**UNIVERSIDADE DE SÃO PAULO
INSTITUTO DE FÍSICA DE SÃO CARLOS**

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**Confinement, ghost sector and geometry
in lattice gauge theories**

São Carlos

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**Confinement, ghost sector and geometry
in lattice gauge theories**

Dissertation presented to the Graduate Program in Physics at the Instituto de Física de São Carlos, Universidade de São Paulo, to obtain the degree of Master in Science.

Concentration area: Basic Physics

Advisor: Profa. Dra. Tereza Cristina da Rocha Mendes

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*I dedicate this work for all students.
Gather yourself together,
for you are the future of the Earth.
We must not let anyone destroy it.*

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“The saddest aspect of life right now is that science gathers knowledge faster than society gathers wisdom.”

Isaac Asimov

“When radium was discovered, no one knew that it would prove useful in hospitals. The work was one of pure science. And this is a proof that scientific work must not be considered from the point of view of the direct usefulness of it.”

Maria Skłodowska-Curie

ABSTRACT

LACHINI, N. P. **Confinement, ghost sector and geometry in lattice gauge theories.** 2019. 188p. Dissertation (Master in Science) - Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, 2019.

In this work we study the Gribov-Zwanziger scenario of confinement through lattice gauge theories. We start by reviewing continuum aspects of quantized Yang-Mills theories and the Faddeev-Popov method. After that, we present the gauge-copies problem and its potential resolution by restricting the path integral to the Gribov region, using the semi-classical computation as an illustration. Then we do a survey on lattice gauge theory and describe the main procedures and algorithms necessary to study the confinement problem numerically. At this point, we do a digress and review general features of confinement, from the well-known phenomenological models to the Green's functions and center dominance approaches. Finally, we present simulations of the ghost-sector and the geometry of gauge-space for $SU(2)$ theory. This includes a prescription for the discretization of BPST instanton backgrounds and the verification of their lattice topological charges. In that aspect, we show results supporting that instantons probably do not contribute to ghost enhancement. Also, using relatively small lattices, we compute the gluon and ghost propagators and the static quark-antiquark potential on vortex-only and vortex-removed ensembles through the so-called center projection and vortex removal procedures. We gather data that reproduce already published work in favor of the center dominance picture. Moreover, we are also able to present preliminary but novel results that numerically verify the localization of center vortices on the Gribov horizon and their probable consistency with massive-type solutions of the Dyson-Schwinger equations, besides a computation of the gluon propagator for pure $SU(2)$ vortices.

Keywords: Lattice gauge theory. Faddeev-Popov Ghosts. Gribov-Zwanziger Scenario. BPST Instantons. Center projection

RESUMO

LACHINI, N. P. **Confinamento, setor fantasma e geometria em teorias de gauge na rede.** 2019. 188p. Dissertação (Mestrado em Ciências) - Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, 2019.

Neste trabalho estudamos o cenário de confinamento de Gribov-Zwanziger através da teoria de calibre na rede. Iniciamos por uma revisão de aspectos da teoria de Yang-Mills quantizada e do método de Faddeev-Popov. Em seguida, apresentamos o problema das cópias de gauge e sua potencial resolução pela restrição da integral de trajetória à região de Gribov, usando o cálculo semi-clássico como ilustração. Então partimos para o estudo de teorias de calibre na rede e descrevemos os principais procedimentos e algoritmos necessários ao estudo numérico do confinamento. Neste ponto fazemos uma digressão para revisar aspectos gerais do confinamento, desde os seus bem conhecidos modelos fenomenológicos até as diferentes abordagens por funções de Green e dominância de centro. Finalmente, apresentamos simulações do setor fantasma e da geometria do espaço de calibre para a teoria $SU(2)$. Isso inclui uma prescrição da discretização de instantons BPST e a verificação de suas cargas topológicas na rede. Neste aspecto, mostramos resultados que indicam a provável não contribuição ao fortalecimento do propagador de fantasmas por configurações de instanton. Também, usando redes relativamente pequenas, calculamos os propagadores do glúon e do fantasma e o potencial estático quark-antiquark em ensembles sem vórtices e somente com vórtices, através dos conhecidos métodos de projeção de centro e remoção de vórtices. Reunimos dados que reproduzem trabalhos publicados anteriormente em favor do cenário de dominância de centro. Ademais, apresentamos resultados preliminares e inéditos que verificam numericamente a localização de vórtices de centro no horizonte de Gribov e sua consistência com soluções do tipo massivas das equações de Dyson-Schwinger, além do cálculo do propagador do glúon para vórtices puros em $SU(2)$.

Palavras-chave: Teoria de calibre na rede. Fantasmas de Faddeev-Popov. Cenário de Gribov-Zwanziger. Instantons BPST. Projeção de centro

CONTENTS

1	INTRODUCTION	17
2	GAUGE THEORIES	23
2.1	Classical Theory	23
2.1.1	Electromagnetic Field	23
2.1.2	Yang-Mills Field	25
2.2	Quantum Theory	28
2.2.1	Electromagnetic Field: Coulomb gauge	29
2.2.2	Electromagnetic Field: Lorenz gauge	30
2.2.3	Path Integrals: Quantum Mechanics	34
2.2.4	Path Integrals: Quantum Field Theory	40
2.3	Faddeev-Popov Method	45
2.3.1	Electromagnetic Case	45
2.3.2	Yang-Mills Case	49
3	GRIBOV-ZWANZIGER SCENARIO	53
3.1	The Problem	53
3.1.1	Gribov Copies	53
3.1.2	Gribov Region	54
3.2	No-Pole Condition	59
3.3	Propagators	63
3.3.1	Gluon Propagator	63
3.3.2	Ghost Propagator	65
3.4	Gribov-Zwanziger Action	66
3.5	BRST symmetry	69
4	LATTICE GAUGE THEORY	75
4.1	Lattice Generalities	75
4.1.1	Regulator	75
4.1.2	Link Variables	76
4.1.3	Observables and Wilson Action	78
4.1.4	Path Integral	80
4.1.5	Strong-Coupling Expansion	81
4.2	Gauge Fixing	84
4.2.1	Lattice Gribov Region	84
4.2.2	Faddeev-Popov Matrix	85

4.2.3	Algorithms	87
4.3	Physical Limits	90
4.4	Monte Carlo Methods	93
4.4.1	Markov Chains	93
4.4.2	Algorithms	95
4.4.3	Thermalization	98
4.4.4	Statistical Errors	100
5	CONFINEMENT	107
5.1	Phenomenological Basis and Models	107
5.1.1	Linear Potential and Wilson Loop	107
5.1.2	Regge Trajectories	109
5.2	Color Confinement in Landau Gauge	111
5.2.1	Kugo-Ojima	111
5.2.2	Zwanziger criterion	113
5.2.3	Functional Approaches	115
5.2.4	Lattice results	117
5.3	Center Dominance	119
5.3.1	Confinement and Color Screening	119
5.3.2	N -ality and Center Symmetry	122
6	APPLICATIONS AND RESULTS	127
6.1	Center Vortices	127
6.1.1	Center Projection	127
6.1.2	Static Quark-Antiquark Potential	129
6.2	BPST Instantons	132
6.2.1	Topology Elements	132
6.2.2	Lattice Topology	134
6.2.3	Instanton Background	135
6.3	Geometry and Ghost Sector	139
6.3.1	Ghost Propagator and Analytical Bounds	139
6.3.2	R functional	147
6.3.3	Crossing the Gribov horizon	149
7	CONCLUSIONS	155
	REFERENCES	157

	APPENDIX	173
	APPENDIX A – NOTATION	175
A.1	Minkowski space	175
A.2	Euclidean space	175
	APPENDIX B – PATH INTEGRAL SUPPLEMENT	177
B.1	Gaussian Integrals	177
B.2	Generating Functional and Correlation Functions	179
B.3	Perturbation Theory	180
	APPENDIX C – GROUP SUPPLEMENT	183
C.1	Haar measure	183
C.2	Integration	184
C.3	SU(2) Conventions and Formulas	184
C.3.1	Pauli Matrices	184
C.3.2	Trace Properties	185
C.3.3	Caley-Klein Parametrization	185
	APPENDIX D – ALGORITHMS	187
D.1	Conjugate Gradient	187
D.2	Power Method	187

1 INTRODUCTION

According to the current paradigm of Physics, Nature is described by four fundamental forces. The most present in our day-to-day life is the *gravitational* force, chronologically the first one to be described: by Newton in the 17th century and revisited by Einstein in the 1910s. Also, the *electromagnetic* force was fundamental to the development of modern society in the 19th century and, headed by Maxwell, was the second one to receive proper physical formalization. Both gravity and electromagnetism are long-range forces. Conversely, the *weak* and *strong* forces are (effectively) short-ranged and were revealed with the exploration of the atomic structure. This dates back to the discovery of the nucleus and the electron at the beginning of the 20th century. Apart from gravity, the other three forces are satisfactorily described within the Standard Model.¹

Figure 1.1 – The Standard Model and the graviton.

Source: GALBRAITH et al.²

At the core of the Standard Model reside the so-called *gauge theories*.³ These permeate physics at least since the conception of Maxwell’s electromagnetic theory, when its manifest gauge invariance was supposed to be accidental. What we can call the first phase of gauge theories started with Einstein’s work and ended just before Yang and Mills’.⁴ This stage consisted in the development of general relativity and its “geometrization” of gravity on one side, and the progressive reinterpretation and use of gauge invariance in electromagnetism and quantum mechanics on the other. In 1918, Weyl was the first one who tried to link gravity and electromagnetism by attaching a scale factor to the

space-time metric.⁴ More than ten years later, after further development of quantum mechanics, he reinterpreted such scale factor as a phase of the wave function. From this reasoning, the *gauge principle* was first used to generate electromagnetic theory from the localization of a global symmetry. Finally, in the 1950s gauge theory was put at the same level of mathematical abstraction as general relativity through the geometrical framework of fiber bundles.⁴

The second phase of gauge theory began with Yang and Mills' work⁵ describing a non-Abelian theory with local $SU(2)$ symmetry. At the time, there was no hope that it could successfully describe nuclear forces. The reason was that, inspired by Yukawa's theory of meson exchanges, the mediators of short-ranged interactions were believed to be very massive, while Yang-Mills' were massless. That picture was revived with the description of the weak force, culminating in the mass generation mechanism⁶⁻⁸ and electroweak theory^{9,10} in the 1960s. At that time, experiments started to show that the neutron, proton and pion were far away from being the only subatomic particles, which led Gell-Mann to propose the Eightfold Way in 1961 to accommodate hadrons in a single framework.¹ Furthermore, the large number of new particles gave a hint that those hadrons could not be as elementary as in the way it was thought before. This gave birth, in 1964, to the quark model,^{11,12} described by the representation of a global symmetry: the non-exact *flavor* $SU(3)$ symmetry. In that description, hadrons are composed of quarks: three quarks for baryons and a quark-antiquark pair for mesons.

The deep-inelastic-scattering experiments at SLAC in the 1960s showed a peculiar scaling invariance called Bjorken scaling. These highly energetic collisions demonstrated that when hit by an electron in this regime, a proton seemed to be composed of point-like and almost free components called *partons*,¹³ and these were subsequently converted into hadrons. The quark was readily included in the parton model, and it seemed that, whatever force was involved in those reactions, it was not the weak force, because of the small time scales involved. This also evidenced the apparently strange *asymptotic-freedom* behavior,^{3,13} i.e., that the quarks should be almost free when very close to each other, something that was not expected for an allegedly strong force.

Returning to the quark model, one of its great flaws was the inconsistency with the Pauli principle when describing resonances, e.g. the Δ^{++} resonance, composed of three identical quarks. This motivated the introduction of an exact gauge symmetry as an *ad hoc* solution at the time by Greenberg, Han and Nambu.³ The quantum number corresponding to the new symmetry was named *color*. In the light of the parton model and deep-inelastic-scattering experiments, the Yang-Mills theory with color symmetry was shown to satisfy the fractional scattering of electron-positron annihilation

$$R = \frac{\sigma(e^+e^- \rightarrow \text{hadrons})}{\sigma(e^+e^- \rightarrow \mu^+\mu^-)},$$

indicating the presence of $N_c = 3$ colors in a theory with 3 or more quark flavors. Moreover, in 1973, Gross, Wilczek and Politzer^{14,15} showed that Yang-Mills theories were asymptotically free, supporting Bjorken scaling. Further consolidation of non-Abelian gauge theories was the proof of their renormalizability given by 't Hooft¹⁶ and the prediction of Bjorken scaling violation at experiments with higher resolutions.¹³ The $SU(N_c = 3)$ Yang-Mills theory mediated by massless bosons called gluons, together with massive quarks, is known as *quantum chromodynamics* (QCD), being the sector of the Standard Model that describes the strong force.

Figure 1.2 – The running of the strong-coupling constant in the perturbative region.

Source: TANABASHI et al.¹⁷

In QCD, gluons are the carriers of the color field between quarks, in resemblance to the photon and the electromagnetic field in QED. A drastic difference is that gluons are color-charged and consequently interact with other gluons as well, unlike the photons. That characteristic leads to vacuum polarization and antiscreening,³ giving rise to the observed asymptotic-freedom. Consequently, as presented in Figure 1.2, the strong-force coupling is small at higher energies (or smaller distances), being suitable for perturbative treatment.^{13,18} However, an apparently weak point of QCD, at the time of its conception, was the fact that we do not observe free quarks in experiments. This phenomenon is called *quark confinement* and is supported by theoretical arguments and computer simulations, although no one was able to derive it directly from QCD yet. As a phenomenon governed by the strong force at long distances, it cannot be described solely by perturbation theory.

The study of the vacuum structure through $SU(N_c)$ Yang-Mills theories without

quarks showed that the essence of confinement is already present in the pure gluon theory. Usually, the complicated aspects of QCD, namely its non-perturbative regime, are traced back to the non-commutativity of $SU(N_c)$ and the highly non-trivial topology of the non-Abelian group. In fact, four-dimensional quantum Yang-Mills theories still lack a rigorous mathematical formulation, this being connected with confinement and the proof of the mass gap in an axiomatic paradigm.¹⁹ Nevertheless, many progresses were possible in the path integral quantization, which includes the Faddeev-Popov gauge fixing.²⁰ One of the first approaches to the infrared behavior of Yang-Mills theories, closely related to confinement, was pioneered in 1978 by Gribov^{21,22} and proposed to extend gauge fixing to non-perturbative regimes. Gribov's gauge fixing and quantization connected long-range effects to the infrared behavior of Green functions, which opened the way for the investigation of confinement from the point of view of *color confinement*.

Following, an almost natural framework for non-perturbative QCD and confinement was introduced in 1974 by Wilson²³ and consists in describing the necessary fields on an Euclidean lattice instead of on the continuum space-time. In lattice gauge theory, the quantum fields are safely defined on the lattice links and sites and can be used in computer simulations to calculate observables in regimes not accessible by perturbation theory. Of course, one needs to do a careful extrapolation to the continuum limit^{24,25} before drawing conclusions from lattice data. Since its primordial days, lattice QCD simulations supported asymptotic-freedom²⁶ and the confinement picture,²⁷ being computations of the static quark-antiquark potential the most striking demonstrations of the latter.²⁸

The lattice approach to quantum field theories offers a first-principles framework for studying confinement from the Gribov-Zwanziger scenario perspective.^{22,29} Mainly, lattice simulations have been providing results on Green functions since the 1980s. Almost as in a symbiotic relation, those results have been used by analytical approaches as a reference guide for the non-perturbative behavior of Yang-Mills theories. Besides the Gribov-Zwanziger scenario and the ideas that stemmed from it, other analytical approaches as the Dyson-Schwinger equations^{30,31} and the functional renormalization group³² have used lattice data, many times as input or reference (good or bad) for calculations. Moreover, the configuration-based approach to confinement³³⁻³⁵ was revitalized by lattice gauge theory in the 1990s,³⁶ showing that quark confinement is most probably related to the unbroken realization of a global center symmetry somehow encoded in QCD through specific field configurations such as center vortices and Abelian monopoles. Analyzing the impact of different semiclassical configurations on confinement turned out to be a popular methodology and it can be explored using other topological objects, e.g. merons and calorons.³⁷ Furthermore, lattice methods can be used to deepen the connection between those configurations and the Gribov-Zwanziger scenario by studying their gauge-geometrical characteristics.³⁸

In this dissertation, the conceptual tools necessary for studying confinement through the Gribov-Zwanziger scenario on the lattice will be reviewed and discussed. In Chapter 2 we will develop the theory of gauge fields, passing by some classical and quantum aspects of electromagnetism and Yang-Mills theories. Following that, we will review the problem of gauge copies and the Gribov-Zwanziger scenario in Chapter 3. Lattice theory and methods applied to pure gauge theories will be introduced and described in Chapter 4, aiming at the Landau gauge-fixing algorithms. Besides discussing what is confinement, a review of the principal approaches for its investigation is made in Chapter 5. Next, in Chapter 6 we present methods for generating different semiclassical configurations on the lattice and characterizing their geometrical aspects. Finally, a brief conclusion is given.

2 GAUGE THEORIES

The basic framework for studying QCD and, more generally, the Standard Model, is the vast field of *gauge theories*. These are characterized by an intrinsic redundancy in the description of the system at the classical level, parametrized by gauge transformations. We can have both global and local symmetries associated to those transformations. We will be interested in the local ones, as they play a key role in the explanation of fundamental interactions.

Nevertheless, we must recall that local gauge transformations are not related to physical symmetries as it happens for the relation between rotations and angular momentum. They are instead an ambiguity that emerges from the description, as we will see in the next sections. In fact, only gauge-invariant quantities are considered to be physical observables. Furthermore, we will need to treat this redundancy when moving on to the quantum theory by gauge fixing the fields, which essentially generates all the problems considered in this thesis.

We will present Yang-Mills theories and their $SU(N_c)$ symmetry as a generalization of covariant electromagnetism at the classical level. Afterwards, we will make a transition to the quantum theory, first outlining canonical approaches to electromagnetism, and then tackling the path integral formalism. Finally, we will cover the Faddeev-Popov gauge-fixing procedure and introduce the so-called Faddeev-Popov ghosts.

2.1 Classical Theory

2.1.1 Electromagnetic Field

Instead of approaching the Yang-Mills theories directly, we start by describing the gauge properties of the classical electromagnetic theory in four dimensions and in the absence of sources. In this case, the Lagrangian density in covariant notation is given by³⁹

$$\mathcal{L}_{\text{EM}} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu}, \quad (2.1)$$

where

$$F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) \quad (2.2)$$

is the electromagnetic field tensor and A_μ is the 4-vector potential embedded in the 3+1 Minkowski space $\mathbb{M}$ (see [A.1](#) for notation conventions). We also define the associated action functional

$$S_{\text{EM}}[A] = \int d^4x \mathcal{L}_{\text{EM}}(A_\mu, \partial_\nu A_\mu). \quad (2.3)$$

Using Euler-Lagrange's equations derived from the principle of least action³⁹ $\frac{\delta S_{\text{EM}}[A]}{\delta A_\nu(x)} = 0$

$$\partial_\mu \left(\frac{\partial \mathcal{L}_{\text{EM}}}{\partial (\partial_\mu A_\nu)} \right) - \frac{\partial \mathcal{L}_{\text{EM}}}{\partial A_\nu} = 0, \quad (2.4)$$

we obtain the classical equations of motion

$$\partial_\mu F^{\mu\nu} = 0 \quad \Leftrightarrow \quad \partial^2 A^\nu = \partial^\nu (\partial \cdot A), \quad (2.5)$$

which correspond to Gauss' and Ampère's laws in vacuum. Furthermore, the antisymmetry of $F_{\mu\nu}$ implies the Bianchi identity

$$\partial^\rho F^{\mu\nu} + \partial^\mu F^{\nu\rho} + \partial^\nu F^{\rho\mu} = 0, \quad (2.6)$$

corresponding to the homogeneous Maxwell's equations.

We know from classical electrodynamics that the potential A_μ is determined by the $\mathbf{E}$ and $\mathbf{B}$ fields in a non-unique way, so that we can add to it a gradient of an arbitrary real function $\theta : \mathbb{M} \rightarrow \mathbb{R}$, namely

$$A_\mu \rightarrow A'_\mu = A_\mu - \partial_\mu \theta, \quad (2.7)$$

which entails

$$\begin{aligned} F_{\mu\nu} \rightarrow F'_{\mu\nu} &= \partial_\mu A_\nu + \partial_\mu \partial_\nu \theta - \partial_\nu A_\mu - \partial_\nu \partial_\mu \theta \\ &= \partial_\mu A_\nu - \partial_\nu A_\mu = F_{\mu\nu}, \end{aligned} \quad (2.8)$$

leaving the physics encoded in $F_{\mu\nu}$ untouched. This phase transformation is known as a *local gauge transformation*.³⁹ In a convenient way, we can write (2.7) as

$$A_\mu \rightarrow A'_\mu = e^{ie_0\theta} \left(A_\mu - \frac{i}{e_0} \partial_\mu \right) e^{-ie_0\theta}, \quad (2.9)$$

and

$$F_{\mu\nu} \rightarrow F'_{\mu\nu} = e^{ie_0\theta} F_{\mu\nu} e^{-ie_0\theta} = F_{\mu\nu}, \quad (2.10)$$

where e_0 is the electromagnetic coupling constant, which is identified with an elementary electric charge when we add matter fields to the theory. On the other hand, if we choose θ to be a constant function of space-time, the gauge transformation is said to be *global*.

We can further define the *covariant derivative* associated with this local gauge symmetry as

$$D_\mu \equiv \partial_\mu + ie_0 A_\mu. \quad (2.11)$$

This derivative takes into account the gauge freedom at each space-time point in a theory with local gauge invariance. More specifically, A_μ defines a *parallel transport* in the space of phase transformations, known as a *connection* within the geometric framework.¹⁸

At this point, it is clear that the Lagrangian density (2.1) or, equivalently, the action (2.3), is invariant under local and global gauge transformations, consequently defining symmetries of the theory. The famous Noether theorem establishes a connection between symmetries and conservation laws in classical field theory. In particular, the invariance of the Lagrangian (2.1) under a global gauge transformation implies the conservation of electric charge when the potential is coupled to a matter field current J_μ .¹⁸ As mentioned before, a local gauge symmetry is a redundancy in our problem and is not generally viewed under the scope of Noether's theorem.⁴⁰

2.1.2 Yang-Mills Field

From the classical electromagnetic theory, we would like to generalize its elements to different types of symmetry. To mathematically visualize this, take the the set of local gauge transformations given in the last section. They are what we call a group.⁴¹ In order to form a group G , a set $\{\mathfrak{g}_i\}$ together with an operation $\circ$ must obey the following axioms

$$\begin{aligned}
\text{Closure :} & & \mathfrak{g}_i, \mathfrak{g}_j \in G & \Rightarrow \mathfrak{g}_i \circ \mathfrak{g}_j \in G \\
\text{Associativity :} & & \mathfrak{g}_i \circ (\mathfrak{g}_j \circ \mathfrak{g}_k) &= (\mathfrak{g}_i \circ \mathfrak{g}_j) \circ \mathfrak{g}_k \in G \\
\text{Existence of identity } \mathbb{1} : & & \mathfrak{g}_i \circ \mathbb{1} = \mathbb{1} \circ \mathfrak{g}_i &= \mathfrak{g}_i, \quad \forall \mathfrak{g}_i \\
\text{Unique inverse } \mathfrak{g}_k^{-1} : & & \mathfrak{g}_k \circ \mathfrak{g}_k^{-1} = \mathfrak{g}_k^{-1} \circ \mathfrak{g}_k &= \mathbb{1}, \quad \forall \mathfrak{g}_k
\end{aligned} \tag{2.12}$$

Then, our set of phase transformations $e^{i\theta}$ at each space-time point is the group of complex numbers with unit absolute value. The group operation is just the usual product of complex numbers, the identity is $\mathbb{1} = 1$ and the inverse is the complex conjugate $\mathfrak{g}_i^{-1} = \mathfrak{g}_i^*$.

More terminologically, the gauge group of electromagnetic theory is called $U(1)$ and it is part of a category of groups associated to continuous symmetries, known as *Lie groups*. From the point of view of topology, Lie groups can be locally mapped onto an appropriate Euclidean space, a property that can identify them as differentiable manifolds. For example, the $U(1)$ group is characterized by only one continuous real parameter θ , which can be mapped onto the closed real line (1-sphere).

We can further generalize this group to the so-called unitary matrix groups $U(N_c)$ of N_c^2 real independent parameters, where the letter U stands for the unitarity of its group elements, i.e., $\mathfrak{g}_i^{-1} = \mathfrak{g}_i^\dagger$. Finally, if we impose the additional condition $\det \mathfrak{g}_i = 1$ we arrive at the desired group $SU(N_c)$ of $N_c^2 - 1$ real independent parameters, defined by its fundamental representation^A of $N_c \times N_c$ unitary matrices with determinant 1. The dimension of $SU(N_c)$ is equal to $N_c^2 - 1$ and we label the group parameters by θ^a , $a = 1, \dots, N_c^2 - 1$.

^A A representation is an operation-preserving map, i.e., a homomorphism between the group and a matrix vector space. The representation with the lowest possible dimension is called fundamental or defining representation.

Considering the importance of continuous symmetries, it should be important to look at infinitesimal transformations defined by Lie groups. For an infinitesimal transformation close to the identity we can write

$$\mathbf{g} = \mathbb{1} + i\theta^a T^a, \quad a = 1, \dots, N_c^2 - 1, \quad (2.13)$$

where $\theta^a \ll 1$. The objects T^a are the *generators* of the Lie group. The number of generators is the same as the number of group parameters and they form a basis for a vector space called *Lie algebra*.

The Lie algebra can be taken as the fundamental space from where the Lie group is generated by an exponentiation map. In fact, it is the cotangent space of the Lie group. From an axiomatic point of view, the Lie algebra is a vector space which must be closed under the binary operation $[\cdot, \cdot]$ (called Lie bracket) and, besides anticommutativity and bilinearity under $[\cdot, \cdot]$, its basis elements obey the Jacobi identity, namely

$$[T^a, [T^b, T^c]] + [T^c, [T^a, T^b]] + [T^b, [T^c, T^a]] = 0. \quad (2.14)$$

Then, the so-called commutation relations are completely defined by

$$[T^a, T^b] = i f^{abc} T^c, \quad (2.15)$$

where f^{abc} are the *structure constants* of the group, a complete antisymmetric tensor ^B. Moreover, we have the freedom to normalize the generators by fixing their trace as

$$\text{Tr}(T^a T^b) = \frac{1}{2} \delta^{ab}. \quad (2.17)$$

For a Lie group of $N_c \times N_c$ matrices the generators can be taken as $N_c \times N_c$ matrices and the Lie bracket is the usual commutator of matrices $AB - BA$. Therefore, the generators of $SU(N_c)$ in the fundamental representation are $N_c^2 - 1$ Hermitian traceless ^C $N_c \times N_c$ matrices and the group is generated by the exponentiation of the Lie algebra $\mathfrak{su}(N_c)$, formally defined by the usual Taylor expansion for matrices

$$\mathbf{g} = e^{i\theta} = \sum_{k=0}^{\infty} \frac{(i\theta)^k}{k!}, \quad \theta^a \in \mathbb{R}, \quad \theta = \theta^a T^a \in \mathfrak{su}(N_c). \quad (2.18)$$

Note that the group elements do not commute in general, as it is implied by (2.15), composing what we call a *non-Abelian* group. Conversely, the $U(1)$ group from electrodynamics is an Abelian group.

^B We can also use (2.15) in (2.14) to arrive at the important relation

$$f^{ade} f^{bcd} + f^{cde} f^{abd} + f^{bde} f^{cad} = 0. \quad (2.16)$$

^C From the identity $\det e^{iT} = e^{i\text{Tr} T}$ and $\det e^{iT} = 1$ we get $\text{Tr} T = 0$. From unitarity, we have $\mathbf{g}_i^{-1} = e^{-iT}$ and $\mathbf{g}_i^\dagger = e^{-iT^\dagger}$, yielding $T = T^\dagger$. Note that we could choose the generators T to be anti-Hermitian by omitting the i in the exponentiation (2.18).

The development of fundamental theories in the last century made extensive use of *local* $SU(N_c)$ symmetry, namely $\mathfrak{g} : \mathbb{M} \rightarrow SU(N_c)$, as the underlying mechanism of interactions. Theories with local $SU(N_c)$ symmetries are called Yang-Mills theories after Yang and Mills' seminal work with $SU(2)$ in the context of quantum field theory (QFT).⁵ We can write Yang-Mills Lagrangian in analogy with the electromagnetic theory,

$$\mathcal{L}_{\text{YM}} = -\frac{1}{2} \text{Tr}(F_{\mu\nu} F^{\mu\nu}) = -\frac{1}{4} F_{\mu\nu}^a F^{a\mu\nu}. \quad (2.19)$$

Here, the trace is taken over the adjoint representation index $a = 1, \dots, N_c^2 - 1$, known in QCD simply as color index, so that $F_{\mu\nu}^a$ is a color component of $F_{\mu\nu}$. Notice that $F_{\mu\nu} = F_{\mu\nu}^a T^a$ is an element of the Lie algebra $\mathfrak{su}(N_c)$.

To infer the form of $F_{\mu\nu}$ in terms of the gauge field A_μ in $SU(N_c)$ theory, we assume that the latter transforms in analogy with the Abelian case (2.9), i.e.

$$A_\mu \rightarrow A'_\mu = \mathfrak{g} A_\mu \mathfrak{g}^\dagger - \frac{i}{g_0} \mathfrak{g} \partial_\mu \mathfrak{g}^\dagger, \quad (2.20)$$

where now $\mathfrak{g} = \mathfrak{g}(x) \in SU(N_c)$ for each $x \in \mathbb{M}$. Naively setting $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ leads to

$$\begin{aligned} \partial_\mu A_\nu - \partial_\nu A_\mu &\rightarrow \partial_\mu (\mathfrak{g}^\dagger A_\nu \mathfrak{g}^\dagger + i g_0^{-1} \mathfrak{g} \partial_\nu \mathfrak{g}^\dagger) - \partial_\nu (\mathfrak{g} A_\mu \mathfrak{g}^\dagger + i g_0^{-1} \mathfrak{g} \partial_\mu \mathfrak{g}^\dagger) = \\ &\mathfrak{g} (\partial_\mu A_\nu - \partial_\nu A_\mu) \mathfrak{g}^\dagger - \frac{1}{g_0} \left\{ i \partial_\mu \mathfrak{g} \partial_\nu \mathfrak{g}^\dagger - i \partial_\nu \mathfrak{g} \partial_\mu \mathfrak{g}^\dagger \right. \\ &\quad \left. + \mathfrak{g} A_\nu \partial_\mu \mathfrak{g}^\dagger + \partial_\nu \mathfrak{g} A_\mu \mathfrak{g}^\dagger - \partial_\nu \mathfrak{g} A_\mu \mathfrak{g}^\dagger - \mathfrak{g} A_\mu \partial_\nu \mathfrak{g}^\dagger \right\}, \end{aligned} \quad (2.21)$$

which clearly does not transform as (2.10) anymore. However, notice that the transformation of the commutator

$$\begin{aligned} i g_0 [A_\mu, A_\nu] &\rightarrow i g_0 \left[\mathfrak{g} A_\mu \mathfrak{g}^\dagger - i g_0^{-1} \mathfrak{g} \partial_\mu \mathfrak{g}^\dagger, \mathfrak{g} A_\nu \mathfrak{g}^\dagger - i g_0^{-1} \mathfrak{g} \partial_\nu \mathfrak{g}^\dagger \right] = \\ &i g_0 \mathfrak{g} [A_\mu, A_\nu] \mathfrak{g}^\dagger - \frac{1}{g_0} \left\{ -i \partial_\mu \mathfrak{g} \partial_\nu \mathfrak{g}^\dagger + i \partial_\nu \mathfrak{g} \partial_\mu \mathfrak{g}^\dagger \right. \\ &\quad \left. - \mathfrak{g} A_\nu \partial_\mu \mathfrak{g}^\dagger - \partial_\nu \mathfrak{g} A_\mu \mathfrak{g}^\dagger + \partial_\nu \mathfrak{g} A_\mu \mathfrak{g}^\dagger + \mathfrak{g} A_\mu \partial_\nu \mathfrak{g}^\dagger \right\} \end{aligned} \quad (2.22)$$

yields a term which cancels the undesired ones from the transformation of $\partial_\mu A_\nu - \partial_\nu A_\mu$ alone. This motivates the definition

$$F_{\mu\nu} \equiv \partial_\mu A_\nu - \partial_\nu A_\mu + i g_0 [A_\mu, A_\nu] \quad (2.23)$$

for the generalized electromagnetic tensor in $SU(N_c)$ gauge theories. Alternatively, we have the equivalent expression for the color components

$$F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a - g_0 f^{abc} A_\mu^b A_\nu^c. \quad (2.24)$$

In this way, $F_{\mu\nu}$ transforms as (2.10), i.e.,

$$F_{\mu\nu}(x) \rightarrow \mathfrak{g}(x) F_{\mu\nu}(x) \mathfrak{g}^\dagger(x), \quad (2.25)$$

and we can straightforwardly verify that the Lagrangian (2.19) is invariant under $SU(N_c)$ gauge transformations

$$\mathcal{L}_{\text{YM}} \rightarrow \mathcal{L}'_{\text{YM}} = -\frac{1}{4} \text{Tr} \left(\mathfrak{g} F_{\mu\nu} \mathfrak{g}^\dagger \mathfrak{g} F^{\mu\nu} \mathfrak{g}^\dagger \right) = -\frac{1}{4} \text{Tr} \left(\mathfrak{g}^\dagger \mathfrak{g} F_{\mu\nu} F^{\mu\nu} \right) = \mathcal{L}_{\text{YM}}, \quad (2.26)$$

where the cyclic property of trace was used .

Using the complete antisymmetry of $F_{\mu\nu}$ we can write the Yang-Mills Lagrangian in terms of the gauge field

$$\mathcal{L}_{\text{YM}} = -\frac{1}{4} \left(\partial_\mu A_\nu^a - \partial_\nu A_\mu^a \right)^2 + g_0 f^{abc} A_\mu^b A_\nu^c \partial_\mu A^{\nu a} - \frac{g_0^2}{4} f^{abc} f^{ade} A_\mu^b A_\nu^c A^{\mu d} A^{\nu e}. \quad (2.27)$$

The g_0 constant is analogous to the elementary electric charge in $U(1)$ theory and it is called coupling constant. It is of central importance in the quantum theory, where it dictates the strength of interaction.¹⁸

Further use of Lagrange's equations (2.4) for the color components A_ν^b leads to the classical equations of motion for Yang-Mills theories, namely

$$\left(\partial^\mu \delta^{ab} + g_0 f^{abc} A^{\mu c} \right) F_{\mu\nu}^b = 0, \quad (2.28)$$

where the term in parenthesis is the covariant derivative in the adjoint representation. This representation of the covariant derivative can be directly identified with the variation of A_μ under infinitesimal gauge transformations of the kind (2.20) with $\mathfrak{g}$ as in (2.13), i.e.

$$\begin{aligned} \delta A_\mu &= (\mathbb{1} + i g_0 \theta) A_\mu (\mathbb{1} - i g_0 \theta) - \frac{i}{g_0} (\mathbb{1} + i g_0 \theta) \partial_\mu (\mathbb{1} - i g_0 \theta) - A_\mu \\ &\approx -\partial_\mu \theta - i g_0 [A_\mu, \theta] = -D_\mu \theta, \end{aligned} \quad (2.29)$$

or, for the color components,

$$(D_\mu)^{ab} = \partial_\mu \delta^{ab} + g_0 f^{abc} A_\mu^c, \quad (2.30)$$

yielding the compact expression $D^\mu F_{\mu\nu} = 0$ for Equation (2.28). There is also a geometrical identity of the type (2.6) but we omit it here due to lack of need.

2.2 Quantum Theory

We now dive into the quantization of gauge theories, a problem that haunts theoretical physicists since the 1950s. In fact, the main question behind this dissertation, regarding the confinement mechanism of QCD, is intricately linked to the question of how we can properly quantize Yang-Mills theories, as we will see in the next chapters.

As suggested in Section 2.1, we adopt the philosophy that the gauge symmetry, even having no physical essence itself, is primary in our description of the strong interaction. Such line of thought enables us to retroactively think of (2.1) and (2.19) as the unique

gauge-invariant Lagrangians that are quadratic in $F_{\mu\nu}$ without higher derivatives of A_μ ^D. We first tackle the problem of defining the case of free quantum electrodynamics, which is the theory of massless particles of light called photons.

2.2.1 Electromagnetic Field: Coulomb gauge

The first question we should ask is: how can we quantize a real 4-vector field A_μ , thus containing *four* real components, if only two internal degrees of freedom of the photon, namely its transverse polarizations, are known to be physical? If questioned on how to proceed with the quantization process, someone used to the canonical procedure⁴² for the scalar field would naturally try to impose the usual canonical commutation relations between the fields A_μ and its conjugate momenta

$$\pi_\mu(x) \equiv \frac{\partial \mathcal{L}_{\text{EM}}}{\partial \dot{A}^\mu} = F_{\mu 0}, \quad \dot{A}^\mu(x) \equiv \partial_0 A^\mu(x). \quad (2.31)$$

In fact, it is possible to canonically quantize the electromagnetic theory with some difficulty in comparison to, say, the scalar field, because we have to choose whether or not we are going to overquantize the non-dynamical degrees of freedom. Maybe, from a naive point of view, one could think that only quantizing the physically relevant degrees of freedom should be best, which is the approach that we briefly review now.

The canonical quantization procedure relies on the Hamiltonian formulation of classical theory. The electromagnetic Hamiltonian is given by

$$H_{\text{EM}} = \int d^4x \left(\pi^\mu \dot{A}_\mu - \mathcal{L}_{\text{EM}} \right) = \int d^4x \left(\frac{1}{2} \pi_j \pi_j + \frac{1}{4} F^{ij} F_{ij} - A_0 \partial_j \pi^j \right), \quad (2.32)$$

where the last term resulted from an integration by parts neglecting a surface term, and from

$$\pi_0 = F_{00} = 0, \quad (2.33)$$

which is so due to the antisymmetry of $F_{\mu\nu}$. Notice that, from the equations of motion (2.5) and the condition (2.33), we have

$$\partial^\mu F_{\mu 0} = \partial^\mu \pi_\mu = 0 \Rightarrow \partial^i \pi_i = \partial^0 \pi_0 = 0, \quad (2.34)$$

which is recognized as Gauss's law $\nabla \cdot \mathbf{E} = 0$ if we notice that $\pi_i = F_{i0} = -E_i$. The conditions (2.33) and (2.34) are called *constraints*.

The theory of *constrained Hamiltonian systems*⁴³ is the proper formalization and generalization of such concepts. When the Hessian matrix of a Lagrangian is singular, it is not possible to uniquely express the generalized velocities $\dot{A}_\mu$ in terms of A_μ and π_μ , preventing one from writing a sensible Hamiltonian without imposing the constraints

^D The absence of third order derivatives or higher is a strong indication that the theory is *local*, an important requirement for a quantum field. Another essential requirement satisfied by the Yang-Mills' Lagrangian is that it must be renormalizable.

emerging from the Lagrangian formulation via Lagrange multipliers. Gauge systems are a kind of constrained systems whose constraints are *generators* of gauge transformations.⁴⁴

Therefore, it is entailed that the fields and their conjugate momenta cannot be treated as independent variables, resulting in the impossibility of naively imposing canonical commutation relations between A_μ and π_μ . A possible way of proceeding is to eliminate the spurious degrees of freedom by fixing the gauge with, say, the Coulomb condition

$$\nabla \cdot \mathbf{A} = 0. \quad (2.35)$$

If we were to use the usual commutation relations, i.e. $[\hat{A}_\mu, \hat{\pi}_\nu] \propto \eta_{\mu\nu}$, we would notice that $\hat{A}_0$ commutes with all the other fields because of (2.33), hence being regarded as a *c*-number instead of an operator. In particular $[\hat{H}, \hat{A}_0] = 0$, entailing that $\hat{A}_0$ is not a dynamical variable, so we can drop all the $[\hat{A}_0, \cdot]$ commutators. However, notice that the remaining commutators are not yet compatible with the Coulomb gauge condition

$$\partial_i^{\mathbf{x}} [\hat{A}_i(\mathbf{x}, t), \hat{E}_j(\mathbf{y}, t)] = [\partial_i^{\mathbf{x}} \hat{A}_i(\mathbf{x}, t), \hat{E}_j(\mathbf{y}, t)] = i \partial_j^{\mathbf{x}} \delta(\mathbf{x} - \mathbf{y}) \neq 0, \quad (2.36)$$

due to the presence of the non-dynamical longitudinal component of $\hat{\mathbf{A}}$. We can correct this by defining the transverse Dirac δ -function⁴⁵

$$\delta_{ij}^{\text{tr}}(\mathbf{x}) \equiv \frac{1}{(2\pi)^3} \int d\mathbf{k} e^{i\mathbf{k} \cdot \mathbf{x}} \left(\delta_{ij} - \frac{k_i k_j}{|\mathbf{k}|^2} \right), \quad (2.37)$$

which is divergenceless by construction. Then the correct commutation relations in Coulomb gauge can be written as

$$[\hat{A}_i(\mathbf{x}, t), \hat{E}_j(\mathbf{y}, t)] = -i \delta_{ij}^{\text{tr}}(\mathbf{x} - \mathbf{y}), \quad (2.38)$$

$$[\hat{A}_i(\mathbf{x}, t), \hat{A}_j(\mathbf{y}, t)] = [\hat{E}_i(\mathbf{x}, t), \hat{E}_j(\mathbf{y}, t)] = 0, \quad (2.39)$$

and we can see that they are compatible with the gauge condition $\nabla \cdot \hat{\mathbf{A}} = 0$. For a detailed account of Coulomb gauge quantization, see Ref. 46. Conversely, for a simplified approach along the lines of our discussion, see Refs. 47, 48.

By quantizing only the physical degrees of freedom, we are implicitly constructing the quantum theory in a Hilbert space where only states with positive norm exist. The downside of Coulomb gauge quantization is that we give up manifest Lorentz covariance to be able to quantize only the dynamical degrees of freedom. The lack of Lorentz covariance complicates many computations and precludes the proof of the renormalizability of the theory, so that we look into a covariant quantization of the electromagnetic field.

2.2.2 Electromagnetic Field: Lorenz gauge

We can treat the pathology in the electromagnetic theory from another perspective. Notice that the classical equations (2.5) are expressed by the kinetic operator

$$K_{\mu\nu} \equiv \eta_{\mu\nu} \partial^2 - \partial_\mu \partial_\nu. \quad (2.40)$$

This operator is singular, i.e., it has *zero eigenvectors*. Take for example the $\partial_\mu \lambda(x)$ mode. Then we have

$$K_{\mu\nu} \partial^\mu \lambda(x) = (\partial^2 \partial^\mu - \partial_\mu \partial_\nu \partial^\mu) \lambda(x) = 0. \quad (2.41)$$

This means that, given a solution $\tilde{A}_\mu$ of (2.5), the family of modes $\tilde{A}_\mu + \partial_\mu \lambda$ are also solutions, preventing us from defining a unique one. As in the previous section, it all boils down to the necessity of imposing a gauge condition, even at the classical level. Let us see how we can covariantly solve that at the quantum level.

Instead of applying the gauge condition directly in the Hamiltonian formulation, we can circumvent the problem by modifying the Lagrangian and then dealing with the emerging issues. One of the first attempts, due to Fermi, is to propose the Lagrangian

$$\mathcal{L}_{\text{Fermi}} = -\frac{1}{2} \partial_\mu A_\nu \partial^\mu A^\nu, \quad (2.42)$$

which gives the equation of motion

$$\partial^2 A_\mu = 0. \quad (2.43)$$

Notice that this equation of motion is the same as Maxwell's one (2.5) if the *Lorenz gauge condition*

$$\partial \cdot A = 0 \quad (2.44)$$

is satisfied. We can further show that the Lagrangian (2.1) plus the term $-\frac{1}{2}(\partial \cdot A)^2$ is equivalent to the Fermi Lagrangian (2.42), i.e.,

$$\mathcal{L}_{\text{EM}} \rightarrow \mathcal{L}'_{\text{EM}} = -\frac{1}{4} (F_{\mu\nu})^2 - \frac{1}{2} (\partial \cdot A)^2 = \mathcal{L}_{\text{Fermi}} - \frac{1}{2} \partial_\mu A_\nu \partial^\nu A^\mu + \frac{1}{2} (\partial \cdot A)^2 \sim \mathcal{L}_{\text{Fermi}}, \quad (2.45)$$

meaning that $\mathcal{L}'_{\text{EM}}$ provides the same classical equations as $\mathcal{L}_{\text{Fermi}}$. The generalization of $\mathcal{L}'_{\text{EM}}$ that we can use is a kind of parametrization for the extra term $-\frac{1}{2}(\partial \cdot A)^2$, namely

$$\mathcal{L}'_{\text{EM}} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} - \frac{1}{2\alpha} (\partial \cdot A)^2, \quad (2.46)$$

so that each α gives a different Lagrangian. The choice of α is called a *gauge choice*. The gauge choice $\alpha = 1$ is known as *Feynman gauge* (choice) and recovers Fermi's theory (2.42).

The new term in (2.46) is called a *gauge-fixing term* and it explicitly breaks the gauge symmetry of the action (2.3), formally making the theory non-singular, as can be seen by the new conjugate momenta

$$\pi'_\mu = F_{\mu 0} - \frac{1}{\alpha} \eta_{\mu 0} (\partial \cdot A) \neq 0, \quad (2.47)$$

which can now be safely used to define the Hamiltonian. Moreover, the modified kinetic operator

$$K'_{\mu\nu} = \eta_{\mu\nu} \partial^2 - \left(1 - \frac{1}{\alpha}\right) \partial_\nu \partial_\mu \quad (2.48)$$

is invertible.

We choose to work with the Feynman gauge choice and finally state the covariant equal-time commutation relations with $\hat{\pi}_\mu = -\dot{\hat{A}}_\mu$

$$[\hat{A}_\mu(\mathbf{x}, t), \hat{A}_\nu(\mathbf{y}, t)] = -i \eta_{\mu\nu} \delta(\mathbf{x} - \mathbf{y}), \quad (2.49)$$

$$[\hat{A}_\mu(\mathbf{x}, t), \hat{A}_\nu(\mathbf{y}, t)] = [\hat{A}_\mu(\mathbf{x}, t), \hat{A}_\nu(\mathbf{y}, t)] = 0. \quad (2.50)$$

These are exactly the commutation relations of a real scalar field replicated four times, except for the minus sign in $[\hat{A}_0, \hat{A}_0]$.

Here, the non-physical character of part of the degrees of freedom is revealed: the states created by $\hat{A}_0$ have negative norm. In the language of creation-annihilation operators⁴² we can write the Fourier expansion as

$$\hat{A}^\mu(x) = \hat{A}^{\mu(+)}(x) + H.C. = \int \frac{d\mathbf{k}}{\sqrt{16\pi^3|\mathbf{k}|}} \left\{ e^{-ik \cdot x} \sum_{s=0}^3 \epsilon_{(s)}^\mu(\mathbf{k}) \hat{a}_{(s)}(\mathbf{k}) + H.C. \right\}, \quad (2.51)$$

where $\epsilon^{(s)}$ are the four polarization 4-vectors. We can choose two of them as the physical ones, namely $\epsilon^{(1)}$ and $\epsilon^{(2)}$, so that they are transversal and the other two are orthogonal to them, i.e.,

$$\epsilon_{(0)}^\mu \equiv (1, \mathbf{0}), \quad \epsilon_{(3)}^\mu \equiv (0, \mathbf{k}/|\mathbf{k}|) \quad \text{and} \quad \epsilon_{(1)} \cdot (0, \mathbf{k}) = \epsilon_{(2)} \cdot (0, \mathbf{k}) = 0. \quad (2.52)$$

We call the polarization with $s = 0$ the scalar polarization, and $s = 3$ the longitudinal polarization and both must be considered as non-physical. Now we can easily deduce the commutation relations for the Fock space operators. In particular, $[\hat{a}_0(\mathbf{k}), \hat{a}_0^\dagger(\mathbf{k}')] = -\delta(\mathbf{k} - \mathbf{k}')$ and the states created by $\hat{a}_0^\dagger(\mathbf{k})$ have negative norm. Take for example the scalar 1-photon state $|1_s\rangle = \int d\mathbf{k} f(\mathbf{k}) \hat{a}_0^\dagger(\mathbf{k}) |0\rangle$, where f is just an arbitrary modulation (e.g. a wave-packet) and $|0\rangle$ is the vacuum of the theory. Its norm is

$$\langle 1_s | 1_s \rangle = - \int d\mathbf{k} d\mathbf{k}' |f|^2 \delta(\mathbf{k} - \mathbf{k}') \langle 0 | 0 \rangle = - \int d\mathbf{k} |f|^2 \leq 0, \quad (2.53)$$

showing that the related Hilbert space has *indefinite metric*, which destroys the usual probability interpretation of quantum mechanics.

It is then clear that we have to slice off the Hilbert sub-space containing states of negative metric, which comes down to imposing the Lorenz condition (2.44) at the quantum level. Remember that we cannot impose $\partial \cdot A = 0$ as an operator equation, for then we would fall into the case of Section 2.2.1, where we solved for the constraints and quantized only the transverse polarization states.

The usual way to covariantly quantize electromagnetic theory in the canonical picture is originally due to Gupta and Bleuler.^{49,50} The idea is to restrict the original Hilbert space $\mathcal{H}_{\text{total}}$ to a new one $\mathcal{H}_{\text{phys}}$ whose states obey the condition⁴⁷

$$(\partial \cdot \hat{A})^{(+)} |\Psi_{\text{phys}}\rangle = 0, \quad (2.54)$$

where $|\Psi_{\text{phys}}\rangle$ is a *physical state*^E. The Gupta-Bleuler prescription preserves the linear character of the original Hilbert space and recovers Maxwell's theory in terms of expected values over physical states

$$\begin{aligned}\langle\Psi_{\text{phys}}|\partial\cdot\hat{A}|\Psi_{\text{phys}}\rangle &= \langle\Psi_{\text{phys}}|(\partial\cdot\hat{A})^{(-)}+(\partial\cdot\hat{A})^{(+)}|\Psi_{\text{phys}}\rangle \\ &= \langle\Psi_{\text{phys}}|(\partial\cdot\hat{A})^{(+)\dagger}+(\partial\cdot\hat{A})^{(+)}|\Psi_{\text{phys}}\rangle = 0.\end{aligned}\quad (2.55)$$

Taking the condition (2.54) together with the decomposition (2.51) yields

$$(\partial\cdot\hat{A})^{(+)}|\Psi_{\text{phys}}\rangle = -i\int\frac{d\mathbf{k}}{\sqrt{16\pi^3|\mathbf{k}|}}e^{-ik\cdot x}|\mathbf{k}|[\hat{a}_{(0)}(\mathbf{k})-\hat{a}_{(3)}(\mathbf{k})]|\Psi_{\text{phys}}\rangle = 0, \quad (2.56)$$

which in turn entails

$$[\hat{a}_{(0)}(\mathbf{k})-\hat{a}_{(3)}(\mathbf{k})]|\Psi_{\text{phys}}\rangle = 0. \quad (2.57)$$

If we sandwich the last equation with its dual partner $\langle\Psi_{\text{phys}}|[\hat{a}_{(0)}(\mathbf{k})-\hat{a}_{(3)}(\mathbf{k})]^\dagger = 0$ we obtain

$$\langle\Psi_{\text{phys}}|\hat{a}_{(0)}^\dagger(\mathbf{k})\hat{a}_{(0)}(\mathbf{k})|\Psi_{\text{phys}}\rangle = \langle\Psi_{\text{phys}}|\hat{a}_{(3)}^\dagger(\mathbf{k})\hat{a}_{(3)}(\mathbf{k})|\Psi_{\text{phys}}\rangle, \quad (2.58)$$

showing that the states of the new Hilbert space $\mathcal{H}_{\text{phys}}$ contain exactly the same number of scalar and longitudinal photons. Notice that the state $|1_s\rangle$ from (2.53) does not obey this condition and so it is eliminated from $\mathcal{H}_{\text{phys}}$. We can further notice that states $|\phi\rangle$ with no transversal photons and obeying (2.57) have zero norm. Then, due to the linearity of the condition (2.54), a physical state $|\Psi_{\text{phys}}\rangle$ can be decomposed in a pure transversal state $|\psi_T\rangle$ and a state $|\phi_n\rangle$ with n scalar and longitudinal photons, i.e., $|\Psi_{\text{phys}}\rangle = |\psi_T\rangle \otimes |\phi_n\rangle$. Unless $n = 0$, all $|\phi_n\rangle$ states have zero norm and no observable significance, being susceptible to exclusion and giving rise to a positive-definite Hilbert state $\overline{\mathcal{H}}_{\text{phys}} = \mathcal{H}_{\text{phys}}/\mathcal{H}_0$ ^F, where $\mathcal{H}_0$ contains only zero norm states.

We should remark that the scalar and longitudinal photons have no particular importance in the free electromagnetic theory but they are fundamental when matter currents are coupled to A_μ , i.e., in full QED. Nevertheless, they appear only in off-shell processes, i.e., as virtual particles that cannot be observed and only indirectly contribute to physical quantities. In fact, it is possible to show that transforming a transversal state as $|\psi_T\rangle \rightarrow |\psi_T\rangle + |\phi\rangle$, where $|\phi\rangle$ is an arbitrary balanced admixture of scalar and longitudinal photons, is equivalent to a gauge transformation, namely $\langle\psi_T|A^\mu|\psi_T\rangle \rightarrow \langle\psi_T|A^\mu + \partial^\mu\lambda|\psi_T\rangle$,⁴² which we know to have no influence on gauge-invariant quantities. Finally, there remains the question of the physicality of asymptotic

^E The form of Gupta-Bleuler condition (2.54) is only possible because (2.43) implies $\square\partial\cdot A = 0$, so that $\partial\cdot A$ can be considered a massless free field and uniquely decomposed in positive and negative frequency parts, just as a scalar field.

^F To be more precise, we should define $\overline{\mathcal{H}}_{\text{phys}} = \overline{\mathcal{H}_{\text{phys}}/\mathcal{H}_0}$, where the bar indicates the inclusion of the limits of the Cauchy sequences defining the space, i.e., completion.

states, i.e., whether or not the physical in-states necessarily evolve to physical out-states. That is related to the unitarity of the relevant S -matrix and will be commented in Section 3.5.

Finally, given that we were able to properly quantize the electromagnetic field in a covariant and consistent way, we should probably try the same reasoning for Yang-Mills theories. However, notice that (2.28) has the extra term $g_0 f^{abc} A_\mu^c F^{\mu\nu b}$ in comparison to its Abelian counterpart (2.5). If we apply ∂^ν to the Fermi-Feynman version of (2.28) obtained by inserting a gauge fixing term in (2.19), i.e., to the classical equation

$$D_\mu^{ab} (F^{\mu\nu})^b + \partial^\nu (\partial \cdot A)^a = 0, \quad (2.59)$$

we get

$$\partial_\nu [\partial_\mu F^{\mu\nu a} + \partial^\nu (\partial \cdot A)^a] = \partial^2 (\partial \cdot A)^a = -g_0 f^{abc} \partial_\nu (A_\mu^c F^{\mu\nu b}), \quad (2.60)$$

showing that $\partial^2 (\partial \cdot A)^a$ is not a free field and we cannot decompose the operator $(\partial \cdot \hat{A})^a$ in positive and negative frequency parts as we did for the Abelian field. As we could have imagined, this indicates that the Gupta-Bleuler prescription is not suitable to non-Abelian gauge theories and we need to find an alternative way to quantize it.

2.2.3 Path Integrals: Quantum Mechanics

The path integral is one of the most important concepts of modern quantum field theory, and will prove itself useful in this dissertation both conceptually and computationally. It first appeared as an alternative formulation of quantum mechanics, seminally suggested by Dirac⁵¹ and then formalized by Feynman.⁵²

We didactically introduce the path integral by its construction in the context of quantum mechanics, starting with the Schrödinger equation

$$i \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle. \quad (2.61)$$

Its formal solution for *time-independent* Hamiltonians is

$$|\Psi(t_f)\rangle = e^{-i(t_f-t_i)\hat{H}} |\Psi(t_i)\rangle, \quad (2.62)$$

where the evolution operator $\hat{U}(t_f - t_i) = e^{-i(t_f-t_i)\hat{H}}$ promotes the time evolution of the state $|\Psi(t_i)\rangle$ to $|\Psi(t_f)\rangle$.

We turn our attention to the matrix elements of $\hat{U}$ between eigenstates $|q\rangle$ of the position operator $\hat{Q}$, i.e.

$$\langle q_f | e^{-i(t_f-t_i)\hat{H}} | q_i \rangle = \langle q_f | e^{-it_f\hat{H}} e^{it_i\hat{H}} | q_i \rangle = \langle q_f, t_f | q_i, t_i \rangle \equiv K(q_f, t_f; q_i, t_i), \quad (2.63)$$

Figure 2.1 – Paths broke into 1, 2 and N partitions.

Source: By the author.

which is known as the *propagator* of the system. The propagator is the Green function of the Schrödinger equation, so that the solution (2.62) in position space can be written as

$$\begin{aligned}\Psi(q_f, t_f) &= \langle q_f | \Psi(t_f) \rangle = \langle q_f | e^{i(t_f - t_i)\hat{H}} \left(\int dq_i |q_i\rangle \langle q_i| \right) | \Psi(t_i) \rangle \\ &= \int dq_i K(q_f, t_f; q_i, t_i) \Psi(q_i, t_i),\end{aligned}\quad (2.64)$$

where we used the trick of inserting the resolution of the identity in position space, $\int dq |q\rangle \langle q|$, after the evolution operator.

The famous reasoning by Feynman follows from successively inserting resolutions of the identity between t_f and t_i in the propagator (2.63). Iterating the process one time yields

$$\begin{aligned}K(q_f, t_f; q_i, t_i) &= \langle q_f | e^{-i(t_f - t_1)\hat{H}} e^{-i(t_1 - t_i)\hat{H}} | q_i \rangle \\ &= \langle q_f | e^{-i(t_f - t_1)\hat{H}} \int dq_1 |q_1\rangle \langle q_1| e^{-i(t_1 - t_i)\hat{H}} | q_i \rangle \\ &= \int dq_1 K(q_f, t_f; q_1, t_1) K(q_1, t_1; q_i, t_i).\end{aligned}\quad (2.65)$$

We can repeat this process as many times as we want (see Figure 2.1), and in the context of the double-slit experiment this would correspond to the insertion of arbitrarily many double slits between the initial one and the target.⁵³ Iterating N times we get

$$\begin{aligned}K(q_f, t_f; q_i, t_i) &= \int dq_1 \dots dq_N K(q_f, t_f; q_N, t_N) \dots K(q_1, t_1; q_i, t_i) \\ &= \int \prod_{j=1}^N dq_j \prod_{j=0}^N K(q_{j+1}, t_{j+1}; q_j, t_j) \\ &= \int \prod_{j=1}^N dq_j K_N(q_f, t_f; q_i, t_i),\end{aligned}\quad (2.66)$$

where $q_{N+1} = q_f$, $t_{N+1} = t_f$, $q_0 = q_i$, $t_0 = t_i$ and $\prod_{j=0}^N K(q_{j+1}, t_{j+1}; q_j, t_j) \equiv K_N(q_f, t_f; q_i, t_i)$.

We wish to compute (2.66) in the limit $N \rightarrow \infty$, i.e., in the limit of continuous paths between q_f and q_i . In such a limit we define the infinitesimal time step $t_{i+1} - t_i = (t_f - t_i)/(N + 1) \equiv \delta t$ and write

$$K(q_{j+1}, t_{j+1}; q_j, t_j) = \langle q_{j+1} | e^{i\delta t \hat{H}} | q_j \rangle \approx \langle q_{j+1} | 1 - i\delta t \hat{H} | q_j \rangle. \quad (2.67)$$

The first term is just

$$\langle q_{i+1} | q_i \rangle = \delta(q_{i+1} - q_i) = \int \frac{dp_i}{2\pi} e^{ip_i(q_{i+1}-q_i)}, \quad (2.68)$$

i.e., the expression of orthogonality between position eigenstates. The second one can be written as

$$\langle q_{i+1} | \hat{H} | q_i \rangle = \int \frac{dp_i}{2\pi} H\left(p_i, \frac{q_{i+1} + q_i}{2} \equiv \tilde{q}_i\right) e^{ip_i(q_{i+1}-q_i)}, \quad (2.69)$$

given that the Hamiltonian $\hat{H}$ is *Weyl ordered*^G. Notice that $H(p_i, \tilde{q}_i)$ is not the operator $\hat{H}$, but a *c*-number function of its eigenvalues. From the last two equations we can write

$$K(q_{j+1}, t_{j+1}; q_j, t_j) \approx \int \frac{dp_i}{2\pi} e^{ip_i(q_{i+1}-q_i)} [1 - i\delta t H(p_i, \tilde{q}_i)] \approx \int \frac{dp_i}{2\pi} e^{ip_i(q_{i+1}-q_i)} e^{-i\delta t H(p_i, \tilde{q}_i)} \quad (2.70)$$

and hence

$$\begin{aligned} K_N(q_f, t_f; q_i, t_i) &= \int \prod_{j=0}^N dp_j \exp [ip_j(q_{j+1} - q_j) - i\delta t H(p_j, \tilde{q}_j)] \\ &= \int \prod_{j=0}^N dp_j \exp i\delta t \left[\sum_{k=0}^N p_k \frac{q_{k+1} - q_k}{\delta t} - H(p_k, \tilde{q}_k) \right]. \end{aligned} \quad (2.71)$$

We finally obtain a first expression for the path integral by substituting (2.71) in (2.66)

$$K(q_f, t_f; q_i, t_i) \approx \int \left(\prod_{i=1}^N dq_i \prod_{j=0}^N \frac{dp_j}{2\pi} \right) \exp i\delta t \left[\sum_{k=0}^N p_k \frac{\delta q_i}{\delta t} - H(p_k, \tilde{q}_k) \right], \quad (2.72)$$

which is denoted by the symbolic expression

$$\int_{q(t_i)=q_i}^{q(t_f)=q_f} \mathfrak{D}q(t) \mathfrak{D}p(t) \exp i \left[\int_{t_i}^{t_f} dt p(t) \dot{q}(t) - H(p(t), q(t)) \right], \quad (2.73)$$

where we spelled out the boundary conditions. This is called the *phase space path integral* or *Hamiltonian path integral* and we loosely interpret $\mathfrak{D}q(t) \mathfrak{D}p(t)$ as an integration measure over trajectories in phase space.

If taken as the limit of a denumerable product of N one-dimensional measures, $\mathfrak{D}p(t) = \prod_i dp_i$ and $\mathfrak{D}q(t) = \prod_i dq_i$ can at least be visualized. The momentum measure, as it does not involve derivatives of $p(t)$, can be taken as a rectangular approximation, where each partition is associated to a constant height $p(t_i) \approx p_i$. For the position measure, we cannot use constant-valued partitions because the integrand involves $\dot{q}$ and thus demands non-zero derivatives, being it sufficient to take any smooth function between q_i and q_{i+1} . The choice corresponding to Weyl ordered Hamiltonians is a linear interpolation between the partition endpoints, where we associate the average $q(t_i) \approx \tilde{q}_i = \frac{q_{i+1} + q_i}{2}$ and the line

^G A Weyl ordered Hamiltonian is symmetrical over operator products, e.g., $\hat{H} = \hat{q}\hat{p} - \hat{p}\hat{q}$.^{46,54}

slope $\dot{q}(t_i) \approx \frac{q_{i+1}-q_i}{\delta t}$ to the measure. Other ordering prescriptions amount to other ways of discretizing the paths.⁴⁶

It is important to notice in (2.73) that the position $q(t)$ is fixed at the endpoints q_f and q_i , but the momentum $p(t)$ is integrated over all possible values in phase space. This happened because we started with the matrix elements of $e^{-it\hat{H}}$ between position eigenstates. Conversely, in momentum space the position coordinates in (2.73) would have fixed endpoints. Fixing both would be inconsistent with the uncertainty principle from quantum mechanics because we would be simultaneously specifying the momentum and the position of a state.

Because $p(t)$ is totally independent of $q(t)$ in (2.73), we cannot yet interpret the expression $p(t)\dot{q}(t) - H(p(t), q(t))$ as the Lagrangian, and for this we have to integrate out the momentum. Take, for example, a simple Hamiltonian $\hat{H} = \hat{p}^2/2m + V(\hat{q})$ quadratic in $\hat{p}$. We can then complete squares in (2.70) and integrate out the momentum p_i

$$\begin{aligned} K(q_{i+1}, t_{i+1}; q_i, t_i) &= \int \frac{dp_i}{2\pi} \exp -i \left[-p_i(q_{i+1} - q_i) + \delta t \frac{p_i^2}{2m} + \delta t V(\tilde{q}_i) \right] \\ &= e^{-i\delta t V(\tilde{q}_i)} \int \frac{dp_i}{2\pi} \exp -i \left[\delta t \frac{p_i^2}{2m} - p_i \delta q_i \pm \frac{m}{2\delta t} \delta q_i^2 \right] \\ &= e^{-i\delta t V(\tilde{q}_i)} e^{\frac{im}{2\delta t} \delta q_i^2} \int \frac{dp_i}{2\pi} \exp \left[-i \frac{\delta t}{2m} \left(p_i - \frac{m}{\delta t} \delta q_i \right)^2 \right] \\ &= \sqrt{\frac{m}{2\pi i \delta t}} \exp i \delta t \left[\frac{m}{2} \left(\frac{\delta q_i}{\delta t} \right)^2 - V(\tilde{q}_i) \right], \end{aligned} \quad (2.74)$$

with $\delta q_i = q_{i+1} - q_i$ and where we used the complex version of the Gaussian integral formula, $\int d\alpha e^{-i\alpha^2} = \sqrt{\frac{\pi}{i}}$.⁵⁵ Using this result in (2.66) yields

$$K(q_f, t_f; q_i, t_i) = \int \left(\prod_{i=1}^N dq_i \right) \left(\sqrt{\frac{m}{2\pi i \delta t}} \right)^{N+1} \exp i \delta t \left[\sum_{k=0}^N \frac{m}{2} \left(\frac{\delta q_k}{\delta t} \right)^2 - V(\tilde{q}_k) \right], \quad (2.75)$$

where we can use instead a more compact and purely symbolic expression

$$\int_{q(t_i)=q_i}^{q(t_f)=q_f} \mathfrak{D}q(t) \exp i \left[\int_{t_i}^{t_f} dt \frac{m}{2} \dot{q}(t)^2 - V(q(t)) \right] = \int_{q(t_i)=q_i}^{q(t_f)=q_f} \mathfrak{D}q(t) \exp i \int_{t_i}^{t_f} dt L(q, \dot{q}). \quad (2.76)$$

If in some sense the limit $N \rightarrow \infty$ can be taken, we can regard the expression in the exponential as the Lagrangian $L(q, \dot{q})$ of the system and its integral between the endpoints as the action functional $S[q, \dot{q}]$. The mnemonic formula $\int \mathfrak{D}q(t) e^{iS[q, \dot{q}]}$ is the so-called Feynman path integral and $\mathfrak{D}q(t)$ is a supposed integration measure over the path space.

We can regard the position measure here in the same way as before for the Hamiltonian path integral. Furthermore, we can estimate the typical paths contributing

to (2.76) if we take its Euclidean (Wick rotated) version

$$K_{\text{Euc}}(q_f, \tau_f; q_i, \tau_i) = \int \left(\prod_{i=1}^N dq_i \right) \left(\sqrt{\frac{m}{2\pi\delta\tau}} \right)^{N+1} \exp \left[-\delta\tau \sum_{k=0}^N \frac{m}{2} \left(\frac{\delta q_k}{\delta\tau} \right)^2 + V(\tilde{q}_k) \right], \quad (2.77)$$

where $\tau = it$ is called the imaginary or Euclidean time, corresponding to a rotation of $\pi/2$ in the complex plane of the relevant analytically continued functions. Then the kinetic energy behaves as $\sim \delta\tau^{-1}$ and the potential energy as $\sim \delta\tau$, so that the former dominates the measure for $\delta\tau \approx 0$. Consequently, typical paths are the ones whose position variations go as $\sim \sqrt{\delta\tau}$ in the $\delta\tau \rightarrow 0$ limit, amounting to continuous but non-differentiable trajectories. Curiously, these are common trajectories in Brownian motion. Indeed, the Wick rotated Schrödinger equation corresponds to a diffusion equation, e.g., the free quantum particle is mapped onto the free Brownian particle.⁵⁶

It is important to stress that the Feynman path integral (2.76) is a derived expression from the Hamiltonian path integral (2.73). In our case, it was assumed that the Hamiltonian was quadratic in momentum to arrive at the exact form of (2.75). When studying quantum systems with more complicated Hamiltonians, say, one with additional constraints or with variable p^2 -coefficients, one should be careful in using Feynman's version of the path integral. An example is the class of systems with Lagrangian $L = f(q) \dot{q}^2/2$, for which the conventional action in (2.76) must be replaced by an effective one containing additional terms so that the correct Hamiltonian path integral can be recovered.^{57,58} As we will see, related problems appear when quantizing gauge theories.

Figure 2.2 – Illustration of a 2D path superposition.

Source: By the author.

We should also remark that expressions (2.73) and (2.76) were derived in a heuristic fashion, i.e., with the “physicist’s way of thinking”. Actually, establishing a rigorous justification for them is a considerably difficult task, which was undertaken by many mathematical physicists such as Kac, Wiener, Nelson, and others.^{59,60} The problem begins with the fact that (2.75) involves an oscillatory integrand and its measure is complex,

without a natural damping mechanism. These points motivate the introduction of the already mentioned Euclidean path integral, mapping the one-dimensional quantum problem onto a diffusion equation. The resulting expression, if periodic boundary conditions are imposed and trace over the position space is taken, is

$$\text{Tr} \left[e^{-(\tau_f - \tau_i) \hat{H}_{\text{Euc}}} \right] = \int dq_{\text{pbc}} \int_{q(\tau_i)=q_{\text{pbc}}}^{q(\tau_f)=q_{\text{pbc}}} \mathfrak{D}q(\tau) \exp \left[- \int_{\tau_i}^{\tau_f} d\tau L_{\text{Euc}}(q, \dot{q}) \right], \quad (2.78)$$

which can be identified with a *partition function* of statistical mechanics. This brings about the mathematical ideas of stochastic processes and Brownian motion, which are treated by probability theory, Wiener integration and the Feynman-Kac formula.^{60–62}

Before we go on to the next section, we should do one last computation that will be important in QFT. Until now, we were able to formally derive path integral expressions for transition amplitudes between arbitrary states, i.e, for $\langle q_f, t_f | q_i, t_i \rangle = K(q_f, t_f; q_i, t_i)$. As we will confirm later, it is desirable to interpolate this amplitude with position operators as

$$\langle q_f, t_f | \hat{q}(t_2) \hat{q}(t_1) | q_i, t_i \rangle, \quad (2.79)$$

where $t_f > t_2 > t_1 > t_i$. Notice that $\hat{q}_H(t) = e^{-it\hat{H}} \hat{q}_S e^{it\hat{H}}$ is the position operator in the Heisenberg picture and we will temporarily make explicit the labels H (for Heisenberg) and S (for Schrödinger) for clarity. Inserting two resolutions of the identity in the position space in (2.79), yields

$$\begin{aligned} \langle q_f | e^{-it_f \hat{H}} \hat{q}_H(t_2) \hat{q}_H(t_1) e^{it_i \hat{H}} | q_i \rangle &= \langle q_f | e^{-i(t_f - t_2) \hat{H}} \hat{q}_S e^{-i(t_2 - t_1) \hat{H}} \hat{q}_S e^{-i(t_1 - t_i) \hat{H}} | q_i \rangle \\ &= \langle q_f | e^{-i(t_f - t_2) \hat{H}} \hat{q}_S \left(\int dq_2 | q_2 \rangle \langle q_2 | \right) e^{-i(t_2 - t_1) \hat{H}} \hat{q}_S \left(\int dq_1 | q_1 \rangle \langle q_1 | \right) e^{-i(t_1 - t_i) \hat{H}} | q_i \rangle \\ &= \int dq_2 \int dq_1 q_2 q_1 \langle q_f | e^{-i(t_f - t_2) \hat{H}} | q_2 \rangle \langle q_2 | e^{-i(t_2 - t_1) \hat{H}} | q_1 \rangle \langle q_1 | e^{-i(t_1 - t_i) \hat{H}} | q_i \rangle \\ &= \int dq_2 \int dq_1 q_2 q_1 \int_{q(t_2)=q_2}^{q(t_f)=q_f} \mathfrak{D}q(t''') e^{i \int_{t_2}^{t_f} dt''' L} \int_{q(t_1)=q_1}^{q(t_2)=q_2} \mathfrak{D}q(t'') e^{i \int_{t_1}^{t_2} dt'' L} \int_{q(t_i)=q_i}^{q(t_1)=q_1} \mathfrak{D}q(t') e^{i \int_{t_i}^{t_1} dt' L} \\ &= \int dq_2 \int dq_1 q_2 q_1 \int_{q(t_i)=q_i}^{q(t_f)=q_f} \mathfrak{D}q(t) e^{i \int_{t_i}^{t_f} dt L} = \int dq_2 \int dq_1 \int_{q(t_i)=q_i}^{q(t_f)=q_f} \mathfrak{D}q(t) e^{i \int_{t_i}^{t_f} dt L} q(t_2) q(t_1) \\ &= \int_{q(t_i)=q_i}^{q(t_f)=q_f} \mathfrak{D}q(t) e^{i \int_{t_i}^{t_f} dt L} q(t_2) q(t_1), \end{aligned} \quad (2.80)$$

where we opted for the Lagrangian representation (2.86) of the transition amplitude, together with all its already mentioned limitations. If we compute $\langle q_f, t_f | \hat{q}(t_1) \hat{q}(t_2) | q_i, t_i \rangle$ with $t_f > t_1 > t_2 > t_i$ instead, we will arrive at the same path integral result. This means that the last line of (2.80) automatically takes into account the time ordering of position operators and we can then write

$$\langle q_f | e^{-i t_f \hat{H}} T \{ \hat{q}_H(t_1) \hat{q}_H(t_2) \} e^{i t_i \hat{H}} | q_i \rangle = \int_{q(t_i)=q_i}^{q(t_f)=q_f} \mathfrak{D}q(t) e^{i \int_{t_i}^{t_f} dt L} q(t_2) q(t_1), \quad (2.81)$$

where T is the time-ordering operator defined by its action on time-dependent operators

$$T \{ \hat{q}(t_1) \hat{q}(t_2) \} = \begin{cases} \hat{q}(t_2) \hat{q}(t_1), & \text{if } t_2 > t_1 \\ \hat{q}(t_1) \hat{q}(t_2), & \text{if } t_1 > t_2 \end{cases}. \quad (2.82)$$

A similar expression appearing in QFT will be of crucial importance.

2.2.4 Path Integrals: Quantum Field Theory

Instead of repeating all the reasoning from last section for the case of fields, our idea now is to intuitively generalize those key concepts to infinite degrees of freedom. Notice that (2.73), (2.76) and (2.77) can be easily modified to take M degrees of freedom into account if we perform the substitution

$$q \rightarrow q_\alpha, \alpha = 1, \dots, M. \quad (2.83)$$

The jump to field theories is an extrapolation of this notation to a continuous index $\alpha \rightarrow x$

$$q_\alpha \rightarrow q(x), \quad (2.84)$$

where now q is a continuous function. For gauge theories in $3 + 1$ dimensions we have four real fields A_μ indexed by μ , each a function of the space-time argument x . In particular, for Yang-Mills fields we also have the color index $a = 1, \dots, N_c^2 - 1$ as additional labels.

There are some field theories that can be interpreted as discrete systems in the limit of infinite and continuous degrees of freedom, e.g., the vibrating string.³⁹ We will not follow this constructive but rather limited approach, instead we just suppose that our formulas (2.73) and (2.76) have their analogous counterparts in field theory and justify them *a posteriori*. So, for a generic field $\hat{\Phi}$ and its conjugate momentum $\hat{\Pi}$ in $3 + 1$ dimensions, the field path integrals are symbolically defined as

$$\langle \Phi^f(\mathbf{x}) | e^{-i(t_f-t_i)\hat{H}} | \Phi^i(\mathbf{x}) \rangle = \int_{\Phi(t_i, \mathbf{x})=\Phi_i(\mathbf{x})}^{\Phi(t_f, \mathbf{x})=\Phi_f(\mathbf{x})} \mathfrak{D}\Phi(x) \mathfrak{D}\Pi(x) \exp \left\{ i \int_{t_i}^{t_f} dt \int d^3x [\Pi \dot{\Phi} - \mathcal{H}(\Phi, \Pi)] \right\} \quad (2.85)$$

and

$$\langle \Phi^f(\mathbf{x}) | e^{-i(t_f-t_i)\hat{H}} | \Phi^i(\mathbf{x}) \rangle = \int_{\Phi(t_i,\mathbf{x})=\Phi_i(\mathbf{x})}^{\Phi(t_f,\mathbf{x})=\Phi_f(\mathbf{x})} \mathfrak{D}\Phi(x) \exp \left[i \int_{t_i}^{t_f} dt \int d^3x \mathcal{L}(\Phi, \partial_\mu \Phi) \right],^{\text{H}} \quad (2.86)$$

where Φ^f and Φ^i are spatial configurations of fields at the fixed times t_f and t_i . Notice that the fields Φ appearing in these formulas are not operators of the second quantized theory, instead they are functionals of the field operators and can be formally defined by the eigenvalue equation

$$\hat{\Phi}(x) |\Phi\rangle = \Phi(x) |\Phi\rangle. \quad (2.87)$$

They can also be taken as classical fields in the sense that they are just c -numbers.

Rather than trying to establish a direct connection between these formulas and the Hamiltonian quantization formulas from QFT^I, we invert the reasoning. Now we take (2.85) or (2.86) as the quantization prescription of our systems. Again, the Hamiltonian path integral (2.85) is the fundamental formula from which the Lagrangian one (2.86) should be derived, and from this point stem many technical difficulties to define the path integral for non-Abelian gauge theories, as will be discussed soon.

From a physical point of view we should try to look at how to compute measurable quantities from path integrals in order to verify quantum theory. With that in mind, we could, for example, compute S -matrix elements, which can be turned into physical amplitudes of scattering experiments. Essentially, we must obtain the basic vacuum expectations of the theory, also called its n -point *Green functions*, in their time-ordered version

$$\langle 0 | \hat{T} \{ \Phi(x_1) \dots \hat{\Phi}(x_n) \} | 0 \rangle, \quad (2.88)$$

and then use the LSZ reduction formula^{48,66} to compute physical amplitudes. Notice that we need vacuum expectation values but until now we have only written down expectation values between arbitrary states at different times, e.g. $\langle \Phi_f | \Phi_i \rangle$. It is possible to express the n -point Green functions in terms of path integrals by breaking up the amplitudes $\langle \Phi_f | \Phi_i \rangle$ into different time slices as we did in Equation (2.80), which corresponds to the QFT expression

$$\langle \Phi_f | e^{-i t_f \hat{H}} \hat{\Phi}(x_2) \hat{\Phi}(x_1) e^{i t_i \hat{H}} | \Phi_i \rangle = \int_{\Phi(t_i,\mathbf{x})=\Phi_i(\mathbf{x})}^{\Phi(t_f,\mathbf{x})=\Phi_f(\mathbf{x})} \mathfrak{D}\Phi(x) \exp \left[i \int_{t_i}^{t_f} d^4x \mathcal{L} \right] \Phi(x_1) \Phi(x_2), \quad (2.89)$$

^H Notice the use of the Hamiltonian and Lagrangian densities instead of, respectively, the Hamiltonian $H = \int d^3\mathcal{H}$ and the Lagrangian $L = \int d^3\mathcal{L}$.

^I It is possible to establish a formal connection between the canonical formulation and the path integral through operator equations and commutation relations⁶³ or through the Symanzik construction.^{64,65} The quantum theory can also be evidenced by obtaining Schrödinger's functional equation.⁴⁸

where again $\hat{\Phi}(x_j)$ are Heisenberg picture operators and $t_f > t_2 > t_1 > t_i$. Furthermore, using a resolution of the identity composed by the eigenstates $|n\rangle$ of the Hamiltonian, i.e., $\hat{H}|n\rangle = E_n|n\rangle$, and supposing $\langle\Phi|0\rangle \neq 0$, we have

$$e^{-it\hat{H}}|\Phi\rangle = \sum_n e^{-itE_n}|n\rangle\langle n|\Phi\rangle \xrightarrow{t \rightarrow \infty(1-i\epsilon)} e^{-itE_0}\langle 0|\Phi\rangle|0\rangle, \quad \epsilon > 0. \quad (2.90)$$

In words, we are taking the infinitesimally Wick rotated limit in time and isolating the overlap of $|\Phi\rangle$ with the vacuum. We can then write

$$|0\rangle = \lim_{t_i \rightarrow -\infty(1-i\epsilon)} \left(e^{it_i E_0} \langle 0|\Phi_i\rangle \right)^{-1} e^{it_i \hat{H}} |\Phi_i\rangle \quad (2.91)$$

$$\langle 0| = \lim_{t_f \rightarrow \infty(1-i\epsilon)} \left(e^{-it_f E_0} \langle 0|\Phi_f\rangle \right)^{-1} \langle \Phi_f| e^{-it_f \hat{H}}, \quad (2.92)$$

and consequently

$$\begin{aligned} \langle 0|\hat{\Phi}(x_2)\hat{\Phi}(x_1)|0\rangle &= \lim_{\substack{t_i \rightarrow -\infty(1-i\epsilon) \\ t_f \rightarrow \infty(1-i\epsilon)}} \langle \Phi_f| e^{-it_f \hat{H}} \hat{\Phi}(x_2)\hat{\Phi}(x_1) e^{it_i \hat{H}} |\Phi_i\rangle \mathcal{N}^{-1} \\ &= \lim_{\substack{t_i \rightarrow -\infty(1-i\epsilon) \\ t_f \rightarrow \infty(1-i\epsilon)}} \mathcal{N}^{-1} \int_{\Phi(t_i, \mathbf{x})=\Phi_i(\mathbf{x})}^{\Phi(t_f, \mathbf{x})=\Phi_f(\mathbf{x})} \mathfrak{D}\Phi(x) \exp \left[i \int_{t_i}^{t_f} d^4 x \mathcal{L} \right] \Phi(x_1)\Phi(x_2). \end{aligned} \quad (2.93)$$

The normalization factor $\mathcal{N} = e^{-i(t_f-t_i)\hat{H}} \langle \Phi_f|0\rangle \langle 0|\Phi_i\rangle$ can be evaluated by

$$\langle 0|0\rangle = \lim_{\substack{t_i \rightarrow -\infty(1-i\epsilon) \\ t_f \rightarrow \infty(1-i\epsilon)}} \int \mathfrak{D}\Phi(x) e^{i \int_{t_i}^{t_f} d^4 x \mathcal{L}} \mathcal{N}^{-1} \quad \therefore \quad \mathcal{N} = \lim_{\substack{t_i \rightarrow -\infty(1-i\epsilon) \\ t_f \rightarrow \infty(1-i\epsilon)}} \int \mathfrak{D}\Phi(x) e^{i \int_{t_i}^{t_f} d^4 x \mathcal{L}}, \quad (2.94)$$

employing the usual normalization of the vacuum $\langle 0|0\rangle = 1$. Finally, we arrive at the path integral expression, recalling that it accounts for both time orderings as in (2.81),

$$\langle 0|T\{\hat{\Phi}(x_1)\hat{\Phi}(x_2)\}|0\rangle = \lim_{\substack{t_i \rightarrow -\infty(1-i\epsilon) \\ t_f \rightarrow \infty(1-i\epsilon)}} \frac{\int \mathfrak{D}\Phi(x) \Phi(x_1)\Phi(x_2) \exp \left[i \int_{t_i}^{t_f} d^4 x \mathcal{L} \right]}{\int \mathfrak{D}\Phi(x) \exp \left[i \int_{t_i}^{t_f} d^4 x \mathcal{L} \right]}, \quad (2.95)$$

where we omitted boundary conditions for simplicity. It is straightforward to generalize this formula to n -point functions and then compute complicated physical amplitudes through the path integral formalism.

Unfortunately, the computation of physical amplitudes, specially if it relies only on perturbation theory, should not satisfy the rigorous theorist. We need at least a way to know we are dealing with a reasonable quantum theory, i.e., that we can extend the techniques to any of its aspects, say, the non-perturbative ones. Note that even if we are using a new quantization prescription, we still have restrictions upon the fields and the Hilbert space of the theory, e.g., locality, unitarity, uniqueness of vacuum, positiveness and, eventually, renormalizability. The branch of theoretical physics called *axiomatic quantum field theory*⁶⁷ treats questions of that kind.

Figure 2.3 – Scheme of Wick rotation and its “infinitesimal” form used in (2.95).

Source: By the author.

In the axiomatic framework, fields are operator-valued distributions and, together with the states of the relevant Hilbert space, have to satisfy a series of axioms which guarantee a well-defined theory from a mathematical perspective. In particular, the *Wightman reconstruction theorem*⁶⁸ shows that it is possible to reconstruct the axiomatic field theory from vacuum expectation values satisfying certain conditions, i.e., the axioms can be formulated in terms of $\langle 0 | \hat{\Phi}(x_1) \dots \hat{\Phi}(x_n) | 0 \rangle$, also called Wightman functions. From the axiomatic formulation one may also derive important properties such as the CPT

symmetry and the spin-statistics connection for general fields.⁶⁷ However, the generality of this approach prevents it from formulating more complicated theories, especially interacting and gauge-invariant ones.

Following the trail of the axiomatic enterprise, another branch of theoretical physics, the *constructive quantum field theory*,^{60,69} was created envisaging a rigorous definition of more specific theories, i.e., specific Lagrangians as the Higgs model and Yang-Mills theory in 2D.⁶⁰ Here comes about an appropriate definition of the probability measure $d\mu = \mathfrak{D}\Phi e^{-S}$ of the Lagrangian path integral (2.86) in its Euclidean version. The Euclidean formulation of quantum field theories was pioneered by Schwinger,⁷⁰ whose suggestion was to construct theories from representations of the Euclidean group, instead of the Lorentz one. Some years later, Symanzik⁷¹ interpreted the Euclidean Green functions,

$$S_n(x_1, \dots, x_n) \equiv \langle \hat{\phi}(\mathbf{x}_1, \tau_1) \dots \hat{\phi}(\mathbf{x}_n, \tau_n) \rangle = \langle 0 | \hat{\phi}(\mathbf{x}_1, \tau_1) \dots \hat{\phi}(\mathbf{x}_n, \tau_n) | 0 \rangle^J, \quad (2.96)$$

also called *correlation functions* or Schwinger functions, as *moments* of the measure $d\mu$, which turned out to be the right connection between quantum field theory and statistical mechanics^K. Finally, the Euclidean formulation was fully established when Osterwalder and Schrader⁷² gave sufficient conditions, e.g. reflection positivity, to reconstruct the Minkowski theory from the Euclidean one, i.e., they stated a set of axioms that the Euclidean Green functions should obey so that one would be able to “undo” the Wick rotation.

Nevertheless, the path integral faces the problem of singularities, e.g. ultraviolet divergences, common to most quantum field theories. The tool we use to treat singularities

^J Here $|0\rangle$ is the ground state with the lowest energy of the Euclidean system.

^K In the Euclidean formulation, because the separations are all space-like, the correlation functions are symmetric in their arguments and the Wick rotated fields ϕ can be viewed as random variables, which is fundamental to the statistical interpretation.

is called *regularization*. In particular, for gauge theories it is of utmost importance that the regularization preserves gauge symmetry so that we can further renormalize the theory. From the constructive point of view, the most prominent regularization to the date is the Euclidean lattice regularization²³ because it preserves gauge invariance and reflection positivity,⁷³ even if some continuous symmetries are obscured by the Euclidean space discretization. This approach consists in the introduction of a finite hypercubic lattice whose sites are separated by a finite distance a . The problem of defining the continuum theory is then equivalent to that of removing the lattice regularization, i.e., by taking the limit of infinite lattice volume and $a \rightarrow 0$. The lattice formalism will be detailed in Chapter 4, focusing on its numerical applications.

Therefore, for the sake of definiteness we will use the path integral in the Euclidean formulation from now on, especially in the Lagrangian form. Using the Wick rotated version of the Lagrangian path integral (2.86), namely,

$$\langle \hat{\phi}_f(\mathbf{x}) | e^{-(\tau_f - \tau_i) \hat{H}_{\text{Euc}}} | \hat{\phi}_i(\mathbf{x}) \rangle = \int_{\phi(\mathbf{x}, \tau_i) = \phi_i(\mathbf{x})}^{\phi(\mathbf{x}, \tau_f) = \phi_f(\mathbf{x})} \mathfrak{D}\phi(x_{\text{Euc}}) \exp \left[- \int_{\tau_i}^{\tau_f} d^4 x_{\text{Euc}} \mathcal{L}_{\text{Euc}} \right], \quad (2.97)$$

the Euclidean version of (2.95) generalized to n fields will be

$$\langle \hat{\phi}(x_1^{\text{Euc}}) \dots \hat{\phi}(x_n^{\text{Euc}}) \rangle = \lim_{\substack{\tau_i \rightarrow -\infty \\ \tau_f \rightarrow \infty}} \frac{\int \mathfrak{D}\phi(x_{\text{Euc}}) \exp \left[- \int_{\tau_i}^{\tau_f} d^4 x_{\text{Euc}} \mathcal{L}_{\text{Euc}} \right] \phi(x_1^{\text{Euc}}) \dots \phi(x_n^{\text{Euc}})}{\int \mathfrak{D}\phi(x_{\text{Euc}}) \exp \left[- \int_{\tau_i}^{\tau_f} d^4 x_{\text{Euc}} \mathcal{L}_{\text{Euc}} \right]}, \quad (2.98)$$

where we again omitted the boundary conditions. In these formulas $d^4 x_{\text{Euc}} = d^3 \mathbf{x} d\tau$, $|0\rangle$ is the ground state of the Euclidean theory and $\mathcal{L}_{\text{Euc}}$ is the Euclidean version of the Lagrangian density $\mathcal{L}$. Notice that the limits for obtaining the vacuum expectation values are now simpler because the Wick rotation already accounts for the fast suppression of $\langle n > 0 | \phi \rangle$ overlaps. From now on we will be working always in the Euclidean formulation, dropping the Euclidean label and using τ and x_4 equivalently.

The measure in our formulas for the path integral (2.97) is loosely defined by the finite product of individual measures at each site of the Euclidean lattice

$$\mathfrak{D}\phi = \prod_{x_i \in \Lambda} d\phi(x_i). \quad (2.99)$$

To be consistent we should also take any derivatives in the Lagrangian density as their discretized version, i.e., a finite difference expression. For example, we could take it as a forward difference

$$\partial_\mu \phi(x) = \frac{\phi(x + a\hat{\mu}) - \phi(x)}{a} + \mathcal{O}(a). \quad (2.100)$$

We can then estimate the profile of the paths (field configurations) contributing to (2.102)

by writing the discretized version of the kinetic operator appearing in the action functional

$$\begin{aligned} \int d^4x (\partial_\mu \phi)^2 &= \sum_{x \in \Lambda} a^4 \left(\frac{\phi(x + a\hat{\mu}) - \phi(x)}{a} \right)^2 + \mathcal{O}(a^6) \\ &\approx \sum_{x \in \Lambda} a^2 (\phi(x + a\hat{\mu}) - \phi(x))^2, \end{aligned} \quad (2.101)$$

where $\hat{\mu}$ is a unitary vector pointing in the μ -direction. We know that the kinetic term dominates the measure $d\mu \sim e^{-S}$, which entails that the typical paths behave as $\delta\phi \sim a^{-1}$ and we see that they are even more singular than in the case of non-relativistic quantum mechanics. In this case, the field configurations will not necessarily be continuous functions, but distributions. Indeed, a finite action means zero measure⁶⁵ and only taking too “smooth” paths into account is not sufficient to describe the physics contained in the path integral.

Finally we should state the QFT version of the partition function (2.78). For the needs of computing correlation functions (2.98) it is immaterial to take the trace or impose temporal boundary conditions. This is justified because we are always going to implicitly take the limits $\tau_f \rightarrow \infty$ and $\tau_i \rightarrow -\infty$ in the path integrals and suppose that respective fixed field configurations have non-zero overlap with the vacuum. Hence we write the partition function (or simply the path integral) as

$$\mathcal{Z} = \int \mathfrak{D}\phi(x) e^{-S[\phi]}, \quad (2.102)$$

which is the expression we are going to use throughout this dissertation.

We will now depart from the general theory of path integrals and focus on its application to the quantization of gauge fields.

2.3 Faddeev-Popov Method

The attentive reader may have noticed that we almost ignored the Hamiltonian path integral and stated the last definitions only using the Lagrangian formulation. In gauge theories it is possible to impose the constraints via the Hamiltonian path integral.⁷⁴ However, the Hamiltonian approach hides the covariance of the theory, one of the virtues of Feynman integration, making calculations very messy and cumbersome. We instead follow the more common practice of integration over all configurations in a covariant language.

2.3.1 Electromagnetic Case

We start with the electromagnetic case and its path integral

$$\mathcal{Z}_{\text{EM}} = \int_{\mathbb{A}} \mathfrak{D}A e^{-S_{\text{EM}}[A]}, \quad (2.103)$$

where the action $S_{\text{EM}}[A] = 1/4 \int d^4x F_{\mu\nu}^2$ (see Appendix A) is the Wick rotated version of (2.3) and the measure, analogous to (2.99), is written as

$$\mathfrak{D}A \equiv \prod_{\mu=1}^4 \prod_{x_i \in \Lambda} dA_\mu(x_i). \quad (2.104)$$

We should recall that we are now working in Euclidean space and we do not need to distinguish between upper and lower indices. The domain of integration $\mathbb{A}$ is just the loosely-defined space of the gauge potentials A_μ in Euclidean space.

Since the path integral (2.103) encodes the Euclidean version of the singular quadratic operator (2.40),

$$K_{\mu\nu} = \square\delta_{\mu\nu} - \partial_\mu\partial_\nu, \quad (2.105)$$

we should suspect that the quantum theory defined by it will be ill-defined if one wants to perturbatively compute Green functions. In fact, as we already discussed, this operator contains zero eigenvectors due to gauge transformations of *physically equivalent* field configurations. For instance, consider configurations obtained by gauge transforming the classical vacuum, i.e.

$$A_\mu^0 = 0 \rightarrow A_\mu^{0'} = \partial_\mu\lambda(x). \quad (2.106)$$

These will compose a family of field configurations with vanishing action due to the gauge invariance of S_{EM} , which will be accounted for in the path integral (2.103) and therefore will make it badly defined.

Indeed, if the main goal is to derive Feynman rules and perturbatively compute, say, S -matrix elements, then one is in trouble. The perturbative approach boils down to the inversion of the kinetic operator (2.40) in order to define the free-theory *propagators*, which is impossible if the former contains zero modes. This is the main motivation of the method by Faddeev and Popov²⁰ in the framework of non-Abelian theories. We will first apply it to the free electromagnetic (Abelian) theory in order to present its concepts.

The essence of the Faddeev-Popov procedure is to directly impose a gauge condition, e.g., Lorenz gauge, to the Feynman path integral through the insertion of a δ -function identity. This procedure selects only one representative from each physical *equivalence class* of field configurations to contribute in the path integral. As a consequence, an infinite constant corresponding to the physically equivalent configurations will be factored out from (2.103). Hopefully, the zero modes are ruled out in this process because we are going to suspend manifest gauge invariance of the action.

Taking one-dimensional⁴⁸ and two-dimensional^{22,75} examples as an intuitive starting point, we can analogously state the “one” of Faddeev-Popov as

$$\Delta_{\text{EM}}[A] \int_{\mathbb{G}} \mathfrak{D}\theta \, \delta(G[A^\theta]) = 1, \quad \theta : \mathbb{E} \rightarrow \mathbb{R}, \quad (2.107)$$

where A^θ is just a notation for the transformed field appearing in (2.7) and (2.9), namely

$$A_\mu^\theta(x) \equiv A_\mu(x) - \partial_\mu\theta(x). \quad (2.108)$$

The path measure in the space of phase transformations is formally defined in terms of the $U(1)$ group parameter $\theta \in \mathbb{R}$,

$$\mathfrak{D}\theta \equiv \prod_{x_i \in \Lambda} d\theta(x_i), \quad (2.109)$$

and integration is done over the large space $\mathbb{G}$ composed of phase transformations $e^{i\theta(x)}$ for all $x \in \mathbb{E}$. The δ -functional appearing in (2.107) is the functional version of the δ -function, formally defined as

$$\int_{\mathbb{G}} \mathfrak{D}\theta \, \delta(G(A^\theta)) \equiv \int_{\mathbb{G}} \prod_{x_i \in \Lambda} d\theta(x_i) \, \delta(G[A^\theta](x_i)), \quad (2.110)$$

where G is a mapping from the space of all the gauge potentials to the restricted space defined by a corresponding gauge-fixing condition. Therefore, here G will take the role of a *gauge condition* through the equation $G[A^\theta] = 0$, for some $\theta = \theta_0$. The last ingredient to be defined is the Faddeev-Popov determinant

$$\Delta_{\text{EM}}[A] = |\det \mathcal{M}_{\text{EM}}|, \quad \mathcal{M}_{\text{EM}}(x, y) = \left. \frac{\delta G[A^\theta](x)}{\delta \theta(y)} \right|_{G[A^{\theta_0}] = 0}, \quad (2.111)$$

which is just the Jacobian of the change of variables from G to θ evaluated on the gauge condition, i.e., for a θ_0 satisfying $G[A^{\theta_0}] = 0$, assuming θ_0 is *unique*.

We go on by inserting (2.107) in the path integral (2.103) and changing the order of integrations

$$\mathcal{Z}_{\text{EM}} = \int_{\mathbb{G}} \mathfrak{D}\theta \int_{\mathbb{A}} \mathfrak{D}A \, e^{-S_{\text{EM}}[A]} \Delta_{\text{EM}}[A] \, \delta(G[A^\theta]). \quad (2.112)$$

To further proceed, notice that the measures $\mathfrak{D}A$ and $\mathfrak{D}\theta$ are both invariant by gauge transformations. In the present $U(1)$ case, this is easy to establish because (2.108) corresponds to a translation in the Abelian group of phase transformations, i.e., in the space parametrized by θ , reflecting in

$$\mathfrak{D}A^\theta = \mathfrak{D}A \quad (2.113)$$

because θ is an arbitrary function and does not depend on the fields. Then, by construction, the group measure, here denoted by the single group parameter, is also gauge invariant

$$\mathfrak{D}(\theta + \theta') = \mathfrak{D}\theta, \quad (2.114)$$

because the transformation parameter θ' is fixed with respect to θ in the translation $d\theta \rightarrow d(\theta + \theta')$. These remarks are important to establish the invariance of the determinant

$$\begin{aligned} \Delta_{\text{EM}}^{-1}[A^{\theta'}] &= \int_{\mathbb{G}} \mathfrak{D}\theta \, \delta(G[A^{\theta\theta'}]) = \int_{\mathbb{G}} \mathfrak{D}(\theta + \theta') \, \delta(G[A^{\theta\theta'}]) \\ &= \int_{\mathbb{G}} \mathfrak{D}\theta'' \, \delta(G[A^{\theta''}]) = \Delta_{\text{EM}}^{-1}[A]. \end{aligned} \quad (2.115)$$

The last observations enable us to perform the transformation $A \rightarrow A^{-\theta}$ in (2.112) and write

$$\begin{aligned} \mathcal{Z}_{\text{EM}} &= \int_{\mathbb{G}} \mathfrak{D}\theta \int_{\mathbb{A}} \mathfrak{D}A^{-\theta} \, e^{-S_{\text{EM}}[A^{-\theta}]} \Delta_{\text{EM}}[A^{-\theta}] \, \delta(G[(A^{-\theta})^\theta]) \\ &= \left(\int_{\mathbb{G}} \mathfrak{D}\theta \right) \int_{\mathbb{F}} \mathfrak{D}A \, e^{-S_{\text{EM}}[A]} \Delta_{\text{EM}}[A] \, \delta(G[A]), \end{aligned} \quad (2.116)$$

where we also used the gauge invariance of the action S_{EM} , besides (2.113) and (2.115). In the last expression we were able to eliminate the θ transformation dependence in the path integral and thus factor out the *gauge space volume*, which can be absorbed in a (infinite) normalization constant. We can further choose a specific gauge condition, e.g. Lorenz condition

$$G[A^\theta] = \partial_\mu A_\mu^\theta = 0, \quad (2.117)$$

which can always be achieved for any A_μ by choosing an appropriate $\theta = \theta_0$.⁴⁷ Because we know the determinant is gauge invariant, we can choose to transform A^θ to A in (2.111), thus satisfying the gauge condition $G[A] = 0$ at $\theta_0 = 0$, and explicitly write the determinant (2.111) by using the transformation (2.108) around the gauge condition ($\theta_0 = 0$)

$$\mathcal{M}_{\text{EM}}(x, y) = \frac{\delta}{\delta\theta(y)} \partial_\mu [A_\mu(x) - \partial_\mu \theta(x)] \Big|_{\theta=0} = -\partial_\mu \partial_\mu \delta(x - y), \quad (2.118)$$

which is the negative Laplace operator in Euclidean space. Therefore, the path integral (2.116) in Lorenz gauge turns out to be

$$\mathcal{Z}_{\text{EM}} = \mathcal{N} \int_{\mathbb{F}} \mathfrak{D}A e^{-S_{\text{EM}}[A]} \delta(\partial \cdot A) \det(\mathcal{M}_{\text{EM}}) = \mathcal{N}' \int_{\mathbb{F}} \mathfrak{D}A e^{-S_{\text{EM}}[A]} \delta(\partial \cdot A), \quad (2.119)$$

where the gauge volume $\mathcal{N} = \int_{\mathbb{G}} \mathfrak{D}\theta$ and the Faddeev-Popov determinant were absorbed into $\mathcal{N}'$. The outgoing integration space $\mathbb{F}$ is just the aforementioned space of gauge potentials restricted to the gauge condition (2.117). Notice that we did not take the absolute value of the determinant because we know the negative Laplacian is a positive-definite operator^L.

Still in Lorenz gauge, we would like to eliminate the annoying δ -function inside the path integral (2.119). A common practice is to lift up to the action any remaining terms other than exponentials. In particular, the trick used here is to extend the Lorenz gauge definition to the same expression up to a function $\xi : \mathbb{E} \rightarrow \mathbb{R}$ independent of A_μ (linear covariant gauge) such as

$$G[A^\theta] = \partial_\mu A_\mu^\theta - \xi, \quad (2.120)$$

and multiply (2.119) by a suitable constant factor (see (B.4)) in terms of the Gaussian functional integral for the bosonic field ξ

$$cst. = \int \mathfrak{D}\xi e^{-(2\alpha)^{-1} \int dx \xi(x)^2}, \quad (2.121)$$

which yields

$$\mathcal{Z}_{\text{EM}} = \mathcal{N}''' \int_{\mathbb{F}} \mathfrak{D}A e^{-S_{\text{EM}}[A]} \int \mathfrak{D}\xi \delta(\partial \cdot A - \xi) e^{-(2\alpha)^{-1} \int d^4x \xi(x)^2} = \mathcal{N}''' \int_{\mathbb{F}} \mathfrak{D}A e^{-S_{\text{FP}}[A]}. \quad (2.122)$$

^L The non-trivial (non-constant) eigenvectors of the negative Laplacian are plane-waves as $\psi(x) = e^{-ik \cdot x}$ whose eigenvalues $\lambda = k^2$ are strictly positive.

The Faddeev-Popov action S_{FP} is the sum of S_{EM} and the gauge fixing term, i.e.

$$S_{\text{FP}}[A] = \int d^4x \left[\frac{1}{4} F_{\mu\nu} F_{\mu\nu} + \frac{1}{2\alpha} (\partial \cdot A)^2 \right], \quad (2.123)$$

whose Lagrangian corresponds to the Euclidean version of the generalized Fermi Lagrangian in (2.46). The parameter α corresponds again to a specific gauge choice and must be fixed at some point.

The path integral (2.122) is much better defined than the initial one (2.103). Undesired equivalent configurations were factored out and we can straightforwardly obtain the free-photon propagator used in perturbation theory.

2.3.2 Yang-Mills Case

We shall now repeat the Faddeev-Popov procedure for non-Abelian theories. Besides their original work,²⁰ Feynman had already noticed the necessity of modifying the usual diagrammatic rules to account for unitarity of the S -matrix in Yang-Mills (and gravitational) theories.⁷⁶ Similar procedures were also developed in complementary works by DeWitt, Mandelstam and Fradkin.^{77–79} The non-Abelian case is very similar to the electromagnetic one and is where the path integral proves its worth. Indeed, the motivation for using this procedure here is the same: defining a free propagator to be used in perturbative computations, i.e., perturbatively quantize the theory.

When considering non-Abelian groups, the physically equivalent configurations are connected by the local $SU(N_c)$ transformation $\mathfrak{g}$,

$$A_\mu^{\mathfrak{g}} \equiv \mathfrak{g}(x) A_\mu(x) \mathfrak{g}^\dagger(x) - \frac{i}{g_0} \mathfrak{g}(x) \partial_\mu \mathfrak{g}^\dagger(x), \quad (2.124)$$

as in (2.20). Each set of equivalent fields is commonly known as a *gauge orbit*. Therefore, our task is to impose a gauge condition by selecting a representative configuration from each orbit. The set of such representatives is called a *gauge slice*. These concepts can be schematically represented as in Figure 2.4.

The Yang-Mills path integral in Euclidean space has the same form of (2.103)

$$\mathcal{Z}_{\text{YM}} = \int_{\mathbb{A}} \mathfrak{D}A e^{-S_{\text{YM}}[A]}, \quad (2.125)$$

with $S_{\text{YM}}[A] = 1/2 \text{Tr} \int d^4x F_{\mu\nu}^2$ (see A.2). In this case, the formal integration measure, namely

$$\mathfrak{D}A \equiv \prod_{x_i \in \Lambda} \prod_{\mu=1}^4 \prod_{a=1}^n A_\mu^a(x_i), \quad (2.126)$$

involves a larger space because it takes into account the dimension of the group $SU(N_c)$. As we should already suspect due to the group structure of non-Abelian gauge potentials, the domain of integration now is, roughly speaking, a copy of the Lie algebra of $SU(N_c)$ over Euclidean space.

We can state the “one” of Faddeev-Popov for Yang-Mills theories as

$$\Delta_{\text{YM}}[A] \int_{\mathbb{G}} \mathfrak{D}\mathfrak{g} \, \delta(G^a[A^{\mathfrak{g}}]) = 1_{\mathbb{G}} \equiv \mathbb{1}, \quad \mathfrak{g} : \mathbb{E} \rightarrow SU(N_c), \quad (2.127)$$

where we use the group element symbol $\mathfrak{g}$ instead of the group parameters. The measure is invariant under left and right non-Abelian transformations, i.e.,

$$\mathfrak{D}\mathfrak{g} = \mathfrak{D}(\mathfrak{g}\mathfrak{g}') = \mathfrak{D}(\mathfrak{g}'\mathfrak{g}), \quad (2.128)$$

which can be defined by an Euclidean space replication of the so-called Haar group measure ^M, therefore contemplating the domain of integration, namely, a replication of $SU(N_c)$ over $\mathbb{E}$.

As in the Abelian case, we regard Δ_{YM} as the Jacobian determinant of the change of variables from G to θ and it is written as in (2.7), but now the Faddeev-Popov operator has color indices, namely

$$\Delta_{\text{YM}}[A] = |\det \mathcal{M}_{\text{YM}}|, \quad (2.129)$$

with

$$\mathcal{M}_{\text{YM}}^{ab}(x, y) \equiv \left. \frac{\delta G^a[A^{\mathfrak{g}}](x)}{\delta \theta^b(y)} \right|_{G^a[A^{\mathfrak{g}_0}] = 0}, \quad (2.130)$$

where θ^b are the $N_c^2 - 1$ group parameters and $\mathfrak{g}_0$ corresponds to the transformation that brings A to the desired gauge slice. Again, this determinant is gauge invariant and the reasoning is similar to (2.115). Besides, notice that we now have one gauge condition for each color component, resulting in $N_c^2 - 1$ equations $G^a[A^{\mathfrak{g}}] = 0$, *which we assume to have a unique solution*.

In close analogy to the last section, we can insert (2.127) into (2.125) and separate the gauge slice from the rest of $\mathbb{A}$ -space integration, resulting in

$$\mathcal{Z}_{\text{YM}} = \left(\int_{\mathbb{G}} \mathfrak{D}\mathfrak{g} \right) \int_{\mathbb{F}} \mathfrak{D}A e^{-S_{\text{YM}}[A]} \Delta_{\text{YM}}[A] \prod_{a=1}^{N_c^2-1} \delta(G^a[A]), \quad (2.131)$$

where the path integral only covers the quotient space $\mathbb{F} = \mathbb{A}/\mathbb{G}$, i.e., the integration is done along the gauge slice defined by the gauge conditions $G^a[A^{\mathfrak{g}}] = 0$.

We again choose to work in Lorenz gauge with the set of conditions

$$G^a[A^{\mathfrak{g}}] = \partial \cdot A^a, \quad a = 1, \dots, N_c^2 - 1, \quad (2.132)$$

Figure 2.4 – One-dimensional cut of a gauge slice and its intersections with various gauge orbits.

Source: By the author.

^M The Haar measure is a group integration measure satisfying (2.128). See Appendix C.1.

and from this express the correspondent Faddeev-Popov determinant. Using the fact that such a determinant is gauge invariant, we can pick A in a way that it “sits” on the gauge condition and then perform the gauge transformation from there. Consequently, because we can choose to be on the gauge slice, we set $\mathfrak{g}_0 = \mathbb{1}$ (which corresponds to $\theta_0^a = 0$) and use only the infinitesimal transformation (2.29) around the gauge condition to evaluate (2.129) in Lorenz gauge, i.e.,

$$\begin{aligned} \mathcal{M}_{\text{YM}}^{ab}(x, y) &= \left. \frac{\delta G^a[A^{\mathbb{1}+i\theta}](x)}{\delta \theta^b(y)} \right|_{\theta=0} = \left. \frac{\delta}{\delta \theta^b(y)} \partial_\mu \left[A_\mu^a - \partial_\mu \theta^a - g_0 f^{abc} A^{\mu c} \theta^b + \mathcal{O}(\theta^2) \right] (x) \right|_{\theta=0} \\ &= -\partial_\mu \left(\partial_\mu \delta^{ab} + g_0 f^{abc} A_\mu^c \right) \delta(x - y) = -\partial_\mu D_\mu^{ab} \delta(x - y), \end{aligned} \quad (2.133)$$

which we simply denote as $\mathcal{M}_{\text{YM}}[A] = -\partial \cdot D$.

We can eliminate the δ -function in (2.131) using the same trick of (2.122), but now extending the set of gauge conditions (2.132) to

$$G^a[A^{\mathfrak{g}}] = \partial \cdot A^a - \xi^a, \quad a = 1, \dots, N_c^2 - 1, \quad (2.134)$$

where each $\xi^a : \mathbb{E} \rightarrow \mathbb{R}$ plays the same role of ξ in the electromagnetic case. Finally, plugging one integral of the kind (2.121) for each color component into (2.131) and integrating out, we arrive at

$$\mathcal{Z}_{\text{YM}} = \mathcal{N} \int_{\mathbb{F}} \mathfrak{D}A e^{-S_{\text{YM}}[A] - (2\alpha)^{-1} \int d^4x (\partial \cdot A^a)^2} |\det \mathcal{M}_{\text{YM}}|. \quad (2.135)$$

Unlike the Abelian case, we cannot take the Faddeev-Popov determinant out of the integration because it depends on A . Nevertheless, we can follow the philosophy of lifting up the non-exponential terms in the path integral, but now using a *fermionic* version of the Gaussian integral (2.121) generalized to an arbitrary Hermitian operator $H^{ab}(x, y)$, see (B.15). Suppose two independent scalar anticommuting fields c^a and $\bar{c}^a$ in the adjoint representation of $SU(N_c)$. We can immediately write down

$$\det \mathcal{M}_{\text{YM}} = \int \mathfrak{D}\bar{c}\mathfrak{D}c e^{\int d^4x d^4y \bar{c}^a(x) \mathcal{M}^{ab}(x, y) c^b(y)}, \quad (2.136)$$

if we assume the determinant is always positive. It is then simple to see that (2.135) turns into

$$\mathcal{Z}_{\text{YM}} = \mathcal{N}' \int_{\mathbb{F}} \mathfrak{D}A \mathfrak{D}\bar{c}\mathfrak{D}c e^{-S_{\text{FP}}[A, \bar{c}, c]}, \quad (2.137)$$

and the gauge-fixed action is now

$$S_{\text{FP}}[A] = \int d^4x \left[\frac{1}{4} F_{\mu\nu}^a F_{\mu\nu}^a + \frac{1}{2\alpha} (\partial \cdot A^a)^2 + \bar{c}^a (\partial \cdot D)^{ab} c^b \right]. \quad (2.138)$$

Figure 2.5 – Ghost-gluon vertex.

Source: DOHSE.⁸⁰

The new fields c^a are called *ghosts of Faddeev-Popov*. They are scalar and anticommuting. Therefore, because of the spin-statistics theorem, we know they cannot stand for a physical particle. Indeed, they are essential to prove the unitarity of perturbation theory even if they do not contribute with external legs in S -matrix calculations. As it would be expected, the new term $\bar{c}(\partial \cdot D)c$ introduces a new three-particle interaction vertex in perturbation theory, the ghost-gluon one, which will eventually appear in loop corrections. This term is not relevant in the electromagnetic theory, where the ghosts decouple from photons and play no role at all. Also, there are certain non-covariant gauges, e.g. the axial gauge, in which the non-Abelian ghosts do not plague the perturbative analysis,^{81,82} but that are very difficult to address when dealing with renormalization aspects.

3 GRIBOV-ZWANZIGER SCENARIO

In Chapter 2, we set the basic framework of quantum field theory and Yang-Mills fields. The path integral formalism and the Faddeev-Popov for non-Abelian fields are conventional methods for dealing with perturbative calculations, which were more or less established in the beginning of the 1970s together with asymptotic-freedom.^{14,15} Of course, the perturbative perspective was very limited and the infrared problem in non-Abelian theories seemed impenetrable.⁸³ In that context, Gribov pointed out a problem in the Faddeev-Popov gauge-fixing procedure and proposed a solution,²¹ which will be covered in this chapter.

3.1 The Problem

In Section 2.3, the first assumption we made when demonstrating the Faddeev-Popov method was that the Landau gauge condition was *ideal*. In terms of geometry of gauge space, this is equivalent to assuming that the chosen gauge slice crosses each gauge orbit exactly once. Unfortunately, this is not true for Yang-Mills theories in general, due to their highly non-trivial topological structure. In fact, in Ref. 84 it was proved that it is impossible to choose a unique representative of each orbit using a continuous gauge condition.

3.1.1 Gribov Copies

The spurious intersection points on the gauge slice are called *Gribov copies* or *ambiguities* and we can define them in Landau gauge as follows. Take a given field configuration A_μ obeying the Landau condition, i.e.,

$$\partial_\mu A_\mu = 0. \quad (3.1)$$

If we can find a configuration A'_μ *physically equivalent* to A_μ and that also satisfies the same gauge condition, namely

$$\partial_\mu A'_\mu = 0, \quad (3.2)$$

then we have a Gribov copy.

In theories with $SU(N_c)$ local symmetry, we know that physically equivalent fields $A'_\mu = A_\mu^{\mathfrak{g}}$ are connected to A_μ through the transformation (2.124) for every $\mathfrak{g} \in \mathbb{G}$. This formally defines the concept of gauge orbit. Now suppose we take an infinitesimal transformation $\mathfrak{g} = \mathbb{1} + i\theta$ along such orbit

$$A_\mu \rightarrow A'_\mu = A_\mu - D_\mu \theta, \quad (3.3)$$

and impose the Landau gauge condition on both A_μ and its transformation A'_μ as in (3.1) and (3.2), i.e.,

$$\partial_\mu A'_\mu = \partial_\mu A_\mu - \partial_\mu D_\mu \theta = -\partial_\mu D_\mu \theta = \mathcal{M}[A] \theta = 0. \quad (3.4)$$

This is a condition for the existence of infinitesimal Gribov copies under the transformation $\mathbf{g}$. Furthermore, the statement of (3.4), here written for clarity as

$$\int d^4y \mathcal{M}^{ab}(x, y) \theta^b(y) = 0, \quad (3.5)$$

is the same as saying that the Faddeev-Popov operator has zero modes, i.e., that it has eigenvectors with null eigenvalues. Therefore, the existence of Gribov copies is directly related to the presence of (non-trivial)^A zero modes in the spectrum of $\mathcal{M}$.

We can further explore this by posing the complete eigenvalue equation for Faddeev-Popov operator

$$\mathcal{M}\gamma = \lambda\gamma. \quad (3.6)$$

This is just a Schrödinger-type equation for the “wave function” $\gamma(x)$, explicitly written as

$$-\partial_\mu \partial_\mu \gamma - i g_0 \partial_\mu [A_\mu, \gamma] = \lambda\gamma, \quad (3.7)$$

with the “energy” eigenvalue λ . Knowing that the negative Laplace operator has only positive eigenvalues, we can say that for sufficiently large (in some sense) gauge fields A_μ , this Schrödinger equation will certainly have zero eigenvalues. Comparing this analysis to condition (3.4) we see that the Landau gauge condition cannot be taken as ideal over the entire gauge space. For explicit examples of Gribov copies, see Refs. 85, 86.

Moreover, recall that we also assumed the Faddeev-Popov determinant (2.129) to be always positive. As the above discussion attests, the Faddeev-Popov operator can clearly have negative eigenvalues for some field configurations, implying that $\det \mathcal{M}$ is not always positive.

From these last remarks, we can conclude that our gauge-fixing procedure through the Faddeev-Popov method is not always satisfactory. As long as we are close enough to the naive vacuum $A_\mu = 0$, infinitesimal copies are not an issue and we can do perturbation theory with a clean conscience. However, for non-perturbative reasoning this quantization process is certainly spoiled.

3.1.2 Gribov Region

As a possible solution to the ambiguity problem, Gribov proposed the restriction of the path integration to the so-called *Gribov region*. This region is defined as

$$\Omega = \{A_\mu \in \mathbb{A} \mid \partial_\mu A_\mu = 0, \mathcal{M}[A] > 0\}, \quad (3.8)$$

^A There will always be trivial zero modes associated to constant eigenvectors.

where $\mathcal{M}[A] > 0$ means positive-definiteness, namely

$$\int d^4x \gamma^a(x) \int d^4y \mathcal{M}^{ab}(x, y) \gamma^b(y) \equiv (\gamma, \mathcal{M}[A]\gamma) > 0, \quad \forall \gamma \neq 0, \quad (3.9)$$

for a given A_μ . Notice that γ^a is not a fermionic variable, but only real test function.

The Gribov region has several geometric properties that endorses the geometric approach characteristic of Gribov's theory. Those properties help concretely define Ω as a suitable region of integration. The most important ones are:

(1) The vacuum belongs to Ω

The Faddeev-Popov operator for the vacuum ($A_\mu^0 = 0$) is just the negative Laplace operator

$$\mathcal{M}[0] = -\square \quad (3.10)$$

and, as we have already commented, it possesses only positive eigenvalues apart from the trivial space. Therefore, the condition (3.1.2) is automatically satisfied and the vacuum is in the Gribov region.

(2) Ω is convex

If a and b and $\rho a + (1 - \rho)b$, $\rho \in [0, 1]$, are inside a region, then such region is said to be *convex*. Graphically, any straight line from a to b is entirely contained inside the region.

In the case of the Gribov region, take two arbitrary configurations $A_\mu^{(1)}, A_\mu^{(2)} \in \Omega$ and a third one defined by $A_\mu^{(3)} \equiv \rho A_\mu^{(1)} + (1 - \rho)A_\mu^{(2)}$, $\rho \in [0, 1]$. Clearly, $\partial_\mu A_\mu^{(3)} = 0$ if $\partial_\mu A_\mu^{(1)} = 0$ and $\partial_\mu A_\mu^{(2)} = 0$. It remains to show that $\mathcal{M}[A^{(3)}]$ is positive-definite. The Faddeev-Popov operator defined by $A_\mu^{(3)}$ is

$$\begin{aligned} \mathcal{M}^{ab}[A^{(3)}] &= \left(-\square \delta^{ab} - g_0 \partial_\mu f^{abc} \rho A_\mu^{c(1)} \right) + \left(-\square \delta^{ab} - g_0 \partial_\mu f^{abc} (1 - \rho) A_\mu^{c(2)} \right) \pm \rho \square \delta^{ab} \\ &= \mathcal{M}^{ab}[\rho A^{(1)}] + \mathcal{M}^{ab}[(1 - \rho)A^{(2)}] = \rho \mathcal{M}^{ab}[A^{(1)}] + (1 - \rho) \mathcal{M}^{ab}[A^{(2)}]. \end{aligned} \quad (3.11)$$

Taking an arbitrary normalized vector γ , notice that

$$(\gamma, \mathcal{M}[A^{(3)}]\gamma) = \rho (\gamma, \mathcal{M}[A^{(1)}]\gamma) + (1 - \rho) (\gamma, \mathcal{M}[A^{(2)}]\gamma) \geq \rho \lambda_1^{(1)} + (1 - \rho) \lambda_1^{(2)} > 0, \quad (3.12)$$

where $\lambda_1^{(1)}$ and $\lambda_1^{(2)}$ are the smallest eigenvalues of $\mathcal{M}[A^{(1)}]$ and $\mathcal{M}[A^{(2)}]$, respectively. Therefore, $\mathcal{M}[A^{(3)}] > 0$ and $A_\mu^{(3)}$ belongs to the Gribov region.

(3) Ω is bounded in every direction

We can show Ω is bounded in every direction in the gauge-space if, given an arbitrary configuration $A_\mu \in \Omega$ (and different from the vacuum), we step out of the Gribov region after a scale transformation of the kind

$$A_\mu \rightarrow \rho A_\mu, \quad \rho \in \mathbb{R}, \quad (3.13)$$

for large enough ρ , i.e., if $\rho A_\mu \notin \Omega$ for some finite ρ .

Indeed, this is very simple to demonstrate.⁸⁷ First decompose the Faddeev-Popov operator as

$$\mathcal{M}[A] = -\square + \mathcal{K}[A], \quad (3.14)$$

where $\mathcal{K}^{ab}[A] = -g_0 f^{abc} A_\mu^c \partial_\mu$. Notice that, using the antisymmetry of the structure constants, $\sum \lambda_{\mathcal{K}} = \text{Tr } \mathcal{K} = 0$, being $\{\lambda_{\mathcal{K}}\}$ the set of eigenvalues of $\mathcal{K}$. Then, at least one of them, say $\lambda_{\mathcal{K}}^{(-)}$, has to be negative in order for their sum to be zero. Consider the eigenvector corresponding to $\lambda_{\mathcal{K}}^{(-)}$ and name it $\gamma^{(-)}$. For the scaled configuration we obtain

$$(\gamma^{(-)}, \mathcal{M}[\rho A] \gamma^{(-)}) = -(\gamma^{(-)}, \square \gamma^{(-)}) + \rho \lambda_{\mathcal{K}}^{(-)} < 0 \quad (3.15)$$

for a large enough value of ρ , meaning that the Faddeev-Popov operator defined by ρA_μ is not positive-definite as in (3.9), i.e., $\rho A_\mu \notin \Omega$, as we wanted to show. Furthermore, it is also possible to prove that the Gribov region is bounded by a hyper-ellipsoid in the gauge-space.⁸⁸

(4) All orbits cross Ω

Another important property of the Gribov region is that every gauge orbit crosses it at least once, which was proved in.⁸⁹ In this way, we make sure that the path integration over Ω includes all the physical configurations.

The enumeration of these properties apparently supports Ω as a region free of copies and suitable for restricting the Yang-Mills path integral. It is also useful to pictorially visualize it as in Figure 3.1. Notice that the boundary $\partial\Omega$ of the (first) Gribov region, known as *Gribov horizon*, is defined by the contiguous line of null eigenvalues of the Faddeev-Popov operator. The subsequent region in the outward direction from $A_\mu = 0$, i.e. Ω_1 , is the geometric locus of field configurations whose Faddeev-Popov operator contains one negative eigenvalue and it is called the second Gribov region. This geometric categorization goes on indefinitely as we walk through $\mathbb{A}$. Actually, we can prove that there are infinitesimally related copies in both sides of each horizon,^{21,85} which further motivates the use of such horizons as separators of ambiguities.

An important formulation of the Gribov region is based on the functional (on the gauge transformations) defined by

$$E[A^{\mathfrak{g}}] = \|A^{\mathfrak{g}}\|^2 \equiv \int d^4x \text{Tr} [A_\mu^{\mathfrak{g}}(x) A_\mu^{\mathfrak{g}}(x)] = \frac{1}{2} \int d^4x A_\mu^{\mathfrak{g}a}(x) A_\mu^{\mathfrak{g}a}(x), \quad (3.16)$$

frequently referred to as minimizing functional. This functional has a different value on each point of a given gauge orbit and the Gribov region is the set of its *local minima* along all orbits.

Figure 3.1 – Representation of the gauge slice (hypersurface) defined by Landau condition (3.1) in $\mathbb{A}$. Note that the gauge orbits pierce the hyperplane at more than one point, representing a non-ideal situation.

Source: By the author.

We can recover (3.1.2) by recalling the conditions on the first and second derivatives of a one-variable function so that a certain point in the domain is a local minimum, and extending these conditions to functionals. We expect that the first and second order (infinitesimal) variations around a local minimum of a certain gauge orbit obey $\delta \|A\|^2 = 0$ and $\delta^2 \|A\|^2 > 0$, where we have fixed $\mathfrak{g} = \mathbb{1}$. Then, the first variation of (3.16) yields

$$\delta \|A\|^2 = \frac{1}{2} \delta \int d^4x A_\mu^a A_\mu^a = \int d^4x A_\mu^a \delta A_\mu^a = - \int d^4x A_\mu^a (D_\mu \theta)^a, \quad (3.17)$$

and using the antisymmetry of the structure constants,

$$\begin{aligned} \delta \|A\|^2 &= - \int d^4x A_\mu^a (\partial_\mu \delta^{ab} + g_0 f^{abc} A_\mu^c) \theta^b = \int d^4x \theta^a \partial_\mu A_\mu^a = 0, \quad \forall \theta \\ &\Rightarrow \partial \cdot A = 0, \end{aligned} \quad (3.18)$$

where we neglected a surface term after an integration by parts. Iterating this process, the second variation yields

$$\begin{aligned} \delta^2 \|A\|^2 &= \delta \int d^4x \theta^a \partial_\mu A_\mu^a = \int d^4x \theta^a (-\partial_\mu D_\mu)^{ab} \theta^b > 0, \quad \forall \theta \\ &\Rightarrow \mathcal{M}[A] = -\partial \cdot D > 0. \end{aligned} \quad (3.19)$$

These two conditions are nothing more than the original definition of the Gribov region.

Unfortunately, the (first) Gribov region still contains copies.^{22,87} This is expected because the functional $\|A\|^2$, being defined on a high-dimensional space (very similar to the energy of a frustrated system), certainly has more than one minimum per gauge orbit. Such problem motivates the introduction of the *fundamental modular region* (FMR), symbolized by Λ .

The FMR is defined as the set of *absolute* minima of (3.16). Then, restricting the path integral to Λ would be the “correct” choice, for it really selects only one representative

configuration from each orbit. Of course, it is rather obscure which set of minima of $\|A\|^2$, absolute or not, should be included in the integration. Conventionally, the region Λ takes into account the minima where $\|A\|^2$ is closest to the naive vacuum up to a *global* gauge transformation, namely (3.16)^B. This adds up to the uniqueness problem of the global minimum of the minimizing functional.

Being a proper subset of the Gribov region, we expect that the FMR have properties very similar to those of Ω . In fact, this is true and they have been proved.^{86,87} Nevertheless, although we know that the interior of the FMR does not contain any Gribov copies, its boundary $\partial\Lambda$ contains continuous degeneracies corresponding to zero modes.⁸⁶ The latter are absolute minima of the minimizing functional (3.16) along the same gauge orbit and they belong to the Gribov horizon as well (see Figure 3.2). In principle, these copies must be identified in order to have a proper fundamental modular region, although they should not pose a problem to the path integration for they have a “zero measure”. Actually, this is rather tricky because the measure is also expected to be concentrated at $\partial\Omega$ in the infinite-volume limit.⁹¹

No one was able to implement the restriction of the Yang-Mills path integral to Λ . One can argue that only copies in the common boundary of the Gribov region and the FMR (see Figure 3.2) should be relevant in the path integral measure.⁹⁰ On the other hand, many lattice studies indicate that the Gribov copies inside Ω are not capable of modifying the qualitative aspect of many results. In that sense, the first calculations by Gribov (further developed by Zwanziger) already provide non-trivial information about the effects of restricting the path integral to Ω .

We should point out that alternatives to the Gribov problem for non-Abelian theories exist. Besides the use of non-covariant gauges,⁸¹ there is the very different possibility of stochastic quantization and gauge fixing.⁹² Also, some work towards averaging over all Gribov copies instead of restricting the path integral to Ω has been advocated,⁹³ or even gauge fixing the theory “by patches” of gauge space in order to avoid Gribov horizons⁹⁴ (for more examples, see Ref. 22).

Figure 3.2 – Depiction of the FMR region and its common boundary with Ω . The topology of $\partial\Omega \cap \partial\Lambda$ is oversimplified.

Source: By the author.

^B Furthermore, we could prescribe an analogous minimizing functional for non-trivial topological sectors of the gauge-space by centering the FMR around an instanton configuration.⁹⁰

3.2 No-Pole Condition

Now we will walk through the semi-classical computation by Gribov in Landau gauge^{21,22} with some detail. This will give us insight on the propagators' infrared behavior entailed by Gribov's formulation. His idea was to implement the restriction of the path integral to Ω as a condition over the gauge fields A_μ . Having that in mind, in a first moment we will treat them as classical (external) fields, maintaining only the ghost degrees of freedom in the path integral. Then, we will integrate them in a convenient way to properly add the effect of the Gribov region to the propagators.

Nevertheless, we first need to gain some insight into how the restriction to Ω contributes to the complete theory. For this we analyze the full ghost propagator. Then we define the full Yang-Mills path integral (2.137) together with a factor $\mathcal{V}(\Omega)$ which suppresses path integration outside the Gribov region

$$\mathcal{Z}_\Omega = \int \mathfrak{D}A \mathfrak{D}c \bar{c} e^{-S_{\text{FP}}[A, \bar{c}, c]} \mathcal{V}(\Omega), \quad (3.20)$$

whereby we drop the argument on the functional measures. In order to compute the ghost propagator we add the corresponding ghost sources and define the generating functional

$$\mathcal{Z}_\Omega[\bar{\eta}, \eta] = \int \mathfrak{D}A e^{-S_{\text{FP}}[A]} \mathcal{V}(\Omega) \mathcal{Z}_{\bar{c}, c}[\bar{\eta}, \eta; A], \quad (3.21)$$

where $\bar{\eta}, \eta$ are also Grassmannian fields and the ghost generating functional is composed of the Faddeev-Popov operator, see (2.136) and (B.15). We can write $\mathcal{Z}_{\bar{c}, c}[\bar{\eta}, \eta]$ in terms of the sources' Fourier components, yielding

$$\tilde{\mathcal{Z}}_{\bar{c}, c}[\bar{\eta}, \eta; A] = \det \mathcal{M} e^{-\int \frac{d^4 q}{(2\pi)^4} \bar{\eta}^a(-q) (\mathcal{M}^{-1})^{ab}(q) \eta^b(q)}, \quad (3.22)$$

where we assumed that $\mathcal{M}$ is invariant under translations and thus $\mathcal{M}(x, y) = \mathcal{M}(x - y)$. From (3.22) and the Fourier version of (3.21), the ghost propagator turns out to be

$$\begin{aligned} \langle \bar{c}^a(k) c^b(-p) \rangle_\Omega &= \frac{1}{\tilde{\mathcal{Z}}_\Omega[0]} \frac{\delta}{\delta \bar{\eta}^b(p)} \frac{\delta}{\delta \eta^a(-k)} \tilde{\mathcal{Z}}_\Omega[\bar{\eta}, \eta] \Big|_{\bar{\eta}=\eta=0} \\ &= (2\pi)^4 \delta(k - p) \frac{\int \mathfrak{D}A e^{-S_{\text{YM}}[A]} \mathcal{V}(\Omega) (\det \mathcal{M}) (\mathcal{M}^{-1})^{ba}(k)}{\int \mathfrak{D}A e^{-S_{\text{YM}}[A]} \mathcal{V}(\Omega) (\det \mathcal{M})} \\ &\equiv (2\pi)^4 \delta(k - p) \mathcal{G}_\Omega^{ab}(k). \end{aligned} \quad (3.23)$$

Now, take the perturbative one-loop result for the same quantity without the restriction of the path integral²²

$$\mathcal{G}_{1L}(k) = \frac{\delta^{ab}}{N_c^2 - 1} \mathcal{G}_{1L}^{ab} = \frac{1}{k^2} \frac{1}{\left(1 - \frac{11N_c g_0^2}{48\pi^2} \ln \frac{\Lambda^2}{k^2}\right)^{9/44}}, \quad (3.24)$$

and notice that it has two poles, one at $k_1^2 = 0$ and another one at $k_2^2 = \Lambda^2 \exp\left(-\frac{48\pi^2}{11N_c g^2}\right)$, where Λ is an ultraviolet cut-off. For $k^2 \gg k_1^2, k_2^2$, the one-loop expression $\mathcal{G}_{1L}$ is positive

and, being in the perturbative regime, we can safely state that the path integration is constrained to the Gribov region. However, if we compare this perturbative result with $\mathcal{G}_\Omega$ in the range of momenta $0 < k^2 < k_2^2$, we see that $\mathcal{G}_{1L}$ is no longer positive and consequently the Faddeev-Popov operator is not positive-definite anymore, which means that we are outside of Ω . Therefore, if we require that the only pole present in the ghost propagator be the one at $k^2 = 0$, then the path integration will be confined to the Gribov region. This is the so-called *no-pole* condition.²¹

Following the above reasoning we will now treat A_μ as an external field and obtain a condition so that $\mathcal{G}$ has no poles for $p > 0$. Thus we shall only need the pure ghost generating functional (3.22) written in a perturbative fashion (see B.3). In terms of Fourier components,

$$\tilde{\mathcal{Z}}_{\bar{c},c}[\bar{\eta}, \eta; A] = \exp \left(i g_0 f^{dec} \int \frac{d^4 l}{(2\pi)^4} \frac{d^4 u}{(2\pi)^4} A_\mu^c(l+u) l_\mu \frac{\delta}{\delta \bar{\eta}^d(l)} \frac{\delta}{\delta \eta^e(u)} \right) \tilde{\mathcal{Z}}_{\bar{c},c}^0[\bar{\eta}, \eta], \quad (3.25)$$

where the $\mathcal{Z}_{\bar{c},c}^0$ is defined in (B.24) and (B.26), whose Fourier version is

$$\tilde{\mathcal{Z}}_{\bar{c},c}^0[\bar{\eta}, \eta] = \mathcal{N} e^{-\int \frac{d^4 q}{(2\pi)^4} \bar{\eta}^a(-q) \mathcal{G}_{(0)}^{ab}(q) \eta^b(q)}. \quad (3.26)$$

The ghost propagator obtained from (3.25) and expressed as a series up to second order is

$$\mathcal{G}(k; A) = \mathcal{G}_{(0)}(k; A) + \mathcal{G}_{(1)}(k; A) + \frac{1}{2} \mathcal{G}_{(2)}(k; A), \quad (3.27)$$

where the zeroth-order term is just the usual free ghost propagator (B.26)

$$\begin{aligned} (2\pi)^4 \delta(k-p) \mathcal{G}_{(0)}(k; A) &= \frac{\delta^{ab}}{N_c^2 - 1} \frac{1}{\tilde{\mathcal{Z}}_{\bar{c},c}^0[0]} \frac{\delta}{\delta \bar{\eta}^b(p)} \frac{\delta}{\delta \eta^a(-k)} \tilde{\mathcal{Z}}_{\bar{c},c}^0[\bar{\eta}, \eta] \Big|_{\bar{\eta}=\eta=0} \\ &= (2\pi)^4 \delta(k-p) \mathcal{G}_{(0)}(k) = (2\pi)^4 \delta(k-p) \frac{1}{k^2}. \end{aligned} \quad (3.28)$$

The higher order terms can be computed by drawing the possible connected diagrams, namely

Figure 3.3 – Connected Feynman diagrams up to $\mathcal{O}(g_0^2)$.

$$\sigma(k; A) = \frac{1}{V} \frac{N_c g_0^2}{(N_c^2 - 1)} \frac{k_\mu}{k^2} \int \frac{d^4 q}{(2\pi)^4} \frac{(k - q)_\nu}{(k - q)^2} A_\mu^c(q) A_\nu^c(-q) \quad (3.34)$$

is called the *ghost form factor*^C. Writing (3.33) as a geometric sum and ignoring the higher order corrections, we find

$$\mathcal{G}(k; A) = \frac{1}{k^2} \frac{1}{1 - \sigma(k; A)}. \quad (3.35)$$

Recalling the discussion following (3.24), we see that the suggestive expression (3.35) provides a compact way of stating the no-pole condition

$$\sigma(k; A) < 1. \quad (3.36)$$

We can then say that (3.36) is a necessary condition (in the semi-classical treatment) for a given configuration A_μ to be inside the Gribov region.

We can further simplify the last expression in order to make practical use of it. First, note that in Landau gauge $q_\mu A_\mu^c(q) A_\nu^c(-q) = q_\nu A_\mu^c(q) A_\nu^c(-q) = 0$, so that the tensor $A_\mu^c(q) A_\nu^c(-q)$ has no longitudinal component. Hence we can write it in terms only of its transverse component A_T , i.e.,

$$A_\mu^c(q) A_\nu^c(-q) = A^T \mathcal{P}_{\mu\nu}^T \quad \therefore \quad A^T = \frac{1}{3} A_\rho^c(q) A_\rho^c(-q), \quad (3.37)$$

obtained after contracting μ and ν , where $\mathcal{P}_{\mu\nu}^T = \delta_{\mu\nu} - q_\mu q_\nu / q^2$ is the transverse projector operator. Consequently, noting that $k_\mu q_\nu \mathcal{P}_{\mu\nu}^T = 0$, we have

$$\begin{aligned} \sigma(k; A) &= \frac{1}{V} \frac{N_c g_0^2}{N_c^2 - 1} \frac{k_\mu}{k^2} \int \frac{d^4 q}{(2\pi)^4} \frac{k_\nu}{(k - q)^2} \frac{1}{3} A_\rho^c(q) A_\rho^c(-q) \mathcal{P}_{\mu\nu}^T \\ &= \frac{1}{3V} \frac{N_c g_0^2}{N_c^2 - 1} \left\{ \int \frac{d^4 q}{(2\pi)^4} \frac{A_\rho^c(q) A_\rho^c(-q)}{(k - q)^2} - \frac{k_\mu k_\nu}{k^2} \int \frac{d^4 q}{(2\pi)^4} \frac{A_\rho^c(q) A_\rho^c(-q)}{(k - q)^2} \frac{q_\nu q_\mu}{q^2} \right\}. \end{aligned} \quad (3.38)$$

One can show in arbitrary dimensions that $\sigma(k; A)$ is a decreasing function of k^2 ,⁹⁵ so that we can safely express the no-pole condition (3.36) as

$$\sigma(0; A) < 1, \quad (3.39)$$

which is much simpler. Finally, the limit $k \rightarrow 0$ is taken by using the identity²²

$$\int d^4 q f(q^2) \frac{q_\mu q_\nu}{q^2} = \frac{\delta_{\mu\nu}}{4} \int d^4 q f(q^2) \quad (3.40)$$

in the second term of the following line, yielding

$$\begin{aligned} \sigma(0; A) &= \frac{1}{3V} \frac{N_c g_0^2}{N_c^2 - 1} \left\{ \int \frac{d^4 q}{(2\pi)^4} \frac{A_\rho^c(q) A_\rho^c(-q)}{q^2} - \lim_{k \rightarrow 0} \frac{k_\mu k_\nu}{k^2} \int \frac{d^4 q}{(2\pi)^4} \frac{A_\rho^c(q) A_\rho^c(-q)}{q^2} \frac{q_\nu q_\mu}{q^2} \right\} \\ &= \frac{1}{3V} \frac{N_c g_0^2}{N_c^2 - 1} \left(1 - \frac{k_\mu k_\nu \delta_{\mu\nu}}{4k^2} \right) \int \frac{d^4 q}{(2\pi)^4} \frac{A_\rho^c(q) A_\rho^c(-q)}{q^2} \\ &= \frac{1}{4V} \frac{N_c g_0^2}{N_c^2 - 1} \int \frac{d^4 q}{(2\pi)^4} \frac{1}{q^2} A_\rho^c(q) A_\rho^c(-q). \end{aligned} \quad (3.41)$$

We shall now implement the no-pole condition in the calculation of the gluon and ghost propagators.

^C The physical volume V comes from the factor $(2\pi)^4 \delta(0)$ in (3.32). This reflects the fact that we are always implicitly considering the limit $V \rightarrow \infty$.

3.3 Propagators

3.3.1 Gluon Propagator

In the last section we obtained (3.39) as a condition so that the ghost propagator has no poles except for $k = 0$. This guaranteed the restriction of the path integral to the Gribov region. Recall that we introduced a factor in Equation (3.20) so that it would filter out the path integral at the first Gribov horizon, as desired. Together with (3.39) we can guess that the simplest way to that is

$$\mathcal{V}(\Omega) = \begin{cases} 1 & \text{if } \sigma(0; A) < 1 \\ 0 & \text{if } \sigma(0; A) > 1 \end{cases} = \theta(1 - \sigma(0; A)), \quad (3.42)$$

i.e., with the Heaviside function. The Heaviside function has the following integral representation

$$\theta(x) = \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{d\beta}{2\pi i} \frac{e^{i\beta x}}{\beta - i\varepsilon} = \lim_{\varepsilon \rightarrow 0^+} \int_{-i\infty+\varepsilon}^{+i\infty+\varepsilon} \frac{d\beta}{2\pi i \beta} e^{\beta x}, \quad (3.43)$$

yielding the path integral

$$\begin{aligned} \mathcal{Z}_\Omega &= \int \mathfrak{D}A \mathfrak{D}c \bar{c} e^{-S_{\text{FP}}[A, \bar{c}, c]} \mathcal{V}(\Omega) \\ &= \int \mathfrak{D}A \mathfrak{D}c \bar{c} \int \frac{d\beta}{2\pi i \beta} e^{\beta} e^{-\beta \sigma(0; A)} e^{-S_{\text{FP}}[A, \bar{c}, c]}, \end{aligned} \quad (3.44)$$

where the limits of the β integral and the limit $\varepsilon \rightarrow 0^+$ are implicit in the notation. As we will be interested in the tree-level contribution to the propagators, we separate the Faddeev-Popov action in quadratic and interacting parts and define

$$\mathcal{Z}_\Omega^0 = \int \frac{d\beta}{2\pi i \beta} e^{\beta} \int \mathfrak{D}A e^{-\beta \sigma(0; A) - S_A^0[A]} \mathcal{Z}_{\bar{c}, c}[\bar{\eta}, \eta; A], \quad (3.45)$$

where, in particular, the free gluon action is

$$\begin{aligned} S_A^0[A] &= \int d^4x \frac{1}{4} (\partial_\mu A_\nu^a - \partial_\nu A_\mu^a)^2 + \frac{1}{2\alpha} (\partial \cdot A^a)^2 \\ &= -\frac{1}{2} \int d^4x A_\mu^a(x) \delta^{ab} \left[\square \delta_{\mu\nu} + \left(\frac{1}{\alpha} - 1 \right) \partial_\mu \partial_\nu \right] \delta(x - y) A_\nu^b(y). \end{aligned} \quad (3.46)$$

Noting the quadratic form of $\sigma(0; A)$, we write the Fourier version of (3.45) as the generating functional ^D

$$\begin{aligned} \tilde{\mathcal{Z}}_\Omega^0[J] &= \int \frac{d\beta}{2\pi i \beta} e^{\beta} \int \mathfrak{D}A e^{-\frac{1}{2} \int \frac{d^4k}{(2\pi)^4} A_\mu^a(-k) K_{\mu\nu}^{ab}(k) A_\nu^b(k) + \int \frac{d^4k}{(2\pi)^4} J_\mu^a(-k) A_\mu^a(k)} \int \mathfrak{D}c \bar{c} e^{-S_{\bar{c}, c}^0[\bar{c}, c]} \\ &= \mathcal{N} \int \frac{d\beta}{2\pi i \beta} (\det K)^{-1/2} e^{\frac{1}{2} \int \frac{d^4k}{(2\pi)^4} J_\mu^a(-k) (K^{-1})_{\mu\nu}^{ab}(k) J_\nu^b(k)} \int \mathfrak{D}c \bar{c} e^{-S_{\bar{c}, c}^0[\bar{c}, c]}, \end{aligned} \quad (3.47)$$

^D The validity of the Faddeev-Popov method in the presence of gluon sources must be taken with a grain of salt since the original action is not gauge-invariant anymore. The answer boils down to the insensitivity of S -matrix elements in the presence of physical sources, see Refs. 65, 96 for details.

where (B.4) was used, and define

$$K_{\mu\nu}^{ab}(k) = \delta^{ab} \left[\frac{\beta N_c g_0^2}{2V(N_c^2 - 1)} \frac{\delta_{\mu\nu}}{k^2} + k^2 \delta_{\mu\nu} + \left(\frac{1}{\alpha} - 1 \right) k_\mu k_\nu \right]. \quad (3.48)$$

Then, the tree-level gluon propagator is given by, see (B.2),

$$\begin{aligned} \langle A_\mu^a(k) A_\nu^b(-k) \rangle_\Omega &= \frac{1}{\tilde{\mathcal{Z}}_\Omega^0[0]} \frac{\delta}{\delta J_\nu^b(p)} \frac{\delta}{\delta J_\mu^a(-k)} \tilde{\mathcal{Z}}_\Omega^0[J] \Big|_{J=0} \\ &= \frac{1}{\tilde{\mathcal{Z}}_\Omega^0[0]} (2\pi)^4 \delta(0) \mathcal{N} \int \frac{d\beta}{2\pi i} \frac{e^\beta}{\beta} (\det K)^{-1/2} (K^{-1})_{\mu\nu}^{ab}(k). \end{aligned} \quad (3.49)$$

The determinant is computed in Ref.²² and we write it down here

$$(\det K)^{-1/2} = \exp \left\{ -\frac{3}{2} (N_c^2 - 1) V \int \frac{d^4 q}{(2\pi)^4} \ln \left(q^2 + \frac{\beta}{2V q^2} \frac{N_c}{N_c^2 - 1} \right) \right\}. \quad (3.50)$$

We proceed in the computation of (3.49) with a steepest-descent⁵⁵ evaluation

$$\langle A_\mu^a(k) A_\nu^b(-k) \rangle_\Omega = V \frac{1}{\tilde{\mathcal{Z}}_\Omega^0[0]} \int \frac{d\beta}{2\pi i} e^{f(\beta)} (K^{-1})_{\mu\nu}^{ab}(k) \approx V (K^{-1})_{\mu\nu}^{ab}(k) \Big|_{\beta=\beta_0}, \quad (3.51)$$

where the saddle-point is defined by the stationary condition $f'(\beta_0) = 0$, with respect to the function

$$f(\beta) = \beta - \ln \beta - \frac{3}{2} (N_c^2 - 1) V \int \frac{d^4 q}{(2\pi)^4} \ln \left(q^2 + \frac{\beta}{2V q^2} \frac{N_c g_0^2}{N_c^2 - 1} \right). \quad (3.52)$$

This yields the *gap equation* in the thermodynamic limit $V \rightarrow \infty$, supposing $\beta_0 \sim V$ so that γ is finite,

$$1 = g_0^2 N_c \frac{3}{4} \int \frac{d^4 q}{(2\pi)^4} \frac{1}{q^4 + 2g_0^2 N_c \gamma^4}, \quad (3.53)$$

which fixes the evaluation point of the steepest-descent and where the mass parameter γ is defined as

$$\gamma^4 \equiv \frac{\beta_0}{4V(N_c^2 - 1)}. \quad (3.54)$$

Finally, using the procedure in B.3 to invert (3.48) we arrive at the gluon propagator according to the Gribov approximation

$$(K^{-1})_{\mu\nu}^{ab}(k) = \delta^{ab} \frac{k^2}{k^4 + 2g_0^2 N_c \gamma^4} \left[\delta_{\mu\nu} + (\alpha - 1) \frac{k^2 k_\mu k_\nu}{k^4 + 2\alpha g_0^2 N_c \gamma^4} \right] \equiv D_{\mu\nu}^{ab}(k), \quad (3.55)$$

which in Landau gauge reduces to

$$D_{\mu\nu}^{ab}(k) = \delta^{ab} \left(\frac{k^2}{k^4 + 2g_0^2 N_c \gamma^4} \right) \mathcal{P}_{\mu\nu}^T \equiv \delta^{ab} D(k) \mathcal{P}_{\mu\nu}^T. \quad (3.56)$$

We see that the mass parameter γ works as a low-momentum regulator of the theory, non-trivially modifying the infrared behavior of the gluon propagator. According to this

result, $D(k)$ is said to be infrared *suppressed* and, in particular, $D(0) = 0$. This result implies that the gluon propagator violates reflection positivity of the theory which, as commented in Section 2.2.4, is necessary for the construction of a sensible Hilbert space and the interpretation of the gluon as an asymptotic particle.⁹⁷ This impossibility should be an indication of gluon confinement and shall be further explored over the next chapters.

3.3.2 Ghost Propagator

The Landau gauge ghost propagator is computed in a similar way by doing the remaining functional integral over the gauge field in (3.35)

$$\begin{aligned} \langle \bar{c}^a(k) c^b(-k) \rangle_\Omega &= (2\pi)^4 \delta(0) \frac{\int \mathfrak{D}A \ e^{-S_A^0[A]} \mathcal{G}^{ab}(k; A) \mathcal{V}(\Omega)}{\int \mathfrak{D}A \ e^{-S_A^0[A]} \mathcal{V}(\Omega)} \\ &= V \frac{1}{k^2} \frac{1}{1 - \langle \sigma(k) \rangle}, \end{aligned} \quad (3.57)$$

where the ghost form factor (3.38) is averaged over the Gribov region

$$\begin{aligned} \langle \sigma(k) \rangle &= \frac{1}{3V} \frac{N_c g_0^2}{N_c^2 - 1} \frac{k_\mu k_\nu}{k^2} \int \frac{d^4 q}{(2\pi)^4} \frac{\langle A_\rho^c(q) A_\rho^c(-q) \rangle}{(k - q)^2} \mathcal{P}_{\mu\nu}^T \\ &= N_c g_0^2 \frac{k_\mu k_\nu}{k^2} \int \frac{d^4 q}{(2\pi)^4} \frac{1}{q^4 + 2g_0^2 N_c \gamma^4} \frac{q^2}{(k - q)^2} \mathcal{P}_{\mu\nu}^T, \end{aligned} \quad (3.58)$$

which is obtained after the use of identity (3.40). To compute $1 - \langle \sigma(k) \rangle$ we write “1” in a convenient way using the gap equation (3.53) and again (3.40),

$$\begin{aligned} 1 - \langle \sigma(k) \rangle &= N_c g_0^2 \delta_{\mu\nu} \frac{k_\mu k_\nu}{k^2} \int \frac{d^4 q}{(2\pi)^4} \frac{1}{q^4 + \chi^4} \left(1 - \frac{1}{4} \right) - N_c g_0^2 \frac{k_\mu k_\nu}{k^2} \int \frac{d^4 q}{(2\pi)^4} \frac{q^2}{q^4 + \chi^4} \frac{1}{(k - q)^2} \mathcal{P}_{\mu\nu}^T \\ &= N_c g_0^2 \frac{k_\mu k_\nu}{k^2} \int \frac{d^4 q}{(2\pi)^4} \frac{1}{q^4 + \chi^4} \left(\delta_{\mu\nu} - \frac{q_\mu q_\nu}{q^2} \right) - N_c g_0^2 \frac{k_\mu k_\nu}{k^2} \int \frac{d^4 q}{(2\pi)^4} \frac{1}{q^4 + \chi^4} \frac{q^2}{(k - q)^2} \mathcal{P}_{\mu\nu}^T \\ &= N_c g_0^2 \frac{k_\mu k_\nu}{k^2} \int \frac{d^4 q}{(2\pi)^4} \frac{1}{q^4 + \chi^4} \left(1 - \frac{q^2}{(k - q)^2} \right) \mathcal{P}_{\mu\nu}^T, \end{aligned} \quad (3.59)$$

with the acronym $\chi^4 = 2g_0^2 N_c \gamma^4$.

Thus the one-loop corrected ghost propagator in Gribov’s approach is given by

$$\mathcal{G}^{ab}(k) = \frac{\delta^{ab}}{k^2} \left\{ N_c g_0^2 \frac{k_\mu k_\nu}{k^2} \int \frac{d^4 q}{(2\pi)^4} \frac{1}{q^4 + 2g_0^2 N_c \gamma^4} \left(1 - \frac{q^2}{(k - q)^2} \right) \mathcal{P}_{\mu\nu}^T \right\}^{-1}, \quad (3.60)$$

and following Ref. 98 we can extract the infrared behavior by the approximation $\left(1 - \frac{q^2}{(k - q)^2} \right) \approx$

$\frac{k^2 - 2k \cdot q}{q^2}$ near $k = 0$, yielding

$$\begin{aligned} \mathcal{G}^{ab}(k) &\approx \frac{\delta^{ab}}{k^2} \left\{ N_c g_0^2 \frac{k_\mu k_\nu}{k^2} \int \frac{d^4 q}{(2\pi)^4} \frac{1}{q^4 + 2g_0^2 N_c \gamma^4} \left(\frac{k^2 - 2k \cdot q}{q^2} \right) \mathcal{P}_{\mu\nu}^T \right\}^{-1} \\ &\approx \frac{\delta^{ab}}{k^2} \left\{ N_c g_0^2 \frac{3}{4} \delta_{\mu\nu} k_\mu k_\nu \int \frac{d^4 q}{(2\pi)^4} \frac{1}{q^4 + 2g_0^2 N_c \gamma^4} \frac{1}{q^2} \right\}^{-1} = \frac{\delta^{ab}}{k^2} \left(g_0 \sqrt{N_c} \frac{k^2}{\gamma^2} \frac{3}{128 \sqrt{2} \pi} \right)^{-1} \\ &= \delta^{ab} \frac{128 \sqrt{2} \pi \gamma^2}{3 g_0 \sqrt{N_c} k^4}, \end{aligned} \quad (3.61)$$

where we used the four-dimensional integrated solid angle $\Omega_4 = 2\pi^2$ together with the spheric integral $\int_0^\infty dr r/(r^4 + \chi^4) = \pi/4\chi^2$. This expression diverges faster than the free ghost propagator (B.26) for vanishing momentum. Such a propagator is then said to be infrared *enhanced*, which supposedly indicates long-range effects of the theory.²¹ We shall further explore the consequences and validity of this kind of statements in Chapter 5.

3.4 Gribov-Zwanziger Action

The results (3.56) and (3.61) were obtained by Gribov in 1978.²¹ As we saw, this already gave non-trivial information on how a restriction of the path integral to Ω could modify the infrared behavior of Yang-Mills theories. Nevertheless, Gribov's computation was semi-classical in its nature and aimed at the imposition of the no-pole condition at lowest order in perturbation theory. That idea was properly extended to an all-order renormalizable action by Zwanziger.⁹⁹

The idea of the so-called *Gribov-Zwanziger action* is to directly impose the definition of the Gribov region, (3.1), on the path integral. This boils down to imposing that the smallest non-trivial eigenvalue of $\mathcal{M}$ is non-negative,

$$\lambda_1 \geq 0. \quad (3.62)$$

It was then imperative to obtain at least an approximate formula for λ_1 . Actually, Zwanziger obtained an expression for the trace of the Faddeev-Popov operator using degenerate perturbation theory at finite volume,^{22,99} given by

$$\text{Tr } \mathcal{M} = 4(N_c^2 - 1)V - H[A], \quad (3.63)$$

where

$$H[A] = g_0^2 \int d^4 x \int d^4 y f^{abc} f^{aed} A_\mu^b(x) [\mathcal{M}^{(-1)}(x, y)]^{cd} A_\mu^e(y) \quad (3.64)$$

is the so-called *horizon function*. If we suppose that, in the infinite-volume limit, the spectrum of $\mathcal{M}$ becomes negative one eigenvalue at a time, we can use the weaker condition $\text{Tr } \mathcal{M} > 0$ to contain the path integral inside Ω , leading to

$$\mathcal{Z}_{\text{GZ}} = \int \mathfrak{D}A \mathfrak{D}c \bar{c} e^{-S_{\text{FP}}[A, \bar{c}, c]} \theta \left(4(N_c^2 - 1)V - H[A] \right). \quad (3.65)$$

To understand the bulk properties of this partition function, let us use a toy model for the GZ action.²² Take the quadratic action for a (free) real scalar field on a large finite volume

$$S_{\text{toy}}[\phi] = \frac{1}{2} \int d^4x (\partial\phi)^2. \quad (3.66)$$

Suppose a fantasy Gribov region bounded by the ϕ -ellipsoid

$$H_{\text{toy}}[\phi] = \frac{1}{2} \int d^4x \phi(x) (-\square)^{-1} \phi(x) = cV, \quad (3.67)$$

where c is a constant. Notice that both S_{toy} and H_{toy} scale with V . The analogous Gribov-Zwanziger path integral of such a theory would then be

$$\mathcal{Z}_{\text{toy}} = \int \mathfrak{D}\phi e^{-S_{\text{toy}}[\phi]} \theta(cV - H_{\text{toy}}[\phi]). \quad (3.68)$$

Notice that, being the integral bounded by a high-dimensional hyperellipsoid, we can expect the integration to be localized close to the fantasy Gribov horizon, near the boundaries of the ellipsoid where most of its volume is concentrated.¹⁰⁰ Therefore, in the infinite-volume limit we should be able to substitute (3.68) by

$$\mathcal{Z}_{\text{toy}} = \int \mathfrak{D}\phi e^{-S_{\text{toy}}[\phi]} \delta(cV - H_{\text{toy}}[\phi]). \quad (3.69)$$

Using the Fourier representation of δ and dislocating the integration to the real axis in similarity with (3.43), we get

$$\mathcal{Z}_{\text{toy}} = \int_{-i\infty+\epsilon}^{+i\infty+\epsilon} \frac{d\beta}{2\pi} \int \mathfrak{D}\phi e^{-S_{\text{toy}}[\phi]} e^{\beta(cV - H_{\text{toy}}[\phi])} = \int_{-i\infty+\epsilon}^{+i\infty+\epsilon} \frac{d\beta}{2\pi} e^{-F(\beta)}, \quad (3.70)$$

where

$$F(\beta) = -\ln \int \mathfrak{D}\phi e^{-S_{\text{toy}}[\phi] + \beta(cV - H_{\text{toy}}[\phi])} \sim V. \quad (3.71)$$

In the infinite-volume limit we can do a saddle-point expansion

$$\mathcal{Z}_{\text{toy}} \approx e^{-F(\beta_0)}, \quad (3.72)$$

with the stationary point defined by

$$\begin{aligned} 0 = \frac{dF}{d\beta} \Big|_{\beta_0} &= - \frac{\int \mathfrak{D}\phi e^{-S_{\text{toy}}[\phi] + \beta(cV - H_{\text{toy}}[\phi])} (cV - H_{\text{toy}}[\phi])}{\int \mathfrak{D}\phi e^{-S_{\text{toy}}[\phi] + \beta(cV - H_{\text{toy}}[\phi])}} \Big|_{\beta_0} \\ &= -cV + \frac{\int \mathfrak{D}\phi e^{-S_{\text{toy}}[\phi] - \beta H_{\text{toy}}[\phi]} H_{\text{toy}}[\phi]}{\int \mathfrak{D}\phi e^{-S_{\text{toy}}[\phi] - \beta H_{\text{toy}}[\phi]}} \Big|_{\beta_0}, \end{aligned} \quad (3.73)$$

resulting in the gap equation

$$\langle H_{\text{toy}}[\phi] \rangle_{\beta_0} = cV \quad (3.74)$$

and

$$\mathcal{Z}_{\text{toy}} \approx \int \mathfrak{D}\phi e^{-S_{\text{toy}}[\phi] - \beta_0 H_{\text{toy}}[\phi]}. \quad (3.75)$$

The last expression is analogous to a canonical ensemble in statistical mechanics where the “energy” H_{toy} admits fluctuations, contrary to the starting microcanonical ensemble expression (3.69), where H_{toy} is fixed. To confirm the equivalence between the canonical and microcanonical ensembles, one can explicitly demonstrate that the relative variance goes to zero as V^{-1} , i.e.,

$$\frac{\langle \Delta H_{\text{toy}}^2 \rangle}{\langle H_{\text{toy}}^2 \rangle} \sim \frac{1}{V}, \quad (3.76)$$

which is consistent with the substitution $\theta \rightarrow \delta$.²²

We can proceed in a similar fashion with the Gribov-Zwanziger path integral (3.65), yielding the *non-local Gribov-Zwanziger action*

$$\mathcal{Z}_{\text{GZ}} = \int \mathfrak{D}A \mathfrak{D}c \mathfrak{D}\bar{c} \, e^{-S_{\text{FP}}[A, \bar{c}, c] - \gamma^4 H[A] + \gamma^4 4(N_c^2 - 1)V}, \quad (3.77)$$

where γ is the saddle-point parameter, defined through the gap equation

$$\langle H[A] \rangle_\gamma = 4(N_c^2 - 1)V. \quad (3.78)$$

The action implicitly defined in (3.77) can be “localized” by introducing a pair of bosonic $\{\bar{\varphi}, \varphi\}$ and ghost $\{\bar{\omega}, \omega\}$ fields, yielding

$$\mathcal{Z}_{\text{GZ}} = \int \mathfrak{D}A \mathfrak{D}c \mathfrak{D}\bar{c} \mathfrak{D}\varphi \mathfrak{D}\bar{\varphi} \mathfrak{D}\omega \mathfrak{D}\bar{\omega} \, e^{-S_{\text{GZ}}[A, \bar{c}, c, \bar{\varphi}, \varphi, \bar{\omega}, \omega]}, \quad (3.79)$$

where the *local Gribov-Zwanziger action* is

$$\begin{aligned} S_{\text{GZ}}[A, \bar{c}, c, \bar{\varphi}, \varphi, \bar{\omega}, \omega] = \int d^4x \left\{ \frac{1}{4} F_{\mu\nu}^a F_{\mu\nu}^a + \frac{1}{2\alpha} (\partial \cdot A)^2 + \bar{c}^a \partial \cdot D_\mu^{ab} c^b \right. \\ \left. - \bar{\varphi}_\mu^{ac} \mathcal{M}^{ab} \varphi_\mu^{bc} + \bar{\omega}_\mu^{ac} \mathcal{M}^{ab} \omega_\mu^{bc} + \gamma^2 g_0 f^{abc} A_\mu^a (\bar{\varphi} + \varphi)_\mu^{bc} - 4\gamma^4 (N_c^2 - 1) \right\} \end{aligned} \quad (3.80)$$

and the gap equation takes the form

$$\langle g_0 f^{abc} A_\mu^a (\bar{\varphi} + \varphi)_\mu^{bc} \rangle_\gamma = 8\gamma^2 (N_c^2 - 1). \quad (3.81)$$

The Gribov-Zwanziger action leads to the same results (3.56) and (3.61) of Gribov’s calculation for the gluon propagator and the ghost propagator.²² Furthermore, it was demonstrated that the no-pole condition leads to the same results as the Gribov-Zwanziger action to all orders in perturbation theory.¹⁰¹

In the quest for showing the validity of the Gribov-Zwanziger approach to quantization of non-Abelian theories, it is natural to ask if its results do not depend on the gauge choice, as it is expected. Originally, the analysis was carried out in Landau and

Coulomb gauge,^{21,102} the latter being not very useful to prove renormalizability properties. In the last years, work has been done in the direction of the maximal Abelian gauge^{98,103} due to its importance in the confinement problem.³⁷ Also, the implementation of the Gribov-Zwanziger action in (general) linear covariant and Curci-Ferrari gauges has been drawing attention of the community.^{98,104,105}

The Gribov-Zwanziger in Landau gauge action has been proved to be renormalizable first in Refs. 99,106 and then in the framework of algebraic renormalization,^{107,108} where it was shown that renormalization properties rules out any kind of ambiguity on the choice of the horizon function. An essential tool for establishing renormalizability of gauge theories is the so-called BRST symmetry, which shall be discussed next.

Last but not least, a refinement of the Gribov-Zwanziger action was proposed in which local composite operators as $A_\mu^a(x)A_\mu^a(x)$ and $\bar{\varphi}_\mu^{ab}(x)\varphi_\mu^{ab}(x) - \bar{\omega}_\mu^{ab}(x)\omega_\mu^{ab}(x)$ were added to (3.80) while keeping its renormalizability intact.¹⁰⁹ The gluon propagator computed from this action does not vanish at zero momentum as in (3.56), but attains a finite value $D(0) \propto M^2$, which characterizes a dynamically generated mass scale. Moreover, in light of lattice results (see Subsection 5.2.4), the novel two-dimensional condensate also entails a free infrared ghost propagator, i.e., not enhanced as in (3.61).

3.5 BRST symmetry

The verification that an action possesses BRST symmetry^{44,110–112} is important to the proof of renormalizability and unitarity of non-Abelian gauge theories, even on the absence of Gribov copies. Furthermore, it is also crucial to the Kugo-Ojima criterion of confinement to be discussed in Chapter 5.

The BRST invariance of the Lagrangian paves the way to the quantization of non-Abelian theories using the canonical (operator) formalism in the asymptotic ultraviolet regime. Actually, we can intuitively view it as a natural generalization of the Gupta-Bleuler procedure reviewed in Section 2.2.2. More specifically, using the Nakanishi-Lautrup formalism,¹¹³ which extends the Gupta-Bleuler quantization in Feynman gauge to covariant gauges, we can rewrite the Lagrangian of electromagnetic theory (2.46) as

$$\mathcal{L}_{\text{EM}} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + B(\partial \cdot A) + \frac{\alpha}{2}B^2, \quad (3.82)$$

where $B = B(x)$ is an auxiliary field (commonly named after Nakanishi and Lautrup), analogous to a Lagrange multiplier^E. Notice that here we are using Minkowski metric, i.e., we are dealing with the theory with Lorentz symmetry.

^E In fact, (2.46) can be recovered in the path integral formulation by completing squares and integrating over B .

The classical equations of motion derived from (3.82) are

$$\partial \cdot A = -\alpha B \quad (3.83)$$

$$\partial^2 B = 0. \quad (3.84)$$

Equation (3.84) implies that $\hat{B}$ can be decomposed into positive and negative frequency parts,

$$\hat{B}(x) = \hat{B}^{(+)}(x) + \hat{B}^{(-)}(x), \quad (3.85)$$

making it possible to consistently impose the subsidiary condition

$$\hat{B}^{(+)}(x) |\Psi_{\text{phys}}\rangle = 0 \quad (3.86)$$

to select physical states. Together with (3.83) this is nothing more than the Gupta-Bleuler condition (2.54) for $\alpha \neq 0$.

In the BRST approach, a pair of anti-commuting fields c and $\bar{c}$ are introduced in an essential way, i.e., at the classical level. They are later identified with the Faddeev-Popov ghosts presented in Section 2.3. As we saw there, ghosts decouple from the electromagnetic theory and are expected to give no contribution to asymptotic or virtual processes. However, there still exist negative norm states plaguing the covariant theory. Directly related to that, the most concise way to prove unitarity of the S -matrix is to use the subsidiary condition

$$\hat{Q}_{\text{BRST}} |\Psi_{\text{phys}}\rangle = 0. \quad (3.87)$$

The conserved charge $\hat{Q}_{\text{BRST}}$ corresponds to the Noether charge associated with the invariance of the extended Lagrangian

$$\mathcal{L}_{\text{EM}} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + B(\partial \cdot A) + \frac{\alpha}{2} B^2 + \partial_\mu \bar{c} \partial^\mu c \quad (3.88)$$

under (Abelian) BRST transformations, operationally defined by

$$\delta B = 0, \quad \delta c = 0, \quad \delta \bar{c} = \lambda B, \quad \delta A_\mu = -\lambda \partial_\mu c, \quad (3.89)$$

where λ is an infinitesimal global anti-commuting parameter.

The explicit expression of Q_{BRST} in terms of negative and positive frequency components in momentum space is

$$\hat{Q}_{\text{BRST}} = i \sum_{\mathbf{k}} \hat{c}^{(-)}(-\mathbf{k}) \hat{B}^{(+)}(\mathbf{k}) - \hat{B}^{(-)}(-\mathbf{k}) \hat{c}^{(+)}(\mathbf{k}). \quad (3.90)$$

Recalling that the fields $\bar{c}$ and c are free from the beginning, we can restrict ourselves to the subspace of states which contains no ghosts at all, i.e., $\mathcal{H}' \otimes |0_{\bar{c},c}\rangle$, where $\mathcal{H}'$ is an indefinite metric space. With that in mind, condition (3.87) turns out to be

$$\begin{aligned} \hat{Q}_{\text{BRST}} |\Psi_{\text{phys}}\rangle &= i \sum_{\mathbf{k}} \left[\hat{c}^{(-)}(-\mathbf{k}) \hat{B}^{(+)}(\mathbf{k}) - \hat{B}^{(-)}(-\mathbf{k}) \hat{c}^{(+)}(\mathbf{k}) \right] |\Psi_{\text{phys}}\rangle \otimes |0_{\bar{c},c}\rangle \\ &= i \sum_{\mathbf{k}} \hat{B}^{(+)}(\mathbf{k}) |\Psi_{\text{phys}}\rangle \otimes |1_{c(-\mathbf{k})}\rangle = 0, \end{aligned} \quad (3.91)$$

which, due to the separability and linear independence of the 1-particle ghost states, recovers the Gupta-Bleuler-Nakanishi-Lautrup condition (in momentum space)

$$(\partial \cdot \hat{A})^{(+)}(x) |\Psi_{\text{phys}}\rangle = 0 \quad (3.92)$$

and its consequences regarding the absence of negative states in the physical spectrum.

In fact, in order to establish a canonical formulation of a theory with indefinite metric state space $\mathcal{H}$, Kugo and Ojima gave the following “physicality criteria”:¹¹⁴

1. Hermiticity of the Hamiltonian: $\hat{H} = \hat{H}^\dagger$
2. Invariance of the subspace $\mathcal{H}_{\text{phys}}$ under (asymptotic) time evolution : $\hat{S}\mathcal{H}_{\text{phys}} = \mathcal{H}_{\text{phys}}$
3. positive semi-definiteness of $\mathcal{H}_{\text{phys}}$.

These criteria enable one to prove the unitarity of the *physical* S -matrix $\hat{S}_{\text{phys}}$ in the quotient space

$$\overline{\mathcal{H}}_{\text{phys}} = \mathcal{H}_{\text{phys}} / \mathcal{H}_0, \quad (3.93)$$

where $\mathcal{H}_0$ is the zero-norm subspace of $\mathcal{H}_{\text{phys}}$. In QED, the transversality condition (3.86) is sufficient to define $\mathcal{H}_{\text{phys}}$ and guarantee the confinement of asymptotic negative norm states (scalar and longitudinal ones) through (3.5).

The story for Yang-Mills theories is much more involved because neither the spurious gauge degrees of freedom nor the ghosts trivially decouple from the physical degrees of freedom. Indeed, only imposing (3.86) is not enough to guarantee that no unphysical states will appear after time development of a many-particle physical state. At best it will serve for one-particle states. We need to use the generalized BRST condition (3.87) in its non-Abelian version to properly guarantee the unitarity of $\hat{S}_{\text{phys}}$ using (3.5).

In Euclidean formulation, the BRST invariant Yang-Mills Lagrangian is just the usual Faddeev-Popov one in (2.138)

$$\mathcal{L}_{\text{YM}} = \frac{1}{4} F_{\mu\nu}^a F_{\mu\nu}^a + B^a (\partial \cdot A^a) - \frac{\alpha}{2} (B^a)^2 + \bar{c}^a (\partial \cdot D)^{ab} c^b, \quad (3.94)$$

where B^a is in the adjoint representation and is analogous to the Nakanishi-Lautrup field in the Abelian theory.¹¹³ The set of BRST transformations in this case is

$$\delta B^a = 0, \quad \delta \bar{c}^a = \lambda B^a, \quad \delta A_\mu^a = -\lambda D_\mu^{ac} c^c, \quad \delta c^a = -\lambda \frac{g_0}{2} f^{abc} c^b c^c. \quad (3.95)$$

It is simple to show that the Lagrangian (3.94) is invariant under BRST transformation,

$$\delta \mathcal{L}_{\text{YM}} = \frac{1}{4} \delta (F_{\mu\nu}^a)^2 + B^a \partial_\mu \delta (A_\mu^a) + \delta (\bar{c}^a \partial_\mu D_\mu^{ab} c^b) = -\bar{c}^a \partial_\mu \delta (D_\mu^{ab} c^b), \quad (3.96)$$

where we used the fact the original Yang-Mills term is invariant under transformations of the type $\delta A_\mu^a = -D_\mu \theta$, see (3.3). We check that the remaining term vanishes by computing

$$\begin{aligned} \delta(D_\mu^{ab} c^b) &= D_\mu^{ab} (\delta c^b) + (\delta D_\mu^{ab}) c^b \\ &= -g_0 \lambda f^{abc} \left\{ \frac{1}{2} (\partial_\mu c^b c^c) + (\partial_\mu c^c) c^b \right\} - g_0^2 \lambda \left\{ \frac{1}{2} f^{bdc} f^{abe} A_\mu^e c^d c^c + f^{abc} f^{ced} A_\mu^d c^e c^b \right\} \\ &= 0 - \lambda \frac{g_0^2}{2} A_\mu^e c^b c^c \left\{ f^{ade} f^{bcd} + f^{cde} f^{abd} + f^{bde} f^{cad} \right\} = 0, \end{aligned} \quad (3.97)$$

using the anticommutativity of the ghost fields and the Jacobi identity (2.16).

The physicality criteria (3.5) are then analyzed.¹¹⁴ The first condition on the Hamiltonian derived from (3.94) is verified by choosing the appropriate Hermiticity of the ghosts fields $\bar{c}^a$ and c^a . To verify the second one, we must *assume* the global BRST charge Q_{BRST} is well-defined and then impose (in the theory properly defined in Minkowski space)

$$\hat{Q}_{\text{BRST}} |\Psi_{\text{phys}}\rangle = 0 \quad (3.98)$$

in order to define $\mathcal{H}_{\text{phys}}$. Knowing that $\hat{Q}_{\text{BRST}}$ is conserved, i.e. $[\hat{Q}_{\text{BRST}}, \hat{H}] = 0$, we can show $\mathcal{H}_{\text{phys}}$ is invariant under time evolution. The proof of the positive semi-definiteness of $\mathcal{H}_{\text{phys}}$ is the most non-trivial one of the criteria and theory-dependent.

We outline the reasons behind the third criterion. For this purpose it is used that the BRST charge operator is *nilpotent*, i.e.

$$\hat{Q}_{\text{BRST}}^2 = 0, \quad (3.99)$$

which can be equivalently verified by taking the BRST variation of (3.96). This property divides the state space of $\hat{Q}_{\text{BRST}}$ into three parts: its *kernel*, $\text{Ker}(\hat{Q}_{\text{BRST}})$, composed of states that are annihilated by the charge operator, $\hat{Q}_{\text{BRST}} |\phi\rangle = 0$ (*closed* ones); its image, $\text{Im}(\hat{Q}_{\text{BRST}}) \subseteq \text{Ker}(\hat{Q}_{\text{BRST}})$, composed of states that can be written as the action of the charge operator in some other state, $|\psi\rangle = \hat{Q}_{\text{BRST}} |\chi\rangle \neq 0$ (*exact* ones); and the states that are neither in $\text{Ker}(\hat{Q}_{\text{BRST}})$ nor in $\text{Im}(\hat{Q}_{\text{BRST}})$. The latter set is the quotient space (3.93), which can also be expressed as

$$\overline{\mathcal{H}}_{\text{phys}} = \text{Ker}(\hat{Q}_{\text{BRST}}) / \text{Im}(\hat{Q}_{\text{BRST}}). \quad (3.100)$$

The space $\overline{\mathcal{H}}_{\text{phys}}$, candidate to be our physical state space, is called the *cohomology* of $\hat{Q}_{\text{BRST}}$, composed of states that are *closed but not exact*.

The demonstration of the semi-definiteness of $\text{Ker}(\hat{Q}_{\text{BRST}})$ is carried out through the so-called *quartet mechanism*,¹¹⁴ which uses a global symmetry of the ghosts under scale transformations

$$c^a \rightarrow e^\zeta c^a, \quad \bar{c}^a \rightarrow e^{-\zeta} \bar{c}^a, \quad (3.101)$$

to define the ghost charge Q_c , plus the additional condition

$$\hat{Q}_c |\Psi_{\text{phys}}\rangle = 0. \quad (3.102)$$

Given these two global charges, the algebra

$$\begin{aligned}\{\hat{Q}_{\text{BRST}}, \hat{Q}_{\text{BRST}}\} &= 0 \\ [\hat{Q}_c, \hat{Q}_{\text{BRST}}] &= \hat{Q}_{\text{BRST}} \\ [\hat{Q}_c, \hat{Q}_c] &= 0\end{aligned}\tag{3.103}$$

dictates the possible representations consistent with BRST symmetry and the subsidiary conditions. Being $\hat{Q}_{\text{BRST}}$ a nilpotent operator, the representations will be at most of dimension two, i.e., singlets or doublets. The BRST-singlets with vanishing ghost number can be identified with physical states, given that the particular theory is verified to not possess BRST-singlets plagued with ghosts, which is true in Yang-Mills theories. On the other hand, the BRST-doublets, always realized in pairs called quartets, are identified with the usual unphysical states. The point is that condition (3.98) implies that the states in $\mathcal{H}_{\text{phys}}$ are always realized in zero-norm combinations of quartet states, i.e., semi-positive states, which verifies the third criterion.

In Yang-Mills theories, BRST-singlets are identified with the transverse degrees of freedom. Conversely, scalar, longitudinal and ghost modes belong to the quartet representation. In this way, we see that the quartet mechanism shows that spurious states are “confined” and cannot appear in asymptotic states. More precisely, we can define a scattering matrix $\hat{S}_{\text{phys}}$ defined in the cohomology of $\hat{Q}_{\text{BRST}}$ which is unitary, implying that the asymptotic time evolution of physical particles cannot contain unphysical modes. Kugo and Ojima also developed a criterion¹¹⁴ in order to describe color confinement in the context of the quartet mechanism, which shall be commented in Chapter 5.

When dealing with the Gribov-Zwanziger action in the light of BRST symmetry, it is known that it *breaks* an extended set of BRST transformations involving the auxiliary fields,^{22,98} i.e.

$$sS_{\text{GZ}} = g_0 \gamma^2 f^{abc} \int d^4x \left[A_\mu^a \omega_\mu^{bc} - D_\mu^{ad} c^d (\bar{\varphi} + \varphi)_\mu^{bc} \right] \neq 0.\tag{3.104}$$

This breaking can be intuitively understood by noting that a BRST transformation as (3.95) includes a gauge transformation (3.3), which means that performing a (infinitesimal) BRST transformation on a field configuration inside the Gribov region results in a configuration no longer inside it. Therefore, restricting the path integral to Ω , i.e. implementing the Gribov-Zwanziger action, should automatically break BRST symmetry as formulated above. However, the breaking is considered *soft* because in the high-momentum limit ($\gamma \rightarrow 0$), the Faddeev-Popov theory is recovered and the symmetry is restored. Nevertheless, it does not prevent one from proving the renormalizability of the Gribov-Zwanziger action through the doublet theorem¹¹⁵ and it even leads to a simple algebraic proof of the statement that γ is a physical parameter of the theory.¹⁰⁹

Finally, we should remark that the original BRST quantization and Kugo-Ojima analysis were made in the context of the Faddeev-Popov action, directly taking into account

only the asymptotic UV regime with support of perturbation theory in Minkowski metric. However, as will be clear in Chapter 5, the main goal of infrared QCD is a resolution for the confinement problem, which is essentially *non-perturbative* and requires techniques beyond scattering theory. This includes contemplating the Gribov problem, which is out of the scope of the ideas presented in this section. For example, it is imperative to come up with a non-perturbative and nilpotent BRST symmetry^{98,116,117} that may guide the identification of a physical state space consistent with confinement and independent of the S-matrix and unitarity paradigm of conventional quantum field theory, possibly taking into account the most probable positivity violation of the gluon propagator and related problems discussed in Chapter 5.

4 LATTICE GAUGE THEORY

The approaches explored until now have an analytical character in the sense that continuum computations were used to derive certain properties starting from fundamental principles or hypotheses. An example was the derivation of the Gribov-Zwanziger propagators in Section 3.3 from the restriction of the path integral to the Gribov region. In order to study the Gribov-Zwanziger scenario and related issues from a numerical perspective, we introduce now lattice gauge theory in the context of pure Yang-Mills and its basic simulation methods.

4.1 Lattice Generalities

4.1.1 Regulator

It is widely known that quantum field theory (QFT) is generally infested by undesired divergences. This can be traced back, in the path integral approach, to the ill-defined measure of integration, as commented on Section 2.2.4. In any case, ultraviolet divergences are directly related to the point-like nature of QFT and require the *renormalization* program to yield sensible physical observables.

In a few words, to renormalize a theory we must first *regularize* it by mutilating the short distance modes through the introduction of some type of *regulator*, a mathematical artifact. Then we systematically reintroduce these modes by redefining the bare parameters of the Lagrangian in such a way that the physical quantities match its experimentally-determined values as the regulator is removed.

The conventional practice since the development of QFT is called perturbative renormalization.^{18,46–48,60,65} In this case, the perturbative Feynman series is computed and the divergences manifest themselves as ill-defined integrals in momentum space, corresponding to specific closed loops in a diagram. As mentioned above, a mathematical artifact, e.g. dimensional regulator, is introduced and one is able to isolate the ultraviolet divergent term of the integral. Finally, the Lagrangian is reparametrized in a way that, if the theory is (perturbatively) renormalizable, one is able to cancel out the divergences systematically and the computation yields finite results with predictive power.

Although the perturbative approach has demonstrated great value for some theories, e.g. QED, it faces many difficulties when applied to a theory displaying strong non-perturbative effects. In particular, Yang-Mills theories and QCD are wildly infrared non-perturbative due to their non-Abelian gauge structure. Thus, direct perturbative computations are of little use when applied to the study of phenomena much below the scale of $\Lambda_{QCD} \sim 1$ GeV, a region very important to the Standard Model's hadronic sector.

One alternative is the so-called *lattice gauge theory*,^{24,25,118–121} introduced by Wilson in 1974.²³ This approach to QFT consists in replacing the continuum (Euclidean) space with a discrete lattice in four dimensions

$$\Lambda = \{x; x/a \in \mathbb{Z}^4\}, \quad (4.1)$$

where the constant a is called *lattice spacing*. The fields are then defined only on the lattice's bonds and sites, the latter identified by the labels

$$x = (x_1, x_2, x_3, x_4). \quad (4.2)$$

The introduction of a minimum distance automatically defines an infrared regulator for the theory, eliminating momenta $|p| \leq \pi/a$. Of course, the lattice spacing a must not be taken as a physical quantity and should be removed at the end of the day, just as any other regulator. We restrict the lattice to a finite volume of sides L_μ , where

$$L_\mu = aN_\mu, \quad \text{with } x_\mu = 1, 2, \dots, N_\mu, \quad \text{and } \mu = 1, 2, 3, 4, \quad (4.3)$$

which introduces a natural infrared cutoff. We then must take the *continuum* limit and the *thermodynamic* limit in order to recover physical observables (see Section 4.3). Furthermore, because we will be dealing most of the times with finite volumes, periodic boundary conditions will always be implied so that border effects are minimized.

We will now specify the concepts necessary to define lattice gauge theory in the path integral approach, which includes link variables, observables and the Wilson action.

4.1.2 Link Variables

After introducing the lattice regulator, one could immediately ask how discretization affects the continuous symmetries of the system. In fact, the introduction of a lattice spacing, for instance, breaks Euclidean symmetry (corresponding to Lorentz symmetry in the case of Minkowski space), reducing it to a symmetry under generalized $\pi/2$ rotations. Anyway, we must recover these symmetries as we take the continuum limit and this condition serves as a primary test for a reasonable lattice model. Nevertheless, keeping local gauge symmetry *intact* is of central importance for the description of interactions involved in Yang-Mills theories.

We succinctly described the objects involved in local gauge symmetry in Section 2.1, e.g., the gauge field A_μ , the strength tensor $F_{\mu\nu}$ and the covariant derivative D_μ . In that framework, each point of space can be viewed as a different reference frame with respect to gauge transformations.³ Of course, because the theory is locally gauge invariant, each point can have arbitrary phase orientation. Thus, from a geometrical point of view,

Figure 4.1 – Scheme of a symmetric 3D lattice.

Source: By the author.

we can see A_μ as an infinitesimal phase comparator between two space points, which is used in the definition of the covariant derivative, making it possible to compare two points in two different gauge reference frames. In this philosophy, the $F_{\mu\nu}$ tensor is defined in a (local) gauge-invariant way.

Given that A_μ is an infinitesimal connection, we can integrate it over an arbitrary path $\mathcal{C}_{xy}$ from x to y and recover the finite parallel transporter²⁴

$$\mathfrak{U}(\mathcal{C}_{xy}) = \mathcal{P} \exp \left\{ i g_0 \int_{\mathcal{C}_{xy}} dx \cdot A(x) \right\}, \quad (4.4)$$

where $\mathcal{P}$ is a path-ordering operator to enforce ordered integration along $\mathcal{C}_{yx}$. This continuum parallel transporter gauge transformation depends only on the endpoints

$$\mathfrak{U}(\mathcal{C}_{xy}) \rightarrow \mathfrak{g}(x) \mathfrak{U}(\mathcal{C}_{xy}) \mathfrak{g}^\dagger(y) \quad (4.5)$$

and thus its trace along a closed path $\mathcal{C}_{xx}$ is gauge invariant

$$\text{Tr} \mathfrak{U}(\mathcal{C}_{xx}) \rightarrow \text{Tr} \mathfrak{g}(x) \mathfrak{U}(\mathcal{C}_{xx}) \mathfrak{g}^\dagger(x) = \text{Tr} \mathfrak{U}(\mathcal{C}_{xx}), \quad (4.6)$$

and is used to define observables of the theory. We can write an elementary parallel transporter along a specific direction, say μ , between two points separated by a distance a as

$$\mathfrak{U}(x \rightarrow x + \hat{\mu}) \equiv \exp \left\{ i g_0 \int_x^{x+\hat{\mu}} dx \cdot A(x) \right\}, \quad (4.7)$$

where $\hat{\mu}$ is a vector in the μ -direction with $|\hat{\mu}| = a$.

The elementary parallel transporter between two neighboring points on a lattice is the fundamental variable of lattice gauge theory and is known as *link variable*. The link variables $\{U_\mu(x)\}$ are defined as oriented objects along the bond between two lattice sites and are elements of the compact group $SU(N_c)$, instead of its algebra $\mathfrak{su}(N_c)$. We thus write down

$$\begin{array}{l} x \xrightarrow{U_\mu(x)} x + \hat{\mu} \\ U_{-\mu}(x + \hat{\mu}) = U_\mu^\dagger \\ x \xleftarrow{\quad} x + \hat{\mu} \end{array}$$

Figure 4.2 – Scheme of a link variable and its conjugate.

$$U_\mu(x) = e^{i\varphi(x)} \in SU(N_c), \quad \varphi(x) \in \mathfrak{su}(N_c). \quad (4.8)$$

We can connect the continuum parallel transporter with the link variables through the expression (4.7). Different approximations may be used to evaluate the integral when it is necessary to directly connect continuum fields with lattice fields. The most common one is to replace the integral by $aA_\mu(x_P)$ where x_P is some point in the line element $x \rightarrow x + \hat{\mu}$,

$$U_\mu(x) = e^{iag_0 A_\mu(x_P)}, \quad (4.9)$$

Source: By the author.

For simplicity, we will use $x_P = x$, but notice that $x_P = x + \hat{\mu}/2$ provides a better estimate of the integral in (4.7). Nevertheless, we expect to obtain the same results in the continuum limit regardless of the choice of x_P .

One could ask if it would be possible to formulate a discretized theory directly using the gauge potential. In fact, a theory along those lines is given in Ref. 122 and it is verified that gauge symmetry is essentially lost. If the theory is not exactly gauge invariant, the couplings of different interactions are not equal and a mass term can appear in the Lagrangian. In this way, it is much more difficult to simulate the original gauge-invariant theory because these parameters would need fine tuning. We will later show that the transformation

$$U_\mu(x) \rightarrow U_\mu^g(x) = \mathbf{g}(x) U_\mu(x) \mathbf{g}^\dagger(x + \hat{\mu}) \quad (4.10)$$

is equivalent to the transformation (2.20) in the continuum.

Nevertheless, we can recover the gauge potential by Taylor expanding the link variable in (4.9) and its adjoint for small a . Therefore we define the (dimensionless) lattice gauge potential as

$$\mathcal{A}_\mu(x) = \frac{U_\mu(x) - U_\mu^\dagger(x)}{2i} - \frac{1}{N_c} \text{Tr} \frac{U_\mu(x) - U_\mu^\dagger(x)}{2i}, \quad (4.11)$$

which will be used along the text. Note that this definition differs from the continuum gauge field by $\mathcal{O}(a^3)$, namely

$$\begin{aligned} \mathcal{A}_\mu(x) &= \frac{1}{2i} \left[\mathbb{1} + i a g_0 A_\mu(x) - \frac{a^2 g_0^2}{2} A_\mu(x)^2 - \mathbb{1} + i a g_0 A_\mu(x) + \frac{a^2 g_0^2}{2} A_\mu(x)^2 \right] + \mathcal{O}(a^3 g_0^3) \\ &= a g_0 A_\mu(x) + \mathcal{O}(a^3 g_0^3). \end{aligned} \quad (4.12)$$

Also, we should emphasize that (4.11) is just one way of defining the gauge potential on the lattice, different combinations of link variables being used to cancel undesired powers of a .

We have defined the most fundamental field in a lattice gauge theory and now will use it to compose observables and a lattice analogue of the Yang-Mills action.

4.1.3 Observables and Wilson Action

In the pure gauge theory, we take observables to be invariant quantities under gauge transformations. Inspired by (4.6), a straightforward way to define an invariant quantity in lattice gauge theory is to take the (normalized) trace of closed circuits of link variables, known as *Wilson loop*, defined as

$$\mathcal{W}(\mathcal{C}) = \frac{1}{N_c} \text{Tr} \prod_{U_i \in \mathcal{C}} U_i, \quad (4.13)$$

a quantity that has a continuum analogue in terms of the gauge transporter in (4.4).¹⁸ If a Wilson loop lies on a plane it is called a planar loop.

Another observable of pure gauge theory important to lattice studies, specially in finite temperature computations, is the *Polyakov loop*, defined in each spatial site as the ordered chain of link variables in the time direction along its entire length. On a periodic lattice with time extension N_t , we write it as the trace of the closed temporal loop

$$\mathcal{P}(\mathbf{x}) = \frac{1}{N_c} \text{Tr} \prod_{x_4=0}^{N_t-1} U_4(\mathbf{x}, x_4), \quad (4.14)$$

which is a gauge-invariant quantity. Notice that, because this loop winds around the time direction, it has a non-trivial topology.

Now we construct the central gauge-invariant object in a path integral theory, the action. Knowing that traces of closed loops form invariant quantities, we take the elementary Wilson loop as the building block of the simplest action. The minimal chain of link variables is called a *plaquette*^A variable

$$U_{\mu\nu}(x) = U_\mu(x) U_\nu(x + \hat{\mu}) U_\mu^\dagger(x + \hat{\nu}) U_\nu^\dagger(x). \quad (4.15)$$

Given this object and noting its similarity with the concept of minimal circuit provided by the continuum strength tensor $F_{\mu\nu}$, we state the following *Ansatz* for the action of pure gauge theory with $SU(N_c)$ symmetry on a lattice

$$S_W[U] = \frac{2}{g_0^2} \sum_{x \in \Lambda} \sum_{\mu > \nu} \text{Re} \text{Tr}[\mathbb{1} - U_{\mu\nu}(x)]. \quad (4.16)$$

This discretized expression was first proposed in Ref. 23 and is called Wilson action.

Figure 4.3 – Scheme of an elementary (planar) Wilson loop, i.e., a plaquette.

Source: By the author.

We should of course at least check if the Wilson action corresponds to the Yang-Mills action in the (naive) continuum limit $a \rightarrow 0$. In order to verify the continuum limit

^A Sometimes we will directly call a minimal Wilson loop, i.e., from (4.13), as plaquette, which is the group-normalized trace of the definition (4.15). Which one to be chosen will be clear from the context.

of the action, we first expand the plaquette operator to order $\mathcal{O}(a^3)$ using (4.2) and the Baker-Campbell-Hausdorff formula three times, yielding

$$\begin{aligned}
U_{\mu\nu}(x) &= e^{i a g_0 A_\mu(x)} e^{i a g_0 A_\nu(x+\hat{\mu})} e^{-i a g_0 A_\mu(x+\hat{\nu})} e^{-i a g_0 A_\nu(x)} \\
&= e^{i a^2 g_0 [\partial_\mu A_\nu(x) - \partial_\nu A_\mu(x)] - \frac{a^2 g_0^2}{2} [A_\mu(x), A_\nu(x)] - \frac{a^2 g_0^2}{2} [A_\mu(x), A_\nu(x)] + a^2 g_0^2 [A_\mu(x), A_\mu(x)] + a^2 g_0^2 [A_\mu(x), A_\nu(x)]} \\
&\quad + a^2 g_0^2 [A_\nu(x), A_\mu(x)] + a^2 g_0^2 [A_\nu(x), A_\nu(x)] + \mathcal{O}(a^3 g_0)} \\
&= e^{i a^2 g_0 (\partial_\mu A_\nu(x) - \partial_\nu A_\mu(x)) - a^2 g_0^2 [A_\mu(x), A_\nu(x)] + \mathcal{O}(a^3 g_0)} = e^{i a^2 g_0 F_{\mu\nu}(x) + \mathcal{O}(a^3 g_0)}, \tag{4.17}
\end{aligned}$$

where the expansion of the continuum gauge field around x is of the form $A_\mu(x + \hat{\nu}) = A_\mu(x) + a \partial_\nu A_\mu(x) + \mathcal{O}(a^2)$ and $F_{\mu\nu}$ is given by (A.3). This result shows us the connection between the plaquette variable and the continuum strength tensor, being an approximation to the continuum gauge transporter over an elementary circuit. Substituting (4.17) in the Wilson action definition and expanding the exponentials up to $\mathcal{O}(a^6)$ we get ^B

$$\begin{aligned}
S_W[U] &= \frac{2}{g_0^2} \sum_{x \in \Lambda} \sum_{\mu > \nu} \left\{ N_c - \frac{1}{2} \text{Tr} e^{i a^2 g_0 F_{\mu\nu}(x) + \mathcal{O}(a^3 g_0)} + e^{-i a^2 g_0 F_{\mu\nu}(x) + \mathcal{O}(a^3 g_0)} \right\} \\
&= \frac{2}{g_0^2} \sum_{x \in \Lambda} \sum_{\mu > \nu} \left\{ N_c - \frac{1}{2} \text{Tr} [2 \mathbb{1} - a^4 g_0^2 F_{\mu\nu}(x)^2 + \mathcal{O}(a^6 g_0^2)] \right\} \\
&= \frac{1}{2} a^4 \sum_{x \in \Lambda} \sum_{\mu, \nu=1}^4 [\text{Tr} F_{\mu\nu}(x)^2 + \mathcal{O}(a^4)], \tag{4.18}
\end{aligned}$$

which corresponds to the Yang-Mills action when $a \rightarrow 0$. Of course, we are supposing that

$$a^4 \sum_{x \in \Lambda} \rightarrow \int d^4 x \tag{4.19}$$

for lattice volume growing as $V = N^4 \rightarrow \infty$. This is just one of many possible discretizations of the continuum action and, using the same reasoning as when defining the lattice gauge field (4.11), it can be improved to progressively cancel powers of a . Although such naive correspondence is necessary, it is not sufficient to show the complete equivalence between the two theories, as we will discuss in the next sections.

4.1.4 Path Integral

Finally, we must define the path integral of the lattice theory in order to compute quantum expected values. Given the Wilson action (4.16) and knowing that the fundamental field is given by the set of link variables, we define the path integral

$$\mathcal{Z}_W[U] = \int \mathfrak{D}U e^{-S_W[U]}. \tag{4.20}$$

The measure of integration is given by

$$\mathfrak{D}U = \prod_{x \in \Lambda} \prod_{\mu=1}^4 dU_\mu(x) \tag{4.21}$$

^B Notice that the errors of odd order cancel in the expansion of the exponential.

and $dU_\mu(x)$ is the unique Haar measure of $SU(N_c)$, see C.1.

Supposing an observable which depends only on the link variables, e.g. Wilson loops, we compute expectation values in the usual way,

$$\langle O[U] \rangle = \frac{1}{\mathcal{Z}_W} \int \mathfrak{D}U e^{-S_W[U]} O[U]. \quad (4.22)$$

Because the Haar measure is invariant under group multiplications, the expectation values are clearly gauge invariant.

Here we make a comment about the form of the Wilson action in comparison to the Yang-Mills one. Notice that we inserted the lattice gauge coupling in front of the summation, unlike in the continuum action. This is so because in non-perturbative computations the coupling is not a (in some sense) small parameter anymore, around which we would perturbatively expand. In lattice theory we are interested in doing mainly non-perturbative computations that resemble the ones in statistical mechanics, with the inverse coupling

$$\frac{2N_c}{g_0^2} \equiv \beta \quad (4.23)$$

corresponding to a kind of *inverse temperature*. Nevertheless, we can obtain the same form for the Yang-Mills action by doing the following transformation

$$A_\mu \rightarrow g_0 A_\mu, \quad (4.24)$$

yielding

$$S_{\text{YM}} = \frac{1}{2g_0^2} \text{Tr} \int d^4x F_{\mu\nu}^2, \quad (4.25)$$

with corresponding modifications in $F_{\mu\nu}$, D_μ and the transformation of A_μ .

Note that if one desires to use the path integral (4.20) to derive lattice Feynman rules and compute a weak-coupling expansion similar to the conventional continuum approach, one is faced with the same problem of the Yang-Mills theory. It is then necessary to perform a lattice version of the Faddeev-Popov method in order to define a free propagator on which a perturbation series is performed.^{24,25} However, as we are going to use non-perturbative methods to compute observables, there is no need to fix the gauge perturbatively. Indeed, when we directly evaluate (4.21), the gauge volume factors out and is canceled by the normalization. Nevertheless, as we will be interested in gauge-dependent objects such as the Faddeev-Popov operator and ghost propagator, we will need to fix the gauge somehow, an issue that is addressed on Section (4.2).

4.1.5 Strong-Coupling Expansion

The advantage of dealing with a theory with an inverse temperature-like term is that we can do a strong-coupling expansion to extract some information for $g \rightarrow \infty$, i.e.,

$\beta \rightarrow 0$. This procedure is very similar to the high-temperature expansion used in statistical mechanics, but here we are dealing with a non-commutative symmetry.

In particular, we can extract the strong-coupling behavior of an arbitrary planar Wilson loop on the lattice.²³ Using (4.22), (4.16) and (4.13), we write the expected value of a Wilson loop in terms of the inverse coupling (4.23) as

$$\langle \mathcal{W}(C) \rangle = \frac{1}{\mathcal{Z}_W} \int \mathfrak{D}U e^{-S_W[U]} \mathcal{W}(C) = \frac{\int \mathfrak{D}U \exp \left[\frac{\beta}{N_c} \sum_{x \in \Lambda, \mu < \nu} \text{Re Tr } U_{\mu\nu}(x) \right] \frac{1}{N_c} \text{Tr} [\prod_{l \in C} U_l]}{\int \mathfrak{D}U \exp \left[\frac{\beta}{N_c} \sum_{x \in \Lambda, \mu < \nu} \text{Re Tr } U_{\mu\nu}(x) \right]}, \quad (4.26)$$

where we have canceled the common constant terms appearing both in the numerator and denominator. Our objective is to expand this expression to leading order in β . The smallest non-vanishing expansion for the denominator is simply given by the zeroth-order expansion of the action term

$$\mathcal{Z}_W = \int \mathfrak{D}U \exp \left[\frac{\beta}{N_c} \sum_{x \in \Lambda, \mu < \nu} \text{Re Tr } U_{\mu\nu}(x) \right] \approx \int \mathfrak{D}U (1 + \mathcal{O}(\beta)) = 1, \quad (4.27)$$

where the conventional normalization of the Haar measure was used (see C.1).

The remaining integral in the numerator can be rewritten by noting that $2 \text{Re Tr } U_{\mu\nu} = \text{Tr } U_{\mu\nu} + \text{Tr } U_{\mu\nu}^\dagger$ and by Taylor-expanding the exponential

$$\begin{aligned} \langle \mathcal{W}(C) \rangle &= \int \mathfrak{D}U \exp \left[\frac{\beta}{2N_c} \sum_{x \in \Lambda, \mu < \nu} \left(\text{Tr } U_{\mu\nu}(x) + \text{Tr } U_{\mu\nu}^\dagger(x) \right) \right] \frac{1}{N_c} \text{Tr} \left[\prod_{l \in C} U_l \right] \\ &\approx \int \mathfrak{D}U \sum_{i,j} \left\{ \frac{1}{i!j!} \left(\frac{\beta}{2N_c} \right)^{i+j} \left[\sum_{x \in \Lambda, \mu < \nu} \text{Tr } U_{\mu\nu}(x) \right]^i \left[\sum_{x \in \Lambda, \mu < \nu} \text{Tr } U_{\mu\nu}^\dagger(x) \right]^j \right\} \frac{1}{N_c} \text{Tr} \left[\prod_{l \in C} U_l \right]. \end{aligned} \quad (4.28)$$

Inspecting this expression in view of (C.10) and (C.14), the latter being conveniently written after plugging in two external links as

$$\int_{SU(N_c)} dU \text{Tr} (VU) \text{Tr} (U^\dagger W) = \int_{SU(N_c)} dU V_{ji} U_{ij} (U^\dagger)_{kl} W_{lk} = \frac{1}{N_c} \delta_{il} V_{ij} \delta_{jk} W_{lk} = \frac{1}{N_c} \text{Tr} (VW), \quad (4.29)$$

we note that only plaquettes with contrary orientation in comparison to $\mathcal{W}$, i.e. $U_{\mu\nu}^\dagger$, can yield a non-vanishing contribution. Furthermore, it is also implied that *all* links from the loop contour must be paired by oppositely oriented ones. In turn, this means that the leading contribution to the integral will come from the smallest possible number of paired plaquettes, each one having an oppositely oriented link in common with the contour of the loop and with its neighboring plaquettes, resulting in the tiling depicted in Figure 4.5. The leading term is then the one corresponding to $j = n_t n_r \equiv n_a$, proportional to the area of the loop,

Figure 4.4 – The result (4.29) is represented in (a), while a generalization to a larger loop is depicted in (b). Trace is implicit in each loop and integration is taken over the paired links.

Source: By the author.

$$\begin{aligned}
 \langle \mathcal{W}(\mathcal{C}) \rangle &\approx \frac{1}{N_c} \int \mathfrak{D}U \sum_j \left\{ \frac{1}{j!} \left(\frac{\beta}{2N_c} \right)^j \left[\sum_{x \in \Lambda, \mu < \nu} \text{Tr } U_{\mu\nu}^\dagger(x) \right]^j \right\} \text{Tr} \left[\prod_{l \in \mathcal{C}} U_l \right] \\
 &= \frac{1}{N_c} \int \mathfrak{D}U \frac{1}{n_A!} \left(\frac{\beta}{N_c} \right)^{n_A} \left[\sum_{x \in \Lambda, \mu < \nu} \text{Tr } U_{\mu\nu}^\dagger(x) \right]^{n_A} \text{Tr} \left[\prod_{l \in \mathcal{C}} U_l \right] \\
 &= \frac{1}{N_c} \left(\frac{\beta}{N_c} \right)^{n_A} \int \mathfrak{D}U \text{Tr} \left[\prod_{j \in A_C} U_j^\dagger \right] \text{Tr} \left[\prod_{l \in \mathcal{C}} U_l \right], \tag{4.30}
 \end{aligned}$$

where we used the fact that there are $n_A!$ different possibilities of tiling the region depicted in Figure 4.5.

Figure 4.5 – Full tiling of a Wilson loop by plaquettes.

Source: By the author.

Finally, we can iterate expression (4.29) to integrate the inner links inside A_C . First we integrate the plaquettes into columns, yielding a factor of $\left(\frac{1}{N_c} \right)^{(n_t-1)n_r}$, and then we iterate the computation on the $n_r - 1$ columns, which leaves the outer loop to be dealt with

$$\begin{aligned}
 \langle \mathcal{W}(\mathcal{C}) \rangle &\approx \left(\frac{\beta}{2N_c} \right)^{n_A} \left(\frac{1}{N_c} \right)^{(n_t-1)n_r} \left(\frac{1}{N_c} \right)^{n_r-1} \int \left[\prod_{i \in \mathcal{C}} dU_i \right] \text{Tr} \left[\prod_{l \in \mathcal{C}} U_l^\dagger \right] \text{Tr} \left[\prod_{l \in \mathcal{C}} U_l \right] \\
 &= \left(\frac{\beta}{2N_c} \right)^{n_A} \left(\frac{1}{N_c} \right)^{n_A-1} \frac{1}{N_c} \text{Tr}(\mathbb{1}) = \left(\frac{\beta}{2N_c^2} \right)^{n_A} = e^{n_A \log(\beta/2N_c^2)}. \tag{4.31}
 \end{aligned}$$

The last result is valid for $N_c > 2$ theories. In the case of $SU(2)$, where $\text{Re Tr } U_{\mu\nu} = \text{Tr } U_{\mu\nu}$, the factor of $1/2$ in (4.28) cancels out and we have

$$\langle \mathcal{W}(\mathcal{C}) \rangle \approx \left(\frac{\beta}{4} \right)^{n_A} = e^{n_A \log(\beta/N_c)}. \quad (4.32)$$

Note that in this limit the Wilson loop obeys an *area law*, which is an indication of confinement (see Chapter 5).

4.2 Gauge Fixing

In order to study gauge-dependent quantities of the continuum theory on the lattice, we must learn a way to gauge-fix a lattice configuration $\{U_\mu(x)\}$. In our case, we will be interested in the Landau gauge condition (3.1), i.e., that all field configurations appearing on the path integral be transverse. Moreover, we are also interested in assessing properties related to the restriction of the path integral to the Gribov region Ω defined in (3.1.2).

4.2.1 Lattice Gribov Region

Recalling the formulation of the Gribov region given by the minimizing functional $\|A^g\|^2$ in (3.16), namely

$$\|A^g\|^2 \equiv \int d^4x \text{Tr} [A_\mu^g(x) A_\mu^g(x)], \quad (4.33)$$

we can analogously define its lattice counterpart

$$\mathcal{E}[U^g] = 1 - \frac{a^4}{4N_c V} \sum_{x \in \Lambda} \sum_{\mu=1}^4 \text{Re Tr } U_\mu^g(x), \quad (4.34)$$

where U^g is given by the gauge transformation (4.10). Using this minimizing functional, we can define the lattice Gribov region by a minimization process over the transformations g .

Of course, we should guarantee that the lattice minimizing functional (4.34) is equivalent to the continuum one in (4.33) when $a \rightarrow 0$. First we show that the transformation of the links in (4.10) is equivalent to the transformation of the gauge potential in the continuum limit, i.e., to (2.20). Using the expansion $g^\dagger(x + \hat{\mu}) = g^\dagger(x) + a\partial_\mu g^\dagger(x) + \mathcal{O}(a^2)$ and the expression (4.9), we get

$$\begin{aligned} U_\mu^g(x) &= \mathbb{1} + i a g_0 A_\mu^g(x) + \mathcal{O}(a^2 g_0^2) \\ &= g(x) \left[1 + i a g_0 A_\mu(x) + \mathcal{O}(a^2 g_0^2) \right] \left[g^\dagger(x) + a\partial_\mu g^\dagger(x) + \mathcal{O}(a^2) \right] \\ &= \mathbb{1} + i a g_0 \left[g(x) A_\mu(x) g^\dagger(x) - i g_0^{-1} g(x) \partial_\mu g^\dagger(x) \right] + \mathcal{O}(a^2), \end{aligned} \quad (4.35)$$

where we confirm that the transformed continuum gauge potential appears between brackets.

With this result, we expand (4.34) to second order and check that

$$\begin{aligned}
a^{-2}g_0^{-2}\mathcal{E}[U^{\mathfrak{g}}] &= a^{-2}g_0^{-2}\frac{a^4}{8VN_c}\sum_{x\in\Lambda}\sum_{\mu=1}^4\mathrm{Tr}\left[2\mathbb{1}-U_{\mu}^{\mathfrak{g}}(x)-U_{\mu}^{\mathfrak{g}\dagger}(x)\right] \\
&= a^{-2}g_0^{-2}\frac{a^4}{8VN_c}\sum_{x\in\Lambda}\sum_{\mu=1}^4\mathrm{Tr}\left[2\mathbb{1}-\mathbb{1}-iag_0A_{\mu}^{\mathfrak{g}}(x)+\frac{a^2g_0^2}{2}(A_{\mu}^{\mathfrak{g}})^2(x)\right. \\
&\quad \left.-\mathbb{1}+iag_0A_{\mu}^{\mathfrak{g}}(x)+\frac{a^2g_0^2}{2}(A_{\mu}^{\mathfrak{g}})^2(x)+\mathcal{O}(a^4g_0^4)\right] \\
&= \left(\frac{1}{8N_cV}\right)a^4\sum_{x\in\Lambda}\sum_{\mu=1}^4\mathrm{Tr}\left[(A_{\mu}^{\mathfrak{g}})^2(x)+\mathcal{O}(a^2g_0^2)\right], \tag{4.36}
\end{aligned}$$

which is proportional to (4.33) when $a \rightarrow 0$ and $V = N^4 \rightarrow \infty$ ^C.

4.2.2 Faddeev-Popov Matrix

Now, to better define the minimization process, we specialize to the case of the $SU(2)$ group, where most of our computations on the lattice will be done. We then use the well-known Caley-Klein parametrization of $SU(2)$ elements (see C.3), namely

$$U_{\mu}(x) = u_{\mu}^4(x) + i\mathbf{u}_{\mu}(x) \cdot \boldsymbol{\sigma}, \tag{4.37}$$

and also parametrize the gauge transformations as exponentials of elements of the algebra

$$\mathfrak{g}(x) = e^{i\boldsymbol{\gamma}(x) \cdot \boldsymbol{\sigma}}, \quad (\boldsymbol{\gamma})_a = \gamma_a : \mathbb{E} \rightarrow \mathbb{R}. \tag{4.38}$$

If we fix $\{\boldsymbol{\gamma}(x)\}$ and define the one-parameter subgroup of $SU(2)$ as

$$\mathfrak{g}(\tau; x) = e^{i\tau\boldsymbol{\gamma}(x) \cdot \boldsymbol{\sigma}}, \quad \tau \in \mathbb{R}, \tag{4.39}$$

it will be possible to explore arbitrary directions of the gauge space by fixing $\{\gamma_a(x)\}$ and varying τ and, consequently, look for minima of the functional (4.34) as a function of this parameter

$$\begin{aligned}
\mathcal{E}(\tau) &= 1 - \frac{a^4}{4V}\sum_{x\in\Lambda}\sum_{\mu=1}^4\mathrm{Re}\mathrm{Tr}U_{\mu}^{\mathfrak{g}(\tau)}(x) \\
&= \frac{1}{8N^4}\sum_{x\in\Lambda}\sum_{\mu=1}^4\mathrm{Tr}\left[\mathbb{1}-\mathfrak{g}(x;\tau)U_{\mu}(x)\mathfrak{g}^{\dagger}(x+\hat{\mu};\tau)\right], \tag{4.40}
\end{aligned}$$

for fixed $\{U_{\mu}(x)\}$.

We now explore the derivatives of $\mathcal{E}$ in analogy to what we did back in Section 3.1.2 using $\|A^{\mathfrak{g}}\|^2$. The first derivative of (4.40) with respect to τ is

$$\mathcal{E}'(\tau) = -\frac{1}{8N^4}\sum_{x\in\Lambda}\sum_{\mu=1}^4\mathrm{Tr}\left\{\mathfrak{g}'(x;\tau)U_{\mu}(x)\mathfrak{g}^{\dagger}(x+\hat{\mu};\tau)+\mathfrak{g}(x;\tau)U_{\mu}(x)\mathfrak{g}^{\dagger\prime}(x+\hat{\mu};\tau)\right\}. \tag{4.41}$$

^C The term between parentheses in the last line of (4.36) is a conventional normalization used on the lattice and does not change the minima of $\mathcal{E}$. Also, notice that we divide $\mathcal{E}$ by a^2 when taking the continuum limit because the former is a dimensionless quantity on the lattice, in contrast to the continuum functional.

Using (4.37), (4.39) and (C.3.2) the last expression evaluated at $\tau = 0$ ($\mathbf{g}(x) = \mathbb{1}$) reduces to (color sums are implicit)

$$\begin{aligned}\mathcal{E}'(0) &= -\frac{1}{8N^4} \sum_{x \in \Lambda} \sum_{\mu=1}^4 \text{Tr} \left\{ i \gamma^a(x) \sigma^a \left(u_\mu^4(x) + i u_\mu^b(x) \sigma^b \right) - i \left(u_\mu^4(x) + i u_\mu^a(x) \sigma^a \right) \gamma^b(x + \hat{\mu}) \sigma^b \right\} \\ &= \frac{1}{8N^4} \sum_{x \in \Lambda} \sum_{\mu=1}^4 \left\{ \gamma^a(x) u_\mu^b(x) - u_\mu^a(x) \gamma^b(x + \hat{\mu}) \right\} \text{Tr} \sigma^a \sigma^b,\end{aligned}\quad (4.42)$$

and we use the fact that the lattice is periodic, which enables us to do $x \rightarrow x - \hat{\mu}$ in the sums over the entire lattice. Then,

$$\mathcal{E}'(0) = \frac{1}{4N^4} \sum_{x \in \Lambda} \sum_{\mu=1}^4 \gamma^a(x) \left[u_\mu^a(x) - u_\mu^a(x - \hat{\mu}) \right] = \frac{1}{4N^4} \sum_{x \in \Lambda} \gamma^a(x) [\nabla_\mu \cdot \mathcal{A}_\mu(x)]^a, \quad (4.43)$$

where we defined the left-sided finite difference

$$\nabla_\mu f(x) \equiv f(x) - f(x - \hat{\mu}), \quad f : \Lambda \rightarrow \mathbb{R}, \quad (4.44)$$

and, together with (4.11), the $SU(2)$ color components

$$\mathcal{A}_\mu^a \equiv \frac{1}{2} \text{Tr} \mathcal{A}_\mu \sigma^a. \quad (4.45)$$

With this expression we see that the stationarity condition for the configuration $\{U_\mu(x)\}$ implies the Landau gauge condition over the corresponding gauge potentials, i.e.,

$$\nabla \cdot \mathcal{A}(x) = 0, \quad \forall x \in \Lambda. \quad (4.46)$$

Using a simplified notation, we obtain the second derivative in a similar computation

$$\begin{aligned}\mathcal{E}''(0) &= -\frac{1}{8N^4} \sum_{x,\mu} \text{Tr} \left\{ -\gamma^a(x) \gamma^b(x) \sigma^a \sigma^b \left[u_\mu^4(x) + i u_\mu^c(x) \sigma^c \right] - \left[u_\mu^4(x) + i u_\mu^a(x) \sigma^a \right] \right. \\ &\quad \times \gamma^b(x + \hat{\mu}) \gamma^c(x + \hat{\mu}) \sigma^b \sigma^c - 2i^2 \gamma^a(x) \sigma^a \left[u_\mu^4(x) + i u_\mu^b(x) \sigma^b \right] \gamma^c(x + \hat{\mu}) \sigma^c \left. \right\} \\ &= \frac{1}{4N^4} \sum_{x,\mu} \left\{ \gamma^a(x) \gamma^b(x) + \gamma^a(x + \hat{\mu}) \gamma^b(x + \hat{\mu}) - 2\gamma^a(x) \gamma^b(x + \hat{\mu}) \right\} u_\mu^4(x) \text{Tr} \sigma^a \sigma^b \\ &\quad + \frac{1}{4N^4} \sum_{x,\mu} \left\{ -2i \gamma^a(x) u_\mu^b(x) \gamma^c(x + \hat{\mu}) \right\} \text{Tr} \sigma^a \sigma^b \sigma^c \\ &= \frac{1}{4N^4} \sum_{x,\mu} \left\{ [\gamma^a(x + \hat{\mu}) - \gamma^a(x)]^2 u_\mu^4(x) + \varepsilon^{abc} [\gamma^a(x + \hat{\mu}) - \gamma^a(x)] \right. \\ &\quad \times [\gamma^b(x + \hat{\mu}) + \gamma^b(x)] u_\mu^c(x) \left. \right\}\end{aligned}\quad (4.47)$$

and this is directly related to the lattice version of the Faddeev-Popov matrix by

$$\mathcal{E}''(0) \equiv \frac{1}{4N^4} \sum_{x,y} \gamma^a(x) \mathcal{M}^{ab}(x, y) \gamma^b(y). \quad (4.48)$$

Of course, requiring $\{U_\mu(x)\}$ to be a local minimum of $\mathcal{E}$ entails

$$\mathcal{M} \geq 0, \quad (4.49)$$

in the positive-definiteness sense.

Therefore, we see that transforming an arbitrary lattice configuration in a way that the new configuration minimizes $\mathcal{E}$ is equivalent to fixing the configuration to the Landau gauge. In this way, we bring the configuration inside the Gribov region.

Furthermore, if we are on a finite lattice and in a theory defined over a compact group, it is clearly implied that each gauge orbit must have a unique configuration satisfying the condition of absolute minimum of $\mathcal{E}$ ^{123,124} on each orbit. We can then define the (absolute) minimal Landau gauge as the lattice analogue of the fundamental modular region. Unfortunately, a multi-dimensional system as a lattice gauge theory is expected to have strong disorder and then have many local minima in $\mathcal{E}$.

4.2.3 Algorithms

We present here the idea behind the computational Landau gauge fixing for a gauge theory with $SU(2)$ symmetry.¹²⁵ The algorithms we consider are local, i.e., they modify one lattice site at a time. This can be a problem if one is interested in minimizing the effect of *critical slowing-down*, which appears when the statistical system is close to a critical point. We will not directly address this here, but we present local algorithms improved in a way to diminish these effects, e.g., by giving larger jumps in configuration space and by introducing stochastic processes. Also, in principle these algorithms do not discriminate between relative and absolute minima, which is not important for we are not directly studying effects of the fundamental modular region here.

In our case, the problem is to minimize the functional in (4.40) each site at a time, i.e., given the position on the lattice, what is the gauge transformation $\mathbf{g}(y)$ which minimizes

$$\begin{aligned}\tilde{\mathcal{E}}[\mathbf{g}(y)] &= -\frac{1}{8N^4} \text{Tr} \mathbf{g}(y) \sum_{\mu=1}^4 \left[U_{\mu}(y) \mathbf{g}^{\dagger}(y + \hat{\mu}) + U_{\mu}^{\dagger}(y - \hat{\mu}) \mathbf{g}^{\dagger}(y - \hat{\mu}) \right] \\ &\equiv -\frac{1}{8N^4} \text{Tr} \mathbf{g}(y) h(y),\end{aligned}\tag{4.50}$$

where $h(y)$ is analogous to an external field acting on $\mathbf{g}(y)$. Notice that h is a sum of $SU(2)$ matrices and so it is *proportional* to an $SU(2)$ matrix.

Our algorithms will be iterative processes that monotonically decrease (4.50). They are expected to converge simply because $\tilde{\mathcal{E}}[\mathbf{g}(y)]$ has a lower bound, given by -1 . Each iteration will consist in updating the gauge transformation $\mathbf{g}(y)$ multiplicatively, namely

$$\mathbf{g}(y) \rightarrow \mathbf{g}^{(\text{update})}(y) \equiv R^{(\text{update})}(y) \mathbf{g}(y),\tag{4.51}$$

where $R(y) \in SU(2)$ and it is specific for each algorithm. In order to measure the efficiency in minimizing the local functional, we introduce its local variation

$$\Delta \tilde{\mathcal{E}}[\mathbf{g}(y)] = -\frac{1}{8N^4} \text{Tr} [\mathbf{g}'(y) - \mathbf{g}(y)] h(y),\tag{4.52}$$

and the normalized displacement in the configuration space

$$\mathcal{D}^2(y) = \frac{1}{2} \text{Tr} [\mathbf{g}(y) - \mathbf{g}'(y)] [\mathbf{g}(y) - \mathbf{g}'(y)]^\dagger = \text{Tr} [\mathbb{1} - \mathbf{g}'(y) \mathbf{g}^\dagger(y)]. \quad (4.53)$$

In order to directly evaluate the iterative process of minimization, it is useful to introduce the positive quantity

$$e_2 = \frac{1}{N^4} \sum_{x \in \Lambda} \sum_{a=1}^3 [\nabla \cdot \mathcal{A}(x)]_a^2, \quad (4.54)$$

which is to be measured at each iteration step and is expected to converge to zero. We generally stop the gauge-fixing steps when it reaches a tolerance value of $e_2^{(\text{tol})} = 10^{-12}$.

Figure 4.6 – Links emanating from y in a 2D lattice.

Los Alamos

The Los Alamos method consists in choosing the $R(y)$ that makes $\tilde{\mathcal{E}}[\mathbf{g}(y)]$ as small as possible, bringing $\tilde{\mathcal{E}}[\mathbf{g}(y)]$ to its absolute minimum in one step. Inspecting (4.50), this is given by the choice

$$\mathbf{g}^{(\text{Alamos})}(y) = \mathcal{P}_{SU(2)} [h^\dagger(y)], \quad (4.55)$$

where $\mathcal{P}_{SU(2)} h^\dagger = h^\dagger / \sqrt{\det h}$ projects $h^\dagger$ onto $SU(2)$, given that the latter is proportional to an element of the group. Thus the update matrix is given by

$$R^{(\text{Alamos})}(y) = \mathcal{P}_{SU(2)} [h^\dagger(y) \mathbf{g}^\dagger(y)]. \quad (4.56)$$

The great advantage of the Los Alamos method is its simplicity, but we should try to locally improve it.

Overrelaxation

One of the ways of locally improving the above method is by generalizing it. In the overrelaxation method the updated link variable is given by

$$\mathbf{g}^{(\text{over})}(y) = \mathcal{P}_{SU(2)} \left[\left(h^\dagger(y) \mathbf{g}^\dagger(y) \right)^\omega \right] \mathbf{g}(y), \quad (4.57)$$

where $\omega \in (1, 2)$ is a tunable parameter. Consequently the update matrix is given by

$$R^{(\text{over})}(y) = \mathcal{P}_{SU(2)} \left[\left(h^\dagger(y) \mathbf{g}^\dagger(y) \right)^\omega \right] = \left[\frac{h^\dagger(y) \mathbf{g}^\dagger(y)}{\sqrt{\det h(y)}} \right]^\omega. \quad (4.58)$$

For $\omega = 1$, the above prescription reduces to Los Alamos method, i.e.

$$\mathbf{g}^{(\text{over})}(y) = \frac{h^\dagger(y) \mathbf{g}^\dagger(y)}{\sqrt{\det h(y) \mathbf{g}(y)}} \mathbf{g}(y) = \frac{h^\dagger(y)}{\sqrt{\det h(y)}} = \mathbf{g}^{(\text{Alamos})}(y), \quad (4.59)$$

Source: By the author.

representing the best local minimization of $\tilde{\mathcal{E}}$ but lacking in mobility through the configuration space. On the other extreme, the case $\omega = 2$ reduces to

$$\mathbf{g}^{(\text{over})}(y) = \frac{(h^\dagger(y) \mathbf{g}^\dagger(y))^2}{\det h(y) \mathbf{g}(y)} \mathbf{g}(y) = \frac{h^\dagger(y) \mathbf{g}^\dagger(y) h^\dagger(y)}{\det h(y)}. \quad (4.60)$$

Notice that the local variation of $\Delta\tilde{\mathcal{E}}$ is then

$$\Delta\tilde{\mathcal{E}}[\mathbf{g}(y)] = \frac{1}{8N^4} \text{Tr} \left[\mathbf{g}(y) h(y) - \frac{h^\dagger(y) \mathbf{g}^\dagger(y) h^\dagger(y) h(y)}{\det h(y)} \right] = 0, \quad (4.61)$$

and the displacement in configuration space is maximally improved. Choosing an intermediate value of ω gives better convergence rate because it tends to spread the local “interactions” faster through the lattice than in the Los Alamos method, i.e., it balances the rate of minimization and the size of the step in configuration space.

In practice, one implements the update (4.58) by truncating the binomial expansion

$$\left[\frac{h^\dagger(y) \mathbf{g}^\dagger(y)}{\sqrt{\det h(y)}} \right]^\omega = \sum_{k=0}^{\infty} \frac{\Gamma(\omega+1)}{k! \Gamma(\omega+1-n)} \left[\frac{h^\dagger(y) \mathbf{g}^\dagger(y)}{\sqrt{\det h(y)}} - \mathbb{1} \right]^k \quad (4.62)$$

at some value of k .¹²⁵ As $\frac{h^\dagger(y) \mathbf{g}^\dagger(y)}{\sqrt{\det h(y)}}$ tends to $\mathbb{1}$ when the algorithm is converging, i.e., the updates are progressively closer to identity, one can safely take into account only the linear term, which results in

$$R^{(\text{over})}(y) = \mathcal{P}_{SU(2)} \left\{ 1(1-\omega) + \frac{h^\dagger(y) \mathbf{g}^\dagger(y)}{\sqrt{\det h(y)}} \right\}, \quad (4.63)$$

where the projection onto $SU(2)$ can be done through a numerical reunitarization.

Stochastic Overrelaxation

This algorithm implements a local update based on the two extremes of the overrelaxation method with complementary probabilities

$$\mathbf{g}^{(\text{stoch})}(y) = \begin{cases} \mathcal{P}_{SU(2)} \left[(h^\dagger(y) \mathbf{g}^\dagger(y))^2 \right] & \text{with probability } p \\ \mathcal{P}_{SU(2)} [h^\dagger(y)] & \text{with probability } 1-p \end{cases}, \quad (4.64)$$

for $0 < p < 1$, which resembles a random-walk through the lattice. Again, the probability p must be tuned for maximal efficiency. We see that this method stochastically alternates between maximum minimizing steps and maximum jumps in configuration space, which can speed up the convergence process by (partially) circumventing critical slowing-down.

We can write the stochastic overrelaxation update as

$$\mathbf{g}^{(\text{stoch})}(y) = \begin{cases} \frac{h^\dagger(y) \mathbf{g}^\dagger(y)}{\det h(y)} \text{Tr} [\mathbf{g}(y) h(y)] - \mathbb{1} & \text{with probability } p \\ \frac{h^\dagger(y)}{\det h(y)} & \text{with probability } 1-p \end{cases}, \quad (4.65)$$

which is a more implementation-friendly form. We will use essentially this gauge fixing method along all our computations, fixing $p = 0.7$ by convention.

4.3 Physical Limits

We have already discussed that it is necessary for a discretized theory to have a naive continuum limit, i.e., to formally correspond to the relevant continuum theory in the limit $a \rightarrow 0$. However, this does not guarantee that the quantum lattice theory will really possess the properties of, in our case, Yang-Mills theory. Furthermore, we must have some guarantee that we are really extracting physical information when using finite values of a , which is the case in real life simulations.

The most important point is that a lattice field theory is a statistical system with a partition function defined by the path integral and whose continuum limit in general corresponds to a critical point (second order phase transition) on the phase space involving the inverse coupling $\beta = 2N_c/g_0^2$.²⁴ This means that we have a characteristic correlation length

$$\xi = \frac{1}{ma}, \quad (4.66)$$

which expresses the smallest mass scale m of the system. In terms of lattice quantities, we have $\hat{\xi} = 1/\hat{m} \rightarrow \infty$ with $\hat{m} = ma \rightarrow 0$, when $a \rightarrow 0$. In the limit of small a , the correlation length then diverges and the system “loses memory” of its grained structure. Moreover, because the physical quantities do not explicitly depend on the regulator a , $g_0 = g_0(a)$ must undergo a specific tuning in order to compensate the effect of varying a . The approach to criticality is then expressed by

$$\hat{\xi}(g_0) \xrightarrow{g_0 \rightarrow g_0^*} \infty, \quad (4.67)$$

where g_0^* is the critical coupling. In particular, the continuum mass scale (if existent) is extracted by using progressively smaller values of a for $a \approx 0$, i.e.

$$m = m(g_0, a) \xrightarrow{g_0 \rightarrow g_0^*} \frac{\hat{m}(g_0)}{a}. \quad (4.68)$$

When $m(g_0, a)$ stops changing we then know that we are in the region of continuum physics.

All the statements above are governed by the renormalization group. In particular, we can determine the dependence of g_0 on the regulator a by using the so-called renormalization-group equation for some observable, say the static quark-antiquark potential (see Section 5.1.1) at a fixed position r , i.e.

$$\left[a \frac{\partial}{\partial a} - \beta_L(g_0) \frac{\partial}{\partial g_0} \right] V(r, g_0, a) = 0. \quad (4.69)$$

Then, through, say, lattice perturbation theory, we can compute V in the small g_0 regime and obtain the (lattice) beta function,^{24,25} which up to second order is given by

$$\beta_L(g_0) = -a \frac{\partial g_0}{\partial a} \approx -\beta_L^{(0)} g_0^3 - \beta_L^{(1)} g_0^5, \quad (4.70)$$

The coefficients for $SU(N_c)$ theory,²⁴

$$\beta_L^{(0)} = \frac{11N_c}{48\pi^2}, \quad \beta_L^{(1)} = \frac{17N_c^2}{384\pi^4}, \quad (4.71)$$

are independent of the regularization scheme and can in fact be calculated using any perturbative method, including continuum ones^D. After integrating (4.70), we obtain the bare coupling's a -dependence

$$a = \frac{1}{\Lambda_L} \exp\left(\frac{-1}{2\beta_L^{(0)} g_0^2}\right) \left(\beta_L^{(0)} g_0^2\right)^{-\beta_L^{(1)}/2(\beta_L^{(0)})^2}, \quad (4.72)$$

where Λ_L is an integration constant corresponding to the asymptotic-freedom scale of the lattice regularization.

The last equation gives us the very important information that the true continuum limit of a non-Abelian lattice theory is obtained by taking the bare coupling constant to zero, i.e., $g_0^* = 0$. Therefore, we must use progressively larger values of the inverse coupling $\beta \sim g_0^{-2}$ in order to make the lattice spacing smaller and access the continuum limit. However, if we use an excessively large value of β in a simulation, given that our lattice side is $L = Na$, the physical dimension probed will perhaps be too small for accessing the phenomena we are interested in. This is especially true when dealing with long-range phenomena and infrared behaviors, because the smallest lattice momentum is $|p_{\min}| \sim L^{-1}$ (see Section 6.3).

On the other hand, if we take β to be too small, then our results will suffer from large discretization errors, which can give rise to the observation of lattice artifacts instead of physical phenomena. Therefore, it is clear that we must remain inside a *scaling window* in order to obtain legitimate physics. How large the window will be depends on the lattice size that we can simulate and on the thermalization, autocorrelation (see next section) and measurement times for a given β , i.e., the computational time available. Moreover, besides taking the continuum limit $a \rightarrow 0$, one should also take the thermodynamical limit, i.e., send the lattice volume to infinity. In practice, computer resources will highly constrain those limits and what we can do is to simulate progressively larger and finer lattices, verifying if the results are self-consistent.

^D We note that, being excessively involved, lattice perturbative calculations generally are only justified when one desires to improve lattice actions through the cancellation of scaling violating terms, obtaining a “faster” continuum limit.

But how large or small should β be? We can exemplify the asymptotic scaling behavior with the string tension σ . This quantity quantifies the linearly rising behavior observed in simulations of the static quark-antiquark potential and is related to the area law behavior of large Wilson loops. A not so precise but instructive way of accessing the string tension is to compute the *Creutz ratios*,²⁶ defined by

$$\chi(I, J) = -\log \frac{\mathcal{W}(I, J)\mathcal{W}(I-1, J-1)}{\mathcal{W}(I-1, J)\mathcal{W}(I, J-1)}. \quad (4.73)$$

The Creutz ratios are designed to cancel out constant and perimeter factors from the Wilson loop. They tend to the (in lattice units) string tension for not too small I and J , i.e., $\chi(I, J) \rightarrow \sigma a^2 \equiv \hat{\sigma}$. In Figure 4.7 we see that, for $I, J > 1$, $\chi(I, J)$ clearly departs from the strong-coupling behavior (green line) and enters the *scaling region*, taken to be roughly $\beta \in [2.1, 2.8]$ for $SU(2)$.¹²⁶ A fit with the form of Equation (4.72) (squared) to $\chi(I, J) = \hat{\sigma}$ for $I = J = 4$ produces the black line in Figure 4.7 and yields the lattice mass scale $\Lambda_L = 0.0113(7)\sqrt{\sigma}$.¹²⁷

The only problem we now have is that we keep expressing all quantities in lattice units. To be able to obtain physical results we must somehow fix the scale with external information. For example, we could use the conventional value for the string tension $\sigma = (440\text{MeV})^2$ taken from phenomenological models to determine a for a given value of β (see Section 5.1.2). However, a probably more reliable method is to use the so-called Sommer parameter to fix a .¹²⁸ In this case, instead of determining a by first computing $\hat{\sigma}$, we use the physical parameter $r_0 = 0.5$ fm for which the string force is known. The force is derived from an effective Schrödinger equation for a heavy quark-antiquark pair, which yields

$$F(r_0)r_0^2 = V'(r_0)r_0^2 = 1.65, \quad (4.74)$$

where $V'(r_0)$ is the derivative of the static potential at r_0 . Using the *Ansatz* $V(r) = c + \gamma/r + \sigma r$ (see Section 5.1.1), we obtain¹¹⁸

$$a = r_0 \sqrt{\frac{\hat{\sigma}}{1.65 + \hat{\gamma}}}, \quad (4.75)$$

Figure 4.7 – Scaling of the string tension evaluated through Creutz ratios. Notice that this extrapolation only works for not too small Wilson loops. The green line is the strong-coupling expansion obtained from (4.32), namely $\log 4/\beta$. The black line is a fit with the form (4.72) squared (in string-tension units).

Source: By the author.

where the hat variables are obtained from a fit of V to the static-potential simulation data (in lattice units). For results exemplifying both ways of fixing a , see Section 6.1.2.

Finally, we should also account for any remaining renormalization effects and this varies with the problem. For renormalizing gluon and ghost propagators we can use a renormalization point at some $p^2 = \mu^2$ to fix the value of the propagators and determine the β -dependent multiplicative renormalizations.^{126,129} Nevertheless, these will not be crucial to our analysis and we will not implement them on the results in Chapter 6.

4.4 Monte Carlo Methods

The set of tools of lattice gauge theory is many times strongly associated to numerical simulations. In fact, due to the formal similarity with statistical systems, a number of strategies come from this field, being the Monte Carlo methods the most important ones. Here we present a description of the essentials of Monte Carlo methods used in lattice gauge theory.

4.4.1 Markov Chains

Our main objective in lattice gauge theory is to compute quantum expected values of observables in Euclidean space given by

$$\langle f[U] \rangle = \frac{\int \mathfrak{D}U e^{-S_W[U]} f[U]}{\int \mathfrak{D}U e^{-S_W[U]}}, \quad (4.76)$$

where $f[U]$ could be some Wilson loop defined in (4.13), or even more complicated quantities.

If analytical methods happen to be not suitable for any reason, we could try to numerically compute all the integrals for each link of the lattice. However, notice that for a lattice with N^4 sites, we have $4N^4$ link variables each with $N_c^2 - 1$ group parameters, yielding a total of $4(N_c^2 - 1)N^4$ integrals. For a simple $N = 8$ lattice and $SU(3)$ group, we then would have ~ 130000 integrations to be done, resulting in a sum of 15^{130000} , if a deterministic method as Simpson's rule is used in a coarse mesh with 15 points. Of course, it is virtually impossible to use that kind of direct method.

Monte Carlo methods have blossomed in the middle of the last century as a way to circumvent problems as those. There are two types of Monte Carlo methods: the static and *dynamic* ones. The dynamic ones are much more suited for systems with many degrees of freedom. The idea of dynamic methods is to approximate the “ensemble” average (4.76) by an average over of n samples generated by a *stochastic process*, i.e.,

$$\langle f \rangle \approx \frac{1}{n} \sum_{i=1}^n f(\{U\}_i) \equiv \bar{f}, \quad (4.77)$$

where $f = f(\{U\}_i)$ is the observable “measured” at the link configuration $\{U\}_i$ and $\bar{f}$ denotes a *sample* average, in contrast to the *ensemble* average $\langle f \rangle$. The stochastic process

used in our computations is called a *Markov chain* and each sample is an element of such chain, preferably after a sufficiently long *thermalization time* n_{therm} . Of course, estimating an average by sampling over the configuration space will introduce statistical errors that go as $1/\sqrt{n}$, by central-limit-theorem arguments and “independent and identically distributed”-variables assumptions.

Considering the state space $\mathbb{U}$ of all possible link configurations and $\mathbb{U}$ -valued random variables X_t , a Markov chain, schematically given by the sequence

$$X_0 \rightarrow X_1 \rightarrow X_2 \rightarrow \dots \rightarrow X_n, \quad (4.78)$$

is composed of two essential ingredients. One is the *initial distribution* $\pi_{(0)}$ on $\mathbb{U}$, which simply gives the probability $P(X_0 = \{U\}_i) = \pi_{(0)}(\{U\}_i) \equiv \pi_{(0)i}$ for the first element of the chain to be equal to some link configuration $\{U\}_i \in \mathbb{U}$. The second ingredient is a *transition probability matrix* given by the elements $p_{ij} = p(\{U\}_i \rightarrow \{U\}_j)$ obeying

$$p_{ij} \geq 0, \quad \forall i, j \quad \text{and} \quad \sum_{j \in \mathbb{U}} p_{ij} = 1, \quad \forall i, \quad (4.79)$$

which gives the time-independent conditional probability $P(X_{t+1} = \{U\}_j | X_t = \{U\}_i) = p_{ij}$ of going to $\{U\}_j$ given that the preceding element is $\{U\}_i$. With this in mind, a Markov chain is totally expressed by the joint probability

$$P(X_n = \{U\}_j | \dots | X_2 = \{U\}_{k_2} | X_1 = \{U\}_{k_1} | X_0 = \{U\}_i) = \rho_i p_{ik_1} p_{k_2 k_3} \dots p_{k_n j}. \quad (4.80)$$

In view of the definitions above, it is clear that the process of generating a new state of a Markov chain does not contain memory of the past, only of the previous state at most. We further define the m -step transition probability

$$P(X_{t+m} = \{U\}_j | X_t = \{U\}_i) = \sum_{\{k\}} p_{ik_1} \dots p_{k_{m-1}j} \equiv p_{ij}^{(m)}. \quad (4.81)$$

A Markov chain is irreducible if from any state we can get to each other state on $\mathbb{U}$ in a finite number of steps, i.e.

$$\exists m \geq 0, \quad p_{ij}^{(m)} > 0, \quad \forall i, j. \quad (4.82)$$

Furthermore, it is said to be *aperiodic* if it is always possible for the chain to go back to the same arbitrary state in any number of steps, i.e.,

$$p_{ii}^{(m)} > 0, \quad \forall i, m. \quad (4.83)$$

These two characteristics are important for our problems and are sometimes known, among physicists, as (strong) *ergodicity*. We will assume that such a class of Markov chains is always compatible with the systems in which we are interested and restrict our attention to it.

For an irreducible and aperiodic Markov chain, there is a theorem¹³⁰ that guarantees that

$$\lim_{m \rightarrow \infty} p_{ij}^{(m)} = \pi_j, \quad (4.84)$$

for a unique distribution π , given that it exists. Furthermore, this distribution is *stationary*, i.e.

$$\sum_i \pi_i p_{ij} = \pi_j, \quad \forall j. \quad (4.85)$$

In the context of the path integrals that we are trying to estimate, we can identify the distribution π , also called equilibrium distribution, with the Boltzmann factor $\propto e^{-S[U]}$. Then, after a sufficiently long Monte Carlo time n_{therm} , we know that the samples in a Markov chain are generated with the correct equilibrium distribution and we can safely *estimate* an expected value from them.

We should now devise practical algorithms obeying the rules above, namely ergodicity (4.82), (4.83) and stationarity (4.85), in order to implement this method through algorithms. We should also try to estimate the rate of convergence to stationarity and the statistical errors made by doing a sampling through a Markov process.

4.4.2 Algorithms

A lot of useful algorithms were designed to satisfy what we call microreversibility, stated by the *detailed balance* condition

$$\pi_i p_{ij} = \pi_j p_{ji}. \quad (4.86)$$

Using (4.79) we see that detailed balance obeys the stationarity condition (4.85) and thus is sufficient for the class of algorithms we want to invent. We restrict ourselves to these.

It is important to note that here we will use *local* algorithms, i.e., we iterate over each link variable of a lattice configuration. This is of practical importance to keep the acceptance rate of the updates high enough to cover a representative part of the configuration space $\mathcal{U}$. When we repeat the steps of the algorithm for each link variable, covering all the lattice, we have what is called a *sweep* and the resulting gauge configuration is the subsequent state in our Markov chain.

Metropolis

The class of algorithms named after Metropolis¹³¹ is given by a transition matrix of the form (no implicit sum)

$$p_{ij} = c_{ij} a_{ij}, \quad (4.87)$$

where c is a given transition rate to a candidate configuration, which is to be accepted with probability ^E

$$a_{ij} = \min \left(1, \frac{\pi_j c_{ji}}{\pi_i c_{ij}} \right). \quad (4.88)$$

It is easy to see that p satisfies detailed balance

$$\pi_i p_{ij} = \min(\pi_i c_{ij}, \pi_j c_{ji}) = \pi_j c_{ji} \min \left(\frac{\pi_i c_{ij}}{\pi_j c_{ji}}, 1 \right) = \pi_j p_{ji}. \quad (4.89)$$

Ergodicity is left to be demonstrated for each specific choice of c .

One very specific and famous version of this algorithm is given by the choice of a symmetric candidate transition $c_{ij} = c_{ji}$, yielding

$$p_{ij} = \min \left(1, \frac{\pi_i}{\pi_j} \right) = \min \left(1, \frac{e^{-S[U_i]}}{e^{-S[U_j]}} \right) = \min(1, e^{-\Delta S}). \quad (4.90)$$

This enables us to formulate simple rules for computing Markov-chain transitions from the state U_i given some proposed state U_j :

- If $\Delta S \leq 0$ then the U_j is accepted right away.
- If $\Delta S \geq 0$, then U_j is accepted with probability $e^{-\Delta S}$.

The last step can be interpreted in QFT as the addition of quantum fluctuations to the classical contributions. As we mentioned, we proposed a transition for an individual link U_i at a time, instead of the whole configuration $\{U\}$, which is done so that the acceptance rate is not too small. See Ref. 118 for a detailed implementation.

Heat bath

A heat-bath algorithm resembles the action of a thermal reservoir in a system on the canonical ensemble.^{127,132} In this case, the heat bath is composed of the neighboring link variables of the one to be modified.

The transition probability is given in the form of a Metropolis-type transition (4.87) with the trial configuration chosen according to the canonical probability distribution

$$c_{ij} = \mathcal{Z}^{-1} e^{-\tilde{S}[U_j]} = \pi(U_j), \quad (4.91)$$

where $\tilde{S}[U_j]$ is the local contribution to the action given by U_j and its fixed neighbors called *staples* (see Equation (6.20)). Notice that this choice implies $a_{ij} = 1$, i.e., the candidate link is always accepted. Moreover, this transition probability is independent of the starting link U_i .

^E Actually, it is not necessary to involve the minimum function, but just a suitable function of $\pi_j c_{ji} / \pi_i c_{ij}$.¹³⁰

As a kind of generalized Metropolis algorithm, the heat-bath method automatically satisfies detailed balance and ergodicity is enforced by $c_{ij} \propto e^{-\tilde{S}[U_j]} > 0$ for any pair i, j .^F A detailed $SU(2)$ implementation is given in Refs. 118, 127, 132^G.

Microcanonical Overrelaxation

The motivation for the overrelaxation algorithm is to locally improve the above ergodic methods against *critical slowing-down*,¹³⁰ which causes the Markov chain to reach the equilibrium distribution very slowly when close to a critical point of the theory, e.g., the continuum limit. This problem may be attributed to the local character of the Metropolis and heat-bath methods, taking too long to communicate their updates to the whole lattice.

Instead of implementing global methods, e.g. multigrid,¹³⁰ one can use a deterministic update as the overrelaxation in order to fight critical slowing-down.^{135, 136} In this case, we propose the candidate link as

$$U_j = V U_i^{-1} V, \quad V \in SU(N_c), \quad (4.92)$$

which means that c_{ij} is symmetric and detailed balance is automatically satisfied. The group element V is chosen so that it is equal to the U_i whose value minimizes the action, i.e.,

$$\tilde{S}_i = \text{Re Tr } U_i A, \quad (4.93)$$

where A are the fixed neighboring links of U_i , its staples.

We can better visualize why this is a good choice to perform a large step in configuration space with the compact $U(1)$ theory, where $U_j = e^{i\theta_j}$, $V = e^{i\varphi}$ and $A = e^{i\alpha}$ and with $\theta_j, \alpha \in [0, 2\pi)$, yielding

$$e^{\theta_j} = e^{i\varphi} e^{-i\theta_i} e^{i\varphi}, \quad (4.94)$$

where we choose $\theta_i \equiv \varphi = \pi - \alpha$ so that it minimizes

$$\tilde{S}_i \propto \text{Re } U_i A = \text{Re } e^{i(\theta_i + \alpha)} = \cos(\theta_i + \alpha) \rightarrow \cos(\theta_i + \alpha) \Big|_{\theta_i = \varphi = \pi - \alpha} = -1. \quad (4.95)$$

Then, the update $\theta_i \rightarrow \theta_j = 2\pi - 2\alpha - \theta_i$ is equivalent to a reflection

$$\cos(\theta_i + \alpha) \rightarrow \cos(2\pi - \alpha - \theta_i) = \cos(-\alpha - \theta_i), \quad (4.96)$$

located in the opposite side of the unit circle and leaves the action unchanged (microcanonical), i.e., it is always accepted.

^F Actually, detailed balance may not hold, depending on how the sweeping of the lattice is done. The method is explicitly valid anyway because it is based on partial resampling (holding most degrees of freedom fixed and sampling the remaining one exactly from the equilibrium distribution.).

^G The $SU(3)$ version is usually executed through the Cabibbo-Marinari algorithm, known also as pseudo-heat bath.^{118, 133, 134} This is also valid for $N_c > 3$.

When translating this algorithm to $SU(N_c)$, it is not always possible to make the updates with probability 1. Only in $SU(2)$ this is possible because the staples are proportional to an element of the group and thus are easily projected onto it. For other groups this projection is only approximate. Nevertheless, this method aims at maximally changing the link variable, corresponding to much larger jumps in configuration space than the Metropolis or heat-bath updates. However, overrelaxation does not introduce fluctuations on the action. Therefore, it must be combined with Metropolis or heat bath in order to efficiently cover configuration space and reduce critical slowing-down. A detailed description of the overrelaxation algorithm for the $SU(2)$ group is given in Refs. 118, 136.

We combine both heat-bath and overrelaxation methods, using the well-established hybrid overrelaxation (HOR) algorithm.¹³⁵ The HOR algorithm was shown to efficiently fight critical slowing-down and is also easy to implement. It consists in performing, for each sweep, N_{over} microcanonical overrelaxation sweeps followed by N_{hb} standard heat-baths sweeps. We adopt the practice of Ref. 123 and fix $N_{\text{over}} = N/2$ and $N_{\text{hb}} = 1$ in all simulations (see Chapter 6).

4.4.3 Thermalization

As we mentioned, given the right conditions, a Markov chain always converges to the equilibrium distribution, namely the Boltzmann distribution, in an infinite number of transitions. However, in a real simulation we are limited to perform a finite number of steps and thus it is important to estimate the rate of convergence to equilibrium from an arbitrary distribution and errors made in this implementation.

Strictly speaking, the function that controls the convergence to equilibrium of some observable f is the normalized *autocorrelation function*

$$\rho_{ff}(t) = \frac{C_{ff}(t)}{C_{ff}(0)} \equiv \frac{\langle f_s f_{s+t} \rangle - \langle f_s \rangle^2}{\langle f_s^2 \rangle - \langle f_s \rangle^2}, \quad (4.97)$$

where t is the Monte Carlo time. In a typical spatial lattice, ρ_{ff} will behave as a series of exponentially decaying modes, so that we define the *exponential autocorrelation time* as

$$\tau_{\text{exp},f} \equiv \lim_{t \rightarrow \infty} \sup \frac{t}{-\log |\rho_{ff}(t)|} \quad (4.98)$$

for the observable f and

$$\tau_{\text{exp}} \equiv \sup \tau_{\text{exp},f} \quad (4.99)$$

for all possible observables. In other words, this means that the autocorrelation time measures the characteristic relaxation time for the slowest mode of the system.

Note that, starting from some arbitrary link configuration, e.g. $\{U\}_i$, which represents a narrow initial distribution $\pi_{(0)i} = \delta(\{U\}_i)$, is obviously going to lead to a transient phase during the process of equilibration. This introduces a *bias* in the result that we get

from the sample average (4.77) when compared to the original ensemble average. We could think it is reasonable to use a thermalization time $n_{\text{therm}} \sim 20\tau_{\text{exp}}$ so that the deviation from equilibrium is $e^{-20} \sim 10^{-9}$. However, we almost never know τ_{exp} and even so, it may be too conservative, there existing algorithms for which it actually diverges. Therefore, we should view τ_{exp} only as an upper bound of n_{therm} .

The best we can do is to try estimating n_{therm} theoretically and empirically.¹³⁰ By theoretically estimation we mean to understand the general physical mechanisms that govern the system's slow modes in order to guarantee that we are close to equilibrium. Nevertheless, in practice we stick to the empirical estimation, which consists basically in plotting the thermalization process for as many observables as possible. It is also useful to start from different configurations, namely ordered (cold) and disordered (hot) ones, and see how much time they take to converge into one another, as exemplified in Figure 4.8.

Figure 4.8 – Thermalization of plaquette observable for different initializations ($\beta = 2.2$, $N = 12$).

Source: By the author.

At the end of the day, we should discard about n_{therm} generated configurations before doing any measurements, where $20\tau_{\text{estimated,exp}} \lesssim n_{\text{therm}} \lesssim n/5$ of a total of n updates, keeping in mind to always have $n_{\text{therm}} \ll n$. The final averages are not very sensitive to this transient because the final bias $\sim 1/n$ is smaller than the statistical errors $\sim 1/\sqrt{n}$ (see next section), so that we have some freedom in choosing n_{therm} from this range ^H.

^H Given that the total run time n is very large, we can also use the first configurations in the average.¹³⁰

4.4.4 Statistical Errors

In simulations we approximate the ensemble average $\langle f \rangle$ by a sample average $\bar{f}$ taken from a dataset composed of n values. Whether we are discarding the n_{therm} first configurations or not, we will need to estimate the errors we are making with that simplification. Assuming the estimate $\bar{f}$ in (4.77) is unbiased, i.e. $\langle \bar{f} \rangle = \langle f \rangle$, its variance will be

$$\begin{aligned}\sigma_{\bar{f}}^2 &= \left\langle \left(\bar{f} - \langle \bar{f} \rangle \right)^2 \right\rangle = \left\langle \left(\frac{1}{n} \sum_{i=1}^n f_i - \frac{1}{n} \sum_{i=1}^n \langle f \rangle \right)^2 \right\rangle \\ &= \frac{1}{n^2} \sum_{i,j=1}^n \left\langle f_i f_j + \langle f \rangle^2 - f_i \langle f \rangle - f_j \langle f \rangle \right\rangle = \frac{1}{n^2} \sum_{i,j=1}^n \left(\langle f_i f_j \rangle - \langle f \rangle^2 \right).\end{aligned}\quad (4.100)$$

In the case of *uncorrelated* configurations, $\langle f_i f_j \rangle - \langle f_i \rangle \langle f_j \rangle = 0$ for $i \neq j$ and we get the variance of the estimator in terms of the ensemble variance

$$\begin{aligned}\sigma_{\bar{f}}^2 &= \frac{1}{n^2} \left(\sum_{i=1}^n \langle f_i f_i \rangle + \sum_{i,j=1, i \neq j}^n \langle f_i f_j \rangle - \sum_{i,j=1}^n \langle f \rangle^2 \right) \\ &= \frac{1}{n} \langle f^2 \rangle + \frac{n(n-1)}{n^2} \langle f \rangle^2 - \langle f \rangle^2 = \frac{1}{n} \left(\langle f^2 \rangle - \langle f \rangle^2 \right) = \frac{1}{n} C_{ff}(0) = \frac{1}{n} \sigma_f^2,\end{aligned}\quad (4.101)$$

with C_{ff} defined in (4.97).

Integrated Autocorrelation Time

Unfortunately, the uncorrelated generation of configurations is not the case in Markov chains. In an algorithm, subsequent *states* generated by the methods in (4.4.2) will retain memory of the past and will not be effectively independent, even if the transition rules are independent in each Monte Carlo step. Returning to (4.100), we can write

$$\sigma_{\bar{f}}^2 = \frac{1}{n^2} \sum_{i,j=1}^n C_{ff}(|t|) \Big|_{t=i-j} \quad (4.102)$$

in terms of the autocorrelation function C_{ff} in (4.97). Writing the above sum as a constrained sum in terms of new variables t, k obeying the substitutions $|i-j| \rightarrow |t|$, $i \rightarrow k$ with the respective ranges $|t| = 0, \dots, n-1$, $k = 1 - |t|, \dots, n - |t|$, yields

$$\begin{aligned}\sigma_{\bar{f}}^2 &= \frac{1}{n^2} \sum_{t=-(n-1)}^{n-1} \sum_{k=1}^{n-|t|} C_{ff}(|t|) = \frac{1}{n} \sum_{t=-n+1}^{n-1} \frac{n-|t|}{n} C_{ff}(0) \rho_{ff}(|t|) \\ &= \frac{\sigma_f^2}{n} \sum_{t=-n+1}^{n-1} \left(1 - \frac{|t|}{n} \right) \rho_{ff}(|t|) \approx \frac{\sigma_f^2}{n} \sum_{t=-n+1}^{n-1} \rho_{ff}(|t|) \\ &= \frac{\sigma_f^2}{n} \left(1 + 2 \sum_{t=1}^n -1 \rho_{ff}(t) \right) = \frac{\sigma_f^2}{n} 2\tau_{\text{int},f},\end{aligned}\quad (4.103)$$

where we implicitly defined the *integrated autocorrelation time* by

$$\tau_{\text{int},f} \equiv \frac{1}{2} + \sum_{t=1}^{n-1} \rho_{ff}(t). \quad (4.104)$$

We then conclude that the variance of the estimator increases by a factor of $2\tau_{\text{int},f}$ when the generated configurations are not independent. It is also possible to interpret $n/2\tau_{\text{int},f}$ as the effective number of Markov chain's states.

Given this information about the algorithm's autocorrelation time, one can choose to discard every $n_{\text{cor}} \approx 2\tau_{\text{int},f}$ configurations after thermalization and use formula (4.101) to compute the error. Equivalently, one can keep all the measurements generated by the simulation and then use formula (4.103). Whether we are using one method or the other, we do not know the ensemble variance σ_f^2 exactly, so we estimate it by the unbiased sample variance ^I

$$\sigma_f^2 \approx \bar{\sigma}_f^2 = \frac{1}{n-1} \sum_{i=1}^n (f_i - \bar{f})^2, \quad (4.105)$$

and take, respectively, the standard deviation $\sigma_{\bar{f}} \approx \bar{\sigma}_f / \sqrt{n}$ or $\sigma_{\bar{f}} \approx \bar{\sigma}_f \sqrt{2\tau_{\text{int},f}/n}$ and write

$$\langle f \rangle = \bar{f} \pm \sigma_{\bar{f}}. \quad (4.106)$$

The integrated autocorrelation time is the quantity that measures the effect of critical slowing-down of the algorithm on the observable we are estimating. When $\tau_{\text{int},f}$ is large, the algorithm tends to be less efficient close to a critical point of the system, which is also a reflection of the algorithm's local character. Of course, to completely measure the efficiency of a method one needs to also take into account the complexity of each algorithm's iteration, i.e., to measure its cost in CPU-time.

In general, the characteristic time for thermalization $n_{\text{therm}} \approx 2\tau_{\text{exp},f}$ is not equal to $2\tau_{\text{int},f}$. The former estimates the time for reaching equilibrium from an arbitrary configuration and the latter estimates the time for producing an independent configuration from the previous. Consequently, $\tau_{\text{int},f}$ is responsible for the determination of the total run length n . If we want error bars of, say $y\%$, we should then choose a total run of $n \sim 2 \times 10^4 \tau_{\text{int},f} / y^2$. We then see how much a precise Monte Carlo simulation costs: too obtain 1% statistical errors, supposing the algorithm has small integrated autocorrelation times, we must generate about 10000 configurations!

After all this discussion, there is still a gap in our approach: we do not know the exact ρ_{ff} and C_{ff} in order to compute $\tau_{\text{int},f}$. We must then estimate them with the finite data provided in a simulation run. The estimator for C_{ff} when we do not know $\langle f \rangle$ (most of the cases) is given by

$$\bar{C}_{ff}(t) \equiv \frac{1}{n-|t|} \sum_{i=1}^{n-|t|} (f_i - \bar{f}) (f_{i+|t|} - \bar{f}), \quad (4.107)$$

^I The sample variance $\bar{\sigma}_f^2$ is a random variable and it is biased because the measurements fall closer to the sample average than to the ensemble average. When the bias is taken into account we must divide the naive $1/n$ factor that would normally be used by $n-1/n$, resulting in (4.105).¹³⁷

which itself is a random number for each t , having its own biases and errors.^{130,138} Its normalized version is naturally $\bar{\bar{\rho}}_{ff}(t) = \bar{\bar{C}}_{ff}(t)/\bar{\bar{C}}_{ff}(0)$. However, the estimate of $\tau_{\text{int},f}$ must be handled with care, because for $|t| \gg \tau_{\text{int},f}$ the signal-to-noise ratio is too small and we will certainly miss the exact value. We define the estimate as

$$\bar{\bar{\tau}}_{\text{int},f} \equiv \frac{1}{2} + \sum_{t=1}^{n-1} \lambda(t) \bar{\bar{\rho}}_{ff}(t), \quad (4.108)$$

where $\lambda(t)$ is some cutoff function of the step-type

$$\lambda(t) = \begin{cases} 1 & \text{if } |t| \leq M \\ 0 & \text{if } |t| > M \end{cases}. \quad (4.109)$$

We should then start with small values of M and progressively increase it and check if the result is consistent with $\bar{\bar{\tau}}_{\text{int},f} \ll M \ll n$. We remark that, if M is too small, the variance of the estimate will be spoiled by bias.^{130,138} Nevertheless, in Ref. 139 an automatic windowing algorithm is introduced which implements the constraints for M by iterating the computation of (4.108) until one finds the smallest value of M that satisfies the dynamical condition

$$M \geq c \bar{\bar{\tau}}_{\text{int},f}(M), \quad c \in \mathbb{R}, \quad (4.110)$$

with c usually taken to lie between 6 and 15 for the sake of consistency. As it is expected, this algorithm needs a long run to be reliable ($n \sim 1000\tau_{\text{int},f}$).

We see that the methods related to a direct computation of $\tau_{\text{int},f}$ rely on large amounts of data. To just obtain an estimate $\tau_{\text{int},f}$ we must run a long simulation without discarding any configurations and even then we cannot know if a reliable estimate for $\tau_{\text{int},f}$ will be obtained, because *a priori* it is not known how large $\tau_{\text{int},f}$ is in comparison to the chosen n . The problem is even worse if we need to compute expected values F which are derived quantities from primary expectation values f_i , e.g. $F(f_1, f_2) = \langle f_1 \rangle / \langle f_2 \rangle$ or even parameters from data fits.^{24,138} Of course we can compute these by defining the relevant autocorrelation matrix $C_{f_i f_j}(t)$ and analogously computing the appropriate autocorrelation times and errors by error propagation^J. We instead present simpler methods that can be mixed with the straightforwardness of the above ones to obtain results with smaller amount of data and work.

Binning

The data binning method is a simple way to estimate the integrated autocorrelation time. Given a dataset of total size n for an observable f

$$\{f\} = \{f_1, f_2, \dots, f_n\}, \quad (4.111)$$

^J We cannot do a simple error propagation of the type $\Delta F = \left| \frac{\partial F}{\partial f_1} \right| \Delta f_1 + \left| \frac{\partial F}{\partial f_2} \right| \Delta f_2$ because this assumes that the expected values are uncorrelated, which is not true in general. One needs to take into account the correlations by computing the complete autocorrelation matrix or, alternatively, use a resampling method of Section 4.4.4.

in each binning step one divides $\{f\}$ in n_b sets of size $b = n/n_b$ each. Then we have, for some $n_b < n$,

$$\{f^{(1)}\}, \{f^{(2)}\}, \dots, \{f^{(n_b)}\}, \quad (4.112)$$

where data are consecutively gathered, i.e.,

$$\{f^{(\alpha)}\} = \{f_{\alpha+(\alpha-1)b}, f_{\alpha+(\alpha-1)b+1}, \dots, f_{\alpha+(\alpha-1)b+b-1}\} = \{f_{\alpha(1+b)-b}, \dots, f_{\alpha(1+b)-1}\}. \quad (4.113)$$

We then collapse each subset to its mean value

$$\{f^{(\alpha)}\} \rightarrow \frac{1}{b} \sum_{j=\alpha(1+b)-b}^{\alpha(1+b)-1} f_j \equiv \tilde{f}_\alpha, \quad \alpha = 1, \dots, n_b. \quad (4.114)$$

Notice that the sample averages are identical, i.e., for every choice of n_b

$$\bar{\tilde{f}} = \frac{1}{n_b} \sum_{\alpha=1}^{n_b} \tilde{f}_\alpha = \frac{1}{n_b b} \sum_{\alpha=1}^{n_b} \sum_{j=\alpha(1+b)-b}^{\alpha(1+b)-1} f_j = \frac{1}{n} \sum_{j=1}^n f_j = \bar{f}. \quad (4.115)$$

When each binning iteration is done, its collapsed values will now have less autocorrelation. For sufficiently large bin size b , the variance over the blocks, given by (4.101) and (4.105)

$$\bar{\sigma}_{f,\text{bin}}^2 = \frac{1}{n_b(n_b - 1)} \sum_{j=1}^{n_b} (\tilde{f}_j - \bar{\tilde{f}})^2, \quad (4.116)$$

will be approximately the variance computed over an uncorrelated set of data. At this point, the block size b will be a rough estimate of the autocorrelation time.

A practical way of executing binning is to plot the variance (4.116) for each bin size. When the variance reaches a plateau we can then pick the autocorrelation time as approximately equal to the bin size. Binning really pays off when we are dealing with derived functions of primary expectation values $F = F(\langle f \rangle, \langle g \rangle, \dots)$, then we can calculate the variance of F using

$$\bar{\sigma}_{F,\text{bin}}^2 = \frac{1}{n_b(n_b - 1)} \sum_{j=1}^{n_b} (F(\tilde{f}_j, \tilde{g}_j, \dots) - \bar{F})^2 \quad (4.117)$$

for each bin size and pick the autocorrelation time by eye in a $\bar{\sigma}_{F,\text{bin}}^2 \times b$ plot. The problem is that many times the bin size can get too small before one reaches the variance plateau and a lot of noise can be present, especially if we are computing correlators, e.g., the Polyakov-loop correlation function $\langle \mathcal{P}(\mathbf{x}_1) \mathcal{P}(\mathbf{x}_2) \rangle$.

Figure 4.9 – Binning procedure for estimating the autocorrelation time ($\beta = 2.2$, $N = 4$).

Source: By the author.

Resampling Methods

When there is not enough data to reliably determine the autocorrelation time and statistical errors solely from binning, we can combine it with the so-called resampling methods. The most used ones are the *jackknife* and *bootstrap* methods,¹⁴⁰ of which we will focus only on the latter.

The idea behind resampling methods is that we can obtain the variance of some estimator $\bar{f}$ by looking at the distribution of a number of different independent realizations of our Markov chain, i.e., different ensembles of finite size. Of course, doing this would cost too much to be useful, but we can do a rather smart move to obtain something that emulates this process.

In the bootstrap method, we recycle our single original ensemble of size n by drawing K new ensembles, each of size m , from it. So, given the original set of measurements (4.111) of some primary observable f , we generate K ensembles

$$\{f\}_i = \{f_{i_1}, f_{i_2}, \dots, f_{i_m}\}, \quad i = 1, \dots, K, \quad (4.118)$$

where each i_j ($j = 1, \dots, m$) is chosen with uniform probability from the set $\{1, \dots, n\}$. With these ensembles at our disposal, we can compute the resampled averages for each $\{f_i\}$ as

$$\hat{f}_i = \frac{1}{m} \sum_{j=1}^m f_{i_j}, \quad i = 1, \dots, K, \quad (4.119)$$

and then estimate $\langle f \rangle$ by the bootstrap average

$$\bar{\hat{f}} = \frac{1}{K} \sum_{j=1}^K \hat{f}_j. \quad (4.120)$$

The estimate of the variance will be given by the bootstrap variance

$$\sigma_{\bar{\hat{f}}}^2 = \frac{1}{K} \sum_{j=1}^K \left(\hat{f}_j - \bar{\hat{f}} \right)^2. \quad (4.121)$$

The jackknife method is a similar process where, instead of sorting out the new ensembles, one creates n new ensembles of size $n - 1$ each by excluding one of the original elements.^{24,118,120,140} Generally, bootstrap is preferable when n is too large, besides being more reliable than jackknife.

Resampling methods are generally stable in the presence of correlations, and by mixing then with binning (with which we can generate a set of roughly independent samples) we can compute both a better estimator for the variance and an approximation for the autocorrelation time of complicated secondary observables. We must then use the bootstrap or jackknife variance as the estimator for the variance in each binning step. This is true specially when computing errors of fit parameters.

5 CONFINEMENT

Since the 1970s, many people have been trying to explain the contrived aspects of QCD and its constituent non-Abelian gauge symmetry. A milestone for the breakthrough of QCD on the explanation of fundamental interactions was the discovery of asymptotic-freedom in 1974,^{14,15} which resulted in a Nobel prize many years later. Nevertheless, as an obstacle for the quark model^{11,12} incorporated to QCD, the behavior of the theory at large distances is obscured by the *confinement problem* until now.

Historically, confinement could be stated as the fact that no asymptotic quarks and gluons are observed in experiments. This is very peculiar if compared to the success of QED, where electrons and photons can be relatively easy to observe. Nevertheless, there are many theoretical models and numerical evidences that support that confinement emerges from QCD, for its essential aspects can be accommodated into a consistent framework. Still, there is no derivation of confinement from a fundamental theory, namely Yang and Mills'. From the perspective of mathematical rigor and axiomatic quantum field theory, the formulation of confinement (and other associated aspects) is actually worth 1 million dollars as a Millenium Prize.¹⁹ In this chapter, we will study confinement from a physical point of view, based on path integrals, gauge fixing and lattice gauge theory, beginning with its phenomenological basis.

5.1 Phenomenological Basis and Models

5.1.1 Linear Potential and Wilson Loop

One very established result is that of Bachas¹⁴¹ regarding the concavity of the (static) quark-antiquark potential $V(r)$. From fundamental considerations of the reflection positivity of correlation functions,²⁸ it was proved that this potential must obey

$$V' > 0 \quad \text{and} \quad V'' \leq 0, \quad (5.1)$$

which means that V is always rising and has a curvature that is at most linear. The bluntest evidence for a linearly rising potential, i.e. $V(r) \propto r$ comes from numerical simulations on the lattice, with and without dynamical fermions.^{28,142} Besides, phenomenological models, e.g. for the charmonium,^{143,144} use with success the so-called Cornell potential

$$V(r) = c + \frac{\gamma}{r} + \sigma r. \quad (5.2)$$

The Coulomb-like term in (5.2), known as Lüscher's term, is expected from perturbative theory²⁴ at short distances. In fact, it is a universal constant derived from a large class of quantum string effective models,¹⁴⁵ assuming the value $\gamma = -\pi/12$ in four dimensional theory, which is a strong theoretical requirement for confinement models (see Section 5.3).

The constant c is a self-energy term that could be set, for instance, to twice the energy of the lightest quark or, more conveniently, to zero.²⁴

In the framework of lattice gauge theory it is possible to relate the Wilson loop to this static potential in a specific limit. For this, we write the Wilson loop defined in Section 4.1.3 distinguishing link variables in (Euclidean) time direction from the spatial ones, i.e.

$$\mathcal{W}(|\mathbf{x} - \mathbf{y}|, t) = \text{Tr} S(\mathbf{x}, \mathbf{y}, t) T(\mathbf{y}, t)^\dagger S(\mathbf{x}, \mathbf{y}, 0)^\dagger T(\mathbf{x}, t), \quad (5.3)$$

where $S(\mathbf{x}, \mathbf{y}, t)$ is an ordered spatial chain of links connecting $\mathbf{x}$ and $\mathbf{y}$ at a fixed time t and $T(\mathbf{y}, t)$ is a temporal line composed of $n_t = t/a$ links at the fixed spatial position $\mathbf{y}$. More precisely,

$$S(\mathbf{x}, \mathbf{y}, t) = \prod_{i \in \mathcal{C}_{x,y}} U^{(i)}, \quad T(\mathbf{y}, n_t) = \prod_{j=0}^{n_t-1} U_4(\mathbf{y}, ja). \quad (5.4)$$

where $\mathcal{C}_{x,y}$ is a spatial path from $\mathbf{x}$ to $\mathbf{y}$.

Recalling that the Wilson loop is a gauge-invariant object, we can use a convenient gauge to relate it to the static potential. In temporal gauge, all links in the time direction are fixed to unity, i.e. $U_4(\cdot) = \mathbb{1}$. In this case, the Wilson loop is expressed as

$$\langle \mathcal{W}(|\mathbf{x} - \mathbf{y}|, t) \rangle = \langle \text{Tr} [S(\mathbf{x}, \mathbf{y}, t) S(\mathbf{x}, \mathbf{y}, 0)^\dagger] \rangle, \quad (5.5)$$

making it clear that the expected value of a Wilson loop is just the correlation function between two spatial lines. If we use the Hamiltonian version of the theory, we can then show

Figure 5.1 – Scheme of a Wilson loop according to (5.3).

Source: By the author.

$$\begin{aligned} \langle \mathcal{W}(|\mathbf{x} - \mathbf{y}|, t) \rangle &= \langle S_{ab}(\mathbf{x}, \mathbf{y}, n_t) S_{ba}(\mathbf{x}, \mathbf{y}, 0)^\dagger \rangle \\ &= \frac{1}{Z} \text{Tr} \left[e^{-a(N_T - n_t)\hat{H}} \hat{S}_{ab}(\mathbf{x}, \mathbf{y}) e^{-an_t\hat{H}} \hat{S}_{ba}(\mathbf{x}, \mathbf{y})^\dagger \right] \\ &= \frac{1}{\text{Tr} [e^{-aN_T\hat{H}}]} \sum_{j,k=0} \langle k | e^{-a(N_T - n_t)\hat{H}} \hat{S}_{ab}(\mathbf{x}, \mathbf{y}) | j \rangle \langle j | e^{-an_t\hat{H}} \hat{S}_{ba}(\mathbf{x}, \mathbf{y})^\dagger | k \rangle \\ &= \frac{1}{\sum_{j=0} e^{-aN_TE_j}} \sum_{j,k=0} \langle k | \hat{S}_{ab}(\mathbf{x}, \mathbf{y}) | j \rangle \langle j | \hat{S}_{ba}^\dagger(\mathbf{x}, \mathbf{y}) | k \rangle e^{-aN_TE_k + an_tE_k} e^{-an_tE_j} \\ &= \frac{\sum_{j,k=0} \langle k | \hat{S}_{ab}(\mathbf{x}, \mathbf{y}) | j \rangle \langle j | \hat{S}_{ba}^\dagger(\mathbf{x}, \mathbf{y}) | k \rangle e^{-aN_T(E_k - E_0) + an_tE_k} e^{-an_tE_j}}{\sum_{j=0} e^{-aN_T(E_j - E_0)}}, \end{aligned} \quad (5.6)$$

where $|j\rangle$ are eigenstates of $\hat{H}$, $S_{ba}(\mathbf{x}, \mathbf{y})$ is a Schrödinger picture operator and N_T is the temporal lattice size. In the limit that $N_T \rightarrow \infty$, only the term $k = 0$ survives

$$\langle \mathcal{W}(|\mathbf{x} - \mathbf{y}|, t) \rangle = \sum_{j=0} e^{-an_t\Delta E_j} \langle 0 | \hat{S}_{ab}(\mathbf{x}, \mathbf{y}) | j \rangle \langle j | \hat{S}_{ba}^\dagger(\mathbf{x}, \mathbf{y}) | 0 \rangle, \quad \Delta E_j = E_j - E_0. \quad (5.7)$$

If $E_0 = 0$ is taken as the energy of the vacuum, and assuming $E_2, E_3, \dots$ are quantum corrections ^A, $E_1 = \Delta E_1$ corresponds to the energy between the color sources located at $\mathbf{x}$ and $\mathbf{y}$, in the limit that they have infinite mass. This shows that the Wilson loop is related to the energy between static (infinite mass) sources at $\mathbf{x}$ and $\mathbf{y}$. Therefore, it is straightforward to obtain the energy between static quark and antiquark in the limit $N_T \gg n_t \gg a$,

$$\langle \mathcal{W}(r, t) \rangle \approx C_0 e^{-a n_t V(r)} \Rightarrow aV(r) \approx \log \left[\frac{\langle \mathcal{W}(r, t) \rangle}{\langle \mathcal{W}(r, t+a) \rangle} \right], \quad (5.8)$$

or even

$$aV(r) \rightarrow -\frac{1}{n_t} \log \langle \mathcal{W}(r, t) \rangle + cst. \quad (5.9)$$

A more satisfactory explanation for this relation involves the introduction of the quark path integral. The idea is that heavy quark propagators, directly related to the static potential, are reduced, using the hopping expansion,¹¹⁸ to chains of link variables whose expected values are Wilson loops.

We can use (5.8) together with the result (4.31) to estimate the asymptotic value for the static quark-antiquark potential in the strong-coupling limit, i.e.,

$$aV(r) \rightarrow \log \left[\left(\frac{\beta}{2N_c^2} \right)^{n_r n_t} \left(\frac{\beta}{2N_c^2} \right)^{-n_r(n_t+1)} \right] = -n_r \log \left(\frac{\beta}{2N_c^2} \right), \quad (5.10)$$

for $SU(N_c > 2)$ and, according to (4.32),

$$aV(r) \rightarrow -n_r \log \left(\frac{\beta}{4} \right) \quad (5.11)$$

for $SU(2)$ theory.

Notice that, in physical units, the potential extracted from the Wilson loop is

$$V(r) \rightarrow -a^{-2} \log \left(\frac{\beta}{4} \right) r = \sigma r, \quad (5.12)$$

where we recognize the coefficient of the linear term in (5.2) in the strong-coupling limit, namely, for $SU(2)$, $\sigma = -a^{-2} \log \beta/4$.

5.1.2 Regge Trajectories

A peculiar behavior is present when we look at how the spins of hadrons are distributed according to their squared mass. More specifically, they tend to fall on linear curves called *Regge trajectories*.^{28,146} We can qualitatively understand them using the (relativistic) spinning stick model. In that model, we imagine two quarks (a meson) to be

^A More specifically, these corrections correspond to excited states of the color flux tube formed between the sources (see next subsection).

effectively bound by a rigid rod.^{28,147} The rod is allowed to relativistically rotate and its angular momentum along a fixed axis will be

$$J = \sigma \int_{-L/2}^{L/2} \gamma(v) r v dr, \quad (5.13)$$

where σ is the linear density of energy (mass) uniformly distributed along the stick and $\gamma(v) = (1 - v^2/c^2)^{-1/2}$ is the relativistic parameter. Considering the rod's ends to be at or approximately at the velocity of light c , we can state

$$\frac{L/2}{r} = \frac{c}{v}, \quad (5.14)$$

which yields

$$J = \sigma \int_{-L/2}^{L/2} \frac{r dr}{\sqrt{1 - (2r/L)^2}} \frac{2rc}{L} = \frac{4c}{L} \int_0^{L/2} \frac{r^2 dr}{\sqrt{1 - 4r^2/L^2}} = \frac{\pi\sigma L^2}{8} c. \quad (5.15)$$

On the other hand, the mass of the rod will be

$$M = \sigma \int_{-L/2}^{L/2} \gamma(v) dr = \sigma \int_0^{L/2} \frac{dr}{\sqrt{1 - 4r^2/L^2}} = \frac{\pi\sigma L}{2}. \quad (5.16)$$

Gathering both results leads to

$$M^2 = \frac{\pi^2 \sigma^2 L^2}{4} = \frac{2\pi\sigma J}{c} \equiv \frac{J}{\alpha}. \quad (5.17)$$

Figure 5.2 – Regge trajectories.

Source: By the author.

The last equation gives a classical qualitative explanation to Regge trajectories. In Figure 5.2 we see the linear relation between J and M^2 estimated by Equation (5.17). The Regge slope in natural units is estimated from the data as being

$$\alpha = \frac{1}{2\pi\sigma} \approx 0.9 \text{ GeV}^{-2}, \quad (5.18)$$

and $\sqrt{\sigma} = 429(2) \text{ MeV}$ for the most linear trajectory ($\rho - a$).²⁸ Conventionally, the so-called *string tension* is fixed at

$$\sigma = (440 \text{ MeV})^2. \quad (5.19)$$

Of course, this is a simplified and effective picture of what happens inside a meson. We should ask ourselves how this stick behavior can be derived from a fundamental theory, i.e., from QCD. One of the ideas consistently explored since the 1970s is that of *flux-tube* formation. This dates back from simplified string^{148,149} and dual superconductor models.^{34,35} In these, the concept of flux tube reflects a picture

of confinement in hadronic interactions where color-electric field lines are concentrated inside a cylindrical object with linear energy density equal to σ , which is consistent with the linearly rising potential. A natural extension of the stick model would be to allow the string to vibrate in transversal directions, which leads to the subject of (bosonic) string theory. In fact, numerical studies with bosonic strings support this picture.¹⁵⁰ Regarding the *dual superconductor* models,^{34,35} in these the QCD vacuum is considered as a type-II superconductor with the roles of electric and magnetic fields interchanged. Therefore, the color-electric charges, or quarks, would be confined through the formation of color-electric *Nielsen-Olesen vortices* through the Meissner effect, which gives rise to the flux tube and the linear potential between them.³⁷ This mechanism, in duality to the regular superconductivity, consists in the condensation of color-magnetic degrees of freedom. Despite its physical appeal, the dual-superconductor approach to confinement is essentially of an Abelian nature, which almost forces one to fix the gauge and single out an Abelian subgroup. That makes it hard to believe that all the richness of confinement could be explained solely in this way.

5.2 Color Confinement in Landau Gauge

Usually when we talk about confinement in the context of Green function approaches, what we are really referring to is *color confinement*. In this case, the main goal is to demonstrate how only color-singlet states manage to appear in experiments and *why* that happens given a fundamental theory, namely QCD. In other words, how and why all observed particles are *color neutral* ^B.

5.2.1 Kugo-Ojima

The criterion

Using the philosophy of color neutrality, the Kugo-Ojima confinement scenario in the context of Landau gauge and BRST symmetry^{112,114,151} aims at giving a sufficient criterion so that the *global* color charge Q^a , given in Euclidean space by

$$Q^a = \int d^3\mathbf{x} \partial_i F_{0i}^a + \{Q_{\text{BRST}}, D_0^{ab} \bar{c}^b\}, \quad (5.20)$$

vanishes for all possibly observed states. We must keep in mind from the beginning that this scenario originally does not take into account Gribov copies or any legitimate non-perturbative effects. In fact, the starting point is the Faddeev-Popov and scattering formalism in *Minkowski space*. Furthermore, the existence of a well-defined BRST charge is *assumed* from the beginning. For these reasons, we emphasize that the following Kugo-Ojima analysis cannot be readily applied to the Gribov-Zwanziger action because, besides

^B In Section 5.3 we will see that the definition of what is confinement itself is a potential problem and it is not really settled.

being formulated in Euclidean space, the restriction to the Gribov region breaks BRST (see Section 3.5).

Using the canonical formalism and the nilpotency of the BRST operator defined in Section 3.5, Kugo and Ojima were able to demonstrate that *localized* physical states in QCD are colorless,

$$\langle \Psi_{\text{phys}} | Q^a | \Psi_{\text{phys}} \rangle = 0, \quad (5.21)$$

given that the global color symmetry is *unbroken*^{114 C}. In principle, this reasoning could be valid also for QED, but the localization restriction is not satisfied by the electromagnetic interaction, which is long-ranged. This is a good check because the validity of the theorem for QED would yield a confined electric charge and we certainly do not observe this.

Using the quartet mechanism for the asymptotic fields of colored states, Kugo and Ojima developed a criterion so that the above situation is realized in a possible solution of QCD.^{114,152} The criterion is composed of the two following parts:

- $u(0) = -1$
- Global color symmetry is unbroken

In the first one we have the quantity $u(p^2)$ implicitly defined by²²

$$\int d^4x e^{ipx} \langle D_\mu^{ac} c^c(x) D_\nu^{bd} \bar{c}^d(0) \rangle_{\text{FP}} = \delta^{ab} \left[\left(\delta_{\mu\nu} - \frac{p_\mu p_\nu}{p^2} \right) u(p^2) - \frac{p_\mu p_\nu}{p^2} \right] \quad (5.22)$$

in Euclidean terms, where FP stands for the expected value using the Faddeev-Popov action. This is essentially a condition for the color charge (5.20) to be well-defined. The second condition is usually assumed to be true.¹¹⁴

Furthermore, the Kugo-Ojima criterion implies particular infrared behaviors for the propagators. Firstly, in order for the color charge (5.20) to be well defined, the first term, related to the gluon propagator, must have no massless poles. This supports a *suppressed* gluon propagator at zero momentum, but not necessarily vanishing.^{114,153} Secondly, in Ref. 152 it was shown that the ghost propagator has an *enhanced* form, which can be written as

$$G(p^2) \propto \frac{1}{p^2} \frac{1}{[1 + u(p^2) + w(p^2)]}. \quad (5.23)$$

where u is given in (5.22), so that the assumption $w(p^2) = 0$ connects this behavior to the Kugo-Ojima criterion.²²

^C Here the word “unbroken” means that the global symmetry is not spontaneously broken, see Section 5.3.

Kugo-Ojima and Gribov-Zwanziger

As stressed above and in Section 3.5, the Kugo-Ojima confinement criterion uses the canonical formalism deduced from the Faddeev-Popov action, which implicitly is to say that it does not take into account Gribov copies and the Gribov-Zwanziger scenario. Furthermore, it is fundamental to notice that the Kugo-Ojima approach assumes a well-defined BRST charge, which is not immediately true for non-perturbative approaches. In fact, in Section 3.5 we saw that the Gribov-Zwanziger action breaks BRST symmetry, making a consistent link between both approaches unfeasible.

Even though there are problems with the original Kugo-Ojima framework, it is interesting to point out that the latter and the Gribov-Zwanziger scenario have a subtle connection. If the confinement criterion $u(0) = -1$, which originally was *deduced* from the Faddeev-Popov theory with BRST symmetry, is imposed from the beginning on the Faddeev-Popov path integral as a boundary condition, we obtain the Gribov-Zwanziger action without BRST symmetry.^{107,108} In this strict sense, we could say that both approaches are equivalent, at least when $u(0) = -1$ is used as a boundary condition on the original Faddeev-Popov theory. Nevertheless, the relation between Kugo-Ojima criterion and color confinement is unclear, since the latter is expected to be inherently explained by non-perturbative effects, which are not explicitly contemplated in the seminal paper.¹¹⁴

5.2.2 Zwanziger criterion

We saw in Chapter 3 that the Gribov-Zwanziger scenario predicts specific behaviors for the gluon and ghost propagators of Yang-Mills theories. First, Gribov's semi-classical computation entailed a vanishing gluon propagator and an enhanced ghost propagator at vanishing momentum transfer, as derived in Section 3.3. Then, Zwanziger extended Gribov's idea to the local and renormalizable Gribov-Zwanziger action, where the so-called horizon condition implies the same behaviors for the propagators on the infrared.^{99,106}

In the 1990s, Zwanziger derived very strict bounds for the free energy on a lattice gauge theory that can be used to relate color confinement to the infrared behavior of the gluon propagator. The free energy W is defined, using continuum notation for convenience, by

$$e^{W[J]} = \int_{\Omega} \mathfrak{D}A \, \rho(A) e^{\int d^4x J_{\mu}^a A_{\mu}^a} = \left\langle e^{J \cdot A} \right\rangle_{\Omega}, \quad (5.24)$$

where integration is limited to the first Gribov region Ω and the gauge copies are weighted with a probability distribution $\rho(A) \geq 0$, which is dependent on the gauge-fixing algorithm (see Section 4.2). Supposing a Euclidean lattice system in the scaling region and with finite volume V , Zwanziger rigorously showed that the free-energy density $w = W/V$ is bounded by a term proportional to the momentum of the external field, which implies

that the color-magnetization under the external field is suppressed in the infrared region,

$$\lim_{k \rightarrow 0} m = 0, \quad (5.25)$$

no matter how strong J is.

To make the discussion a bit more concrete, we write the external source for a particular Fourier mode modulated by a color-magnetic external field h along the directions e_μ^a

$$J_\mu^a(x) = H_\mu^a \cos(kx_1) = h \cos(kx_1) e_\mu^a, \quad (5.26)$$

where k is chosen to be aligned with x_1 , and the free energy becomes

$$e^{W(J)} = \langle e^{\cos(kx_1)H \cdot A} \rangle \equiv e^{W_k(H)}. \quad (5.27)$$

The first bound obtained for the free energy^{97,154} and a stricter one,^{22,155} are

$$\frac{W_k(H; k)}{V} = w_k(H) \leq 2^{-1/2} k \operatorname{Tr} \sqrt{H^a H^a} \leq (2D)^{1/2} k |H|, \quad (5.28)$$

valid in the infinite-volume limit and d dimensions. They imply

$$\lim_{k \rightarrow 0} w_k(h) = 0 \quad (5.29)$$

and also that the color-magnetization $m_k(h) = \frac{\partial w_k(h)}{\partial h}$ obeys²²

$$\lim_{k \rightarrow 0} m_k(h) = 0, \quad (5.30)$$

meaning that the system of color spins does not respond to the external color field, which should characterize color confinement.

Notice that the gluon propagator can be written as a double derivative of w_k at $h = 0$

$$2 \frac{\partial^2 w_k}{\partial H_\mu^a \partial H_\nu^b} \Big|_{h=0} = V^{-1} \langle A_\mu^a(k) A_\nu^b(-k) \rangle_\Omega = \delta^{ab} \delta_{\mu\nu} D(k), \quad (5.31)$$

which essentially is a color-magnetic susceptibility at vanishing external field. The bounds (5.28) entail that the gluon propagator in Coulomb and Landau gauges, as all derivatives of the free energy, should vanish at zero momentum, i.e. $D(0) = 0$, which is the result predicted by the continuum Gribov-Zwanziger scenario (see Section 3.3). This result was obtained in Refs. 97, 154 by supposing that the free energy is analytic in H at $k = 0$. If this assumption is relaxed and the free energy is allowed to have non-analytic behavior, then the gluon propagator can assume a finite value at $k = 0$, i.e., $D(0) \neq 0$. In Refs. 22, 156 models were presented in which the gluon propagator can have a finite value at the deep infrared. As we will see in Section 5.2.4, the consideration of non-analyticity of the free energy was proposed after confrontation with lattice simulations indicating that $D(0) \neq 0$ in 3 and 4 dimensions.

idea of *infrared slavery*^D. In this case, the truncations in Landau gauge neglected all ghost contributions. By that time it was believed that the gluon propagator was solely responsible for the area law leading to the static quark-antiquark potential, which is consistent with a naive, i.e. up to some regularization, Fourier transform of a linear potential.^{82,153}

In the late 1990s, the study of infrared exponents through Dyson-Schwinger equations indicated that the role of ghosts in the infrared was much more important than anticipated in early studies,³⁰ a prediction in agreement with the Gribov-Zwanziger scenario¹⁰⁶ and the Kugo-Ojima criterion.¹⁵² In this case, the ghost contribution was not neglected in the truncations and, followed by many other refined analysis in the infrared limit, led to the so-called *scaling* solution of the Dyson-Schwinger equations for $d = 2, 3$ and 4 dimensions. This is expressed by the asymptotic formulas

$$D(p) \sim p^{-2\kappa_{gluon}-2} \quad \text{and} \quad G(p) \sim p^{-2\kappa_{ghost}-2}, \quad (5.35)$$

for $p \rightarrow 0$. The scaling solution entails a relation between the infrared exponents

$$\kappa_{gluon} = -2\kappa_{ghost} + \frac{d-4}{2} \quad (5.36)$$

for $d = 2, 3$ and 4.¹⁶² The results for $d = 4$ are given by $D(p) \sim p^{4\kappa-2}$ and $G(p) \sim p^{-2\kappa-2}$, with $\kappa_{gluon} = -2\kappa_{ghost} \equiv -2\kappa$. For $\kappa > 0.5$, this represents an *enhanced ghost* propagator and a *vanishing gluon* propagator, being $\kappa \approx 0.595$ the most accepted value in the four-dimensional case.^{157,158,162} Additionally, the scaling solution also predicts finite behavior for the ghost-gluon vertex, besides infinite behavior for the three-gluon and four-gluon vertices at vanishing momentum.^{162,163} Furthermore, one should note that the scaling solution is *unique*, which means that no other solution with a scaling behavior is admitted.¹⁶⁴

Albeit the large support from Kugo-Ojima and Gribov-Zwanziger approaches, there is an alternative solution to the Dyson-Schwinger equations which does not have a scaling character. This is the *decoupling* or *massive* solution, where κ_{gluon} and κ_{ghost} are not tied to each other as in (5.36) for dimensions $d = 3, 4$.^{31,165,166} The decoupling solutions predict

$$\kappa_{gluon} = -1 \quad \text{and} \quad \kappa_{ghost} = 0, \quad (5.37)$$

i.e., a finite gluon propagator and an essentially free ghost propagator at vanishing momentum^E. They also entail a finite value for the ghost-gluon vertex.¹⁶⁷ In fact, the decoupling solutions form a one-parameter family of solutions,^{168,169} where the value of

^D The theoretical proposal in which confinement would be accounted for by infrared divergencies in QCD.⁸³

^E It is common in the literature to study the *dressing function* of the ghost propagator defined by $p^2 G(p)$, which measures its deviation from a free ghost. In this notation, an enhanced ghost propagator would correspond to a divergent dressing function ($\kappa_{ghost} > 0$) and a free ghost propagator to a finite dressing function ($\kappa_{gluon} = 0$).

the ghost propagator at zero momentum can be viewed as a boundary condition of the equations.

In this framework, it is not very clear how and if Gribov copies are accounted for. Zwanziger¹⁵⁷ showed that the Gribov horizons can be viewed as *nodal* surfaces in the region of integration (5.33). If this integration is somehow limited by this surface, e.g. by an appropriate boundary condition,¹⁵⁸ then the computation will correspond to the Gribov gauge fixing. However, after writing the corresponding differential equations, the dependence on any region of integration disappears and it comes into question if a solution obtained by this approach is indeed taking only the first Gribov region into account.

We should mention another functional method that uses a non-perturbative flow equation for the effective action, many times used in conjunction to the Dyson-Schwinger equations. This is the so-called *functional* (or exact) *renormalization group* approach and it is very close in spirit to the Dyson-Schwinger equations. In practice, one has a system of coupled equations for all Green functions involving dressed (full) vertices and propagators, which then must be appropriately truncated and solved. The aforementioned scaling solution is consistent with this approach.³² Nevertheless, the one-parameter family of decoupling solutions is also found as a possible solution in the framework of the functional renormalization group.¹⁶⁹

5.2.4 Lattice results

In the search for an explanation of color confinement, lattice simulations have been used almost as a semi-experimental reference to test continuum results. The first simulation of the gluon propagator dates back from 1985¹⁷⁰ when indications were presented against the $1/k^4$ infrared behavior¹⁵⁹ for the $SU(3)$ theory in Landau gauge. Through the 1990s, computational power progressively increased and larger and finer lattices started to be simulated using $SU(2)$ and $SU(3)$ symmetries, yielding more conclusive results favoring the suppression of the infrared gluon propagator for $D = 3, 4$.^{129,171–173} By that time, at least in the strong-coupling regime, it seemed possible for the gluon to vanish at $p = 0$, but this was very uncertain. Again for $SU(3)$ and $SU(2)$, computations of the lattice ghost propagator started somewhat later for $D = 3, 4$ ^{123,126,174,175} using numerical inversions of the Faddeev-Popov matrix (see Section 6.3). The general trend indicated an enhanced infrared behavior for the ghost propagator. Nevertheless, extracting the deep infrared behavior on a relatively small lattice yields results not reliable enough to make quantitative predictions of infrared exponents. Therefore, larger lattices and a careful analysis of finite volume effects were necessary to make an extrapolation to the infinite-volume limit, which is strictly important for computations at vanishing momentum.

Up to this time, computations were performed using linear lattice sizes of no more

than $L \sim 6$ fm for $D = 4$ and $L \sim 11$ fm for $D = 3$ in $SU(2)$ ^{126,173 F}, corresponding to a minimum lattice momentum of $p_{min} \sim 250$ MeV and $p_{min} \sim 110$ MeV, respectively. Furthermore, a study using a lattice linear size of $L \sim 25$ fm ($p_{min} \sim 50$ MeV)¹⁷⁸ was able to satisfactorily determine a *turnover* momentum^G as $p_{to} \sim 350$ MeV for $D = 3$ in $SU(2)$, but even with such a physical volume the infrared exponents could not be fitted without ambiguity. Moreover, a lattice size of ~ 10 fm was unable to detect a decreasing behavior for the gluon propagator for the $D = 4$ - $SU(2)$ case.¹⁷⁹ Those works were followed by the first computation of $D = 2$ - $SU(2)$ propagators using huge lattices of $L \sim 43$ fm,¹⁸⁰ strongly supporting vanishing gluon and enhanced ghost propagators at the infrared region after a careful infinite-volume extrapolation. At the same time, analytical results from Dyson-Schwinger equations on a four-dimensional compact manifold (4-torus)¹⁸¹ predicted that the onset of infrared effects should take place at $L \sim 10 - 15$ fm and only at 40 fm would the infinite-volume limit be properly evaluated. Those endeavors motivated the implementation of huge lattices at higher dimensions.

Huge-lattice studies appeared almost simultaneously²⁹ for $D = 4$ in both $SU(2)$ and $SU(3)$, and $D = 3$ in $SU(2)$, with lattice sides of ~ 27 fm,¹⁸² $\sim 13, 16, 19$ fm^{183–185} and ~ 85 fm,¹⁸² respectively. These simulations immediately ruled out the scaling solution predicted by Dyson-Schwinger equations and supported the decoupling-type solution (see Section 5.2.3). Furthermore, a new study of $D = 2$ - $SU(2)$ theory at a ~ 70 fm lattice side^{186,187} confirmed that in this case the scaling solution is supported by the lattice.¹⁸⁰

Of course, lattice computations in the Landau gauge also suffer from the Gribov problem because the compact gauge orbits contain a large number of copies corresponding to different local minima of the minimizing functional $\mathcal{E}$ defined in (4.34). In Section 4.2, a number of ways were presented to numerically select those minima from $\mathcal{E}$ that fixes a given lattice configuration to a *minimal* Landau gauge. What copies are selected depends on each algorithm used and until now there is no satisfactory procedure to compute the global minimum of a given orbit on the lattice. Nevertheless, the bias introduced by the arbitrary selection of minima is translated into a *Gribov noise* in the order of the statistical errors in early simulations.^{123,124,188} These were thought to be unimportant, but since then various computations related different sets of minima to different behaviors for the propagators in the infinite-volume limit, which could call into question the validity of lattice results.^{189,190} Until now no qualitative change was verified and the lattice still supports a massive behavior of Yang-Mills theories.

Another important result from the lattice is the confirmation that the gluon degree of freedom violates the reflection positivity axiom of quantum field theory in Euclidean space,^{191,192} which is a strong indication of confinement.¹⁵³ Finally, we should also stress

^F Even smaller sizes were used for the $SU(3)$ theory.^{176,177}

^G The value p_{to} of momentum where the gluon propagator starts to decrease for decreasing p .

that post-2007 lattice results are in qualitative agreement with the so-called refined Gribov-Zwanziger action¹⁰⁹ (also see Section 3.4). There, neither is the gluon propagator null nor is the ghost propagator enhanced at vanishing momentum, but instead they attain a finite value and act as a free field, respectively, supporting the massive or decoupling picture for confinement. Lastly, the gluon propagator in the refined version also violates reflection positivity.

5.3 Center Dominance

We return now to the general discussion of confinement in QCD. Beginning with Cornwall,³³ Mandelstam³⁴ and 't Hooft³⁵ in the 1970s, a configuration-based approach to confinement was introduced. This means that some specific classes of gauge configurations, as the center vortex or the Abelian monopole, would dominate the QCD's path integral and be responsible for confinement,^{37,193,194} an endeavor that gained considerable momentum in the 1990s with lattice simulations.³⁶

5.3.1 Confinement and Color Screening

Configuration-based approaches generally assume that confinement is connected to a specific phase in the coupling-constant space. In a gauge theory, more specifically in lattice gauge theory, it is possible to characterize different phases corresponding to different behaviors of large rectangular Wilson loops. In the massive and massless phases, the Wilson loop falls off with a perimeter law, while in the *magnetic disorder* phase it obeys an area law. One can think of order-disorder transitions in an Ising model as an intuitive guide for what happens in the magnetic disorder phase. There, we have an order parameter, the magnetization, that vanishes for sufficiently high temperatures (disordered) and, conversely, attains a non-vanishing value for low temperatures (ordered), given that a certain global symmetry is spontaneously broken. In gauge theories, the “magnetic” degrees of freedom just refer to their analogues in electromagnetism.

Going back to the Wilson loop, its area-law decay implies an asymptotically linear static quark-antiquark potential, as in Section 5.1.1. Magnetic disorder just means that large Wilson loops are uncorrelated and can be expressed by a larger one involving them (see Figure 4.5), in similarity to Stokes' theorem. In Sections 4.1.5 and 5.1.1 we did exactly that, but only in the strong-coupling regime $\beta \rightarrow 0$, i.e., $g \rightarrow \infty$. Of course this does not mean that when we go to higher values of β the area law will still hold. In fact, this is always true for two-dimensional non-Abelian theories, and for higher dimensions this is not necessarily verified^H. Finally, the point is that in non-Abelian theories there should exist an *order parameter* that indicates if the theory is in a magnetic disorder (confinement)

^H An Abelian example where an area law is not verified at small couplings is QED, where we definitely do not predict a linear potential in an electron-positron pair.

phase or not.¹⁹⁵ However, this is not really guaranteed and waits for further theoretical clarification.

By Elitzur's theorem,¹⁹⁶ we know that a *local gauge symmetry cannot break spontaneously*, meaning that gauge non-invariant local quantities must vanish. Therefore, a satisfactory order parameter in gauge theories should be a gauge-invariant quantity that indicates magnetic disorder. Before looking for an order parameter, we should notice some properties of confinement in gauge theories in the presence of massive fields.

The first problem of dealing with confinement in real QCD is connected with the quark-antiquark pair creation that happens when we try to separate the components of, say, a meson. This is known as *string breaking* and it refers to what happens to the conjectured flux tube when sufficiently stretched to the point of storing enough energy for creating a pair, namely $\sim 2m_q$. Consequently, we never really have an ever linearly rising quark-antiquark potential. Instead, at large distances it reaches a plateau where more and more pairs pop out from the QCD vacuum. String breaking is then a kind of screening effect that prevents us from directly relating confinement to a linear potential, at least in the full theory. Therefore, we consider that confinement should be a property of pure gauge vacuum.

Another obstacle, strongly advocated by Greensite,³⁷ is that it is quite hard if not impossible to distinguish between Higgs-like and confinement-like phases in a gauge-Higgs theory. The argumentation is based on the works by Osterwalder and Seiler⁷³ and Fradkin and Shenker.¹⁹⁷ To understand it, take an $SU(2)$ gauge-Higgs theory given by the action

$$S[\phi, U] = \frac{\beta}{2} \sum_{x \in \Lambda, \mu > \nu} \text{Tr} \left[\mathbb{1} - U_\mu(x) U_\nu(x + \hat{\mu}) U_\mu^\dagger(x + \hat{\nu}) U_\nu^\dagger(y) \right] + \frac{\gamma}{2} \sum_{x \in \Lambda, \mu} \text{Tr} \left[\phi^\dagger(x) U_\mu(x) \phi(x + \hat{\mu}) \right], \quad (5.38)$$

where the first term is just the Wilson action 4.16 and the second one couples the lattice gauge field to a massive scalar Higgs field in the fundamental representation. In such a theory, the $\gamma \ll 1$ regime corresponds to the usual QCD with flux-tube formation and string breaking, while $\gamma \gg 1$ is just as a weak-like theory with color screening. What the works in Refs. 73, 197 show is that one can always choose a path in the (β, γ) space where gauge-invariant quantities and Green functions evolve analytically from one phase to another, without any kind of characteristic transition. In other words, there is no abrupt jump from the spectrum of QCD to a Higgs-like spectrum: both are very alike from the

Figure 5.3 – Scheme of flux tube and string breaking.

Source: By the author.

color-confinement point of view.³⁷ In the gauge-Higgs theory, massive scalars are created near a source of color charge and generate color singlets through a flux tube when in the confinement phase, while in the Higgs phase they also generate color singlets but through a screening mechanism in resemblance to vacuum polarization. From a conceptual perspective, *color confinement* misses an important part of the confinement characterized by the Regge trajectories in the hadron spectrum.

Figure 5.4 – Color confinement in a gauge-Higgs theory.

Source: GREENSITE.¹⁹⁴

Given the above discussion, what order parameter could satisfactorily distinguish confinement (magnetic disorder) from other phases in a Higgs-like theory? Moreover, does it correspond to an unbroken phase of some global symmetry? Related to the Green-function approaches to confinement, we have the Kugo-Ojima criterion discussed in Section 5.2.1 and also the Coulomb confinement criterion.¹⁹⁸ The former considers the theory fixed to the Landau gauge, and the confined phase is related to the unbroken realization of a global symmetry remnant from Landau gauge fixing, besides the global color one. In the latter, the characterization of confinement

is given by the unbroken realization of the remnant symmetry from Coulomb gauge fixing. The problem with both symmetries is that their order parameters, respectively the spatial average of the Higgs field and the spatial average of time-like links on a given time slice, indicate that the respective symmetries break at different points on the (β, γ) space, which is somewhat inconsistent.³⁷

A gauge-invariant quantity we just mentioned that indicates a magnetic disorder phase through an area-law decay is the Wilson loop²³

$$\langle \mathcal{W}(C) \rangle = \begin{cases} e^{-\sigma A_C}, & \text{confined phase} \\ e^{-\sigma P_C}, & \text{unconfined phase} \end{cases}, \quad (5.39)$$

where $\langle \mathcal{W}(C) \rangle$ is defined in (4.13). The problem is that in a gauge-Higgs theory as (5.38) we have a perimeter law everywhere, except along the line $\gamma = 0$. Another issue is that of string breaking, i.e., the presence of matter fields that can mask the confining behavior at large distances. We see that a complete account of confinement in this approach must deal with string breaking and the similarity between different phases in a gauge-Higgs theory. We will now discuss the best candidate for a unbroken global symmetry that can characterize confinement in a given theory.

5.3.2 N -ality and Center Symmetry

The first consideration we must make to characterize confinement is to effectively eliminate string breaking from the theories we are considering. The obvious move is to let all the field masses go to infinity, so that pair production is suppressed. However, only fields in specific color representations can attach to color sources and give rise to string breaking. Suppose an $SU(2)$ gauge theory with color sources in the fundamental representation, namely **2**. If there are massive fields in the adjoint color representation **3**, a simple Young-tableau calculation yields

$$\mathbf{2} \otimes \mathbf{3} = \mathbf{2} \oplus \mathbf{4}, \quad (5.40)$$

therefore no color-singlet states in the **1** representation are possible and string breaking cannot occur. Conversely, if we have massive fields in the fundamental representation, as in the gauge-Higgs theory (5.38), string breaking is possible and we must send this field mass to infinity before verifying magnetic disorder. The latter is what happens with quarks and antiquarks in QCD but for $SU(3)$ color symmetry, i.e., quarks in the fundamental representation **3** can combine with antiquarks in the conjugate representation $\mathbf{3}^*$,

$$\mathbf{3} \otimes \mathbf{3}^* = \mathbf{1} \oplus \mathbf{8}, \quad (5.41)$$

and form a color-singlet.

There is a property of $SU(N_c)$ group representations that characterizes the possibility of string breaking between massive fields in Yang-Mills theory, which is called N -ality. The N -ality of a $SU(N_c)$ group representation is defined as the number of boxes in the corresponding Young tableau modulo N . For instance, the adjoint representation of $SU(2)$ ($\square \square$) has N -ality $k = 0$, while the fundamental representation ($\square$) has $k = 1$. If we suppose that our color sources *always* have non-zero N -ality, then it is sufficient to freeze out only the massive fields that have non-zero N -ality in order to rule out string breaking. This is true because zero N -ality fields cannot glue to a non-zero N -ality field to compose a state with vanishing N -ality characteristic of a color-singlet representation. Therefore, it is not necessary to remove zero N -ality fields from the theory. We can then say, according to Ref. 37, that *confinement is characterized by a linearly rising potential between non-zero N -ality color sources in the limit that the masses of all non-zero N -ality fields go to infinity.*

The N -ality of an $SU(N_c)$ group representation is associated to the representation of a subgroup called *center*. The center of a group is the set of its elements that commute with all other group elements. Therefore, the center of $SU(N_c)$ contains all elements proportional to the identity, i.e., it is the subgroup Z_{N_c} ¹. While there are infinite representations of

¹ For example, we have $Z_2 = \{1, -1\}$ and $Z_3 = \{1, 1e^{2i\pi/3}, 1e^{4i\pi/3}\}$.

$SU(N_c)$, its center only admits N_c possible representations. All $SU(N_c)$ representations with the same Z_{N_c} representation possess the same N -ality, i.e., the same label $k = 0, \dots, N_c - 1$.

Hopefully, the unbroken realization of the symmetry associated to center transformations, namely a *global center symmetry*, implies the magnetic disorder phase of gauge theories. For an element $\mathfrak{g} \in SU(2)$, the action of a center element $\mathfrak{z} \in Z_{N_c}$ in a representation R is given by

$$R[\mathfrak{z} \mathfrak{g}] = \mathfrak{z}^k R[\mathfrak{g}]. \quad (5.42)$$

If we take the center transformation

$$U_4(\mathbf{x}, t_4) \rightarrow \mathfrak{z} U_4(\mathbf{x}, t_4) \quad (5.43)$$

defined over time-like links on a lattice time slice $t = t_4$, we can easily show that the Wilson action is necessarily invariant and then the theory has a global center symmetry^J. However, when we couple the gauge field to a Higgs field in a representation with $k \neq 0$, just as in (5.38), we have

$$R[\phi^\dagger(\mathbf{x}, t_4) U_4(\mathbf{x}, t_4) \phi(\mathbf{x}, t_4)] \rightarrow \mathfrak{z}^k R[\phi^\dagger(\mathbf{x}, t_4) U_4(\mathbf{x}, t_4) \phi(\mathbf{x}, t_4)], \quad (5.44)$$

and center symmetry is explicitly broken. As we have seen for the fundamental-representation Higgs field, when the N -ality is non-vanishing string breaking occurs and we only have a magnetic disorder phase under some energy scale. Thus, we must have an unbroken center symmetry in order to properly observe confinement. Moreover, the global center symmetry cannot be a trivial one or be spontaneously broken by some adjoint-representation field or high-temperature conditions³⁷ in order for a magnetic disorder phase to exist.

Therefore, we can consider order parameters that can assess the unbroken realization of the center symmetry. Besides the Wilson loop in a pure gauge theory, there is a dual Wilson loop called 't Hooft loop which exhibits a perimeter law in the disordered phase,

$$\langle \mathcal{B}(\mathcal{C}) \rangle = \begin{cases} e^{-\sigma P_{\mathcal{C}}}, & \text{confined phase} \\ e^{-\sigma A_{\mathcal{C}}}, & \text{unconfined phase} \end{cases}. \quad (5.45)$$

In the canonical formulation, the 't Hooft loop can be viewed as the creation operator of *thin center vortices*. The Polyakov loop parameter defined in (4.14) is not invariant under (5.43),

$$U_4(\mathbf{x}, 0) \dots U_4(\mathbf{x}, t_4) \dots U_4(\mathbf{x}, N_t - 1) \rightarrow \mathfrak{z} U_4(\mathbf{x}, 0) \dots U_4(\mathbf{x}, t_4) \dots U_4(\mathbf{x}, N_t - 1), \quad (5.46)$$

so we can use it as a true order parameter for the global center symmetry phases,

$$\langle \mathcal{P} \rangle \begin{cases} = 0, & \text{unbroken } Z_{N_c} \\ \neq 0, & \text{broken } Z_{N_c} \end{cases}. \quad (5.47)$$

^J Note that in the Wilson action the number of dagger links inside the trace is the same as the ones with no dagger.

It can also be demonstrated that the Polyakov loop is associated to the free energy F of a color source in a lattice gauge theory at finite temperature by $\langle \mathcal{P} \rangle = e^{-N_T F}$,³⁷ which indicates that in the unbroken phase, $\langle \mathcal{P} \rangle = 0$, F diverges as expected in a confinement scenario. Finally, we should mention that there is also the vortex free energy,³⁷ which presents an area-law falloff when the global center symmetry is unbroken.

Given all these order parameters, we can verify if a given system is in a magnetic disorder phase. But the question is *why*? A consistent answer would probably contain an explanation of confinement (and color confinement). According to Ref. 37, any explanation of confinement should also predict, besides a linearly rising quark-antiquark potential,^{28,141} at least three more behaviors supported by theoretical and numerical evidence: Casimir scaling;¹⁹⁹ N -ality dependence;³⁶ string behavior.¹⁴⁵

Figure 5.5 – In 4D, the creation of a thin center vortex, with the effect $U_i \rightarrow \mathfrak{z}_i U_i$, $\mathfrak{z}_i \in Z_{N_c}$, can be associated to the topological linking of the corresponding Wilson loop and the center vortex, which in this case is a surface. They are characterized by the number of times they intertwine: the topologically invariant linking number.³⁷

Source: GREENSITE.³⁷

In particular, the N -ality dependence condition imposes that a pair of supposed adjoint sources should have a vanishing string tension. It is then possible to motivate the introduction of a specific field configuration related to the 't Hooft loop, the center vortex, which can topologically link to Wilson loops and produce an area law that depends on the N -ality of the source representation.²⁰⁰ More specifically, if we take a Wilson loop $\mathcal{W}(\mathcal{C})$ in the fundamental representation ($k = 1$), we can attach (thin) center vortices to it, acting as $U_i \rightarrow \mathfrak{z}_i U_i$, $\mathfrak{z}_i \in Z_{N_c}$ for link variables U_i in the path $\mathcal{C}$. Then, taking the trace (or the group character for arbitrary representations), the Wilson loop is modified as

$$\mathcal{W}(\mathcal{C}) \rightarrow \mathfrak{z}_1^k \mathfrak{z}_2^k \dots \mathcal{W}(\mathcal{C}), \quad (5.48)$$

in view of (5.42). If we decompose the chain of links (a holonomy) into a center-only part $\mathfrak{Z}$ and another one, u , containing the remains,

$$\mathcal{W}(\mathcal{C}) = \mathfrak{Z}^k(\mathcal{C}) u(\mathcal{C}), \quad (5.49)$$

it is possible to show, under certain uncorrelation assumptions, that the area law comes solely from the vortex component $\mathfrak{Z}$ identified in thermalized link configurations.²⁰⁰ Together with strong numerical and model evidence, this yields the so-called center-vortex confinement scenario, which is the statement that center vortices are the configurations responsible for confinement. For this reason, center vortices will be explored in the next chapter in connection with the Gribov-Zwanziger scenario.

6 APPLICATIONS AND RESULTS

Given all the ideas and methods of the last chapters, we now propose to study the ghost sector of $SU(2)$ Yang-Mills theory through lattice methods. Inspired by Ref. 201, we will analyze the relevance of topological configurations, namely center vortices and instanton backgrounds, to confinement in the light of the Gribov-Zwanziger scenario.

We begin by introducing the center projection and vortex removal methods and reviewing milestone results. Secondly, we will comment on continuum and lattice topology aspects and several discretizations of BPST instantons. Finally, we study the lattice ghost propagator and define the necessary tools for analyzing the Gribov region's geometry,²⁰² applying them to the previously introduced configurations and ensembles.

6.1 Center Vortices

The decomposition of lattice gauge configurations in a vortex-only part, which is allegedly “confining”, and a non-confining part, is supported by various numerical simulations.^{203–205} The method is generally called *center projection* and *vortex removal* and in general begins with some center gauge fixing.

There are many ways of performing vortex decomposition on the lattice. For instance, we can use an *indirect maximal center gauge*, where the lattice is fixed to the center gauge after being fixed in the Abelian subgroup of $SU(N_c)$.³⁶ There are also the Laplacian center gauges, which can deal with the Gribov copy problem.³⁷ Here we will implement the most direct and established one, the $SU(2)$ *direct maximal center gauge*.²⁰³

6.1.1 Center Projection

The idea behind direct maximal center gauge is to bring a given $SU(N_c)$ lattice configuration, say $\{U_\mu\}$, as close as possible to an element of the center Z_{N_c} . Then it is possible to use the decomposition¹⁹⁴ at each lattice site

$$U_\mu^g(x) = Z_\mu(x) U_\mu^{(\text{rem})}(x), \quad (6.1)$$

where $Z_\mu(x) \in Z_{N_c}$ and $U_\mu^{(\text{rem})}(x) \in SU(N_c)/Z_{N_c}$. Here, $Z_\mu(x)$ is the center element closest to $U_\mu^g(x)$. As mentioned in Section 5.3, for the $SU(2)$ case the center elements are just $\mathbb{1}$ and $-\mathbb{1}$. Then, for $N_c = 2$ we have

$$Z_\mu(x) = \text{sgn} \left[\text{Tr } U_\mu^g(x) \right] \mathbb{1}. \quad (6.2)$$

From now on we will only specify the procedure for $SU(2)$ theory.

At the end of the day, the gauge-fixing philosophy is the same of Section 4.2 for Landau gauge. We must maximize the functional²⁰³

$$\mathcal{E}_{\text{MCG}}[U^{\mathfrak{g}}] = \frac{1}{4} \sum_{x \in \Lambda} \sum_{\mu=1}^4 \left(\text{Tr} [U_{\mu}^{\mathfrak{g}}] \right)^2, \quad (6.3)$$

which is equivalent to an adjoint Landau gauge fixing.³⁷ We achieve this by maximizing the local contribution

$$\mathcal{E}_{\text{MCG}}^x = \sum_{\mu=1}^4 \left\{ \text{Tr} [\mathfrak{g}(x) U_{\mu}(x) \mathfrak{g}^{\dagger}(x + \hat{\mu})]^2 + \text{Tr} [\mathfrak{g}(x - \hat{\mu}) U_{\mu}(x - \hat{\mu}) \mathfrak{g}^{\dagger}(x)]^2 \right\} \quad (6.4)$$

through a local algorithm with an overrelaxation step. We follow the procedure devised in Ref. 203, where the gauge transformation is done sequentially to a $\mathfrak{g}(x)$ update, i.e., we transform each link “touching” $\mathfrak{g}(x)$ by

$$U_{\mu}(x) \rightarrow \mathfrak{g}(x) U_{\mu}(x) \mathfrak{g}^{\dagger}(x + \hat{\mu}), \quad U_{\mu}(x) \rightarrow \mathfrak{g}(x - \hat{\mu}) U_{\mu}(x - \hat{\mu}) \mathfrak{g}^{\dagger}(x) \quad (6.5)$$

with $\mathfrak{g}^{\dagger}(x + \hat{\mu}) = \mathbb{1}$ and $\mathfrak{g}(x - \hat{\mu}) = \mathbb{1}$. With this in mind, we can write (6.4) as

$$\mathcal{E}_{\text{MCG}}^x = \sum_{\mu=1}^4 \left\{ \text{Tr} [\mathfrak{g}(x) U_{\mu}(x)]^2 + \text{Tr} [U_{\mu}(x - \hat{\mu}) \mathfrak{g}(x)^{\dagger}]^2 \right\} \quad (6.6)$$

and, using (4.37) together with

$$\mathfrak{g}(x) = g^4(x) \mathbb{1} + i \boldsymbol{\sigma} \cdot \mathbf{g}, \quad \mathbf{g} = (g^1, g^2, g^3), \quad (6.7)$$

we arrive at

$$\mathcal{E}_{\text{MCG}}^x = \sum_{\mu=1}^4 \left\{ [2g^4(x) u_{\mu}^4(x) - 2\mathbf{g}(x) \cdot \mathbf{u}_{\mu}(x)]^2 + [2g^4(x) u_{\mu}^4(x - \hat{\mu}) + 2\mathbf{g}(x) \cdot \mathbf{u}_{x-\mu}(x)]^2 \right\}. \quad (6.8)$$

For convenience we then define a vector y as follows

$$\mathbf{y}(l) = \begin{cases} -\mathbf{u}_{\mu}(x), & \mu = l = 1, \dots, 4 \\ \mathbf{u}_{\mu}(x - \hat{\mu}), & \mu + 4 = l = 5, \dots, 8 \end{cases}, \quad y^4(l) = \begin{cases} u_{\mu}^4(x), & \mu = l = 1, \dots, 4 \\ u_{\mu}^4(x - \hat{\mu}), & \mu + 4 = l = 5, \dots, 8 \end{cases} \quad (6.9)$$

and rewrite (6.8) as

$$\mathcal{E}_{\text{MCG}}^x = \sum_{l=1}^4 \left[\sum_{k=1}^4 g^k(x) y^k(l) \right]^2 + \sum_{l=5}^8 \left[\sum_{k=1}^4 g^k(x) y^k(l) \right]^2 = \sum_{l=1}^8 \left[\sum_{k=1}^4 g^k(x) y^k(l) \right]^2. \quad (6.10)$$

Our aim is to minimize the expression in the last equation given that $\mathfrak{g} \in SU(2)$, i.e. $\det \mathfrak{g} = \sum_{k=1}^4 (g^k)^2 = 1$, which we implement through the Lagrange multiplier λ as

$$\tilde{\mathcal{E}}_{\text{MCG}}^x = \mathcal{E}_{\text{MCG}}^x + \lambda \left(1 - \sum_{k=0}^3 (g^k)^2 \right). \quad (6.11)$$

Finally, setting the derivative $\tilde{\mathcal{E}}_{\text{MCG}}^x$ with respect to g^i equal to zero we arrive at the following condition for the local maximum

$$\sum_{k=1}^4 Y^{ik} g^k = \lambda g^i, \quad (6.12)$$

where $Y^{ik} = \sum_{l=1}^8 y^i(l) y^k(l)$ is a 4×4 real symmetric matrix. The condition is then translated into the eigenvalue equation

$$Y\mathbf{G} = \lambda\mathbf{G}, \quad \mathbf{G} \equiv (g, g^4) \quad (6.13)$$

and the eigenvector with the largest eigenvalue corresponds to the $\mathbf{g}$ that maximizes $\tilde{\mathcal{E}}_{\text{MCG}}^x$ locally.²⁰³ The eigenvector can be obtained through any conventional method, e.g., a power method.²⁰⁶ Given the local gauge transformation, we use the overrelaxation step $\mathbf{g} \rightarrow \mathbf{g}^\omega$ in similarity to (4.62)^A,

$$\mathbf{g}^\omega = \mathcal{P}_{SU(2)} [\mathbb{1} + \omega (\mathbf{g} - \mathbb{1})], \quad (6.14)$$

and update the corresponding links according to (6.5). We iterate this process until the global variation $\Delta\mathcal{E}_{\text{MCG}}$ is less than some numerical tolerance. With the gauge fixed, we proceed to the $SU(2)$ center projection given by (6.2). This yields the center lattice configuration $\{Z_\mu\}$ containing only $\mathbb{1}$ and $-\mathbb{1}$ elements.

A procedure for removing the vortex content of a given lattice configuration was devised in Ref. 204 and it is generally called *vortex removal*. We first fix the gauge to the aforementioned direct maximal center gauge, resulting in a configuration $\{U_\mu^{\mathfrak{g}}\}$, and then project it onto a center lattice configuration $\{Z_\mu\}$. Then we “cancel” the center component by doing

$$U_\mu^{(\text{rem})}(x) = Z_\mu^\dagger(x) U_\mu^{\mathfrak{g}}(x) = Z_\mu(x) U_\mu^{\mathfrak{g}}(x), \quad (6.15)$$

where the last equality is only valid for $SU(2)$. Then it is easy to show that the vortex content in $\{U_\mu^{(\text{rem})}\}$ is trivial²⁰⁴

$$Z_\mu^{(\text{rem})}(x) = \text{sgn} [\text{Tr } U_\mu^{(\text{rem})}(x)] = \text{sgn} [Z_\mu(x) U_\mu^{\mathfrak{g}}(x)] = \text{sgn} [U_\mu^{\mathfrak{g}}(x)]^2 = \mathbb{1}. \quad (6.16)$$

6.1.2 Static Quark-Anqtiquark Potential

We have mentioned the string tension in Section 4.3 and have seen that, as any physical quantity, it must enter the region of asymptotic scaling for some value of the coupling. A good indication that there exists a sensible string tension in a vortex-projected ensemble is to check its scaling. The Figure 6.1 (left) shows that already for small loops the string tension enters the asymptotic scaling regime of $SU(2)$ theory.

^A As in Section 4.2, $\omega \in (1, 2)$ and the ideal value must be calibrated for each problem. We fixed $\omega = 1.7$ in all simulations.

Figure 6.1 – Asymptotic scaling of string tension in center-projected ensemble, where $\chi(4, 4)$ is fitted using (4.72) to yield $\Lambda_L = 0.0177(4)\sqrt{\sigma}$ (left), see also Figure 4.7. Comparison of string-tension convergence between full, center projected and vortex removed ensembles, the black line indicating the string-tension result from Ref. 207 (right).

Source: By the author.

Another aspect of the center dominance confinement scenario that we can demonstrate on the lattice is that the center-projected ensemble is, in a certain way, responsible for almost all the string tension. We have an indication that this is true already by noting the Creutz ratios for the full, center projected and vortex removed ensembles in Figure 6.1 (right). Here, using a coupling in the scaling region of the theory we see that the full Creutz ratio extrapolates to the string tension taken from Ref. 207, while in the removed ensemble it seems to extrapolate to zero. Conversely, the center projected lattice quickly converges to the value of the full $SU(2)$ theory.

As a last check of center dominance and of our center projection procedure, we reproduce the results for the quark-antiquark static potential using the method in Ref. 205. Essentially, we use the result in (5.9) to adjust the curve (in lattice units)

$$-\log \langle \mathcal{W}(r, t) \rangle = \gamma(r)t + \delta(r) \quad (6.17)$$

using a linear regression for various $(\mathcal{W}(r, t), t)$ pairs with fixed r . Then we make the identification $\gamma(r) \rightarrow V(r)$. The explicit expression for an individual Wilson loop on the $\hat{\mu}\hat{\nu}$ -plane is

$$\begin{aligned} \mathcal{W}(r, t) = & \frac{1}{2} \text{Tr} \prod_{j=0}^{r-1} U_{\mu}(x + j\hat{\mu}) \prod_{j=0}^{t-1} U_{\nu}(x + r\hat{\mu} + j\hat{\nu}) \\ & \times \prod_{j=-r}^0 U_{\mu}^{\dagger}(x + t\hat{\nu} + (r+j)\hat{\mu}) \prod_{j=-t}^0 U_{\nu}^{\dagger}(x + (t+j)\hat{\nu}). \end{aligned} \quad (6.18)$$

It is important to note that if the lattice is treated asymmetrically in some direction, say in time, then $\mu = 1, 2, 3$ and $\nu = 4$. This will be true when using the following smearing technique.

In order to enhance the convergence of relation (6.17) and avoid large values of t , we use a version of APE smearing^{207,208} in which we perform the “thick” spatial link substitution

$$U_i(x) \rightarrow \alpha U_i(x) + s_i, \quad (6.19)$$

where the staple variable s is defined by

$$s_i(x) = \sum_{\substack{j=1 \\ j \neq i}}^3 U_j(x + \hat{i}) U_i^\dagger(x + \hat{j}) U_j^\dagger(x) + U_j^\dagger(x + \hat{i} - \hat{j}) U_i^\dagger(x - \hat{j}) U_j(x - \hat{j}), \quad (6.20)$$

which consists of the surrounding (spatial) links touching $U_i(x)$. This enhances the overlap with the ground state in the computation of the Wilson loops,²⁰⁷ so that (6.17) converges well even for the first values of t . In the simulations we chose $\alpha = 2$ and iterated the smearing steps $n_{\text{smear}} = 50$ times in each measurement.

We gather the results for the static potential in Figure 6.2. Notice how the linear character at large distances is almost fully transferred to the center-projected ensemble, while the vortex-removed ensemble stays only with the Coulombic behavior at small distances. Indeed, we found that the vortex-only system is able to reproduce 94(2)% of the original string tension, while the vortex-removed counterpart vanishes.

Figure 6.2 – Static quark-antiquark potential extracted from full, center-projected and vortex-removed ensembles. The scale was fixed using the Sommer parameter (see Table 1) and fits are represented by (dashed) lines.

Source: By the author.

In Table 1 we summarize the results for the potential simulation, where hatted symbols were obtained through fits to lattice data. Notice that the Lüscher term's theoretical value ($\gamma \approx -0.26$) is better approximated for larger lattices and smaller a . The lattice spacing was determined using the string tension value $\sigma = (440 \text{ MeV})^2$ directly in $\hat{\sigma} = \sigma a^2$ (see Eq. 5.19), but we also determined it through the Sommer parameter (see Section 4.3). We stick to the Sommer parameter determination for all other results.

Table 1 – Information of lattices used for computing the potential and fixing the scale. We determined a both directly through the string tension and also using the Sommer parameter. Hatted symbols are quantities extracted from the lattice.

β	N	N_{cf}	N_{therm}	N_{cor}	$\hat{\sigma}$	$\hat{\gamma}$	$a_{\sigma}[fm]$	$a_{\text{Sommer}}[fm]$
2.0	10	250	3000	200	0.518(11)	-0.158(24)	0.323(3)	0.295(5)
2.2	16	50	2000	200	0.238(5)	-0.241(14)	0.218(2)	0.206(3)
2.2	24	30	1500	150	0.245(2)	-0.231(7)	0.222(1)	0.208(1)
2.5	24	20	1000	100	0.039(1)	-0.225(4)	0.089(1)	0.083(1)

Source: By the author.

6.2 BPST Instantons

It is well known that most essential features of QCD can be attributed to the non-trivial topology of non-Abelian gauge theories. In particular, topological properties are important for phenomenological reasons, namely the axial anomaly and the η' mass contribution.²⁰⁹ We will now discuss lattice definitions for the topological charge and describe how instanton background configurations can be realized on the lattice.

6.2.1 Topology Elements

In very general words, topology is related to geometrical and continuity properties. We can say that two objects are topologically equivalent if they can be deformed continuously into one another, i.e., without ripping apart any surfaces. This can be made more precise by saying that two continuous functions $A_1, A_2 : X \rightarrow Y$ are *homotopic* if there is a continuous function $G : X \times [0, 1] \rightarrow Y$ that identifies A_1 and A_2 respectively at 0 and 1, namely $G(x, 0) = A_1(x)$ and $G(x, 1) = A_2(x)$, $x \in X$. Then A_1 and A_2 are said to live in the same homotopy classes (homotopic) and to be topologically equivalent.

If $X = S^n$ ^B, we see that a suitable topological property then divides A -maps into disjoint homotopy classes $\pi_n(Y)$. When $Y = S^n$, we call this property the *winding number*, which labels the homotopy classes as an integer, $\pi_n(S^n) = \mathbb{Z}$. We can loosely understand the winding number, also called Pontryagin index, as the number of times a mapping A winds around Y as X is covered by x . A very simple example are the functions

^B S^n denotes the the n -sphere, i.e., the n -dimensional spherical surface.

$a_\xi : S^1 \rightarrow S^1$ (from and to the closed unit circle) defined by

$$a_\xi(\theta) = e^{i(n\theta + \xi)}, \quad \theta \in [0, 2\pi]. \quad (6.21)$$

Here, n is the winding number and for all values of ξ the corresponding a_ξ 's have the same n and thus are all in the same homotopy class. Equivalently, we can write this as a map from the real line $x \in (-\infty, \infty)$ to the complex unit circle $a(x, y) = x + iy$, given that $x = -\infty$ and $x = \infty$ are identified and $x^2 + y^2 = 1$.

Important for QCD are the mappings $S^3 \rightarrow S^3$, where the domain is a four-dimensional Euclidean sphere characterized by three angles and the image is the $SU(2)$ group manifold, both topologically equivalent to a 3-sphere. The $SU(2)$ elements are characterized by the Caley-Klein parametrization, namely four parameters $g^i, i = 0, \dots, 3$ and a constraint $\sum_{i=1}^3 (g^i)^2 = 1$ (see C.3.3). This analysis can be extended to $SU(N_c)$ by the embedding of $SU(2)$ subgroups.

For completeness, we write down the winding number for Yang-Mills fields in its final form ^C

$$\begin{aligned} Q &= \frac{g_0^2}{16\pi^2} \int d^4x \operatorname{Tr} [F_{\mu\nu}(x) \tilde{F}_{\mu\nu}(x)] \\ &= \frac{g_0^2}{32\pi^2} \int d^4x \sum_{\mu, \nu, \rho, \sigma=1}^4 \varepsilon_{\mu\nu\rho\sigma} \operatorname{Tr} [F_{\mu\nu}(x) F_{\rho\sigma}(x)], \end{aligned} \quad (6.22)$$

commonly known as *topological charge*. In this expression it is also implied the topological charge density

$$Q(x) = \frac{g_0^2}{32\pi^2} \sum_{\mu, \nu, \rho, \sigma=1}^4 \varepsilon_{\mu\nu\rho\sigma} \operatorname{Tr} [F_{\mu\nu}(x) F_{\rho\sigma}(x)], \quad (6.23)$$

which will be used in the next discussion.

An essential non-Abelian field configuration with unit topological charge is the *instanton*, characterized by a local form in Euclidean space. The instanton is a solution of the Euclidean classical Yang-Mills field equations (2.28) with finite action, i.e., satisfying $F_{\mu\nu}(x) \rightarrow 0$ as $|x| \rightarrow \infty$. In view of (2.20), namely

$$A_\mu(x) \rightarrow \mathfrak{g}(x) A_\mu(x) \mathfrak{g}^\dagger(x) - \frac{i}{g_0} \mathfrak{g}(x) \partial_\mu \mathfrak{g}^\dagger(x), \quad (6.24)$$

we see that it is sufficient to require

$$A_\mu(x) \rightarrow -\frac{i}{g_0} \mathfrak{g}(x) \partial_\mu \mathfrak{g}^\dagger(x), \quad (6.25)$$

i.e., A_μ tends to a pure gauge transformation of the vacuum $A_\mu = 0$ as $|x| \rightarrow \infty$. This is what we call a pure gauge field. In this case, the winding occurs at $|x| \rightarrow \infty$, being

^C This definition corresponds to the Euclidean action with no explicit g_0 , i.e., (A.13). The strength field $F_{\mu\nu}$ is defined in A.1 and A.2.

the 3-sphere localized at infinity. Here the mappings are the gauge transformations $\mathfrak{g}(x)$. Proposed in 1975,²¹⁰ the BPST instanton

$$A_\mu(x) = \frac{-i}{g_0} \frac{|x|^2}{|x|^2 + \varrho^2} \mathfrak{g}(x) \partial_\mu \mathfrak{g}^\dagger(x), \quad (6.26)$$

where $|x|^2 = \sum_{i=1}^4 (x_i)^2$ and with

$$\mathfrak{g}(x) = \frac{x_4 + i \boldsymbol{\sigma} \cdot \mathbf{x}}{|x|}, \quad (6.27)$$

satisfies the above requirements. The arbitrary radius ϱ characterizes the scale invariance of the BPST instantons and suggests that they play a role in long-range effects.

6.2.2 Lattice Topology

It is immediate to ask if non-trivial topology can be studied on the lattice: discretized fields are not continuous and in principle we can continuously deform a configuration into any other. However, as noticed by Lüscher,²¹¹ this is a quite restrictive and naive perspective as we are interested in the continuum limit of lattice gauge theories. We must remember that the lattice spacing is a regulator and, as in any other quantum field theory, it must be removed in order to obtain physical predictions. Therefore, it is only necessary to give a definition for topology and topological charge density having the correct continuum limit, e.g.

$$\mathcal{Q}(x) = -\frac{1}{32\pi^2} \sum_{\mu, \nu, \rho, \sigma=1}^4 \varepsilon_{\mu\nu\rho\sigma} \text{Tr} [U_{\mu\nu}(x) U_{\rho\sigma}(x)]^{\text{D}} \quad (6.28)$$

and that in some way reproduces the last section's properties for periodic configurations on a finite lattice. This is done in Ref. 211 by separating distinct topological classes by exceptional configurations with action larger than a certain value, also called *dislocations*.

Inspired by Lüscher's definition for the lattice topological charge, its first implementations were called “geometrical methods”.²¹² They were designed to reconstruct the principal bundle from an interpolation of the link variables, being the topological charge obtained from it through combinatorial analysis. The corresponding computations presented asymptotic scaling, e.g., for the topological susceptibility,²¹³ but systematical errors were almost impossible to estimate. The interpolation involved was rather arbitrary, so this method did not survive the 1990s. In fact, today there are a plethora of other ways for computing topological quantities, most involving smoothing techniques or zero-eigenvalues of the overlap Dirac operator.²¹⁴ The later one uses the relation between the topological charge and the number of Dirac's zero eigenmodes through the Atiyah-Singer theorem. We will explore the former, known as *field theoretic* definition.

The field theoretic approach directly uses the lattice gauge fields, for instance through (6.28), to compute the topological charge of a link configuration. We should

^D The plaquette operator $U_{\mu\nu}$ is defined in (4.15).

remark that any definition with the appropriate continuum limit is valid in principle. If we take (6.28) as the definition, a straightforward expansion shows that discretization errors are of order $\mathcal{O}(a^6)$ so that improved definitions, i.e. involving more loops, could be used to cancel these artifacts.^{214,215} In this way, as we always work with finite lattice spacing a , the topological charge can never be an integer, but only approximate the corresponding one in the continuum limit. Moreover, it was shown that the topological charge in the true continuum limit suffers from a multiplicative renormalization depending on the coupling^{216,217}

$$\mathcal{Q}(x) \rightarrow a^4 Z(\beta) Q(x) + \mathcal{O}(a^6), \quad (6.29)$$

which is related to short-range fluctuations. Through a perturbative analysis it is possible to estimate Z , which is then confirmed by a non-perturbative heating method,²¹⁷ where smooth configurations (BPST instantons) with well-defined topological charge are thermalized without destroying the configuration's original topology.

One way of measuring the topological charge from a thermalized lattice configuration is by the *cooling* method.²¹⁸ To implement cooling, one substitutes each link variable by the inverse staple projected onto the group, i.e.,

$$U_\mu(x) \rightarrow \mathcal{P}_{SU(2)} \left[s_\mu^\dagger(x) \right] = \frac{s_\mu^\dagger(x)}{\sqrt{\det s_\mu^\dagger(x)}}, \quad (6.30)$$

with the staple variable defined in (6.20). This process locally minimizes the action and quickly reduces short-range fluctuations without affecting long-range properties drastically. Then the topological charge can be measured through a field theoretic definition with $Z \approx 1$. Of course, if one applies too many cooling steps, the underlying topological charge can be artificially modified, so that it must be executed carefully.

Following, we will directly use the definition (6.28) to verify the topological charge of a discretized BPST instanton with well-defined topology. Then, cooling will be used only to better implement periodic boundary conditions.

6.2.3 Instanton Background

The instanton solution of Yang-Mills theories is well-known in low-energy QCD by its phenomenological importance. They are relevant in taking into account the spontaneous breaking of chiral symmetry and topological vacua, in particular with the instanton liquid model in the 1980s.²⁰⁹

We shall build BPST instanton solutions on a periodic lattice in order to evaluate their gauge-geometrical properties. There are at least two ways of proceeding according to the literature. One by Teper and Pugh²¹⁹ and the other by Fox et al.²²⁰ In the following we will present only the former and comment on the later.

First, we write (6.27) using the convenient symbol $\tau_\mu = (\boldsymbol{\sigma}, 1)$ (see C.3.3)

$$\mathfrak{g}(x) = \frac{x \cdot \tau}{|x|}, \quad (6.31)$$

and then rewrite the BPST solution (6.26) in a convenient and lattice-friendly notation (omitting constants)

$$\begin{aligned} \frac{|x|^2}{|x| + \varrho^2} \mathfrak{g}^\dagger(x) \partial_\mu \mathfrak{g}(x) &= \frac{|x|^2}{|x| + \varrho^2} \frac{(x \cdot \tau)^\dagger}{|x|} \left[\frac{\tau_\mu}{|x|} - (x \cdot \tau) \frac{x_\mu}{|x|^2} \right] \\ &= \frac{1}{|x|^2 \varrho^2} \left[\tau_\mu (x \cdot \tau)^\dagger - (x \cdot \tau)^\dagger (x \cdot \tau) \frac{x_\mu}{|x|} \right] \\ &= \frac{1}{|x|^2 \varrho^2} \left[\tau_\mu (x \cdot \tau)^\dagger - x_\mu \right] \equiv A_\mu^{\text{reg}}(x), \end{aligned} \quad (6.32)$$

which we will call *regular* BPST solution. This can be written in a straightforward way as²²¹

$$A_\mu^{\text{reg}}(x) = \frac{1}{|x|^2 + \varrho^2} (y_\mu)^k i \sigma^k \quad (6.33)$$

with

$$\text{Instanton: } \begin{cases} y_1 = (x_4, x_3, -x_2) \\ y_2 = (-x_3, x_4, x_1) \\ y_3 = (x_2, -x_1, x_4) \\ y_4 = (-x_1, -x_2, -x_3) \end{cases}, \quad \text{Anti-instanton: } \begin{cases} y_1 = (-x_4, x_3, -x_2) \\ y_2 = (-x_3, -x_4, x_1) \\ y_3 = (x_2, -x_1, -x_4) \\ y_4 = (x_1, x_2, x_3) \end{cases}, \quad (6.34)$$

Teper's Instanton

This is the most simplest way of putting an instanton on a periodic lattice.^{219, 221, 222} It consists first in computing $A_\mu^{\text{reg}}(x)$ centered at, say, the lattice's central hypercube, i.e., mapping $x_\mu \rightarrow x_\mu - N/2$ with N even (in lattice units). The link variables are then calculated through the definition (4.7) of an elementary gauge transporter, namely

$$U_\mu^{\text{reg}}(x) = \mathcal{P} \left[\int_x^{x+\hat{\mu}} d^4x \exp A_\mu^{\text{reg}}(x) \right]. \quad (6.35)$$

We naturally approximate the integral by some interpolation between points x and $x + \hat{\mu}$, i.e., we calculate partial links $\Delta U^{\text{reg}}(x_i) = e^{\Delta x_i A_\mu^{\text{reg}}(x_i)}$, where the Δx_i 's are an arbitrary number of partitions, and then take the product of all $\Delta U^{\text{reg}}(x_i)$'s to be $U_\mu^{\text{reg}}(x)$.

The most important step is to bring the winding surface inside the lattice. This is done through a *singular* gauge transformation given by (6.31). On the lattice this amounts to doing

$$U_\mu^{\text{reg}}(x) \rightarrow U_\mu^{\text{sing}}(x) = \mathfrak{g}(x) U_\mu^{\text{reg}}(x) \mathfrak{g}^\dagger(x + \hat{\mu}). \quad (6.36)$$

It is fundamental to not impose periodic boundary conditions before this stage, i.e., to not use $\mathfrak{g}(x) = \mathfrak{g}(x + N)$ or $A_\mu^{\text{reg}}(x) = A_\mu^{\text{reg}}(x + \hat{\mu})$ in the above steps. Only after doing

the singular transformation does one impose the boundary conditions. In practice, this is done by performing some cooling steps next to the borders so that the difference between the endpoints smooths out. Additionally, one can also implement the method in Ref. 221, where one does the same process for an $N + 2$ lattice side and at the end the remaining links are set to $U_\mu(N, \cdot) \rightarrow \sqrt{U_\mu(N, \cdot)U_\mu(0, \cdot)}$ and used as the ones connecting the lattice endpoints, which simulates a periodic boundary condition. We implemented the last steps and the difference was minimal, so we stayed with the simpler one. It is important to remember to put the instanton's center offsite, say dislocated 0.1 from the central lattice site, so that no singularity from (6.36) is manifest.

Figure 6.3 – BPST 1D-profiles compared with the continuum densities for various lattice volumes. The instanton radius here is always $\varrho = N/3$, the one that gives the topological charge closest to 1. Non-periodic effects on large lattices can be smoothed out through further cooling, which in excess can decrease ϱ too much and spoil the configuration. Instantons with $\varrho \approx 1$ “fall” through the lattice and must be avoided.

Source: By the author.

We show here some topological density profiles obtained from Teper’s instanton. In Figure 6.3 the topological charge density given by (6.28) is integrated to a 1D-slice and compared to the correspondent continuum expression

$$Q_{1D}(x) = \frac{3\varrho^4}{4(x^2 + \varrho^2)^{5/2}} \quad \text{E.} \quad (6.37)$$

^E Q_{1D} is obtained after substituting the instanton field into (6.23), which yields $Q(x) =$

In Figure 6.4 we plot the topological charge density integrated to a $2D$ -slice for various instanton configurations on a $N = 48$ lattice. Notice that the instantons are not superposed but sufficiently spaced, so that each whole configuration can still be considered a classical solution of the non-linear Yang-Mills equations. Furthermore, we numerically verified that the lattice instantons generated are indeed in Landau gauge, as can be analytically computed using Equations (6.26) and (6.27).

Figure 6.4 – BPST $2d$ -profiles for different multi-instanton configurations. From top to bottom and left to right: a large instanton; a large anti-instanton; a small instanton and anti-instanton; four small instantons; five small instantons; one medium instanton and three small anti-instantons.

Source: By the author.

$\frac{6\rho^2}{\pi^2(|x|^2+\rho^2)^4}$,²⁵ and then integrating out three of the four x_μ components.

Fox's Instanton

The Fox discretization of the instanton appears to get some topological properties right,^{220,223} so we mention it here. It is very similar to the above procedure, except for two steps. The first difference is that it compresses the continuum instanton configuration using the map

$$x_\mu \rightarrow \frac{N^3}{(N - x_\mu)^2 - x_\mu^2}, \quad (6.38)$$

which means that the lattice spacing is not constant. The second difference is a division of the lattice into two regions separated by a given boundary. In the inner region one discretizes the instanton using the regular expression (6.33). Conversely, to the outer region is attributed the singular expression found through (6.36), namely

$$A_\mu^{(\text{reg})}(x) = \frac{\varrho^2}{|x|^2 + \varrho^2} \frac{1}{2} \left(\tau_\mu^\dagger \tau_\nu - \tau_\nu^\dagger \tau_\mu \right) \frac{x_\nu}{|x|^2}, \quad (6.39)$$

which decays faster than the regular one for large $|x|$. Moreover, on the interface between the two regions one does an “incomplete” singular gauge transformation (6.36), i.e., a transformation only over the link’s endpoints sitting on the interface, ignoring the other endpoint inside the inner region. Therefore, this method is an interpolation between the expressions (6.33) and (6.39). In practice, it yields a very bizarre topological density concentrated around the boundary between the regions²²² and that depends on the location of the interface, besides not using a constant lattice spacing. For these reasons we do not present the data regarding this configuration here.

6.3 Geometry and Ghost Sector

In this section we describe a characterization of the geometry of the Gribov region through quantities that indicate a configuration’s proximity to the Gribov horizon in Landau gauge. We also review and implement analytical bounds that help in indicating the type of configurations that can give rise to a scaling solution (see Sections 5.2.3 and 5.2.4) and their non-perturbative relevance.

6.3.1 Ghost Propagator and Analytical Bounds

As we have seen in Chapter 5, the gluon and ghost propagators have gained relevance over the years as a tool to explain color confinement in Landau gauge. More specifically in the four-dimensional theory, there are approaches that support the scaling solution (vanishing gluon and enhanced ghost propagators at zero momentum) while others, including most lattice simulations, point to a massive-type solution (finite gluon and free ghost propagators at zero momentum).

Full Propagators and Vortex Removal

The computation of the momentum-space gluon propagator is achieved by the Monte Carlo average¹²³

$$\mathcal{D}(0) = \frac{1}{12N^4} \sum_{\mu=1}^4 \sum_{a=1}^3 \left\langle \left| \sum_{x \in \Lambda} \mathcal{A}_\mu^a(x) \right|^2 \right\rangle \quad (6.40)$$

at zero lattice momentum and

$$\mathcal{D}(k) = \frac{1}{9N^4} \sum_{\mu=1}^4 \sum_{a=1}^3 \left\langle \left| \sum_{x \in \Lambda} \mathcal{A}_\mu^a(x) \cos(2\pi k \cdot x) \right|^2 + \left| \sum_{x \in \Lambda} \mathcal{A}_\mu^a(x) \sin(2\pi k \cdot x) \right|^2 \right\rangle \quad (6.41)$$

for non-zero momentum. This can be translated to the lattice momentum expression, given (in lattice units) by

$$p_\mu = 2 \sin(\pi k_\mu), \quad (6.42)$$

so that it is possible to identify p^2 with the eigenvalues of the (negative) lattice Laplacian operator^F. Here, each component of k varies as $k_\mu = 1/N, \dots, (N-1)/N$. In particular, we choose $k = (0, 0, 0, k_4)$ with $k_4 = 1/N, \dots, (N-1)/N$ for simplicity and also to avoid diagonal directions on the lattice and consequently errors due to breaking of rotational symmetry.²²⁴

For the ghost propagator, we again use $k = (0, 0, 0, k_4)$ with k_4 given above and the Monte Carlo average is¹²³

$$\mathcal{G}(k) = \frac{1}{3N^4} \sum_{x, y \in \Lambda} e^{-2\pi i k \cdot (x-y)} \sum_{a=1}^3 \left\langle (\mathcal{M}^{-1})^{aa}(x, y) \right\rangle, \quad (6.43)$$

so we must somehow compute the inverse of the Faddeev-Popov matrix (6.46). We use a *conjugate gradient* (CG) method to invert $\mathcal{M}$ applied to a specific source, namely a plane-wave or a point source.^{174, 176} We choose the former and we proceed by setting as source, for each k_4 value, a plane-wave vector

$$\xi_k^a(x) = \delta^{ac} e^{-2\pi i k \cdot x} \quad (6.44)$$

for $c = 1, 2, 3$, one at a time. For each value of c we then use CG to solve the $3V \times 3V$ sparse linear system (see D.1)

$$\sum_{b=1}^3 \sum_{y \in \Lambda} \mathcal{M}^{ab}(x, y) \gamma^b(y) = \psi_k^a(x), \quad (6.45)$$

^F The lattice Laplacian operator action corresponds to the Faddeev-Popov matrix in (6.46) for the trivial vacuum, i.e., for $U_\mu(x) = \mathbb{1}$ for all x, μ and for each value of the color index.

where we can compute the action of the Faddeev-Popov matrix on an arbitrary vector γ by comparing (4.47) and (4.48), which yields

$$(\mathcal{M}\gamma)^a(x) = \sum_{\mu=1}^4 \left\{ u_{\mu}^4(x) [\gamma^a(x) - \gamma^a(x + \hat{\mu})] + u_{\mu}^4(x - \hat{\mu}) [\gamma^a(x) - \gamma^a(x - \hat{\mu})] \right. \\ \left. + \sum_{a,b=1}^3 \epsilon^{abc} [u_{\mu}^b(x) \gamma^c(x + \hat{\mu}) - u_{\mu}^b(x - \hat{\mu}) \gamma^c(x - \hat{\mu})] \right\}. \quad (6.46)$$

The application of the algorithm results in an approximation to

$$\gamma^a(x) = \sum_{y \in \Lambda} (\mathcal{M}^{-1})^{ab}(x, y) \xi_k^b(y) \quad (6.47)$$

and consequently, after averaging over b , we obtain

$$\mathcal{G}(k) = \frac{1}{3N^4} \left\langle \sum_{a=1}^3 \sum_{x \in \Lambda} \xi_k^a(x) \gamma^{a*}(x) \right\rangle. \quad (6.48)$$

Figure 6.5 – Momentum-space gluon and ghost propagators in physical units from lattice sizes $N = 10, 16, 24$ and $N = 10, 16$, respectively. The blue plot corresponds to vortex-removed ensembles and the red one to full ensembles. The ghost propagator was fitted to ap^{-b} for both cases, yielding $b = 2.53(9)$ (red line) and $b = 2.33(8)$ (blue line), respectively. The orange (triangle, left) data are preliminary results for the gluon propagator evaluated on pure vortex configurations fixed to the Landau gauge (see Ref. 226).

Source: By the author.

In Figure 6.5 we show preliminary results for the gluon and ghost propagators using full, vortex-removed and vortex-only ensembles. Notice that, for the lattice sizes simulated, it is not possible to observe the turn-over momentum of the gluon propagator. Moreover, the infrared behavior of the ghost propagator cannot be well assessed because

there are not a considerable number of infrared points available. Nevertheless, we see that the qualitative aspects of the vortex-removed ensembles obtained in Ref. 225 are clearly reproduced. We note that when the vortex content is removed, the gluon propagator loses its bulge next to $p \sim 0.5$ GeV. Moreover, the ghost propagator turns out to be less enhanced than in the full case, as demonstrated by the infrared fits.

Results for the center-projected ensembles in Figure 6.5 (left, orange, triangle) were done only for the gluon propagator due to the available CPU-time and are novel for $SU(2)$ gauge theory. The vortex-only gluon propagator retains most of the contribution from the full ensemble, around 60%, as computed in Ref. 226 for the $SU(3)$ group.

Ghost sector bounds

As we have seen in Section 5.2.4, besides the issue of the Gribov copies, one of the great controversies from lattice results concerns the infinite-volume limit necessary to extract infrared information from Green functions. Besides direct results from large volume lattice data,^{29,182} constraints to control the infinite-volume extrapolation were developed both for the gluon and for the ghost propagators.^{186,187,202} In both cases, the analytical bounds still indicate a massive-type solution for $D = 4$. For the gluon, the bounds are given by magnetization-like quantities.¹⁸⁶ We specify the bounds for the ghost propagator here.

Following the reasoning of Section 3.4 in Landau gauge, it is believed that in the infinite-volume limit the functional integration is localized on the boundary of the Gribov region, the Gribov horizon $\partial\Omega$. This follows the intuitive thinking that the volume of a hypersphere gets concentrated near its boundaries the larger the system's dimensionality gets.¹⁰⁰ On the lattice, the Gribov horizon corresponds to Faddeev-Popov's near-zero modes, which translates to the smallest eigenvalue of $\mathcal{M}$ going to zero as the volume increases, i.e., $\lambda_1 \rightarrow 0$.²²⁷ Therefore, it seems relevant to study the rate at which λ_1 vanishes in the infinite-volume limit.

A first inequality between the ghost propagator $\mathcal{G}$, the Faddeev-Popov's smallest eigenvalue λ_1 and its corresponding eigenvector ψ_1 was obtained in Ref. 187. Assuming $0 < \lambda_1 < \lambda_2 < \dots$ and working in the space orthogonal to the kernel of $\mathcal{M}$, we can rigorously show that

$$\frac{1}{3\lambda_1} \sum_{a=1}^3 \left| \tilde{\psi}_1^a(p) \right|^2 \leq \mathcal{G}(p) \leq \frac{1}{\lambda_1}, \quad (6.49)$$

where we specified the formula for $SU(2)$, and

$$\tilde{\psi}_i(p)^a = \frac{1}{N^2} \sum_{x \in \Lambda} \psi_i^a(x) e^{-2\pi i k \cdot x} \quad (6.50)$$

is a Fourier transform. This bound can be systematically improved to involve higher

eigenvalues and eigenvectors, yielding²⁰²

$$\frac{1}{3\lambda_1} \sum_{a=1}^3 |\tilde{\psi}_1^a(p)|^2 \leq \frac{1}{3} \sum_{a=1}^3 \left[\frac{1}{\lambda_1} |\tilde{\psi}_1^a(p)|^2 + \frac{1}{\lambda_2} |\tilde{\psi}_2^a(p)|^2 \right] \leq \dots \leq \mathcal{G}(p) \quad (6.51)$$

as new lower bounds, and

$$\mathcal{G}(p) \leq \dots \leq \left(\frac{1}{\lambda_1} - \frac{1}{\lambda_2} \right) \frac{1}{3} \sum_{a=1}^3 |\tilde{\psi}_1^a(p)|^2 + \frac{1}{\lambda_2} \leq \frac{1}{\lambda_1} \quad (6.52)$$

as the new upper ones. We should stress that these constraints are valid for any momentum p , including $p_{\min} = 2 \sin(\pi/N)$, which is the dominant lattice momentum in the infrared region, and to any configuration inside $\partial\Omega$.

In Refs. 187, 202 it was numerically shown that indeed $\mathcal{G}(p_{\min}) \rightarrow \frac{1}{\lambda_1}$ as the lattice gets larger, which means that the upper bound in (6.49) seems to saturate in the infinite-volume limit. Also, it was verified that $\lambda_2 \rightarrow \lambda_1$ and that the first improved upper bound involving λ_2 in (6.52) also approaches saturation as N grows, which is a verification that all Gribov horizons correspond to one horizon.¹⁰⁰ On the other hand, it was also verified that the above lower bound and its first improvement are very far from saturating the inequalities (6.51) and that the gap gets larger for growing N . Indeed, in a spectral decomposition of the ghost propagator hundreds of low-lying eigenvectors are needed to reasonably reproduce its full value.²²⁷

Another bound that helps control the infrared behavior of the ghost propagator was proposed in Ref. 202. It consists of a lower bound for λ_1 and explicitly relates $\mathcal{G}(p)$ to the geometry of gauge-space. Consider the Gribov region's properties given in Section 3.1.2. In particular, if we set $A^{(1)} = \rho A$ and $A^{(2)} = 0$ with $\rho \in [0, 1]$ in Equation (3.11), we then have (in continuum notation)

$$\mathcal{M}[\rho A] = (1 - \rho) (-\square) + \rho \mathcal{M}[A], \quad (6.53)$$

which by the convexity property gives $\rho A \in \Omega$. If we consider this same equation for a configuration $\rho A' \in \partial\Omega$, i.e. sitting on the Gribov horizon, and look at its smallest eigenvalue, then we can rewrite

$$\lambda_1 \{\mathcal{M}[\rho A']\} = \lambda_1 \{(1 - \rho) (-\square) + \rho \mathcal{M}[A']\} = \min_{\gamma} (\gamma, [(1 - \rho) (-\square) + \rho \mathcal{M}[A']] \gamma), \quad (6.54)$$

where $(\gamma, \gamma) = 1$ and the minimum function was used excluding the trivial null space of $\mathcal{M}$. In a finite volume, of course λ_1 stays positive if $\rho \in [0, 1]$. We can use the last formula together with the concavity property of the minimum function to state the inequality²⁰²

$$\begin{aligned} \lambda_1 \{\mathcal{M}[\rho A']\} &= \min_{\gamma} \{\gamma, [(1 - \rho) (-\square) + \rho \mathcal{M}[A']] \gamma\} \\ &\geq (1 - \rho) \min_{\gamma} \{(\gamma, -\square \gamma)\} + \rho \min_{\gamma} \{(\gamma, \mathcal{M}[A'] \gamma)\} \\ &= (1 - \rho) \lambda_1 \{-\square\} + \rho \lambda_1 \{\mathcal{M}[A']\} \\ &= (1 - \rho) \lambda_1 \{-\square\} = (1 - \rho) p_{\min}^2, \end{aligned} \quad (6.55)$$

where at the end we used that p^2 are eigenvalues of the Laplacian operator and that $\lambda_1 = 0$ on the Gribov horizon, by definition. Therefore, translated to lattice notation, we have the following set of upper bounds for the ghost propagator

$$\mathcal{G}(p) \leq \frac{1}{\lambda_1} \leq \frac{1}{(1 - \rho) p_{\min}^2}. \quad (6.56)$$

Inspecting (6.55), we notice that the bound involving ρ is saturated when the problem reduces to the Abelian case, i.e., when $\mathcal{M}$ is equal to the negative Laplacian operator and $\lambda_1 = p_{\min}^2$. This essentially means that all the non-Abelian effects from a given configuration A are contained in the factor $1 - \rho$.

If we follow the demonstration of property (3) in Section 3.1.2, we know that if we choose $\rho > 1$ we can get a gauge configuration outside Ω for large enough ρ . This gives us the intuition that ρ should be related to some kind of distance in the Gribov region and defined over the gauge-space. In fact, this can be shown by considering the distance function in the gauge-space

$$d^2[A^{(1)}, A^{(2)}] = \frac{1}{12N^4} \sum_{x \in \Lambda} \sum_{\mu=1}^4 \text{Tr} \left\{ [A_\mu^{(1)}(x) - A_\mu^{(2)}(x)]^\dagger [A_\mu^{(1)}(x) - A_\mu^{(2)}(x)] \right\}. \quad (6.57)$$

If we consider again $A^{(1)} = 0, A^{(2)} = \rho A'$ with $\rho \in [0, 1]$ and $A'_\mu \in \Omega$, and apply the distance formula, then

$$d^2[0, \rho A'] = \frac{\rho^2}{12N^4} \sum_{x \in \Lambda} \sum_{\mu=1}^4 \sum_{a=1}^3 (A'_\mu{}^a)^\dagger A'_\mu{}^a \equiv \rho^2 \|A'\|^2, \quad (6.58)$$

which means that ρ can in fact be viewed as a normalized distance of $\rho A' \in \Omega$ from the origin of the gauge-space, i.e.,

$$\rho = \sqrt{\frac{d^2[0, \rho A']}{\|A'\|^2}}. \quad (6.59)$$

Moreover, $1 - \rho$ can be viewed as a distance of $\rho A'$ from the Gribov horizon. Thus, the ρ bound in (6.56) tells us that the infrared behavior of the Landau ghost propagator is indeed constrained by the geometry of the Gribov region.

In view of the scaling-massive solution discussed in Sections 5.2.3 and 5.2.4, one can use the proposed infrared power-law for the ghost propagator, namely $\mathcal{G}(p) \sim p^{-2-2\kappa}$ for $p \rightarrow 0$, to numerically study the infrared exponents associated to the above bounds. Assuming the behavior $\lambda_1 \sim p^{2+\alpha} \sim N^{-2-\alpha}$ ^G, we can say that a necessary condition to obtain an enhanced ghost propagator is that $\alpha > 0$, i.e., $\kappa > 0.5 > 0$ implies $\alpha > 0$. Moreover, considering the last bound and the fact that $p_{\min}^2 \sim N^{-2}$, we know that λ_1 cannot vanish faster than $(1 - \rho)p_{\min}^2$ when $N \rightarrow 0$ or, equivalently, that $\eta \geq \alpha$ for $1 - \rho \sim N^{-\eta}$ in the infrared.

^G The eigenvalues for the free case are p^2 and of course $p \sim 1/N$.

In Figure 6.6 we present preliminary results for the behavior of the bounds as N gets larger. Here we compute the bounds in Equation (6.56) using simple arbitrary copies of the corresponding configurations, i.e., we further fix them to minimal Landau gauge using the stochastic overrelaxation algorithm described in Section 4.2.3. We notice that all bounds are verified considering numerical imprecision. In Tables 3 and 4 we report fitting exponents from the data with a fit function of the form aN^{-b} . Further description for the lattice computation of ρ and details of the simulation will come in the next section.

Figure 6.6 – Bounds in (6.56) for full, center-projected and vortex-removed ensembles on lattices with sizes $N = 4, 8, 12$ (left). The same for single-instanton configurations using $N = 4, 8, 12, 16, 24, 32$. Fits to the data were done using the form aN^{-b} and the results for the exponents are presented in Tables 3 and 4.

Source: By the author.

Table 2 – Lattices used in Figures 6.6, 6.7, 6.9 with $\beta = 2.2$.

N	N_{cf}	N_{therm}	N_{cor}
4	500	500	50
8	25	500	50
12	15	700	50

Source: By the author.

For the center vortex scenario (Figure 6.6 (left), Table 3) we note that, for the small lattice sizes considered, the full ensemble supports an enhanced propagator, as in early lattice simulations. For the vortex-only ensemble the exponents decrease drastically and enhancement is most probably lost. On the other hand, the vortex-removed ensemble seems to carry most of the contribution from the full counterpart but appears to possess less than a free-like pole, at least for the small lattice sizes used, being the geometric bound in this case the most saturated one.²⁰² These data are to be taken with a grain of salt for they were extracted from small lattices, being simulations up to $N \sim 80$ necessary in order to draw more definitive conclusions. For instance, we know from huge lattice simulations that most probably enhancement disappears on huge lattices,^{29,182} which is supported by the bound analysis in Refs. 187,202. Moreover, we clearly see that, at least for the vortex-only and vortex-removed cases, the extrapolation indicates $\mathcal{G}^{-1}(p_{\min}) < \lambda_1$ for $N \rightarrow \infty$, similarly to data in Ref. 202, in contradistinction with the expected exponents from the analytical bounds. How such bounds are realized for large lattices waits for larger simulations and more reliable fits.

Table 3 – Fit information for the bounds (6.56) in full, vortex-removed and projected ensembles, see Figure 6.6 (left).

Ensemble Type	$\mathcal{G}(p_{\min})^{-1}$	λ_1	$p_{\min}^2(1 - \rho)$
Full	2.10(9)	2.69(6)	3.79(11)
Projected	0.62(21)	0.31(6)	1.91(1)
Removed	1.89(1)	1.74(1)	2.056(2)

Source: By the author.

For the BPST case (Figure 6.6 (right), Table 4), we verify that $\kappa, \alpha < 0$, implying that enhancement of the ghost propagator is not supported for instanton background configurations. The geometric bound is far from being saturated just as in Ref. 202 for thermalized configurations. Nevertheless, the fits show a reasonable infinite-volume extrapolation, especially if the small lattices are progressively eliminated. When only the largest lattices are considered, the ghost propagator seems to have at most a free-like pole. Simulations on larger lattices and different background configurations should extend and confirm these results.

Table 4 – Fit information for the bounds (6.56) in single instanton configurations, see Figure 6.6 (right). Different N sets were used to estimate the infrared behavior.

Used N	$\mathcal{G}(p_{\min})^{-1}$	λ_1	$p_{\min}^2 (1 - \rho)$
$4, \dots, 32$	1.811	1.700	2.811
$16, \dots, 32$	1.981	1.899	2.539
$24, 32$	1.992	1.952	2.515

Source: By the author.

6.3.2 R functional

Back in Section 4.2 we presented the lattice minimizing functional $\mathcal{E}$ that was used to define the Gribov region on the lattice. There we show that its local minima correspond to different Gribov copies, i.e., that

$$\mathcal{E}'(\tau = 0) = 0 \quad (6.60)$$

corresponds to a Gribov copy at $\tau = 0$. Furthermore, we derived the Faddeev-Popov matrix from the second derivative of $\mathcal{E}$.

We can use further information from this functional around a given copy to characterize the local geometry of the Gribov region. If we expand it to the fourth order around $\tau = 0$, we have¹²⁴

$$\begin{aligned} \mathcal{E}(\tau) &= \mathcal{E}(0) + \tau \mathcal{E}'(0) + \frac{\tau^2}{2} \mathcal{E}''(0) + \frac{\tau^3}{3!} \mathcal{E}'''(0) + \frac{\tau^4}{4!} \mathcal{E}''''(0) + \mathcal{O}(\tau^5) \\ &= \mathcal{E}(0) + \frac{\tau^2}{2} \left[\mathcal{E}''(0) + \frac{\tau}{3} \mathcal{E}'''(0) + \frac{\tau^2}{12} \mathcal{E}''''(0) \right] + \mathcal{O}(\tau^5), \end{aligned} \quad (6.61)$$

and we can write it as (omitting higher orders)

$$\mathcal{E}(\tau) = \mathcal{E}(0) + \frac{\tau^2 \mathcal{E}''(0)}{2} \left[1 + \frac{1}{3} \frac{\tau \mathcal{E}'''(0)}{\mathcal{E}''(0)} + \frac{1}{12R} \left(\frac{\tau \mathcal{E}'''(0)}{\mathcal{E}''(0)} \right)^2 \right], \quad (6.62)$$

where the R functional is

$$R \equiv \frac{\mathcal{E}'''(0)^2}{\mathcal{E}''(0) \mathcal{E}''''(0)}. \quad (6.63)$$

With this we see that the quadratic equation in the variable $x = \frac{\tau \mathcal{E}'''(0)}{\mathcal{E}''(0)}$,

$$\frac{x^2}{R} + 4x + 12 = 0, \quad (6.64)$$

gives a profile of $\mathcal{E}$ around a Gribov copy.^{90,124}

We compute the expressions for the third and fourth derivatives on the lattice at $\tau = 0$ in order to access the R functional for arbitrary configurations along some chosen ψ_i . In view of its geometrical importance in the ghost sector, we choose to compute the

smallest eigenvalue λ_1 and the associated eigenvector $\gamma = \psi_1$. This is achieved first by computing $\mathcal{E}''(0) = 4N^4\lambda_1$ through a power iteration method (see D.2), which also gives ψ_1 as an output. The third derivative at $\tau = 0$, following the notation of Section 4.2 and setting $\gamma = \psi_1$, is given by

$$\mathcal{E}'''(0) = -\frac{1}{N^4} \sum_{x \in \Lambda} \sum_{\mu=1}^4 \sum_{a=1}^3 \left\{ \frac{3}{4} [\gamma^2(x + \hat{\mu}) - \gamma^2(x)] [\gamma^a(x + \hat{\mu}) + \gamma^a(x)] u_\mu^a(x) \right. \\ \left. + \gamma^2(x) \gamma^a(x) [u^a(x) - u^a(x - \hat{\mu})] \right\}. \quad (6.65)$$

The fourth derivative, similarly, is

$$\mathcal{E}''''(0) = \frac{1}{N^4} \sum_{x \in \Lambda} \sum_{\mu=1}^4 \left\{ [\gamma^2(x + \hat{\mu}) - \gamma^2(x)]^2 u_\mu^4(x) \right. \\ \left. - \gamma^2(x) \sum_{a=1}^3 \left[\gamma^a(x) \sum_{y \in \Lambda} \sum_{a=1}^3 \mathcal{M}^{ab}(x, y) \gamma^b(y) \right] \right\}. \quad (6.66)$$

Here, the Faddeev-Popov matrix applied to γ is given by (6.46).

Following the lines of Ref. 202, we can interpret the effect of removing the vortex content on the third derivative (6.65). A null value for $\mathcal{E}'''(0)$ indicates that the configuration is close to the common boundary of the first Gribov region and the fundamental modular region or, at least, is a good candidate for being on it.¹⁰⁶ In Figure 6.7 we gather histograms on the (absolute value of the) third derivative along ψ_1 for the configurations in Table 5. We notice that the center-projection procedure makes $\mathcal{E}'''(0)$ a factor of 100 smaller than in full configurations, indicating that the former are closer to $\partial\Omega \cap \partial\Lambda$ than the full ones.

Third Derivative - Frequence Histograms

Figure 6.7 – Frequence of third derivative in full and vortex-removed ensembles.

Source: By the author.

6.3.3 Crossing the Gribov horizon

We can follow Ref. 202 and “simulate” the demonstration of property (3) of the Gribov region. This consists in walking a given Monte Carlo configuration out of Ω by slightly scaling the lattice gauge field $\mathcal{A}$ by some factor $\gtrsim 1$. Explicitly, for the i -th scaling step we do

$$\mathcal{A} \rightarrow \mathcal{A}^{(i)} = \tau_i \mathcal{A}, \quad (6.67)$$

where τ_i follows the prescription

$$\tau_i = \tau_{i-1} \delta, \quad \tau_0 = 1, \quad \delta = \begin{cases} 1.001, & \text{if } \lambda_1 \geq 5 \times 10^{-3} \\ 1.0005, & \text{if } 5 \times 10^{-3} \geq \lambda_1 \geq 5 \times 10^{-4} \\ 1.0001, & \text{if } \lambda_1 < 5 \times 10^{-4} \end{cases} . \quad (6.68)$$

We know that, after executing enough steps, the configuration $\mathcal{A}^{(n)}$ for some n will have a negative eigenvalue and then be outside the Gribov region. On the lattice, the R functional is the only one of the Landau gauge-fixing quantities that shows an abrupt change when crossing the Gribov horizon, i.e., when λ_1 goes to zero and changes signal. Therefore it can be used as an indication that the gauge field “crossed” the Gribov horizon.

Walking the configurations to the Gribov horizon through the procedure above also enable us to compute an estimate of ρ on lattice simulations,²⁰² where $\rho \in [0, 1]$ is a normalized distance of a gauge configuration to $\partial\Omega$ (see Equation (6.59)). Supposing the R functional abruptly changes its value going from step $n-1$ to step n , we prescribe that the configuration

$$\mathcal{A}' \equiv \frac{\mathcal{A}^{(n-1)} + \mathcal{A}^{(n)}}{2} = \frac{\tau_{n-1} + \tau_n}{2} \mathcal{A} \quad (6.69)$$

is the closest one to $\partial\Omega$ in the chain $\{\mathcal{A}^{(i)}\}$. Therefore, having (6.59) in mind,

$$\rho = \left(\frac{\tau_{n-1} + \tau_n}{2} \right)^{-1}. \quad (6.70)$$

This enables us to study the chain of bounds given in (6.56) on the lattice and to directly characterize the geometry of arbitrary gauge configurations.

As an example of this procedure, in Figure 6.8 instantons of varied sizes on different lattices are explicitly walked out of Ω . The bump in the value of R indicates that the horizon has been crossed. We note that progressively larger instantons need fewer steps for crossing $\partial\Omega$, which means that the larger an instanton is, the closer to the horizon it gets. A naive extrapolation of the data suggests that $\rho \sim 1$ for lattices of size $N \sim 70$ and instanton radius $R \sim 20$, but only larger-lattice simulations can really confirm that.

Figure 6.8 – Progressive rescaling of instanton configurations for different lattice sizes, until an abrupt change in R is noticed. The instanton radii are denoted by large ($N/2$), best ($N/3$) and small ($N/4$). The value of ρ for the large R instantons on $N = 4, 8, 16$ lattices corresponds to $\rho = 0.61, 0.74, 0.89$, respectively.

Source: By the author.

Table 5 – Below are listed some relevant average values of the geometric-like quantities for different kinds of ensembles, configurations and lattice sizes, where $\bar{\psi}_1$ is defined in (6.71). The thermalized configurations were generated at $\beta = 2.2$ (see Table 2). Instanton information was not taken from ensembles but for a single configuration each time, so that there are no errors associated to it.

	N	$\langle \lambda_1 \rangle$	$\langle \rho \rangle$	$\langle n \rangle$	$\langle \bar{\psi}_1(p_{\min}) \rangle$
Full	4	0.252(6)	0.877(3)	139(4)	0.0275(3)
	8	0.040(3)	0.967(2)	39(2)	0.0174(7)
	12	0.012(2)	0.987(2)	20(2)	0.013(1)
Proj.	4	0.015(4)	0.991(3)	53(31)	0.0210(4)
	8	0.0076(1)	0.99516(1)	9.08(8)	0.0097(5)
	12	0.0067(1)	0.99512(2)	9.9(4)	0.0068(5)
Rem.	4	0.968(2)	0.564(1)	576(1)	0.03638(4)
	8	0.296(3)	0.641(3)	451(3)	0.0375(1)
	12	0.1426(8)	0.660(2)	424(2)	0.03856(9)
BPST	16	0.1057	0.8739	139	0.0267
	24	0.0492	0.8996	114	0.0290
	32	0.0281	0.9136	101	0.0299

Source: By the author.

We can also use the lattices specified in Table 2 to analyze the various quantities presented above under the center projection and vortex removal procedures. In Figure 6.9 (left), we verify two quantities indicating the proximity of a given configuration to

the Gribov horizon. It is noticeable how the spreading character of the full ensembles is removed in the vortex-only and vortex-removed ensembles, where the data becomes clustered. More specifically, center-projection makes λ_1 as small as possible and ρ as close as possible to 1, indicating that center vortex configurations (blue, violet and cyan) are indeed localized on $\partial\Omega$ when transformed to minimal Landau gauge ^H. Conversely, the configurations where vortices are canceled (orange) present the opposite behavior, i.e., they are brought far from the Gribov horizon. In this view, they are closer to the perturbative region compared to the thermalized ensemble, at least for the copies considered.

Figure 6.9 – Scatter plot of the normalized distance from $\partial\Omega$ and the smallest eigenvalue for full, projected and vortex-removed ensembles.

Source: By the author.

In Figure 6.9 (right), we present the behavior of two quantities that can be related to the proximity of the common boundary of Ω and Λ . Small values of the third derivative $\mathcal{E}'''$, as we mentioned before, can indicate configurations on $\partial\Omega \cap \partial\Lambda$. Moreover, R presents a similar behavior for configurations next to the common boundary.²⁰² We can thus read the considerably systematic decrease of $\mathcal{E}'''$ and R in center-projected configurations as an indication that center vortices are closer to $\partial\Omega \cap \partial\Lambda$ when compared to their unprojected counterparts. This is consistent with the fact that center vortices correspond to singular points on $\partial\Omega \cap \partial\Lambda$ when brought to the *absolute* minimal Landau gauge and in fact could possibly be used to triangulate this complicated region.^{22,38} Due to such a singularity of the vortex-only configurations, we also proposed, after transforming them using stochastic overrelaxation with random start (see Subsection 4.2.3), to slightly scale down the obtained

^H By using the degeneracy of center-related gauge orbits, in Refs. 22,38 it was shown that, when brought to minimal Landau gauge, center vortices lie on $\partial\Omega$.

$\mathcal{A}$ as in (6.67) with $\tau = 0.995$. This greatly improved the near-singular matrix inversions¹, which indicates the presence of a non-trivial null space besides the trivial one associated to constant vectors.^{22,38} We shall further explore these issues in a future work.

Figure 6.10 – Average projection on plane-wave versus the inverse of smallest eigenvalue.

Source: By the author.

Finally, we remark that, as pointed out in Ref. 202, configurations that tend to saturate the geometric bound (6.56) and the lower one in (6.49) probably support an enhanced ghost propagator and thus the scaling solution of Dyson-Schwinger equations. In Figure 6.6, we note that the geometric bound in the center-projected ensemble is very far from being saturated. Contrarily, the vortex-removed ensemble approximates well-enough the geometric bound and suggests that they will maybe retain an enhanced behavior for larger lattices. Furthermore, also in Ref. 202 it was noted that those configurations' low-lying eigenvector should have a considerable overlap with the ones for the free case (Abelian), measured by the average overlap with the $p_{\min}$ plane-wave

$$\bar{\psi}_1(p_{\min}) \equiv \frac{1}{12N^4} \sum_{\mu=1}^4 \sum_{a=1}^3 \left| \sum_{x \in \Lambda} \psi_1^b(x) e^{-2i\pi x_\mu/N} \right|^2. \quad (6.71)$$

Here, that is evidenced in Figure 6.10, where it is shown that vortex-removed configurations cluster at the highest value of the average projection on plane-waves, while the vortex-only

¹ This rescaling is the reason why the value of ρ is very close to but not exactly 1 in the vortex configurations considered.

ones approximately preserve the thermalized spreading. This is further confirmed by the proximity of the vortex-removed configurations' smallest eigenvalue to the free (Laplacian) eigenvalues (indicated by black arrows).

7 CONCLUSIONS

In this work we attempted to reunite the basic conceptual and computational tools necessary to numerically study confinement from Gribov's perspective through lattice gauge theory. Also, we related the Gribov approach to the configuration-like approach, where confinement is attributed to certain classes of configurations, following the suggestion of Ref. 228.

We reviewed how to discretize a BPST instanton and measure its topological charge on the lattice, being this a semi-classical configuration once thought to be intimately related to confinement. We reproduced the essential results of Refs. 203–205. These support that center vortices are indeed responsible for the linearly rising potential between static quark and antiquark, a classical indicator of confinement. We also partially reproduced the results of Ref. 225 and also presented preliminary data similar to Ref. 226 but for the $SU(2)$ theory. Only simulations on larger lattices will say if similar conclusions can be drawn or if data must be reinterpreted.

Following the lines of Refs. 187, 202, we analyzed the gauge-geometric properties of the aforementioned configurations through analytical bounds relating the ghost propagator to the smallest eigenvalue of the Faddeev-Popov operator and to the normalized distance of a configuration from the Gribov horizon. Regarding instanton backgrounds, we conclude that it is highly improbable that they can contribute to an enhanced ghost propagator, being similar to typical thermalized configurations in Ref. 202. Moreover, we numerically verify that center vortices are localized on the Gribov horizon when transformed to minimal Landau gauge and that most probably they are closer to the common boundary of the Gribov and the fundamental modular regions^{22,38} when compared to thermalized configurations.

We also conclude that the generated vortex-removed ensembles have the characteristics of configurations that almost saturate the geometric bound and have large eigenvector overlap with free modes. For large enough lattices, their progressive proximity to the horizon can lead to an enhanced ghost propagator. In this perspective, the center dominance picture of confinement hinders the lattice realization of a scaling solution, which extends the discussion of Ref. 202 on why it is not possible to obtain an enhanced ghost propagator on the lattice. Of course, more definite conclusions wait for simulations with high statistics and on sufficiently large lattices, as well as a possible study of the fractal dimension of such topological defects,²²⁹ work that will be presented elsewhere.

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Appendix

APPENDIX A – NOTATION

A.1 Minkowski space

In most of Chapter 2 we use the standard Minkowski metric in field theory

$$\eta^{\mu\nu} = \text{diag}(1, -1, -1, -1), \quad \mu, \nu = 0, 1, 2, 3. \quad (\text{A.1})$$

Thus, the Yang-Mills action is

$$S_{\text{YM}} = -\frac{1}{2} \int d^4x \, \text{Tr} F_{\mu\nu}(x) F^{\mu\nu}(x), \quad (\text{A.2})$$

the strength tensor is

$$F^{\mu\nu}(x) = \partial^\mu A^\nu(x) - \partial^\nu A^\mu(x) + i g_0 [A^\mu(x), A^\nu(x)], \quad (\text{A.3})$$

the transformation of the gauge field is

$$A^\mu(x) \rightarrow A^{\mu'}(x) = \mathfrak{g}(x) \left[A^\mu(x) - \frac{i}{g_0} \partial^\mu \right] \mathfrak{g}^\dagger(x) \quad (\text{A.4})$$

and the covariant derivative in the adjoint representation is

$$D^{\mu ab} = \partial^\mu \delta^{ab} + g_0 f^{abc} A^{\mu c}. \quad (\text{A.5})$$

Here we represent the Laplace operator by

$$\partial^2 = \partial_\mu \partial^\mu. \quad (\text{A.6})$$

A.2 Euclidean space

Yet in Section 2.3 we start using the Euclidean metric, which is given by

$$\delta_{\mu\nu} = \text{diag}(1, 1, 1, 1), \quad \mu, \nu = 1, 2, 3, 4. \quad (\text{A.7})$$

The implementation of the Wick rotation can be pragmatically viewed as the exchange

$$x_0 \rightarrow -i x_4. \quad (\text{A.8})$$

Furthermore, we must do the following substitutions

$$A_0^a \rightarrow i A_4^a \quad (\text{A.9})$$

$$F_{0i}^a \rightarrow i F_{4i}^a \quad (\text{A.10})$$

$$D_0^{ab} \rightarrow i D_4^{ab}. \quad (\text{A.11})$$

The action is then

$$\begin{aligned}
i S_{\text{YM}}^{\mathbb{M}} &= \frac{i}{2} \text{Tr} \int d^3x d x_0 \left(F_{ij}^a F_{ij}^a - F_{0i}^a F_{0i}^a - F_{i0}^a F_{i0}^a \right)^{\mathbb{M}} \\
&\rightarrow -\frac{i}{2} \text{Tr} \int d^3x (-i d x_4) \left(F_{ij}^a F_{ij}^a + F_{4i}^a F_{4i}^a + F_{i4}^a F_{i4}^a \right)^{\mathbb{E}} \\
&= -\frac{1}{2} \text{Tr} \int d^4x^{\mathbb{E}} (F_{\mu\nu}^a F_{\mu\nu}^a)^{\mathbb{E}} \equiv -S_{\text{YM}}^{\mathbb{E}},
\end{aligned} \tag{A.12}$$

where we drop the Euclidean identifier and simply write

$$S_{\text{YM}}^{\mathbb{E}} = \frac{1}{2} \int d^4x F_{\mu\nu}^a(x) F_{\mu\nu}^a(x). \tag{A.13}$$

From the substitutions in (A.9) we reach at the Euclidean forms for $F_{\mu\nu}$, A_μ and D_μ with identical expression to (A.3), (A.4) and (A.5), but with the indices running from 1 to 4.

APPENDIX B – PATH INTEGRAL SUPPLEMENT

B.1 Gaussian Integrals

Here we present useful formulas for treating Gaussian (quadratic in the fields) path integrals.

Bosonic Variables

The bosonic Gaussian integrals are based on the basic one-dimensional integral

$$\int da e^{-ca^2} = \sqrt{\frac{\pi}{c}}. \quad (\text{B.1})$$

Consider the finite dimensional Gaussian integral defined by the $N \times N$ real symmetric matrix (K_{ij}) , with lower indices indicating position or any other degree of freedom. If K is real and symmetric, there exists an orthogonal matrix S so that $SKS^T = K_D$ is a similar diagonal matrix whose elements are the eigenvalues of K . Then, using matrix notation, we change variables in the following integral from a to $a' = Sa$

$$\begin{aligned} z_0 &= \int \left(\prod_i^N da_i \right) e^{-\frac{1}{2}a^T K a} = \int \left(\prod_{i=1}^N da_i \right) e^{-\frac{1}{2}a^T S^T (SKS^T) S a} \\ &= \int \left(\prod_{i=1}^N da'_i \right) \left| \det \frac{\partial a}{\partial a'} \right| e^{-\frac{1}{2}a'^T K_D a'} = \prod_{i=1}^N \left(\int da'_i e^{-\frac{1}{2}a'^2_i (K_D)_{ii}} \right) = \sqrt{\frac{(2\pi)^N}{\det K}}, \end{aligned} \quad (\text{B.2})$$

where we used $\det \frac{\partial a}{\partial a'} = \det S = \pm 1$ and (B.1). Including N external sources j_i and completing squares through the substitution $a \rightarrow a + K^{-1}j$, we get

$$\begin{aligned} z_0[j] &= \int \left(\prod_{i=1}^N da_i \right) e^{-\frac{1}{2}a^T K a + j^T a} \rightarrow z_0[j] = \int \left(\prod_{i=1}^N da_i \right) e^{-\frac{1}{2}a^T K a + \frac{1}{2}j^T K^{-1}j} \\ &= \left(\int \prod_{i=1}^N da'_i e^{-\frac{1}{2}a'^2_i (K_D)_{ii}} \right) e^{\frac{1}{2}j^T K^{-1}j} = \sqrt{\frac{(2\pi)^N}{\det K}} e^{\frac{1}{2}j^T K^{-1}j}. \end{aligned} \quad (\text{B.3})$$

Using the notation of the free gauge fields, the generalization to path integrals is

$$\begin{aligned} \mathcal{Z}_A^0[J] &= \int \mathfrak{D}A e^{-\frac{1}{2} \int d^4x d^4y A_\mu^a(x) K_{\mu\nu}^{ab}(x,y) A_\nu^b(y) + \int d^4x J_\mu^a(x) A_\mu^a(x)} \\ &= \mathcal{N} (\det K)^{-1/2} e^{\frac{1}{2} \int d^4x d^4y J_\mu^a(x) (K^{-1})_{\mu\nu}^{ab}(x,y) J_\nu^b(y)}, \end{aligned} \quad (\text{B.4})$$

where here $\det K$ is the functional determinant of the operator K and $\mathcal{N}$ is a (infinite) constant (which generally cancels out in computations and thus is omitted most of the times).

Fermionic variables

We can define the properties of a finite set of N Grassmann variables $\{n_i\}$ by their anticommutation relations

$$\{c_i, c_j\} = 0. \quad (\text{B.5})$$

We call them the generators of a Grassmann algebra. Derivatives in this space are defined operationally by

$$\left\{ \frac{\partial}{\partial c_i}, c_j \right\} = \delta_{ij}, \quad \left\{ \frac{\partial}{\partial c_i}, \frac{\partial}{\partial c_j} \right\} = 0, \quad (\text{B.6})$$

and integrals by

$$\int dc_i = 0 \quad \text{and} \quad \int dc_i c_i = 1. \quad (\text{B.7})$$

Take a set of $2N$ complex Grassmann variables $\{\bar{c}_1, \dots, \bar{c}_N, c_{N+1}, \dots, c_{2N}\}$. Using this convenient notation, we want to calculate the fermionic Gaussian integral defined by

$$z_0^e = \int \left(\prod_i d\bar{c}_i dc_i \right) e^{-\bar{c} H c}, \quad (\text{B.8})$$

where H is an $N \times N$ Hermitian matrix. We can proceed in the following way.²⁵ Spelling out the summations, we express the exponential as the simple fermionic Taylor series,

$$\begin{aligned} e^{-\sum_{i=1}^N \bar{c}_i \sum_{j=1}^N H_{ij} c_j} &= \prod_{i=1}^N e^{-\bar{c}_i \sum_{j=1}^N H_{ij} c_j} = \prod_{i=1}^N \left(1 - \bar{c}_i \sum_{j=1}^N H_{ij} c_j \right) \\ &= \left(1 - \bar{c}_1 \sum_{j_1=1}^N H_{1j_1} c_{j_1} \right) \dots \left(1 - \bar{c}_N \sum_{j_N=1}^N H_{Nj_N} c_{j_N} \right) = \sum_{j_1, \dots, j_N=1}^N c_{j_1} \bar{c}_1 \dots c_{j_N} \bar{c}_N H_{1j_1} \dots H_{Nj_N}, \end{aligned} \quad (\text{B.9})$$

where we used the anticommutation relations (B.5) and kept only non-vanishing terms after integration (B.8). Notice that this summation is antisymmetric under permutations of the indices and it contains only terms for which all the j 's are different. Thus, we can express it using the totally antisymmetric N -dimensional tensor $\epsilon_{j_1 \dots j_N}$ as

$$e^{-\sum_{i=1}^N \bar{c}_i \sum_{j=1}^N H_{ij} c_j} = c_1 \bar{c}_1 \dots c_N \bar{c}_N \sum_{j_1, \dots, j_N=1}^N \epsilon_{j_1 \dots j_N} H_{1j_1} \dots H_{Nj_N} = c_1 \bar{c}_1 \dots c_N \bar{c}_N (\det H), \quad (\text{B.10})$$

where we identified the tensorial definition of determinant. Finally, using the rules for fermionic integrals in (B.7) we can compute (B.8)

$$z_0^e = \det H \prod_{i=1}^N \left(\int d\bar{c}_i dc_i c_i \bar{c}_i \right) = \det H \quad (\text{B.11})$$

It is also possible to define the “hyperbolic” fermionic Gaussian integral (in opposition to the ‘elliptic’ one (B.8)) by modifying the order of integration

$$z_0^h = \int \left(\prod_i dc_i d\bar{c}_i \right) e^{\bar{c} H c}, \quad (\text{B.12})$$

Repeating the steps leading to the “elliptic” integral, we arrive at

$$z_0^h = \det H \prod_{i=1}^N \left(\int d\bar{c}_i d c_i \bar{c}_i c_i \right) = \det H. \quad (\text{B.13})$$

From now on we will mainly use the “hyperbolic” version of the integral.

We can add the complex sources $\bar{n}, n$ and, doing the substitutions $c \rightarrow c - H^{-1}n$ and $\bar{c} \rightarrow \bar{c} - H^{-1}\bar{n}$, we get

$$z_0^h[\bar{n}, n] = \int \left(\prod_i d\bar{c}_i d c_i \right) e^{\bar{c} H c + \bar{n} c + \bar{c} n} = \det H e^{-\bar{n} H^{-1} n}. \quad (\text{B.14})$$

The generalization to path integrals, using ghost notation, is

$$\begin{aligned} \mathcal{Z}_{\bar{c}, c}[\bar{\eta}, \eta] &= \int \mathcal{D}\bar{c} \mathcal{D}c e^{\int d^4x d^4y \bar{c}^a(x) \mathcal{H}(x, y) c^b(y) + \bar{\eta}^a(x) c^a(x) + \bar{c}^a(x) \eta^a(x)} \\ &= \det \mathcal{H} e^{-\int d^4x d^4y \bar{\eta}^a(x) (\mathcal{H}^{-1})^{ab}(x, y) \eta^a(y)}. \end{aligned} \quad (\text{B.15})$$

B.2 Generating Functional and Correlation Functions

The complete generating functional of Yang-Mills theory is given by

$$\mathcal{Z}_{\text{YM}}[J, \bar{\eta}, \eta] = \int \mathcal{D}A \mathcal{D}\bar{c} \mathcal{D}c e^{-S_{\text{FP}}[A, \bar{c}, c]}, \quad (\text{B.16})$$

where S_{FP} corresponds to the Faddeev-Popov action (2.138).

The general correlation function of $2n$ ghosts and m gauge fields is formally given by the analogue of (2.98), written in terms of the complete generating functional (B.16) as

$$\begin{aligned} &\left\langle \bar{c}^{a_1}(x_1) \dots \bar{c}^{a_n}(x_n) c^{b_1}(y_1) \dots c^{b_n}(y_n) A_{\rho_1}^{c_1}(z_1) \dots A_{\rho_m}^{c_m}(z_m) \right\rangle = \\ &\frac{1}{\mathcal{Z}_{\text{YM}}[0, 0, 0]} \frac{\delta}{\delta J_{\rho_m}^{c_m}(z_m)} \dots \frac{\delta}{\delta J_{\rho_m}^{c_m}(z_m)} \frac{\delta}{\delta \bar{\eta}^{b_n}(y_n)} \dots \frac{\delta}{\delta \bar{\eta}^{b_1}(y_1)} \frac{\delta}{\delta \eta^{a_n}(x_n)} \dots \frac{\delta}{\delta \eta^{a_1}(x_1)} \mathcal{Z}_{\text{YM}}[J, \bar{\eta}, \eta]. \end{aligned} \quad (\text{B.17})$$

We can obtain the correlation functions in momentum space by evaluating the Fourier transform of the above expressions. Alternatively, if we express all fields and sources using their Fourier integrals and correspondent Fourier components, the general correlation function in momentum space is directly obtained by

$$\begin{aligned} &\left\langle \bar{c}^{a_1}(k_1) \dots \bar{c}^{a_n}(k_n) c^{b_1}(p_1) \dots c^{b_n}(p_n) A_{\rho_1}^{c_1}(q_1) \dots A_{\rho_m}^{c_m}(q_m) \right\rangle = \\ &\frac{1}{\tilde{\mathcal{Z}}_{\text{YM}}[0, 0, 0]} \frac{\delta}{\delta J_{\rho_m}^{c_m}(q_m)} \dots \frac{\delta}{\delta J_{\rho_1}^{c_1}(q_1)} \frac{\delta}{\delta \bar{\eta}^{b_n}(p_n)} \dots \frac{\delta}{\delta \bar{\eta}^{b_1}(p_1)} \frac{\delta}{\delta \eta^{a_n}(k_n)} \dots \frac{\delta}{\delta \eta^{a_1}(k_1)} \tilde{\mathcal{Z}}_{\text{YM}}[J, \bar{\eta}, \eta], \end{aligned} \quad (\text{B.18})$$

where we define $\tilde{\mathcal{Z}}$ for a generic field $\phi(x)$ as

$$\mathcal{Z} = \int \frac{d^4k}{(2\pi)^4} e^{i k \cdot x} \int \mathcal{D}\phi(k) e^{-S[\phi]} \equiv \int \frac{d^4k}{(2\pi)^4} e^{i k \cdot x} \tilde{\mathcal{Z}}, \quad (\text{B.19})$$

and also normalize the functional derivative with respect to the Fourier components so that

$$\frac{\delta}{\delta\phi(k)}\phi(p) = (2\pi)^4\delta(k-p). \quad (\text{B.20})$$

B.3 Perturbation Theory

Series Expansion

The interacting theory can be approached by the perturbative method where we extract the interacting part of the action in terms of functional derivatives, namely, for a generic field ϕ

$$\mathcal{Z}[J] = \int \mathfrak{D}\phi e^{-S_0[\phi]-S_I[\phi]+\int d^4x J(x)\phi(x)} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-S_I \left[\frac{\delta}{\delta J} \right] \right)^n \int \mathfrak{D}\phi e^{-S_0[\phi]+\int d^4x J(x)\phi(x)}, \quad (\text{B.21})$$

or, using (B.19),

$$\tilde{\mathcal{Z}}[J] = \int \mathfrak{D}\phi e^{-S_0[\phi]-S_I[\phi]+\int \frac{d^4k}{(2\pi)^4} J(-k)\phi(k)} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-S_I \left[\frac{\delta}{\delta J} \right] \right)^n \int \mathfrak{D}\phi e^{-S_0[\phi]+\int \frac{d^4k}{(2\pi)^4} J(-k)\phi(k)}. \quad (\text{B.22})$$

For example, we can factorize the interacting term of the ghost Lagrangian and write $\mathcal{Z}_{\bar{c},c}$ as a Fourier expansion

$$\begin{aligned} \mathcal{Z}_{\bar{c},c}[\bar{\eta}, \eta; A] &= \int \mathfrak{D}c\bar{c} e^{-\int d^4x d^4y \bar{c}^a(x) \partial_\mu D_\mu^{ab}(x,y) c^b(y) + \int d^4x \bar{\eta}^a c^a + \bar{c}^a \eta^a} \\ &= \int \mathfrak{D}c\bar{c} e^{-g_0 f^{abc} \int d^4x A_\mu^c(x) \bar{c}^a(x) \partial_\mu c^b(x)} e^{-\int d^4x d^4y \bar{c}^a(x) \square^x \delta^{ab} \delta(x-y) c^b(y) + \int d^4x \bar{\eta}^a c^a + \bar{c}^a \eta^a} \\ &= \sum_{m=0}^{\infty} \frac{1}{m!} \left[-g_0 f^{abc} \int d^4x A_\mu^c(x) \frac{\delta}{\delta \eta^a(x)} \partial_\mu \frac{\delta}{\delta \bar{\eta}^b(x)} \right]^m \mathcal{Z}_{\bar{c},c}^0[\bar{\eta}, \eta], \end{aligned} \quad (\text{B.23})$$

where

$$\begin{aligned} \mathcal{Z}_{\bar{c},c}^0[\bar{\eta}, \eta] &= \int \mathfrak{D}c\bar{c} e^{-\int d^4x d^4y \bar{c}^a(x) \square^x \delta^{ab} \delta(x-y) c^b(y) + \int d^4x \bar{\eta}^a c^a + \bar{c}^a \eta^a} \\ &= \det L e^{-\int d^4x d^4y \bar{\eta}^a(x) \mathcal{G}_{(0)}^{ab}(x-y) \eta^a(y)}, \end{aligned} \quad (\text{B.24})$$

is the generating function of the free ghost theory and $[\mathcal{G}_{(0)}^{ab}]^{-1}(x-y) = -\delta^{ab} \square^x \delta(x-y)$ is the ghost kinetic operator.

Free Ghost Propagator

The free ghost propagator is obtained from the inverse of L in (B.24), which in momentum space reads as

$$[\mathcal{G}_{(0)}^{ab}]^{-1}(k) = -\delta^{ab} \int d^4z e^{-ik \cdot z} \square \delta(z) = \delta^{ab} k^2, \quad (\text{B.25})$$

which straightforwardly leads us to

$$\mathcal{G}_{(0)}^{ac}(k) [\mathcal{G}_{(0)}^{cb}]^{-1}(k) = \delta^{ab} \quad \therefore \quad \mathcal{G}_{(0)}^{ab}(k) = \frac{\delta^{ab}}{k^2}. \quad (\text{B.26})$$

Free Gluon Propagator

The free gluon propagator is derived in a similar way by inverting the Euclidean version of (2.48) in momentum space

$$K_{\mu\nu}^{ab}(k) = \delta^{ab} (\Gamma \delta_{\mu\nu} + \Lambda k_\mu k_\nu), \quad \text{with } \Gamma = k^2 \text{ and } \Lambda = 1/\alpha - 1. \quad (\text{B.27})$$

As the tensorial structure of this kinetic operator is slightly more complicated than in the ghost case, we take the following ansatz for the inverse

$$(K^{-1})_{\mu\nu}^{ab} = \delta^{ab} [A(k) \delta_{\mu\nu} + B(k) k_\mu k_\nu] \equiv \mathcal{D}_{(0)\mu\nu}^{ab}(k) \quad (\text{B.28})$$

we get

$$\delta_{\mu\nu} \delta^{ab} = K_{\mu\rho}^{ac}(k) \mathcal{D}_{(0)\rho\nu}^{cb}(k) = \delta^{ab} \Gamma A \delta_{\mu\nu} + \delta^{ab} (\Gamma B + \Lambda A + \Lambda B k^2) k_\mu k_\nu, \quad (\text{B.29})$$

resulting in $A = \Gamma^{-1}$, $B = -\Lambda \Gamma^{-1}/\Gamma + \Lambda k^2$ and, consequently,

$$\mathcal{D}_{(0)\mu\nu}^{ab}(k) = \delta^{ab} \left[\frac{\delta_{\mu\nu}}{k^2} + (\alpha - 1) \frac{k_\mu k_\nu}{k^4} \right]. \quad (\text{B.30})$$

APPENDIX C – GROUP SUPPLEMENT

C.1 Haar measure

In order to perform integrals over a $SU(N_c)$ group, it is advisable to formally define the invariant Haar measure.^{118,119} On a lattice Λ , the functional Haar measure corresponds to

$$\mathfrak{D}U = \prod_{x \in \Lambda} \prod_{\mu=1}^4 dU_\mu(x), \quad U_\mu(x) \in SU(N_c). \quad (\text{C.1})$$

We shall demand $\mathfrak{D}U$ to be invariant under right and left multiplication

$$dU = d[UV] = d[VU], \quad U, V \in SU(N_c) \quad (\text{C.2})$$

and fix

$$\int_{SU(N_c)} dU = \mathbb{1} \quad (\text{C.3})$$

as the normalization of the gauge volume.

We can express the Haar measure for $SU(N_c)$ through the $N_c^2 - 1$ independent parameters of the group, i.e. θ_j , $j = 1, 2, \dots, N_c^2 - 1$. We can write the metric on the group manifold as

$$ds^2 = g_{jk}(\theta) d\theta_j d\theta_k, \text{ where } g_{jk}(\theta) = \text{Tr} \left[\frac{\partial U(\theta)}{\partial \theta_j} \frac{\partial U(\theta)^\dagger}{\partial \theta_k} \right]. \quad (\text{C.4})$$

Then, dU is defined in terms of $d\theta$ as

$$dU = \mathcal{N} \sqrt{\det g} d\theta_1 \cdots d\theta_{N_c^2-1}, \quad (\text{C.5})$$

$\mathcal{N}$ being chosen so that the normalization condition (C.3) is satisfied. To verify that the last definition is left and right invariant we note that, by definition of a Lie group, $U(\theta_1, \dots, \theta_{N_c}) V(\alpha) = W(\tilde{\theta}_1, \dots, \tilde{\theta}_{N_c}; \alpha)$ such that $\tilde{\theta}_k = \tilde{\theta}_k(\theta_1, \dots, \theta_{N_c-1})$ is invertible, where $U, V, W \in SU(N_c)$. Therefore, the Jacobian corresponding to the change of variables $\theta \rightarrow \tilde{\theta}$ is $\det[J]$, with

$$J_{jk} = \frac{\partial \theta_j}{\partial \tilde{\theta}_k}. \quad (\text{C.6})$$

But

$$g_{jk}(\tilde{\theta}) = \text{Tr} \left[\frac{\partial U(\tilde{\theta})}{\partial \tilde{\theta}_j} \frac{\partial U(\tilde{\theta})^\dagger}{\partial \tilde{\theta}_k} \right] = \text{Tr} \left[\frac{\partial U(\theta)}{\partial \theta_n} \frac{\partial U(\theta)^\dagger}{\partial \theta_m} \right] \frac{\partial \theta_n}{\partial \tilde{\theta}_j} \frac{\partial \theta_m}{\partial \tilde{\theta}_k} = g_{nm}(\theta) J_{nj} J_{mk} \quad (\text{C.7})$$

$$= (J^T)_{jn} \left(g(\theta) \right)_{nm} (J)_{mk} = \left(J^T g(\theta) J \right)_{jk}, \quad (\text{C.8})$$

so that

$$dW(\tilde{\theta}) = \mathcal{N} \sqrt{\det[g(\tilde{\theta})]} \prod_j d\tilde{\theta}_j = \mathcal{N} \sqrt{\det[g(\theta)]} \underbrace{\sqrt{\det[J]^2} \prod_j d\tilde{\theta}_j}_{\prod_j d\theta_j} = dU(\theta). \quad (\text{C.9})$$

C.2 Integration

Some group integrals may be straightforwardly computed using (C.2) and (C.3). For example, integrals over matrix elements U_{ij} over the whole group can be expressed as

$$\begin{aligned} \int_{\text{SU}(N_c)} dU U_{ij} &= \int_{\text{SU}(N_c)} d[WU] (WU)_{ij} = \int_{\text{SU}(N_c)} dU (WU)_{ij} = W_{ik} \int_{\text{SU}(N_c)} dU U_{kj} \\ &\Rightarrow \int_{\text{SU}(N_c)} dU U_{ij} = 0, \end{aligned} \quad (\text{C.10})$$

because $dU = d[WU]$ and W is arbitrary, since the integral is necessarily null. A similar reasoning works for $\int_{\text{SU}(N_c)} dU U_{ij} U_{kl}$, etc.

A non-trivial and useful case is $\int_{\text{SU}(N_c)} dU U_{ij} (U^\dagger)_{kl}$. If $j \neq k$, then

$$\begin{aligned} \int_{\text{SU}(N_c)} dU U_{ij} (U^\dagger)_{kl} &= \int_{\text{SU}(N_c)} d[WU] (WU)_{ij} (U^\dagger W^\dagger)_{kl} = W_{in} (W^\dagger)_{ml} \int_{\text{SU}(N_c)} dU U_{nj} (U^\dagger)_{km} \\ &\Rightarrow \int_{\text{SU}(N_c)} dU U_{ij} (U^\dagger)_{kl} = 0. \end{aligned} \quad (\text{C.11})$$

To solve the case $j = k$, we write the contraction for the case $N_c = 2$

$$\int_{\text{SU}(2)} dU \left(U_{i1} (U^\dagger)_{1l} + U_{i2} (U^\dagger)_{2l} \right) = \int_{\text{SU}(2)} dU (UU^\dagger)_{il} = \delta_{il}, \quad (\text{C.12})$$

and note that each term contributes symmetrically to the integral. If, for instance, the labels 1 and 2 are interchanged, U will not be the same element of $\text{SU}(2)$, which does not matter because the integral is over the whole group. So, each of the terms contributes with one-half of the integral and, finally

$$\int_{\text{SU}(2)} dU U_{ij} (U^\dagger)_{kl} = \frac{1}{2} \delta_{il} \delta_{jk}, \quad (\text{C.13})$$

and naturally

$$\int_{\text{SU}(N_c)} dU U_{ij} (U^\dagger)_{kl} = \frac{1}{N_c} \delta_{il} \delta_{jk} \quad (\text{C.14})$$

for any N_c .

C.3 $\text{SU}(2)$ Conventions and Formulas

C.3.1 Pauli Matrices

Beginning in Chapter 4, we frequently use the particular 2-color Lie group $\text{SU}(2)$. We choose a specific basis for its Lie algebra, namely

$$T^a = \frac{\sigma^a}{2}, \quad a = 1, 2, 3, \quad (\text{C.15})$$

where σ^a are the Pauli matrices

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (\text{C.16})$$

Their commutation relation is given by the totally antisymmetric (Levi-Civita) symbol

$$[\sigma^a, \sigma^b] = 2i \varepsilon^{abc} \sigma^c. \quad (\text{C.17})$$

C.3.2 Trace Properties

We list here their basic trace properties

$$\text{Tr}(\sigma^a) = 0 \quad (\text{C.18})$$

$$\text{Tr}(\sigma^a \sigma^b) = 2\delta^{ab} \quad (\text{C.19})$$

$$\text{Tr}(\sigma^a \sigma^b \sigma^c) = 2i \varepsilon^{abc} \quad (\text{C.20})$$

$$\text{Tr}(\sigma^a \sigma^b \sigma^c \sigma^d) = 2(\delta^{ab}\delta^{cd} - \delta^{ac}\delta^{bd} + \delta^{ad}\delta^{bc}). \quad (\text{C.21})$$

C.3.3 Caley-Klein Parametrization

The Caley-Klein parametrization⁵⁵ of 2×2 complex matrices maps $\text{SU}(2)$ matrices in a real quadruplet. For $U \in \text{SU}(2)$ we may write down, for a fixed μ ,

$$U_\mu = u_\mu^4 \mathbb{1} + i u_\mu^a \sigma^a \equiv u_\mu^\rho \tau^\rho, \quad \text{where } u_\mu^\rho \in \mathbb{R}, \quad \rho = 1, 2, 3, 4 \quad (\text{C.22})$$

with the introduced $\text{SU}(2)$ basis given by

$$\tau^\rho = \tau_\rho = (i\sigma^1, i\sigma^2, i\sigma^3, \mathbb{1}) = (i\boldsymbol{\sigma}, \mathbb{1}). \quad (\text{C.23})$$

APPENDIX D – ALGORITHMS

Most of the computational work in this dissertation was implemented in *C*, being some fits done using *gnuplot*. All the computations were executed in a couple of cloud machines, each one with ~ 4 GB/RAM and a virtual CPU corresponding to a single thread of an Intel Xeon E5 ($\sim 2,0$ GHz). At the end, the total CPU-time sums up to a couple of weeks.

D.1 Conjugate Gradient

We use a standard conjugate gradient algorithm (CG)²⁰⁶ to invert the $(N_c^2 - 1)^2 V^2$ Faddeev-Popov matrix in the form of the linear system (see Equation (6.45))

$$\mathcal{M}\gamma = \psi, \quad (\text{D.1})$$

for some suitable source vector ψ . The CG routine is suitable to sparse systems and convergence is only guaranteed for symmetric and positive definite matrices. This is the case for the Faddeev-Popov operator in Landau gauge.⁹¹

We must remember that $\mathcal{M}$ possesses a trivial null-space corresponding to constant eigenvectors. It can be eliminated through the process devised in Ref. 174. Given a routine 'fpCG($\mathcal{M}, \gamma_0, \psi$)' that implements the conjugate gradient method, the removal of the null-space can be written as

```

Input:  $\gamma_0, \psi$ 
Output:  $x_0$ 
1 Function fpOrtCG( $\mathcal{M}, \gamma_0, \psi$ )
2    $b := \mathcal{M}\psi$ 
3    $a_0 := \text{cg\_guess}()$ 
4    $\text{fpCG}(\mathcal{M}, a_0, b)$ 
5    $x_0 := \text{cg\_guess}()$ 
6    $\text{fpCG}(\mathcal{M}, x_0, \psi)$ 

```

The subroutine `cg_guess()` chooses a suitable starting vector for the CG algorithm whose optimal value depends on each case.

D.2 Power Method

The smallest eigenvalue of $\mathcal{M}$ is computed through a power method algorithm.²⁰⁶ The power method is generally used to find the largest eigenvalue of a diagonalizable matrix. Nevertheless, we can combine it with a conjugate gradient routine in order to

compute the smallest eigenvalue of $\mathcal{M}$, what we call an inverse iteration method. This can be written as

```

Input:  $v'$ 
Output:  $v', \mu'^{-1}$ 
1 Function  $pmLambda1(\mathcal{M}, v')$ :
2    $v' := \text{eigenvector\_guess}()$ 
3    $\mu := 1$ 
4    $\mu' := 1$ 
5   while  $|\mathcal{M}v' - \mu'^{-1}v'| > \lambda_{tol}$  do
6      $\gamma_0 := \text{cg\_guess}()$ 
7      $\text{fpOrtCG}(\mathcal{M}, \gamma_0, v')$ 
8      $\mu := \mu'$ 
9      $\mu' := \frac{(v, v')}{(v, v)}$ 
10     $v' := \frac{v'}{|v'|}$ 
11   $v := v'$ 

```

The subroutine `eigenvector_guess()` chooses a suitable starting vector for the power method algorithm whose optimal value depends on each case. The algorithm stops when the eigenvalue has at least the precision given by λ_{tol} . Note that the power method yields the smallest eigenvalue as well as its associated eigenvector.