiral symmetry, in fact in this case eq. (1.93) gives $M_\pi = 0$;
- since the u, d and s quarks are light with respect to the Λ_{QCD} scale, i.e. $m_{u,d,s} \ll \Lambda_{QCD}$, we can say that the chiral symmetry is only approximate, so that the octet mesons are only approximate Goldstone bosons, in this case eq. (1.93) establish that $M_\pi^2 \propto m_q$.
- Using current algebra and pion pole dominance, Weinberg showed in 1966 [11] that chiral symmetry fully determines the interaction among pions of low energy, in terms of the pion decay constant: at leading order in the expansion in powers of the pion momenta and the pion mass, the amplitude of the elastic collision $\pi + \pi \to \pi + \pi$ can be expressed in terms of the function:
$$A(s,t,u) = \frac{s - M_\pi^2}{F_\pi^2} + \ldots \tag{1.96}$$
where s, t, u are the Mandelstam variables of the reaction. At low energies, the pions only interact weakly: if the relative velocity of the incoming particles tends to zero, the square of the center of mass energy, s, approaches $4M_\pi^2$, so that $A(s,t,u)$ tends to $3M_\pi^2/F_\pi^2$ and hence disappears in the chiral limit thus at zero energy, Nambu-Goldstone bosons behave like free particles.

1.4 Anomalous Ward Identities

We analyze in the following section the case of the anomalous axial singlet Ward identity which gives an explanation of the origin of the mass of the η' meson, then we will discuss the Witten–Veneziano formula that, with some important differences, plays for the η' the role that eq. (1.93) plays for the octet mesons.

We now study the anomalous version of the Ward identities obtained above. In QFT the fundamental object is the generating functional of the Green functions, this generator can be written as a path integral with the classical action in it. When the classical action is invariant under a given symmetry we would expect this symmetry and the subsequent classical conservation laws to be preserved also at the quantum level. Nevertheless it can happen that the integral measure, is not invariant under the same transformation. This situation is verified for chiral transformations, giving rise to the *chiral anomaly*.

As we said after eq. (1.70), at a classical level a transformation which is a symmetry of the action leaves the physics invariant, i.e. performing the change:

$$\begin{aligned} \psi &\to \psi' \approx \psi + \delta\psi \\ \bar{\psi} &\to \bar{\psi}' \approx \bar{\psi} + \delta\bar{\psi} \end{aligned} \tag{1.97}$$

leads to the following invariance:

$$\text{(classical symmetry)} \qquad S_F[\psi', \bar{\psi}'] = S_F[\psi, \bar{\psi}] \tag{1.98}$$

At the quantum level the object of interest is the path integral, if the transformation (1.97) leaves both the measure and the action invariant then the following invariance is implied:

$$\text{(QM symmetry)} \qquad \int \mathcal{D}\psi' \mathcal{D}\bar{\psi}' e^{-S_F[\psi', \bar{\psi}']} = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-S_F[\psi, \bar{\psi}]} \tag{1.99}$$

Performing the same calculations as in the previous we can arrive to the anomalous Ward identities, which can be written as:

$$\langle \delta S_F[\psi', \bar{\psi}'] \mathcal{O}[\psi', \bar{\psi}'] \rangle = \langle \delta \mathcal{O}[\psi', \bar{\psi}'] \rangle + \langle Q \mathcal{O}[\psi', \bar{\psi}'] \rangle \tag{1.100}$$

This is the case for chiral symmetry in the massless fermionic action: while still leaving the action invariant the chiral transformation transforms the measure of the generating functional in an anomalous way.

It can be shown that the anomaly is:

$$Q(x) = -\frac{g^2}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \operatorname{Tr}\{F_{\mu\nu} F_{\rho\sigma}\} \tag{1.101}$$

1.5 The Witten–Veneziano Formula

We derive in the following section the Witten–Veneziano formula which relates the mass of the η' particle with the topological charge Q. In our treatment we follow closely [17].

The topological charge is given by:

$$Q = \int d^4x Q(x) = \int d^4x \left[-\frac{g^2}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \operatorname{Tr}\{F_{\mu\nu} F_{\rho\sigma}\} \right] \tag{1.102}$$

The anomalous Ward identity reads:

$$\langle \partial_\mu j^5_\mu(x) q(0) \rangle = 2m \langle P(x) q(0) \rangle + 2N_f \langle q(x) q(0) \rangle \tag{1.103}$$

where, for simplicity, we assumed the case of degenerate masses $M = m \cdot \mathbb{1}$, and we have chosen $\mathcal{O}[\psi, \bar{\psi}] = q(x)$ as defined in eq. (1.102).

In the chiral limit ($m \to 0$) the Fourier transform of the above leads to:

$$\begin{aligned} ip_\mu \int d^4x e^{-ipx} \langle j^5_\mu(x) q(0) \rangle = \\ 2N_f \int d^4x e^{-ipx} \langle q(x) q(0) \rangle \equiv 2N_f \chi(p) \end{aligned} \tag{1.104}$$

We have defined the topological susceptibility:

$$\chi(x) = \int d^4x \langle q(x) q(0) \rangle \tag{1.105}$$

and its Fourier transform:

$$\chi(p) = \int d^4x e^{ipx} \langle q(x) q(0) \rangle \tag{1.106}$$

The absence of massless particles in the singlet pseudoscalar channel implies that:

$$\chi(0) = 0 \qquad \text{(full QCD, } m \to 0\text{)} \tag{1.107}$$

this relation says that the topological susceptibility is zero in the chiral limit:

$$\chi(0) = \langle q(x)q(0) \rangle = 0 \tag{1.108}$$

Now we introduce the parameter u, given by:

$$u = \frac{N_f}{N_c} \tag{1.109}$$

we are interested to study the case where:

$$u \to 0 \tag{1.110}$$

$$p \to 0 \tag{1.111}$$

i.e. the "large N_c" expansion ($N_c \to \infty$, keeping $g^2 N_c$ and N_f fixed) and the chiral ($p \to 0$) limit. The two limits above do not commute.

It can be shown that $\chi(p)$ can be written as:

$$\chi(p) = \chi(0) + \chi'(0)p^2 + \chi''(0)(p^2)^2 + I(p^2)^3 \tag{1.112}$$

where I is the dispersion integral involving the imaginary part of $\chi(p)$. In particular the contribution for η' can be written as:

$$I = \frac{R^2_{\eta'}}{(m^2_{\eta'})(p^2 + m^2_{\eta'})} + \tilde{I} \tag{1.113}$$

where $-R_{\eta'}$ is the residue at the η' pole which is negative in the Euclidean metric.

We then take the limit $u \to 0$, this consists in eliminating the contributions from the fermionic determinant, so we can write:

$$\lim_{u \to 0} \chi(p) = \chi(p)|_{\text{quenched}} \tag{1.114}$$

If in the r.h.s. of eq. (1.112), keeping p^2 fixed we write the contribution of η' in terms of powers of $\frac{m^2_{\eta'}}{p^2}$, if we suppose that

$$m^2_{\eta'} \propto \frac{N_f}{N_c} \tag{1.115}$$

hence $\frac{m^2_{\eta'}}{p^2} = \mathcal{O}\left(\frac{u}{p^2}\right)$, and thus we obtain:

$$\chi(0)\big|_{\text{quenched}} = \lim_{u \to 0} \frac{R^2_{\eta'}}{m^2_{\eta'}} \tag{1.116}$$

from the previous equations, if we assume that the quantities on the r.h.s. are finite when $u \to 0$ and we conclude that:

$$\frac{R^2_{\eta'}}{m^2_{\eta'}} = \chi(0)|_{\text{quenched}} + \mathcal{O}(u) \tag{1.117}$$

We have the following:

$$\langle 0|\partial_\mu j^5_\mu|\eta'\rangle = \sqrt{2N_f}F_{\eta'}m^2_{\eta'} \tag{1.118}$$

In the chiral limit:

$$2N_f\langle 0|Q|\eta'\rangle = \langle 0|\partial_\mu j^5_\mu|\eta'\rangle \tag{1.119}$$

and also the following relation holds:

$$R^2_{\eta'} = |\langle 0|Q|\eta'\rangle|^2 \tag{1.120}$$

So we obtain:

$$\left.\frac{R^2_{\eta'}}{m^2_{\eta'}}\right|_{u=0} = \left.\frac{F^2_{\eta'}m^2_{\eta'}}{2N_f}\right|_{u=0} = \left.\frac{F^2_\pi m^2_{\eta'}}{2N_f}\right|_{u=0} \tag{1.121}$$

we recall that $F_\pi = \mathcal{O}(\sqrt{N_c})$ and then:

$$\left.\frac{R^2_{\eta'}}{m^2_{\eta'}}\right|_{u=0} = \mathcal{O}(1) \tag{1.122}$$

We finally obtain the following relation:

$$m^2_{\eta'} = \frac{2N_f}{F^2_\pi}\chi^{\mathrm{YM}}(0) + \mathcal{O}(u^2) \tag{1.123}$$

which is the *Witten–Veneziano formula* for the η' mass.

Some comments to eq. (1.123) are in order:

- reminding that the topological susceptibility is $\chi^{\mathrm{YM}} = \mathcal{O}(1)$ and $F = \mathcal{O}(\sqrt{N_c})$ thus $m_{\eta'} \propto \frac{N_f}{N_c}$ we can verify with eq. (1.123) that the assumption made in eq. (1.115) is valid.
- in the chiral limit, $m \to 0$ eq. (1.123) shows that in the large N_c limit, $m_{\eta'} \to 0$ and the η' meson is a Goldstone boson.
- the analogy between the topological susceptibility in eq. (1.123) and the condensate in eq. (1.93) is not complete. In fact, as we said after eq. (1.93), the condensate Σ and the pion decay constant F_π describe the pion-pion scattering at all orders, in case of multi-pion scattering (e.g. $4\pi \to 4\pi$ and so on), these constants appear. Instead, in the scattering of multiple η' particles, higher momenta of the distribution of the topological charge appear.

In the context of large N_c expansion the higher momenta of the distribution of the topological charge can be studied, in particular the following result holds:

$$\frac{\langle Q^4\rangle^{\mathrm{YM}}_{\mathrm{con}}}{\langle Q^2\rangle^{\mathrm{YM}}} \propto \frac{1}{N_c^2} \tag{1.124}$$

and more generally the normalized cumulants should scale asymptotically as N_c^{2-2n} (where $n = 1, 2, \dots$) [12].

1.6 The Dilute Instanton Gas

In 1976 't Hooft proposed a solution for the $U(1)_A$ problem based on the use of instantons [15]. An instanton is a solution of the equations of motion of the classical field theory on a Euclidean spacetime with a finite, non-zero action. In such a theory, solutions to the equations of motion may be thought of as extremes the action.

Approximating the action in the factorized form:

$$S_G = (n + \bar{n})S_0 \tag{1.125}$$

where n is the number of instantons and $\bar{n}$ is the number of anti-instantons of the system and

$$S_0 = \frac{8\pi^2}{g^2} \tag{1.126}$$

Using the Atiyah–Singer index theorem the topological charge of the system can be defined as:

$$\nu = n - \bar{n} \tag{1.127}$$

With these definitions we can write the partition function of the system as:

$$Z[\theta] = \frac{1}{Z[0]} \sum_{n,\bar{n}} e^{i\theta(n-\bar{n})} e^{-(n+\bar{n})S_0} \int \mathcal{D}A_\mu \delta(N - n)\delta(\bar{N} - \bar{n}) \tag{1.128}$$

Putting this system in a large box with side of length L, in the dilute gas approximation, i.e. requesting that instantons have a small radius and are separated we have that:

$$\int \mathcal{D}A_\mu \delta(N - n)\delta(\bar{N} - \bar{n}) = \frac{(KVT)^{(n+\bar{n})}}{n!\bar{n}!} \tag{1.129}$$

where $V = L^3$ So we can write:

$$Z[\theta] = e^{VT\left(2Ke^{-S_0}\right)\cos\theta} \tag{1.130}$$

which can be written equivalently:

$$Z[\theta] = e^{-F[\theta]} \tag{1.131}$$

with:

$$F[\theta] = -VT\left(2Ke^{-S_0}\right)\cos\theta \tag{1.132}$$

It can be shown [15] that the following relations hold:

$$\frac{\langle Q^n \rangle_{\text{con}}}{VT} = (-i)^n \frac{d^n}{d\theta^n}\left[-\frac{F[\theta]}{VT}\right] \tag{1.133}$$

then we have arrive to the following results:

$$\frac{\langle Q^2 \rangle}{VT} = 2e^{-S_0} K \cos\theta \tag{1.134}$$

$$\frac{\langle Q^4 \rangle_{\text{con}}}{VT} = 2e^{-S_0} K \cos\theta \tag{1.135}$$

thus in this model the ratio between $\frac{\langle Q^2\rangle}{VT}$ and $\frac{\langle Q^4\rangle_{\text{con}}}{VT}$ is exactly:

$$\frac{\langle Q^4\rangle_{\text{con}}}{\langle Q^2\rangle} = 1 \qquad \forall\theta \tag{1.136}$$

In this model the quantity $2Ke^{-S_0}$ can be fixed to meson mass. Nevertheless the same quantity appear in the evaluation of higher order momenta of the distribution of the topological charge. In particular the prediction made in eq. (1.136) differs from the one made in eq. (1.124) in the setting of the large N_c expansion and the Witten–Veneziano formula.

1.7 Light Mesons

The presence of non-null quark masses has led us to eq. (1.93), in view of which the mesons of the octet are interpreted as the Goldstone bosons ensuing the spontaneous breaking of the axial generators.

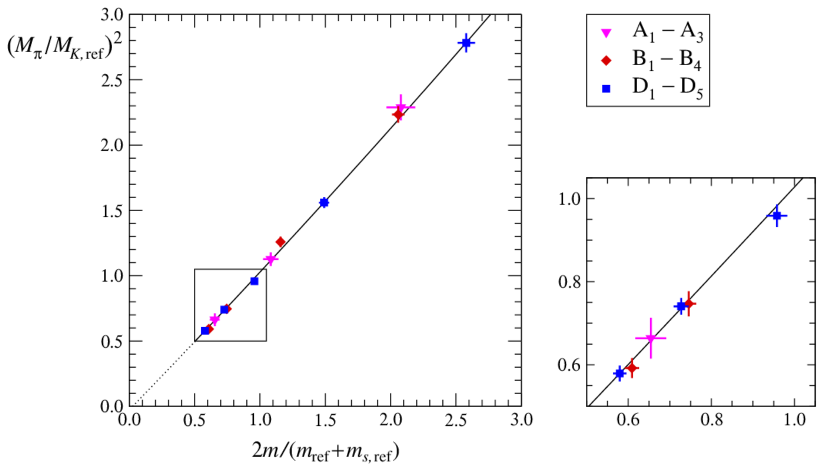

Figure 1.1: Dependence of the square of the pion mass M_π^2 on the sea-quark mass m. The solid curve is a quadratic least-squares fit (with constant term) of all data points, and the plot on the right is a blowup of the region enclosed by the little box. This plot is taken from Del Debbio et al. [18] (fig. 4).

Eq. (1.93) had a striking numerical confirmation in [18] from which fig. 1.1 is reported.

The linear proportionality expected by the GMOR relation is thus verified and the logic of the reasoning can be reversed: if the GMOR relation holds then the quark masses must be small with respect to Λ_{QCD}. This picture explains correctly why the mesons of the octet have smaller masses than the nucleons.

In the massless case the Lagrangian possess also the $U(1)_A$ symmetry, which should imply a parity doubling [19] in the hadronic spectrum, where any particle should possess a chirality quantum number and a chiral partner, with equal quantum numbers but opposite parity. Such doubling is not observed but on the other hand a broken $U(1)_A$ symmetry would imply the existence of a ninth Goldstone boson.

It can be argued that the η' is thus the required particle, arising from the breakdown of the chiral axial symmetry, but it is considerably heavier than the pion, whilst it should have a compable mass. This limit can be made more explicit, in fact in 1975 Weinberg showed [19] that the following limit on the candidate Goldstone boson mass should hold:

$$m_{\eta'} \leq \sqrt{3} m_\pi \tag{1.137}$$

thus a broken $U(1)_A$ would require a neutral pseudoscalar spinless boson with mass less than $\sqrt{3}m_\pi$. Using the masses reported in table (1.1) it can be seen that this inequality does not hold for the η' meson, thus it can not be the aforementioned Goldstone boson.

This problem has become known in literature as the $U(1)$ problem [13, 14, 19]. In this chapter we have shown that the Witten–Veneziano formula and the dilute instanton model propose two different mechanisms to explain the value of the η' mass.

I	I_3	S	Meson	Quark content	Mass (MeV)
1	-1	0	π^-	$d\bar{u}$	140
1	1	0	π^+	$u\bar{d}$	140
1	0	0	π^0	$d\bar{d} - u\bar{u}/\sqrt{2}$	135
$\frac{1}{2}$	$\frac{1}{2}$	$+1$	K^+	$u\bar{s}$	494
$\frac{1}{2}$	$-\frac{1}{2}$	$+1$	K^0	$d\bar{s}$	498
$\frac{1}{2}$	$-\frac{1}{2}$	-1	K^-	$s\bar{u}$	494
$\frac{1}{2}$	$\frac{1}{2}$	-1	$\bar{K}^0$	$s\bar{d}$	498
0	0	0	η	$\cos\theta\eta_8 + \sin\theta\eta_0$	547
0	0	0	η'	$\cos\theta\eta_8 - \sin\theta\eta_0$	958

$$\eta_8 = (d\bar{d} + u\bar{u} - 2s\bar{s})/\sqrt{6}$$
$$\eta_0 = (d\bar{d} + u\bar{u} + s\bar{s})/\sqrt{3}$$
$$\theta \simeq -11^\circ$$

Table 1.1: The small masses of the mesons in the octet support the hypothesis that these particles are Goldstone bosons of the spontaneously broken chiral symmetry, but $m_{\eta'}$ can not be explained in this way. This has become known as the $U(1)_A$ problem.

Chapter 2

Lattice Field Theory

The natural framework to quantize the lattice theory is the path integral formalism; in this formulation the system takes the form of a classical four-dimensional statistical model. The gauge fields are treated as classical stochastic variables assigned to the points of the lattice and are associated to the links, while the matter fields are Grassman variables. In this analogy, the Euclidean action of the quantum field theory corresponds to the classical Hamiltonian of the statistical system and the mass of the lightest particle corresponds to the inverse of the correlation length.

The lattice furnishes a regularization of the theory by providing an ultraviolet cutoff proportional to the inverse lattice spacing and this is actually the only known non-perturbative regularization of quantum field theory.

The crucial question is whether the theory formulated on the lattice is well defined in the limit when the lattice spacing a is sent to zero. The physical continuum limit corresponds to holding the values of physical quantities fixed while letting $a \to 0$; the renormalization group equation describes how the parameters behave by changing the scale of the theory (in this case the lattice spacing). Since the theory is asymptotically free, the continuum limit is realized when the bare gauge coupling g_0 is sent to zero.

An important advantage of the lattice formulation is that the path integrals which correspond to expectation values of physical observables can be computed numerically via Monte Carlo simulations. The idea is to generate samples consisting of a large number of field configurations according to the Boltzmann distribution and to evaluate the observables as sample averages.

Since the first work by Creutz [20] on SU(2) this method was successfully applied to lattice pure gauge theories and in recent years to full QCD with two and three light flavors of dynamical fermions; during this period, increasing precision and reliability due to theoretical improvement of the techniques has been accompanied by an enhanced computing power.

In this chapter we review the discretization of a field theory on the lattice. We start with a naive discretization of the fermion field, which will lead us to the problem of the appearance of "fermion doublers" which are lattice artifact that possess no continuum counterpart, we will introduce then the Wilson action which solves the problem of doublers at the expense of breaking chiral symmetry explicitly. From this staring point we discuss the discretization of gauge fields on the lattice and then we introduce the Ginsparg–Wilson fermions, which allow to implement exact chiral symmetry on the lattice. The Nielsen–Ninomiya theorem is avoided asking a milder constrain on the anti-commutation relation between the Dirac operator and the γ_5 matrix.

2.1 Naive Discretization

Our treatment will follow closely that of [25].

The starting point is the continuum fermionic action, in its euclidean version:

$$S = \int d^4x \bar{\psi}(x)(\gamma_\mu \partial_\mu + M)\psi(x) \tag{2.1}$$

the fields transform under a global $SU(N_c)$ symmetry as:

$$\psi \to \psi'(x) = G\psi(x) \tag{2.2}$$
$$\bar{\psi} \to \bar{\psi}'(x) = \bar{\psi}(x)G^{-1} \tag{2.3}$$

where $G \in SU(N_c)$, and we can write $G = e^{i\Lambda}$ with $\Lambda \in \mathbf{su}(N_c)$.

The symmetry can be promoted to be local, introducing a quadrivector $A_\mu(x)$ and the covariant derivative:

$$D_\mu = \partial_\mu + igA_\mu \tag{2.4}$$

then the action becomes:

$$S_F = \int d^4x \bar{\psi}(x)(\gamma_\mu D_\mu + M)\psi(x) \tag{2.5}$$

and the fields ψ, $\bar{\psi}$ and A_μ transform under the gauge, $G(x) \in SU(N_c)$:

$$\psi \to \psi'(x) = G(x)\psi(x) \tag{2.6}$$
$$\bar{\psi} \to \bar{\psi}'(x) = \bar{\psi}(x)G(x)^{-1} \tag{2.7}$$
$$A_\mu \to A'_\mu(x) = G(x)A_\mu(x)G^{-1} + gG(x)\partial_\mu G^{-1}(x) \tag{2.8}$$

where every $G(x) \in SU(3)$ for each x, we can generalize the previous transformation to be $G(x) = e^{i\Lambda(x)}$ with $\Lambda(x) \in \mathbf{su}(3)$ for each x. The covariant derivate when gauge transformed becomes:

$$D_\mu \to D'_\mu = G(x)D_\mu G^{-1}(x) \tag{2.9}$$

The full action is given by:

$$S_{\text{QCD}} = \frac{1}{4}\int d^4x F_{\mu\nu}F_{\mu\nu} + \int d^4x \bar{\psi}(x)(D + m)\psi(x) \tag{2.10}$$

where $D = \gamma_\mu D_\mu$. The generating functional is given by:

$$Z[j, \eta, \bar{\eta}] = \int \mathcal{D}A\mathcal{D}\psi\mathcal{D}\bar{\psi} e^{-S_{\text{QCD}} - \int d^4x j^\mu A_\mu - \int d^4x (\bar{\eta}\psi + \bar{\psi}\eta)} \tag{2.11}$$

The Green functions of the theory are obtained differentiating with respect to the sources $j^\mu(x)$, $\eta(x)$ and $\bar{\eta}(x)$, where j^μ is a current and η and $\bar{\eta}$ are Grassman variables.

We now discretize the theory on the lattice, as in fig. 2.1, making the following requests:

- the lattice action has to be invariant under the same symmetry of the original theory (for QCD the gauge group is $SU(3)$);
- the lattice action should reproduce correctly the continuum action when the lattice spacing is sent to zero, i.e. $a \to 0$.

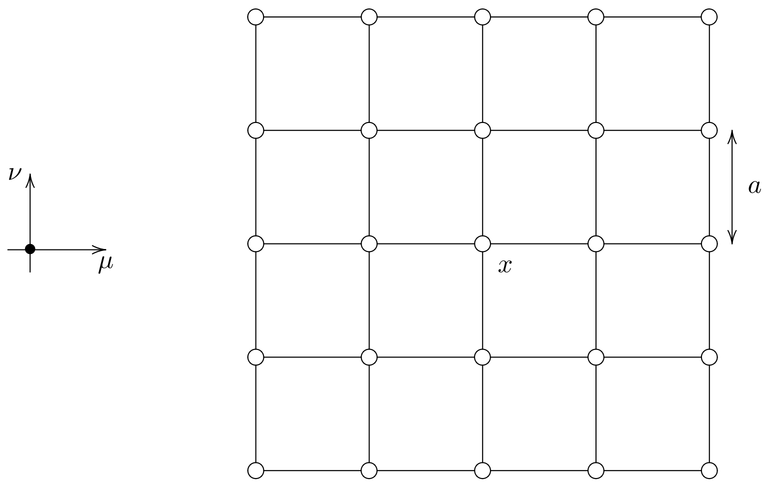

Figure 2.1: Lattice with spacing a.

The lattice spacing will be denoted with a and, where not otherwise noted, it should be set to one ($a = 1$), this factor can be reinserted in the formulas when needed using dimensional analysis. Every point on the 4-dimensional lattice can be labeled with a four-tuple of integers:

$$n \equiv (n_1, n_2, n_3, n_4) \tag{2.12}$$

where n_4 is the Euclidean time. We can perform now the following substitutions:

$$x_\mu \to n_\mu a \tag{2.13}$$

$$\psi_\alpha(x) \to \frac{1}{a^{3/2}} \hat{\psi}(na) \tag{2.14}$$

$$\bar{\psi}_\alpha(x) \to \frac{1}{a^{3/2}} \hat{\bar{\psi}}(na) \tag{2.15}$$

The integrals and the field integration measure become:

$$\int d^4x \to a^4 \sum_n \tag{2.16}$$

$$\mathcal{D}\psi\mathcal{D}\bar{\psi} \to \prod_{\alpha,n} d\hat{\psi}_\alpha(na) \prod_{\beta,m} d\hat{\bar{\psi}}_\beta(ma) \tag{2.17}$$

Dimensional analysis suggests to perform the following substitution for the mass term:

$$M \to \frac{1}{a}\hat{M} \tag{2.18}$$

and the derivatives become:

$$\partial_\mu \psi_\alpha(x) \to \frac{1}{a^{3/2}} \hat{\partial}_\mu \hat{\psi}_\alpha(n) \tag{2.19}$$

more explicitly the lattice derivative $\hat{\partial}_\mu$ is given by:

$$\hat{\partial}_\mu \hat{\psi}_\alpha(n) = \frac{1}{2}\left[\hat{\psi}_\alpha(n+\hat{\mu}) - \hat{\psi}_\alpha(n-\hat{\mu})\right] \tag{2.20}$$

where we use the notation $(n+\hat{\mu})$ as a shorthand for $(\dots, n_\mu + 1, \dots)$ given $n \equiv (\dots, n_\mu, \dots)$ where $\mu = 1, 2, 3, 4$. The lattice version of $S_F^{(\mathrm{eucl})}$ is:

$$S_F = \sum_{\substack{n,m \\ \alpha,\beta}} \bar{\hat{\psi}}_\alpha(n) K_{\alpha\beta}(m,n) \hat{\psi}_\beta(m) \tag{2.21}$$

with:

$$K_{\alpha\beta}(m,n) = \sum_\mu \frac{1}{2}(\gamma_\mu)_{\alpha\beta}\left[\delta_{m,n+\hat{\mu}} - \delta_{m,n-\hat{\mu}}\right] + \hat{M}\delta_{\mu\nu}\delta_{\alpha\beta} \tag{2.22}$$

The correlation functions are obtained in the following way:

$$\langle \hat{\psi}_\alpha(n) \dots \bar{\hat{\psi}}_\beta(m) \dots \rangle = \frac{\int \mathcal{D}\bar{\hat{\psi}} \mathcal{D}\hat{\psi} \; \hat{\psi}_\alpha(n) \dots \bar{\hat{\psi}}_\beta(m) \dots e^{-S_F}}{\int \mathcal{D}\bar{\hat{\psi}} \mathcal{D}\hat{\psi} \; e^{-S_F}} \tag{2.23}$$

where

$$\mathcal{D}\bar{\hat{\psi}} \mathcal{D}\hat{\psi} = \prod_{n,\alpha} \bar{\hat{\psi}}_\alpha(n) \prod_{m,\beta} \hat{\psi}_\beta(m). \tag{2.24}$$

We can derive these correlation functions directly from the generating functional:

$$Z[\eta, \bar{\eta}] = \int \mathcal{D}\bar{\hat{\psi}} \mathcal{D}\hat{\psi} e^{-S_F + J[\eta,\bar{\eta}]} \tag{2.25}$$

with

$$J[\eta, \bar{\eta}] = \sum_{n,\alpha} [\bar{\eta}_\alpha \hat{\psi}_\alpha(n) + \bar{\hat{\psi}}_\alpha(n) \eta_\alpha(n)] \tag{2.26}$$

It can be shown that integrating eq. 2.25 the following expression can be obtained:

$$Z[\eta, \bar{\eta}] = \det K e^{\sum_{n,m,\alpha,\beta}\left(\bar{\eta}_\alpha(n) K^{-1}_{\alpha,\beta}(n,m) \eta_\beta(m)\right)} \tag{2.27}$$

2.1.1 The Doubling Problem

The two-point correlation function is given by:

$$\langle \hat{\psi}_\alpha(n) \bar{\hat{\psi}}_\beta(m) \rangle = K^{-1}_{\alpha\beta}(n,m) \tag{2.28}$$

When the lattice spacing is sent to zero ($a \to 0$) the theory must reproduce correctly the physical theory, in particular in the free theory:

$$\langle \psi_\alpha(x) \bar{\psi}_\beta(y) \rangle = \lim_{a \to 0} \frac{1}{a^3} G_{\alpha\beta}\left(\frac{x}{a}, \frac{y}{a}; Ma\right) \tag{2.29}$$

where $G_{\alpha\beta}(n, m, \hat{M}) \equiv K^{-1}_{\alpha\beta}(n, m)$ and we have written explicitly the dependence from the mass. The following completeness relation holds:

$$\sum_{\lambda,l} K^{-1}_{\alpha\lambda}(n, l) K_{\lambda\beta}(l, m) = \delta_{\alpha\beta}\delta_{nm} \tag{2.30}$$

thus we arrive at the following limit:

$$\langle\psi_\alpha(x)\bar{\psi}_\beta(y)\rangle = \lim_{a\to 0} \int_{-\pi/a}^{\pi/a} \frac{d^4p}{(2\pi)^4} \frac{\left[-i\sum_\mu \gamma_\mu \tilde{p}_\mu + M\right]_{\alpha\beta}}{\sum_\mu \tilde{p}_\mu^2 + M^2} e^{ip(x-y)} \tag{2.31}$$

with

$$\tilde{p}_\mu = \frac{1}{a}\sin(p_\mu a) \tag{2.32}$$

Eq. 2.32 gives rise to the so-called *doubling problem*, in fact that equation, given periodic boundary conditions, admits two solutions at $x = 0$ and $x = \pm\frac{\pi}{a}$, see fig. 2.2.

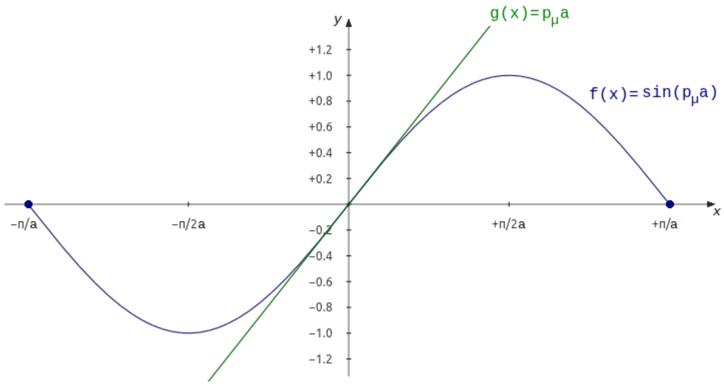

Figure 2.2: An illustration of the doubling problem arising from eq. 2.32 which admits two solutions (Points at $x = \pm\frac{\pi}{a}$ are identified imposing periodic boundary conditions).

In d dimensions we would have found 2^d solutions. The insurgence of this problem can be reconducted to the symmetric form of the derivative that we have chosen in eq. 2.20. More explicitly, we can rewrite eq. 2.31 as:

$$\langle\psi_\alpha(x)\bar{\psi}_\beta(y)\rangle = \sum_{\bar{p}} e^{ip(n-m)} \int_{-\pi/2a}^{\pi/2a} \frac{d^4p}{(2\pi)} \frac{\left[-i\sum_\mu \delta_{\bar{p}_\mu}\gamma^\mu \tilde{p}_\mu + M\right]_{\alpha\beta}}{\sum_\mu \tilde{p}_\mu^2 + M^2} e^{ip(x-y)} \tag{2.33}$$

where $x = na$, $y = ma$ and $\delta_{\bar{p}_\mu} = e^{i\bar{p}_\mu}$. The first summation runs over $\bar{p}$ given, in lattice units, by:

$$(0, 0, 0, 0)\ ;\ (\pi, 0, 0, 0)\ ;\ (\pi, \pi, 0, 0)\ ;\ (\pi, \pi, \pi, 0)\ ;\ (\pi, \pi, \pi, \pi) \text{ and permutations}$$

and we have 16 possibilities in total (i.e. 2^4 as expected). only the one given by $(0, 0, 0, 0)$ gives the correct continuum limits in fact the others all give a factor $(-1)^{n-m}$, which arise from the term $e^{i\bar{p}(n-m)}$.

2.2 Wilson Fermions

It is possible to obtain the correct continuum limit from different discretizations on the lattice, now we can use this ambiguity to modify the action:

$$S_F = \sum_{\substack{n,m \\ \alpha,\beta}} \bar{\hat{\psi}}_\alpha(n) K_{\alpha\beta}(n,m) \hat{\psi}_\beta(m) \tag{2.34}$$

with $K_{\alpha\beta}$ as in eq. (2.22). The purpose of our modification is to modify the poles in the denominator of eq. (2.33) to move them of an amount proportional to the inverse lattice spacing, in this way we will solve the doubling problem at cost of explicitly breaking chiral invariance. Let the Wilson action be:

$$S_F^{(\mathrm{W})} = S_F - \frac{r}{2} \sum_n \bar{\hat{\psi}}(n) \hat{\Box} \hat{\psi}(n) \tag{2.35}$$

where r is called *Wilson parameter* and the box operator is defined by:

$$\hat{\Box}\psi(\hat{n}) = \sum_\mu \left[\hat{\psi}(n+\hat{\mu}) + \hat{\psi}(n-\hat{\mu}) - 2\hat{\psi}(n) \right] \tag{2.36}$$

and

$$\Box \to a^2 \hat{\Box} \tag{2.37}$$

in this way we obtain:

$$S_F^{(\mathrm{W})} = \sum_{m,n} \bar{\hat{\psi}}_\alpha(n) K_{\alpha\beta}^{(\mathrm{W})}(n,m) \hat{\psi}_\beta(m) \tag{2.38}$$

with

$$K_{\alpha\beta}^{(\mathrm{W})}(n,m) = (\hat{M} + 4r)\delta_{nm}\delta_{\alpha\beta} - \frac{1}{2} \sum_\mu \left[(r-\gamma_\mu)_{\alpha\beta} \delta_{m,n+\hat{\mu}} + (r+\gamma_\mu)_{\alpha\beta} \delta_{m,n-\hat{\mu}} \right] \tag{2.39}$$

even in the massless case ($\hat{M} = 0$) this expression explicitly breaks the chiral symmetry. Computing the two point function we find that:

$$\langle \psi_\alpha(x) \bar{\psi}_\beta(y) \rangle = \lim_{a \to 0} \int_{-\pi/a}^{\pi/a} \frac{d^4p}{(2\pi)^4} \frac{[-i\gamma_\mu \tilde{p}_\mu + M(p)]_{\alpha\beta}}{\sum_\mu \tilde{p}_\mu^2 + M^2(p)} e^{ip(x-y)} \tag{2.40}$$

with

$$\tilde{p}_\mu = \frac{1}{a} \sin(p_\mu a) \tag{2.41}$$

and

$$M(p) = M + \frac{2r}{a} \sum_\mu \sin^2\left(\frac{p_\mu a}{2}\right) \tag{2.42}$$

That the doubling phenomenon must occur in a lattice regularization which respect the usual hermiticity, locality and translational invariance requirements follows from a theorem by Nielsen and Ninomiya, which will be analyzed in further detail in the following.

2.3 Gauge Fields on the Lattice

In this section we derive the form of the pure gauge term of the QCD action. In practice we need to find a way to write gauge transformations as eq. (2.6) on the lattice.

We start with the Wilson version of the fermionic action, inserting (2.39) in eq. (2.38) we obtain the following[1]:

$$S_F = (\hat{M}+4r)\sum_n \bar{\psi}(n)\psi(n) - \frac{1}{2}\sum_{n,\mu}[\bar{\psi}(n)(r-\gamma_\mu)\psi(n+\hat{\mu})+\bar{\psi}(n+\hat{\mu})(r+\gamma_\mu)\psi(n)] \tag{2.43}$$

where a summation over flavor indexes $a = 1, \ldots, N_f$ is intended.

On the lattice the global symmetry of eq. (2.2) becomes, with $G \in SU(N)$:

$$\psi(n) \to G\psi(n) \tag{2.44}$$

$$\bar{\psi}(n) \to \bar{\psi}(n)G^{-1} \tag{2.45}$$

Now the symmetry 2.44 has to be promoted to a local gauge symmetry, to do so we analyze how the bilinear $\bar{\psi}(x)\psi(y)$ transforms under a gauge transformation, in the continuum we have:

$$\psi(x)\psi(y) \to \bar{\psi}(x)G^{-1}(x)G(y)\psi(y) \tag{2.46}$$

where the problem of eq. (2.46) is that the gauge transformations are taken at different points thus a factor, known as *Schwinger line integral*, must be introduced. This term, under gauge transformation, must transform in the following way:

$$U(x,y) \to G(x)U(x,y)G^{-1}(y) \tag{2.47}$$

to compensate for the change in eq. (2.46), furthermore we need that $U(x,y) \in SU(N_f)$.

We can suppose that x and y are separated by a small distance ε, then the bilinear must be modified as follows:

$$\bar{\psi}(x)\psi(x+\varepsilon) \to \bar{\psi}(x)U(x,x+\varepsilon)\psi(x+\varepsilon)\bar{\psi}(x+\varepsilon)\psi(x) \to \bar{\psi}(x+\varepsilon)U^\dagger(x,x+\varepsilon)\psi(x) \tag{2.48}$$

where $U(x, x+\varepsilon)$ can be written as:

$$U(x,x+\varepsilon) = e^{ig\varepsilon\cdot A(x)} \tag{2.49}$$

and $\varepsilon \cdot A(x) = \sum_\mu \varepsilon_\mu A_\mu$.

These considerations suggest to make the following changes to eq. (2.43) to arrive at a gauge-invariant expression:

$$\begin{aligned} \bar{\psi}(n)(r-\gamma_\mu)\psi(n+\hat{\mu}) &\to \bar{\psi}(n)(r-\gamma_\mu)U_{n,n+\hat{\mu}}\psi(n+\hat{\mu}) \\ \bar{\psi}(n+\hat{\mu})(r+\gamma_\mu)\psi(n) &\to \bar{\psi}(n+\hat{\mu})(r+\gamma_\mu)U_{n+\hat{\mu},n}\psi(n) \end{aligned} \tag{2.50}$$

where the following relation holds:

$$U_{n+\hat{\mu},n} = U^\dagger_{n,n+\hat{\mu}} \tag{2.51}$$

[1]We drop the superscript W, since hereinafter we will always use the Wilson action. We also drop the hat from lattice fields for simplicity.

and $U_{n+\hat{\mu},n} \in SU(N_f)$.

The discretized version of $U(x,y)$ can then be written as:

$$U_{n+\hat{\mu},n} = e^{i\phi_\mu(n)} \tag{2.52}$$

where is a matrix belonging to the Lie algebra of $SU(3)$, i.e. $\phi_\mu(n) \in \mathbf{su}(3)$.

The quantities $U_{n,n+\hat{\mu}}$, $U^\dagger_{n,n+\hat{\mu}}$ in fig. 2.3 are defined between two neighboring lattice sites, for this reason they are referred as *links*.

Figure 2.3: Links among the lattice sites x and $x+\widehat{\mu}$.

We can introduce for the links the following notation:

$$U_\mu(n) \equiv U_{n,n+\hat{\mu}} = e^{igaA_\mu(n)} \tag{2.53}$$

where in the continuum limit $aA_\mu(n)$ becomes the gauge field $A_\mu(x)$.

Thus the gauged version of eq. (2.43) is:

$$\begin{aligned} S_F = {} & (\hat{M}+4r)\sum_n \bar{\psi}(n)\psi(n) + \\ & - \frac{1}{2}\sum_{n,\mu}[\bar{\psi}(n)(r-\gamma_\mu)U_\mu(n)\psi(n+\hat{\mu}) + \\ & + \bar{\psi}(n+\hat{\mu})(r+\gamma_\mu)U^\dagger_\mu(n)\psi(n)] \end{aligned} \tag{2.54}$$

which is invariant under a gauge transformation, which is now implemented on the lattice as:

$$\psi(n) \to G(n)\psi(n) \tag{2.55}$$

$$\bar{\psi}(n) \to \bar{\psi}(n)G^{-1}(n) \tag{2.56}$$

$$U_\mu(n) \to G(n)U_\mu(n)G^{-1}(n+\hat{\mu}) \tag{2.57}$$

$$U^\dagger_\mu(n) \to G(n+\hat{\mu})U^\dagger_\mu(n)G^{-1}(n) \tag{2.58}$$

We have to define a discretized version of the field tensor $F_{\mu\nu}$, to do so we need to build a gauge invariant quantity, using the links as building blocks. The gauge-invariant product of links involving the least number of links is:

$$U_{\mu\nu}(n) = U_\mu(n)U_\nu(n+\hat{\mu})U^\dagger_\nu(n+\hat{\nu})U^\dagger_\nu(n). \tag{2.59}$$

The quantity in eq. (2.59) is called a “plaquette” (see fig. 2.4) around lattice point n. Since the group $SU(N_c)$ to which the links belong is not abelian the order in which the link are traversed is important.

In a similar way to eq. (2.53) for the plaquette we can write:

$$U_{\mu\nu}(n) = e^{iga^2\mathcal{F}_{\mu\nu}(n)} \tag{2.60}$$

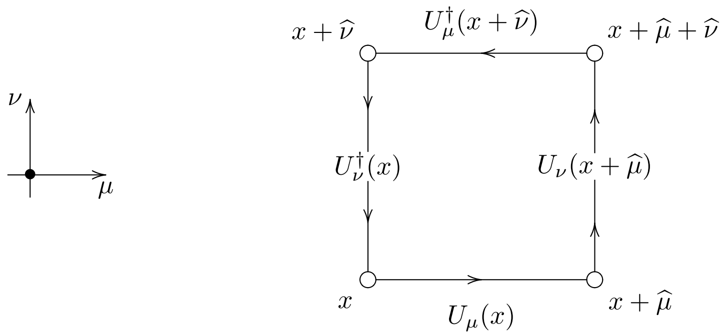

Figure 2.4: A plaquette $U_{\mu\nu}(x) \equiv U_P$ is defined, as in eq. (2.59), as the product of four links.

and in the continuum limit $\mathcal{F}_{\mu\nu}(n)$ can be shown to reduce to the correct continuum expression of the field strength:

$$\mathcal{F}_{\mu\nu} \underset{a\to 0}{\longrightarrow} F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + ig[A_\mu, A_\nu] \tag{2.61}$$

More explicitly, on the lattice the field tensor can defined as:

$$F_{\mu\nu}(n) = \frac{1}{4}\mathcal{P}\{Q_{\mu\nu}(n)\} \tag{2.62}$$

where $\mathcal{P}$ projects any 3×3 matrix to $\mathbf{su}(3)$:

$$\mathcal{P}\{M\} = \frac{1}{2}(M - M^\dagger) - \frac{1}{6}\,\mathrm{Tr}\{M - M^\dagger\} \tag{2.63}$$

and $Q_{\mu\nu}(n)$ is defined as:

$$\begin{aligned} Q_{\mu\nu}(n) = {} & U_\mu(n)U_\nu(n+\hat{\mu})U_\mu(n+\hat{\nu})^\dagger U_\nu(n)^\dagger + \\ & + U_\nu(n)U_\mu^\dagger(n-\hat{\mu}+\hat{\nu})U_\nu^\dagger(n-\hat{\mu})U_\mu(n-\hat{\mu}) + \\ & + U_\mu^\dagger(n-\hat{\mu})U_\nu^\dagger(n-\hat{\mu}-\hat{\nu})U_\mu(n-\hat{\mu}-\hat{\nu})U_\nu(n-\hat{\nu}) + \\ & + U_\nu^\dagger(n-\hat{\nu})U_\mu(n-\hat{\nu})U_\nu(n+\hat{\mu}-\hat{\nu})U_\mu^\dagger(n). \end{aligned} \tag{2.64}$$

For small lattice spacing the following approximation can be shown to hold:

$$\mathrm{Tr}\left\{\sum_n \sum_{\substack{\mu,\nu \\ \mu<\nu}} \left[1 - \frac{1}{2}(U_{\mu\nu}(n) + U_{\mu\nu}^\dagger(n))\right]\right\} \approx \frac{1}{4}\sum_{\substack{\mu,\nu \\ \mu<\nu}} a^4 F_{\mu\nu}(n)F_{\mu\nu}(n) \tag{2.65}$$

thus we can define:

$$S_G = c\,\mathrm{Tr}\left\{\sum_n \sum_{\substack{\mu,\nu \\ \mu<\nu}} \left[1 - \frac{1}{2}(U_{\mu\nu}(n) + U_{\mu\nu}^\dagger(n))\right]\right\}. \tag{2.66}$$

The action (2.66) has continuum limit:

$$S_G \to c\frac{g^2}{2} S_G^{(\mathrm{cont})} \tag{2.67}$$

thus we have to choose:

$$c = \frac{2}{g^2} \tag{2.68}$$

Introducing the quantity:

$$\beta = \frac{2N}{g^2} \tag{2.69}$$

we can finally write:

$$S_G^{(SU(N))} = \beta \sum_P \left[1 - \frac{\mathrm{Tr}}{2N} \left\{(U_P(n) + U_P^\dagger(n))\right]\right\} \tag{2.70}$$

where we have written the sum U_P is the product of the link composing a plaquette, as in fig. 2.4, and the sum runs over all plaquettes P.

We can now write the full action for QCD on the lattice, for the case $N_c = 3$, as:

$$S_{\mathrm{QCD}} = S_G[U] + S_F^{(\mathrm{W})}[U, \psi, \bar{\psi}] \tag{2.71}$$

where

$$S_G[U] = \frac{6}{g^2} \sum_P \left[1 - \frac{\mathrm{Tr}}{6}(U_p + U_P^\dagger)\right] \tag{2.72}$$

and

$$\begin{aligned} S_F^{(\mathrm{W})}[U, \psi, \bar{\psi}] = (\hat{M} + 4r) \sum_n \bar{\psi}(n)\psi(n) + \\ - \frac{1}{2} \sum_{n,\mu} [\bar{\psi}(n)(r - \gamma_\mu) U_\mu(n) \psi(n + \hat{\mu}) + \\ + \bar{\psi}(n + \hat{\mu})(r + \gamma_\mu) U_\mu^\dagger(n) \psi(n)]. \end{aligned} \tag{2.73}$$

2.3.1 Explicit form of the Wilson Action

In this section we write a more explicit form of the gauge term (2.72) of the Wilson action on the lattice for a non-abelian $SU(3)$ gauge theory, since we need it in the next chapter to define the Wilson Flow. Furthermore in this section we will label the lattice sites with x instead of the usual n.

Starting from:

$$S_W^{(SU(N_c))} = \beta \sum_P \left[1 - \frac{\mathrm{Tr}}{2N_c} \left(U_P + U_P^\dagger\right)\right] = \beta \sum_P \left[1 - \frac{\Re}{N_c} \left\{ \mathrm{Tr}(U_P) \right\}\right] \tag{2.74}$$

For $N_c = 3$, also setting $\beta = \dfrac{6}{g_0^2}$, this becomes:

$$\begin{aligned} S_W^{(SU(3))} &= \frac{6}{g_0^2} \sum_x \sum_{\substack{\mu,\nu \\ \mu<\nu}} \left[1 - \frac{\mathrm{Tr}}{6} \left\{ U_{\mu\nu}(x) + U_{\mu\nu}^\dagger(x) \right\}\right] = \\ &= \frac{6}{g_0^2} \sum_x \sum_{\substack{\mu,\nu \\ \mu<\nu}} \left[1 - \frac{\mathrm{Tr}}{6} \left\{ U_\mu(x) U_\nu(x + \widehat{\mu}) U_\nu^\dagger(x + \widehat{\nu}) U_\nu^\dagger(x) + \right.\right. \\ &\left.\left. + U_\nu(x) U_\mu(x + \widehat{\nu}) U_\nu^\dagger(x + \widehat{\mu}) U_\mu^\dagger(x) \right\}\right] \end{aligned} \tag{2.75}$$

where we have written the plaquette U_P as defined before; $U_P^\dagger$ is given by:

$$U_{\mu\nu}^\dagger = U_\nu(x) U_\mu(x + \widehat{\nu}) U_\nu^\dagger(x + \widehat{\mu}) U_\mu^\dagger(x). \tag{2.76}$$

2.4 Ginsparg-Wilson Fermions

As introduced before, the Nielsen–Nynomiya theorem, also known as no-go theorem, states that on the lattice for a Dirac operator the following properties can not hold simultaneously [26, 27]:

1. $D(x)$ is local, i.e. it is limited by $Ce^{-\gamma|x|}$ for some γ;
2. $\hat{D}(p) = i\gamma_\mu p_\mu + \mathcal{O}(ap^2)$ for $p \ll \frac{\pi}{a}$;
3. $\hat{D}(p)$ is invertible for $p = 0$, i.e. no doublers arise;
4. $\gamma_5 D + D\gamma_5 = 0$;

where $\hat{D}(p)$ is the Fourier transform of $D(x)$.

This theorem seems to leave no possibility for the implementation of chiral symmetry on the lattice, but it turns out that it is possible to break standard chiral symmetry in a controlled way; this possibility has been proposed by Ginsparg and Wilson in 1982 [25] and the ensuing formulation is nowadays known as *Ginsparg-Wilson (GW) fermions.*

For GW fermions the fermionic action is of the form:

$$S_F = \sum_{x,y} \bar{\psi}(x)(D(x,y) + M\delta_{xy})\psi(y) \tag{2.77}$$

where the Dirac operator $D(x,y)$ is 4×4 matrix in Dirac space which breaks the standard chiral symmetry and, since the lattice action must possess the correct continuum limit, when $a \to 0$ $D(x,y)$ becomes the usual continuum Dirac operator.

While in the continuum, or in a naive discretization, the Dirac operator anticommutes with γ_5, the GW-Dirac operator satisfies the following relation:

$$\gamma_5 D + D\gamma_5 = aD\gamma_5 RD \tag{2.78}$$

where R is an Hermitian non-singular operator [22] which is local on position space and proportional to the unit matrix in Dirac space. For our purposes we can set $R = \mathbb{1}$ and rewrite eq. (2.78) as:

$$\{\gamma_5, D\} = aD\gamma_5 D \tag{2.79}$$

The following relation also holds:

$$\{\gamma_5, D^{-1}\} = a\gamma_5 \tag{2.80}$$

A Dirac operator satisfying the GW relation alone however does not ensure the absence of species doubling. Any matrix of the form:

$$D = \frac{1}{a}(1 - V) \tag{2.81}$$

where the matrix V satisfies the following properties:

$$\begin{aligned} V^\dagger V &= \mathbb{1} \\ V^\dagger &= \gamma_5 V \gamma_5 \end{aligned} \tag{2.82}$$

solves the GW relation. It was only in 1998 that an explicit expression for D was given that is free of doublers and local [28, 29, 30]. It also satisfies an exact index theorem [31, 32] a lattice version of the Atiyah-Singer index theorem. In the continuum the Dirac operator for massless fermions in a smooth background field carrying non-vanishing topological charge Q possess left- and right- handed zero modes. The difference $n_L - n_R$ equals the topological charge of the background field. The Neuberger solution is obtained by choosing:

$$V = A(A^\dagger A)^{-\frac{1}{2}} \tag{2.83}$$

with

$$A = 1 - aK^{(\mathrm{W})} \tag{2.84}$$

where $K^{(\mathrm{W})}$ is the Wilson-Dirac operator defined in eq. 2.39.

Thus the decomposition into left- and right-handed components can be adapted to the lattice, we define a new couple of projectors:

$$\hat{P}_R = \frac{1+\hat{\gamma}_5}{2}\psi \qquad \hat{P}_L = \frac{1-\hat{\gamma}_5}{2} \tag{2.85}$$

where $\hat{\gamma}_5$ is given by:

$$\hat{\gamma}_5 = \gamma_5(1 - aD) \tag{2.86}$$

Using eq. (2.79) one can verify the following properties:

$$\hat{\gamma}_5^\dagger = \hat{\gamma}_5 \qquad \hat{\gamma}_5^2 = 1 \tag{2.87}$$

and thus the usual relations among the new projectors hold:

$$\begin{aligned} \hat{P}_R^2 &= \hat{P}_R \\ \hat{P}_L^2 &= \hat{P}_L \\ \hat{P}_R\hat{P}_L &= \hat{P}_L\hat{P}_R = 0 \\ \hat{P}_L + \hat{P}_R &= 1 \end{aligned} \tag{2.88}$$

and

$$\begin{aligned} D\hat{P}_R &= P_L D \\ D\hat{P}_L &= P_R D \end{aligned} \tag{2.89}$$

We can now define on the lattice the left- and right-handed components of the field:

$$\begin{aligned} \psi_R &= \hat{P}_R\psi \qquad & \psi_L &= \hat{P}_L\psi \\ \bar{\psi}_R &= \bar{\psi}P_L \qquad & \bar{\psi}_L &= \bar{\psi}P_R \end{aligned} \tag{2.90}$$

and, as before, the action can be decomposed into a left- and a right-handed part:

$$\bar{\psi}D\psi = \bar{\psi}_L D\psi_L + \bar{\psi}_R D\psi_R \tag{2.91}$$

and the mass term breaks the chiral symmetry:

$$M(\bar{\psi}_R\psi_L + \bar{\psi}_L\psi_R) = M\bar{\psi}(P_L\hat{P}_L + P_R\hat{P}_R)\psi = M\bar{\psi}\left(1 - \frac{a}{2}D\right)\psi \tag{2.92}$$

One important difference is that in the continuum chirality is a strictly local concept where the projectors involve a single spacetime point x. On the lattice, instead, the projectors contain the Dirac operator D and consequently the chirality of a lattice fermion is determined using informations from the gauge field and from neighboring lattice sites.

The GW action posses an exact chiral symmetry which differs from the standard chiral symmetry (1.35), but it is possible to define a modified symmetry which allows to study the regime of small quark masses and resolves the general problem of putting chiral gauge theories on the lattice. This symmetry is given by the following transformation:

$$\begin{aligned} \psi &\to \psi'(x) = e^{i\beta\hat{\gamma}_5}\psi(x) \\ \bar{\psi} &\to \bar{\psi}'(x) = \bar{\psi}(x)e^{i\beta\gamma_5} \end{aligned} \tag{2.93}$$

The infinitesimal transformations are:

$$\begin{aligned} \delta\psi &= \psi' - \psi = i\beta\hat{\gamma}_5\psi(x) \\ \delta\bar{\psi} &= \bar{\psi}' - \bar{\psi} = i\beta\bar{\psi}(x)\gamma_5 \end{aligned} \tag{2.94}$$

The Lagrangian density for massless fermions is invariant under the transformation 2.93:

$$\begin{aligned} \delta\mathcal{L} &= \mathcal{L}[\psi', \bar{\psi}'] - \mathcal{L}[\psi, \bar{\psi}] = \bar{\psi}' D\psi' = \\ &= \delta\bar{\psi} D\psi + \bar{\psi} D\delta\psi = \\ &= i\beta\bar{\psi}(x)\gamma_5 D\psi(x) + i\beta\bar{\psi}(x)D\hat{\gamma}_5\psi = \\ &= i\beta\bar{\psi}(x)\gamma_5 D\psi(x) - i\beta\bar{\psi}(x)\gamma_5 D\psi = 0 \end{aligned} \tag{2.95}$$

where we have made use of the relation:

$$D\hat{\gamma}_5 = -\gamma_5 D \tag{2.96}$$

which is a rewriting of (2.79).

Chapter 3

The fourth cumulant of the topological charge

3.1 The Axial Singlet Anomalous Ward Identity on the Lattice

We now have a formulation of quantum chromodynamics on the lattice which:

1. reproduces the correct continuum limit;
2. is gauge invariant;
3. has a local Dirac operator;
4. is free of doublers;

moreover, thanks to the Ginsparg-Wilson relation (2.78) we are able to define the chiral component of the fields and to restore explicitly the chiral symmetry on the lattice.

It can be proven [25] that any lattice discretization with the properties 1-4 enumerated above reproduces the axial anomaly in the continuum limit.

We can recover the anomaly à la Fujikawa [41, 42], i.e. from the non-trivial Jacobian resulting from the change in the integration measure of the functional integral when applying a global axial singlet symmetry transformation.

We can write the singlet axial rotation transform as:

$$\begin{pmatrix} \psi' \\ \bar{\psi}' \end{pmatrix} = \begin{pmatrix} e^{i\beta(x)\hat{\gamma}_5} & 0 \\ 0 & e^{i\beta(x)\gamma_5} \end{pmatrix} \begin{pmatrix} \psi \\ \bar{\psi} \end{pmatrix} \tag{3.1}$$

We have that the following relation holds:

$$\mathcal{D}\bar{\psi}'\mathcal{D}\psi' \to \mathcal{D}\bar{\psi}'\mathcal{D}\psi' \equiv \mathcal{J}[\beta]^{-1}\mathcal{D}\bar{\psi}\mathcal{D}\psi \tag{3.2}$$

where $\mathcal{J}[\beta]$ in the Jacobian of the transformation $\psi \to \psi', \bar{\psi} \to \bar{\psi}'$. In eq. (3.2) the inverse Jacobian appears because ψ,$\bar{\psi}$ are Grassman variables.

Using the matrix form defined above we can write:

$$\prod_{x,c,s,f} d\psi'(x)d\bar{\psi}'(x) = \left[\det \begin{pmatrix} e^{i\beta(x)\hat{\gamma}_5} & 0 \\ 0 & e^{i\beta(x)\gamma_5} \end{pmatrix}\right]^{-1} \prod_{x,c,s,f} d\psi(x)d\bar{\psi}(x) \tag{3.3}$$

and we obtain:

$$\prod_{x,c,s,f} d\psi'(x)d\bar{\psi}'(x) = e^{-i\beta(x)\,\mathrm{Tr}\{\hat{\gamma}_5\}N_f} \prod_{x,c,s,f} d\psi(x)d\bar{\psi}(x) \tag{3.4}$$

The following equality holds:

$$a^4 q_N(x) = -\frac{\bar{a}}{2}\,\mathrm{Tr}\{\gamma_5 D(x,x)\} = \frac{1}{2}\,\mathrm{Tr}\{\hat{\gamma}_5\} \tag{3.5}$$

where $\bar{a} = \frac{a}{\rho}$ with $0 < \rho < 2$. The trace is taken over the spin and color indexes, we may simply write $\mathrm{Tr}\{\gamma_5 D\}$ and we have added the subscript N to stress the fact that this definition of the topological charge is using the GW Dirac operator and in the form proposed by Neuberger:

$$D_N = \bar{a}\left(1 + X\frac{1}{\sqrt{X^\dagger X}}\right) \tag{3.6}$$

with

$$X = D_W - \frac{1}{\bar{a}} \tag{3.7}$$

where

$$D_W = \frac{1}{2}\left[\gamma_\mu(\nabla_\mu + \nabla^*_\mu) - a\nabla^*_\mu\nabla_\mu\right] \tag{3.8}$$

and ∇_μ, ∇^*_μ are the gauge covariant forward and backward derivatives on the lattice:

$$\begin{aligned} \nabla_\mu p(x) &= \frac{1}{a}\left[U_\mu(x)p(x+a\hat{\mu}) - p(x)\right] \\ \nabla^*_\mu p(x) &= \frac{1}{a}\left[p(x) - U^\dagger_\mu(x-a\hat{\mu})p(x-a\hat{\mu})\right] \end{aligned} \tag{3.9}$$

Now we will justify the first equality in eq. (3.5) showing that it reproduces the one given in eq. (1.102). We will also explicitly connect it with the index theorem and thus with the dilute instanton gas model. Our presentation will follow mainly [21, 22].

We require the Dirac operator to satisfy the following property:

$$\gamma_5 D\gamma_5 = D^\dagger \tag{3.10}$$

called γ_5-hermiticity. It can be shown that the Wilson Dirac operator complies with this request, which leads to the following relation on his characteristic polynomial $P(\lambda)$:

$$\begin{aligned} P(\lambda) &= \det[D - \lambda\mathbb{1}] = \det[\gamma_5^2(D - \lambda\mathbb{1})] = \det[\gamma_5(D - \lambda\mathbb{1})\gamma_5] = \\ &= \det[D^\dagger - \lambda\mathbb{1}] = \det[D - \lambda^*\mathbb{1}]^* = P(\lambda^*)^* \end{aligned} \tag{3.11}$$

where the superscript $(^*)$ indicates the complex conjugation.

Thus the Wilson Dirac operator spectrum can be decomposed as:

- real eigenvalues λ with eigenvectors u_λ such that $(u_\lambda, \gamma_5 u_\lambda) \neq 0$
- complex eigenvalues ζ and $\bar{\zeta}$ with eigenvectors u_ζ such that $(u_\zeta, \gamma_5 u_\zeta) = 0$

Now, we ask that the Dirac operator satisfies also the GW relation 2.78 thus we find that, in addition to γ_5-hermiticity, the following hold:

$$D_N + D_N^\dagger = aD_N D_N^\dagger = aD_N^\dagger D_N \tag{3.12}$$

thus D is a normal operator and eigenvector corresponding to different eigenvalues are orthogonal. Multiplying this equation with a normalized eigenvector v_λ from the right and with $v_\lambda^\dagger$ from the left we obtain:

$$\lambda^* + \lambda = a\lambda^*\lambda \tag{3.13}$$

Writing $\lambda = x + iy$ this equation becomes:

$$\left(x - \frac{1}{a}\right)^2 + y^2 = \frac{1}{a^2} \tag{3.14}$$

which that the spectrum of a Ginsparg-Wilson Dirac operator lies on the circle in the complex plane with center $(\frac{1}{a}, 0)$ and a radius of $\frac{1}{a}$. We can parametrize this circle as:

$$\lambda = 1 - e^{i\varphi} \qquad \text{with}\, \varphi \in (-\pi, \pi] \tag{3.15}$$

So we have three kinds of eigenvalues:

- $\lambda = 0$: with eigenvectors with definite chirality, such that $\gamma_5 u_\lambda = \pm u_\lambda$, we denote with n^+ and n^- their respective multiplicity;
- $\lambda = \frac{2}{a}$: with eigenvectors with definite chirality, we denote with $\tilde{n}^+$ and $\tilde{n}^-$ their respective multiplicity;
- complex eigenvalues ζ and $\bar{\zeta}$, with eigenvectors u_ζ such that $\gamma_5 u_\zeta = u_\zeta$

The following relation holds:

$$\tilde{n}^+ - \tilde{n}^- = -(n^+ - n^-) \tag{3.16}$$

Now, reminding that the Neuberger definition of the Dirac operator satisfies the GW relation, we have that the following relation holds:

$$\begin{aligned} q_N(x) &\equiv \frac{a}{2}\,\mathrm{Tr}\{\gamma_5 D_N\} = -\frac{1}{2}\,\mathrm{Tr}\{\gamma_5(2 - aD_N)\} = \\ &= -\frac{1}{2}\sum_\lambda (2 - a\lambda)(u_\lambda, \gamma_5 u_\lambda) = \\ &= n^- - n^+ \end{aligned} \tag{3.17}$$

the difference between the number of the negative and positive zero modes of the Dirac operator is also called from the Atiyah-Singer theorem the index of the operator:

$$\mathrm{index}(D_N) = n^- - n^+ \tag{3.18}$$

thus we have that the following relation holds:

$$q_N(x) = \mathrm{index}(D_N) \tag{3.19}$$

eq. (3.19) expresses the index theorem on the lattice.

It can be showed [22] that for smooth lattice configurations the following equality holds:

$$q_N(x) = -\frac{1}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}\,\mathrm{Tr}\{F_{\mu\nu}F_{\mu\nu}\} + \mathcal{O}(a^2) \tag{3.20}$$

since $q_N(x)$ is a gauge invariant pseudoscalar of dimension four in the continuum limit we obtain again the topological charge as defined in the previous sections.

Thus we have completely justified the following equivalence:

$$Q = \sum_x a^4 q(x) = \frac{1}{2}\,\mathrm{Tr}\{\hat{\gamma}_5\} \tag{3.21}$$

and we can write:

$$\prod_{x,c,s,f} d\psi'(x)d\bar{\psi}'(x) = e^{-i\beta(x)2N_f Q}\prod_{x,c,s,f} d\psi(x)d\bar{\psi}(x) \tag{3.22}$$

We can rewrite the Ward identities on the lattice[1]:

$$\langle\partial^*_\mu j^5_\mu(x)\mathcal{O}\rangle = N_f\langle\mathrm{Tr}\{\gamma_5 D_N(x,x)\}\rangle + \langle\delta_x\mathcal{O}\rangle \tag{3.23}$$

Integrating the l.h.s. of 3.23 and assuming the absence of a $U(1)_A$ massless Goldstone boson we obtain:

$$2N_f a^4\sum_x\langle q(x)\mathcal{O}\rangle + \langle\delta\mathcal{O}\rangle = 0 \tag{3.24}$$

3.2 Renormalization on the Lattice

The lattice acts as a regulator of the theory in an Euclidean path integral, converting a quantized gauge theory in an equivalent classical statistical system with is well suited to numerical simulation using established techniques [20]. The inverse lattice spacing can be interpreted as a ultraviolet cutoff $\frac{1}{a}\sim\Lambda$.

The regularization on the lattice needs to be followed by a renormalization procedure to obtain the physical results. The goal of renormalization is to remove ultraviolet divergences from a field theory: the bare parameters become functions of the ultraviolet cutoff in such a manner that physical quantities have a finite limit as the cutoff is removed. A renormalization scheme begins with the selection of an arbitrary set of physical measurables which is sufficiently complete to determine the bare parameters when the cutoff is in place. Then these given measurables have to remain fixed.

To restore the physical theory we can take the *continuum limit*, i.e. we must send the lattice spacing to zero $a\to 0$, holding the aforementioned quantities fixed.

If we want to calculate on the lattice an observable O of dimension d, the result we will obtain from the lattice calculation is of the form:

$$\langle O_P\rangle = a^d\cdot\overline{O_L(a;g,M)} \tag{3.25}$$

where O_L is the number obtained from the lattice simulation. We added the subscript O_P to the observable to indicate that it is the physical values (with

[1] The definition of the quantity $\partial^*_\mu j^5_\mu(x)$ is involved, for further details see [23].

the appropriate unit of measure). The bar over O_L indicates that its value is mediated over a (usually large) number of configurations.

We have written explicitly that, in general, O_L is a dimensionless function of the lattice spacing, and of the free parameters of the theory thus the coupling constant g and the mass of the quarks M. Note that even if the factor a^d appears in eq. (3.25) O_L can still contain a dependence on the lattice spacing which in higher powers of a, this contribution goes to zero in the continuum limit and it is generally referred to as *discretization errors* at finite lattice spacing. The relation in eq. (3.25) can be rewritten as:

$$a^{-d} O_P = O_L(a; g, M) \tag{3.26}$$

in this formula the quantities on both sides are adimensional, and it is a convenient starting point when writing the relation between lattice quantities and physical quantities. If we also set $a = 1$ we speak of *lattice units*.

When sending the lattice spacing to zero, we thus have to find particular combinations of the variables to hold fixed, we need as many of them as the number of free parameters in $O_L(a; g, M)$.

Some observables like hadron masses can be measured directly on the lattice as am_{phys}. By comparing such number with the physical mass m_{phys} of that particle one may determine the lattice spacing and establish the scale of the system. The value of low-energy parameters as quark masses depends on their definitions in some renormalization scheme. Since one wants to compare with physical, experimentally measured quantities one has to relate these to the parameters of the underlying formulation of the quantized theory. For that purpose one has to determine the scaling properties, i.e. the dependence on scale a, of the observable and their behavior under renormalization.Many quantities are intrinsically scale dependent and are even divergent when the cutoff parameter is removed.

If we take the case of two quarks, as we have seen above in general we have to find three parameters to specify completely the continuum limit of a generic observable O_L. Typical parameters used in lattice QCD are the squared pion mass m_π^2 and the neutron mass m_N. The conversion of the lattice spacing is achieved choosing the value of β, thus fixing the value of the coupling constant g, and calculating the value of the ratio among the lattice spacing and a reference scale r_0.

In the regularization some symmetries of the original theory are lost. In the lattice approach these are the continuous spacetime transformations. We have seen in the previous chapter that there are also many lattice discretization where chiral symmetry is lost. Chiral symmetry is very useful in this context since it implies several relations between renormalization constants. In order to compute renormalization constants non-perturbatively on the lattice one needs a renormalization scheme which can be implemented in lattice Monte Carlo simulations and in the continuum theory.

There exist mass-independent renormalization schemes where it is possibly to the define the coupling constant as a function of the lattice spacing alone.

Summarizing, to extract physical values from lattice computations three steps are needed:

- define the quantities we are interested in computing on the lattice. Usually many equivalent definitions can be given.

- the numerical results must be related to the physical quantities via a renormalization process.
- several computations at different lattice spacing must be performed to extrapolate the continuum limit.

3.2.1 Renormalization of the Topological Charge

From the analogous in the continuum of eqs. (3.23) and (3.24) it can be shown that $\mathrm{Tr}\{\gamma_5 D(x,x)\}$ and $\partial_\mu j^5_\mu$ are not limited, but the quantity

$$\int d^4x \langle \mathrm{Tr}\{\gamma_5 D(x,x)\}\rangle \equiv 2N_f Q$$

is finite.

From this we conclude that to renormalize $\mathrm{Tr}\{\gamma_5 D(x,x)\}$ we can use only operators of dimension $d \leq 4$ with null integral. The natural choice for this is $\partial_\mu j^5_\mu$ and we have:

$$\tilde{q}(x) = \mathrm{Tr}\{\gamma_5 D(x,x)\} - \frac{Z}{2N_f}\partial_\mu j^5_\mu(x) \tag{3.27}$$

and

$$\partial_\mu \tilde{j}^5_\mu = (1-Z) j^5_\mu(x) \tag{3.28}$$

where $\tilde{q}(x)$ and $\tilde{j}^5_\mu$ are the renormalized quantities. Z is logarithmically divergent in perturbation theory and for $u = \dfrac{N_f}{N_c} \to 0$, i.e. in the large N_c limit it is null, so no further renormalization of $q(x)$ is needed.

3.3 The Wilson Flow

The Wilson flow has been introduced by M. Lüscher in [34] as a mean to generate smooth gauge configurations on the lattice, from which the topological charge can be defined. For any $t > 0$ the correlation functions are finite, i.e. do not require additional renormalization, once the theory in four dimensions is renormalized in the usual way [36]. The flow thus maps the gauge field to a one-parameter family of smooth renormalized fields. Thus the definition of the topological charge definition is free of power divergences and so it does not need any ultraviolet renormalization after the renormalized parameters have been fixed.

The flow used in this work is defined as:

$$\dot{B} = D_\nu G_{\mu\nu}, \qquad \text{with } B_\mu|_{t=0} = A_\mu \tag{3.29}$$

and

$$G_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu] \tag{3.30}$$

the derivative is defined by:

$$D_\mu = \partial_\mu + [B_\mu, \cdot] \tag{3.31}$$

Recent theoretical and numerical studies of the Wilson flow suggest that the gauge field obtained at flow time $t > 0$ is a smooth renormalized field. More precisely, the gauge potential is averaged over a spherical range in space whose mean-square radius in four dimensions is equal to $\sqrt{8t}$. Thus the expectation values of local gauge-invariant expressions in this field are well-defined physical quantities that probe the theory at length scales on the order of $\sqrt{t}$.

We choose as our QCD action the Wilson action:

$$S_W[U] = \frac{1}{g_0^2} \sum_p \Re \operatorname{Tr}\{1 - U(p)\} \tag{3.32}$$

where the sum runs over all the plaquettes on the lattice, g_0 is the bare coupling constant and $U(p)$ is the product of the link variables around p.

The associated flow $V_t(x,\mu))$ of lattice gauge fields (i.e. the Wilson flow) is then defined by the equations:

$$V_t(x,\mu) = -g_0 \left(\partial_{x,\mu} S_W(V_t)\right) V_t(x,\mu) \tag{3.33}$$

with the initial condition:

$$V_t(x,\mu)|_{t=0} = U(x,\mu) \tag{3.34}$$

$\partial_{x,\mu}$ is the differential operator on $\mathbf{su}(3)$ with respect to the link variable $V_t(x,\mu)$. The notation is clarified in the next section.

The existence, uniqueness and smoothness of the Wilson flow at all positive and negative times t is rigorously guaranteed on a finite lattice [34, 35].

The one-loop calculation at small coupling suggests that the fields obtained at positive flow time are renormalized fields for any number of quark flavors [37]. The question has been studied numerically in the pure gauge theory.

Using the Wilson flow and eq. (3.20) we can define the topological charge as:

$$q^t_{\mathrm{WF}}(x) = -\frac{1}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \operatorname{Tr}\{F^t_{\mu\nu} F^t_{\mu\nu}\} + \mathcal{O}(a^2) \tag{3.35}$$

where the superscript t reminds that this is calculated at "flow time" t.

The equivalence between the Wilson flow definition, eq. (3.35), and the Neuberger definition, 3.5, is yet to be proven analytically. Although the analytical proof of this equivalence is needed, there are recent numerical results [43] which agree, within errors, with computations of the susceptibility based on the use of the two definitions.

3.3.1 Differential equation

In this section we derive the explicit form of the differential equation satisfied by the Wilson flow. We have that for the Wilson flow the following differential equation holds [37], where the subscript t appearing here refer to flow time[2]:

$$\dot{V}_t(x,\mu) = -g_0^2 \Big\{ \partial_{x,\mu} S_W[U_t(\tilde{x},\tilde{\mu})] \Big\} V_t(x,\mu) \tag{3.36}$$

[2]We will write in this section $U(x,\mu) \equiv U_\mu(x)$ to simplify the notation.

with the initial condition $V_t(x,\mu)$ where the dot is the derivative with respect to flow time and for clarity we have explicitly written the U's as a function of lattice point x and direction μ. Equation (3.36) can be written as:

$$\dot{V}_t = Z(V_t)V_t \tag{3.37}$$

having put $Z(V_t)$ equal to:

$$\begin{aligned} Z(V_t) &= -g_0^2 \partial_{\tilde{x},\tilde{\mu}} S_W[V_t(x,\mu)] = \\ &= -g_0^2 \frac{6}{g_0^2} \sum_x \sum_{\substack{\mu,\nu \\ \mu\neq\nu}} \partial_{\tilde{x},\tilde{\mu}} \left[1 - \frac{1}{6} \Re \operatorname{Tr}\left\{U_\mu(x) T^\dagger_{\mu\nu}(x)\right\}\right] \\ &= \partial_{\tilde{x},\tilde{\mu}} \sum_x \sum_{\substack{\mu,\nu \\ \mu\neq\nu}} \Re \operatorname{Tr}\left\{U_\mu(x) T^\dagger_{\mu\nu}(x)\right\} \end{aligned} \tag{3.38}$$

we also note that V_t and $\dot{V}_t \in SU(3)$ and $Z(V_t) \in \mathbf{su}(3)$.

In [37], the derivative of the gauge field functions $\partial_{x,\mu} f(U)$ is defined as:

$$\partial_{\tilde{x},\tilde{\mu}} f(U) = \sum_a T^a \partial^a_{\tilde{x},\tilde{\mu}} f(U) \tag{3.39}$$

where T^a are the generator of the $\mathbf{su}(3)$ Lie algebra.[3] The derivative $\partial^a_{\tilde{x},\tilde{\mu}} f(U)$ is defined as:

$$\partial^a_{\tilde{x},\tilde{\mu}} f(U) = \frac{d}{ds} f\left(e^{sX(y,\rho)}U\right)\Big|_{s=0} \tag{3.40}$$

with

$$X(y,\rho) = \begin{cases} T^a & \text{if } (y,\rho) = (\tilde{x},\tilde{\mu}) \\ 0 & \text{else} \end{cases}$$

We need to find the dependence of the action with respect to a given link $U_\mu(x)$, to do so we introduce the quantities $V^\dagger_{\mu\nu}(x)$, $V_{\mu\nu}(x)$ as the product the three remaining links in the plaquette (fig. 3.1):

$$V^\dagger_{\mu\nu}(x) = U_\nu(x+\hat{\mu}) U^\dagger_\mu(x+\hat{\nu}) U^\dagger_\nu(x) \tag{3.41}$$

$$V_{\mu\nu}(x) = U_\nu(x) U_\mu(x+\hat{\nu}) U^\dagger_\nu(x+\hat{\mu}) \tag{3.42}$$

so that $U_{\mu\nu}(x) = U_\mu V^\dagger_{\mu\nu}(x)$.

We see from fig. 3.2 that the dependency from $U_\mu(x)$ in the Wilson action is given by the term:

$$\begin{aligned} &\sum_x \sum_{\substack{\mu,\nu \\ \mu\neq\nu}} \Re \operatorname{Tr}\left\{U_\mu(x) V^\dagger_{\mu\nu}(x)\right\} = \\ &= \ldots \Re \operatorname{Tr}\left\{U_\mu(x) V^\dagger_{\mu\nu}(x)\right\} + \Re \operatorname{Tr}\left\{U^\dagger_\mu(x-\hat{\nu}) T_{\mu\nu}(x-\hat{\nu})\right\} + \cdots = \\ &= \cdots + \Re \operatorname{Tr}\left\{U_\mu(x) U_\nu(x+\hat{\mu}) U^\dagger_\mu(x+\hat{\nu}) U^\dagger_\nu(x)\right\} + \\ &+ \Re \operatorname{Tr}\left\{U_\mu(x) U^\dagger_\nu(x+\hat{\mu}-\hat{\nu}) U^\dagger_\mu(x-\hat{\nu}) U_\nu(x-\hat{\nu})\right\} + \ldots \end{aligned} \tag{3.43}$$

[3] While different choices can be made about the generators of $\mathbf{su}(3)$, the combination $\sum_a T^a \partial^a_{\tilde{x},\tilde{\mu}}$ can be shown to be basis independent.

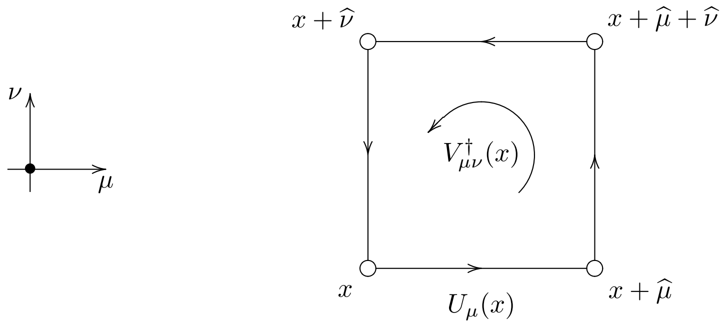

Figure 3.1: A staple $V^\dagger_{\mu\nu}$ is the product of 3 links and a plaquette can be defined as the product $U_{\mu\nu}(x) = U_\mu(x)V^\dagger_{\mu\nu}(x)$.

where in the last equality we have used the cyclic property of the Tr operator. So we can write $f(U(x,\mu))$ as:

$$f(U(x,\mu)) = \frac{1}{2}\sum_x \sum_{\substack{\mu,\nu \\ \mu\neq\nu}} \Re\,\mathrm{Tr}\{U_\mu(x)V^\dagger_{\mu\nu}(x)\} \tag{3.44}$$

with $V^\dagger_{\mu\nu}(x) = U_\nu(x+\widehat{\mu})U^\dagger_\mu(x+\widehat{\nu})U^\dagger_\nu(x) + U^\dagger_\nu(x+\widehat{\mu}-\widehat{\nu})U^\dagger_\mu(x-\widehat{\nu})U_\nu(x-\widehat{\nu})$.

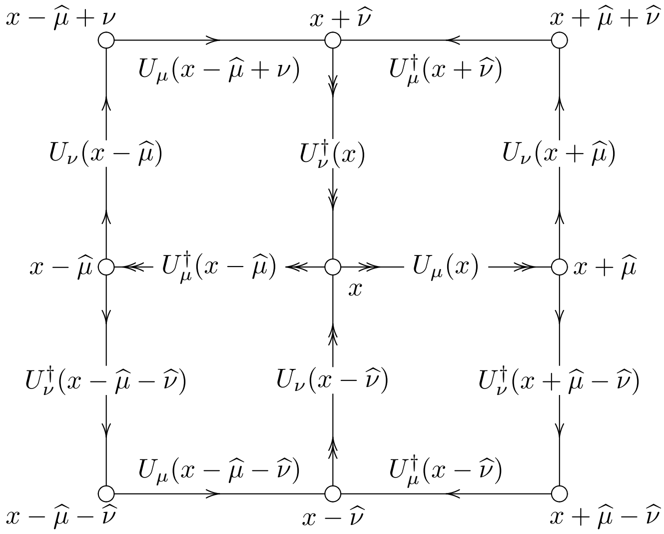

Figure 3.2: The links around the lattice point x.

Equation (3.40) becomes:

$$\begin{aligned}
\partial^a_{\tilde{x},\tilde{\mu}} f(U) = {} & \frac{d}{ds} \sum_x \sum_{\substack{\mu,\nu \\ \mu\neq\nu}} \frac{1}{2} \Re \operatorname{Tr} \left\{ e^{sX} U_\mu(x) V^\dagger_{\mu\nu}(x) \right\} \Bigg|_{s=0} = \\
= {} & \sum_x \sum_{\substack{\mu,\nu \\ \mu\neq\nu}} \frac{d}{ds} \frac{1}{2} \Re \operatorname{Tr} \left\{ \left(1 + sX + \frac{s^2}{2} X^2 \right) U_\mu(x) V^\dagger_{\mu\nu}(x) \right\} \Bigg|_{s=0} = \\
= {} & \sum_{\substack{\nu \\ \nu\neq\tilde{\mu}}} \frac{1}{2} \Re \operatorname{Tr} \left\{ T^a U_\mu(x) V^\dagger_{\mu\nu}(x) \right\}
\end{aligned} \tag{3.45}$$

and $Z(U_t)$ from equation 3.38 becomes:

$$Z(U_t(\tilde{x},\tilde{\mu})) = \frac{1}{2} \sum_a \sum_{\substack{\nu \\ \nu\neq\tilde{\mu}}} T^a \Re \operatorname{Tr} \left\{ T^a U_{\tilde{\mu}}(\tilde{x}) V^\dagger_{\tilde{\mu}\nu}(\tilde{x}) \right\} \tag{3.46}$$

$Z(U_t)$ as given by (3.46) is an element of $\mathbf{su}(3)$ as expected.

Chapter 4

Numerical Simulations, Results and Conclusions

In this chapter we present the results of the numerical simulations on the lattice.

4.1 Lattice Units and Conversion Factors

The length reference scale for our lattice simulations is[1]:

$$r_0 = 0.5 \text{ fm} \tag{4.1}$$

We need now to find a conversion coefficient to express this quantity in lattice units. This is provided by the parametrization (2.18) given in [44] and reported below:

$$\ln\left(\frac{a}{r_0}\right) = 1.6805 + 1.7139(\beta - 6) - 0.8155(\beta - 6)^2 + 0.6667(\beta - 6)^3 \tag{4.2}$$

Following the prescriptions of [44] we found the ratio r_0/a and its uncertainty to be:

$$\left[\frac{r_0}{a}\right](\beta = 5.96) = 5.00 \pm 0.02 \tag{4.3}$$

Following the same reasoning of the previous section, and reminding that the topological susceptibility χ has the dimensions of (energy)^4 we can write the following dimensionless quantity:

$$a^4\chi \equiv \chi_l \tag{4.4}$$

where χ_l is the result of the lattice computation, i.e.:

$$\chi_l = \langle Q^2 \rangle = \frac{1}{N_{\text{conf}}} \sum_{i=1}^{N_{\text{conf}}} (Q_i)^2 \tag{4.5}$$

[1]For convenience we will express the result in natural units, we used the following conversion factor [45]:

$$\hbar c = 197.3269631 \text{ MeV} \cdot \text{fm}$$

then:

$$\chi = \frac{\chi_l}{a^4} = \chi_l \cdot \left(\frac{r_0}{a} \cdot \frac{1}{r_0}\right)^4 \tag{4.6}$$

For convenience we will present our results as $\chi^{1/4}$ which has the dimension of an (energy).

The ratio $r = \dfrac{\langle Q^4\rangle_{\text{con}}}{\langle Q^4\rangle}$ is dimensionless, so no conversion factors are needed. For the fourth cumulant $\langle Q^4\rangle_{\text{con}}$ we used the following formula:

$$\langle Q^4\rangle_{\text{con}} = \frac{1}{N_{\text{conf}}} \sum_{i=1}^{N_{\text{conf}}} (Q_i)^4 - 3\langle Q^2\rangle \tag{4.7}$$

4.2 Integration Method

Ensembles of representative gauge fields are generated on a lattice, using the Wilson gauge action and a combination of well-known link-update algorithms.

To integrate the Wilson flow equation eq. (3.37):

$$\dot{V}_t = Z(V_t)V_t \tag{4.8}$$

a Runge-Kutta third order method has been used, it is detailed in appendix A.

Using the notation:

$$Z_i = \varepsilon Z(W_i) \qquad (\text{for } i = 0, 1, 2) \tag{4.9}$$

the rules for the integration from time t to $t + \varepsilon$ are:

$$\begin{cases} W_0 = V_t \\ W_1 = \exp\left\{\frac{1}{4}Z_0\right\} W_0 \\ W_2 = \exp\left\{\frac{8}{9}Z_1 - \frac{17}{36}Z_0\right\} W_1 \\ V_{t+\varepsilon} = \exp\left\{\frac{3}{4}Z_2 - \frac{8}{9}Z_1 + \frac{17}{36}Z_0\right\} W_2 \end{cases} \tag{4.10}$$

in total we can write:

$$V_{t+\varepsilon} = \exp\left\{\frac{3}{4}Z_2 - \frac{8}{9}Z_1 + \frac{17}{36}Z_0\right\} \exp\left\{\frac{8}{9}Z_1 - \frac{17}{36}Z_0\right\} \exp\left\{\frac{1}{4}Z_0\right\} V_t \tag{4.11}$$

This Runge-Kutta scheme obtains the solution of the flow equation at times $t = n\varepsilon$, with $n = 1, 2, 3, \ldots$, recursively, starting from the initial configuration at $t = 0$.

This integration scheme is accurate up to errors of order ε^4 per step. The total error of the integration up to a specified flow time thus scales like ε^3. The integration is also numerically stable in the direction of positive flow time [37], with the integration errors in the link variables being on the order of 10^{-6} if $\varepsilon = 0.01$.

4.3 Choice of the Simulation Parameters

In this section we explain the reasons behind the choice of the simulation parameters.

Figs. 4.1 and 4.2 show the results of the estimation of $\chi^{\mathrm{YM}(0)}$ with the alternative using Neuberger fermions obtained for various lattice spacings.

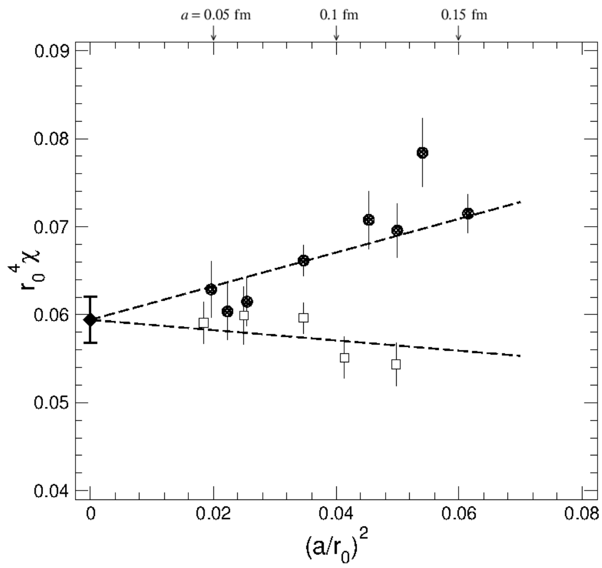

Figure 4.1: Continuum extrapolation of the adimensional product $r_0\chi$, using the Neuberger definition for the topological charge $q_N(x)$ (see eq. 3.20). The filled diamond at $a = 0$ is the extrapolated value in the continuum limit. This plot is taken from Del Debbio et al. [46] (fig. 3).

While the continuum limit is independent on the discretization chosen, numerical results at finite lattice spacing are affect by discretization errors which depend on the action and on the particular form of the observables on the lattice. Nevertheless since the definition of the topological charge using the Wilson and the Neuberger one are affacted by discretization errors of the order $\mathcal{O}(a^2)$ it is reasonable to expect that in our setting the effect of this errors should be of the same order of magnitude. In particular from the data reported in figs. 4.1 and 4.2 it can be seen that for in our case, i.e. for lattice spacing $a \approx 1\,\mathrm{fm}$ (corresponding to $(a/r_0)^2 \approx 0.04$) discretization errors due to the lattice spacing are expected to be contained within the 15% from the extrapolated continuum value.

Fig. 4.3 explains that the value we computed is fairly independent from the lattice size and volume effects should be contained within a 5% error band. Finite volume effects are independent both from the regularization and the operator form; thus the square point in fig. 4.4 also shows that lattice size effects do not alter significantly the final result in a setting comparable to ours.

Fig. 4.4 shows that the discretization errors on the ratio $\dfrac{\langle Q^4\rangle_{\mathrm{con}}}{\langle Q^2\rangle}$ are negligi-

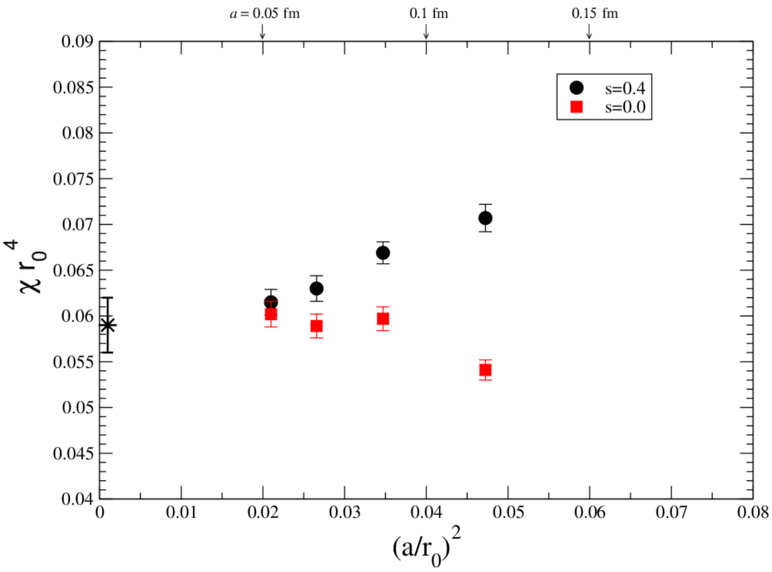

Figure 4.2: Topological susceptibility as a function of the square of the lattice spacing at a fixed value of the lattice size $L = 1.304\,\mathrm{fm}$. The continuum limit point is the result quoted in [46]. This plot is taken from Giusti et al. [48] (fig. 2).

ble withting the statistical significance of the results at different lattice spacings.

Finally fig. 4.5 shows that the reference scale chosen for the Wilson time integration t_0 is stable at different values of the lattice size and extrapolates smoothly to the continuum value. Also in this case discretization errors are shown to be contained within the 10% with respect to the continuum limit.

The parameters used in the final simulation are shown in table 4.1. Table 4.2 presents the lattice spacing, the lattice size and other relevant quantities in physical units.

paramter	value
V	12×12^3
n_{cfg}	102000
β	5.96
n_{hb}	1
n_{or}	6
level	0
n_{th}	1500
n_{it}	100

parameter	value
n_{cy}	5
n_{evol}	71
ε	$1.0 \cdot 10^{-2}$

Table 4.1: The parameter used in the numerical simulation. The lattice volume V is given by $T \times L^3$ lattice sites. The table on the right gives the parameters specific to the Wilson flow integration.

parameter	value
a	≈ 0.1 fm
L	≈ 1.2 fm
r_0	0.5 fm
t_0	$(0.16845 \text{ fm})^2$
t_0/r_0^2	0.1135

parameter	value
τ_1 $(n_{cy} = 1; n_{evol} = 71)$	$\approx (0.08426\,\text{fm})^2$
τ_2 $(n_{cy} = 2; n_{evol} = 142)$	$\approx (0.11916\,\text{fm})^2$
τ_3 $(n_{cy} = 3; n_{evol} = 213)$	$\approx (0.14595\,\text{fm})^2$
$\tau_4 \equiv t_{max}$ $(n_{cy} = 4; n_{evol} = 284)$	$\approx (0.16852\,\text{fm})^2$

Table 4.2: The table on the left reports the lattice spacing and the reference scale expressed in physical units. On the right the table shows the Wilson flow time at which the topological charge has been computed.

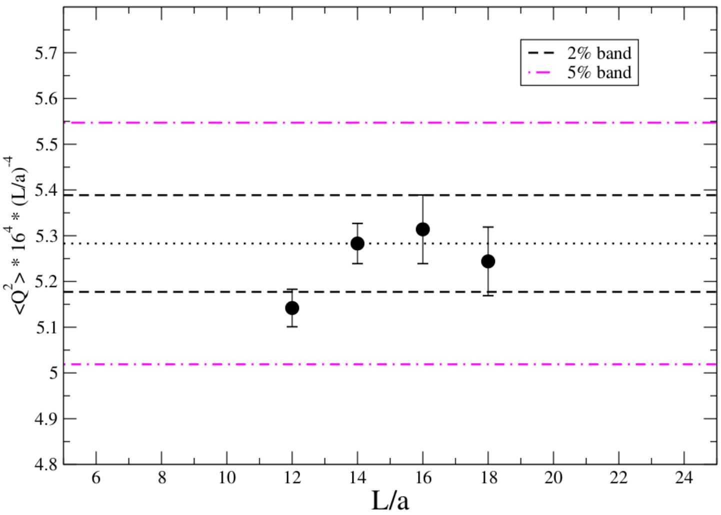

Figure 4.3: Rescaled topological charge as a function of the lattice size. Bands of $\pm 2\%$ (dashed lines) and $\pm 5\%$ (dot-dashed lines) centered at the value measured at $L = 14$ are shown. This plot is taken from Giusti et al. [48] (fig. 1).

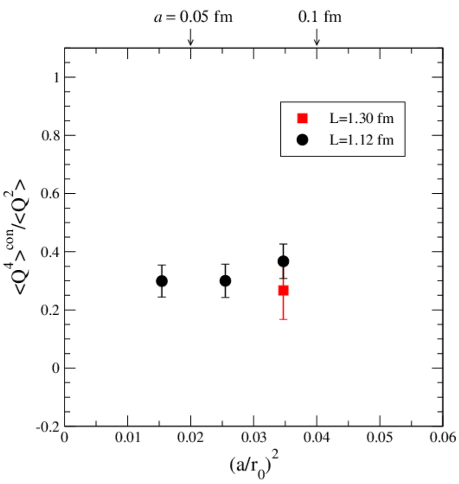

Figure 4.4: Ratio of the first two cumulants vs the lattice spacing. This plot is taken from Giusti et al. [47] (fig. 2).

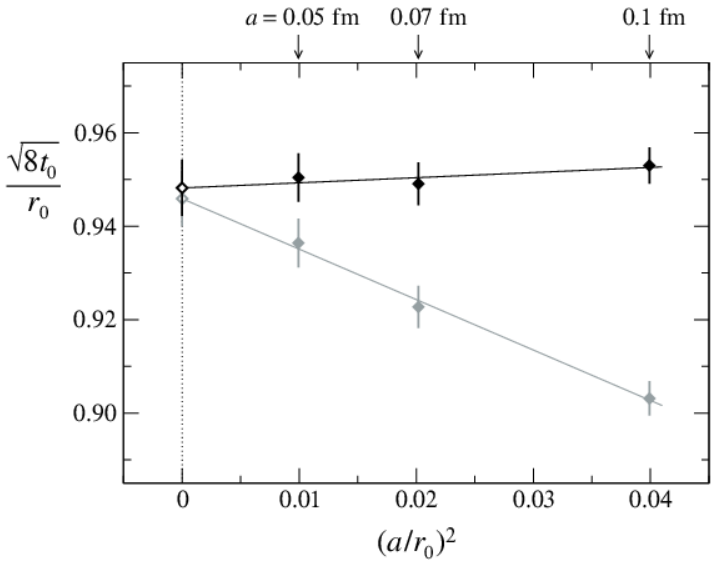

Figure 4.5: Extrapolation of the dimensionless ratio $\sqrt{8t_0}/r_0$ of the Wilson flow and the lattice reference scales to the continuum limit (open data points). Black and grey data use two alternative definitions for the evaluation of the ratio $\frac{\sqrt{8t_0}}{r_0}$, both are show to extrapolate smoothly to the continuum value. This plot is taken from Lüscher [37] (fig. 3).

4.4 Results

Our work has been based on the `CSyYM package` on top of which we implemented from scratch the Wilson flow integration method described above. This program has been written in C using only standard libraries, and the package is compliant with the standard ANSI X3.159-1989 - "Programming Language C"[2].

The simulations of this work where run on the TURING cluster at the Theoretical Division of the Physics Department at University of Milan-Bicocca, on Dual-Core AMD Opteron Processors. The data has been generated during two runs on respectively 9 and 8 nodes, using 36 and 32 cores respectively. Each noded generated 1500 configurations in parallel. An average configuration took $\sim 300\,s$ for its generation and processing, and 8.9 MB of data has been generated in total.

The lattice initial configuration was "cold" (all links set to zero), and was evolved till the thermalization of the system making n_{th} update steps. The update of the fields has been performed using a well-known update algorithm called "heat bath" with over-relaxation, for the number of over-relaxation steps n_{or} and heat-bath steps n_{hb} typical values were chosen.

In order to safely suppress any residual statistical correlations of the n_{cfg} generated fields, the separation in simulation time of the fields was taken to be at least 10 times the integrated autocorrelation time of the topological charge.

The total number of configurations generated was n_{cfg} and for each the value of the average plaquette was collected.

Then, for each configuration, the Wilson flow integrator described in section 4.2 was applied for n_{evol} steps with an increment of $\varepsilon = 0.01$. At this point the topological charge Q and the total lattice energy were calculated and their values collected. The process was then repeated n_{cy} times, thus collecting data at flow times $0, \tau_1, \tau_2, \tau_3$ and τ_4 (see table 4.2 for the corresponding values expressed in physical units). The number of evolution steps n_{evol} was chosen with respect to a reference time t_0 reported in table 4.2 and such to ensure the necessary smoothing of the fields.

The data analysis and the computation $(\chi^t)^{\mathrm{YM}}$ and $\langle Q^4\rangle^{\mathrm{YM}}_{\mathrm{con}}/\langle Q^2\rangle^{\mathrm{YM}}$ has been run completely off-line. The results are reported in table 4.3.

Fig. 4.6 plots the values of the topological susceptibility χ^{YM} measured at different values of the flow time. From this plot we see the discretization are contained withing the $\approx 6\%$ of the value calculated at the greatest Wilson flow time. The differences among these values are originated only by discretization errors since in the continuum limit the values calculated at any flow time $t > 0$ must converge to the continuum value. This observation confirms the estimation made in the previous section that the discretization errors should be within the 15% of the continuum value.

Fig. 4.7 plots the values of the ratio $\langle Q^4\rangle^{\mathrm{YM}}_{\mathrm{con}}/\langle Q^2\rangle^{\mathrm{YM}}$ measured at different values of the flow time.

Fig. 4.8 plots the values of the topological charge Q measured at greatest flow time. As can be seen the values of Q concentrates (discarding discretization errors around integer values), the profile of the peaks is a gaussian centered

[2] This version of the language is more widely known as `C89`.

t_{WF}	χ_t^{YM} (MeV)	r_t^{YM} $(\cdot 10^{-1})$
τ_1 $\approx (0.11916\,\mathrm{fm})^2$	173.7 ± 0.7	1.5 ± 0.5
τ_2 $\approx (0.11916\,\mathrm{fm})^2$	179.3 ± 0.7	1.8 ± 0.6
τ_3 $\approx (0.14595\,\mathrm{fm})^2$	182.0 ± 0.7	1.9 ± 0.7
$\tau_4 \equiv t_{max} \approx t_0$ $\approx (0.16852\,\mathrm{fm})^2$	183.6 ± 0.7	1.9 ± 0.7

Table 4.3: Results of the numerical simulation.

around zero with:

$$\begin{aligned} &\langle Q \rangle : (-6 \pm 39) \cdot 10^{-4} \\ &\langle Q^2 \rangle : 1.547 \pm 0.007 \end{aligned} \tag{4.12}$$

both results are presented in lattice units.

These results are compatible with the known values from the literature, as presented in fig. 4.9.

In particular:

- the result we found is statistically equivalent to the values reported in [47].
- in the previous section we argued that the systematic errors due to finite size effects should be under control.
- our estimation of the discretization errors seems to be compatible with the values we found. For the topological susceptibility this claim is supported by other studies in literature [43].

Thus we claim that value we found for r has a significance of its own, within its statistical error.

This result for r strongly supports the scenario obtained from large N_c scaling arguments, and in particular the Witten–Veneziano mechanism to explain the origin of the η' mass, while the dilute instanton gas model seems to be inconsistent with these results.

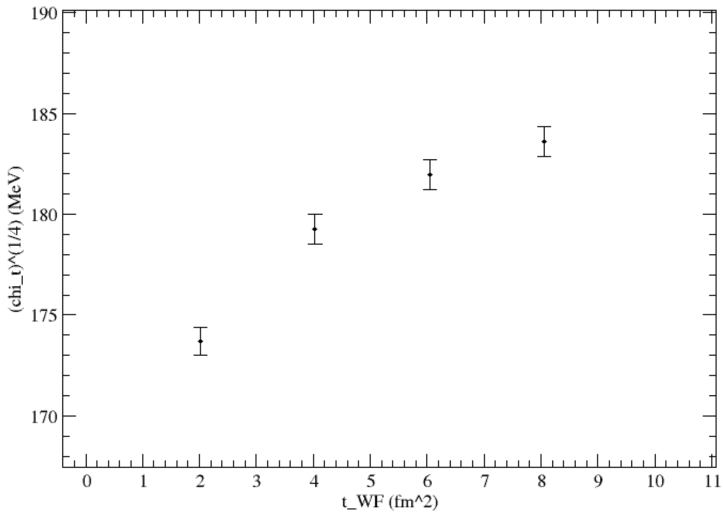

Figure 4.6: The topological charge χ_t^{YM} at different flow times.

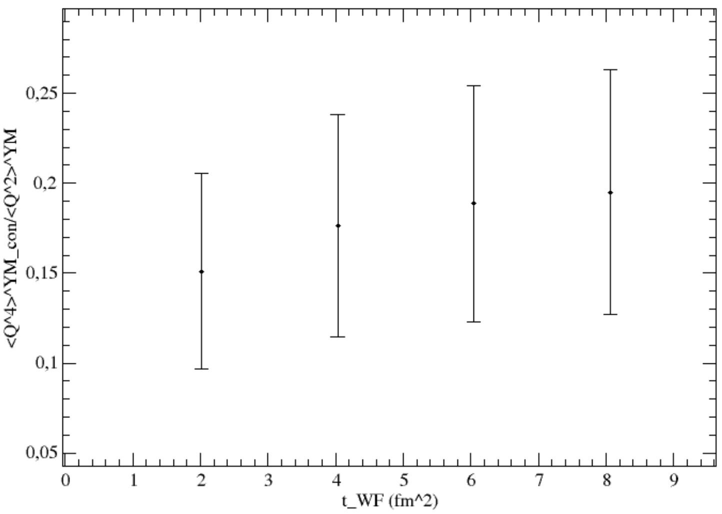

Figure 4.7: The ratio $r = \frac{\langle Q^4 \rangle_{\mathrm{con}}^{\mathrm{YM}}}{\langle Q^2 \rangle^{\mathrm{YM}}}$ at different flow times.

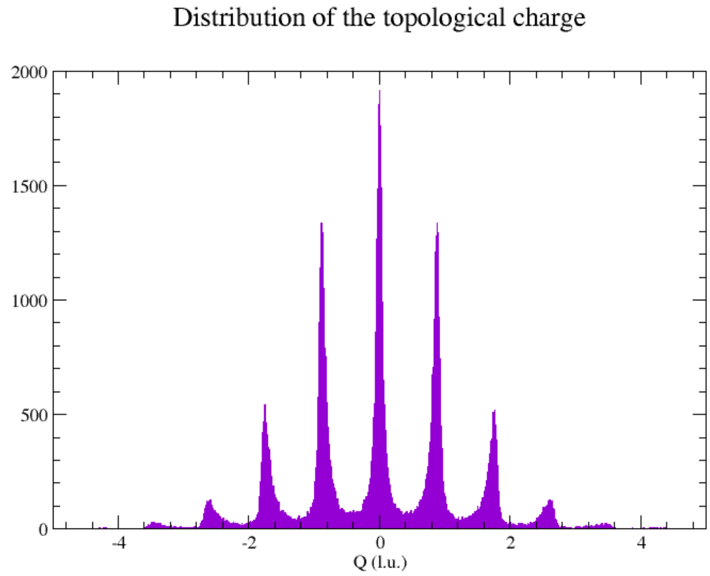

Figure 4.8: Distribution of the topological charge Q, the histogram is plot with 100 bins in the interval $(-5, 5)$.

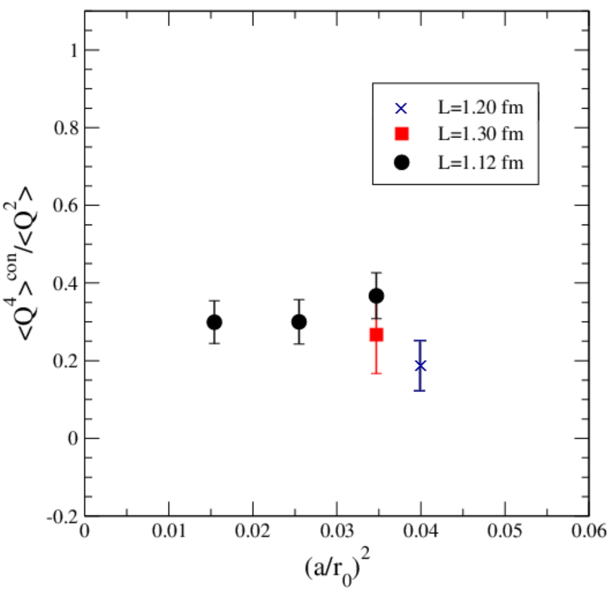

Figure 4.9: Ratio of the first two cumulants vs the lattice spacing. The result we found (cross) is compared with the results reported in 4.4 /fig. 2 in Giusti et al. [47]).

4.5 Conclusions and Outlook

The η' meson was discovered independently by two groups in 1964: Kalbfleisch et al. [49] (paper submitted 9th April) and Goldberg et al. [50] (paper submitted 15th April). In that year the quark model was proposed and the Ω^- ($S = 3$) particle was discovered.

The QCD Lagrangian with three massless flavors possess a symmetry under the chiral group

$$U(N_f)_L \times U(N_f)_R = SU(N_f)_L \times SU(N_f)_R \times U(1)_V \times U(1)_A \tag{4.13}$$

which leaves the action invariant under separate transformations of the chiral components of the fields ψ,$\bar{\psi}$.

This symmetry, if manifest, would imply a parity doubling in the hadronic spectrum where every particle should have a parity partner with the same quantum numbers, but opposite parity. Since this parity doubling is not observed, one must conclude that the chiral symmetry is spontaneously broken in QCD. The Goldstone theorem provides the existence of spinless and massless particles, called Goldstone bosons, equal to the number of broken generators of the symmetry which underwent spontaneous breakdown.

In chapter 1 we specified the meaning of this claim thanks to the Gell-Mann–Oakes–Renner relation (GMOR), eq. (1.93), obtained from the chiral Ward identities, in which, in the chiral limit, the squared masses of the pions (and the other mesons in the octet) are proportional to the quark masses and to the fermionic condensate Σ. In the massless case, the pions, kaons and the η meson are Goldstone bosons arising from the spontaneous breakdown of the chiral symmetry.

For chiral singlet rotations in the group $U(1)_A$ one may expect the η' meson to be the Goldstone boson following the spontaneous breaking of this symmetry. Nevertheless the η' meson has a mass too big to be this missing Goldstone boson: in 1976 Weiberg showed that if the η' mass would be explained in the same way the following limit should hold:

$$m_{\eta'} < \sqrt{3} m_\pi \tag{4.14}$$

Recalling that $m_\pi = 140\,\text{MeV}$ and $m_{\eta'} = 958\,\text{MeV}$ it is evident that this inequality is violated thus the η' can not be the aforementioned Goldstone boson and the origin of its mass can not be explained with the same mechanism used for the pions. This has become known as the $U(1)_A$ problem in literature.

In the '70s it was clarified that the η' meson could acquire its mass from an anomalous contribution to the chiral singlet Ward identity, the chiral anomaly is given by:

$$\mathcal{A} = -\frac{g^2}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \operatorname{Tr}\{F_{\mu\nu} F_{\mu\nu}\} \tag{4.15}$$

Then, in 1976, 't Hooft proposed a solution to the $U(1)_A$ problem, based on the "dilute instanton gas" model, a particularity of which consisted in the introduction of a quantity, called *topological charge*, which could be used to classify the instantonic configurations in the system of interest:

$$Q = \int d^4x q(x) = -\int d^4x \frac{g^2}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \operatorname{Tr}\{F_{\mu\nu} F\rho\sigma\} \tag{4.16}$$

Independently, in 1979, Witten and Veneziano proposed an alternative solution to the $U(1)_A$ problem which made use of a method called "large N_c" expansion (always proposed by 't Hooft [15] in another context), where an action with symmetry $SU_c(N_c)$ is expanded in series of $1/N_c$ in the limit $N_c \to \infty$. This expansion leads to a prediction on the η' mass which is known as *Witten-Veneziano formula*:

$$m_{\eta'}^2 = \frac{2N_f}{F_\pi^2}\chi^{\text{YM}}(0) + \mathcal{O}\left(\frac{1}{N_c^2}\right) \tag{4.17}$$

where the topological susceptibility is defined as:

$$\chi^{\text{YM}}(x) = \int d^4x \langle q(x)q(0)\rangle^{\text{YM}} \tag{4.18}$$

and it is calculated in the pure gauge limit.

From the two mechanism two different predictions on the distribution of the topological charge can be derived, the most simple quantity we can define to highlite the differences between the two models is the ratio:

$$r = \frac{\langle Q^4\rangle_{\text{con}}}{\langle Q^2\rangle}. \tag{4.19}$$

The dilute instanton gas model predicts:

$$\frac{\langle Q^4\rangle_{\text{con}}}{\langle Q^2\rangle} = 1 \tag{4.20}$$

while the prediction for the large N_c expansion is:

$$\frac{\langle Q^4\rangle_{\text{con}}}{\langle Q^2\rangle} \propto \frac{1}{N_c^2} \tag{4.21}$$

thus the two models formulate competing predictions that can be tested through a simulation on the lattice.

In chapter 2 we reviewed the lattice formulation of a gauge field theory and the description of fermions on the lattice. A naive discretization of fermions leads to the appearance of non-physical solutions called "doublers". This problem can be solved in various way, one of which is the Wilson formulation in which doublers are absent, but chiral symmetry is explicitly broken, even if the fermion mass is set to zero. Furthermore, the Nielsen-Ninomiya theorem states that the standard chiral symmetry on the lattice cannot be implemented on the lattice without giving up some important property like locality or gauge invariance. Nevertheless it is possible to break chiral invariance in a mild way, in the sense of eq. (2.78) and obtain a discretized version of the fermions, known as Ginsparg-Wilson fermions, such that is possible to define a chiral transformation on them which is a symmetry for the Lagrangian.

In chapter 3 we showed how the anomaly appears in the lattice formulation and the equivalence of the definition of the topological charge with the one given in chapter 1. Then we presented the method of the Wilson flow and we showed how it can be used to measure the topological charge and topological susceptibility on the lattice.

The results of our numerical simulation are reported in figs. 4.6 and 4.7, in particular we quote here the values at the greatest "Wilson flow time" measured ($t \approx (0.16852\,\mathrm{fm})^2$):

$$
\begin{aligned}
&(\chi^{\mathrm{YM}})^{-1/4} = 183.6 \pm 0.7 \text{ MeV}, \\
&r = \frac{\langle Q^4 \rangle^{\mathrm{YM}}_{\mathrm{con}}}{\langle Q^2 \rangle^{\mathrm{YM}}} = (1.9 \pm 0.7) \cdot 10^{-1}.
\end{aligned}
\tag{4.22}
$$

we recall that this simulation was performed at $\beta = 5.96$.

These results are compatible with the known values of $\chi^{\mathrm{YM}})^{-1/4}$ and r present in literature and calculated with other methods (see fig. 4.9)-

We stress that the evaluation of the ratio r using the Wilson flow is novel, and the precision we reached on the estimate of $\chi^{\mathrm{YM}})^{-1/4}$ is unprecedented.

We justified that the value of the ratio r we found has a significance of its own since the systematic errors should be under control.

The value we found for r, with the other results in literature, strongly supports support the scenario obtained by general large N_c scaling arguments and eq. (4.21), thus the numerical results support the Witten–Veneziano mechanism for the explanation of of the large η' mass observed in nature. Instead, the value expected using the dilute instanton gas mechanism and recalled in eq. (4.20) is inconsistent with our findings. Thus the dilute instanton gas model description is disproven by our results.

This work can be expanded in the future performing simulations on bigger lattices and at a smaller lattice spacing. These are needed to determine the continuum (physical) value of the aforementioned quantities and to have a better understanding of the systematic errors ensuing the lattice discretization.

Appendix A

Runge-Kutta Methods

A.1 Runge-Kutta Method for ODEs

Runge-Kutta methods (RK) are a family of well-known methods [38, 39] for numerical integration of ordinary differential equations (ODEs) such as the following initial-value problem:

$$\begin{cases} \dot{x}(t) = f(x,t) \\ x(t=0) = x_0 \end{cases} \tag{A.1}$$

in the following we will use the notation $x_t := x(t)$.

Every RK is a "one-step method" since the approximate values η_i of the exact solution $x(t_i)$ can be obtained by means of:

$$\begin{aligned} &\eta_0 = x_0 \\ &\quad \text{for } i = 0, 1, 2, \cdots : \\ &\qquad \eta_{i+1} = \eta_i + \epsilon \cdot \Phi(t, x; \epsilon; f) \\ &\qquad t_{i+1} := t_i + \epsilon. \end{aligned}$$

where $\Phi(t, x; \epsilon; f)$ is the function describing the method. If we call $z(t)$ the exact solution of A.1 and define the quantity:

$$\Delta(t, x; \epsilon; f) = \begin{cases} \dfrac{z(t+\epsilon) - z(t)}{\epsilon} & \text{if } \epsilon \neq 0 \\ f(x,t) & \text{if } \epsilon = 0 \end{cases} \tag{A.2}$$

we can say that Δ represents the difference quotient of the exact solution $z(t)$ of A.1 for step size ϵ, while $\Phi(t, x; \epsilon; f)$ is the same for the approximate solutions η_i

Thus defining the difference (we omit the dependence on f for simplicity):

$$\tau(t, x; \epsilon) := \Delta(t, x; \epsilon) - \Phi(t, x; \epsilon) \tag{A.3}$$

then we call a method of order p when:

$$\tau(t, x; \epsilon) = \mathcal{O}(\epsilon^p) \tag{A.4}$$

In particular the Runge-Kutta third and fourth order method method can be written as:

$$x_{t+\epsilon} = x_t + \epsilon \cdot (ak_1 + bk_2) + \mathcal{O}(\epsilon^3) \tag{A.5}$$

$$x_{t+\epsilon} = x_t + \epsilon \cdot (ak_1 + bk_2 + ck_3) + \mathcal{O}(\epsilon^4) \tag{A.6}$$

$$x_{t+\epsilon} = x_t + \epsilon \cdot (ak_1 + bk_2 + ck_3 + dk_4) + \mathcal{O}(\epsilon^5) \tag{A.7}$$

where:

$$k_i = f\left(x_t + \epsilon \cdot \sum_{j=1}^{s} \beta_{ij} k_j, t_n + \alpha_i \epsilon\right) \tag{A.8}$$

are increments obtained evaluating the derivatives of x_t at the i-th order, and s is the order of the method.

We derive the value of the coefficients a, b, ... for A.5, A.6 and A.7 in the next sections.

A.1.1 2nd Order

We develop the derivation evaluated at the starting point and at the mid-point and of any interval $(t, t+\epsilon)$, thus we choose:

$$\begin{array}{cc} \alpha_i & \beta_i \\ \alpha_1 = 0 & \beta_{11} = 0 \\ \alpha_2 = \frac{1}{2} & \beta_{21} = \frac{1}{2} \end{array}$$

and $\beta_{ij} = 0$ otherwise.

We begin with the following Taylor expansion:

$$x_{t+\epsilon/2} = x_t + \frac{\epsilon}{2}\dot{x}_t + \frac{\epsilon^2}{8}\ddot{x}_t \tag{A.9}$$

We can also write the following expansion which are correct up to $\mathcal{O}(\epsilon^2)$:

$$x_{t+\epsilon} = x_{t+\epsilon/2} + \frac{\epsilon}{2}\dot{x}_{t+\epsilon/2} + \frac{\epsilon^2}{8}\ddot{x}_{t+\epsilon/2} \tag{A.10}$$

$$x_t = x_t - \frac{\epsilon}{2}\dot{x}_{t+\epsilon/2} + \frac{\epsilon^2}{8}\ddot{x}_{t+\epsilon/2} \tag{A.11}$$

subtracting A.10 and A.10 we obtain the following relation which is correct up to $\mathcal{O}(\epsilon^3)$:

$$x_{t+\epsilon} = x_t + \epsilon\dot{x}_{t+\epsilon/2} = x_t + f(x_{t+\epsilon/2}) \tag{A.12}$$

Expanding A.12 using A.9 and discarding terms of order $\mathcal{O}(\epsilon^3)$ we obtain:

$$x_{t+\epsilon} = x_t + f\left(x_t + \frac{\epsilon}{2}k_1\right) \tag{A.13}$$

where we have called $k_1 = f(x_t) = \dot{x}_t$. The expression A.13 can be immediately compared with A.5 to give:

$$\begin{cases} a = 0 \\ b = \dfrac{1}{2} \end{cases} \tag{A.14}$$

A.1.2 3rd Order

We develop the derivation evaluated at the starting point, the mid-point and the end point of any interval $(t, t+\epsilon)$, thus we choose:

$$\begin{array}{cc} \alpha_i & \beta_i \\ \alpha_1 = 0 & \beta_{21} = \frac{1}{2} \\ \alpha_2 = \frac{1}{2} & \beta_{32} = 2 \\ \alpha_3 = 1 & \beta_{31} = -1 \end{array}$$

and $\beta_{ij} = 0$ otherwise.

We begin by defining the following quantities:

$$x^1_{t+\epsilon} = x_t + \epsilon \dot{x}_t = x_t + \epsilon f\left(x_t, t\right) \tag{A.15}$$

$$x^2_{t+\epsilon} = x_t + \epsilon f\left(x_t, t\right) + 2f\left(x^1_{t+\epsilon/2}, t + \frac{\epsilon}{2}\right) \quad \text{where } x^1_{t+\epsilon/2} = \frac{x_t + x^1_{t+\epsilon}}{2} \tag{A.16}$$

If we the define:

$$k_1 = f(x_t, t) \tag{A.17}$$

$$k_2 = f\left(x^1_{t+\epsilon/2}, \frac{\epsilon}{2}\right) = f\left(x_t + \frac{\epsilon}{2}k_1, t + \frac{\epsilon}{2}\right) = f(x_t, t) + \frac{\epsilon}{2}\frac{d}{dt}f(x_t, t) \tag{A.18}$$

$$k_3 = f\left(x^2_{t+\epsilon}, \epsilon\right) = f(x_t - \epsilon k_1 + 2\epsilon k_2, t + \epsilon) = \tag{A.19}$$

$$= f(x_t, t) - \epsilon\frac{d}{dt}f(x_t, t) + 2\epsilon\frac{d}{dt}\left[f(x_t) + \frac{\epsilon}{2}\frac{d}{dt}f(x_t, t)\right]$$

If we now express A.6 using A.17 and the following, we obtain:

$$\begin{aligned} x_{t+\epsilon} &= x_t + \epsilon\left\{af(x_t, t) + b\left[f(x_t, t) + \frac{\epsilon}{2}\frac{d}{dt}f(x_t, t)\right] + \right. \\ &\quad \left. + c\left[f(x_t, t) - \epsilon\frac{d}{dt}f(x_t, t) + 2\epsilon\frac{d}{dt}\left[f(x_t, t) + \frac{\epsilon}{2}\frac{d}{dt}f(x_t, t)\right]\right]\right\} = \\ &= x_t + \epsilon a f(x_t, t) + b\epsilon f(x_t, t) + \frac{\epsilon^2}{2}b\frac{d}{dt}f(x_t, t) + c\epsilon f(x_t, t) + \\ &\quad + c\epsilon^2\frac{d}{dt}f(x_t, t) + 2c\epsilon\frac{d}{dt}f(x_t, t) + 2c\frac{\epsilon^3}{2}\frac{d}{dt}f(x_t, t) + \mathcal{O}(\epsilon^4) \end{aligned} \tag{A.20}$$

Now we compare A.20 with the the Taylor series of $x_{t+\epsilon}$ around x_t:

$$\begin{aligned} x_{t+\epsilon} &= x_t + \epsilon\dot{x}_t + \frac{\epsilon^2}{2}\ddot{x}_t + \frac{\epsilon^3}{6}x^{(3)}_t + \mathcal{O}(\epsilon^4) = \\ &= x_t + \epsilon f(x_t, t) + \frac{\epsilon^2}{2}\frac{d}{dt}f(x_t, t) + \frac{\epsilon^3}{6}\frac{d^2}{dt^2}f(x_t, t) + \mathcal{O}(\epsilon^4) \end{aligned} \tag{A.21}$$

we obtain a system of constraints on the coefficients:

$$\begin{cases} a + b + c = 1 \\ \frac{1}{2}b - c + 2c = \frac{1}{2} \\ c = \frac{1}{6} \end{cases} \tag{A.22}$$

which solved gives $a = \frac{1}{6}, b = \frac{2}{3}, c = \frac{1}{6}$ and A.6 becomes:

$$x_{t+\epsilon} = x_t + \epsilon \cdot \frac{1}{6}(k_1 + 4k_2 + k_3) + \mathcal{O}(\epsilon^4) \tag{A.23}$$

A.1.3 4th Order

We develop the derivation[1] for the RK4 using A.8 evaluated at the starting point, the mid-point and the end point of any interval $(t, t+\epsilon)$, thus we choose

$$\begin{array}{ll} \alpha_i & \beta_i \\ \alpha_1 = 0 & \beta_{21} = \frac{1}{2} \\ \alpha_2 = \frac{1}{2} & \beta_{32} = \frac{1}{2} \\ \alpha_3 = \frac{1}{2} & \beta_{43} = 1 \\ \alpha_4 = 1 & \end{array}$$

and $\beta_{ij} = 0$ otherwise. We begin by defining the following quantities:

$$x^1_{t+\epsilon} = x_t + f\left(x_t, t\right) \tag{A.24}$$

$$x^2_{t+\epsilon} = x_t + f\left(x^1_{t+\epsilon/2}, t + \frac{\epsilon}{2}\right) \qquad \text{where } x^1_{t+\epsilon/2} = \frac{x_t + x^1_{t+\epsilon}}{2} \tag{A.25}$$

$$x^3_{t+\epsilon} = x_t + f\left(x^2_{t+\epsilon/2}, t + \frac{\epsilon}{2}\right) \qquad \text{where } x^2_{t+\epsilon/2} = \frac{x_t + x^2_{t+\epsilon}}{2} \tag{A.26}$$

If we define:

$$k_1 = f(x_t, t) \tag{A.27}$$

$$k_2 = f\left(x^1_{t+\epsilon/2}, t + \frac{\epsilon}{2}\right) \tag{A.28}$$

$$k_3 = f\left(x^2_{t+\epsilon/2}, t + \frac{\epsilon}{2}\right) \tag{A.29}$$

$$k_4 = f\left(x^3_{t+\epsilon}, t + \epsilon\right) \tag{A.30}$$

and for the previous A.28-A.30 we can show that the following equalities holds up to $\mathcal{O}(\epsilon^2)$:

$$\begin{aligned} k_2 &= f\left(x^1_{t+\epsilon/2}, t + \frac{\epsilon}{2}\right) = f\left(x_t + \frac{\epsilon}{2}k_1, t + \frac{\epsilon}{2}\right) \qquad (A.31) \\ &= f\left(x_t, t\right) + \frac{\epsilon}{2}\frac{d}{dt}f\left(x_t, t\right) \\ k_3 &= f\left(x^2_{t+\epsilon/2}, t + \frac{\epsilon}{2}\right) = f\left(x_t + \frac{\epsilon}{2}f\left(x_t + \frac{\epsilon}{2}k_1, t + \frac{\epsilon}{2}\right), t + \frac{\epsilon}{2}\right) \qquad (A.32) \\ &= f\left(x_t, t\right) + \frac{\epsilon}{2}\frac{d}{dt}\left[f\left(x_t, t\right) + \frac{\epsilon}{2}\frac{d}{dt}f\left(x_t, t\right)\right] \\ k_4 &= f\left(x^3_{t+\epsilon}, t + \epsilon\right) = f\left(x_t + \epsilon f\left(x_t + \frac{\epsilon}{2}k_2, t + \frac{\epsilon}{2}\right), t + \epsilon\right) \qquad (A.33) \\ &= f\left(x_t + \epsilon f\left(x_t + \frac{\epsilon}{2}f\left(x_t + \frac{\epsilon}{2}f\left(x_t, t\right), t + \frac{\epsilon}{2}\right), t + \frac{\epsilon}{2}\right), t + \epsilon\right) \\ &= f\left(x_t, t\right) + \frac{\epsilon}{2}\frac{d}{dt}\left[f\left(x_t, t\right) + \frac{\epsilon}{2}\frac{d}{dt}\left[f\left(x_t, t\right) + \frac{\epsilon}{2}\frac{d}{dt}f\left(x_t, t\right)\right]\right] \end{aligned}$$

where:

$$\frac{d}{dt}f(x_t, t) = \frac{\partial}{\partial x}f(x_t, t)\dot{x}_t + \frac{\partial}{\partial t}f(x_t, t) = f_x(x_t, t)\dot{x}_t + f_t(x_t, t) := \ddot{x}_t \tag{A.34}$$

[1] This derivation follows closely the one presented in the following notes: *Numerical Simulation of Space Plasmas (I) Appendix C by Ling-Hsiao Lyu - September 2007*
This resource is accessible at the url: `http://www.ss.ncu.edu.tw/~lyu/lecture_files_en/lyu_NSSP_Notes/Lyu_NSSP_AppendixC.pdf`

is the total derivative of f with respect to time.

If we now express A.7 using A.27 and A.31-A.33 we obtain:

$$
\begin{aligned}
x_{t+\epsilon} &= x_t + \epsilon \Bigg\{ a \cdot f(x_t,t) + b \cdot \left[f\left(x_t,t\right) + \frac{\epsilon}{2}\frac{d}{dt} f\left(x_t,t\right) \right] + \\
&+ c \cdot \left[f\left(x_t,t\right) + \frac{\epsilon}{2}\frac{d}{dt} \left[f\left(x_t,t\right) + \frac{\epsilon}{2}\frac{d}{dt} f\left(x_t,t\right) \right] \right] + \\
&+ d \cdot f\left(x_t,t\right) + \frac{\epsilon}{2}\frac{d}{dt} \left[f\left(x_t,t\right) + \frac{\epsilon}{2}\frac{d}{dt} \left[f\left(x_t,t\right) + \frac{\epsilon}{2}\frac{d}{dt} f\left(x_t,t\right) \right] \right] \Bigg\} + \mathcal{O}(\epsilon^5) \\
&= x_t + a \cdot \epsilon f_t + b \cdot \epsilon f_t + b \cdot \frac{\epsilon^2}{2}\frac{df_t}{dt} + c \cdot \epsilon f_t + c \cdot \frac{\epsilon^2}{2}\frac{df_t}{dt} + \qquad \text{(A.35)} \\
&+ c \cdot \frac{\epsilon^3}{4}\frac{d^2 f_t}{dt^2} + d \cdot \epsilon f_t + d \cdot \epsilon \frac{df_t}{dt} + d \cdot \frac{\epsilon^2}{2}\frac{d^2 f_t}{dt^2} + d \cdot \frac{\epsilon^4}{4}\frac{d^3 f_t}{dt^3} + \mathcal{O}(\epsilon^5)
\end{aligned}
$$

and comparing A.35 with the Taylor series of $x_{t+\epsilon}$ around x_t:

$$
\begin{aligned}
x_{t+\epsilon} &= x_t + \epsilon \dot{x}_t + \frac{\epsilon^2}{2}\ddot{x}_t + \frac{\epsilon^3}{6} x_t^{(3)} + \frac{\epsilon^4}{24} x_t^{(4)} + \mathcal{O}(\epsilon^5) = \\
&= x_t + \epsilon f(x_t,t) + \frac{\epsilon^2}{2}\frac{d}{dt} f(x_t,t) + \frac{\epsilon^3}{6}\frac{d^2}{dt^2} f(x_t,t) + \frac{\epsilon^4}{24}\frac{d^3}{dt^3} f(x_t,t) + \mathcal{O}(\epsilon^5)
\end{aligned} \qquad \text{(A.36)}
$$

we obtain a system of constraints on the coefficients:

$$
\begin{cases}
a + b + c + d = 1 \\
\frac{1}{2} b + \frac{1}{2} c + d = \frac{1}{2} \\
\frac{1}{2} d + \frac{1}{4} c = \frac{1}{6} \\
\frac{1}{4} d = \frac{1}{24}
\end{cases} \qquad \text{(A.37)}
$$

which solved gives $a = \frac{1}{6}, b = \frac{1}{3}, c = \frac{1}{3}, d = \frac{1}{6}$ and A.7 becomes:

$$
x_{t+\epsilon} = x_t + \epsilon \cdot \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) + \mathcal{O}(\epsilon^5) \qquad \text{(A.38)}
$$

A.2 Runge-Kutta Method for the Flow Equation

In [37] is shown that the flow equation can be written as an ordinary first-order differential equation:

$$
\dot{V}_t = Z(V_t) V_t \qquad \text{(A.39)}
$$

with $V_t \in \mathcal{G}$, and $Z(V_t) \in \mathbf{g}$ are respectively elements of a gauge (Lie) group and of the associated Lie algebra.

A.2.1 2nd Order

In this section we solve the equation A.39 to the second order method to show the explicit steps which are applied in higher order methods. We won't make any a priori assumption on the form of the solution but we impose that this solution is closed respect to the group $SU(N)$.

We begin with the following Taylor expansion:

$$\begin{aligned} V_{t+\epsilon/2} &= V_t + \frac{\epsilon}{2}\dot{V}_t + \mathcal{O}(\epsilon^2) = \\ &= V_t + \frac{\epsilon}{2}[Z(V_t)V_t] + \mathcal{O}(\epsilon^2) = \\ &= \left(1 + \frac{\epsilon}{2}Z(V_t)\right) V_t + \mathcal{O}(\epsilon^2) = \\ &= e^{\left\{\frac{\epsilon}{2}Z(V_t)\right\}} V(t) + \mathcal{O}(\epsilon^2) \end{aligned} \tag{A.40}$$

where in the second row we have used A.39 and in the last raw we have added terms of order $\mathcal{O}(\epsilon^2)$ to have a closed expression in $SU(N)$, having $Z(V_t) \in \mathbf{g}$ and thus $\exp\{\frac{\epsilon}{2}Z(V_t)\} \in \mathcal{G}$.

Writing the following Taylor expansions around $V_{t+\epsilon/2}$ up to order $\mathcal{O}(\epsilon^3)$:

$$V_{t+\epsilon} = V_{t+\epsilon/2} + \frac{\epsilon}{2}\dot{V}_{t+\epsilon/2} + \frac{\epsilon^2}{8}\ddot{V}_{t+\epsilon/2} \tag{A.41}$$

$$V_t = V_{t+\epsilon/2} - \frac{\epsilon}{2}\dot{V}_{t+\epsilon/2} + \frac{\epsilon^2}{8}\ddot{V}_{t+\epsilon/2} \tag{A.42}$$

we get:

$$\begin{aligned} V_{t+\epsilon} &= V_t + \dot{V}_{t+\epsilon/2} + \mathcal{O}(\epsilon^3) = V_t + \epsilon Z(V_{t+\epsilon/2})V_{t+\epsilon/2} + \mathcal{O}(\epsilon^3) = \\ &= \left(1 + \epsilon Z(V_{t+\epsilon/2}) \exp\left\{\frac{\epsilon}{2}Z(V_t)\right\}\right) V_t + \mathcal{O}(\epsilon^3) \end{aligned} \tag{A.43}$$

where we used A.40 in the last equality. Now we have to unitarize the result so we impose the following condition:

$$V_{t+\epsilon} := e^A e^{\left\{\frac{\epsilon}{2}Z(V_t)\right\}} V_t \tag{A.44}$$

Introducing the notation:

$$\begin{cases} Z_i = \epsilon Z(W_i) \\ \text{where:} \\ W_0 = V_t \\ W_1 = \exp\left\{\frac{1}{2}Z_0\right\} W_0 = V_{t+\epsilon/2} \end{cases} \tag{A.45}$$

we can rewrite A.44 up to order $\mathcal{O}(\epsilon^3)$ as:

$$(1 + Z_1(1 + \frac{1}{2}Z_0)) = (1 + A + \frac{1}{2}A^2)(1 + \frac{1}{2}Z_0 + \frac{1}{8}Z_0^2) \tag{A.46}$$

from A.46, equation the l.h.s. with the r.h.s. order by order in ϵ, we obtain the following system of equations:

$$\begin{cases} Z_1 = A + \frac{1}{2}Z_0 & (\epsilon) \\ \frac{1}{2}Z_1 Z_0 = \frac{1}{2}A^2 + \frac{1}{2}AZ_0 + \frac{1}{8}Z_0^2 & (\epsilon^2) \end{cases} \tag{A.47}$$

Expanding $Z(V_t)$ in series and write:

$$\begin{aligned} Z_1 - Z_0 &= Z(W_1) - Z(W_0) = Z(W_0 + \Delta W) - Z(W_0) = \\ &= \sum_{n=1}^{+\infty} \frac{z_n}{n!}(W_0 + \Delta W)^n - \sum_{n=1}^{+\infty} \frac{z_n}{n!}(W_0)^n = \\ &= \sum_{n=1}^{+\infty}\sum_{i=0}^{n-1} \frac{z_n}{n!}(W_0)^i \Delta W (W_0)^{n-i-1} + \dots \end{aligned} \tag{A.48}$$

where we have set $\Delta W = W_1 - W_0$. We can note that the difference ΔW is of $\mathcal{O}(\epsilon)$ in fact:

$$\Delta W = W_1 - W_0 := V_{t+\epsilon/2} - V_t = \frac{\epsilon}{2}\dot{V}_t + \dots = \frac{\epsilon}{2} Z(V_t)V_t + \mathcal{O}(\epsilon^2) \tag{A.49}$$

so in the equation of order ϵ^2 of A.47 we can set $Z_1 \simeq Z_0$, and we would be discarding only terms of $\mathcal{O}(\epsilon^3)$.

Thus we obtain that the second equation of A.47 is an identity and from the first equation we get: $A = Z_1 - Z_0$.

Then we can write the solution of A.39 up to $\mathcal{O}(\epsilon^3)$ as:

$$\begin{cases} W_0 = V_t \\ W_1 = \exp\left\{\frac{1}{2}Z_0\right\} W_0 = V_{t+\epsilon/2} \\ V_{t+\epsilon} = \exp\left\{Z_1 - \frac{1}{2}Z_0\right\} W_1 \end{cases} \tag{A.50}$$

A.2.2 3rd Order

Now we present the explicit derivation third order method presented in [37] and used for our simulations.

First of all we need to ensure that the method will not break gauge symmetry, so we require that given $V_t \in \mathcal{G}$, $Z(V_t) \in \mathbf{g}$ we have $V_{t+\epsilon} \in \mathcal{G}$.

We write the solution of the flow equation A.39 as:

$$V_{t+\epsilon} = e^{\mathcal{C}} e^{\mathcal{B}} e^{\mathcal{A}} V_t \tag{A.51}$$

with $\mathcal{A}, \mathcal{B}, \mathcal{C} \in \mathbf{g}$ and $e^{\mathcal{A},\mathcal{B},\mathcal{C}} \in \mathcal{G}$. We then define:

$$W_0 = V_t \tag{A.52}$$

$$W_1 = e^{\mathcal{A}} \cdot W_0 = \exp\{a_0 Z_0\} \cdot W_0 \tag{A.53}$$

$$W_2 = e^{\mathcal{B}} \cdot W_1 = \exp\{b_1 Z_1 + b_0 Z_0\} \cdot W_1 \tag{A.54}$$

$$W_3 = e^{\mathcal{C}} \cdot W_2 = \exp\{c_2 Z_2 + c_1 Z_1 + c_0 Z_0\} \cdot W_2 \tag{A.55}$$

where $Z_i = \epsilon Z(W_i)$ with $i = 0, 1, 2$ and we have borrow from the standard Runge-Kutta method the idea that the solution of A.39 can be written as the product of three separate exponential where are function of only Z_0, Z_0 and Z_1, and Z_0, Z_1, Z_2 respectively:

$$\mathcal{A} = \mathcal{A}(Z_0) = a_0 Z_0 \tag{A.56}$$

$$\mathcal{B} = \mathcal{B}(Z_0, Z_1) = b_1 Z_1 + b_0 Z_0 \tag{A.57}$$

$$\mathcal{C} = \mathcal{C}(Z_0, Z_1, Z_2) = c_2 Z_2 + c_1 Z_1 + c_0 Z_0 \tag{A.58}$$

We can expand each exponential map in A.51 and write:

$$
\begin{aligned}
V_{t+\epsilon} = \Bigg\{ \Bigg[& 1 + (c_2 Z_2 + c_1 Z_1 + c_0 Z_0) + \frac{1}{2}(c_2 Z_2 + c_1 Z_1 + c_0 Z_0)^2 + \\
+ & \frac{1}{6}(c_2 Z_2 + c_1 Z_1 + c_0 Z_0)^3 \Bigg] \times \\
\times & \left[1 + (b_1 Z_1 + b_0 Z_0) + \frac{1}{2}(b_1 Z_1 + b_0 Z_0)^2 + \frac{1}{6}(b_1 Z_1 + b_0 Z_0)^3 \right] \times \\
\times & \left[1 + (a_0 Z_0) + \frac{1}{2}(a_0 Z_0)^2 + \frac{1}{6}(a_0 Z_0)^3 \right] + \mathcal{O}(\epsilon^4) \Bigg\} V_t
\end{aligned}
\tag{A.59}
$$

Now we need to write the expansion of $Z(V_t)$ around W_0, we can write Z as series:

$$
Z(W) = \sum_{n=1}^{+\infty} \frac{z_n}{n!} W^n \tag{A.60}
$$

with $z_n = \frac{d}{d\mathcal{W}} Z(W)$. Noting that the quantity $\Delta W = W_1 - W_0$ does not commute with W_0 and is of order $\mathcal{O}(\epsilon)$, then we can write the difference between $Z_1 = Z(W_1)$ and $Z_0 = Z(W_0)$ as:

$$
\begin{aligned}
Z_1 - Z_0 = & \, Z(W_0 + \Delta W) - Z(W_0) = \\
= & \sum_{n=1}^{+\infty} \frac{z_n}{n!}(W_0 + \Delta W)^n - \sum_{n=1}^{+\infty} \frac{z_n}{n!}(W_0)^n = \\
= & \sum_{n=1}^{+\infty} \sum_{i=0}^{n-1} \frac{z_n}{n!}(W_0)^i \Delta W (W_0)^{n-i-1} + \\
+ & \sum_{n=1}^{+\infty} \sum_{i=0}^{n-1} \sum_{j=i+1}^{n-1} \frac{z_n}{n!}(W_0)^i \Delta W (W_0)^{j-i-1} \Delta W (W_0)^{n-j-1} + \\
+ & \, \mathcal{O}\left((\Delta W)^3\right)
\end{aligned}
\tag{A.61}
$$

Thus we see that the initial series is reproduced for each term. In the following the we consider only the terms of the form $(\Delta W), (\Delta W)^2, \ldots,$ then we can write:

$$
Z_1 - Z_0 = \frac{dZ_0}{d\mathcal{W}}(W_1 - W_0) + \frac{1}{2}\frac{d^2 Z_0}{d\mathcal{W}^2}(W_1 - W_0)^2 + \mathcal{O}(\epsilon^4) \tag{A.62}
$$

$$
Z_2 - Z_1 = \frac{dZ_1}{d\mathcal{W}}(W_2 - W_1) + \frac{1}{2}\frac{d^2 Z_1}{d\mathcal{W}^2}(W_2 - W_1)^2 + \mathcal{O}(\epsilon^4) \tag{A.63}
$$

$$
\begin{aligned}
Z_2 - Z_0 = & \frac{dZ_0}{d\mathcal{W}}(W_1 - W_0) + \frac{dZ_1}{d\mathcal{W}}(W_2 - W_1) + \frac{1}{2}\frac{d^2 Z_0}{d\mathcal{W}^2}(W_1 - W_0)^2 \\
& + \frac{1}{2}\frac{d^2 Z_1}{d\mathcal{W}^2}(W_2 - W_1)^2 + \mathcal{O}(\epsilon^4)
\end{aligned}
\tag{A.64}
$$

where we have defined $Z'_i = \epsilon \cdot \dfrac{dZ(W_i)}{d\mathcal{W}}$. We are also using the fact that $Z_i \sim \mathcal{O}(\epsilon)$, $Z'_i \sim \mathcal{O}(\epsilon)$ and $(W_i - W_j) \sim \mathcal{O}(\epsilon)$ with $i, j = 0, 1, 2;\ i \neq j$.

In fact the following Taylor expansions hold:

$$W_1 - W_0 = \exp\{a_0 Z_0\} W_0 - W_0 = (\exp\{a_0 Z_0\} - 1) \cdot W_0 =$$
$$= \left[a_0 Z_0 + \frac{1}{2}(a_0 Z_0)^2 + \frac{1}{6}(a_0 Z_0)^3 + \mathcal{O}(\epsilon^4) \right] \cdot V_t \tag{A.65}$$
$$W_2 - W_1 = \exp\{b_1 Z_1 + b_0 Z_0\} \cdot W_1 - W_1 = (\exp\{b_1 Z_1 + b_0 Z_0\} - 1) \cdot W_1 =$$
$$= \left\{ \left[(b_1 Z_1 + b_0 Z_0) + \frac{1}{2}(b_1 Z_1 + b_0 Z_0)^2 + \frac{1}{6}(b_1 Z_1 + b_0 Z_0)^3 \right] \times \right.$$
$$\left. \times \left[a_0 Z_0 + \frac{1}{2}(a_0 Z_0)^2 + \frac{1}{6}(a_0 Z_0)^3 \right] + \mathcal{O}(\epsilon^4) \right\} \cdot V_t \tag{A.66}$$

What we obtained from A.59 and following must be compared with Taylor series of the evoluted flow $V_{t+\epsilon}$:

$$V_{t+\epsilon} = V_t + \epsilon \dot{V}_t + \frac{\epsilon^2}{2} \ddot{V}_t + \frac{\epsilon^3}{3!} V_t^{(3)} + \mathcal{O}(\epsilon^3) \tag{A.67}$$

where the dot indicates the time derivative and $^{(n)}$ the n-th time derivative respectively. If we insert repeatedly A.39 in A.67 we get:

$$V_{t+\epsilon} = V_t + \epsilon Z(V_t) V_t + \frac{\epsilon^2}{2} \frac{d}{dt} [Z(V_t) V_t] + \frac{\epsilon^3}{3!} \frac{d^2}{dt^2} [Z(V_t) V_t] + \mathcal{O}(\epsilon^4) =$$
$$= \left[1 + \epsilon \tilde{Z}_0 + \frac{\epsilon^2}{2} (\widetilde{\dot{Z}_0} + \tilde{Z}_0^2) + \frac{\epsilon^3}{6} (\widetilde{\ddot{Z}_0} + 2 \widetilde{\dot{Z}_0} \tilde{Z}_0 + \tilde{Z}_0 \widetilde{\dot{Z}_0} + \tilde{Z}_0^3) + \mathcal{O}(\epsilon^4) \right] \cdot V_t \tag{A.68}$$

where we have introduced $\tilde{Z}$'s to write explicitly epsilons and to factor out V_t:

$$Z_0 = \epsilon \tilde{Z}_0 \tag{A.69}$$
$$\dot{Z}_0 = \epsilon^2 \widetilde{\dot{Z}_0} = Z_t' Z_t \tag{A.70}$$
$$\ddot{Z}_0 = \epsilon^3 \widetilde{\ddot{Z}_0} = Z_t'' Z_t V_t Z_t + (Z_t')^2 Z_t V_t + Z_t' Z_t^2 \tag{A.71}$$

furthermore:

$$\dot{Z}_t = \frac{dZ}{dt}(V_t) = \frac{dZ(V_t)}{dV_t} \dot{V}_t = Z_t' Z_t V_t \tag{A.72}$$
$$\ddot{Z}_t = \frac{d^2 Z}{dt^2}(V_t) = Z_t'' (Z_t V_t)^2 + (Z_t')^2 Z_t V_t^2 + Z_t' Z_t^2 V_t \tag{A.73}$$

are total derivatives of $Z(V_t)$ with respect to time.

Finally, equating A.68 and A.59 at each order and eliminating redundant equations (e.g. equations from the terms $\tilde{Z}_0(\epsilon)$, $\tilde{Z}_0^2(\epsilon^2)$, $\tilde{Z}_0^3(\epsilon^2)$ give the same equations) we obtain the following equations on the coefficients:

$$\begin{cases} c_2 a_0 + c_2 b_1 + c_2 b_0 + c_1 a_0 + b_1 a_0 = \dfrac{1}{2} & \widetilde{\dot{Z}_0}(\epsilon^2) \\ \dfrac{1}{2} \left[c_2 (a_0 + b_1 + b_0)^2 + a_0^2 (c_1 + b_1) \right] = \dfrac{1}{6} & \widetilde{\ddot{Z}_0}(\epsilon^3) \\ \dfrac{1}{2} c_2 (c_2 + c_1 + c_0)(a_0 + b_0 + b_1) + \left(\dfrac{1}{2} c_1 + b_1 \right) (c_2 + c_1 + c_0) a_0 + & \\ + \dfrac{1}{2} (b_1 + b_0) b_1 a_0 = \dfrac{1}{6} & \tilde{Z}_0 \widetilde{\dot{Z}_0}(\epsilon^3) \end{cases} \tag{A.74}$$

We see that we obtain an equation for each term with zero, one or two derivatives. From these equation we could obtain the following equalities:

$$\begin{cases} b_0 = \dfrac{-1+3x+3y-6xy+6x^2y}{6(-1+x)x} \\ b_1 = \dfrac{1-3x-3y}{6(-1+x)x} \\ c_1 = \dfrac{2-5x+3x^2-4y+6xy+3y^2}{6\left(-x+x^2\right)y} \\ c_2 = \dfrac{2-3x}{6y(x+y)} \end{cases} \tag{A.75}$$

where we have defined $x = a_0$, $y = b_0 + b_1$, $z = c_0 + c_1 + c_2$.

As in the standard Runge-Kutta method and as can be seen from A.75 we have some freedom in the choice of the parameter, this residual freedom consists in setting the values of where to expand the series, we can choose two points since the final point is fixed at $t + \epsilon$. In [37] the following values are chosen:

$$\begin{cases} a_0 = \dfrac{1}{4} \\ b_0 + b_1 = \dfrac{5}{12} \to a_0 + b_0 + b1 = \dfrac{2}{3} \\ c_0 + c_1 + c_2 = \dfrac{1}{3} \to c_2 + c_1 + c_0 + b_1 + b_0 + a_0 = 1 \end{cases} \tag{A.76}$$

where on the right side we noted the terms interested in the comparison and in parenthesis the order of ϵ involved.

Appendix B

The Axial Current in Two Dimensions

In the following section we analyze the current conservation equation for the axial current in the contest of two-dimensional massless QED. This theory will serve as an introduction to the more complex theory of massless four-dimensional QCD.

The Lagrangian of two-dimensional QED is:

$$\mathcal{L} = \bar{\psi}(i\not{D})\psi - \frac{1}{4}(F_{\mu\nu})^2 \tag{B.1}$$

where, being in two dimensions, the possible values for the indices μ, ν are $0, 1$ and the covariant derivative is given by $D_\mu = \partial_\mu + ieA_{mu}$. The Dirac matrices are 2×2 matrices. The following representation:

$$\gamma^0 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \gamma^1 = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \tag{B.2}$$

satisfies the dirac algebra:

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu} \tag{B.3}$$

The matrix γ_5 is defined as the product of the Dirac matrices and commutes with each γ_μ

$$\gamma_5 = \gamma^0\gamma^1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{B.4}$$

We can define the following currents:

$$j^\mu = \bar{\psi}\gamma_\mu\psi \qquad j^{\mu 5} = \bar{\psi}\gamma_\mu\gamma_5\psi \tag{B.5}$$

which are conserved if there is no mass term in the Lagrangian.

To make the conservation law more explicit, we can write the fermion field ψ in the spinor basis, i.e.:

$$\psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} \tag{B.6}$$

where the subscript indicates the γ_5 eigenvalue. Using the explicit form of the Dirac matrices and of the fermion field written in (B.2) and (B.6), we can rewrite

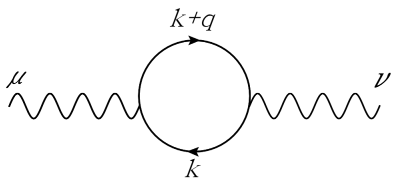

Figure B.1: The vacuum polarization Feynman diagram in QED, $i\Pi_2^{\mu\nu}(q)$

the Lagrangian as:

$$\mathcal{L} = \psi_+^\dagger i(D_0 + D_1)\psi_+ + \psi_-^\dagger i(D_0 - D_1)\psi_- \tag{B.7}$$

In the free theory, we would obtain for the fields ψ_+ and ψ_- the following equations:

$$\begin{aligned} i(\partial_0 + \partial_1)\psi_+ = 0 \\ i(\partial_0 - \partial_1)\psi_- = 0 \end{aligned} \tag{B.8}$$

The solution for ψ_+ and ψ_- are, respectively, waves that move to the right or to the left in one-dimensional space. Thus ψ_+ can conveniently be re-labelled as right-moving fermion (or ψ_R) and ψ_- can conveniently be re-labelled as left-moving fermion (or ψ_L).

If the fields are massless the Lagrangian contains no terms that mix the "right" and "left" fields defined above thus it would be natural to find that the currunt for those fields are separately conserved:

$$\partial_\mu \left(\bar{\psi}\gamma_\mu \left(\frac{1-\gamma_5}{2} \right) \psi \right) = 0 \tag{B.9}$$

$$\partial_\mu \left(\bar{\psi}\gamma_\mu \left(\frac{1+\gamma_5}{2} \right) \psi \right) = 0 \tag{B.10}$$

In two-dimesional spacetime the following relation holds among the γ_μ's and the matrix γ_5:

$$\gamma_\mu \gamma_5 = -\varepsilon^{\mu\nu}\gamma_\nu \tag{B.11}$$

where $\varepsilon^{\mu\nu}$ is a total antisimmetric tensor, with $\varepsilon^{01} = 1$. The currents $j^{\mu 5}$ and j^μ have the same relation.

B.1 The Vaacum Polarization Diagram

We report here the calculation of the vacuum polarization diagram for QED.

The electron loop is given by:

$$\begin{aligned} i\Pi_2^{\mu\nu}(q) &= (-ie)^2(-1)\int \frac{d^2k}{(2\pi)^2} \operatorname{Tr}\left[\gamma_\mu \frac{i}{(\not{k}-m)} \gamma^\nu \frac{i}{\not{k}+\not{q}-m} \right] \\ &= -(-ie)^2 \int \frac{d^2k}{(2\pi)^2} \operatorname{Tr}\left[\gamma_\mu \frac{i(\not{k}+m)}{k^2-m^2} \gamma^\nu \frac{i(\not{k}+\not{q}+m)}{(k+q)^2-m^2} \right] \\ &= -\operatorname{Tr}[\mathbb{1}]e^2 \int \frac{d^2}{(2\pi)^2} \frac{k^\mu (k+q)^\nu + k^\nu (k+q)^\mu - g^{\mu\nu}(k\cdot(k+q)-m^2)}{(k^2-m^2)((k+q)^2-m^2)} \end{aligned} \tag{B.12}$$

Where it is possible to use the renormalized parameters e, m in stead of the bare coupling costants e_0, m_0 since the difference would give a contribution of order α^2.

Making use of the following identity, obtained introducing a Feynman parameter:

$$\begin{aligned}\frac{1}{(k^2-m^2)((k+q)^2-m^2)} &= \int_0^1 dx \frac{1}{(k^2+2xk\cdot q+xq^2-m^2)^2} \\ &= \int_0^1 dx \frac{1}{(\ell^2+x(1-x)q^2-m^2)^2}\end{aligned} \tag{B.13}$$

with $\ell = k + xq$. Performing a Wick rotation such that $l^0 = i\ell_E^0$ we have:

$$i\Pi_2^{\mu\nu}(q) = -\operatorname{Tr}[\mathbb{1}]ie^2 \int_0^1 dx \int \frac{d^d\ell_E}{(2\pi)^d} \frac{(-\frac{2}{d}+1)g^{\mu\nu}\ell_E^2}{(\ell_E^2+\Delta)^2} \tag{B.14}$$

Using some known formulæ [51] we obtain:

$$\begin{aligned}i\Pi_2^{\mu\nu}(q) &= \frac{-1}{(4\pi)^{d/2}}\left(1-\frac{d}{2}\right)\Gamma\left(1-\frac{d}{2}\right)\left(\frac{1}{\Delta}\right)^{1-\frac{d}{2}} g^{\mu\nu} = \\ &= \frac{1}{(4\pi)^{d/2}}\Gamma\left(2-\frac{d}{2}\right)\left(\frac{1}{\Delta}\right)^{2-\frac{d}{2}}\cdot(-\Delta g^{\mu\nu})\end{aligned} \tag{B.15}$$

Then in two dimensions we have:

$$\begin{aligned}i\Pi^{\mu\nu}(q) &= -i(q^2g^{\mu\nu}-q^\mu q^\nu)\frac{2e^2}{(4\pi)^{d/2}}\operatorname{Tr}[\mathbb{1}] \\ &\times \int_0^1 dx x(1-x)\frac{\Gamma(2-\frac{d}{2}}{(-x(1-x)q^2)^{2-d/2}}\end{aligned} \tag{B.16}$$

In two dimensions, $d = 2$ we have $\operatorname{Tr}[\mathbb{1}] = 2$, and the above expression becomes:

$$\begin{aligned}i\Pi^{\mu\nu}(q) &= i(q^2g^{\mu\nu}-q^\mu q^\nu)\frac{2e^2}{4\pi}\cdot 2\cdot\frac{1}{q^2} \\ &= i\left(g^{\mu\nu}-\frac{q^\mu q^\nu}{q^2}\right)\frac{e^2}{\pi}\end{aligned} \tag{B.17}$$

The term in (B.17) has the structure of a photon mass term, so the photon receives the mass:

$$m_\gamma^2 = \frac{e^2}{\pi} \tag{B.18}$$

The possibility of having a non-zero mass vector field in two dimension was for showed by J. Schwinger in [40].

Once we have an explicit expression for the vacuum polarization, we can find the expectation value of the current induced by a background electromagnetic field.

This quantity is given by the diagram in fig. which gives:

$$\int d^2x e^{iq\cdot x}\langle j^\mu(x)\rangle = \frac{i}{e}\left(i\Pi^{\mu\nu}(q)\right)A_\nu(q) = \\ = -\left(g^{\mu\nu} - \frac{q^\mu q^\nu}{q^2}\right)\cdot \frac{e}{\pi}A_\nu(q) \tag{B.19}$$

where $A_\nu(q)$ is the Fourier transform of the background field. This quantity manifestly satisfies the relation $q_\mu\langle j^\mu(q)\rangle = 0$.

Making use of the relation (B.11) we can rewrite the preceding relation as:

$$\langle j^{\mu 5}(q)\rangle = -\varepsilon^{\mu\nu}\langle j_\nu(q)\rangle = \\ = \varepsilon^{\mu\nu}\frac{e}{\pi}\left(A_\nu(q) - \frac{q_\nu q^\lambda}{q^2}A_\lambda(q)\right) \tag{B.20}$$

If the axial vector current were conserved, this object would satisfy the Ward identity. Instead we have:

$$q_\mu\langle j^{\mu 5}(q)\rangle = \frac{e}{\pi}\varepsilon^{\mu\nu}q_\mu A_\nu(q) \tag{B.21}$$

This is the Fourier transform of the field equation:

$$\partial_\mu j^{\mu 5} = \frac{e}{2\pi}\varepsilon^{\mu\nu}F_{\mu\nu} \tag{B.22}$$

Apparently, the axial vector current is not conmserved in the presence of electromagnetic fields, as the result of an anomalous behaviour of its vacuum polarization diagram.

The problem come in the regularization of the vacuum polarization diagram. By dimensional analysis we can write in general:

$$i\Pi^{\mu\nu} = ie^2\left(Ag^{\mu\nu} - B\frac{q^\mu q^\nu}{q^2}\right) \tag{B.23}$$

the coefficient B is a definite integral and is, in any event, unambiguosly determined by the low-energy structure of the theory since it is the residue of the pole in q^2. However, the integral A is logarithmically divergent so its value depends on the regularization. Dimesional regularization automatically subtracts this integral to set $A = B$, then the vector current Ward identity is satisfied. Another possibility was to set directly $A = 0$, this would lead to the following consequences:

$$q_\mu\langle j^\mu(q)\rangle = \frac{e}{\pi}q^\nu A_\nu(q) \tag{B.24}$$

This results would depend on the unphysical gauge degrees of freedom of the vector potential. We must conclude, then, that it is not possible to regularize two dimensional QED so that, simultaneously, the theory is gauge invariant and the axial vector current is conserved.

The last argument shows clearly that requiring gauge invariance for the theory lead to the anomalous nonconservation of the axial vector current.

B.2 Axial Current Non-Conservation

Another possible viewpoint on the problef of the anomaly of the axial current is to study the operator equation for the divergence of $j^{\mu 5}$. The variation of the Lagrangian(B.1) leads to the following two equations of motion for the fermion fields:

$$\partial\!\!\!/\psi = -ieA\!\!\!/\psi \tag{B.25}$$

$$\partial_\mu \bar{\psi}\gamma_\mu = ie\bar{\psi}A\!\!\!/ \tag{B.26}$$

Summing these equations one would easily conclude that the following conservation law holds:

$$\partial_\mu j^{\mu 5} = 0 \tag{B.27}$$

Nevertheless, the explicit construction of the divergence of $j^{\mu 5}$ shows some subtleties which will alter the final conclusion, and that will reproduce the result of eq. (B.22).

A way to construct the axial current is to place the two fields ψ, $\bar{\psi}$ at two distinct spacetime point, separated by an infinitesimal distance ϵ and then take the limit for $\epsilon \to 0$:

$$j^{\mu 5} = \text{Symm}\lim_{\epsilon\to 0}\left\{\bar{\psi}\left(x+\frac{\epsilon}{2}\right)\gamma_\mu\gamma_5 \exp\left[-ie\int_{x-\epsilon/2}^{x+\epsilon/2} dz\cdot A(z)\right]\psi\left(x-\frac{\epsilon}{2}\right)\right\} \tag{B.28}$$

in the previous equation we have inserted a term

$$\exp\left[-ie\int_{x-\epsilon/2}^{x+\epsilon/2} dz\cdot A(z)\right]$$

called a *Wilson line*, to ensure the local gauge invariance of $j^{\mu 5}$. The form of the Wilson line term will be derived explicitly in the next chapters.

The limit has to be taken symmetrically to obtain the correct transformation propertied of $j^{\mu 5}$ under Lorentz transformations, this implies the following relations:

$$\begin{aligned} &\underset{\epsilon\to 0}{\text{sylim}}\left\{\frac{\epsilon^\mu}{\epsilon^2}\right\} = 0 \\ &\underset{\epsilon\to 0}{\text{sylim}}\left\{\frac{\epsilon^\mu\epsilon^\nu}{\epsilon^2}\right\} = \frac{1}{d}g^{\mu\nu} \end{aligned} \tag{B.29}$$

where sylim denotes the symmetric limit. Taking the divergence of (B.28) we obtain:

$$\partial_\mu j^{\mu 5} = \operatorname*{sylim}_{\epsilon\to 0}\left\{\left(\partial_\mu\bar{\psi}\left(x+\frac{\epsilon}{2}\right)\right)\gamma_\mu\gamma_5\exp\left[-ie\int\limits_{x-\epsilon/2}^{x+\epsilon/2} dz\cdot A(z)\right]\psi\left(x-\frac{\epsilon}{2}\right)+\right.$$
$$+\bar{\psi}\left(x+\frac{\epsilon}{2}\right)\gamma_\mu\gamma_5\exp\left[-ie\int\limits_{x-\epsilon/2}^{x+\epsilon/2} dz\cdot A(z)\right]\left(\partial_\mu\psi\left(x-\frac{\epsilon}{2}\right)\right)+$$
$$\left.+\bar{\psi}\left(x+\frac{\epsilon}{2}\right)\gamma_\mu\gamma_5\left[-ie\epsilon^\nu\partial_\mu A_\nu(x)\right]\left(\partial_\mu\psi\left(x-\frac{\epsilon}{2}\right)\right)\right\} \tag{B.30}$$

Using the equations of motion and keeping terms up to order ϵ, we obtain:

$$\begin{aligned}\partial_\mu j^{\mu 5} = \operatorname*{sylim}_{\epsilon\to 0}&\left\{\bar{\psi}\left(x+\frac{\epsilon}{2}\right)\left[ie\not{A}\left(x+\frac{\epsilon}{2}\right)-ie\not{A}\left(x-\frac{\epsilon}{2}\right)\right.\right.\\ &\left.\left.-ie\epsilon^\nu\gamma_\mu\partial_\mu A_\nu(x)\right]\gamma_5\psi\left(x-\frac{\epsilon}{2}\right)\right\}\end{aligned} \tag{B.31}$$

and finally:

$$\partial_\mu j^{\mu 5} = \operatorname*{sylim}_{\epsilon\to 0}\left\{\bar{\psi}\left(x+\frac{\epsilon}{2}\right)\left[-ie\gamma_\mu\epsilon^\nu\left(\partial_\mu A_\nu-\partial_\nu A_\mu\right)\right]\gamma_5\psi\left(x-\frac{\epsilon}{2}\right)\right\} \tag{B.32}$$

This expression seems to vanish in the limit $\epsilon\to 0$, but the contraction of the fermion field in two dimensions gives:

$$\begin{aligned}\psi(y)\bar{\psi}(x) &= \int\frac{d^2k}{(2\pi)^2}e^{-ik\cdot(y-z)}\frac{i\not{k}}{k^2} =\\ &= -\not{\partial}\left(\frac{i}{4\pi}\log(y-z)^2\right) =\\ &= \frac{-i}{2\pi}\frac{\gamma^\alpha(y-z)_\alpha}{(y-z)^2}\end{aligned} \tag{B.33}$$

Thus

$$\bar{\psi}\left(x+\frac{\epsilon}{2}\right)\not{A}\psi\left(x-\frac{\epsilon}{2}\right) \tag{B.34}$$

because the contraction of the fermion fields is singular as $\epsilon\to 0$ the term in eq. (B.32) can give a finite contribution, and we find:

$$\begin{aligned}\partial_\mu j^{\mu 5} &= \operatorname*{sylim}_{\epsilon\to 0}\left\{\frac{-i}{2\pi}\operatorname{Tr}\left[\frac{\gamma^\alpha\epsilon_\alpha}{\epsilon^2}\gamma_\mu\gamma_5\right]\cdot\left(-ie\epsilon^\nu(\partial_\mu A_\nu-\partial_\nu A_\mu)\right)\right\}\\ &= \operatorname*{sylim}_{\epsilon\to 0}\left\{\frac{-i}{2\pi}\operatorname{Tr}\left[\frac{\gamma^\alpha\epsilon_\alpha}{\epsilon^2}\gamma_\mu\gamma_5\right]\cdot\left(-ie\epsilon^\nu F_{\mu\nu}\right)\right\}\end{aligned} \tag{B.35}$$

Using the relation, valid in two dimensions:

$$\operatorname{Tr}\left[\gamma^\alpha\gamma_\mu\gamma_5\right] = 2\varepsilon^{\alpha\mu} \tag{B.36}$$

we finally arrive to:

$$\begin{aligned}\partial_\mu j^{\mu 5} &= \frac{e}{2\pi} \operatorname*{sylim}_{\epsilon\to 0} \left\{ 2\frac{\epsilon_\mu \epsilon^\nu}{\epsilon^2} \varepsilon^{\mu\alpha} F_{\nu\alpha} \right\} \\ &= \frac{e}{2\pi} 2 \cdot \frac{1}{2} g^{\mu\nu} \varepsilon^{\mu\alpha} F_{\nu\alpha} = \\ &= \frac{e}{2\pi} \varepsilon^{\nu\alpha} F_{\nu\alpha}\end{aligned} \tag{B.37}$$

Acknowledgements

I wish to thank prof. Claudio Destri and prof. Carlo Oleari for their assistance with the setup and run of TURING. I also wish to thank Dr. Paolo Dini for the support provided with my INFN account and related matters. I am indebted to Dr. Michele Pepe, for giving me the priority on the use of TURING for the last run of my simulations.

Ringraziamenti (II)

Mal: «Well, we're still flying.»
Simon: «That's not much.»
Mal: «It's enough.»

Firefly (ep. 1 - Serenity)

Detesto il rischio di dimenticare qualcuno degno di essere citato, ma mi lancerò lo stesso nei ringraziamenti personali. Lo spazio qui è limitato, ma sappiate che vi ho pensati tutti.

L'università, prima di tutto, mi ha permesso di conoscere alcune persone che adesso hanno un posto importante nella mia vita: senza di voi non ce l'avrei mai fatta e non credo di riuscire a spiegare in quali e quanti modi mi avete aiutato durante questo percorso. Un ringraziamento speciale va a Chiara, la sorella che mi sono scelto, Davide e Veronica. Grazie per esserci stati dal primo all'ultimo giorno, dentro e fuori dall'università. Anche Rocco, Alice e Claudio meritano di essere menzionati.

Un ringraziamento va ai miei amici: Federico, Stefano, Emanuele "Master", Roberto, Mattia, Andrea e Monica sono i primi che mi vengono in mente (ecco, adesso avrò fatto arrabbiare un sacco di gente!) Lia, spero ti piacerà la citazione di Firefly.

La banda, intesa nel senso peggiore del termine, di Wikimedia Italia, di Wikipedia, del mondo Wikimedia, e dell'universo FLOSS meriterebbe un capitolo a parte, ma mi sto già dilungando troppo: scelgo Frieda ed Andrea come destinatari di tutti i miei strali `=P`.

Grazie alla mia famiglia, per il supporto (o la sopportazione?). Spero che gli zii, e soprattutto le zie, capiranno che non posso citarli tutti a meno di non riempire un'altra pagina intera. Tra i cugini, ringrazio Elena e Giulia per tutti.

Un ringraziamento va a tutti i miei insegnanti e a tutti coloro i quali mi hanno insegnato qualcosa in questi anni (sono tanti, anche solo tra le persone che ho citato qui sopra), ne scelgo alcuni rappresentativi: la mia maestra Anna Pagnoncelli, la mia prof. di Economia aziendale Erminia Pini ed il prof. di Matematica Sergio Dell'Orto.

Ultimi, ma solo perché sono i più importanti, i miei genitori, ai quali questa tesi è dedicata.

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