Lattice vs. Continuum: Landau Gauge Fixing and 't Hooft-Polyakov Monopoles

A Dissertation Submitted for the Degree of Doctor of Philosophy

by

Dhagash B. Mehta

Supervisors: Dr. Lorenz von Smekal and Prof. Anthony G. Williams

Centre for the Subatomic Structure of Matter, School of Chemistry and Physics, University of Adelaide. March, 2009. To my family and friends ...

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List of Acronyms

- 1. BKK Bernstein-Khovanskii-Kushnirenko
- 2. BRST Becchi-Rouet-Stora-Tyutin
- 3. CAD Cylindrical Algebraic Decomposition
- 4. CBB Classical Bezout Bound
- 5. CGB Comprehensive Groebner Basis
- 6. DSE Dyson-Schwinger Equation
- 7. FMR Fundamental modular region
- 8. LSZ Lehmann-Symanzik-Zimmermann
- 9. MLLG Modified lattice Landau gauge
- 10. NAG Numerical Algebraic Geometry
- 11. NPHC Numerical Polynomial Homotopy Continuation
- 12. QE Qunatifier Elimination
- 13. QED Quantum Electrodynamics
- 14. QCD Quantum Chromodynamics
- 15. RPXYM Random phase XY model
- 16. SLLG Standard lattice Landau gauge
- 17. SMV Stable Mixed Volume

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Abstract

In this thesis we study the connection between continuum quantum field theory and corresponding lattice field theory, specifically for two cases: Landau gauge fixing and 't Hooft-Polyakov monopoles.

To study non-perturbative phenomena such as the confinement mechanism of quarks and gluons and dynamical chiral symmetry breaking in Quantum Chromodynamics (QCD), there are two major approaches: the Dyson-Schwinger equations (DSEs) approach, which is based on the covariant continuum formulation, and lattice gauge theory. The strength and beauty of lattice gauge theory is due to the fact that gauge invariance is manifest and fixing a gauge is not required. In the covariant continuum formulation of gauge theories, on the other hand, one has to deal with the redundant degrees of freedom due to gauge invariance and has to fix gauge (most popularly, Landau gauge). There, the gauge-fixing machinery is based on the so-called Faddeev-Popov procedure or more generally, the Becchi-Rouet-Stora-Tyutin (BRST) symmetry. Beyond perturbation theory this is aggravated by the existence of so-called Gribov copies, however, that satisfy the same gauge-fixing condition, but are related by gauge transformations, and are thus physically equivalent. When attempting to fix Landau gauge on the lattice to make a connection with its continuum counterpart, this ambiguity manifests itself in the Neuberger 0/0 problem that asserts that the expectation value of any physical observable will always be of the indefinite form 0/0. We explain the topological nature of this problem and how the complete cancellation of Gribov copies can be avoided in a modified lattice Landau gauge based on a new definition of gauge fields on the lattice as stereographically projected link variables. For compact U(1), where the Gribov copy problem is related to the classification the local minima of XY spin glass models, we explicitly show that there still remain Gribov copies but their number is exponentially reduced in lower dimensional models. We then formulate the corresponding Faddeev-Popov procedure on the lattice, for these models. Moreover, we explicitly demonstrate that the proposed modification circumvents the Neuberger 0/0 problem for lattices of arbitrary dimensions for compact U(1). Applied to the maximal Abelian subgroup this will avoid the perfect cancellation amongst the remaining Gribov copies for SU(N), and so the corresponding BRST formulation is also then possible for generic SU(N), in particular, for the Standard Model groups.

For higher dimensional lattices, the gauge fixing conditions for both the standard and the modified lattice Landau gauges are systems of multivariate nonlinear equations, solving which in general is a highly non-trivial task. However, we show that these systems can be interpreted as systems of polynomial equations. They can then be solved exactly by computational Algebraic Geometry, the Groebner basis technique in particular, and numerically by the Polynomial Homotopy Continuation method.

't Hooft-Polyakov monopoles play an important role in high energy physics due to their presence in grand unified theories and their usefulness in studying non-perturbative properties of quantum field theories through electric-magnetic dualities. In the second part of the thesis, we study adjoint Higgs models, which exhibit 't Hooft-Polyakov monopoles, and have been extensively analyzed using semi-classical analysis in the continuum. However, to study them in a fully nonperturbative fashion, it is essential to put the theory on the lattice. Here, we investigate twisted C-periodic boundary conditions in SU(N) gauge field theory with an adjoint Higgs field and show that for even N with a suitable twist one can impose a non-zero magnetic charge relative to each of N - 1 residual U(1)'s in the broken phase, thereby creating 't Hooft-Polyakov magnetic monopoles. This makes it possible then to use lattice Monte-Carlo simulations to study the properties of these monopoles in the full quantum theory and compare them with the existing results in the continuum.

Statement of Originality

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Dhagash B. Mehta

Acknowledgements

Firstly, I am very thankful to my primary supervisor, Lorenz von Smekal, who first convinced me and then helping and supporting me to work on these extremely interesting problems. Mainly due to countless discussions with him and his encouragements this thesis has made thus far.

I thank my co-supervisor, Anthony G. Williams, who supported me in many ways including providing me assistance and support in many administrative problems. I am also very thankful to my both supervisors for giving me the creative freedom. I thank Arttu Rajantie who invited me to visit Imperial College London to work in collaboration with him and being my co-supervisor for more than 8 months during my ph.d.; Martin Schaden for very fruitful discussions at early and very important stage of this thesis during his visit to Adelaide; and Jon-Ivar Skullerud for his critical remarks on the thesis.

I thank Andre Sternbeck and Samuel Edwards for their wonderful collaborations, discussions, inputs and great help in proof-reading this thesis. Thanks to my friends at the CSSM, Ahmed Bakry, Marco Bartolozzi, Jonathan Carroll, Ben Crouch, Tat Chew, Marco Ghiotti, John Hedditch, Mariusz Hoppe, Antonio Laguna, Ben Lasscock, Selim Mehbub, Peter Moran, Alan O'Cais, Maria Parapilly, Skye Platten et al. who made my stay at CSSM a wonderful experience and also proof-read my thesis. Thanks to my office-mates at Theoretical Division at Imperial College London who made my visit to London a memorable experience.

I thank my postgraduate coordinator Rodney Crewther and Max Lohe for their kind help and guidance at many stages; to Varghese Mathai and all the postgraduate students in the Mathematics department of University of Adelaide; to Billy Hanan for his kind help in proof-reading a draft of this thesis; to Ramona Adorjan, Patrick Fitzhenry and the whole SAPAC team for their numerous technical help related to computers; and to Sara Boffa, Brownyn Gibson, Sharon Johnson, and Silvana Santucci for their tremendous administrative help.

I acknowledge the E-IPRS scholarships administrators who financially supported me throughout my ph.d. candidature and British Council and the University of Adelaide who funded me for my visit to London.

At personal level, I acknowledge the love and encouragement from my parents, wife, brother and my extended family. Thanks to my friends spread across the globe for their love, support and friendship.

Chapter 1

Introduction

1.1 Motivation

Quantum field theory [1] has provided the basis of the current understanding of particle physics first developed in the quantization of electrodynamics. Subsequent developments of the covariant perturbation expansion and renormalization made it clear that the local quantum field theory description of Quantum Electrodynamics (QED) is very accurate and immensely useful in explaining Lamb shift, higher order corrections to the elementary processes of electrons and photons etc. Since then this local quantum field theory approach has been applied to elementary particles together with collision theory, or more specifically, the so-called Lehmann-Symanzik-Zimmermann (LSZ) formalism, to theories such as Quantum Chromodynamics (QCD), the immensely successful theory of strong interactions. In the weak coupling regime of QCD, perturbative calculations in this approach have been shown to impressively match with experiments. In fact, there is now hardly a doubt that QCD is *the* theory of strong interactions [2, 3, 4].

Though the perturbative approach has been extremely successful, there are many important physical phenomena which need a non-perturbative treatment: the fundamental degrees of freedom of QCD, i.e., quarks and gluons have not been detected as isolated particles experimentally. This is quite a challenging puzzle, namely confinement, and a satisfactory understanding of the confinement mechanism is yet to be achieved even after numerous attempts [5]. Another example of a purely non-perturbative phenomenon which still needs to be better understood is dynamical chiral symmetry breaking in QCD. To understand such a non-perturbative phenomenon, a genuine non-perturbative approach to QCD is essential.

An immensely useful approach to study such non-perturbative phenomena is lattice field theory, which is a Euclidean space-time formulation of quantum field theory on the lattice [6, 7, 8]. In this approach, firstly, the space-time is transferred from Minkowski space to Euclidean space where time is imaginary. Then the Euclidean space-time is discretized, so the four-dimensional space-time integral is replaced by a discrete sum over all lattice points while derivatives are replaced by finite differences. Finally, methods used in statistical mechanics can be applied to calculate the expectation values of observables and the physical properties can be extracted using computer simulations on a finite lattice space-time grid.

In the continuum, well-developed methods like perturbation theory, semiclassical analysis or $\frac{1}{N}$ -expansions can be used to study field theories in general [1]. However, in the non-perturbative domain, the connection between the continuum and the corresponding lattice field theory is still under-developed. In this thesis we study this connection in two specific cases in the continuum and on the lattice: Landau gauge-fixing and 't Hooft-Polyakov monopoles.

1.2 Landau Gauge-fixing

In the continuum, a promising approach to study non-perturbative phenomena in QCD is to study truncated systems of Dyson-Schwinger equations (DSEs) [9], i.e., the equations of motion for QCD Green's functions. Here, a truncation requires additional sources of information such as Slavnov-Taylor identities, as entailed by gauge invariance, to specify vertex functions and higher *n*-point functions in terms of the elementary 2-point functions, i.e., the quark, ghost and gluon propagators. The basic quantity here is the generating functional, which requires gauge-fixing to remove redundant degrees of gauge freedom, in the so-called functional-integral formalism. The investigation of the gauge-dependent QCD Green's functions at low momentum can give a coherent description of hadronic states and processes and it is also important for an understanding of confinement in the so-called Kugo-Ojima confinement scenario. Most of the work in relation to the Kugo-Ojima scenario have been done in covariant gauges, more specifically, in Landau gauge.

The standard approach of gauge-fixing in the perturbative limit is called the Faddeev-Popov procedure [10]. There, a gauge-fixing device which is called the gauge-fixing partition function, Z_{GF} , is formulated. With an ideal gauge-fixing condition, Z_{GF} is equal to one. This unity is inserted in the measure of the generating functional so that the redundant degrees of freedom are removed after appropriate integration. The generalization of the Faddeev-Popov procedure is the Becchi-Rouet-Stora-Tyutin (BRST) formulation [11]. The assumption that the gauge-fixing condition is ideal, i.e., the gauge-fixing condition has a unique solution, is crucial here. A very important work of V. N. Gribov, in 1978, conveyed that in non-Abelian gauge theories a generalized Landau gauge-fixing condition would have multiple solutions, called Gribov copies [12, 13, 9]. In the perturbative limit, where perturbations around the trivial configuration of gauge fields are considered, the corresponding gauge-fixing condition has a unique solution, and

hence the BRST formulation in this limit is well-defined. In the non-perturbative regime, however, the effects of Gribov copies should be properly taken into account.

Now, the DSE approach has an unprecedented advantage in the low momenta region of QCD. However, lattice QCD provides an opportunity to do *first principle* calculations of non-perturbative quantities in QCD: the approximations involved in lattice QCD can be systematically removed, unlike the truncations of DSEs. Thus, lattice simulations can provide an independent check on the results obtained in the DSE approach. A gauge field theory put on the lattice is manifestly gauge invariant, i.e., one does not need to fix a gauge on the lattice to calculate gauge invariant observables. However, to study the DSE approach, Kugo-Ojima scenario and hadron phenomenology related to this approach on the lattice, gauge-dependent quantities and hence gauge fixing on the lattice are desired. Mainly for this reason, the lattice Landau gauge studies have gained a huge amount of interest recently (see, e.g., Ref. [9, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25] for both continuum and lattice DSE studies).

On the lattice, Landau gauge fixing is nowadays formulated as a functional minimization problem. That is, instead of solving the gauge-fixing condition, one numerically minimizes a gauge-fixing functional, called the lattice Landau gauge-fixing functional, whose first derivative with respect to gauge transformation is the gauge-fixing condition. Numerical functional minimization for the lattice Landau gauge-fixing functional can be done using variants and/or combinations of Simulated Annealing, Overrelaxation, Fourier acceleration etc. It is important to note that this is the same as finding minima, maxima or saddle points of a classical Hamiltonian [26, 27, 28] of a spin glass system, and the extrema and saddle points are Gribov copies of the lattice Landau gauge. Here one faces a major computational problem: finding the absolute minimum of a spin glass system becomes exponentially harder when increasing the lattice size.

There is one more obstacle on the lattice. A very important work of H. Neuberger conveyed that when performing the gauge-fixing procedure analogous to the Faddeev-Popov procedure on the lattice, which needs to take all extrema of the gauge fixing functional into account, the lattice analogue of the aforementioned unity, or Z_{GF} , turns out to be zero [29, 30, 31, 32, 33, 34] due to a perfect cancellation among Gribov copies. Thus, the expectation value of a gauge-fixed observable turns out to be of the indeterminate form 0/0. This problem is known as the Neuberger 0/0 problem. In other words, BRST formulations on the lattice can not be constructed. This is a severe problem: the continuum DSE studies of gauge theories are based on BRST formulations. But the Neuberger 0/0 problem prevents us from constructing the BRST formulation on the lattice. The lattice implementations of the Landau gauge are thought to have avoided this problem because there one hopes to find the absolute minimum of the gauge-fixing functional numerically. Since it is not feasible to find the absolute minimum, one settles for local minima, the set of which is called the first Gribov region, among which there is no cancellation. However, for the BRST formulation, sampling from all the possible gauge-fixed configurations, an averaging (say, Monte-Carlo averaging) over all extrema and saddle points of the gauge-fixing functional must be performed which for the standard definition of the lattice Landau gauge (which we call the standard lattice Landau gauge (SLLG)), will suffer from the Neuberger 0/0 problem.

Though early lattice studies of the gluon and ghost propagators for the SLLG supported their infrared behaviour predicted by the DSE approach qualitatively well, recently, large lattices have been used to study the finite-volume effects in the SU(2) theory to study observed puzzling discrepancies¹ in the infinite volume limit [36, 37, 38] and raised doubt on the Kugo-Ojima confinement criterion. This study suggested that the finite-volume effects appear to be ruled out as the dominant cause of the observed discrepancies between the continuum and lattice DSE studies. This poses the obvious question whether there is something fundamentally wrong with our general understanding of continuum covariant gauge theory or whether we are comparing two different scenarios, one in the continuum and another on the lattice. Thus, it is very important to have a proper Landau gauge-fixing procedure on the lattice for which the BRST formulation can be constructed, and therefore to settle down the issues related to the Kugo-Ojima confinement criterion from lattice studies [35].

The first important step in this direction was put forward by M. Schaden [39]. Schaden carried forward the Witten-type topological field theory on the lattice to show that Z_{GF} calculates the Euler characteristic χ , a topological invariant which counts holes of a manifold, of the group manifold G, at each site of the lattice in the SLLG. That is, for a lattice with n lattice-sites,

$$Z_{GF} = (\chi(G))^n. \tag{1.1}$$

For compact U(1) or any SU(N) the group manifolds are odd-dimensional spheres for which χ is zero. Thus, $Z_{GF} = (0)^n = 0$, for all the Standard Model groups. For SU(2) gauge theory, Schaden proposed to construct a BRST formulation for the coset space SU(2)/U(1) for which $\chi(SU(2)/U(1)) \neq 0$. This has been a remarkable achievement. This procedure can be generalized to fix the gauge of an SU(N) lattice gauge theory to the maximal Abelian subgroup $(U(1))^{N-1}$, since $\chi(SU(N)/SU(N-1)\times U(1)) \neq 0$ as well. This indicates that the Neuberger 0/0 problem for an SU(N) lattice gauge theory actually lies in $(U(1))^{N-1}$, and hence can be evaded if that for compact U(1) is evaded combined with Schaden's approach. For compact U(1), Gribov copy problem is purely a lattice artifact. In the present study, we propose a modification of the group manifold of compact

¹A discussion on the details about these discrepancies is beyond the scope of this thesis. The reader is referred to Ref. [35] for a recent review. Note that in this thesis, we do not comment on nor compare the results from both the continuum and lattice DSE scenarios. Instead, we simply study the connection between the essential framework (BRST formulation) in the continuum and on the lattice.

U(1), i.e., a circle S^1 , via stereographic projection at each lattice site. For such a stereographically projected manifold the corresponding χ is 1 and thus the Neuberger 0/0 problem is completely avoided. Applying the same technique to the maximal Abelian subgroup $(U(1))^{N-1}$, the generalization to SU(N) lattice gauge theories is possible when the odd-dimensional spheres S^{2k+1} , $k = 1, \ldots, N-1$ 1, of its parameter space are stereographically projected to the real projective space $\mathbb{R}P(2k)$ which is the set of all lines in \mathbb{R}^{2k+1} passing through the origin. In the absence of the cancellation of the lattice artifact Gribov copies along the U(1)circles, the remaining cancellations between copies in SU(N), which will persist in the continuum limit, are then necessarily incomplete because $\chi(\mathbb{R}P(2k)) = 1$. The precise implementation of the modified lattice Landau gauge (MLLG) is described in this thesis. In particular, we will establish that the Neuberger 0/0problem is completely evaded for an arbitrary dimensional lattice via the MLLG for compact U(1). Furthermore, we will show that in lower dimensional models for compact U(1), by solving the corresponding gauge-fixing equations analytically for different boundary conditions, the MLLG suppresses the number of Gribov copies compared to that for the SLLG.

The gauge-fixing equations for higher dimensional lattices are highly nonlinear and hence difficult to deal with. However, in this thesis we show that the non-linearity of these equations is *polynomial-like*. That is, the system of equations can be transformed in terms of multivariate polynomial equations. Then we can use some of the powerful results and algorithms of Algebraic Geometry and demonstrate how these equations can be solved exactly. We, moreover, use the Polynomial Homotopy Continuation method to solve these polynomial equations numerically.

Note that the Landau gauge-fixing functional for the SLLG for compact U(1) can be considered as the classical Hamiltonian of the random phase XY model (RPXYM) in condensed matter theory (see, e.g., [40, 41]). The special case, known as the trivial orbit case where all link variables are trivial, corresponds to the classical XY model. The classical XY model stands alongside the famous Ising and Heisenberg models as one of the most intensely studied models in statistical mechanics and condensed matter theory. The model has been widely studied as the simplest model of classical superconductivity and for several aspects of high- T_c superconductors [42], to describe the XY magnet with random Dzyaloshinski-Moriya interactions [43] or to describe a positional disordered Josephson junction array [44, 45]. In all cases, the calculations (related to Domain Wall Renormalization Group studies) again boil down to obtaining all local extrema of the above Hamiltonian. The calculations require an exact form of the ground state energies of this system with different boundary conditions and take the average of the difference between them, $\langle \delta E \rangle$, called the *defect energy* [46, 47].

1.3 't Hooft-Polyakov Monopoles

We move on to another problem where the lattice counterpart of the continuum needs special attention. The so-called 't Hooft-Polyakov monopoles [48, 49] play an important role in high energy physics for two reasons: their existence is a general prediction of grand unified theories and they provide a way to study non-perturbative properties of quantum field theories through electric-magnetic dualities [50]. In the continuum, the existence of 't Hooft-Polyakov monopole configurations have been demonstrated in Georgi-Glashow like models for any SU(N) with adjoint Higgs fields. They were studied via continuum semi-classical analysis [48, 49]. However, as a matter of fact, semi-classical continuum analysis might not always be a good guide to what happens in the fully fluctuating quantum ensemble as studied in Euclidean lattice field theory. There, the mass of 't Hooft-Polyakov monopoles in the three-dimensional SU(2) adjoint Higgs model has been demonstrated to vanish in both so-called confinement and Coulomb phases [51, 52]. We therefore study and generalize such a fully non-perturbative description of 't Hooft-Polyakov monopoles on the lattice for generic SU(N) and its relation with the continuum counterpart.

On the lattice, non-trivial boundary conditions, called twisted boundary conditions, can be chosen to insert 't Hooft-Polyakov monopoles and then one can study their nonperturbative quantum properties. This trick has been successfully demonstrated for the SU(2) model [51, 52]. The generalization of this trick to SU(N) is highly non-trivial since the elements of SU(2) group are quite special in several ways, e.g., there exist various representations of SU(2) to parameterize the corresponding S^3 in 3 parameters, the change of sign of the adjoint SU(2) Higgs field is a symmetry of the corresponding renormalized action density etc. In SU(N), for N > 2, one has neither of them in general. We discuss these aspects and explain our results. Specifically, we generalize this trick for all even N and we prove rigorously that the twisted C-periodic boundary conditions do not admit monopoles for odd N. We also relate the available continuum results with the results on the lattice.

1.4 Structure Of The Thesis

The thesis is organized as follows. In Chapter 2, we briefly describe the general Landau gauge fixing procedure both in the continuum and on the lattice. After discussing Gribov copies and the Neuberger 0/0 problem on the lattice, we explain their topological interpretation and provide the general idea behind the proposed MLLG. In Chapter 3, we specialize to the compact U(1) case. For the corresponding SLLG, we demonstrate the Gribov copy problem and the Neuberger 0/0 problem explicitly in lower dimensional models with both periodic and anti-periodic boundary conditions. We then show how the MLLG circum-

vents the Gribov copy problem in lower dimensional models and the Neuberger 0/0 problem in arbitrary dimension for compact U(1). We then summarize the chapter.

Solving the lattice Landau gauge fixing equations for higher dimensional lattices is a highly non-trivial problem. In Chapter 4, we transform the problem in terms of Algebraic Geometry. We devote the chapter to introducing several basic notions of Algebraic Geometry and the so-called Groebner basis technique, and demonstrate their usefulness to solve the gauge fixing equations exactly. We carry forward this discussion in Chapter 5 and introduce a numerical technique which is called the Polynomial Homotopy Continuation method. There, we obtain *all* solutions of the gauge fixing equations numerically for the SLLG on a two-dimensional lattice and analyze the solutions. We also translate many other problems in terms of Algebraic Geometry in a related Appendix for future work and conclude the chapter.

In Chapter 6, we study how different boundary conditions on the lattice for adjoint Higgs Grand Unified models admit 't Hooft-Polyakov monopoles in generic SU(N) models, for even N. We work out several important results and discuss the connection to the available continuum results.

Finally, in Chapter 7 we conclude the thesis and mention the related future research directions.

Chapter 2

Landau Gauge Fixing

In this chapter, we first introduce gauge field theories, describe the standard Faddeev-Popov gauge-fixing procedure in the continuum and pose the Gribov copy problem. After briefly introducing lattice field theory, we describe how gauge-fixing is done on the lattice. There, in addition to Gribov copies, one encounters the Neuberger 0/0 problem. We explain the topological interpretation of this problem. Motivated by the topological interpretation, we propose a modified lattice Landau gauge and go through the topological arguments again to show why we expect that this modification will circumvent the Neuberger 0/0 problem on the lattice.

2.1 Gauge Field Theories

Quantum Electrodynamics (QED), the quantum field theory of electromagnetism, has been remarkably successful in describing the interactions of electrons and photons. The classical Lagrangian of QED possesses a local Abelian (U(1)) gauge symmetry and hence QED is also called an Abelian gauge theory. The local U(1) gauge symmetry approach of QED has been extended to SU(N) formally, for any N, where the N = 3 case is known as Quantum Chromodynamics (QCD). QCD very successfully describes the strong interactions, however, it is fundamentally different than QED: the gauge boson of QED, the photon, does not carry any electric charge and therefore does not interact with other photons. On the other hand, the gluons, the gauge bosons of QCD, interact with each other and these self interactions are known to be responsible for asymptotic freedom in QCD. We briefly describe gauge field theory for SU(N) below [1].

Let T^a be the generators of the Lie algebra of SU(N), where $a = 1, ..., N^2 - 1$, with the commutation relations $[T^a, T^b] = if^{abc}T^c$, where f^{abc} are the totally antisymmetric structure constants of SU(N). The normalization of the generators is given by $Tr(T^aT^b) = C\delta^{ab}$ where the constant C depends on the representation of the generators. We use the fundamental representation here. The general form of the Lagrangian density of a pure Yang-Mills gauge theory in the Euclidean space, for SU(N), is

$$L_G = -\frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} , \qquad (2.1)$$

where $F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g_s f^{abc} A^b_\mu A^c_\nu$ are the field strengths, with $A_\mu = A^a_\mu T^a$ and $F_{\mu\nu} = F^a_{\mu\nu} T^a$. Note that for our discussion we are only interested in the pure gauge Lagrangian density. This Lagrangian density is invariant under arbitrary local gauge transformations $g(x) = \exp[ig_s\omega^a(x)T^a] \in \mathrm{SU}(N)$, where ω^a are spacetime dependent gauge transformations, i.e., under the transformation $A_\mu \to$ $(A_\mu)^g = g(x)A_\mu g^{\dagger}(x) + \frac{1}{g_s}g(x)\partial_\mu(g^{\dagger}(x))$, and g_s is the bare coupling constant. This local gauge-invariance has been a guiding principle to derive the QCD Lagrangian density. The corresponding pure gauge action, $S_G[A]$, is

$$S_G[A] = -\frac{1}{4} \int d^4 x F^a_{\mu\nu} F^{a\mu\nu}.$$
 (2.2)

Now to quantize this theory we use the functional-integral formalism introduced by Feynman [1]. There, the fields are taken to be c-numbers and the Lagrangian density (or just Lagrangian) takes its classical form. Now, a quantum field theory can be completely characterized by the infinite hierarchy of *n*-point functions (or Green's functions) which are a basis of the Dyson-Schwinger equations (DSEs) approach. In the functional-integral formalism in Euclidean space, these Green's functions can be obtained by a so-called generating functional or the path integration, which in the above pure gauge theory is formally¹ given as

$$Z = \int DA \ e^{-S_G[A]}.$$
(2.3)

Moreover, a vacuum expectation value of some gauge-invariant observable O[A] is formally defined as a functional integral, i.e.,

$$\langle O \rangle = \frac{\int DA \ O[A] \exp[-S_G[A]]}{\int DA \exp[-S_G[A]]} \ . \tag{2.4}$$

Here, $\int DA$ is to be understood as an integration over all gauge fields. Now, due to the gauge invariance of $S_G[A]$, the integration measure is ill-defined because of an infinite number of gauge fields corresponding to identical action, i.e., for each value of A there exists an infinite number of values A^g which give the same action. Thus, in Eq. (2.4) the numerator and the denominator are both infinite, giving $\langle O \rangle = \infty/\infty$.

Now, we say A and all A^g are equivalent and the set of all such equivalent gauge fields to A form an equivalence class, called the gauge orbit of A. Two

¹It is important to note that this is a *sourceless* generating functional. We omit a discussion of the source term since the rest of the discussion is independent of it. The reader is referred to Ref. [1] for related details.

gauge fields lying on different orbits are called inequivalent gauge fields, say A^{ineq} . Thus, formally, the functional integral over A can be thought of as

$$\int DA = \int DA^{\text{ineq}} \int Dg.$$
(2.5)

To get rid of the infinity in Eq. (2.4), the integration should be somehow restricted to only one gauge field per gauge orbit. That is, one needs to introduce an appropriate constraint into the integration that restricts the integral to one only over A^{ineq} . This can be done by introducing a constraint equation, say f[A] = 0, called gauge-fixing condition, via a delta functional in the integral. Ideally, the gauge-fixing condition should be satisfied at exactly one A per gauge orbit. With such an ideal gauge-fixing condition, the corresponding integral becomes welldefined. In practice, gauge fixing is done via the Faddeev-Popov procedure which we describe below.

2.1.1 Faddeev-Popov Gauge-fixing Procedure

Here, we briefly explain the Faddeev-Popov procedure [53, 54, 55, 10]. Firstly, recall from multivariable calculus the identity

$$\int d^{n}f \,\,\delta^{(n)}(\vec{f}) = 1, \tag{2.6}$$

where \vec{f} is a vector of real numbers with *n* components and $\delta^{(n)}(\vec{f})$ is a *n*dimensional delta function. If \vec{f} is specified by *n* functions $f_i(\vec{x})$ of *n* variables $\vec{x} = (x_1, \ldots, x_n)^T$, the integration is the product over integrations over all functions f_i and the above identity turns out to be

$$\int d^n f \,\,\delta^{(n)}(\vec{f}(\vec{x})) = \int d^n x \,\,\delta^{(n)}(\vec{f}(\vec{x})) \,\left| \det \frac{\partial f_i}{\partial x_j} \right|_{\vec{f}=\vec{0}} = 1, \tag{2.7}$$

where we have changed the integration variables from \vec{f} to \vec{x} and inserted the absolute value of the Jacobian determinant for this change of variables. Note that the last identity is true as long as $\vec{f}(\vec{x})$ has one zero within the integration range. To generalize this to the functional integration, we begin with the identity

$$\int Df \,\delta[f([A],x)] = 1, \qquad (2.8)$$

where Df is the functional integration measure and f([A], x) means that f is a functional of A and a function of x. Now, changing the variables from f to gauge transformation g in the above identity, we get

$$\int Dg \,\delta[f([A], x)] \,\Delta_{FP}[A] = 1, \qquad (2.9)$$

where $\Delta_{FP}[A]$ is called the Faddeev-Popov determinant. $\Delta_{FP}[A]$ is defined as the determinant of the Jacobian for the change of variables $M_{FP}([A])$, called the Faddeev-Popov operator, and defined as² $M_{FP}^{ab}([A], x, y) = \frac{\delta f([A^a], x)}{\delta g^b(y)}|_{f=0}$.

A very crucial assumption in the above equation is that f([A], x) has exactly one zero within the appropriate integration range. Using the unity in Eq. (2.9), we get

Using the unity in Eq. (2.9), we get

$$\int DA^{\text{ineq}} = \int DA^{\text{ineq}} \int Dg \,\delta[f([(A^{\text{ineq}})^g], x)] \,\Delta_{FP}[(A^{\text{ineq}})^g]$$
$$= \int DA \,\delta[f([A], x)] \,\Delta_{FP}[A].$$
(2.10)

Thus, the aforementioned path integration after inserting the unity of Eq. (2.9) and using Eq. (2.10), can be written as

$$Z = \int DA \,\,\delta[f([A], x)] \,\,\Delta_{FP}[A] \,\,e^{-S_G[A]} \,\,, \tag{2.11}$$

called the gauge-fixed partition function. Similarly, the gauge-fixed expectation value of O[A] reads as

$$\langle O \rangle = \frac{\int DA \ O[A] \ \delta[f([A], x)] \ \Delta_{FP}[A] \ e^{-S_G[A]}}{\int DA \ \delta[f([A], x)] \ \Delta_{FP}[A] \ e^{-S_G[A]}} \ .$$
(2.12)

Thus, both of them are now definite quantities. This is the essence of the Faddeev-Popov procedure of gauge fixing. One can also express Δ_{FP} in terms of Grassmann variables, for an ideal gauge-fixing condition, as

$$\Delta_{FP} = \int D\overline{c} \ Dc \ \exp\left[\left(-\int d^4x d^4y \ \overline{c}^a(x) M_{FP}^{ac}([A], x, y) c^c(y)\right)\right], \qquad (2.13)$$

where c and \overline{c} are Lorentz scalar, anti-commuting fields called Faddeev-Popov ghosts. These additional fields violate the spin-statistics theorem and thus do not correspond to physical particles.

Now, for the generalized Landau gauge $f([A], x) = \partial_{\mu}A_{\mu}(x) - k(x)$, with k(x) being an arbitrary function, we arrive at the expression for the expectation value of O[A] as

$$\langle O \rangle = \frac{\int DA \ Dc \ D\overline{c} \ O[A] e^{-S_{GF}[A,c,\overline{c}]}}{\int DA \ Dc \ D\overline{c} \ e^{-S_{GF}[A,c,\overline{c}]}}, \qquad (2.14)$$

where

$$S_{GF}[A,c,\bar{c}] = S_G[A] + \int d^4x \left(\frac{1}{2\xi} (\partial_\mu A^a_\mu)^2\right) + \int d^4x \ d^4y \ (\bar{c}^a(x)\partial^\mu D^{ac}_\mu c^c(y)) \ , \ (2.15)$$

²Note that usually Δ_{FP} is defined as the absolute value of the determinant of the Faddeev-Popov operator. However, for an ideal gauge fixing condition, the absolute sign can be ignored.

with ξ being the width of the Gaussian which is introduced to perform a Gaussian weighted average over the generalized covariant gauges. In the limit $\xi \to 0$, the Gaussian width vanishes and we recover the Landau gauge $\partial_{\mu}A_{\mu} = 0$.

Now, introducing the so-called Nakanishi-Lautrup [56] auxiliary fields b^a , we can write down the gauge-fixed Lagrangian as

$$L(A, c, \overline{c}, b) = -\frac{1}{4} (F^a_{\mu\nu})^2 - \frac{\xi}{2} (b^a)^2 - b^a \partial_\mu A^a_\mu + \overline{c}^a \partial_\mu D^{ac}_\mu c^c.$$
(2.16)

This Lagrangian is no longer gauge invariant due to the addition of gauge-fixing terms, i.e., the gauge invariance has been removed. This is what we desired in order to remove the infinities from $\langle O \rangle$. However, this Lagrangian is invariant under Becchi-Rouet-Stora-Tyutin (BRST) transformation [11],

$$sA^{a}_{\mu} = D^{ac}_{\mu}c^{c}, \ sc^{a} = -\frac{1}{2}g_{s}f^{abc}c^{b}c^{c}, \ s\overline{c}^{a} = b^{a}, \ sb^{a} = 0,$$
(2.17)

where s is the BRST operator³ which is nilpotent, i.e., $s^2 = 0$ [56].

The above Lagrangian can be obtained by starting from the ungauge-fixed action and requiring BRST invariance. Thus, the BRST invariance can be thought of as a generalization of gauge invariance because BRST symmetry implies gauge symmetry, though the reverse is not true. However, a little thought reveals that the expectaction value of any physical observable is independent of the gauge, even though the BRST symmetric Lagrangian is not. Note that the assumption of unique zero of the gauge-fixing conditions is perfectly fine in the perturbative limit since there we deal with perturbation around A = 0 only and so the Faddeev-Popov procedure or the BRST formulation works well.

2.1.2 Gribov Copies

We have been cautious about the assumption of an ideal gauge-fixing condition in the above discussion. A remarkable result of V. N. Gribov conveyed that for non-Abelian theories, even after fixing gauge with a generalized gauge fixing condition $f([A], x) = \partial_{\mu}A_{\mu}(x) - k(x)$ with Landau or Coulomb gauge being its special cases, there exist residual gauge copies which are physically equivalent to each other and related by non-trivial gauge transformations [12, 57, 58, 59]. In other words, these gauge fixing conditions do not fix the gauge uniquely for non-Abelian theories, or in general for a compact gauge group [13]. These copies are called Gribov copies which are classified according to the eigenvalues of the corresponding M_{FP} : the set of Gribov copies at which M_{FP} is positive definite is called the first Gribov region, denoted as C_0 , and the set of Gribov copies at which M_{FP} has exactly *i* negative eigenvalues is called the (i+1)th Gribov region, denoted as C_i . The Gribov horizons are defined as the boundaries between two

³Strictly speaking, this BRST transformation is called the off-shell BRST transformation.

consecutive Gribov regions where eigenvalues of M_{FP} go through zero. Thus, Gribov regions are separated by the Gribov horizons. The fundamental modular region (FMR) is defined as the set of unique representatives of every gauge orbit which is moreover convex and bounded in every direction.

Now, we should revisit the above mentioned Faddeev-Popov procedure. In the presence of Gribov copies, instead of Eq. (2.9), we get [60, 61]

$$Z_{GF} := \int Dg \,\delta[F([A], x)] \,\Delta_{FP}[A] = n_{GC}[A], \qquad (2.18)$$

where $n_{GC}[A]$ is an integer which counts the sign-weighted intersections of the gauge orbit with the gauge fixing surface, and we have denoted the gauge fixing device as Z_{GF} . In the perturbative limit, the effect of Gribov copies can be ignored. However, in the non-perturbative domain, Gribov copies should be taken into account. In a continuum formulation of QCD it seems unlikely that a systematic elimination of gauge copies is possible at all. However, their presence may or may not be a serious problem, since gauge-fixing without elimination of Gribov copies can be formulated systematically in terms of a (Witten type) topological quantum field theory on the gauge group, on compact manifolds [9]. There, the standard Faddeev- Popov procedure of inserting unity into the unfixed generating functional generalizes to inserting the above mentioned sign-weighted average over all Gribov copies.

2.2 Gauge Field Theory On The Lattice

A gauge field theory can be successfully studied nonperturbatively by discretizing the Euclidean space-time and putting the gauge and matter fields and observables of the theory on a four-dimensional lattice space-time grid [6, 7, 8]. A lattice grid consists of lattice nodes, called lattice sites, and joints connecting any two adjacent nodes of length a in each direction, called links. The gauge fields are usually defined through link variables $U_{i,\mu} \in G$ where the discrete variable idenotes site index, μ is directional index and G is the corresponding group of the theory. The gauge transformations $g_i \in G$ are defined at each lattice site. The relation of the gauge-fields on the lattice to its continuum counter-part, with the standard definition, is

$$aA_{\mu}(x) = \frac{1}{2i}(U_{i,\mu} - U_{i,\mu}^{\dagger})|_{\text{traceless}}$$
 (2.19)

The classical action on the lattice can be constructed such that in the limit $a \rightarrow 0$ it reproduces the classical action of the corresponding continuum theory. There are infinitely many ways to define a lattice action for QCD. The fermionic part of the action on the lattice is very subtle and we avoid the related discussion as

the discussion in the rest of thesis is independent of it. For the remaining pure gauge action on the lattice, a popular choice is the so-called Wilson action,

$$S_G[U] := \beta \sum_i \sum_{\mu < \nu} \left(1 - \frac{1}{N} \operatorname{Re} \operatorname{Tr} \Box_{i,\mu\nu} \right), \qquad (2.20)$$

where *i* lables lattice sites and μ and ν take values from $1, \ldots, d$, with *d* being the lattice dimension. *N* is the number of color charges, and $\beta = \frac{2N}{g_s^2}$ where g_s is the bare coupling. $\Box_{i,\mu\nu} := U_{i,\mu}U_{i+\hat{\mu},\nu}U_{i+\hat{\nu},\mu}^{\dagger}U_{i,\nu}^{\dagger}$ is the plaquette at the *i*th site in a μ - ν plane, where $\hat{\mu}$ and $\hat{\nu}$ are the unit vectors in the μ and ν directions respectively. In the limit $a \to 0$, $S_G[U]$ tends to be the classical action $S_G[A]$ as in Eq. (2.2).

The lattice expectation value of O is

$$\langle O \rangle_L = \frac{\int \prod_{i,\mu} dU_{i,\mu} \exp[-S_G[U]] O[U_{i,\mu}]}{\int \prod_{i,\mu} dU_{i,\mu} \exp[-S_G[U]]}.$$
 (2.21)

In Monte-Carlo simulations of a lattice gauge theory, a finite number of link configurations $[U^j]$, $j = 1, ..., N_k$ are generated with a probability distribution of $\exp[-S_G[U]]$. Then, $\langle O \rangle_L$ is estimated as the average value of O over these configurations, that is,

$$\langle O \rangle_L = \frac{1}{N_k} \sum_{i=1}^{N_k} O[U^i]$$
(2.22)

whose statistical error decreases with larger N_k . To recover the continuum limit, we take the limit $a \to 0$ to obtain $\langle O \rangle$.

We should mention here that due to the finiteness of the lattice, one needs to specify some boundary conditions on both the gauge fields and the gauge transformations. The most popular choices are periodic and anti-periodic boundary conditions. We will be more specific in defining boundary conditions in Chapter 3. There are also other non-trivial boundary conditions used for various purposes. We will discuss them at length in Chapter 6.

2.2.1 Landau Gauge Fixing On The Lattice

The lattice formalism of a gauge field theory is manifestly gauge-invariant because the gauge fields take values from the compact Lie group and the functional integration measure is well-defined. That is, gauge-fixing is not required on the lattice. In particular, we can simply sample configurations in the numerical simulations and can be sure that no finite ensemble will ever sample the same orbit twice. However, gauge-dependent quantities are the basis of the different confinement scenarios such as Kugo-Ojima and Gribov-Zwanziger [56, 12] scenarios and the DSEs studies in general for the QCD hadron phenomenology [9] in the continuum and hence it is essential to have a lattice analogue of Landau gauge fixing to compare the corresponding results: in practical calculations in the continuum DSE approach where one has to deal with infinitely many integral equations, a truncation scheme is used. On the other hand, the approximations involved in gaugedependent QCD Green's functions calculations can be systematically removed on the lattice, unlike the truncations of the continuum DSEs. So, the corresponding lattice simulations can provide an independent check on the results obtained in the continuum DSE approach [14, 9, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25]. Because the DSEs are studied mostly in Landau gauge, we are mainly interested in the lattice analogue of Landau gauge here. Below we first re-formulate Landau gauge-fixing in the continuum as a functional minimization problem since its lattice analogue is used in the lattice computations. We then describe how standard Landau gauge-fixing is done in the actual lattice computations.

We can formulate the problem of solving Landau gauge conditions in the continuum,

$$\partial_{\mu}A_{\mu} = 0 , \qquad (2.23)$$

as a functional minimization problem [62, 63]. Specifically, the first derivatives of the functional, called norm functional or Landau gauge fixing functional,

$$||A^{g}||^{2} = -\int d^{4}x Tr((gA_{\mu}g^{\dagger} - g\partial_{\mu}g^{\dagger})^{2})$$
 (2.24)

with respect to gauge parameters g are shown to give Eq. (2.23), where A_{μ} is the usual gauge field. The second derivative matrix, or the Hessian matrix, of this functional is the Faddeev-Popov operator M_{FP} . As mentioned above, there appear many extrema and saddle points of the gauge-fixing functional, i.e., Gribov copies, in the non-perturbative domain. The first Gribov region C_0 then is the set of local minima. The set of absolute minima is the FMR which is contained within C_0 . Moreover, Gribov copies are non-degenerate in the interior of C_0 . However, at the first Gribov horizon, degenerate minima exist. Similarly, the set of all saddle points at which the corresponding M_{FP} has exactly *i* negative eigenvalues is the (i + 1)th Gribov region C_i and the set of degenerate extrema which constitute the boundary between C_i and C_{i+1} is the (i + 1)th Gribov horizons.

On the lattice, the corresponding lattice Landau gauge-fixing functional, that is iteratively minimized with respect to the corresponding gauge transformations g_i , is

$$F_U(g) = \sum_{i,\mu} (1 - \frac{1}{N} \text{Re Tr } g_i^{\dagger} U_{i,\mu} g_{i+\hat{\mu}}), \qquad (2.25)$$

where the sum runs over all lattice sites i and lattice directions μ and $g_i^{\dagger} U_{i,\mu} g_{i+\hat{\mu}} \equiv U_{i,\mu}^g$ the gauge transformed link variables. The gauge-fixing equations on the lattice are then the first derivatives of $F_U(g)$ with respect to the gauge transforma-

tions, i.e.,

$$f_i(g) = \frac{\partial F_U(g)}{\partial g_i} = 0 \tag{2.26}$$

for each lattice site *i*. At each lattice site, these f_i give the lattice divergence of the lattice gauge fields defined in Eq. (2.19) and in the naive continuum limit recover the Landau gauge $\partial_{\mu}A_{\mu} = 0$. This is called the standard lattice Landau gauge (SLLG). The corresponding Faddeev-Popov operator M_{FP} is the Hessian matrix of $F_U(g)$, with respect to the gauge transformations, and $\Delta_{FP} = \det M_{FP}$. We can then use the well-established numerical methods of functional minimization such as Simulated Annealing, Overrelaxation, Fourier acceleration, etc. to minimize $F_U[g]$ [64, 65, 66].

On the lattice, the presence of Gribov copies has been explicitly established [67, 68, 69] and the effects of Gribov copies on the lattice in various confinement scenarios have been extensively studied (see [70] for a review). However, the difference here is that since the lattice gauge fixing is usually done by numerically minimising the gauge fixing functional, Gribov copies are restricted to C_0 only. One obvious way of fixing the gauge uniquely on the lattice is to find the absolute minimum out of all minima found numerically. However, the number of minima increases exponentially with increasing lattice size and so it becomes hopeless to ever find the absolute minimum in practice.

It is important to mention at this point that to overcome the Gribov copy problem, an alternative gauge to Landau gauge, called Laplacian gauge, was proposed in Ref. [71]. However, there the renormalizability yet remains to be shown explicitly.

2.2.2 The Neuberger 0/0 Problem

There is one more and rather crucial problem on the lattice: while fixing the usual Landau gauge via the Faddeev-Popov procedure, the lattice analogue of Eq. (2.9) turns out to be zero, for a compact U(1) or SU(N) theory. Specifically, Z_{GF} , with gauge parameter $\xi = 0$ in the lattice analogue of Eq. (2.15), on the lattice turns out to be⁴

$$Z_{GF} = \sum_{i} \operatorname{sign} (\Delta_{FP})_{i} , \qquad (2.27)$$

where the sum runs over all Gribov copies and $(\Delta_{FP})_i$ denotes the value of Δ_{FP} evaluated at an *i*th Gribov copy. For compact U(1) or SU(N), $Z_{GF} = 0$, called the Neuberger zero. Consequently, the corresponding partition function itself becomes zero after inserting this gauge-fixing device and the gauge-fixed observables

⁴A full discussion related to the topological field theoretical derivation of this very interesting result is avoided in this thesis as it is well-documented in the original papers cited in this subsection and in Ref. [32].

are of the indefinite form 0/0. This means that the standard Faddeev-Popov procedure can not be performed on the lattice. This problem is called the Neuberger 0/0 problem [29, 30].

We should pause here and summarize the problem. As mentioned above and in the Introduction, gauge-fixing on the lattice is essential to study related confinement scenarios and QCD Green's functions that are fundamental building blocks of hadron phenomenology in the continuum Landau gauge DSE studies [14, 9, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25]. To study them on the lattice, the lattice BRST formulation is essential since the continuum covariant formalism of a gauge theory is based on BRST formulations. But the Neuberger 0/0 problem prevents us from constructing the BRST formulation on the lattice. The lattice implementations of the Landau gauge are thought to have avoided this problem because the numerical procedures are based on minimizations of a gauge fixing potential and one settles on the local minima which samples gauge copies from C_0 among which there is no cancellation. However, for the BRST formulation sampling from all the possible gauge-fixed configurations, i.e., not only from C_0 but an averaging (say, Monte-Carlo averaging) over all Gribov copies must be performed [35]. But doing so for the standard definition of the Landau gauge (i.e., with the standard lattice Landau gauge-fixing functional $F_U(q)$) will leave the expectation value of a gauge-fixed observable ill-defined and thus the results in the continuum and on the lattice can not be compared straightforwardly. Below we discuss the Neuberger 0/0 problem in terms of topology to get a better understanding of the origin of this problem.

2.3 Topological Interpretation

Here, we briefly describe Morse theory and interpret Gribov copies and the Neuberger 0/0 problem in Morse theoretical terms. Specifically, with the Witten-type topological field theory [72, 73] interpretation, the gauge-fixing partition function Z_{GF} for the lattice Landau gauge-fixing was shown, in Ref. [39], to be calculating a topological invariant, namely the Euler characteristic χ of a manifold $\mathbb{M}(\chi(\mathbb{M}))$ which is a topological invariant (i.e., it does not depend on the Riemannian metric) that counts the number of holes in \mathbb{M} . For more technical details on the relation between topological field theory and Z_{GF} the reader is referred to [32]. Following this interpretation, we will propose a modification to the SLLG.

2.3.1 Morse Theory and The Neuberger 0/0 Problem

Morse theory deals with functions called height functions, $h(\vec{x})$, defined from a compact, differentiable and orientable manifold \mathbb{M} to \mathbb{R} , with \vec{x} being a vector consisting of the corresponding variables. The solutions to the equations obtained by equating first derivatives of $h(\vec{x})$ with respect to all its variables to zero are

called the critical points of \mathbb{M} . The second derivative matrix, or the Hessian, of $h(\vec{x})$ is then used to classify the critical points: if the Hessian is singular at a critical point, then the critical point is called degenerate, otherwise it is non-degenerate. $h(\vec{x})$ is called a non-degenerate height function if all of its critical points are non-degenerate.

Now, the Poincaré-Hopf theorem asserts that $\chi(\mathbb{M})$ is equal to the sum of signs of Hessian determinants at all critical points of the function, i.e.,

$$\chi(\mathbb{M}) = \sum_{i} \text{ sign } (\det(\text{Hessian of } h(\vec{x})))_{i} .$$
 (2.28)

for a non-degenerate $h(\vec{x})$, where the sum runs over all critical points. This is a very interesting result since on the left hand side there appears a topological invariant and on the right hand side there appears a quantity from analysis.

Now, in the aforementioned procedure of lattice Landau gauge fixing we can immediately identify the gauge-fixing functional (2.25) as a height function, Gribov copies as the critical points and M_{FP} as the corresponding Hessian matrix [39]. Thus, finally we can achieve

$$Z_{GF} = \sum_{i} \operatorname{sign} (\Delta_{FP})_{i} = (\chi(\mathbb{M})) , \qquad (2.29)$$

where now \mathbb{M} is the corresponding manifold depending on the boundary conditions used for the lattice and the sum runs over all Gribov copies. On the lattice with *n* lattice sites, \mathbb{M} is the cartesian product space $G \times G \cdots \times G$ where *G* is the manifold of the gauge-transformed link variable at each site and the number of factors in this expression depends on whether the global gauge freedom is fixed or unfixed. Using the fact that for a cartesian product space of manifolds *X* and *Y* we have $\chi(X \times Y) = \chi(X)\chi(Y)$, Eq. (2.29) turns out to be Eq. (1.1) if the global gauge freedom is fixed. With an unfixed global gauge freedom, $Z_{GF} = (\chi(G))^{n-1}$.

For the compact U(1) case⁵ for the SLLG $G = S^1$. It follows that because (2.25) can be viewed as a height function from $S^1 \times S^1 \cdots \times S^1$ to \mathbb{R} in this case, and since $\chi(S^1) = 0$, we have $Z_{GF} = 0$. For the compact U(1) case, as we will explicitly see in Chapter 3, anti-periodic boundary conditions fixes the global gauge freedom, so the corresponding manifold is $(S^1)^n$. For the periodic boundary conditions case the corresponding manifold is $(S^1)^{n-1}$. Thus, for any boundary conditions, we have $Z_{GF} = 0$. In fact, for all the Standard Model groups the Euler characteristic is zero as their group manifolds consist of odd-dimensional spheres, e.g., $\chi(SU(2) \cong S^3) = 0$, $\chi(SU(3) \cong S^3 \times S^5) = 0$ etc., yielding the Neuberger zero. Moreover, another important conclusion of this discussion is that the Euler characteristic of the manifold at each site contributes to the Neuberger zero.

⁵We should note here that there are two alternatives for U(1) group: compact U(1) and non-compact U(1). Though compact QED is not a physical theory, it exhibits most of the features of an SU(N) on the lattice due to the compactness of the group manifold. We will return to this in Chapter 3.

2.3.2 Modification Via Stereographic Projection

After interpreting the Neuberger 0/0 problem in terms of Morse theory, Schaden proposed to construct a BRST formulation for SU(2) gauge theory within the coset space SU(2)/U(1) for which $\chi(SU(2)/U(1)) \neq 0$ [39]. This procedure can be generalized to fix the gauge of an SU(N) lattice gauge theory to the maximal Abelian subgroup, $(U(1))^{N-1}$, since $\chi(SU(N)/SU(N-1)\times U(1)) \neq 0$ as well. This also indicates that the Neuberger 0/0 problem for an SU(N) lattice gauge theory actually lies in $(U(1))^{N-1}$, and can be evaded if that for compact U(1) is evaded combined with Schaden's approach. Thus, in this subsection we concentrate on the lattice Landau gauge for compact U(1).

As seen in the previous section, since the Euler characteristic of the manifold at each lattice site contributes to the Neuberger zero, we first note that the height function for a single S^1 is

$$h(t) = \cos t. \tag{2.30}$$

This function can be viewed as the standard lattice Landau gauge-fixing functional (2.25) for the single lattice site case: in Eq.(2.25), for compact U(1) at an *i*th lattice site, we have $U_{i,\mu} = e^{i\phi_{i,\mu}}$ and $g_i = e^{i\theta_i}$ where $\phi_{i,\mu}$ and θ_i both take values from $(-\pi, \pi]$, and N = 1. So, $U_{i,\mu}^g = e^{i(\phi_{i,\mu} + \theta_{i+\hat{\mu}} - \theta_i)}$ where the exponent here is defined modulo 2π . Thus, by identifying t as $(\phi_{i,\mu} + \theta_{i+\hat{\mu}} - \theta_i)$ in the above height function, we have $\cos t = \operatorname{Tr} U_{i,\mu}^g$. Note that since we are considering a single lattice site here, we formally omit explicitly mentioning indices for t. Now, h(t) is known to have two points at infinity: the north pole and the south pole. They both are the critical points of this circle but have opposite sign of the Hessian determinant, giving their sum to be 0. Our central idea is to modify this height function in an appropriate way to resolve the Neuberger 0/0 problem.

We can immediately think of at least two choices. Firstly, we can project out the south pole (equivalently, the north pole) to infinity stereographically⁶⁷, called stereographic projection [74]. Thus, the modified manifold is an open interval or just \mathbb{R} . The corresponding height function, or the lattice Landau gauge, is then

$$h^{s}(t) = -2\ln(\cos\frac{t}{2})$$
 (2.31)

It is easy to see that there is only one critical point for this case, which is when $\tan \frac{t}{2} = 0$, i.e., t = 0 and at this point the Hessian determinant, $\sec^2(\frac{t}{2})$, is 1.

Ānother choice is to take the absolute value of the height function as,

$$h^{\rm abs}(t) = |\cos t| , \qquad (2.32)$$

⁶Stereographic projection of a circle is a standard textbook topic and the reader is referred to a standard textbook on topology, e.g., Ref. [74].

⁷It must be emphasized at this stage that this modification is on the manifold of the gaugetransformed link angle at each site, i.e., the gauge group of the gauge transformations is, of course, left unchanged here.

where again there is only one critical point here, which is when $(\tan t)|\cos t| = 0$, i.e., t = 0 and the Hessian determinant $|\cos t|$ at this point is 1. However, we refer to the former case as the modified lattice Landau gauge (MLLG) throughout this thesis.

In practice, we will modify the corresponding term at each lattice site in the SLLG, as discussed in Chapter 3, and will show rigorously that the MLLG indeed evades the Neuberger 0/0 problem in an arbitrary dimensional lattice. However, from the topological arguments, since $\chi(\mathbb{R})$ is non-zero at each lattice site, we can clearly expect at this stage that there should be no Neuberger 0/0 problem in the compact U(1) case with such a modification. Below, we continue extracting some important results related to the number of Gribov copies using Morse theory.

2.3.3 Betti Numbers and Gribov Copies

Here, we show how the Morse theoretical interpretation of the lattice Landau gauge can give a lower bound on the number of Gribov copies⁸ N_{GC} . We briefly explain the Morse indices, Betti numbers and their relationship with $\chi(\mathbb{M})$ via the so-called Poincaré polynomial P(z) of \mathbb{M} along with Morse inequalities. We then obtain an expression for the lower bound on N_{GC} at a given orbit and calculate⁹ it explicitly for compact U(1), SU(2) and SU(N). The ultimate goal of this discussion is to show that the lower bound on N_{GC} is exponentially suppressed in the MLLG compared to the SLLG.

Let K_i be the number of critical points of a height function $h(\vec{x})$ with its Hessian at these critical points having *i* negative eigenvalues. Then $\chi(\mathbb{M}) = \sum_i (-1)^i K_i$, where now the sum over *i* runs from 0 to the dimension of \mathbb{M} .

In addition to the Euler characteristic, the so-called Betti numbers are closely related topological invariants of a manifold. Firstly, a Homology group is a measure of the hole structure of a manifold, or more specifically, a topological space. There may be several Homology groups of a manifold. Now, an *i*th Betti number b_i is defined as the rank of the *i*th Homology group (the reader is referred to [73] for details on Betti numbers and their relation to the Euler characteristic).

The Poincaré polynomial is defined as $P(z) = \sum_i b_i z^i$ for an arbitrary real variable z. Then, it turns out that

$$P(1) = \sum_{i} b_i \& P(-1) = \sum_{i} (-1)^i b_i = \chi(\mathbb{M}) , \qquad (2.33)$$

where the sum runs over the dimension of \mathbb{M} .

Now, there are two types inequalities, called Morse inequalities, that relate

⁸Note that n_{GC} is formally a sign-weighted sum of the Faddeev-Popov determinants over all Gribov copies and N_{GC} is the number of Gribov copies. They may or may not coincide.

⁹Here, we omit the explicit mention of the orbit-dependence of N_{GC} .

 b_i 's and K_i 's. The weak Morse inequality states that

$$\sum_{i} K_i \ge \sum_{i} b_i \tag{2.34}$$

and the strong inequality states that

$$K_i \ge b_i \tag{2.35}$$

for all *i*. Now, due to the weak Morse inequality and using the fact that $\sum_i K_i$ is the total number of critical points which is N_{GC} for a lattice Landau gauge fixing functional, we have

$$P(1) = \sum_{i} b_{i} \le \sum_{i} K_{i} = N_{GC}, \qquad (2.36)$$

where the sum runs over all gauge-fixed variables, i.e., i = 0, ..., n for the antiperiodic boundary conditions case and i = 0, ..., n-1 for the periodic boundary conditions case.

To calculate the corresponding P(z), first note that $P_{X \times Y}(z) = P_X(z)P_Y(z)$ for a product space manifold $X \times Y$ of X and Y, where $P_X(z)$ and $P_Y(z)$ are the Poincaré polynomials of X and Y respectively. For the SLLG for the compact U(1) case with anti-periodic boundary conditions, the corresponding manifold is $(S^1)^n$ and the corresponding Poincaré polynomial is

$$P_{(S^1)^n}(z) = \prod_{k=1}^n P_k(z) = \prod_{k=1}^n (1+z) = (1+z)^n = \sum_{i=0}^n \binom{n}{i} z^i$$

$$\therefore P_{(S^1)^n}(1) = 2^n \le \sum_{i=0}^n K_i = N_{GC} , \qquad (2.37)$$

where we have abbreviated $P_{k,S^1}(z)$ as $P_k(z)$ and we have used the fact that $P_{S^1}(z) = 1 + z$, with the Betti numbers $b_0 = 1 = b_1$ and all others being zero for S^1 . Thus, N_{GC} must be greater than or equal to 2^n in this case. Moreover, we can verify that $P(-1) = (1-1)^n = 0 = \chi((S^1)^n)$ as expected. Also, we identify the Betti numbers of this *n*-torus as $b_i = {n \choose i}$, for all i = 0, ..., n, by comparing the above equation with Eq. (2.33). Similarly, for the periodic boundary conditions case, the corresponding manifold is $(S^1)^{n-1}$, i.e.,

$$P_{(S^{1})^{(n-1)}}(z) = \prod_{k=1}^{n-1} P_{k}(z) = \prod_{k=1}^{n-1} (1+z) = (1+z)^{n-1} = \sum_{i=0}^{n-1} \binom{n-1}{i} z^{i}$$

$$\therefore P_{(S^{1})^{(n-1)}}(1) = 2^{n-1} \le \sum_{i=0}^{n-1} K_{i} = N_{GC}.$$
(2.38)

So, the corresponding Betti numbers for $(S^1)^{n-1}$ are $b_i = \binom{n-1}{i}$ for i = 0, ..., n-1.

For SU(2), the group manifold is S^3 and the corresponding Poincaré polynomial is $P_{S^3}(z) = (1+z^3)$. Thus, for the SLLG with periodic boundary conditions the corresponding Poincaré polynomial is

$$P_{(S^3)^{(n-1)}}(z) = \prod_{k=1}^{n-1} (1+z^3) = (1+z^3)^{n-1}$$

$$\therefore P_{(S^3)^{(n-1)}}(1) = 2^{n-1} \le N_{GC}^{SU(2)}, \qquad (2.39)$$

giving the same lower bound for the number of Gribov copies as that of the compact U(1) case.

For a generic SU(N) with N > 2, the group manifold is $S^3 \times S^5 \times ...S^{2N-1}$ and the corresponding Poincaré polynomial is $(1+z^3)(1+z^5)...(1+z^{2N-1})$. Thus, for the SLLG with periodic boundary conditions,

$$P_{(S^3 \times \dots \times S^{2N-1})^{(n-1)}}(z) = ((1+z^3)(1+z^5)\dots(1+z^{2N-1}))^{n-1}$$

$$P_{(S^3 \times \dots \times S^{2N-1})^{(n-1)}}(1) = 2^{(N-1)(n-1)} \le N_{GC}^{SU(N)}, \qquad (2.40)$$

giving a larger lower bound than that of the compact U(1) and SU(2) cases.

On the other hand, the corresponding manifold for the MLLG is \mathbb{R}^n for the compact U(1) case with anti-periodic boundary conditions. Here, $b_0 = 1$, for \mathbb{R} , and all other $b_i = 0$ for $i = 1, \ldots$ So the corresponding Poincaré polynomial, with $P_{\mathbb{R}}(z) = 1$, is

$$P_{\mathbb{R}^n}(z) = \prod_{k=1}^n (1) = 1^n = 1$$

: $P_{\mathbb{R}^n}(-1) = P_{\mathbb{R}^n}(1) = 1 \le N_{GC}$. (2.41)

Thus, the lower bound on the number of Gribov copies is exponentially suppressed from 2^n in the standard case to 1 in the modified case for compact U(1). Similarly, with periodic boundary conditions,

$$P_{\mathbb{R}^{n-1}}(z) = \prod_{k=1}^{n-1} (1) = 1^{n-1} = 1$$

$$\therefore P_{\mathbb{R}^{n-1}}(-1) = P_{(\mathbb{R})^{n-1}}(1) = 1 \le N_{GC} .$$
(2.42)

Furthermore, the corresponding Betti numbers of \mathbb{R}^{n-1} are $b_0 = 1$ and $b_i = 0$ for i = 1, ..., n for the anti-periodic boundary conditions case and $b_0 = 1$ and $b_i = 0$ with i = 1, ..., n-1 for the periodic boundary conditions case.

2.4 Remarks

1. We briefly revisit the definition of gauge fields on the lattice and point out how the modification of the lattice Landau gauge corresponds to a new definition of the gauge fields on the lattice. The gauge fields in the continuum in the standard definition is given by Eq. (2.19). In the proposed modification, we have implicitly proposed a different lattice definition of the gauge fields as

$$aA_{\mu}(\vec{x}) = \frac{1}{2i}(\tilde{U}_{i,\mu} - \tilde{U}_{i-\hat{\mu},\mu}), \text{ with } \tilde{U}_{i,\mu} \equiv \frac{2U_{i,\mu}}{1 + \frac{1}{2} \operatorname{Tr} U_{i,\mu}}, \qquad (2.43)$$

where $U_{i,\mu} \in G$ for G being compact U(1) or SU(N). For any of these lattice definition of gauge fields, say $aA_{\mu}(\vec{x}) = X_{i,\mu}$, the lattice Landau gauge at each lattice site reads as

$$f_i = \sum_{\mu} (X_{i,\mu}^g - X_{i-\hat{\mu},\mu}^g) = 0, \qquad (2.44)$$

where $X_{i,\mu}^g$ is the gauge transformed $X_{i,\mu}$. Thus, both definitions give the divergence at each site for a lattice. Moreover, both definitions have the same continuum limit.

2. In the SLLG, the corresponding Z_{GF} is 0 independent of the orbit considered, i.e., random values of $U_{i,\mu}$ in Eq.(2.25). This is called orbitindependence. For the MLLG, we need to show such an orbit-independence, i.e., the corresponding Z_{GF} for the MLLG is constant for a given lattice for any orbit. In the lower dimensional models considered in Chapter 3 we explicitly demonstrate such orbit-independence for the MLLG.

2.5 Summary

- 1. Gauge-fixing in the continuum is essential to remove the redundant gauge freedom to study gauge-dependent quantities which are the basis of the continuum covariant field theory formulation [56, 12] and the QCD hadron phenomenology [9]. To study them on the lattice, it is essential to fix a gauge.
- 2. The standard procedure for gauge-fixing in the continuum is the Faddeev-Popov procedure, which suffers from Gribov copies in the non-perturbative domain. On the lattice, an analogous procedure suffers from the Neuberger 0/0 problem, i.e., the expectation value of a gauge-fixed observable turns out to be of the indefinite form 0/0, due to Gribov copies. Schaden interpreted the Neuberger 0/0 problem in terms of Witten-type topological field theory and asserted that the problem persists because the gauge fixing partition function calculates the Euler characteristic χ of the group manifold at each site of the lattice, which is zero for compact U(1) and SU(N) for the SLLG. Schaden also constructed a BRST formulation for the coset

space SU(2)/U(1), for the SU(2) case, for which χ is non-zero. We argued that together with Schaden's approach, the Neuberger 0/0 problem can be evaded if that for compact U(1) is evaded. We proposed a modification of the lattice Landau gauge-fixing definition, via stereographic projection of the manifold at each lattice site, which is expected to evade the Neuberger 0/0 problem since χ is non-zero in this case.

3. We showed that a lower bound on the number of Gribov copies, N_{GC} , on the lattice can be computed by calculating the corresponding Poincaré polynomial. For the SLLG on a lattice with *n* lattice sites, we found this lower bound to be 2^n for the compact U(1) case with anti-periodic boundary conditions, 2^{n-1} for compact U(1) and SU(2) with periodic boundary conditions and $2^{(n-1)(N-1)}$ for any SU(N) for N > 2 with periodic boundary conditions, for a lattice with *n* lattice sites. This lower bound for the MLLG for the compact U(1) case is exponentially reduced and is 1.
Chapter 3

Lattice Landau Gauge For Lower Dimensional Models

As discussed in Chapters 1 and 2, the Neuberger 0/0 problem can be evaded for the SU(N) case if that for compact U(1) is evaded together with Schaden's coset space BRST formulation. In the present chapter, we discuss the SLLG and the proposed MLLG for compact U(1) explicitly. In particular, we analytically solve the corresponding gauge-fixing equations for both the SLLG and the MLLG with anti-periodic and periodic boundary conditions on a one-dimensional lattice. We demonstrate the presence of Gribov copies and the Neuberger 0/0 problem in this toy model explicitly for the SLLG. We also show how the MLLG circumvents the Neuberger 0/0 problem there. We then discuss the complete Coulomb gauge for 1 + 1 dimensions, use our results of the one-dimensional MLLG and formulate the Faddeev-Popov gauge-fixing procedure for compact QED via the MLLG in these lower dimensional models. Finally, we mention a few important remarks and summarize the chapter.

3.1 Lattice Landau Gauge Fixing for Compact U(1)

The group manifold of compact U(1) is topologically a circle S^1 . The gauge fixing functional for the SLLG, Eq. (2.25), in this case reduces to

$$F_{\phi}(\theta) = \sum_{i,\mu} (1 - \cos(\phi_{i,\mu} + \theta_{i+\hat{\mu}} - \theta_i)), \qquad (3.1)$$

where $\hat{\mu}$ is a unit vector in the μ -direction, index $i \equiv (i_1, \ldots, i_d)$ for a *d*-dimensional lattice runs over all lattice sites, and μ runs from 1 to *d*. Here, we have used the fact that for the compact U(1) case, $U_{i,\mu} = e^{i\phi_{i,\mu}}$ and $g_i = e^{i\theta_i}$ with $\phi_{i,\mu} \mod 2\pi \in (-\pi, \pi]$ and $\theta_i \mod 2\pi \in (-\pi, \pi]$ being link-angles and gauge transformations

respectively. Following on from the discussion in Section 2.3.2, the gauge-fixing functional for the MLLG can be written as,

$$F_{\phi}^{s}(\theta) = -2\sum_{i,\mu} \ln(\cos(\phi_{i,\mu} + \theta_{i+\hat{\mu}} - \theta_{i})/2).$$
(3.2)

We should mention here that a given random set of $\phi_{i,\mu}$ is called a *random orbit* or a *hot configuration*. The special case when all $\phi_{i,\mu}$ are zero is called the *trivial* orbit, or cold configuration. The extrema and saddle points of a gauge-fixing functional are referred to as the gauge fixed configurations or Gribov copies. The gauge-fixing conditions are the first derivatives of the given functional with respect to all gauge transformations equated to zero. That is, for the SLLG they read as

$$f_{i}(\theta) = -\sum_{\mu=1}^{d} \left(\sin(\phi_{i,\mu} + \theta_{i+\hat{\mu}} - \theta_{i}) - \sin(\phi_{i-\hat{\mu},\mu} + \theta_{i} - \theta_{i-\hat{\mu}}) \right) = 0, \quad (3.3)$$

for all i. For the MLLG, the corresponding gauge-fixing equations are

$$f_i^s(\theta) = -\sum_{\mu=1}^d \left(\tan((\phi_{i,\mu} + \theta_{i+\hat{\mu}} - \theta_i)/2) - \tan((\phi_{i-\hat{\mu},\mu} + \theta_i - \theta_{i-\hat{\mu}})/2) \right) = 0, \quad (3.4)$$

for all lattice sites i.

The Faddeev-Popov operator is the Hessian of the gauge-fixing functional with respect to all gauge transformations, and for compact U(1) for the SLLG it is

$$(M_{FP})_{i,j} = \sum_{\mu} \left(-\cos \phi_{i,\mu}^{\theta} \delta_{i+\hat{\mu},j} + (\cos \phi_{i,\mu}^{\theta} + \cos \phi_{i-\hat{\mu},\mu}^{\theta}) \delta_{i,j} - \cos \phi_{i-\hat{\mu},\mu}^{\theta} \delta_{i-\hat{\mu},j} \right),$$

$$(3.5)$$

where $\phi_{i,\mu}^{\theta} = \phi_{i,\mu} + \theta_{i+\hat{\mu}} - \theta_i \mod 2\pi \in (-\pi,\pi]$. Similarly, for the MLLG, the Faddeev-Popov operator reads as

$$(M_{FP}^{s})_{i,j} = \sum_{\mu} \left(-\sec^2 \frac{\phi_{i,\mu}^{\theta}}{2} \delta_{i+\hat{\mu},j} + (\sec^2 \frac{\phi_{i,\mu}^{\theta}}{2} + \sec^2 \frac{\phi_{i-\hat{\mu},\mu}^{\theta}}{2}) \delta_{i,j} - \sec^2 \frac{\phi_{i-\hat{\mu},\mu}^{\theta}}{2} \delta_{i-\hat{\mu},j} \right).$$

$$(3.6)$$

We should also note here that for periodic boundary conditions, in the compact U(1) case,

$$\theta_{i+n\hat{\mu}} = \theta_i, \ \phi_{i+n\hat{\mu},\mu} = \phi_{i,\mu}, \ \phi^{\theta}_{i+n\hat{\mu},\mu} = \phi^{\theta}_{i,\mu} ,$$
(3.7)

and for anti-periodic boundary conditions,

$$\theta_{i+n\hat{\mu}} = -\theta_i, \ \phi_{i+n\hat{\mu},\mu} = -\phi_{i,\mu}, \ \phi^{\theta}_{i+n\hat{\mu},\mu} = -\phi^{\theta}_{i,\mu} ,$$
 (3.8)

with n being the total number of lattice sites in the μ -direction.

We concentrate on the one-dimensional case below. Though this model does not have any dynamics, most of the features present in its higher dimensional counterparts appear here.

3.2 Anti-periodic Boundary Conditions In One Dimension

Consider a one-dimensional lattice chain of length n with gauge transformations $\theta_i \mod 2\pi \in (-\pi, \pi]$ at lattice sites and gauge transformed link variables $\phi_i^{\theta} = \phi_i + \theta_{i+1} - \theta_i \mod 2\pi \in (-\pi, \pi]$ between neighboring sites, where $i = 1, \ldots, n$, with anti-periodic boundary conditions. We deal with the SLLG and the MLLG separately below.

3.2.1 Standard Lattice Landau Gauge (SLLG)

According to Eq. (3.1), $F_{\phi}(\theta)$ in one dimension reduces to

$$F_{\phi}(\theta) = \sum_{i} (1 - \cos(\phi_i + \theta_{i+1} - \theta_i)), \qquad (3.9)$$

where now $i = 1, \ldots, n$.

Similarly, the gauge-fixing equations for the one-dimensional SLLG are

$$f_i(\theta) = -\left(\sin(\phi_i + \theta_{i+1} - \theta_i) - \sin(\phi_{i-1} + \theta_i - \theta_{i-1})\right) = 0,$$
(3.10)

for all i = 1, ..., n. Note that these equations are a variant of the Kuramoto model which is a popular model to model synchronization in complex networks [75]

A simple way to solve these gauge-fixing conditions for the anti-periodic boundary conditions case is first to change the variables to $s_i = \phi_i + \theta_{i+1} - \theta_i \mod 2\pi \in (-\pi, \pi]$, for all $i = 1, \ldots, n$, and then to solve the system for these new variables. Anti-periodic boundary conditions for the new variables, i.e., $s_{n+1} = -s_1$ and $s_0 = -s_n$, ensure that the Jacobian matrix M for this change of variables is non-zero. In particular, det $\frac{\partial s_i}{\partial \theta_j} = \det \frac{\partial(\phi_i + \theta_{i+1} - \theta_i)}{\partial \theta_j} = \det(\delta_{i+1,j} - \delta_{i,j}) =$ det $M_{i,j}$. In fact, it can be easily seen that

$$\det M = (-1)^{n+1}2. \tag{3.11}$$

This non-singularity of M is simply because anti-periodic boundary conditions rule out the global zero or the constant zero mode. The factor 2 here also reflects the fact that the map is two-to-one when taken all s_i modulo 2π . Thus, Eq. (3.10) can be written as

$$\tilde{f}_i(s) = -(\sin s_i - \sin s_{i-1}) = 0,$$
(3.12)

for all i = 1, ..., n. This can be written in matrix form as $M\vec{S} = \vec{0}$, where $\vec{S} = (\sin(s_1), ..., \sin(s_n))^T$ is a column vector, and $\vec{0}$ is the zero vector. Since M is non-singular here, this matrix equation only has a trivial solution, $\vec{S} = \vec{0}$, i.e., $\sin s_i = 0$ and hence $s_i \in \{0, \pi\}$, for all i = 1, ..., n. Thus, after gauge fixing, $\vec{s} = \vec{\eta}$, where $\vec{\eta}$ is the vector consisting of only 0 and π as its elements and $\vec{s} = (s_1, ..., s_n)^T$ is a column vector. Thus, there are 2^n possible configurations which are *Gribov copies* [12]. It should be mentioned here that because there is no dynamics in this one-dimensional model, effectively all 2^n copies of the gauge-fixed configuration $\vec{s} = \vec{0}$ are related to each other by permutations of 0's and π 's for all s_i 's, and so they are trivial copies of each other. In terms of θ_i 's, we get

$$\vec{\theta} = M^{-1}(-\vec{\phi} + \vec{\eta}),$$
 (3.13)

where $\vec{\phi} = (\phi_1, \dots, \phi_n)^T$ and $\vec{\theta} = (\theta_1, \dots, \theta_n)^T$ are column vectors.

For the trivial orbit case, i.e., $\vec{\phi} = \vec{0}$, we get

$$\vec{\theta} = M^{-1}\vec{\eta}.\tag{3.14}$$

After taking modulo 2π in the right hand side, it is easy to show that we have two classes of solutions for θ_i 's, i.e., Gribov copies: (a) 2^n sequences with all $\theta_i \in \{0, \pi\}$ and (b) 2^n sequences with all $\theta_i \in \{\pi/2, -\pi/2\}$. There are thus in total 2^{n+1} solutions in terms of θ_i 's. Type (a) solutions are easily seen to always lead to a Gribov copy with an even number of s_i 's being π , while type (b) solutions always leads to a Gribov copy with odd number of s_i 's being π . Thus, the double counting of link configurations with 2π -periodicity corresponds to identifying pairs of θ_i 's related by a swapping of all components, in each of the two types separately.

Faddeev-Popov Operator and The Neuberger 0/0 Problem

For the one-dimensional lattice, using Eq. (3.5), we get

$$(M_{FP})_{i,j} = \frac{\partial f_i(\theta)}{\partial \theta_j} = \frac{\partial f_i(s)}{\partial s_k} \frac{\partial s_k}{\partial \theta_j} = -\cos s_i \delta_{i+1,j} + (\cos s_i + \cos s_{i-1}) \delta_{i,j} - \cos s_{i-1} \delta_{i-1,j}. \quad (3.15)$$

Ideally we would prefer the usual diagonalization of M_{FP} with some orthogonal matrix since the diagonal elements of the resulting diagonal matrix are then the eigenvalues of M_{FP} and a classification of the solutions would be straight-forward. However, the explicit form of both the diagonalizing and the diagonal matrices get cumbersome for large n in this case. Moreover, for higher dimensional lattices, it is very difficult to diagonalize M_{FP} . We instead notice that M_{FP} can be written in the following form,

$$M_{FP} = M^T D(c_1, c_2, \dots, c_n) M, (3.16)$$

where $D(c_1, c_2, \ldots, c_n)$ or just D is a diagonal $n \times n$ matrix with entry $c_i = \cos s_i$ at the *i*-th diagonal position¹. Thus,

$$\det M_{FP} = \det(M^T D M) = \det M^T (\prod_{i=1}^n c_i) \det M = 4 \prod_{i=1}^n c_i,$$
(3.17)

where we have used the fact that det $M = \det M^T = (-1)^{n+1}2$. Now, out of 2^n Gribov copies of the form $\vec{s} = \vec{\eta}$ for 2^{n-1} Gribov copies det M_{FP} is 4 and for the remaining 2^{n-1} Gribov copies it is -4. Thus, following the topological field theoretical interpretation of the lattice Landau gauge fixing procedure [39], in this case, Eq. (2.18) gives

$$Z_{GF} = \sum_{k=1}^{2^{n}} \operatorname{sign} \left(\det M_{FP} \right) \Big|_{\vec{s}=\vec{s}_{k}}$$

= $(2^{n-1} - 2^{n-1})$
= 0, (3.18)

where \vec{s}_k is the k-th Gribov copy, and the factor 2 arising due to the over-counting is ignored. This is the Neuberger zero [29, 30] which gives rise to the Neuberger 0/0 problem.

Here, since M_{FP} is a real and symmetric matrix, all eigenvalues are real. A very important consequence of the decomposition Eq. (3.16) is that M_{FP} can be viewed as congruent to the diagonal matrix D via the invertible real symmetric matrix M. Now, Sylvester's law of inertia states that in such a case the number of positive (negative) elements of D is exactly equal to the number of positive (negative) eigenvalues [76]. The possibility of having any $c_i = 0$ is already ruled out, and so is the possibility of zero eigenvalues. Thus, for the solution $\vec{s} = \vec{0}$, all c_i 's are +1 and M_{FP} is positive definite. This configuration is the FMR which corresponds to the absolute minimum of $F_{\phi}(\theta)$.

Now, take exactly one of the s_i 's in this FMR configuration, say s_j , from 0 to π , and so the corresponding $c_j = -1$. For such a new configuration, which is also a Gribov copy, exactly one eigenvalue of M_{FP} will be negative and all others positive. The set of all n such Gribov copies with exactly one negative eigenvalue

¹It should be emphasized here that this is *not* the usual diagonalization. The diagonal elements of D here are *not* the eigenvalues of M_{FP} . However, this is still very useful for our purposes due to Sylvester's law of inertia. I am thankful to Max Lohe for pointing out this interesting result.

is the second² Gribov region C_1 . In general, the set of all $\binom{n}{r}$ Gribov copies with r out of $n s_i$'s being π and all remaining s_i 's being 0 is the (r+1)th Gribov region C_r , at which M_{FP} has exactly r negative eigenvalues.

In terms of θ_i 's, for the trivial orbit case, we can now observe the Z_2 structure: we can define a gauge transformation which when applied to any copy of type (a) or (b) leads to a copy of the other type, and returns the original configuration when applied twice. For odd n for example, a *chequer-board* gauge transformation $\vec{\theta} + \left(\frac{\pi}{2}, -\frac{\pi}{2}, \ldots, \frac{\pi}{2}\right)^T$ changes every link by π and therefore swaps the overall sign of M_{FP} . For odd n, this then also swaps the sign of the Faddeev-Popov determinant which gives the Neuberger zero. For even n, because we know all the solutions, the Neuberger zero can be explicitly seen here. However, for higher dimensional lattices where it is difficult to obtain all solutions, the issue related to the Z_2 structure becomes more involved.

3.2.2 Modified Lattice Landau Gauge (MLLG)

The MLLG functional for the one-dimensional lattice is,

$$F_{\phi}^{s}(\theta) = -2\sum_{i} \ln \cos\left((\phi_{i} + \theta_{i+1} - \theta_{i})/2\right), \qquad (3.19)$$

where the sum is over i = 1, ..., n, and the corresponding gauge-fixing conditions are

$$f_i^s(\theta) = -\left(\tan((\phi_i + \theta_{i+1} - \theta_i)/2) - \tan((\phi_{i-1} + \theta_i - \theta_{i-1})/2)\right) = 0, \quad (3.20)$$

for i = 1, ..., n.

To solve these equations we use the same trick as before, i.e., change the variables to s_i 's, to get

$$\tilde{f}_i^s(s) = -\left(\tan\frac{s_i}{2} - \tan\frac{s_{i-1}}{2}\right) = 0,$$
(3.21)

for i = 1, ..., n, or equivalently, $M\vec{S}^s = \vec{0}$, with $\vec{S}^s = (\tan(s_1/2), \ldots, \tan(s_n/2))^T$. We finally obtain $s_i = 0 \mod 2\pi$, for all i = 1, ..., n. Thus, the allowed unique configuration is $\vec{s} = \vec{0}$, giving the FMR.

In terms of θ_i 's, the solutions are

$$\vec{\theta} = M^{-1}(-\vec{\phi} + \vec{0}). \tag{3.22}$$

Thus, there are only two solutions in terms of the θ_i 's. For the trivial orbit case, there are no type (b) solutions here, and only two solutions of type (a), $\vec{\theta} = (0, 0, \dots, 0)$ and (π, π, \dots, π) survive, both of which lead to the same trivial link configuration modulo 2π . One can also show that for a random orbit, both copies also lead to the same configuration. There are thus no more Gribov copies for the one-dimensional MLLG with anti-periodic boundary conditions.

²Note that here the FMR and C_0 are the same in this case.

Faddeev-Popov Operator and No Neuberger 0/0 Problem

The Faddeev-Popov operator for the MLLG in terms of new variables is

$$(M_{FP}^{s})_{i,j} = \frac{\partial f_{i}^{s}(\theta)}{\partial \theta_{j}} = \frac{\partial f_{i}^{s}(s)}{\partial s_{k}} \frac{\partial s_{k}}{\partial \theta_{j}}$$

$$= -\sec^{2} \frac{s_{i}}{2} \delta_{i+1,j} + (\sec^{2} \frac{s_{i}}{2} + \sec^{2} \frac{s_{i-1}}{2}) \delta_{i,j} - \sec^{2} \frac{s_{i-1}}{2} \delta_{i-1,j}$$
(3.23)

for i, j = 1, ..., n. For anti-periodic boundary conditions we can decompose M_{FP}^s as

$$M_{FP}^s = M^T D^s M, (3.24)$$

where $D^{s} = D(\sec^{2} \frac{s_{1}}{2}, \dots, \sec^{2} \frac{s_{n}}{2})$ and $\det M^{s}_{FP} = 4 \prod_{i=1}^{n} \sec^{2} \frac{s_{i}}{2}$.

Thus, at $\vec{s} = \vec{0}$, D^s is the identity matrix and so M_{FP}^s is positive definite according to Sylvester's law of inertia. In particular, det $M_{FP}^s = 4$. So, the corresponding $Z_{GF} = 1$ (up to the trivial over-counting). Thus, the Neuberger 0/0 problem is solved in this toy model. In Appendix E we present another alternative to modify the lattice Landau gauge.

3.3 Periodic Boundary Conditions In One Dimension

With periodic boundary conditions, the corresponding system of gauge fixing equations has exactly one free parameter for the one-dimensional lattice from the ungauge-fixed global gauge transformation. The general solutions can be simply stated as $\sin \phi_1^{\theta} = \cdots = \sin \phi_n^{\theta}$ for the equations (3.10) and $\tan \frac{\phi_1^{\theta}}{2} = \cdots = \tan \frac{\phi_n^{\theta}}{2}$ for the equations (3.20), in the periodic boundary conditions case. However, this is still of little help and we should solve the corresponding equations for both the SLLG and the MLLG more explicitly.

We first note that, without loss of generality, we can get rid of a free variable, say θ_n , by taking $\theta_n = 0$ and removing a linearly dependent equation (*n*th equation in this case) from the system. This eliminates the constant zero mode and we are left with n - 1 equations in n - 1 variables. In Appendix B, the corresponding equations are solved explicitly for both the SLLG and the MLLG.

3.3.1 SLLG

For the SLLG, as shown in Appendix B, the solutions are given as

$$\tilde{\phi}_{i}^{\theta} = \left(q_{i-1} + \sum_{l=0}^{i-2} q_{l} \left(\prod_{k=l}^{i-2} (-1)^{q_{k+1}}\right)\right) \pi + \tilde{\phi}_{n}^{\theta} \prod_{l=0}^{i-1} (-1)^{q_{l}}, \qquad (3.25)$$

for i = 1, ..., n - 1, with

$$\tilde{\phi}_{n}^{\theta} = \frac{n(\overline{\phi} - \frac{2\pi r}{n}) - \left(\sum_{i=1}^{n-1} (q_{i-1} + \sum_{l=0}^{i-2} q_{l}(\prod_{k=l}^{i-2} (-1)^{q_{k+1}}))\right)\pi}{\left(\sum_{i=1}^{n-1} (\prod_{l=0}^{i-1} (-1)^{q_{l}}) + 1\right)},$$
(3.26)

where all $q_i \in \{0, 1\}$ with $q_0 = q_n$, $\tilde{\phi}_i^{\theta} = \phi_i^{\theta} + 2\pi l_i$ and $\tilde{\phi}_i = \phi_i + 2\pi l_i$, and with l_i being integers for all i = 1, ..., n. Also, r runs from 0 to n - 1 and the average link-angle is $\overline{\phi} := \frac{1}{n} \sum_{i=1}^{n} \phi_i$. There are $\sum_{i=0}^{\frac{n-1}{2}} (n-2i) {n \choose i}$ Gribov copies if n is odd, and $\sum_{i=0}^{\frac{n-2}{2}} (n-2i) {n \choose i}$ Gribov copies if n is even. After eliminating the constant zero mode, it is easy to show that for the SLLG

with periodic boundary conditions,

$$(M_{FP})_{ij} = \frac{\partial f_i}{\partial \theta_j}, \ i, j = 1, \dots, n-1,$$
(3.27)

i.e.,

$$M_{FP} = \begin{pmatrix} c_1 + c_n & -c_1 & 0 & \dots & 0 \\ -c_1 & c_2 + c_1 & -c_2 & 0 \\ & & \dots & & \\ 0 & & -c_{n-3} & c_{n-2} + c_{n-3} & -c_{n-2} \\ 0 & \dots & 0 & -c_{n-2} & c_{n-1} + c_{n-2} \end{pmatrix}, \quad (3.28)$$

where $c_i = \cos \phi_i^{\theta}$ for $i = 1, \ldots, n$. The determinant of this matrix can be straightforwardly computed and is

$$\det M_{FP} = (\prod_{k=1}^{n} \cos \phi_k^{\theta}) (\sum_{i=1}^{n} \sec \phi_i^{\theta}).$$
(3.29)

Now, for even n, the gauge transformation $\phi_i^{\theta} \to \phi_i^{\theta} + \pi$ satisfies the SLLG conditions, if the ϕ_i^{θ} 's do, because

$$f_{i}(\theta) = -(\sin(\phi_{i}^{\theta} + \pi) - \sin(\phi_{i-1}^{\theta} - \pi))$$

$$= \sin(\phi_{i}^{\theta}) - \sin(\phi_{i-1}^{\theta})$$

$$= 0, \qquad (3.30)$$

for all $i = 1, \ldots, n-1$, where the last equality comes because the ϕ_i^{θ} 's are assumed to satisfy the gauge fixing conditions, and so using Eq. (3.29),

$$\det M'_{FP} = \left(\prod_{k=1}^{n} \cos(\phi_k^{\theta} + \pi)\right) \left(\sum_{i=1}^{n} \sec(\phi_i^{\theta} + \pi)\right)$$
$$= -\left(\prod_{k=1}^{n} \cos\phi_k^{\theta}\right) \left(\sum_{i=1}^{n} \sec\phi_i^{\theta}\right)$$
$$= -\det M_{FP}.$$
(3.31)

Thus, for even n, every Gribov copy comes in pairs with opposite signs of det M_{FP} , and so the sum over all Faddeev-Popov determinants is a zero, i.e., $Z_{GF} = 0$. Thus, for even n, we have an *exact symmetry* in a certain sense because this $\pm \pi$ chequerboard transformation flips the sign of the Faddeev-Popov determinant. However, such an *exact symmetry* does not exist when n is odd since the corresponding M_{FP} is an even dimensional matrix after eliminating the constant zero mode. However, in this case, we can use the classification of Gribov copies according to the number of negative eigenvalues of the corresponding M_{FP} as explained in Appendix B.1.1. It is then easy to see that there are $\frac{1}{2} \sum_{i=1}^{\frac{n-1}{2}} (n-2i) \binom{n}{i}$ solutions for which det M_{FP} is positive and for the remaining same number of solutions it is negative, though the absolute value of det M_{FP} may be different. Thus the sum of *signs* of the Faddeev-Popov determinants is zero, even though the determinants themselves may not add up to be zero.

3.3.2 MLLG

The solutions of the corresponding gauge fixing equations for the MLLG, as shown in the Appendix B, are

$$\tilde{\phi}_n^\theta = \overline{\phi} - \frac{2\pi r}{n},\tag{3.32}$$

for $r = 0, \ldots, n - 1$, together with

$$\begin{split} \tilde{\phi}_{i}^{\theta} &= \overline{\phi} - \frac{2\pi}{n}r, \\ \text{i.e.,} \\ \phi_{i}^{\theta} &= \overline{\phi} - \frac{2\pi}{n}r + 2\pi l_{i}, \end{split} \tag{3.33}$$

for i = 1, ..., n - 1 and where l_i are integers. There are n Gribov copies in this case.

The corresponding Faddeev-Popov operator³ is, after removing the constant zero mode,

$$(M_{FP}^s)_{ij} = \frac{\partial f_i}{\partial \theta_j}, \ i, j = 1, \dots, n-1,$$
(3.34)

and

$$M_{FP}^{s} = \begin{pmatrix} t_{1} + t_{n} & -t_{1} & 0 & \dots & 0 \\ -t_{1} & t_{2} + t_{1} & -t_{2} & 0 \\ & & \dots & & \\ 0 & & -t_{n-3} & t_{n-2} + t_{n-3} & -t_{n-2} \\ 0 & \dots & 0 & -t_{n-2} & t_{n-1} + t_{n-2} \end{pmatrix}.$$

³Note that we use the superscript s for the stereographically MLLG.

where $t_i = \sec^2 \frac{\phi_i^{\theta}}{2}$ for i = 1, ..., n. It is easy to verify that

det
$$M_{FP}^{s} = (\prod_{k=1}^{n} \sec^{2} \frac{\phi_{k}^{\theta}}{2}) (\sum_{i=1}^{n} \cos^{2} \frac{\phi_{i}^{\theta}}{2}),$$
 (3.35)

which is strictly positive definite for $\phi_i^{\theta} \in (-\pi, \pi)$ for $i = 1, \ldots, n$ so there can be no Neuberger zero in this case.

In particular, for each r = 0, ..., n - 1, det $M_{FP}^s = n \left(\sec^2\left(\frac{\overline{\phi} - \frac{2\pi r}{n}}{2}\right) \right)^{n-1}$ which is positive definite. So,

$$Z_{GF} = \sum_{r=0}^{n-1} \operatorname{sign}\left(\left(\sec^2\left(\frac{\overline{\phi} - \frac{2\pi r}{n}}{2}\right)\right)^{n-1}\right) = n.$$
(3.36)

If we define $\overline{\phi}_r := \overline{\phi} - \frac{2\pi r}{n}$, then the absolute minimum here is given by the copy for which $\overline{\phi}_r \mod 2\pi \in (-\frac{\pi}{n}, \frac{\pi}{n})$. The FMR here is the set of configurations with constant link-angles of a value in this range, and its boundary is given by the values $\pm \frac{\pi}{n}$. The boundary is reached along gauge orbits for configurations for which the average link angle, before gauge fixing, happens to be $\overline{\phi} = \frac{\pi}{n} + \frac{\pi}{n}r$ for $r = 0, \ldots, n - 1$. Thus there are two degenerate absolute minima, the copies for which $\overline{\phi}_r = \pm \frac{\pi}{n}$. This should be counted only once to have gauge orbit space correspond to the $\overline{\phi}$ -interval $[-\frac{\pi}{n}, \frac{\pi}{n}]$ for the average gauge angle. In every other case, before gauge fixing, $\overline{\phi} \neq \frac{\pi}{n} \mod \frac{2\pi}{n}$, the gauge orbits pass through the interior of the FMR and there is a unique absolute minimum as expected.

If we allow $\phi \in (-\pi, \pi]$, we will average over all Gribov copies which are the set of all local minima (only minima because the functional is convex and only bounded from below) of the modified functional along the gauge orbits. As we will verify explicitly below, averaging over all copies is equivalent to restricting to the FMR for the one-dimensional U(1) chain.

In Appendix A, we also prove that the Faddeev-Popov operator for the MLLG is positive semi-definite and positive definite for any dimensional lattice with both periodic and anti-periodic boundary conditions, respectively.

3.4 Topological Interpretation Revisited

In Chapter 2, we mentioned the topological interpretation of lattice gauge-fixing in terms of Morse theory. Here, we explicitly show that all Gribov copies can be classified in terms of Morse indices K_i i.e., the number of negative eigenvalues of the corresponding Faddeev-Popov operator. We recall that K_i is the number of Gribov copies in C_i . In general, following the discussion in Section 2.3, we can state the strong Morse inequalities given in Eq. (2.35), as

$$K_i = \gamma_i b_i, \tag{3.37}$$

with $\gamma_i \geq 1$ for all *i*. We already know the Betti numbers for both the SLLG and the MLLG from Section 2.3. Thus, we can compute K_i 's and figure out the γ_i 's accordingly, as done below.

3.4.1 One-dimensional SLLG

Following the discussion below Eq. (3.18) for the one-dimensional SLLG with antiperiodic boundary conditions, there are $\binom{n}{i}$ Gribov copies at which the Faddeev-Popov operator has *i* negative eigenvalues, i.e., $K_i = \binom{n}{i}$, for $i = 0, \ldots, n$. The sum over all K_i 's of course correctly (up to the trivial over-counting) returns the total number of Gribov copies, N_{GC} ,

$$N_{GC} = \sum_{i=0}^{n} K_i = \sum_{i=0}^{n} \binom{n}{i} = 2^n, \qquad (3.38)$$

and similarly the Euler characteristic, defined as the signed sum over K_i 's, is

$$\chi((S^1)^n) = \sum_{i=0}^n (-1)^i K_i = \sum_{i=0}^n (-1)^i \binom{n}{i} = 0,$$
(3.39)

where we have used the properties of binomial coefficients. And since in this case $b_i = \binom{n}{i}$ for $i = 0, \ldots, n$, we get

$$\gamma_i = 1, \tag{3.40}$$

for i = 0, ..., n.

Similarly, for the periodic chain, all Gribov copies for the SLLG for the onedimensional case are classified in terms of the negative eigenvalues of the corresponding Faddeev-Popov operator, in Appendix B.1.1. Thus, for odd n,

$$N_{GC} = \sum_{i=0}^{\frac{n-1}{2}} \frac{n\left(\frac{n+1}{2}-i\right)}{n-i} \binom{n-1}{i} + \sum_{i=\frac{n+1}{2}}^{n-1} \frac{n\left(i-\frac{n-1}{2}\right)}{i+1} \binom{n-1}{i}$$
$$= \sum_{i=0}^{n-1} K_i.$$
(3.41)

The signed sum over these n-1 K_i 's is 0, giving the correct Euler characteristic. So,

$$\gamma_i = \begin{cases} \frac{n\left(\frac{n+1}{2}-i\right)}{n-i} & \text{if } i = 0, \dots, \frac{(n-1)}{2} \\ \frac{n\left(i-\frac{n-1}{2}\right)}{i+1} & \text{if } i = \frac{(n+1)}{2}, \dots, n-1, \end{cases}$$
(3.42)

since $b_i = \binom{n-1}{i}$ for all i = 0, ..., n-1. For even n, similarly,

$$N_{GC} = \sum_{i=0}^{\frac{n-2}{2}} \frac{n\left(\frac{n}{2}-i\right)}{n-i} \binom{n-1}{i} + \sum_{i=\frac{n}{2}}^{n-1} \frac{n\left(i-\frac{n-2}{2}\right)}{i+1} \binom{n-1}{i}$$
$$= \sum_{i=0}^{n-1} K_i.$$
(3.43)

Thus, $\sum_{i=0}^{n-1} (-1)^i K_i = 0$, i.e., the Neuberger zero, and also,

$$\gamma_i = \begin{cases} \frac{n\left(\frac{n}{2}-i\right)}{n-i} & \text{if } i = 0, \dots, \frac{(n-2)}{2} \\ \frac{n\left(i-\frac{n-2}{2}\right)}{i+1} & \text{if } i = \frac{(n)}{2}, \dots, n-1. \end{cases}$$
(3.44)

3.4.2 One-dimensional MLLG

For the MLLG with anti-periodic boundary conditions, the corresponding Faddeev-Popov operator is positive definite and there is only one gauge-fixed configuration. Thus, $K_0 = 1$ and all other $K_i = 0$ for i = 1, ..., n - 1. Thus,

$$N_{GC} = \sum_{i=0}^{n} K_i = \binom{n}{0} = 1.$$
(3.45)

Now, since in this case, as shown in Section 2.3, $b_0 = 1$ and $b_i = 0$ for all i = 1, ..., n, we get $\gamma_0 = 1$.

Similarly, for the periodic boundary conditions case, there are n solutions for which the corresponding Faddeev-Popov operator is positive definite, i.e., $K_0 = n$ and $K_i = 0$ for all i = 1, ..., n - 1. Thus,

$$N_{GC} = \sum_{i=0}^{n-1} K_i = n, \qquad (3.46)$$

and so, the corresponding $\gamma_0 = n$.

3.5 Faddeev-Popov Procedure for the MLLG

The U(1) group is a special case where one can either choose to work with compact U(1) or non-compact U(1). Now, the study of compact QED on the lattice cannot be motivated to understand any physical phenomenon in particle physics. However, compact QED on the lattice has been extensively studied (see, e.g., Ref. [77, 78, 79, 80, 81, 82]) for several reasons: (1) We first note that compact QED is an Abelian gauge theory and may serve as the prototype for all compact gauge theories on the lattice in 4 dimensions. (2) Compact QED exhibits a twofold phase structure, separated by a mass gap: one phase with a massless photon, called the Coulomb phase and the other phase called the confining phase. Though the QED confining phase is unphysical it shares many qualitative features with QCD. (3) In the confining region, where the coupling becomes strong, compact QED exhibits a rich structure of topological defects such as monopoles, Dirac sheets, Dirac plaquettes etc. Their possible connection to the appearance of zero modes of the Dirac operator is of special interest. With the results in the previous section, we are now ready to formulate the Faddeev-Popov procedure for the MLLG for compact QED in one dimension, with periodic boundary conditions.

We first note that

$$Z_{GF} = \frac{1}{n} \prod_{i=1}^{n-1} \int_{0}^{2\pi} d\theta_{i} \left(\prod_{k=1}^{n-1} \delta(f_{k}(\phi^{\theta})) \right) \det M_{FP}^{s}$$

$$= \frac{1}{n} \sum_{r=0}^{n-1} \left(\prod_{i=1}^{n-1} \left(\int_{0}^{2\pi} d\theta_{i} \, \delta_{P}(\theta_{i} - \theta_{i}^{(0)} + \frac{2\pi}{n}r) \right) \right)$$

$$= 1, \qquad (3.47)$$

where δ_P is the periodic delta function, and in the second equality we used

$$\prod_{k=1}^{n-1} \delta(f_k(\phi^\theta)) \det M_{FP}^s = \sum_{r=0}^{n-1} \left(\prod_{k=1}^{n-1} \sum_{m \in Z} \delta(\theta_k - \theta_k^{(0)} + \frac{2\pi}{n}r + 2\pi m_k) \right)$$
$$= \sum_{r=0}^{n-1} \prod_{k=1}^{n-1} \delta_P(\theta_k - \theta_k^{(0)} + \frac{2\pi}{n}r), \qquad (3.48)$$

where m_k are integers for k = 1, ..., n - 1. We then integrate the n - 1 gauge angles θ_i over an interval of 2π in each term.

Now, the partition function for the one-dimensional compact QED on the periodic chain can be formally written as,

$$Z_{1d} = \prod_{i=1}^{n} \int_{S^1} dU_i \ e^{-S_{1d}[U]}.$$
(3.49)

Inserting the unity from Eq. (3.47) into Eq. (3.49), using the gauge invariance of measure, the action and the corresponding det M_{FP}^s , and factorizing the volume of the gauge group, we obtain

$$Z_{1d} = \frac{(2\pi)^{n-1}}{n} \prod_{i=1}^{n} \int_{S^1} dU_i \Big(\prod_{k=1}^{n-1} \delta(f_k(\phi)) \Big) \det M_{FP}^s e^{-S_{1d}[U]}$$

$$= \frac{(2\pi)^{n-1}}{n} \prod_{i=1}^{n} \int_0^{2\pi} \frac{d\phi_i}{2\pi} \Big(\prod_{k=1}^{n-1} \delta_P(\phi_k - \phi_n) \Big) \Big| \det \frac{\partial f}{\partial \phi} \Big|^{-1} \det M_{FP}^s e^{-S_{1d}[U]},$$

(3.50)

where the prefactor $(2\pi)^{n-1}$ is the volume of the gauge group and arises from the integration of the n-1 gauge angles θ_i 's. In the second equality, we again used the properties of the δ -function. Now,

$$\frac{\partial f}{\partial \phi} = - \begin{pmatrix} t_1 & 0 & 0 & \dots & 0 \\ -t_1 & t_2 & 0 & & 0 \\ & & \dots & & \\ 0 & & -t_{n-3} & t_{n-2} & 0 \\ 0 & \dots & 0 & -t_{n-2} & t_{n-1} \end{pmatrix},$$
(3.51)

where now $t_i = \sec^2 \frac{\phi_i}{2}$ for all $i = 1, \ldots, n-1$. So,

$$\left|\det\frac{\partial f}{\partial\phi}\right| = \prod_{i=1}^{n-1}\sec^2\frac{\phi_i}{2}.$$
(3.52)

Moreover, since all $\phi_i = \phi_n \mod 2\pi$ because of the periodic δ -functions in Eq. (3.50), we get

$$\left|\det\frac{\partial f}{\partial\phi}\right|^{-1}\det M_{FP}^s = \sec^2\frac{\phi_n}{2}\left(\sum_{i=1}^n\cos^2\frac{\phi_i}{2}\right) = n.$$
(3.53)

We can now simplify Eq. (3.50) as below,

$$Z_{1d} = \frac{1}{2\pi} \int_0^{2\pi} d\bar{\phi} \ e^{-S_{1d}(\bar{\phi})}, \tag{3.54}$$

after integration of the n-1 periodic δ -functions and renaming $\phi_n \to \overline{\phi}$. Moreover, we have taken $U_i = e^{i\overline{\phi}}$ for all $i = 1, \ldots, n$.

Here, we also need to specify the action $S_{1d}[U]$ for the one-dimensional periodic chain. In this case, since there is no plaquette, the only gauge invariant operator is $l = \sum_{i=1}^{n} \phi_i$ and so

$$S_{1d}[U] = \beta n(1 - \cos(n\overline{\phi})) = \beta n(1 - \cos l), \qquad (3.55)$$

is the physical action in this case.

We can evaluate the partition function in Eq. (3.54) in two ways: restricting the integration range to the FMR or taking all Gribov copies into account. With the former approach,

$$Z_{1d} = \frac{n}{2\pi} \int_{-\frac{\pi}{n}}^{\frac{\pi}{n}} d\bar{\phi} \ e^{-S_{1d}(\bar{\phi})} = \frac{1}{2\pi} \int_{0}^{2\pi} dl \ e^{-\beta n(1-\cos l)} = e^{-\beta n} I_0(\beta n) , \quad (3.56)$$

where $I_0(x)$ is the n = 0 Bessel function of the first kind (with $I_0(0) = 1$ in agreement with our normalization in the original partition function Z_{1d} in Eq. (3.49) which tends to 1 for $\beta \to 0$). The other way is to average over all n Gribov copies, i.e.,

$$Z_{1d} = \frac{1}{2\pi} \int_0^{2\pi} d\overline{\phi} e^{-S_{1d}(\overline{\phi})} = \frac{1}{2\pi n} \int_0^{2\pi n} dl \ e^{-S_{1d}(\frac{l}{n})} = e^{-\beta n} I_0(\beta n), \qquad (3.57)$$

where the periodicity of the action in the loop $l = n\overline{\phi}$ and $\frac{l}{n} = \overline{\phi}$ have been used. Thus, for the MLLG, exactly the same result can be obtained either by averaging over all Gribov copies or when working within the FMR.

3.6 1+1 Complete Coulomb Gauge

It is a highly non-trivial task to solve the two-dimensional lattice Landau gaugefixing equations for both the SLLG and the MLLG. We will devote Chapters 4 and 5 to discuss the related issues for the two-dimensional case. However, a very interesting application of the MLLG on a two-dimensional lattice using the onedimensional results is the complete Coulomb gauge in 1+1 dimensions. A d+1dimensional complete Coulomb gauge on the lattice means the following: first fix the *d*-dimensional Coulomb gauge while leaving the time direction ungauge-fixed. This is nothing but the *d*-dimensional Landau gauge in spatial dimensions. Then, fix the residual gauge freedom for the temporal links in the spatial directions. The Coulomb gauge studies have been of great importance in the Hamiltonian formalism of lattice gauge field theories and in the Gribov-Zwanziger confinement scenario [83, 84, 85, 86, 87, 88]. In particular, the Coulomb gauge in 1 + 1dimensions has recently gained a renewed interest [89]. Here, we can use all the results for the one-dimensional lattice Landau gauge obtained so far to study this two-dimensional system. In this section, we discuss the 1 + 1 complete Coulomb gauge with both periodic and anti-periodic boundary conditions and formulate an analogous Faddeev-Popov procedure for the two-dimensional lattice.

3.6.1 Anti-periodic Boundary Conditions

First, we fix the spatial Coulomb gauge which turns out to be the one-dimensional Landau gauge in each time slice. The corresponding gauge fixing functional for the modified case for a $n_x \times n_t$ lattice, at each time slice t, is

$$(F_{\phi}^{\rm S}(\theta))_t = -2\sum_{x=1}^{n_x} \ln\cos(\frac{\phi_{(x,t),\hat{x}} + \theta_{x+1,t} - \theta_{x,t}}{2}), \qquad (3.58)$$

where we have slightly changed our notations: the lattice site index is (x, t) in x-t plane, $\phi_{(x,t),\hat{x}}$ is the link in the x-direction starting at the site (x, t) and $\theta_{x,t}$ is the gauge transformation at site (x, t). The corresponding gauge fixing conditions,

$$f_{(x,t)}^{s}(\theta) = \tan \frac{(\phi_{(x,t),\hat{x}} + \theta_{x+1,t} - \theta_{x,t})}{2} - \tan \frac{(\phi_{(x-1,t),\hat{x}} + \theta_{x,t} - \theta_{x-1,t})}{2} = 0, \quad (3.59)$$

for $x = 1, ..., n_x$ for each time-slice t. For the anti-periodic boundary conditions case, as we already know, $\phi_{(x,t),\hat{x}}^{\theta} = 0 \mod 2\pi$ for $x = 1, ..., n_x$ at each time slice t. So, at each time slice there is no Gribov copy. We still have the residual gauge freedom

$$\phi_{(x,t),\hat{t}} \to \phi^{\theta}_{(x,t),\hat{t}} = \phi_{(x,t),\hat{t}} + \theta_{x,t+1} - \theta_{x,t}$$
 (3.60)

for all $x = 1, ..., n_x$, all $\theta_{x,t}$'s being spatially constant. This residual gauge transformation basically just changes the spatial average over the *t*-links between neighboring time slices. If $\check{\phi}_{(t),\hat{t}}$ is the average over all *t*-links in a given time slice *t*, then

$$\breve{\phi}_{(t),\hat{t}} := \frac{1}{n_x} \sum_{x=1}^{n_x} \phi_{(x,t),\hat{t}} \to \breve{\phi}_{(t),\hat{t}}^{\theta} = \breve{\phi}_{(t),\hat{t}} + \theta_{x,t+1} - \theta_{x,t}.$$
(3.61)

To fix this residual gauge freedom, we can write the MLLG functional for this one-dimensional chain of the time-link averages $\check{\phi}_{(t),\hat{t}}$ as,

$$\ddot{F}_{\phi}^{s}(\theta) = -2\sum_{t=1}^{n_{t}} \ln \cos(\frac{\breve{\phi}_{(t),\hat{t}} + \theta_{x,t+1} - \theta_{x,t}}{2}), \qquad (3.62)$$

with the corresponding gauge fixing conditions

$$\check{f}_t^s = \tan\frac{\check{\phi}_{(t),\hat{t}} + \theta_{x,t+1} - \theta_{x,t}}{2} - \tan\frac{\check{\phi}_{(t-1),\hat{t}} + \theta_{x,t} - \theta_{x,t-1}}{2} = 0,$$
(3.63)

for t = 1, ..., n, finally giving, for anti-periodic boundary conditions in the time direction, $\check{\phi}^{\theta}_{(t),\hat{t}} = 0 \mod 2\pi$, for all t = 1, ..., n. Here, one can also consider the SLLG and deduce that in the first step there are 2^{n_x} Gribov copies at each time-slice and there are again 2^{n_t} Gribov copies in the second step. Thus in the modified approach, the number of Gribov copies is exponentially suppressed in each step of the complete Coulomb gauge in 1 + 1 dimensions.

3.6.2 Periodic Boundary Conditions

For the periodic boundary conditions case, the gauge-fixing functional for the MLLG in the first step is the same as Eq. (3.58) and the gauge fixing conditions as Eq. (3.59), formally. Here, we formulate the Faddeev-Popov gauge-fixing procedure for this case. In the first step, in terms of average over x-links at each time slice, $\overline{\phi}_{(t),\hat{x}} = \frac{1}{n_x} \sum_{x=1}^{n_x} \phi_{(x,t),\hat{x}}$, for all $t = 1, \ldots, n_t$, we have n_x solutions at each time slice t, as we already know. Thus, we had $2n_tn_x$ link variables (two for each of $n_x n_t$ sites) initially, out of which, after fixing this partial gauge, there are $n_t(n_x + 1)$ variables left, i.e., all $n_t n_x$ t-links $\phi_{(x,t),t}$ and n_t x-links $\overline{\phi}_{(t),x}$.

Such a partially gauge fixed partition function for 2d compact QED is

$$Z_{2d} = \prod_{t=1}^{n_t} \int_0^{2\pi} \frac{d\overline{\phi}_{(t),\hat{x}}}{2\pi} \prod_{x=1}^{n_x} \int_0^{2\pi} \frac{d\phi_{(x,t),\hat{t}}}{2\pi} e^{-S_{2d}(\overline{\phi},\phi)}.$$
 (3.64)

The partially gauge fixed plaquettes are

$$\Box_{(x,t)} = \phi_{(x+1,t),\hat{t}} - \phi_{(x,t),\hat{t}} - (\overline{\phi}_{(t+1),\hat{x}} - \overline{\phi}_{(t),\hat{x}}), \qquad (3.65)$$

and so the usual compact QED, up to a constant, can then be written as

$$S_{2d}(\overline{\phi}, \phi) = -\beta \sum_{x,t} \cos \Box_{(x,t)}$$

= $-\beta \sum_{x,t} \cos(\phi_{(x+1,t),\hat{t}} - \phi_{(x,t),\hat{t}} - (\overline{\phi}_{(t+1),\hat{x}} - \overline{\phi}_{(t),\hat{x}})).$ (3.66)

Now, there is still residual gauge freedom left as given in Eq. (3.60). To fix these residual gauge transformations, we can write the MLLG for this onedimensional chain of time-link averages $\check{\phi}_{(t),\hat{t}}$ as Eq. (3.62) and the gauge fixing conditions as Eq. (3.63). And simply using the known results for the onedimensional chain, we get n_t solutions,

$$\breve{\phi}^{\theta}_{(t),\hat{t}} = \breve{\phi} - \frac{2\pi}{n_t}r + 2\pi q_t, \text{ with}
\breve{\phi} = \frac{1}{n_t} \sum_{t=1}^{n_t} \breve{\phi}_{(t),\hat{t}},$$
(3.67)

for $t = 1, ..., n_t$. Here, $r = 0, ..., n_t - 1$ refers to the number of Gribov copies. This constrains the n_t spatial averages $\check{\phi}_{(t),\hat{t}}$ over the *t*-links between neighboring slices to be all the same, $\check{\phi}$.

We can again insert a one-dimensional MLLG fixing partition function of the form,

$$Z_{GF} = \frac{1}{n_t} \prod_{t=1}^{n_t-1} \int_0^{2\pi} d\theta_{x,t} \Big(\prod_{k=1}^{n_t-1} \delta(\check{f}_k^s(\theta)) \Big) \det M_{FP}^s = 1,$$
(3.68)

where now $\check{f}_k^s(\theta)$ are the gauge fixing conditions given in Eq. (3.63) for $k = 1, \ldots, n_t - 1$, with periodic boundary conditions after appropriately eliminated constant zero mode. So, finally, the partition function for compact QED is

$$Z_{2d} = \int_0^{2\pi} \frac{d\breve{\phi}}{2\pi} \prod_{t=1}^{n_t} \left(\int_0^{2\pi} \frac{d\overline{\phi}_{(t),\hat{x}}}{2\pi} \prod_{x=1}^{n_x} \int_0^{2\pi} \frac{d\phi_{(x,t),\hat{t}}}{2\pi} \delta_P(\breve{\phi}_{(t),\hat{t}} - \breve{\phi}) \right) e^{-S_{2d}(\overline{\phi},\phi)}.$$
 (3.69)

Here, there are n_t periodic δ -function constraints which will eliminate one $\phi_{(x,t),\hat{t}}$ from each time slice t, i.e., in total n_t variables are eliminated. However, finally it has one independent average variable $\check{\phi}$, and hence there are in total $n_t - 1$ variables eliminated, i.e., there are

$$n_t(n_x+1) \to n_t(n_x+1) - (n_t-1) = n_t n_x + 1$$
 (3.70)

variables left.

This is *almost* as much as we can do in eliminating the redundant degrees of freedom in the two-dimensional theory when fixing the gauge up to the global gauge transformations. Thus, it is an only *almost* complete elimination of the gauge freedom in that it still contains all Gribov copies of the two-dimensional compact U(1) lattice gauge theory of which there are $n_t n_x^{n_t}$. This finalizes the Faddeev-Popov procedure of the two-dimensional compact QED in 1+1 complete Coulomb gauge. It is then straightforward to construct the corresponding BRST formulation.

To restrict the theory to the FMR, as we did in the one-dimensional case, we can alternatively write

$$Z_{2d} = n_x^{n_t} n_t \int_{-\frac{\pi}{n_t}}^{\frac{\pi}{n_t}} \frac{d\breve{\phi}}{2\pi} \prod_{t=1}^{n_t} \left(\int_{-\frac{\pi}{n_x}}^{\frac{\pi}{n_x}} \frac{d\overline{\phi}_{(t),\hat{x}}}{2\pi} \prod_{x=1}^{n_x} \int_{0}^{2\pi} \frac{d\phi_{(x,t),\hat{t}}}{2\pi} \delta_P(\breve{\phi}_{(t),\hat{t}} - \breve{\phi}) \right) e^{-S_{2d}(\bar{\phi},\phi)}.$$
(3.71)

3.7 Remarks

- 1. In the one-dimensional lattice, since for the MLLG the corresponding N_{GC} is the same for all random orbits, i.e., random ϕ_i 's before gauge-fixing, we used the prefactor $\frac{1}{n}$ in the gauge fixing partition function in Eq. (3.47). In the higher dimensional case, we have already shown that the Faddeev-Popov operator is positive (semi-)definite, in Appendix A. However, what we have not shown so far for the higher dimensional case is if the corresponding N_{GC} for the MLLG is orbit-independent. If it is, then in those cases too we can use the prefactor $1/N_{GC}$ in the expression of the corresponding Z_{GF} , and the Faddeev-Popov procedure can be elegantly formulated there. If not, then it would be cumbersome to formulate an analogous procedure due to the orbit-dependent prefactor. Establishing a precise statement in one way or another will thus be very important.
- 2. We know that if all elements of an odd dimensional square matrix change their signs, then the determinant of this matrix flips its sign leaving the absolute value unchanged. We show in what follows that by taking the so-called chequer-board transformation on a gauge-fixed configuration of a lattice with odd number of sites with anti-periodic boundary conditions, all elements of the corresponding M_{FP} change the sign, and hence give an opposite signed Faddeev-Popov determinant, for the SLLG. We define the chequer-board transformation as adding and subtracting π to alternate link

angles $\phi^{\theta}_{i,\mu}$'s, i.e., $\phi^{\theta}_{i,\mu} \to \phi^{\theta}_{i,\mu} \pm \pi$ and so

$$f_{i}(\theta) \rightarrow -\sum_{\mu=1}^{d} (\sin(\phi_{i,\mu}^{\theta} + \pi)) - \sin((\phi_{i-\hat{\mu},\mu}^{\theta} - \pi))$$
$$= \sum_{\mu=1}^{d} (\sin\phi_{i,\mu}^{\theta} - \sin\phi_{i-\hat{\mu},\mu}^{\theta})$$
(3.72)

where *i* runs over all lattice sites. Such a gauge-transformed configuration is also a solution of the gauge fixing equations. Note that the same applies to all the boundary points as well, taking proper care of anti-periodic boundary conditions. Thus, the sum of all the determinants is always zero, yielding the Neuberger zero. For an even number of lattice sites, this symmetry does not flip the sign of the Faddeev-Popov determinant since there are an even number of eigenvalues involved there. Finding such a sign-changing transformation becomes much more involved in that case.

With periodic boundary conditions, the chequer-board transformation flips the sign of the Faddeev-Popov determinant leaving the same absolute value, for the even lattice sites case. This is because in this case the Faddeev-Popov operator has an odd number of eigenvalues after eliminating the constant zero mode.

- 3. Apparently, in one dimension, the solutions of the gauge-fixing equations for the MLLG are a subset of the solutions of the SLLG case. Moreover, in the anti-periodic boundary conditions case, the solution for the MLLG case is the FMR (or C_0 , since both are the same in this case) of the SLLG. In the periodic boundary conditions case, the solutions for the MLLG case are the extrema of the SLLG, i.e., the saddle points of the SLLG are eliminated in the MLLG in one dimension. This is a very important result and it would be very interesting to see if it holds for higher dimensional lattices.
- 4. Recently, the MLLG for SU(2) has been used in lattice simulations [90, 91] and it has been shown that there is no advantage that the SLLG has over the MLLG, as expected, since both have the same continuum limit and so any differences between SLLG and MLLG at finite lattice-spacing are only lattice artifacts. However, the most important advantage of the MLLG is that it provides a way to perform lattice gauge-fixed Monte-Carlo simulations sampling *all* Gribov copies of either sign of Faddeev-Popov operator in BRST fashion.

3.8 Summary

We summarize the results obtained so far:

- 1. The gauge fixing equations for both the SLLG and the MLLG can be solved exactly for a one-dimensional lattice with n lattice sites. For the SLLG case, we have explicitly demonstrated that the Neuberger 0/0 problem persists in this simple toy model and there are exactly 2^n Gribov copies in terms ϕ_i^{θ} 's with anti-periodic boundary conditions. For the proposed MLLG with anti-periodic boundary conditions, we proved that there is no Neuberger 0/0 problem since the Faddeev-Popov operator is strictly positive definite. There, we also showed that the corresponding N_{GC} is 1 in terms of the ϕ_i^{θ} 's. Thus, N_{GC} is exponentially suppressed in this case, compared to the SLLG.
- 2. For the periodic boundary conditions case in one dimension, we showed in Appendix B that for the SLLG the corresponding N_{GC} is $\sum_{i=0}^{\frac{n-1}{2}} (n-2i) {n \choose i}$ for odd n and $\sum_{i=0}^{\frac{n-2}{2}} (n-2i) {n \choose i}$ for even n. Moreover, the corresponding Faddeev-Popov operator is an indefinite matrix and the sum of signs of the Faddeev-Popov determinants is zero, i.e., $Z_{GF} = 0$. In addition, we have completely classified the Gribov copies in this case in terms of Morse indices. On the other hand, for the MLLG with periodic boundary conditions, we have shown that there are exactly n Gribov copies. Thus, N_{GC} is exponentially suppressed compared to the SLLG. We also showed that there the Faddeev-Popov operator is always positive semi-definite with exactly one constant zero mode due to the global gauge freedom. Furthermore, the Faddeev-Popov operator, after eliminating the global zero mode, is strictly positive definite and so there is no Neuberger zero.
- 3. We have formulated the Faddeev-Popov gauge-fixing procedure on the lattice for the 1- and (1 + 1)-dimensional compact QED, respectively, via the MLLG.
- 4. Dealing with the gauge fixing equations for higher dimensional lattices is highly non-trivial and the same techniques used for the one-dimensional counter-part does not work any longer. However, in Appendix A we have shown that the Faddeev-Popov operator for the MLLG is positive semidefinite or positive definite for an arbitrary dimensional lattice with both periodic and anti-periodic boundary conditions, respectively. That is, the Neuberger 0/0 problem is solved for compact U(1).

Chapter 4

Algebraic Geometry and Lattice Landau Gauge Fixing

As we saw in the previous chapter, the Landau gauge fixing conditions corresponding to both the SLLG and the MLLG are highly non-linear for higher dimensional lattices. In general, systems of non-linear equations are difficult to solve. However, in this chapter¹ we translate the systems of equations arising in the cases at hand to polynomial equations which can then use many of the results from Algebraic Geometry. Here, we introduce some necessary concepts of Algebraic Geometry. We will follow [92, 93] unless otherwise stated explicitly. We will introduce a relatively recent field of Computational Algebraic Geometry and show how the systems can then be solved using related techniques, specifically the Groebner basis technique. Moreover, we will show that this Algebraic Geometry interpretation gives a deep insight to the Gribov copy problem on the lattice in the standard and modified definitions. Though our goal is to solve the gauge fixing conditions for higher dimensional lattices, we will mainly analyze the one-dimensional case because: (1) we already know the exact solutions for this case and so the results from the new approach will have a precise comparison, and (2) the one-dimensional case, interpreted as an Algebraic Geometry problem, provides all the essence of the higher dimensional generalizations (unlike the same case treated as a linear algebra problem as in Chapter 3). After making a few remarks, we will conclude the chapter.

4.1 Landau Gauge Fixing Equations as Polynomial Equations

Here, we explain the procedure of transforming the Landau gauge-fixing equations into polynomial form. We start with restating the SLLG equations for compact

¹I am thankful to Fernando Hernando for his critical and expert remarks on this chapter.

U(1) in one dimension,

$$f_i(\phi^\theta) = \sin(\phi_i^\theta) - \sin(\phi_{i-1}^\theta) = \sin(\phi_i + \theta_{i+1} - \theta_i) - \sin(\phi_{i-1} + \theta_i - \theta_{i-1})$$

= 0 (4.1)

with i = 1, ..., n. Using trigonometric identities, we can expand the equations as,

$$f_{i}(\phi^{\theta}) = \cos(\theta_{i})(\cos(\phi_{i-1})\sin(\theta_{i-1}) + \cos(\phi_{i})\sin(\theta_{i+1}))$$

$$-\cos(\theta_{i-1})\sin(\phi_{i-1}) + \cos(\theta_{i+1})\sin(\phi_{i}))$$

$$+\sin(\theta_{i})(-\cos(\theta_{i-1})\cos(\phi_{i-1}) - \cos(\theta_{i+1})\cos(\phi_{i}))$$

$$-\sin(\theta_{i-1})\sin(\phi_{i-1}) + \sin(\theta_{i+1})\sin(\phi_{i}))$$

$$= 0.$$
(4.2)

For simplicity, we take the trivial orbit case (i.e., all $\phi_i = 0$), and writing $\cos \theta_i \equiv c_i$ and $\sin \theta_i \equiv s_i$, we get

$$f_i(c,s) = c_i(s_{i+1} + s_{i-1}) - s_i(c_{i+1} + c_{i-1}) = 0 , \qquad (4.3)$$

for all i = 1, ..., n. This is merely a change of notation. However, we add additional equations in the system for each site i,

$$g_i(c,s) = s_i^2 + c_i^2 - 1 = 0, (4.4)$$

for all i = 1, ..., n. Now, the combined system of all $f_i(c, s)$ and $g_i(c, s)$ is not just a change of notation but all the c_i and s_i are algebraic variables and the equations are multivariate polynomial equations, i.e., the fact that c_i and s_i are originally $\sin \theta_i$ and $\cos \theta_i$ is taken care of by the constraint equations (4.4). For example for the n = 3 SLLG case with anti-periodic boundary conditions, we get

$$f_{1}(c,s) = -c_{2}s_{1} - c_{3}s_{1} + c_{1}s_{2} - c_{1}s_{3}$$

$$f_{2}(c,s) = c_{2}s_{1} - c_{1}s_{2} - c_{3}s_{2} + c_{2}s_{3}$$

$$f_{3}(c,s) = -c_{3}s_{1} + c_{3}s_{2} - c_{1}s_{3} - c_{2}s_{3}$$

$$g_{1}(c,s) = c_{1}^{2} + s_{1}^{2} - 1$$

$$g_{2}(c,s) = c_{2}^{2} + s_{2}^{2} - 1$$

$$g_{3}(c,s) = c_{3}^{2} + s_{3}^{2} - 1.$$
(4.5)

Thus, our problem of solving the gauge fixing conditions in terms of θ_i is transformed into that of solving a system of polynomial equations for variable s_i and c_i . In general, for the one-dimensional lattice with n lattice sites, we have in total 2n polynomial equations and 2n variables.

Similarly, for the MLLG via stereographic projection,

$$f_i(\phi^{\theta}) = \frac{\tan(\theta_{i+1}/2) - \tan(\theta_i/2)}{1 + \tan(\theta_{i+1}/2)\tan(\theta_i/2)} - \frac{\tan(\theta_i/2) - \tan(\theta_{i-1}/2)}{1 + \tan(\theta_i/2)\tan(\theta_{i-1}/2)} = 0 , \quad (4.6)$$

where we have taken the trivial orbit case for simplicity². Now, since the tangents of half angles can take values from $-\infty$ to ∞ for angles in $(-\pi, \pi]$, they can readily be treated as *algebraic* variables. However, to get the equations in the *polynomial shape*, we clear out the denominators after multiplying them with the numerators appropriately. To ensure that none of those denominators is zero, we also add one more constraint equation as 1 - yx = 0, where x is the product of all denominators. Thus, in the modified case we have to add only one additional equation and one more variable, y. Then the equations are again polynomial equations with variables $T_i = \tan \frac{\theta_i}{2}$ and y.

For the n = 3 trivial orbit case with anti-periodic boundary conditions, the corresponding MLLG equations are

$$f_{1}(\phi^{\theta}) = T_{2}T_{1}^{2} - T_{3}T_{1}^{2} + 2T_{2}T_{3}T_{1} + 2T_{1} - T_{2} + T_{3}$$

$$f_{2}(\phi^{\theta}) = -T_{1}T_{2}^{2} - T_{3}T_{2}^{2} + 2T_{1}T_{3}T_{2} - 2T_{2} + T_{1} + T_{3}$$

$$f_{3}(\phi^{\theta}) = -T_{1}T_{3}^{2} + T_{2}T_{3}^{2} + 2T_{1}T_{2}T_{3} + 2T_{3} + T_{1} - T_{2}$$

$$f_{4}(\phi^{\theta}) = 1 - y(T_{1}T_{2} + 1)(T_{1}T_{3} - 1)(T_{2}T_{3} + 1).$$
(4.7)

We observe that the systems (4.5) and (4.7) have a striking difference. Though the number of polynomials and variables in (4.5) is less than those in (4.7), the degree of each polynomial equation is 2 in the former case and in the latter it is 3 for all equations except the additional equation that has degree 7.

In general, when transforming the equations of trigonometric functions to equations in polynomial forms we must take care of a few things. Firstly, our original equations are composed of trigonometric functions of some variable angles θ_i . Since the ranges and the domains of trigonometric functions are defined over \mathbb{R} , the solutions of the equations are obviously in \mathbb{R}^n (where n is the number of variables). But the corresponding polynomial equations including the constraint equations, can be defined over any field, e.g., \mathbb{R} , \mathbb{C} , \mathbb{Q} , and the corresponding solutions may be in \mathbb{R}^n , \mathbb{C}^n or \mathbb{Q}^n respectively. So, while dealing with such systems of polynomial equations, we must specify a field over which the new variables are defined. The obvious choice is to take all the new variables in \mathbb{R}^n so that in the end we can have a one-to-one correspondence between the solutions in terms of the original trigonometric variables and the new algebraic variables. However, Algebraic Geometry over the real variables, called Real Algebraic Geometry is a highly complicated subject in contrast to Complex Algebraic Geometry. This is mainly because of the Fundamental Theorem of Algebra which asserts that every non-zero polynomial with complex coefficients can be decomposed into irreducible components of degree one if defined over complex variables. For example, a polynomial $x^2 + 1$ is uniquely factorized if $x \in \mathbb{C}$ as (x+i)(x-i), but it is not factorizable if $x \in \mathbb{R}$. Mainly due to this important result, Algebraic Geometry has been traditionally studied extensively over complex variables and many

²For a random orbit case one follows the same procedure, simply remembering to use trigonometric identities to expand the trigonometric functions of the sum of three angles.

important results are available therein. Thus, though Real Algebraic Geometry is a fertile, exciting and rapidly emerging area of research in pure and applied Mathematics, it has limited applications.

Having said that, we are still not in too much trouble. We can take each of the corresponding polynomial variables from \mathbb{C} , use all the well-developed techniques in Complex Algebraic Geometry, and get all complex solutions which obviously include real solutions. Then we can throw out the complex solutions while keeping only real solutions and we are done. For example, for the equation $x(x^2+1) = 0$, all complex solutions are x = 0, x = i, x = -i and so its real solution is x = 0. This is a standard procedure used in Robotics, Protein Folding, etc. and related problems.

We introduce a few basic notions of Algebraic Geometry below. This technical jargon will lead to a very useful result: we can transform a given system of multivariable polynomial equations to another one which has the same solutions but is easier to solve, roughly speaking. Here, the original system is considered as a basis of an algebraic object, called an *ideal*, and then an important result, that an appropriate change of this basis leaves the solution space unchanged, is used.

Polynomial Rings

First of all, a polynomial f is defined as $f = \sum_{\alpha} a_{\alpha} x^{\alpha}$. Here, the sum is over a finite number of m-tuples $\alpha = (\alpha_1, \ldots, \alpha_m)$, $a_{\alpha} \in K$ (for example, $\mathbb{Q}, \mathbb{R}, \mathbb{C}$) and $x^{\alpha} = x_1^{\alpha_1} \ldots x_m^{\alpha_m}$ is a monomial with all α_i being non-negative integers. The coefficients a_{α} , take values from a field, K. Similarly, the variables x_i can, in general, take values from $\mathbb{Q}, \mathbb{R}, \mathbb{C}$, etc. Thus, each equation in (4.5) is a polynomial in $c_1, c_2, c_3, s_1, s_2, s_3$ and each equation (4.7) is a polynomial in T_1, T_2, T_3, y . For a random orbit, where the parameters are in symbolic form $\sin \phi_i$, $\cos \phi_i$ and $\tan \frac{\phi_i}{2}$, ideally $K = \mathbb{R}$. However, to use the results of Algebraic Geometry to its full extent, we choose $K = \mathbb{C}$. This means that all allowed coefficients are complex numbers having imaginary part zero.

Now, if $K[x_1, \ldots, x_m]$ is the set of all polynomials in variables x_1, \ldots, x_m with coefficients in K, then f can be viewed as a function $f : K^m \longrightarrow K$ where K^m is the affine space of all coefficients. Thus, the sum and product of two polynomials is a polynomial, and a polynomial f divides a polynomial g if g = fhfor some $h \in K[x_1, \ldots, x_m]$. Using this, it can be shown that under addition and multiplication, $K[x_1, \ldots, x_m]$ satisfies all of the field axioms except, the existence of multiplicative inverse because $\frac{1}{x}$ is not a polynomial. $K[x_1, \ldots, x_m]$ is called a commutative ring, or more precisely a polynomial ring (For a nice discussion on related topics, the reader is referred to [92, 93].). Thus, the polynomial system in Eq. (4.5) is defined in the polynomial ring $\mathbb{C}[c_1, c_2, c_3, s_1, s_2, s_3]$ and in Eq. (4.7) is defined in the polynomial ring $\mathbb{C}[T_1, T_2, T_3, y]$.

Ideal

One can now view all the polynomials of a system of polynomial equations as elements of a polynomial ring. From there on, one can also define a corresponding vector space, called an ideal. More specifically an ideal, say I, is a subset of $K[x_1, \ldots, x_m]$ with the following operations: (1.) $0 \in I$, (2.) $f + g \in I$ for all $f, g \in I$ and (3.) $hf \in I$ for $f \in I$ and $h \in K[x_1, \ldots, x_m]$. Now, for all $h_i \in K[x_1, \ldots, x_m]$, $i = 1, \ldots, t$, $I = \langle h_1, \ldots, h_t \rangle$ is an ideal of $K[x_1, \ldots, x_m]$, called an ideal generated by h_1, \ldots, h_t , and if t is finite then I is called finitely generated. The polynomials h_1, \ldots, h_t then form a basis of I.

Thus, for the polynomials in Eq. (4.5), the corresponding ideal is

$$I_{3} = \langle -c_{2}s_{1} - c_{3}s_{1} + c_{1}s_{2} - c_{1}s_{3}, c_{2}s_{1} - c_{1}s_{2} - c_{3}s_{2} + c_{2}s_{3}, -c_{3}s_{1} + c_{3}s_{2} - c_{1}s_{3} - c_{2}s_{3}, c_{1}^{2} + s_{1}^{2} - 1, c_{2}^{2} + s_{2}^{2} - 1, c_{3}^{2} + s_{3}^{2} - 1 \rangle.$$

$$(4.8)$$

Similarly, for polynomials in Eq. (4.7), the ideal is

$$J_{3} = \langle T_{2}T_{1}^{2} - T_{3}T_{1}^{2} + 2T_{2}T_{3}T_{1} + 2T_{1} - T_{2} + T_{3}, -T_{1}T_{2}^{2} - T_{3}T_{2}^{2} + 2T_{1}T_{3}T_{2} - 2T_{2} + T_{1} + T_{3}, -T_{1}T_{3}^{2} + T_{2}T_{3}^{2} + 2T_{1}T_{2}T_{3} + 2T_{3} + T_{1} - T_{2}, 1 - y(T_{1}T_{2} + 1)(T_{1}T_{3} - 1)(T_{2}T_{3} + 1) \rangle .$$

$$(4.9)$$

Affine Variety

So far we have introduced the algebraic counterpart of Algebraic Geometry. Now, roughly speaking, the solution space of a given ideal is called a *variety*. Specifically, an affine variety of an ideal $I = \langle h_1, \ldots, h_t \rangle$ is the set of common zeros of polynomials $h_1 \ldots, h_t$ in affine space, denoted as $V(h_1, \ldots, h_t)$ or V(I).

All this technical jargon turns out to be very helpful. Interpreting the polynomials h_i as a basis of I, we can change the basis to, say, $\langle H_1, \ldots, H_s \rangle$. Then it can be shown that the solution space remains unchanged in an appropriate change of basis, that is, $V(h_1, \ldots, h_t) = V(H_1, \ldots, H_s)$. So, we just look for a basis that is easier to deal with than the original one, in a certain sense³. Such a basis is called a Groebner basis.

³Our aim here is very practical: we wish to solve the system of polynomial equations. However, the Groebner basis technique, introduced in the next section, helps to solve even more general problems which are impossible to handle otherwise, for example, to check if a polynomial is within the given ideal (ideal membership problem), parametrization of the solution space, etc. For more details, the reader is referred to Ref. [92, 93].

4.2 Groebner Basis

We have seen that we can change a basis to the one that is *easier* to solve, called a Groebner basis, such that the corresponding variety remains unchanged. In linear algebra, such a change of basis can be done via Gaussian-Elimination and the new basis is of the so-called Row-Echelon form. In general, an algorithm to obtain a Groebner basis performs a specific set of algebraic operations including factorizing and dividing the polynomials. There, the division requires one to set a *preference* among the variables. This is called a *monomial ordering*.

Formally, a monomial ordering is a relation, say ' \succ ', on the set of monomials x^{α} , $\alpha \in \mathbb{Z}_{\geq 0}^{n}$, satisfying: (1) the ordering always tells which of two distinct monomials is greater, (2) the relative order of two monomials does not change when they are each multiplied by the same monomial and (3.) every strictly decreasing sequence of monomials eventually terminates [94].

There are different types of ordering, for example, lexicographic, graded lexicographic, graded reverse lexicographic, degree lexicographic etc. Some of the most useful orderings are those which compare monomials by their degrees, that is, if $|\alpha| > |\beta|$ then $x^{\alpha} \succ x^{\beta}$, called *graded orderings*. The lexicographic orderings will be primarily used throughout our discussion. To learn more about monomial ordering, the reader is referred to [92, 93].

By fixing a monomial order, we get a *leading term* for each polynomial of a given ideal, denoted as $\langle LT(h_1), \ldots, LT(h_t) \rangle$. One can always find a finite subset $G = \langle H_1, \ldots, H_s \rangle$ of an ideal I, except for $I = \langle 0 \rangle$, such that every leading term of $f \in I$ can be generated by $\langle LT(H_1), \ldots, LT(H_s) \rangle$ (where $f \in I$ means that f is an algebraic combination of h_1, \ldots, h_t). Such a subset G is called a Groebner basis with respect to the specific monomial order⁴.

There may be different Groebner bases for different monomial orderings for the same ideal. However, it can be shown that for any given monomial order, every nontrivial ideal $I \subset K[x_1, \ldots, x_m]$, has a Groebner basis and that any Groebner basis for an ideal I is a basis of I. It can also be shown that V(I) can be computed by any basis of I, and so the solutions of I are the same as that of any of its Groebner basis for any monomial ordering.

There is a well defined procedure to compute a Groebner basis for any given ideal and monomial ordering, called the Buchberger algorithm. It should be noted that the Buchberger algorithm reduces to Gaussian elimination in the case of linear equations, i.e., it is a generalization of the latter. Similarly it is a generalization of the Euclidean algorithm for the computation of the Greatest Common Divisors of a univariate polynomial. Recently, faster algorithms have been developed to obtain a Groebner basis, e.g., F4 [95], F5 [96] and In-

⁴It should be noted here that a Groebner basis may not be unique for a fixed monomial ordering. So, we call it *a* Groebner basis rather than *the* Groebner basis. However, the so-called reduced Groebner basis is unique for a given monomial ordering. The reader is referred to Ref. [92, 93] for more details.

volution Algorithms [97]. Symbolic computation packages such as Mathematica, Maple, Reduce, etc., have built-in commands to calculate a Groebner basis for a given monomial. Singular [98], COCOA [99] and McCauley2 [100] are specialized packages for finding a Groebner basis and Computational Algebraic Geometry, available as freeware. MAGMA [101] is also such a non-free specialized package. Rather than going into the details of the specifics and technicalities of this algorithm, we dive into the practical applications of the Groebner basis technique relevant to our problem and refer the reader to the above mentioned references for further details.

4.2.1 SLLG

We now provide a practical example of how the Groebner basis technique can be used for our systems. For the ideal in Eq. (4.8), a Groebner basis for the lexicographic ordering $c_1 \succ s_1 \succ c_2 \succ s_2 \succ c_3 \succ s_3$ is

$$G_{3} = \langle -s_{3} + s_{3}^{3}, c_{3}s_{3}, -1 + c_{3}^{2} + s_{3}^{2}, -s_{2} + s_{2}s_{3}^{2}, c_{3}s_{2}, s_{2}^{2} - s_{3}^{2}, c_{2}s_{3}, c_{2}s_{2}, \\ -1 + c_{2}^{2} + s_{3}^{2}, -s_{1} + s_{1}s_{3}^{2}, c_{3}s_{1}, c_{2}s_{1}, s_{1}^{2} - s_{3}^{2}, c_{1}s_{3}, \\ c_{1}s_{2}, c_{1}s_{1}, -1 + c_{1}^{2} + s_{3}^{2} \rangle .$$

$$(4.10)$$

It can be shown that the leading term of every polynomial in I_3 is generated by the ideal generated by the leading terms of G_3 , with the chosen monomial ordering. As noted earlier, the solutions of this system are the same as the original system. Here, the first equation in G_3 is a univariate polynomial in variable s_3 and solving it is simple because it can be factorized as $s_3(s_3^2 - 1) = 0$ giving $s_3 = 0$ and $s_3 = \pm 1$. Using this and back-substitution, we can find all the solutions as

$$(c_1, c_2, c_3, s_1, s_2, s_3) = \{(0, 0, 0, \pm 1, \pm 1, \pm 1), (\pm 1, \pm 1, \pm 1, 0, 0, 0)\}.$$
 (4.11)

Thus, $V(G_3)$ is the above mentioned set of 16 isolated points in a 6-dimensional affine space.

From our discussion in Chapter 3, we already know the solutions for this case in terms of θ_i 's, i.e.,

$$(\theta_1, \theta_2, \theta_3) = \{ \text{all } 2^3 \text{ permutations of } 0/\pi \} \\ \cup \{ \text{all } 2^3 \text{ permutations of } -\frac{\pi}{2}/\frac{\pi}{2} \}.$$
 (4.12)

All of these are correctly reproduced in Eq. (4.11) with $s_i = \sin \theta_i$ and $c_i = \cos \theta_i$.

For the periodic boundary conditions case after removing the global gauge freedom, for the trivial orbit, n = 3 case, the corresponding ideal for the SLLG is,

$$I_3^p = \langle -s_1 - c_2 s_1 + c_1 s_2, c_2 s_1 - s_2 - c_1 s_2, c_2 s_1 - c_1 s_2 - s_2, -c_2 s_1 - s_1 + c_1 s_2, c_1^2 + s_1^2 - 1, c_2^2 + s_2^2 - 1 \rangle,$$
(4.13)

with $\theta_3 = 0$. A Groebner basis for $c_1 \succ s_1 \succ c_2 \succ s_2$ lexicographic ordering is

$$G_3^p = \langle 4s_2^3 - 3s_2, 2c_2s_2 + s_2, c_2^2 + s_2^2 - 1, s_1 + s_2, 2c_1s_2 + s_2, c_1^2 + s_2^2 - 1 \rangle .$$
(4.14)

Here, again, we find that the first polynomial is univariate. Solving it and the remainder of the system using back-substitution we arrive at the solutions

$$(\theta_1, \theta_2) = \{(0, 0), (0, \pi), (\pi, 0), (\pi, \pi), (-\frac{2\pi}{3}, \frac{2\pi}{3}), (\frac{2\pi}{3}, -\frac{2\pi}{3})\}.$$
 (4.15)

Thus, we reproduce the known results of Chapter 3.

This approach to solving the periodic boundary conditions case becomes much more interesting as soon as we try to solve the n = 5 trivial orbit because with lexicographic ordering $c_1 \succ s_1 \succ c_2 \succ s_2 \succ c_3 \succ s_3 \succ c_4 \succ s_4$, the first univariate polynomial (For a zero-dimensional ideal, with a lexicographic ordering one can always find a Groebner basis in an upper diagonal form, analogous to the Gaussian Elimination method, such that at least one polynomial is univariate and others having increasing number of variables.) in a Groebner basis $64s_4^7 - 128s_4^5 +$ $80s_4^3 - 15s_4$ is of degree 6, effectively, in s_4 . Now, the Abel-Ruffini theorem yields that a polynomial of degree higher than 4 is not exactly solvable in terms of the radicals of its coefficients [102], and we end up solving the first polynomial numerically. However, numerical procedures to solve univariate polynomials are well developed and highly accurate results can be obtained. We observe that for the trivial orbit case with anti-periodic boundary conditions, the degree of the univariate polynomial in a Groebner basis is 3 for any n, though we have not proven this rigorously. However, for the periodic boundary conditions case with trivial orbit, the degree of this univariate polynomial increases with larger n. We will return to this in the remarks.

4.2.2 MLLG

For the MLLG ideal in Eq. (4.9), a Groebner basis with respect to lexicographic ordering $T_1 \succ T_2 \succ T_3 \succ y$ is $\langle -1 + y, T_3, T_2, T_1 \rangle$ and solving it gives $y = 1, T_1 = T_2 = T_3 = 0$. This reproduces the known result; $\tan(\theta_1/2) = \tan(\theta_2/2) = \tan(\theta_3/2) = 0$. We may now, of course, ignore the *auxiliary* variable y.

An important remark: from Chapter 3, we know that there are always two solutions of the one-dimensional MLLG equations with anti-periodic boundary conditions for any orbit in terms of θ_i 's. But here we find only one solution. The reason is that the variables of these polynomial equations are tangents of site angles, $T_i = \tan(\frac{\theta_i}{2})$ and so whenever we have a solution where some of the original θ_i are π , the corresponding T_i are ∞ , i.e., a solution at infinity. This infinity is difficult to handle computationally. A nice way out is to homogenize the ideal by taking all $T_i = \frac{s_i}{c_i}$ and then clearing the denominator, and the same for the constraint equation. The new equations are now homogeneous, i.e., each monomial of an equation has the same degree, in terms of s_i and c_i . By adding the constraint equations as $c_i^2 + s_i^2 - 1 = 0$ for each i = 1, ..., n and then calculating a Groebner basis for the corresponding ideal, one includes solutions where some of the c_i 's vanish, which correspond to solutions at infinity. Thus, *all* solutions are recovered. In short, by homogenizing the equations by the above method, one can obtain the *solutions at infinity* as regular solutions. There, one should keep in mind that the s_i and c_i are now $\sin \frac{\theta_i}{2}$ and $\cos \frac{\theta_i}{2}$. We should mention here that the trivial orbit case is quite a special case, where solutions at infinity will occur, but for other random orbits this problem should not appear.

For the trivial orbit, periodic boundary conditions case, after removing the global gauge freedom, for n = 3 the corresponding ideal is

$$J_3^p = \langle -T_2T_1^2 - 2T_1 + T_2, -T_1T_2^2 - 2T_2 + T_1, 1 - y(T_1T_2 + 1) \rangle, \qquad (4.16)$$

and a Groebner basis for $y \succ T_1 \succ T_2$ lexicographic ordering is $\langle T_2^3 - 3T_2, T_1 + T_2, T_2^2 + 2y - 2 \rangle$ giving solutions

$$(\theta_1, \theta_2) = \{(0, 0), (\frac{2\pi}{3}, -\frac{2\pi}{3}), (-\frac{2\pi}{3}, \frac{2\pi}{3})\},$$
(4.17)

as expected.

We have obtained a Groebner basis for the one-dimensional systems with n = 10, comfortably, on a desktop machine for both the SLLG and the MLLG. However, since we have already solved these cases for any n analytically, we avoid giving the details here.

4.2.3 Random Orbit Case

For a random orbit, i.e., $\phi_i \neq 0$, the corresponding equations become more complicated. Moreover, due to factorization and division of the polynomials involved in the Buchberger algorithm, the coefficients in a Groebner basis blow up. For this and the related technical reasons, the Groebner basis technique is mainly used for rational coefficients, i.e., for $\mathbb{Q}[x_1, \ldots, x_m]$ and a random orbit case is very difficult to handle.

A natural question to ask is if it is possible to get a Groebner basis for a given monomial ordering in terms of the symbolic form of the coefficients in ϕ_i , valid for all its special cases, called *specializations*, as well. In Ref. [103] the first step was laid down to get such a Groebner basis, called a Comprehensive Groebner Basis (CGB). Since then there has been much progress in this area although it is computationally expensive and much more involved (see, e.g., Ref. [104, 105]). Hence, so far it is restricted to smaller systems only⁵. In the next chapter, we will show that this difficulty in dealing with a parametric system using symbolic

 $^{^5\}mathrm{I}$ thank Antonio Montes and Akira Suzuki for their efforts in computing CGB for the one-dimensional systems.

techniques can be highly efficiently overcome with the help of the Polynomial Homotopy Continuation method.

4.2.4 Higher Dimensional Lattices

Interpreting the gauge fixing equations in terms of Algebraic Geometry allowed us to deal with the *actual non-linearity* of the equations, rather than treating them as linear equations as shown in Chapter 3. Specifically, in this interpretation the corresponding method does not make any distinction between the equations arising from a one-dimensional lattice or those arising from a higher dimensional lattice. In theory, as long as one can obtain a Groebner basis, the equations can be exactly solved. However, obtaining a Groebner basis for a system of gauge-fixing equations for bigger lattices is very difficult due to an algorithmic complexity, known as Exponential Space complexity (we will explain this explicitly in the Remarks at the end of this chapter). In particular, on a regular single desktop machine with 2 GB RAM, we could not obtain a Groebner basis for the SLLG with trivial orbit (i.e., the classical XY model) and with anti-periodic boundary conditions for a 3×3 lattice, using Singular 3.2. The corresponding system is made of 18 equations, each of degree 2, in 18 variables. However, a bigger machine with larger RAM should be able to obtain a Groebner basis for these systems. Recently⁶, V. Gerdt and Daniel Robertz have kindly computed a Groebner Basis for us for this system over $F_2 = \{0, 1\}$ using a Linux machine with AMD Opteron (TM) processor 285 2600 MHz, 4 cores, 16 GB memory and with Magma (V2.14.14) in 31994.250s machine time with degree reverse lexicographic ordering. This is a very important step towards solving the system. However, since the computation is over F_2 not all the solutions over \mathbb{C}^{18} can be obtained.

For the MLLG with anti-periodic boundary conditions on a 3×3 lattice with the trivial orbit, the system consists of 10 equations in 10 variables including the auxiliary one. This system has a smaller number of equations but each equation has a higher degree compared to the aforementioned SLLG case. A Groebner basis for this system can also not be obtained by our machine.

Although so far, this Algebraic Geometry method has not produced any new results in our problem in the sense of solving the corresponding equations for higher dimensional lattices, the Algebraic Geometry interpretation will prove to be immensely helpful and we will be actually able to solve some of these systems in the next chapter.

4.3 More About The Solution Space

Here, we discuss some features of the solution spaces, i.e., the variety of a given ideal. With the help of the terminology introduced below, we then give an Alge-

 $^{^{6}\}mathrm{I}$ am thankful to V. Gerdt and Daniel Robertz for their kind help.

braic Geometry interpretation of Gribov copies and related issues that will prove to be very helpful in the next chapter and in the future work.

Dimension of a Variety

The dimension of a variety is an important concept in Algebraic Geometry. In linear algebra, we know that for n linearly independent equations in n variables there exist isolated solutions. In other words, it is a zero-dimensional variety. A system of n - 1 linearly independent equations in n variables has one free parameter. The solution space is then a line in n-dimensional space, so it is a one-dimensional variety, and so on. This linear independence can be checked by calculating the Jacobian matrix of these equations: if the rank of the Jacobian matrix is n, then all equations are linearly independent, and if it is r < n, then there are n - r linearly dependent equations and the solution space is (n - r)dimensional.

When defining the dimension of a variety of a system of non-linear multivariate polynomial equations, this intuition can be extended, except that now the linear independence of the linear equations is replaced by an algebraic independence of the polynomial equations. For an arbitrary variety $V(h_1, \ldots, h_r) \subset \mathbb{C}^n$, let the rank of its Jacobian $J(h_1, \ldots, h_r)$ be r, then dimension of $V(h_1, \ldots, h_r)$ is n - r. For r = n, the dimension is 0. It can also be said that the dimension of a variety is the largest of the dimensions of its irreducible components. Moreover, it can be shown that a variety consists of finitely many points, or isolated solutions, if and only if its dimension is 0.

Thus, the variety corresponding to the Landau gauge fixing equations (for both SLLG and MLLG) in terms of polynomial equations is zero-dimensional for both the anti-periodic and periodic (after removing the global gauge freedom) boundary conditions.

Multiplicity Of Solutions

The dimension of a variety at a point p, denoted as dim V_p , is also an important concept for our purposes. If the rank of its Jacobian $J_p(h_1, \ldots, h_r)$ at a point $p \in V(h_1, \ldots, h_r)$ is k, then the dimension of $V(h_1, \ldots, h_r)$ at p, denoted as dim V_p , is n - (r + k) with n being the number of variables.

Now, for a univariate polynomial $f(x) \in \mathbb{C}[x]$, the multiplicity of a solution $x^* \in V(f)$ is the integer $\mu > 0$ such that $f(x) = (x - x^*)^{\mu}g(x)$ for a polynomial g(x) with $g(x^*) \neq 0$. Here, x^* is called a *multiple point*. Similarly, for the multivariate case, for a zero-dimensional variety, if at some solution p the rank of $J_p(h_1, \ldots, h_r)$ is k, k > 0, then p is a singular isolated solution and thus a multiple point. This multiplicity of solutions of polynomial equations corresponds to the concept of degenerate critical points in Morse theory.

For a positive-dimensional variety, dim V_p is the maximum dimension of an irreducible component of V containing p. dim $V_p = 0$ means that p is a non-singular point of the variety and lies on a unique irreducible component of the variety.

One can similarly define the dimension of the tangent space of a variety at a point p, denoted as dim T_pV . Then a point p in the affine variety V is non-singular provided dim $T_pV = \dim_p V$, otherwise p is a singular point.

Radical of An Ideal

In general, by the radical of an ideal, we mean the ideal generated by radicals of the polynomials of the original ideal, i.e., all solutions with multiplicity one. Specifically, the set of all $f \in K[x_1, \ldots, x_m]$ for which $f^k \in I$ for any integer $k \geq 1$, then such an ideal is called a *radical* ideal, denoted as \sqrt{I} , and \sqrt{I} is also always an ideal. E.g., the radical of the ideal $I = \langle (x+1)^2 \rangle$ is $\sqrt{I} = \langle x+1 \rangle$. A little thought will reveal that we always have $I \subset \sqrt{I}$. Moreover, \sqrt{I} has no multiple solutions, i.e., have all solutions with multiplicity 1.

Number of Zeroes of An Ideal

For large systems, even after obtaining a Groebner basis it may be cumbersome to solve the corresponding equations. In many cases, it may be sufficient to know the number of solutions and not the solutions themselves.

Firstly, polynomials $h, g \in K[x_1, \ldots, x_m]$ are called congruent modulo I for some ideal I, if $h - g \in I$. It can be shown that a congruent modulo is an equivalence class relation on $K[x_1, \ldots, x_m]$. So, all polynomials h_i following $h_i - g \in I$ are equivalent in this sense and are written as [g]. Now a set of all such equivalence classes is called a quotient of $K[x_1, \ldots, x_m]$ modulo I, denoted as $K[x_1, \ldots, x_m]/I$. These equivalence classes can be obtained using Groebner basis techniques. Now, if V(I) is a zero-dimensional variety and I is defined over an algebraically closed field K, e.g., \mathbb{C} , then the number of zeros of I in K^n is equal to dim $(K[x_1, \ldots, x_m]/I)$, counted with multiplicity.

This is a very interesting result, though we shall refrain from any further discussion on how this quotient ring is related to the number of solutions of the original equations. The interested reader is encouraged to refer to [92] for details.

Using Singular3.2 for the ideal in Eq. (4.8), dim $(\mathbb{C}[s_1, s_2, s_3, c_1, c_2, c_3]/I)$ is found to be 16, and for the ideal in Eq. (4.9), dim $(\mathbb{C}[T_1, T_2, T_3, y]/I)$ is found to be 1 as expected.

4.3.1 Gribov copies and Algebraic Geometry

Now, we are ready to pose the Landau gauge fixing problem, for compact U(1), in terms of the terminology we have introduced:

- 1. Firstly, dim $\mathbb{C}[\{s_i, c_i\}]/I_{SLLG}^{\phi}$ is the total number of real and complex solutions⁷, where I_{SLLG}^{ϕ} is the ideal generated by the SLLG conditions for some random orbit $\{\phi\}$ and variables s_i and c_i for all lattice sites *i*. Moreover, dim $\mathbb{RR}[\{s_i, c_i\}]/I_{SLLG}^{\phi}$, i.e., the number of real solutions of I_{SLLG}^{ϕ} with all its coefficients in \mathbb{R} , is the number of Gribov copies for the SLLG. By calculating this quantity, we count the corresponding N_{GC} for the orbit $\{\phi\}$.
- 2. dim $\mathbb{C}[\{s_i, c_i\}]/I_{SLLG}^{\phi}$ and dim $\mathbb{RR}[\{s_i, c_i\}]/I_{SLLG}^{\phi}$ both depend on the specific values of $\{\phi\}$ as we shall explicitly see in Chapter 5. This corresponds to the orbit-dependence of N_{GC} in the SLLG.
- 3. The set of all Gribov horizons is the set of real multiple solutions, called the *real singular locus* of I_{SLLG}^{ϕ} .
- 4. For the SLLG for higher dimensional lattices at Gribov horizons dim $T_pV > \dim_p V$. That is, the tangent space has at least one flat direction at the Gribov horizon.
- 5. $\sqrt{I_{SLLG}^{\phi}}$ is the corresponding ideal with each Gribov copy having multiplicity one, i.e., the Gribov horizons of the SLLG are removed.
- 6. For the MLLG, since the Faddeev-Popov operator is positive (semi-)definite, the ideal I^{ϕ}_{MLLG} with variables T_i and y and all the coefficients defined over \mathbb{R} is a radical ideal. However, the concept of a *real radical ideal* is more involved and discussed in the remarks at the end of this chapter.
- 7. The topological field theory interpretation asserts that for the MLLG, Z_{GF} counts the number of solutions, since the Faddeev-Popov operator is always positive definite. We now establish one more relation here:

$$Z_{GF} = \dim_{\mathbb{R}} \mathbb{R}[\{T_i, y\}] / I^{\phi}_{MLLG}.$$

$$(4.18)$$

This is remarkable because it establishes a relationship between the lattice topological field theory and Algebraic Geometry.

8. The orbit-independence would then mean that dim $_{\mathbb{R}}\mathbb{R}[\{T_i, y\}]/I^{\phi}_{MLLG}$ is constant with respect to $\{\phi\}$ for the MLLG case.

4.4 Remarks

1. For the SLLG in one dimension, we noted that the maximum degree of a Groebner basis is 3 for the chosen monomial order, and this cubic univariate

⁷For the one-dimensional lattice all the solutions are real but this is not the case for the higher dimensional lattice as will be shown in Chapter 5.

equation is exactly solvable in terms of its radicals. However, in general it is quite possible that the maximum degree of the resulting univariate polynomial of a Groebner basis is 5 or more. Now, the Abel-Ruffini theorem says that the solutions in terms of radicals of the univariate polynomial equation of degree more than 4 can not be obtained. A natural question now is if there is any restriction on the maximum degree of the univariate polynomial for some monomial order that can be known from the original ideal. If such a restriction implies that the maximum degree of the univariate polynomial will be less than 5, then it will indicate that the whole problem can be exactly solved at least in theory. There have been many efforts to find such a precise restriction, but so far there are only a few upper bounds [106, 107, 108, 109] depending on the number of variables and the degrees of each polynomial in the original ideal. These upper bounds in our one-dimensional systems have turned out to be much higher than the obtained ones. However, we recognize that further work is required to refine these bounds for our systems.

- 2. The main problem in this Groebner basis scenario is that the Buchberger algorithm and its variants are known to have *exponential space* complexity. That is, the RAM required by the machine gets exponentially higher for linear increase in number of variables or equations. For this reason, even the simplest non-trivial cases of the two-dimensional SLLG or MLLG for the trivial orbit case are not yet tractable. With a more powerful machine, it is anticipated that the Groebner basis method is a very promising way to exactly solve these cases as well as bigger systems for the two-dimensional lattice. Moreover, the Burchberger algorithm is highly sequential. So, parallelization of the algorithm is highly non-trivial task.
- 3. Real Radical Ideal⁸: The concept of a real radical ideal is very subtle. If we want to check if an ideal I is a real radical, we need to check if for every sum of squares of polynomials $p_i \in \mathbb{R}[x_1, \ldots, x_m], \sum p_i^2 \in I \Rightarrow p_i \in$ I [110]. There is an algorithmic way of checking this by verifying the positive semi-definiteness of a so-called quasi Hankel matrix. Though an efficient implementation of this algorithm still poses challenges, a promising attempt is underway [111, 112].
- 4. Another interesting method for dealing with non-linear equations including those with inequalities, is called *Quantifier Elimination* (QE). The so-called Cylindrical Algebraic Decomposition (CAD) method, which is a special case of the QE, specializes to polynomial equations including inequalities with variables defined over \mathbb{R} . For example, for the equation $x^2 + y^2 - 1 = 0$, a CAD is $-1 \leq x \leq 1$ and $y = \sqrt{1 - x^2}$ or $-\sqrt{1 - x^2}$. The CAD ap-

 $^{^{8}\}mathrm{I}$ am thankful to P. Rosaltski to clarify this important point to me.

pears to be the most appropriate method for our purpose. However, the complexity of the related algorithms severely affects its applicability in bigger systems [113]. Recently, a very sophisticated technique called the discriminant variety, used to reduce the computation in the CAD method, is developed which can give generic real solutions of a system of polynomial equations for generic values of parameters [114, 115, 116]. A parametric CAD for our one-dimensional systems for n = 3 for both the SLLG and the MLLG with periodic and anti-periodic boundary conditions have been kindly computed by Guillaume Moroz and Hirokazu Anai for us⁹. They have also shown that the computation time is efficiently reduced with this new method. This is a remarkable step towards obtaining all the real solutions of a two-dimensional system. In particular, efforts to solve the MLLG with anti-periodic boundary conditions on the 3×3 lattice and to verify if the number of solutions (N_{GC}) depends on the values of parameters (orbit-dependence) are underway.

- 5. We have turned several other systems in lattice field theory and condensed matter theory into polynomial ones, several of which we have solved using the Groebner basis technique in Appendix C. This should serve in two ways: for the particle/condensed matter theorists in general, this provides a database of examples for transforming the equations in terms of polynomials, while for the computational/numerical Algebraic Geometrists it provides a rich test-suite for their respective algorithmic implementations.
- 6. It should be mentioned in passing that in the Dirac constraint formalism and light cone Yang-Mills Mechanics [117, 118] and in finding the global minimum of the Minimal Supersymmetric Standard Model Higgs potential [119, 120, 121], the Groebner basis techniques have been used successfully. Both of them are interesting applications of the Groebner basis techniques in general.

4.5 Summary

In summary:

1. We noticed that the nonlinearity of the gauge-fixing conditions, in both the SLLG and the MLLG cases, for higher dimensional lattices is *polynomial-like*. By using additional constraint equations, the combined system of

⁹I am grateful to Hirokazu Anai and Guillaume Moroz for kindly solving the systems for me and their ongoing efforts for solving the corresponding systems for higher dimensional lattices. It should be noted that this remarkable success has been reported just before submitting this thesis.

equations can be treated as a system of polynomial equations with all variables defined over \mathbb{C} . Though we are interested in only real solutions of these polynomial systems, we rather used Complex Algebraic Geometry concepts over Real Algebraic Geometry due to the stronger results available in the former.

- 2. To solve the systems for both the SLLG and the MLLG exactly, we used an elegant algorithm, called the Buchberger algorithm, implemented on various computer algebra packages. Though the algorithm works well for the one-dimensional lattice, for the 3 × 3 lattice a more powerful machine is required. Recently, a Groebner basis for the SLLG for anti-periodic boundary conditions for the 3 × 3 lattice is computed by V. Gerdt and D. Robertz with a more powerful machine, with a few constraints on the system. We recognize that this is an important first step towards exactly solving this system. For the corresponding MLLG ideal, we continue our efforts with implementation on powerful machines, though we acknowledge that for bigger lattices and in higher dimensions, even the currently most powerful machines may not be able to solve the corresponding ideals due to an algorithmic complexity issue.
- 3. However, we have laid down all the stepping stones to solve the twodimensional gauge-fixing equations so that we can subsequently use a very recent method called Polynomial Homotopy Continuation which can give *all* solutions of a polynomial system numerically. This method does not suffer from the technical difficulties of the Buchberger algorithm or its sophisticated variants, and in principle this method can solve the corresponding ideals for both the SLLG and the MLLG for those which may be intractable for the Groebner basis techniques. Specifically, we solve the ideal mentioned in the previous point in the next chapter.
Chapter 5

Polynomial Homotopy Continuation Method

In the previous chapter we saw that the Algebraic Geometry interpretation offers deep insight into the lattice Landau gauge fixing, and the Groebner basis technique can be used to exactly solve the corresponding equations. For higher dimensional lattices, however, it is difficult to compute a Groebner basis for both the SLLG and the MLLG. Still, it turns out that interpreting the original trigonometric equations as polynomial equations is of great help. In particular, there exists a numerical method, called the Polynomial Homotopy Continuation method¹, that gives *all* solutions of a system of multivariable polynomial equations up to a numerical accuracy. The word *all* makes the difference here between this and other numerical methods. We first introduce this method in general terms starting from the univariate case, and then apply it to our problems, in this chapter.

5.1 Polynomial Homotopy Continuation

For a single variable equation, $f(x) = \sum_{i=0}^{k} a_i x^i$, with coefficients a_i and the variable x both defined over \mathbb{C} , the number of solutions is exactly k if $a_k \neq 0$, counting multiplicities. This powerful result comes from the Fundamental Theorem of Algebra. To get all roots of such single variable polynomials, there exist many numerical methods such as the *companion matrix* trick for low degree polynomials, and divide-and-conquer techniques for high degree polynomials. Here we present another method called Numerical Polynomial Homotopy Continuation (NPHC), which can then be extended to the multivariate case in a straightforward manner. We follow Refs. [94, 122] throughout this chapter unless specified otherwise.

¹I am very grateful to Jan Verschelde, the developer of PHCpack, for clarifying many of the aspects of this method and related issues to me, with a great patience.

5.1.1 Homotopy Continuation

The basic strategy behind homotopy continuation is: first put the equation or the system of equations to be solved into a family of problems depending on parameters, then solve the problem for some appropriate point in the parameter space where usually the corresponding system is easy to solve, and finally track the solutions of the system at this appropriate point in parameter space to the original problem. This approach can be applied to many types of equations (e.g., non-algebraic equations) which exhibit a continuous dependence of the solutions on the parameters, but there exist many difficulties in making this method a primary candidate method to solve any given equation or set of equations. However, for reasons that will be clear below, this method works exceptionally well for polynomial equations.

To clarify how the method works, we first take a univariate polynomial², say $z^2 - 5 = 0$, pretending that we do not know its solutions, i.e., $z = \pm \sqrt{5}$. We first define a family of problems as

$$H(z,t) = (1-t)(z^2 - 1) + t(z^2 - 5) = z^2 - (1+4t) = 0$$
(5.1)

where $t \in [0, 1]$ is a parameter. For t = 0, we have $z^2 - 1 = 0$ and at t = 1 we recover our original problem. The problem of getting all solutions of the original problem now reduces to tracking solutions of H(z,t) = 0 from t = 0 where we know the solutions, i.e., $z = \pm 1$, to t = 1. The choice of the piece $z^2 - 1$ in Eq. (5.1), called the *start system*, should be clear now: this system has the same number of solutions as the original problem and is easy to solve. For multivariable systems, a clever choice of a start system is essential in reducing the computation, and the discussion about this issue will follow soon. Here, we briefly mention the numerical methods used in path-tracking from t = 0 to t = 1. One of the ways to track the paths is to solve the differential equation that is satisfied along all solution paths, say $z_i^*(t)$ for the *i*th solution path,

$$\frac{dH(z_i^*(t),t)}{dt} = \frac{\partial H(z_i^*(t),t)}{\partial z} \frac{dz_i^*(t)}{dt} + \frac{\partial H(z_i^*(t),t)}{\partial t} = 0.$$
 (5.2)

This equation is called the Davidenko differential equation. Inserting (5.1) in this equation, we have

$$\frac{dz_i^*(t)}{dt} = -\frac{2}{z_i^*(t)}.$$
(5.3)

We can solve this initial value problem numerically (again, pretending that an exact solution is not known) with the initial conditions as $z_1^*(0) = 1$ and $z_2^*(0) = -1$. The other approach is to use Euler's predictor and Newton's corrector methods.

 $^{^{2}}$ We have taken this example and the one in the next section from Ref. [94] to make this discussion self-consistent. The reader is encouraged to refer to Ref. [94] for more details on the NPHC method.

This approach works well too. We do not intend to discuss the actual path tracker algorithm used in practice, but it is important to mention that in the path tracker algorithms used in practice, almost all apparent difficulties have been resolved, such as tracking singular solutions, multiple roots, solutions at infinity, etc. For the sake of completeness, we should also mention here that in the actual path tracker algorithms the homotopy is randomly complexified to avoid singularities. This is called the *gamma trick*, i.e., taking

$$H(z,t) = \gamma(1-t)(z^2-1) + t(z^2-5) = 0, \qquad (5.4)$$

where $\gamma = e^{i\theta}$ with $\theta \in \mathbb{R}$ chosen randomly.

There are several sophisticated numerical packages well-equipped with path trackers such as PHCpack [123], PHoM [124], HOMPACK [125] and HOM4PS2 [126, 127]. They all are available as freewares from the respective research groups.

In the above example, the PHCpack with its default settings gives the solutions

$$z = (-2.23606797749979, 0.0000000000000)$$

$$z = (2.23606797749979, 0.0000000000000), (5.5)$$

where the first component is the real part and the second component is the imaginary part in each solution, z. Thus, it gives the expected two solutions of the system with a very high numerical precision.

5.1.2 Multivariable Polynomial Homotopy Continuation

We can generalize the NPHC method to a system of multivariable polynomial equations, say P(x) = 0, where $P(x) = (p_1(x), \ldots, p_m(x))^T$ and $x = (x_1, \ldots, x_m)^T$, that is known to have isolated solutions (i.e., a 0-dimensional variety). To do so, we first need to have some knowledge about the expected number of solutions of the system. There is a classical result, called the *Classical Bezout Theorem*, that asserts that for a system of m polynomial equations in m variables, for generic values of coefficients, the maximum number of solutions in \mathbb{C}^m is $\prod_{i=1}^m d_i$, where d_i is the degree of the *i*th polynomial. This bound is exact for generic values (i.e., roughly speaking, non-zero random values) of coefficients. The genericity is well-defined and the interested reader is referred to Ref. [94] for details.

Based on this bound on the number of complex solutions, we can construct a *homotopy*, or a set of problems, similar to the aforementioned one-dimensional case, as

$$H(x,t) = \gamma(1-t)Q(x) + t P(x),$$
(5.6)

where Q(x) is a system of polynomial equations, $Q(x) = (q_1(x), \ldots, q_m(x))^T$ with the following properties:

- 1. The solutions of Q(x) = H(x, 0) = 0 are known or can be easily obtained. Q(x) is called the *start system* and the solutions are called the *start solutions*.
- 2. The number of solutions of Q(x) = H(x, 0) = 0 is equal to the Classical Bezout bound for P(x) = 0.
- 3. The solution set of H(x,t) = 0 for $0 \le t \le 1$ consists of a finite number of smooth paths, called homotopy paths, each parameterized by $t \in [0, 1)$.
- 4. Every isolated solution of H(x, 1) = P(x) = 0 can be reached by some path originating at a solution of H(x, 0) = Q(x) = 0.

We can then track all the paths corresponding to each solution of Q(x) = 0 from t = 0 to t = 1 and reach P(x) = 0 = H(x, 1). By implementing an efficient path tracker algorithm, we can get all isolated solutions for a system of multivariable polynomials system just as in the univariate case.

The homotopy constructed using the Classical Bezout bound is called the *Total* Degree Homotopy. The start system Q(x) = 0 can be taken as, e.g.,

$$Q(x) = \begin{pmatrix} x_1^{d_1} - 1 \\ x_2^{d_2} - 1 \\ \vdots \\ \vdots \\ \vdots \\ x_m^{d_m} - 1 \end{pmatrix} = 0,$$
(5.7)

where d_i is the degree of the *i*th polynomial of the original system P(x) = 0. Eq. (5.7) is easy to solve and guarantees that the total number of start solutions is $\prod_{i=1}^{m} d_i$, all of which are non-singular. The Total Degree Homotopy is a very effective and popular homotopy whose variants are used in the actual path trackers.

The Total Degree Homotopy works fine for all cases, with negligible efforts to solve the start system itself. The drawback of this homotopy is that it does not take the *sparsity* of the system into account: the systems found in practice do not have all the coefficients *generic* but many of them may be zero. Such systems are called *sparse*: the total number of solutions for a sparse system can be much lower than the Bezout bound, and so many of the solution-paths do not end up being solutions of the original system. That is, the computation done for many of the paths is wasted. A better strategy to solve such sparse systems is to get a tighter bound for the number of solutions than the Bezout bound, and construct a homotopy based on it. There have been many improved homotopies developed other than the Total Degree Homotopy, such as Multihomogeneous Homotopy, Linear Product Homotopy, Monomial Product Homotopy, etc. Here, we will discuss the most important and efficient one, known as the Polyhedral Homotopy.

5.1.3 Polyhedral Homotopy

As mentioned above, polynomial equations in polynomial systems arising in reallife problems may contain zero coefficients. In general, the Bezout bound becomes an upper bound on the number of solutions for such cases. What we are looking for is a tighter bound that takes the sparsity of the system into account. There has been a huge amount of work done on related issues using Resultants and Algebraic Geometry, but the most important result for us is Bernstein's theorem. In order to state it clearly, we need to introduce three notions: Laurent Polynomials, Newton Polytopes and Mixed Volume.

A Laurent polynomial allows negative exponents for the monomials, unlike an ordinary polynomial. Due to that, none of the variables is allowed to be zero. So, multiplication of any Laurent polynomial by a monomial does not change the root count in $(\mathbb{C}^*)^m = \mathbb{C}^m / \{0\}$. Formally, let $S_i \subset \mathbb{Z}^m$ be a set of vectors whose elements are the exponents of the monomials of the *i*th polynomial. S_i is called the support of the *i*th polynomial. Then a polynomial (say, *i*th polynomial) of the form $f_i(x) = \sum_{\alpha \in S_i} c_{i,\alpha} x^{\alpha}$ is called a Laurent polynomial. Here, $c_{i,\alpha} \in \mathbb{C}$ are the coefficients of the monomial x^{α} with $x \in (\mathbb{C}^*)^m$.

Now, a set of points is called a convex set if for every pair of points within the set (or more formally, the mathematical object made by the set), every point on the straight line segment that joins them is also within the set. The convex hull of a set X is the minimal convex set containing X. We note that the convex hull of support S_i of a polynomial, say $Q_i = \text{conv}(S_i)$, is called the *Newton polytope* of $f_i(x)$.

For example, consider a two-variable system,

$$f_1(x,y) = 1 + ax + bx^2y^2 = 0,$$

$$f_2(x,y) = 1 + cx + dy + exy^2 = 0.$$
(5.8)

The Bezout bound of this system is $4 \times 3 = 12$, i.e., there can be a maximum of 12 solutions for this system in \mathbb{C}^2 . Now, the supports of these equations are $S_1 = \{(0,0), (1,0), (2,2)\}$ and $S_2 = \{(0,0), (1,0), (0,1), (1,2)\}$ respectively. The Newton polytopes for $f_1(x, y)$ is $Q_1 = \operatorname{conv}(S_1) = \{(0,0), (1,0), (2,2)\}$ and for $f_2(x, y)$ it is $Q_2 = \operatorname{conv}(S_2) = \{(0,0), (1,0), (0,1), (1,2)\}$.

A Minkowski sum of any two Newton polytopes can be defined as

$$Q_1 + Q_2 = \{q_1 + q_2 \colon q_1 \in Q_1, q_2 \in Q_2\}.$$
(5.9)

The Minkowski sum is equivalent to multiplying the corresponding polynomials algebraically.

Also, as is well-known, an *m*-dimensional volume of a simplex (i.e., roughly speaking, an *m*-dimensional analogue of a triangle) having vertices v_0, v_1, \ldots, v_m , is

$$\operatorname{Vol}_{m}(\operatorname{conv}(v_{0},\ldots,v_{m})) = \frac{1}{m!} |\det[v_{1}-v_{0},\ldots,v_{m}-v_{0}]|.$$
(5.10)

From there on, one can show that the *m*-dimensional volume $\operatorname{Vol}_m(\lambda_1 Q_1 + \cdots + \lambda_m Q_m)$, where $0 \ge \lambda_i \in \mathbb{R}$, is a homogeneous polynomial of degree *m* in variables λ_i . The mixed volume of convex polytopes Q_1, \ldots, Q_m is defined as

$$M(Q_1, \dots, Q_m) = \sum_{i=1}^m (-1)^{m-i} \operatorname{Vol}_m(\sum_{j \in \Omega_i^m} Q_j),$$
 (5.11)

where the inner sum is a Minkowski sum of polytopes and Ω_i^m are the combinations of *m*-objects (i.e., *m*-dimensional geometrical objects made of *m*-simplices) taken *i* at a time. Moreover, it can be shown that the mixed volume is always an integer for a system of Laurent polynomials. For the case of two polynomials in two variables,

$$M(Q_1, Q_2) = \operatorname{Vol}_2(Q_1 + Q_2) - \operatorname{Vol}_2(Q_1) - \operatorname{Vol}_2(Q_2).$$
(5.12)

For the system in Eq. (5.8),

٦

$$Vol_{2}(Q_{1}) = 1,$$

$$Vol_{2}(Q_{2}) = \text{ area of } \|\text{-gram. made by } \{(0,0), (1,0), (0,1), (1,1)\}$$

$$+ \text{ area of triangle made by } \{(1,1), (1,0), (1,2)\}$$

$$= 1 + \frac{1}{2} = \frac{3}{2},$$

$$Vol_{2}(Q_{1} + Q_{2}) = \frac{13}{2}.$$
(5.13)

Thus, the mixed volume for this system is 4. Why is it important? The Bernstein theorem or Bernstein-Khovanskii-Kushnirenko theorem [128, 129, 130] says that for generic coefficients, the number of solutions in $(\mathbb{C}^*)^m$ of a Laurent system is exactly equal to the mixed volume of this system counting with multiplicity for generic coefficients and is an upper bound for it in general. This is also called the BKK root count.

This result is very interesting. One can get a very tight upper bound, on the number of solutions in $(\mathbb{C}^*)^m$ of a polynomial system by knowing the exponent vectors of monomials. This result originates from toric varieties and related issues in Algebraic Geometry. We do not intend to go into further details, rather we discuss its application to the problems at hand.

For the system in Eq. (5.8) there can be a maximum of 4 solutions in $(\mathbb{C}^*)^m$. In contrast, the Bezout bound dictates a bound to be 12 in \mathbb{C}^m .

What about a BKK-like count in \mathbb{C}^m ? An extension of the mixed volume, is the *stable mixed volume* which is the corresponding root count³ in C^m . This

³Because of the highly technical nature of the stable mixed volume, the bound in C^m which has been commonly used and implemented in the community is the bound given in Ref. [131]. This bound is quite easy to state: Add a constant term to polynomials in the system which do not have constant term, and the mixed volume of the resulting augmented system serves as a bound in C^m for the original system. The stable mixed volume is a little bit more general then this augmented mixed volume. I would like to thank TY Li to clarify this point.

ensures that we have all necessary solutions in \mathbb{C}^m [132, 131, 133, 134]. A discussion on the stable mixed volume is beyond the scope of this thesis, although its calculation is similar to that of the mixed volume with some formal complications. However, it should be noted that a highly sophisticated implementation of an algorithm to calculate the mixed volume of a given system is MixedVol [126] which is transplanted in HOM4PS2 and PHCpack.

Now, after calculating the stable mixed volume of the original system P(x) =0, Polyhedral homotopy requires a start system, Q(x) = 0, such that Q(x) has the same stable mixed volume, where of course solutions of Q(x) = 0 should be known or can be obtained easily. Such a homotopy is called the Polyhedral Homotopy. The biggest advantage of this homotopy is that the number of paths to be tracked is much less than that for the Total Degree Homotopy. The apparent drawback here is that to solve the start system itself, the Polyhedral Homotopy requires some computational effort. However, for large systems, the difference between the number of paths to be tracked for both homotopies suppresses this drawback of the Polyhedral Homotopy by saving a huge amount of computational effort. We first performed the checks over the one-dimensional lattice for the SLLG and the MLLG cases and reproduced the known results. However, rather than discussing these cases, we go directly to the cases that we are interested in, i.e., the twodimensional lattice. We note that we were able to reproduce all the known results for the one-dimensional cases for both the SLLG and the MLLG, with a very high numerical precision.

5.2 Results

Here, we present our results obtained so far.

5.2.1 SLLG With Anti-periodic Boundary Conditions

We are now in a position to explore the simplest non-trivial case in higher dimensional lattices, i.e., the SLLG on a 3×3 lattice with the trivial orbit and antiperiodic boundary conditions. We can solve this case using PHCpack, Bertini or HOM4PS2. The summary of results is given in the table (5.1) using HOM4PS2.

CBB	SMV	Reg.	Real
262144	148480	10738	2968

Table 5.1: Summary of the 3×3 lattice, SLLG with anti-periodic boundary conditions, trivial orbit.

Here, CBB denotes the Classical Bezout Bound, SMV denotes the Stable Mixed Volume, Reg. denotes the number of all real and complex regular solutions and Real denotes the number of real solutions. The HOM4PS2 took around 65 minutes to run this system on a linux single-processor desktop machine⁴.

It is important at this stage to mention a few specifics about these solutions:

- 1. A solution here means that it satisfies each of the 18 equations with tolerances 1×10^{-10} . All these solutions come with real and imaginary parts, i.e., as a complex number. A solution is a real solution if the imaginary part of each of 18 variables (i.e., all s_i and c_i) is less than or equal to the tolerance 1×10^{-6} . We also verified that the original equations are satisfied with tolerance 1×10^{-10} after s_i and c_i are transformed back to θ_i . It is important to note that all these solutions can be further refined, if required, with an *arbitrary precision*. This is a remarkable success of the method because then these solutions are close to the *exact solutions*.
- 2. The sum of the Faddeev-Popov determinants at all 2968 real solutions is ~ 10^{-8} , which is numerically zero. Similarly, in terms of θ_i variables, the sum of the Faddeev-Popov determinants is ~ 10^{-11} , again giving the expected Neuberger zero.
- 3. There are exactly 1152 real solutions which have zero Faddeev-Popov determinant (equivalently the Jacobian determinant of the system) with tolerance 1 × 10⁻⁸. These solutions constitute the set of singular locus or the Gribov horizons⁵. They can be further classified in terms of the number of zero eigenvalues of the Faddeev-Popov operator at each of the solutions. This amounts to classifying the singular solutions of the polynomial system in terms of their multiplicities. To study the multiplicity structure, we need to use the so-called deflation technique⁶ for isolated singular solutions [135, 136].
- 4. The remaining 1816 real solutions have nonsingular Faddeev-Popov determinant. They constitute the set of all Gribov regions (excluding Gribov horizons). We can classify all of them by the number of negative eigenvalues (Table 5.2), which shows the expected two-fold symmetry giving rise to the Neuberger zero. Thus, we have obtained the Morse indices, K_i . Figures (5.1) give a pictorial representation of the results..

⁴Note that we do not have any intention of comparing the efficiency of these available packages.

⁵It is important to note that since there are degenerate solutions for the trivial orbit case, the corresponding SLLG functional/Classical XY model is a Morse-Bott function. For a random orbit, one does not encounter these Gribov horizons in general and so there, the function is a usual Morse function.

⁶The work in progress in collaboration with the HOM4PS2 group.

i	0	1	2	3	4	5	6	7	8	9
K_i	2	18	216	342	330	330	342	216	18	2

Table 5.2: Summary of the number of solutions with *i* negative eigenvalues, for the SLLG, 3×3 lattice, trivial orbit, anti-periodic boundary conditions.



Figure 5.1: The horizontal axis denotes the solution number (arbitrarily given) and the vertical axis has the polynomial version (the determinants for the trigonometric version differers by a constant factor only in any case) of the Faddeev-Popov determinant, for the 3×3 lattice for the SLLG, trivial orbit, anti-periodic boundary conditions case. As with all other plots hereafter, this plot does not include the two global maxima and two global minima, since these four points have considerably higher magnitude, an obstacle to viewing the rest of the symmetry clearly. However, the Faddeev-Popov determinants at those solutions as well cancel each other exactly.

Special Random Orbit Case

In our preliminary study, we take a special random orbit case, where the $\phi_{i,\mu}$ are constrained to take values from $\{-\frac{\pi}{2}, 0, \frac{\pi}{2}, \pi\}$. This ensures that the sine and cosine of these angles, i.e., the coefficients of the system, are integers and so contribute little to the numerical errors. The summary of this run is given in Table (5.3).

CBB	S.M.V.	Reg.	Real
262144	148480	17072	2688

Table 5.3: Summary of the solutions for the SLLG, 3×3 lattice, special random orbit, anti-periodic boundary conditions.

1. The sum of the Faddeev-Popov determinants at all the real solutions in



Figure 5.2: Special random orbit, 3×3 lattice, SLLG, anti-periodic boundary conditions, with the polynomial version of the Faddeev-Popov determinant. The randomness is now apparent here compared to the trivial orbit case.

terms of polynomial variables is $\sim 10^{-8}$ which is numerically zero, i.e., the Neuberger zero. Similarly, in terms of θ_i variables, the sum of the Faddeev-Popov determinants is $\sim 10^{-12}$, yielding the expected Neuberger zero. It should be noted that in this case, there is no solution having zero eigenvalue of the Faddeev-Popov operator, i.e., no Gribov horizon.

2. The summary of corresponding Morse indices is given in Table 5.4. (See also Fig. (5.2)).

i	0	1	2	3	4	5	6	7	8	9
K_i	4	46	176	448	670	670	448	176	46	4

Table 5.4: Summary of the number of solutions with i negative eigenvalues for the SLLG, 3×3 lattice, anti-periodic boundary conditions, special random orbit.

Random Orbit Case

Finally, we solve the equations for a random orbit case, i.e., all links $\phi_{i,\mu}$ take some random values from $(-\pi, \pi]$ and the results are summarized in Table (5.5). The sum of determinants is ~ 10⁻⁸ for the polynomial version of the Faddeev-Popov operator and ~ 10⁻¹¹ for the trigonometric version. The summary of the eigenvalues is given in Table (5.6).

Again the two-fold symmetry is apparent here. Moreover, there is no solution with zero eigenvalue. This result is quite remarkable: the Groebner basis technique is too restrictive for the random coefficients in a system as discussed in Section

CBB	SMV	Reg.	Real
262144	148480	20558	2480

Table 5.5: Summary of the solutions for the SLLG, 3×3 lattice, random orbit, anti-periodic boundary conditions.

i	0	1	2	3	4	5	6	7	8	9
K_i	2	58	202	402	576	576	402	202	58	2

Table 5.6: Summary of the number of solutions with *i* negative eigenvalues for the SLLG, 3×3 lattice, anti-periodic boundary conditions, random orbit.

4.2.3, whereas polynomial homotopy continuation works perfectly fine (see Fig. (5.3)).

5.2.2 SLLG With Periodic Boundary Conditions

After eliminating the constant zero mode in the SLLG for the 3×3 lattice case with periodic boundary conditions, we have 14 equations and 14 variables. The number of solutions is 270 out of which 218 are non-singular and 52 are singular (see Fig. (5.4)). The sum of signs of the Faddeev-Popov determinants is zero, with the following summary of eigenvalues of the Faddeev-Popov operator, which is now a 7×7 dimensional matrix. The results are summarized in Table (5.7) and Table (5.8).

i	0	1	2	3	4	5	6	7
P_i	1	7	38	56	42	38	28	8

Table 5.7: Summary of the number of solutions with i positive eigenvalues, denoted as P_i , for the SLLG, 3×3 lattice, trivial orbit, periodic boundary conditions.

Similarly, for a random orbit the number of real solutions is 224 and again the sum of signs of Faddeev-Popov determinants is 0 with the summary of the eigenvalues given in Table (5.9), Table (5.10) and Fig. (5.5).

5.2.3 MLLG

For both the trivial and random orbit cases for the MLLG on the 3×3 lattice, the stable mixed volume is 814880. This is a large number compared to the stable mixed volumes for which the current packages such as PHCpack and HOM4PS2 are scaled for. Moreover, the number of monomials in each equation is also very large compared to SLLG for the current versions of the packages. These two technical difficulties have made the results for the MLLG inaccessible to us so far. This of course does not mean that the NPHC method is not capable of



Figure 5.3: A random orbit, 3×3 lattice, SLLG, anti-periodic boundary conditions, with the polynomial version of the Faddeev-Popov determinant.



Figure 5.4: Trivial orbit, 3×3 lattice, SLLG, periodic boundary conditions, with the polynomial version of the Faddeev-Popov determinant.

i	0	1	2	3	4	5	6	7
K_i	8	28	38	42	56	38	7	1

Table 5.8: Summary of the number of solutions with *i* negative eigenvalues for the SLLG, 3×3 lattice, trivial orbit, periodic boundary conditions.

i	0	1	2	3	4	5	6	7
P_i	1	8	38	72	61	30	12	2

Table 5.9: Summary of the number of solutions with *i* positive eigenvalues, P_i , for the SLLG, 3×3 lattice, random orbit, periodic boundary conditions.

solving such systems, but that in general the current packages are made to deal with smaller systems⁷.

5.3 Some Remarks

- 1. The NPHC method is strikingly different than the Groebner basis technique in that the algorithm for the former suffers from no known major complexities. Moreover, the path tracking is *embarrassingly parallelizable*, because all the start solutions can be tracked completely independently to each other! This very feature along with the rapid progress towards the improvements of the algorithms makes the NPHC well suited for physical problems arising in condensed matter theory, lattice QCD, etc. In short, though it may be very difficult or impossible to solve a system exactly, in theory one can get all solutions for such systems numerically with the NPHC method. This can also prove very useful in the recent studies of the Potential Energy Landscapes of classical Hamiltonians and their relation to the classical phase transitions [137, 138].
- 2. A new hybrid method has been developed to solve the polynomial equations arising from trigonometric equations in Ref. [139]. This method is very efficient, and has the potential to solve bigger systems. There, first a part of the system is solved and then the results are used in the remaining part.

⁷There is a lot of work currently being done to make the respective packages compute these systems. I am very grateful to the HOM4PS2 group, specifically Tsung-Lin Lee and Tien-Yien Li, for their efforts towards solving these systems.

i	0	1	2	3	4	5	6	7
K_i	2	12	30	61	72	38	8	1

Table 5.10: Summary of the number of solutions with *i* negative eigenvalues for the 3×3 lattice, random orbit, periodic boundary conditions.



Figure 5.5: Random orbit, 3×3 lattice, SLLG, periodic boundary conditions, with the polynomial version of the Faddeev-Popov determinant.

For the case at hand, we are in the process of applying this method to bigger lattices, e.g., the 4×4 SLLG with anti-periodic boundary conditions which consists of 32 equations in 32 variables. It is important to note that for the trivial orbit case 4×4 standard Landau Gauge, the stable mixed volume is 878182400. This is quite a challenge for a single machine. However, it seems achievable with the parallel version of the HOM4PS2, called paraHOM4PS2.0, though the public version is as yet unavailable.

- 3. For many practical problems, e.g., motion planning of a robot or chemical reactions, only real solutions are required. Thus, a huge amount of computational effort in getting the other types of solutions is wasted in the NPHC method. It would be much more useful if there was a way of getting only real solutions. However, a path tracker does not know if a given start solution will end up being a real solution of the original system, for a number of technical reasons nicely discussed in Ref. [94]. Moreover, one can wonder if a root count exists only for the real solutions of a system. The main problem to be resolved there is in obtaining Descartes rule of signs for the multivariate case [113, 140]. This, however, has yet to be achieved.
- 4. The NPHC Method and Minimization: Most of the usual methods to minimize a function are based on the Newton-Raphson method, where a start solution is guessed and then is refined by successive iterations. By performing this algorithm several times on the functions, one can obtain several minima of the original function. However, it does not give all extrema, even after a huge number of iterations. There are also many efficient refinements of this procedure such as Simulated Annealing to obtain global minima of the functional. However, they are not always successful (it can easily get

trapped at a local minimum instead of the global minimum). But if the function has a polynomial-like nonlinearity, in theory the NPHC method can give all extrema. It is then easy to separate out the global minima or maxima. This is quite a remarkable achievement and justifies transforming our problem, and other important particle physics and condensed matter theory problems, into polynomial form, as done in Appendix C.

- 5. Recently Akino and Kosterlitz [47] have used a clever trick (first demonstrated in lower dimensional models in Ref. [46]) to obtain the global minimum of the RPXYM: first take a duality transform of the Hamiltonian and then perform numerical minimization so that a minimization algorithm has to find the global minimum from the space of the local minima only. Though this method gives much more confidence in the final results with less numerical effort, finding the global minimum still has to rely on the numerical algorithms which are known to fail for larger systems. Thus, in addition to the usual error from the numerical precision of the machine, there can be an error of an *unknown* order. The present Algebraic Geometry approach has a sharp difference there. Instead of finding the global minimum using a numerical minimization method, we first try finding a Groebner basis of the corresponding polynomial system, and then we can get the global minimum, global maximum and all other extrema and saddle points analytically. Furthermore, for bigger systems, it is certainly difficult to get a Groebner basis; however, using the NPHC method, one can get all the local and global extrema and saddle points up to a numerical precision. Thus, the numerical error in finding the global minimum is just the numerical precision of the machine but no error of unknown order can be added⁸.
- 6. As we saw in the above examples, the stable mixed volume remains the same for any random orbit including trivial orbit case for the SLLG for a given lattice. Thus, it would be very interesting to verify if this number can be used as a *topological invariant* for the gauge-fixing.
- 7. Cheater's homotopy: In the previous chapter on the Groebner basis techniques, we mentioned that our systems were parametric systems, say $f(\vec{q}, \vec{x})$ where \vec{q} are parameters and \vec{x} are variables. To solve such a system algebraically, we discussed the CGB technique. There it was very difficult to obtain a CGB. With the NPHC method, on the other hand, it is rather easier to solve a parametric system. An important observation is that the stable mixed volume remains constant for most values of parameters because the monomials themselves remain the same, except in special cases. Ideally, our strategy should be first to solve the system for a specific value of parameters, e.g., say $f(\vec{q}^*, \vec{x})$, by the usual homotopy continuation method

 $^{^{8}\}mathrm{I}$ am thankful to J. M. Kosterlitz for clarifying these issues to me.

with polyhedral homotopy. Then using $f(\vec{q}^*, \vec{x})$ as the start system and its solutions as start solutions we can construct a general homotopy for all other allowed random values of \vec{q} . Then we can get all solutions for different points in the parameter space using this homotopy [141, 142]. The name, Cheater's homotopy, is thus justified! Both the SLLG and the MLLG have parameters as trigonometric functions of the link variables $\phi_{i,\mu}$ and so they are perfectly suited for the Cheater's homotopy. We have not used this trick in our above mentioned preliminary results so far, but identifying those systems as parametric equations appears to be very useful.

- 8. For most of the systems of polynomial equations in practice, we do not know the actual number of solutions from the beginning. So even after obtaining all solutions through the homotopy continuation method, we would still prefer to have some kind of verification of the solutions. For the SLLG, we used the Neuberger zero as a necessary condition. However, this is certainly not a sufficient condition and further checks may be required for bigger systems. This is called *certifying* the solutions, which is recently developed using the so-called Tropical Algebraic Geometry [143, 144]. We anticipate that our results mentioned above will serve as ideal test systems for all such new ideas.
- 9. To solve the corresponding equations for the periodic boundary conditions case, another method is to leave the constant zero modes in the system and use the Numerical Algebraic Geometry (NAG), which we explain in Appendix C. However, the NAG implemented on the available packages requires improvements to obtain positive dimensional real solutions, though the first step is already laid down [145].

5.4 Summary

We conclude this chapter:

- 1. We have shown that the multivariate polynomial version of the gauge fixing equations can be numerically solved, up to a numerical precision, with the so called NPHC method: for a given system of polynomial equations that are known to have only isolated solutions, the NPHC method gives *all* solutions numerically.
- 2. We demonstrated that the 3×3 SLLG anti-periodic boundary conditions system for the trivial and a random orbit, which were previously intractable, can be solved using the NPHC method. We have also shown the exact cancellation (not only the signs) of the Faddeev-Popov determinants in this case, i.e., the Neuberger zero. We classified all the solutions in terms of their Morse indices.

3. The MLLG on the 3×3 lattice is not yet tractable by the available packages. However, the NPHC method does not have any restriction, in theory, for these systems and our work is in progress to solve these systems. Solving these systems will directly clarify if the number of Gribov copies for the MLLG on the two-dimensional lattice is orbit-independent.

Chapter 6

't Hooft-Polyakov Monopoles In Lattice SU(N)+adjoint Higgs Theory

Another case where the continuum and lattice formulations need special attention is 't Hooft-Polyakov monopoles¹. 't Hooft-Polyakov monopoles [48, 49] play an important role in high energy physics for two reasons: their existence is a general prediction of grand unified theories, such as SU(N)+adjoint Higgs theory, and they provide a way to study non-perturbative properties of quantum field theories through electric-magnetic dualities [50]. However, most of the existing studies of monopoles in non-supersymmetric theories have been restricted to the level of classical solutions. Calculation of even leading-order quantum corrections is difficult, and can usually only be done in simple one-dimensional models [146]. Lattice Monte Carlo simulations provide an alternative, fully non-perturbative approach [147].

There are two general approaches to calculating properties of monopoles in Monte Carlo simulations. One can either define suitable creation and annihilation operators and measure their correlators [148, 149, 150], or one can impose boundary conditions which restrict the path integral to a non-trivial topological sector [151]. The former approach is closer in spirit to usual Monte Carlo simulations and in principle it gives access to a wide range of observable including, e.g., the vacuum expectation value of the monopole field. However, monopoles are surrounded by a spherical infinite-range magnetic Coulomb field and so it is difficult to find a suitable operator and separate the true ground state from excited states. Though the non-trivial boundary conditions provide access to a more limited set of observables, they ensure that the monopole is always in its ground state. Early attempts to simulate monopoles were based on fixed boundary con-

¹I am grateful to Arttu Rajantie for inviting me to Imperial College London for this work and kind and continuous support. I thank Tanmay Vachaspati for helpful suggestions and comments. A special thanks goes to Samuel Edwards for his collaboration in this work.

ditions, but this introduced large finite-size effects. To avoid them, one needs to use boundary conditions which are periodic up to the symmetries of the theory. Such boundary conditions were introduced for the SU(2) theory in Ref. [51], and they were used to calculate the mass of the monopoles in Refs. [52, 152]. They are used also in various related contexts (see, e.g., [153, 154, 155, 156, 157]).

Here, we generalize this result to SU(N) gauge group with N > 2. This is important for several reasons. Many analytical results are only valid in the large-N limit, and for grand unified theory monopoles one needs SU(5) or larger groups. The SU(2) group is also somewhat special, and a richer theoretical structure with new questions arises for N > 2. For example, there can be several different monopole species and unbroken non-Abelian gauge groups.

In the SU(2) case, monopoles were *created* on the lattice by boundary conditions which consist of complex conjugation and topologically non-trivial gauge transformations. Here we generalize this to SU(N) but only for even N. The boundary conditions treat all monopole species in the same way, so we cannot single out one for creation. Instead of actually fixing the magnetic charge, we can only choose between odd and even charges. However, even with these limitations, the boundary conditions make it possible to measure the monopole mass.

Here, we first review the definitions of the magnetic field and magnetic charge in the SU(N)+adjoint Higgs theory in the continuum and on the lattice, respectively. We then show how the monopole mass is expressed in terms of partion functions for different topological sectors. We introduce twisted C-periodic boundary conditions and show that they can be used to calculate the monopole mass, and describe our results.

6.1 Magnetic Charges In The Continuum

The most general renormalizable Lagrangian for the SU(N) gauge field theory A_{μ} with an adjoint Higgs field Φ is

$$L = -\text{Tr}G^{\mu\nu}G_{\mu\nu} + \text{Tr}[D_{\mu}, \Phi][D^{\mu}, \Phi] -m^{2}\text{Tr}\Phi^{2} - \kappa\text{Tr}\Phi^{3} - \lambda_{1}(\text{Tr}\Phi^{2})^{2} - \lambda_{2}\text{Tr}\Phi^{4}, \qquad (6.1)$$

where we have used the covariant derivative and field strength tensor defined by

$$D_{\mu} = \partial_{\mu} + igA_{\mu}, \quad G_{\mu\nu} = -\frac{i}{g}[D_{\mu}, D_{\nu}]$$
 (6.2)

respectively, and g being the coupling strength. Both Φ and A_{μ} are Hermitian and traceless $N \times N$ matrices, which can be expanded in terms of the group generators² T^{A} ,

$$\Phi(x) = \phi^A(x)T^A, \quad A_\mu(x) = A^A_\mu(x)T^A, \tag{6.3}$$

²Notations have been slightly changed here to be consistent with the literature. We use lower case Latin letters for a = 1, ..., N and upper case Latin letters for $A = 1, ..., (N^2 - 1)$. Greek letters represent Lorentz indices.

with real coefficients ϕ^A and A^A_μ . The fields can therefore also be thought of as $N^2 - 1$ component vectors.

For N = 2, the group generators can be chosen to be the Pauli matrices,

$$T^A = \frac{\sigma^A}{2}.\tag{6.4}$$

Because of the properties of the Pauli matrices, $\text{Tr}\Phi = \text{Tr}\Phi^3 = 0$ and $(\text{Tr}\Phi^2)^2 = 2\text{Tr}\Phi^4$, and therefore we can choose $\kappa = \lambda_2 = 0$ without any loss of generality and $\lambda_1 = \lambda$.

In the broken phase, where $m^2 < 0$, the Higgs field has a vacuum expectation value

$$\langle \text{Tr}\Phi^2 \rangle = \frac{1}{2} \langle \phi^A \phi^A \rangle = \frac{m^2}{\lambda}.$$
 (6.5)

The SU(2) symmetry is spontaneously broken to U(1). To represent the direction of symmetry breaking, we define

$$\hat{\Phi}(x) = \frac{\Phi(x)}{\sqrt{2\mathrm{Tr}\Phi(x)^2}},\tag{6.6}$$

which is well defined whenever $\Phi \neq 0$. Following 't Hooft [48], we use this to define the field strength

$$F_{\mu\nu} = 2\text{Tr}\hat{\Phi}G_{\mu\nu} - \frac{4i}{g}\text{Tr}\hat{\Phi}[D_{\mu},\hat{\Phi}][D_{\nu},\hat{\Phi}]$$

$$= \partial_{\mu}(\hat{\phi}^{A}A_{\nu}^{A}) - \partial_{\nu}(\hat{\phi}^{A}A_{\mu}^{A}) + \frac{\epsilon_{ABC}}{g}\hat{\phi}^{A}(\partial_{\mu}\hat{\phi}^{B})\partial_{\nu}\hat{\phi}^{C}.$$
(6.7)

Fixing the unitary gauge, in which $\Phi \propto \sigma^3$, makes this definition more transparent. The gauge fixing is achieved by the gauge transform R(x), such that the transformed field $\tilde{\Phi}$ is diagonal

$$\tilde{\Phi}(x) \equiv R^{\dagger}(x)\Phi(x)R(x) = \sqrt{2\mathrm{Tr}\Phi^2}\frac{\sigma^3}{2}.$$
(6.8)

In terms of the transformed gauge field,

$$\tilde{A}_{\mu} = R^{\dagger} A_{\mu} R - \frac{i}{g} R^{\dagger} \partial_{\mu} R, \qquad (6.9)$$

the field strength tensor has the usual Abelian form,

$$F_{\mu\nu} = \partial_{\mu}\tilde{A}^{3}_{\nu} - \partial_{\nu}\tilde{A}^{3}_{\mu}.$$
(6.10)

Alternatively, we can express this in terms of the diagonal elements of the transformed gauge field,

$$F^a_{\mu\nu} = \partial_\mu \tilde{A}^{aa}_\nu - \partial_\nu \tilde{A}^{aa}_\mu. \tag{6.11}$$

This defines a two-component vector of field strength tensors, but tracelessness of A_{μ} implies $F_{\mu\nu}^2 = -F_{\mu\nu}^1$. The conventional field strength $F_{\mu\nu}$ is given by $F_{\mu\nu} = F_{\mu\nu}^1 - F_{\mu\nu}^2$.

The conserved magnetic current corresponding to the residual U(1) group is defined as

$$j^a_\mu = \partial^{\nu \star} F^a_{\mu\nu}, \tag{6.12}$$

where ${}^{\star}F^a_{\mu\nu}$ is the dual tensor,

$${}^{\star}F^{a}_{\mu\nu} = \frac{1}{2} \epsilon_{\mu\nu\rho\sigma} F^{a\,\rho\sigma}.\tag{6.13}$$

Like the field strength, the magnetic currents satisfy $j_{\mu\nu}^2 = -j_{\mu\nu}^1$, so there is only one monopole species.

Substituting Eq. (6.7), one finds

$$j^{1}_{\mu} = \frac{1}{4g} \epsilon_{\mu\nu\rho\sigma} \epsilon_{ABC} (\partial^{\nu} \hat{\phi}^{A}) (\partial^{\rho} \hat{\phi}^{B}) (\partial^{\sigma} \hat{\phi}^{C}) = -j^{2}_{\mu}.$$
(6.14)

This vanishes when $\Phi \neq 0$, but is generally non-zero when Φ vanishes. The magnetic charge inside volume V bounded by a closed surface S that encloses a zero is

$$Q = \int_{V} d^{3}x \ j_{0} = \pm \frac{2\pi}{g} (1, -1).$$
(6.15)

This can be generalized to SU(N) [158]. The matrices $\{T^A\}$ in Eq. (6.3) are now the generators of SU(N) in the fundamental representation, and we assume the usual normalization $\text{Tr}T^AT^B = \frac{1}{2}\delta^{AB}$. As in Eq. (6.8), consider a gauge transformation R(x) that diagonalizes $\Phi(x)$ and places the eigenvalues in descending order,

$$\tilde{\Phi}(x) = R^{\dagger}(x)\Phi(x)R(x) = \operatorname{diag}(\lambda_1, \dots, \lambda_N), \qquad (6.16)$$

where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N$.

In classical field theory one usually finds that there are only two distinct eigenvalues, and consequently only one residual U(1) group. In that case one can use Eq. (6.7) to define the corresponding field strength. However, as we will discuss in Section 6.2, in lattice Monte Carlo simulations all the eigenvalues are distinct. In that case, $\tilde{\Phi}(x)$ is invariant under gauge transformations generated by the N-1 diagonal generators of SU(N). Thus we are left with a residual U(1)^{N-1} gauge invariance corresponding the Cartan subgroup of SU(N). It is then convenient to follow 't Hooft [158] and define the residual U(1) field strengths by Eq. (6.11), with $a \in \{1, \ldots, N\}$. The corresponding magnetic currents j^a_{μ} are then given by Eq. (6.12). They satisfy the tracelessness condition

$$\sum_{a=1}^{N} F^{a}_{\mu\nu} = \sum_{a=1}^{N} j^{a}_{\mu\nu} = 0, \qquad (6.17)$$

so that there are only N-1 independent U(1) fields and magnetic charges.

The set of points in which two eigenvalues coincide $\lambda_j = \lambda_{j+1}$ is generally pointlike in three dimensions and behaves like a magnetic charge with respect to the SU(2) subgroup involving only the *j*th and (j + 1)th components of a fundamental representation [158]. That is, it behaves like a magnetic monopole with charge $Q = \pm \hat{q}_j$, where the elementary magnetic charges are

$$\hat{q}_{j}^{a} = \frac{2\pi}{g} \left(\delta_{a,j} - \delta_{a,(j+1)} \right), \tag{6.18}$$

or in vector notation

$$\hat{q}_j = \frac{2\pi}{g} \left(\overbrace{0, \dots, 0}^{j-1}, 1, -1, \overbrace{0, \dots, 0}^{N-j-1} \right).$$
 (6.19)

6.2 Magnetic Charge On The Lattice

On the lattice, the Higgs field is defined on sites³ \vec{x} while the gauge degrees of freedom are encoded in SU(N) valued link variables $U_{\mu}(\vec{x})$. The Lagrangian is given by

$$L = \frac{1}{g^2} \sum_{\mu\nu} \text{Tr} U_{\mu}(\vec{x}) U_{\nu}(\vec{x} + \hat{\mu}) U_{\mu}^{\dagger}(\vec{x} + \hat{\nu}) U_{\nu}^{\dagger}(\vec{x}) + 2 \sum_{\mu} \left[\text{Tr} \Phi(\vec{x})^2 - \text{Tr} \Phi(\vec{x}) U_{\mu}(\vec{x}) \Phi(\vec{x} + \hat{\mu}) U_{\mu}^{\dagger}(\vec{x}) \right] + m^2 \text{Tr} \Phi^2 + \kappa \text{Tr} \Phi^3 + \lambda_1 (\text{Tr} \Phi^2)^2 + \lambda_2 \text{Tr} \Phi^4.$$
(6.20)

Again, we diagonalize Φ by a gauge transformation $R(\vec{x})$,

$$\tilde{\Phi}(\vec{x}) = R^{\dagger}(\vec{x})\Phi(\vec{x})R(\vec{x}).$$
(6.21)

Link variables are transformed to

$$\tilde{U}_{\mu}(\vec{x}) = R^{\dagger}(\vec{x})U_{\mu}(\vec{x})R(\vec{x}+\hat{\mu}).$$
(6.22)

The diagonalized field $\tilde{\Phi}$ is still invariant under diagonal gauge transformations,

$$D(\vec{x}) = \text{diag}(e^{i\Delta_1(\vec{x})}, \dots, e^{i\Delta_N(\vec{x})}), \quad \sum_{a=1}^N \Delta_a = 0,$$
 (6.23)

which form the residual $U(1)^{N-1}$ symmetry group.

³The lattice site index is changed from i in the previous chapters to \vec{x} . Lattice spacing is taken to be 1 for simplicity.

To identify the corresponding U(1) field strength tensors, we need to decompose \tilde{U}_{μ} [159],

$$\tilde{U}_{\mu}(\vec{x}) = C_{\mu}(\vec{x})u_{\mu}(\vec{x}),$$
(6.24)

where $u_{\mu}(\vec{x})$ represents the residual U(1) gauge fields and transforms as

$$u_{\mu}(\vec{x}) \to D^{\dagger}(\vec{x})u_{\mu}(\vec{x})D(\vec{x}+\hat{\mu}).$$
 (6.25)

 $C_{\mu}(\vec{x})$ represents fields charged under the U(1) groups.

This decomposition is not unique on the lattice [159]. A simple choice is to define Abelian link variables as the diagonal elements of \tilde{U}_{μ} in direct analogy with Eq. (6.11),

$$u_{\mu}(\vec{x}) = \operatorname{diag} \tilde{U}_{\mu}(\vec{x}). \tag{6.26}$$

In practice, it is often more convenient to work with link angles and define an N-component vector

$$\alpha^a_\mu(\vec{x}) = \arg u^{aa}_\mu. \tag{6.27}$$

As angles, these are only defined modulo 2π , and we choose them to be in the range $-\pi < \alpha_{\mu}^{a} \leq \pi$. As in the continuum, the angles α_{μ}^{a} satisfy

$$\sum_{a} \alpha^a_\mu(\vec{x}) = 0 \mod 2\pi.$$
(6.28)

Therefore it has only N-1 independent components, corresponding to the N-1 residual U(1) gauge groups.

Next, we construct plaquette angles as

$$\alpha^{a}_{\mu\nu}(\vec{x}) = \alpha^{a}_{\mu}(\vec{x}) + \alpha^{a}_{\nu}(\vec{x} + \hat{\mu}) - \alpha^{a}_{\mu}(\vec{x} + \hat{\nu}) - \alpha^{a}_{\nu}(\vec{x})$$
(6.29)

which are the lattice analogs of the Abelian field strength. In the continuum limit, they are related by

$$F^{a}_{\mu\nu} = \frac{1}{g} \alpha^{a}_{\mu\nu}.$$
 (6.30)

Because the links α^a_μ are only defined modulo 2π , the same applies to the plaquette, and again, we choose $-\pi < \alpha^a_{\mu\nu} \leq \pi$.

Using Eq. (6.29), the corresponding lattice magnetic currents are

$$j^a_\mu = \frac{1}{g} \Delta_\nu \alpha^{a\star}_{\mu\nu} \tag{6.31}$$

where

$$\alpha^{a\star}_{\mu\nu} = \frac{1}{2} \epsilon_{\mu\nu\rho\sigma} \alpha^a_{\rho\sigma} \tag{6.32}$$

These are integer multiples of 2π , because each contribution of $\alpha^a_\mu(\vec{x})$ is cancelled by a $-\alpha^a_\mu(\vec{x})$ modulo 2π . In particular, the Abelian magnetic charge inside a single lattice cell is given by

$$q^{a}(\vec{x}) = j_{0}^{a} = \frac{1}{2g} \sum_{ijk} \epsilon_{ijk} \left(\alpha_{ij}^{a}(\vec{x} + \hat{k}) - \alpha_{ij}^{a}(\vec{x}) \right).$$
(6.33)

Each component of this vector is an integer multiple of $(2\pi/g)$, and they all add up to zero. The elementary charges, corresponding to individual monopoles, are the same as in the continuum (6.19). Other values of the charge vector qcorrespond to composite states made of elementary monopoles.

The diagonalization procedure in Eq. (6.16) is ill defined whenever the Higgs field has degenerate eigenvalues, but on the lattice the set of field configurations in which this happens has zero measure in the path integral. Physically this means that the core of the monopole never lies exactly at a lattice site. Therefore these configuration do not contribute to any physical observable and do not have to be considered separately.

6.3 Monopole Mass

The Abelian magnetic charge Q of any lattice field configuration is well defined by adding up the contributions (6.33) from each lattice cell,

$$Q = \sum_{x} q(\vec{x}). \tag{6.34}$$

Because it is discrete, one can define separate partition functions Z_Q for each magnetic charge sector. The full partition function is simply the product

$$Z = \prod_Q Z_Q.$$

The ground state energy of a given charge sector may be defined by

$$E_Q = -\frac{1}{T} \ln \frac{Z_Q}{Z_0},$$
 (6.35)

where Z_0 is the partition function of the charge zero sector and T is the length of the lattice in the time direction.

The mass M_j of a single monopole \hat{q}_j is given by the ground state energy of the corresponding charge sector

$$M_j = E_{\hat{q}_j}.\tag{6.36}$$

In order to calculate the energies E_Q , we need to impose boundary conditions which enforce non-trivial Abelian magnetic charge. It is important that these boundary conditions preserve the translational invariance of the system, because otherwise our calculations are tainted by boundary effects. Because they are generally proportional to the surface area they will completely swamp the contribution from a point-like monopole which we want to measure.

Gauss's law rules out periodic boundary conditions since they fix the charge to zero. However, translational invariance only requires periodicity up to the symmetry of the Lagrangian (6.20). Since the magnetic current is conserved, we only need to consider spatial boundary conditions.

For SU(2), it was found in Ref. [51] that the following boundary conditions force an odd value for the magnetic charge,

$$\Phi(\vec{x} + n\hat{j}) = -\sigma_{j}\Phi(\vec{x})\sigma_{j} = (\sigma_{2}\sigma_{j})^{\dagger}\Phi^{*}(\vec{x})(\sigma_{2}\sigma_{j}) U_{\mu}(\vec{x} + n\hat{j}) = \sigma_{j}U_{\mu}(\vec{x} + n\hat{j})\sigma_{j} = (\sigma_{2}\sigma_{j})^{\dagger}U_{\mu}^{*}(\vec{x})(\sigma_{2}\sigma_{j}).$$

$$(6.37)$$

These are examples of twisted C-periodic boundary conditions, as introduced by Kronfeld and Wiese [160]. Note that twisted C-periodic and twisted periodic boundary conditions are equivalent for the gauge links. On the other hand, the Higgs field requires an additional anti-periodicity when we convert from one form to the other. Physically, this means that the charge conjugation is carried only by the Higgs field in SU(2). We will come back to this important point when we discuss the boundary conditions in terms of the flux sectors of pure SU(2) gauge theory.

It turns out that untwisted C-periodic boundary conditions (no σ_j 's) are compatible with any even value of magnetic charge [51]. Assuming that monopoles do not form bound states, the weight of the multi-monopole configurations in the path integral is exponentially suppressed

$$Z_Q = e^{-MT} Z_0, (6.38)$$

where M is the monopole mass. In the infinite-volume limit, $T \to \infty$, only the configurations with the minimum number of monopoles contribute to the path integral. So the partition function Z_{odd} for twisted C-periodic boundary conditions will be dominated by configurations with a single monopole, while the partition function Z_{even} will be dominated by configurations with no monopoles. Therefore the monopole mass is given my

$$M = -\lim_{T \to \infty} \frac{1}{T} \ln Z_{\text{odd}} / Z_{\text{even}}.$$
 (6.39)

This was used to calculate the non-perturbative mass of the 't Hooft-Polyakov monopole in Ref. [52, 152], with good agreement with classical expectations.

6.4 Twisted Boundary Conditions

Let us now generalize the boundary conditions (6.37) to SU(N) with N > 2. To avoid boundary effects, the boundary conditions must preserve translation invariance, and they will therefore have to be periodic up to the symmetries of the theory. In the case of Eq. (6.20), the available symmetries are complex conjugation of the fields and gauge invariance. When $\kappa = 0$, reflection of the Higgs field $\Phi \rightarrow -\Phi$ is also a symmetry, but in general it is not, and so we do not consider it. The appropriate extension of (6.37) is then a combination of complex conjugation and gauge transformations.

6.4.1 Fully C-periodic Boundary Conditions

It is natural to impose complex conjugation in all three spatial directions, in which case we have

$$\Phi(\vec{x} + n\hat{j}) = \Omega_{j}^{\dagger}(\vec{x})\Phi^{*}(\vec{x})\Omega_{j}(\vec{x}),$$

$$U_{\mu}(\vec{x} + n\hat{j}) = \Omega_{j}^{\dagger}(\vec{x})U_{\mu}^{*}(\vec{x})\Omega_{j}(\vec{x} + \hat{\mu}),$$
(6.40)

where the SU(N) gauge transformation matrix $\Omega_j(\vec{x})$ can in general be position dependent. We refer to these as (fully) C-periodic boundary conditions [160].⁴

To avoid contradiction at the edges, it should not matter in which order the boundary conditions are applied. Therefore, the gauge transformations must satisfy [160]

$$\Omega_{j}^{\dagger}(\vec{x}+n\hat{k})\Omega_{k}^{T}(\vec{x})\Phi(\vec{x})\Omega_{k}^{*}(\vec{x})\Omega_{j}(\vec{x}+n\hat{k})$$

$$=\Phi(\vec{x}+n\hat{j}+n\hat{k})$$

$$=\Omega_{k}^{\dagger}(\vec{x}+n\hat{j})\Omega_{j}^{T}(\vec{x})\Phi(\vec{x})\Omega_{j}^{*}(\vec{x})\Omega_{k}(\vec{x}+n\hat{j}),$$
(6.41)

and

$$\Omega_{j}^{\dagger}(\vec{x} + n\hat{k})\Omega_{k}^{T}(\vec{x})U_{\mu}(\vec{x})\Omega_{k}^{*}(\vec{x} + \hat{\mu})\Omega_{j}(\vec{x} + n\hat{k} + \hat{\mu}) = U_{\mu}(\vec{x} + n\hat{j} + n\hat{k}) = \Omega_{k}^{\dagger}(\vec{x} + n\hat{j})\Omega_{j}^{T}(\vec{x})U_{\mu}(\vec{x})\Omega_{j}^{*}(\vec{x} + \hat{\mu})\Omega_{k}(\vec{x} + n\hat{j} + \hat{\mu}).$$
(6.42)

Since our fields are blind to center elements, Eq. (6.41) implies the cocycle condition

$$\Omega_i^* \Omega_j = z_{ij} \Omega_j^* \Omega_i, \quad z_{ij} = e^{i\theta_{ij}} \in \mathbb{Z}_{\mathbb{N}}.$$
(6.43)

The antisymmetric *twist tensor* $z_{ij} = z_{ji}^*$ consists of Nth roots of unity and therefore we can write

$$\theta_{ij} = \frac{2\pi n_{ij}}{N} \mod 2\pi, \quad n_{ij} \in \mathbb{Z}.$$
(6.44)

Furthermore, Eq. (6.42) implies that z_{ij} has to be independent of position.

⁴In fact, in the terminology of Ref. [160], these correspond to C-periodic boundary conditions with C = -1, and C = 1 corresponds to boundary conditions without complex conjugation.

All choices of $\Omega_j(\vec{x})$ which give the same twist tensor z_{ij} are gauge equivalent [160], and therefore we can assume without any loss of generality that the matrices Ω_j are independent of position.

Let us now consider the effect of the boundary conditions (6.40) on the residual U(1) fields. Because the eigenvalues of the Higgs field Φ are real, they are unaffected by the boundary conditions, and therefore the diagonalized field $\tilde{\Phi}$ defined in Eq. (6.21) is periodic. Therefore,

$$\Phi(\vec{x} + n\hat{j}) = \Omega_{j}^{\dagger} \Phi^{*}(\vec{x}) \Omega_{j}
= \Omega_{j}^{\dagger} \left(R(\vec{x}) \tilde{\Phi}(\vec{x}) R^{\dagger}(\vec{x}) \right)^{*} \Omega_{j}
= \Omega_{j}^{\dagger} R^{*}(\vec{x}) \tilde{\Phi}(\vec{x} + n\hat{j}) R^{T}(\vec{x}) \Omega_{j}.$$
(6.45)

Compatibility with

$$\Phi(\vec{x}+n\hat{j}) = R(\vec{x}+n\hat{j})\tilde{\Phi}(\vec{x}+n\hat{j})R^{\dagger}(\vec{x}+n\hat{j})$$
(6.46)

then implies the boundary conditions for $R(\vec{x})$,

$$R(\vec{x} + n\hat{j}) = \Omega_{j}^{\dagger} R^{*}(\vec{x}).$$
(6.47)

When we have multiple translations, we find a different transformation depending on which boundary condition we apply first,

$$R(\vec{x} + n\hat{j} + n\hat{k}) = \Omega_{j}^{\dagger}\Omega_{k}^{T}R(\vec{x}) = z_{kj}\Omega_{k}^{\dagger}\Omega_{j}^{T}R(\vec{x})$$
$$= z_{kj}R(\vec{x} + n\hat{j} + n\hat{k}).$$
(6.48)

This does not mean an inconsistency because both transformations have the same effect on the fields, but in our calculations we have to choose one or the other consistently. Hereafter we will always choose the x direction first, followed by y and then z.

Applying this to the gauge fixed link variables we find that the twist is absorbed for all links

$$\tilde{U}_{\mu}(\vec{x}+n\hat{j}) = R^{\dagger}(\vec{x}+n\hat{j})U_{\mu}(\vec{x}+n\hat{j})R(\vec{x}+\mu+n\hat{j})
= R^{T}(\vec{x})U_{\mu}^{*}(\vec{x})R^{*}(\vec{x}+\hat{\mu})
= \tilde{U}_{\mu}^{*}(\vec{x}),$$
(6.49)

except for those spatial links at the corners whose endpoints involve two translations as in Eq. (6.48). For them, we obtain for any two directions \hat{i} and \hat{j}

$$U_{j}(\vec{x} + n\hat{i} + (n - 1)\hat{j})$$

$$= R^{\dagger}(\vec{x} + n\hat{i} + (n - 1)\hat{j})U_{j}(\vec{x} + n\hat{i} + (n - 1)\hat{j}) \times$$

$$\times R(\vec{x} + n\hat{i} + n\hat{j})$$

$$= \begin{cases} \tilde{U}_{j}^{*}(\vec{x} + 0\hat{i} + (n - 1)\hat{j}) & \text{if } i < j \\ z_{ij}\tilde{U}_{j}^{*}(\vec{x} + 0\hat{i} + (n - 1)\hat{j}) & \text{if } i > j. \end{cases}$$
(6.50)



Figure 6.1: Integration curve used to calculate the flux through half of the box.

where the notation i < j denotes ordering for \hat{i} and \hat{j} directions in the chosen ordering.

6.4.2 Magnetic Flux

If the decomposition (6.24) commutes with complex conjugation, the boundary conditions (6.40) imply anti-periodicity of $\alpha^a_{\mu}(\vec{x})$. So, the Abelian projected fields inherit the boundary conditions

$$\alpha^{a}_{\mu}(\vec{x}+n\hat{j}) = -\alpha^{a}_{\mu}(\vec{x}), \tag{6.51}$$

except for the special cases

$$\alpha_j^a(\vec{x} + n\hat{\imath} + (n-1)\hat{\jmath}) = \begin{cases} -\alpha_j^a(\vec{x}) & \text{if } i < j\\ \theta_{ij} - \alpha_j^a(\vec{x}) & \text{if } i > j \end{cases}.$$
 (6.52)

It follows that the fluxes

$$\alpha^{a}_{\mu\nu}(\vec{x}) = \alpha^{a}_{\mu}(\vec{x}) + \alpha^{a}_{\nu}(\vec{x} + \hat{\mu}) - \alpha^{a}_{\mu}(\vec{x} + \hat{\nu}) - \alpha^{a}_{\nu}(\vec{x})$$
(6.53)

are always anti-periodic, since the twist angles θ_{ij} cancel when we compare fluxes on opposite sides of the lattice. This means that when we cross the boundary we enter a charge conjugated copy of the same lattice from the opposite side.

To determine the magnetic charge we repeat the trick of [51]. The curve shown Figure 6.1 divides the boundary into two halves. We denote the magnetic flux through them by Φ_+ and Φ_- choosing the positive direction to be pointing outwards. The two halves are related by the boundary conditions, and in particular, the anti-periodicity (6.53) of the field strength implies that they are equal $\Phi_- = \Phi_+$. The magnetic charge inside the lattice is given by the total flux, which is the sum of the two contributions, i.e.

$$Q = \Phi_+ + \Phi_- = 2\Phi_+. \tag{6.54}$$

Applying Stokes's theorem, we can write

$$\Phi_{+}^{a} = \frac{1}{g} \left(\sum_{x=0}^{n-1} \alpha_{1}^{a}(x,n,0) - \sum_{y=0}^{n-1} \alpha_{2}^{a}(n,y,0) + \sum_{z=0}^{n-1} \alpha_{3}^{a}(n,0,z) - \sum_{x=0}^{n-1} \alpha_{1}^{a}(x,0,n) + \sum_{y=0}^{n-1} \alpha_{2}^{a}(0,y,n) - \sum_{z=0}^{n-1} \alpha_{3}^{a}(0,n,z) \right).$$
(6.55)

When we apply the boundary conditions, all terms cancel except those involving the special cases (6.52),

$$\Phi_{+}^{a} = \frac{1}{g} \left(\alpha_{1}^{a}(n-1,n,0) - \alpha_{2}^{a}(n,n-1,0) + \alpha_{3}^{a}(n,0,n-1) - \alpha_{1}^{a}(n-1,0,n) + \alpha_{2}^{a}(0,n-1,n) - \alpha_{3}^{a}(0,n,n-1) \right) \\
= \frac{1}{g} \left(\theta_{21} + \theta_{13} + \theta_{32} \right) \mod \frac{2\pi}{g},$$
(6.56)

where because the link angles α^a_{μ} are defined modulo 2π , the flux is only defined modulo $(2\pi/g)$. Therefore we find

$$Q^{a} = \frac{2}{g}(\theta_{21} + \theta_{13} + \theta_{32}) \mod \frac{4\pi}{g}.$$
 (6.57)

6.4.3 Allowed Magnetic Charges

It is obvious from Eq. (6.57) that the possible charges one can create using the boundary conditions is quite restricted. As in the continuum (6.19), the components are quantized in units of $2\pi/g$. This can be seen explicitly by considering the effect of the cocycle condition (6.43) on the product $\Omega_i \Omega_j^* \Omega_k$ [160]. On one hand, we have

$$\Omega_i \Omega_j^* \Omega_k = z_{jk} \Omega_i \Omega_k^* \Omega_j
= z_{jk} z_{ki} \Omega_k \Omega_i^* \Omega_j
= z_{jk} z_{ki} z_{ij} \Omega_k \Omega_j^* \Omega_i,$$
(6.58)

but applying the condition in the opposite order we find

$$\Omega_{i}\Omega_{j}^{*}\Omega_{k} = z_{ji}\Omega_{j}\Omega_{i}^{*}\Omega_{k}$$

$$= z_{ji}z_{ik}\Omega_{j}\Omega_{k}^{*}\Omega_{i}$$

$$= z_{ji}z_{ik}z_{kj}\Omega_{k}\Omega_{j}^{*}\Omega_{i}.$$
(6.59)

Therefore the twist tensor must satisfy the constraint

$$z_{ji}^2 z_{jk}^2 z_{ki}^2 = 1, (6.60)$$

which implies

$$2(\theta_{21} + \theta_{13} + \theta_{32}) \in 2\pi\mathbb{Z}.$$
(6.61)

Substituting this into Eq. (6.57) gives the charge quantization condition

$$Q^{a} = \frac{2}{g}(\theta_{21} + \theta_{13} + \theta_{32}) \in \frac{2\pi}{g}\mathbb{Z}.$$
(6.62)

On the other hand, because the right hand side does not depend on a at all, every component Q^a has to have the same charge, modulo $(4\pi/g)$. Combining this with Eq. (6.62), we conclude that in terms of multiples of $2\pi/g$, either every component Q^a is odd,

$$Q^a = \frac{2\pi}{g} \mod \frac{4\pi}{g} \text{ for all } a, \tag{6.63}$$

in which case there is an odd number of each magnetic monopole species, or every component is even,

$$Q^a = 0 \mod \frac{4\pi}{g} \text{ for all } a, \tag{6.64}$$

in which case there is an even number of each magnetic monopole species. As was discussed in Section 6.3, the former case always corresponds to one monopole in practice, and the latter to no monopoles.

However, the components of the magnetic charge vector must add up to zero,

$$\sum_{a} Q^a = NQ_a = 0 \mod \frac{4\pi}{g}.$$
(6.65)

If N is odd, Eq. (6.63) violates this constraint, which means that with the boundary conditions in Eq. (6.40), the number of monopoles is always even (i.e., zero). If N is even, both (6.63) and (6.64) satisfy this constraint.

A convenient choice for an odd number of monopoles with Eq. (6.63) is

$$\Omega_1 = \operatorname{diag}(i\sigma_3, \dots, i\sigma_3)$$

$$\Omega_2 = \operatorname{diag}(I, \dots, I)$$

$$\Omega_3 = \operatorname{diag}(i\sigma_1, \dots, i\sigma_1).$$
(6.66)

These are simply the SU(2) matrices from Eq. (6.37) repeated in block diagonal form. They satisfy

$$\Omega_i^* \Omega_j = -\Omega_j^* \Omega_i, \ i \neq j, \tag{6.67}$$

corresponding to a π twist angle in each plane. An even number of monopoles, corresponding to Eq. (6.64), is obtained by simply choosing

$$\Omega_1 = \Omega_2 = \Omega_3 = 1. \tag{6.68}$$

We have therefore found that the twisted boundary conditions (6.40) allow us to impose a non-zero magnetic charge, but with several restrictions. It is, in fact, fairly natural that we cannot specify the exact charge but only whether it is odd or even. To avoid boundary effects our boundary conditions have to preserve translation invariance, but in order to be compatible with Gauss law, they must include charge conjugation. If we had a way to fix the magnetic charge to some particular value Q, a translation by n would therefore change it to -Q, but then translation invariance requires Q = -Q and therefore Q = 0. Another way to see this is to imagine picking one monopole and moving it through to boundary so that it appears from the opposite side of the lattice with the opposite sign, changing the magnetic charge by two units.

The other restriction, that all the charges must have the same value, arises because our boundary conditions are linear operations on the fields. The transformation matrices Ω_j are therefore independent of the direction of symmetry breaking Φ , which defines the different residual U(1) groups. Therefore the boundary conditions cannot treat any U(1) group differently from the others. It may be possible to avoid this restriction by considering non-linear transformations. In practice, one can specify the boundary conditions in the unitary gauge in which the different U(1) groups can be treated separately. However, it is not clear if it is possible even then to impose translation invariant boundary conditions which give different values to different magnetic charges.

Imposing complex conjugation in all three directions has the advantage of preserving the invariance of the theory under 90-degree rotations. However, it is not necessary for a non-zero magnetic charge. It is enough to have complex conjugation in one direction, so that the flux can escape through at least one face. However, it turns out that with such *mixed* boundary conditions, the allowed magnetic charges are constrained exactly as in Section 6.4.3. The proof, which is very similar to that above, is given in Appendix D.

In spite of their limitations, the boundary conditions (6.40) allow us to define the partition functions Z_{odd} and Z_{even} in Eq. (6.39) using the gauge transformation (6.66) and (6.68), respectively. The ratio Z_{odd}/Z_{even} gives the difference in the ground state energies between the two sectors of the theory, i.e., the lightest states compatible with the odd or even magnetic charges. It is obvious that Z_{even} will give the vacuum state, but the interpretation of Z_{odd} is slightly more difficult. If there is only one residual U(1) group, only the monopole species which corresponds to it is massive, and therefore Eq. (6.39) gives the monopole mass, just as in SU(2). If there are several residual U(1) groups, Z_{odd} represents a state that contains one of each monopole species. Depending on which configuration has the lowest energy, they may either be as separate free particles, in which case Eq. (6.39) gives the sum of their masses, or as a bound state in which case it gives the energy of the bound state.

6.4.4 Relation To The Continuum and Zeroes of Higgs

It is interesting to see how twisted C-periodic (and mixed) boundary conditions relate back to Abelian magnetic charge in the continuum theory. Here we look at how the charge forcing boundary conditions translate in the continuum SU(2)case.

Recall that Abelian projected magnetic charge is located at zeroes of the Higgs field in the continuum. Thus, boundary conditions which force an odd number of monopoles must force an odd number of zeroes of Φ . This is easiest to see for the case of C-periodic boundary conditions with twist in each direction. First write these boundary conditions in the form

$$\Phi(\vec{x} + n\hat{i}) = -\sigma_i \Phi(\vec{x})\sigma_i. \tag{6.69}$$

It is then clear from the anticommutativity properties of the Pauli matrices that the components of the Higgs field in the adjoint representation $\Phi = \vec{\phi} \cdot \vec{\sigma}$ inherit the boundary conditions

$$\begin{aligned}
\phi_1(\vec{x} + n1) &= -\phi_1(\vec{x}), \\
\phi_2(\vec{x} + n\hat{2}) &= -\phi_2(\vec{x}), \\
\phi_3(\vec{x} + n\hat{3}) &= -\phi_3(\vec{x}),
\end{aligned}$$
(6.70)

while all other components are periodic. This is as we should expect, as the Higgs field should have a hedgehog configuration near the boundary.

The boundary conditions (6.70) ensure that ϕ_1 has an odd number of zeroes on every line through the box in the x direction. By continuity, these combine to form surfaces pinned to the boundary in the orthogonal plane. Similarly, there are an odd number of surfaces through the other two directions where ϕ_2 and ϕ_3 are respectively zero. Because of their relative orthogonality, these surfaces intersect in an odd number of points where all three components are zero. So we have an odd number of monopoles.

To see how this works, first consider the surfaces where ϕ_1 and ϕ_2 are zero. These intersect to form an odd number of lines in the z direction on which ϕ_1 and ϕ_2 are both zero. By (6.70) there must be an odd number of points on each of these lines where ϕ_3 is zero, and hence an odd number of points in total where ϕ vanishes.

It is straightforward to check that all of the boundary conditions which force an odd magnetic charge have this property. Conversely, those with trivial magnetic charge modulo 4π are found to permit only an even number points where the Higgs field is zero. This can extend to forcing degenerate number of eigenvalues for Higgs corresponding to the appropriate SU(2) subgroups when we go to SU(2N). There the twist is just SU(2) twist in block diagonal form. It is not quite so trivial though since we have to partially diagonalize the Higgs first and further work is required.

6.5 Summary

In summary:

- 1. 't Hooft-Polyakov monopoles are studied extensively using continuum semiclassical analysis, however, to understand their non-perturbative properties it is essential to put the concerned theory on the lattice. In this chapter, we studied an extension of anti-periodic boundary conditions for SU(N) which are called C-periodic boundary conditions. C-periodic boundary conditions for SU(N) have very rich structure. These boundary conditions with nontrivial gauge transformations were used to *insert* magnetic monopoles in the SU(2)+adjoint Higgs theory to study the deconfinement phase transitions in the so-called Grand Unified Theories on the lattice in Ref. [51].
- 2. We have shown how C-periodic boundary conditions (6.40) consisting of complex conjugation and gauge transformations can be used to impose a non-zero magnetic charge in SU(N)+adjoint Higgs theory while preserving translation invariance. This method has significant restrictions: it only works for SU(N) with even N, the charges can only be constrained to be odd or even, and every residual U(1) group has to have the same charge. Nevertheless, even with these restrictions, the boundary conditions make it possible to study magnetic monopoles in lattice Monte Carlo simulations. In particular, it will be straightforward to measure the monopole mass in the same way as in Ref. [152] and to compare the results with their continuum counter-part.

Chapter 7 Conclusions

There is little doubt that Quantum Chromodynamics (QCD), which is based on the quantum field theory framework, is *the* theory of strong interactions. For continuum quantum field theory, known reliable methods include perturbation theory, semi-classical expansions or large N expansions. However, to study many important physical phenomena such as confinement and dynamical chiral symmetry breaking in QCD, a fully non-perturbative approach is essential. Lattice field theory is such a non-perturbative approach that has been immensely successful in practical calculations of non-perturbative quantities in QCD. However, in the non-perturbative domain, the connection between the lattice and the continuum methods is still under-developed. The main aim of this thesis was to study this connection, specifically in two cases: Landau gauge fixing and 't Hooft-Polyakov monopoles.

Landau Gauge Fixing

There are two major approaches to studying non-perturbative phenomena in QCD: the Dyson-Schwinger Equations (DSEs) approach, which is based on a covariant continuum formulation, and lattice gauge theory. In the covariant continuum formulation of gauge theories, one has to fix a gauge, most popularly Landau gauge, to remove the redundant degrees of freedom. There, gauge-fixing is based on the so-called Faddeev-Popov procedure, or in more sophisticated language, the Becchi-Rouet-Stora-Tyutin (BRST) formulation [9]. In non-Abelian field theories, however, this procedure does not fix the gauge uniquely but leaves copies of physically equivalent gauge fields, called Gribov copies [12]. In the perturbative limit, where perturbations around the trivial configuration of gauge fields are considered, the corresponding gauge fixing condition has no Gribov copies. However, in the non-perturbative domain, Gribov copies do appear. Lattice field theory, on the other hand, offers an opportunity to perform *first principle* calculations of physical quantities in the non-perturbative domain. However, when following an analogous gauge fixing procedure on the lattice, one encounters, in addition to Gribov copies, the Neuberger 0/0 problem [29, 30]: the expectation value of a gauge-fixed observable turns out to be of the indefinite form 0/0.

In Chapter 2, we explained the Morse theoretical interpretation of Gribov copies and the Neuberger 0/0 problem on the lattice. That is, the standard lattice Landau gauge (SLLG) fixing device, which needs to be inserted in the gauge-invariant measure of the theory in the Faddeev-Popov procedure, calculates the Euler characteristic of the group manifold for the gauge-fixed link variables at each site, which is zero for compact U(1) and a generic SU(N) [39]. We argued that the Neuberger 0/0 problem can be solved for SU(N) if that for compact U(1) is solved together with Schaden's coset space BRST formulation which fixes the gauge to the maximal Abelian group U(1)^{N-1} [39]. We proposed a modification of the gauge-fixing functional via stereographic projection of compact U(1) circles of each gauge-fixed link angles, which has no difference with the SLLG in the continuum limit but resolves the Neuberger 0/0 problem for the compact U(1) case. Moreover, the modified lattice Landau gauge (MLLG) restricts the lower bound on the number of Gribov copies N_{GC} to polynomial increase with respect to the lattice size as compared to exponential increase for the SLLG.

In Chapter 3, we worked with lower dimensional lattice toy models employing either periodic or anti-periodic boundary conditions, for compact U(1). We analytically solved the gauge fixing conditions corresponding to both the SLLG and MLLG. For the SLLG, we explicitly demonstrated the topological origin of the Neuberger 0/0 problem in these simple toy models, by classifying all Gribov copies in terms of Morse theory, and also showed that N_{GC} exponentially grows with the lattice size. For the MLLG, we showed that N_{GC} increases polynomially with the lattice size and so is exponentially suppressed compared to the SLLG, in these lower dimensional models. Furthermore, we constructed the corresponding Faddeev-Popov procedure for these lower dimensional models via the MLLG. For the MLLG, we also showed that there is no cancellation among Gribov copies for an arbitrary dimensional lattice and so the Neuberger 0/0 problem is no longer present in the compact U(1) case. It is then straightforward to construct the corresponding BRST formulations for these models.

The gauge-fixing equations for higher dimensional lattices are highly nonlinear and hence difficult to solve. In Chapter 4, we transformed these (trigonometric) equations to polynomial equations and interpreted the problem in terms of Algebraic Geometry. This interpretation then allowed us to use sophisticated Computational Algebraic Geometry techniques, specifically the Groebner basis technique. This technique computationally solves a system of polynomial equations exactly. Though the corresponding algorithm suffers from the so-called Exponential Space complexity and solving large systems is difficult, we reported that the simplest non-trivial case of the SLLG on a two-dimensional lattice (i.e., a 3 lattice with anti-periodic boundary conditions) has been recently solved in a restrictive sense, in collaboration with V. Gerdt and D. Robertz. Furthermore, we interpreted Gribov copies and related issues in terms of Algebraic Geometry terminology. We have also pointed out that this method can be applicable to many problems in particle physics and statistical mechanics such as solving the classical equations of motion for compact QED on the lattice, representations of Lie groups etc.

The Algebraic Geometry interpretation of the lattice Landau gauge fixing equations opens up an opportunity to use a very recent method, the Numerical Polynomial Homotopy Continuation (NPHC) method, to solve the corresponding system numerically. Using the NPHC method, up to a numerical precision, one can obtain *all* solutions of a system of multivariate polynomial equations. In Chapter 5 we introduced the method and then solved the above mentioned 3×3 lattice case, for the trivial orbit and for random orbits with both periodic and anti-periodic boundary conditions. The NPHC method looks very promising for lattice field theory computations where it promises to find all the local and global extrema and the saddle points if the given functional is in the polynomial form. Moreover, this method is readily parallelizable.

't Hooft-Polyakov Monopoles

't Hooft-Polyakov monopoles have been studied extensively using continuum semi-classical analysis. However, to understand their non-perturbative properties it is essential to study them on the lattice. On the lattice, non-trivial boundary conditions, called C-periodic boundary conditions, were used to ensure the presence of 't Hooft-Polyakov monopoles inside the lattice in Ref. [51]. This construction then was used to study the deconfinement phase transitions in the so-called grand unified theories, such as adjoint Higgs models, for the SU(2) adjoint Higgs model. In Chapter 6, we studied an extension of C-periodic boundary conditions to SU(N). C-periodic boundary conditions for SU(N) have a very rich structure. We showed how C-periodic boundary conditions, consisting of complex conjugation and gauge transformations, can be used to impose 't Hooft-Polyakov monopoles in the SU(N) case while preserving the translation invariance. This method has significant restrictions: it only works for SU(N) with even N, the charges can only be constrained to be odd or even, and every residual U(1)group has to have the same charge. Nevertheless, even with these restrictions, the boundary conditions make it possible to study magnetic monopoles in lattice Monte Carlo simulations for the SU(N) model with N > 2. In particular, it will be straightforward to measure the monopole mass in the same way as in Ref. [152].

Future Research Plans

With the proposed MLLG, it should now be possible to implement the gauge-fixed Monte-Carlo simulations on the lattice: the current gauge-fixed Monte-Carlo
simulations done via the SLLG, samples the first Gribov region, i.e., the set of all local and global minima of the gauge-fixing functional, and do not take the rest of the Gribov copies into account. By using the MLLG, one can sample from all Gribov copies without encountering the Neuberger 0/0 problem. It will be very interesting to compare the existing results in the continuum DSE approach to those obtained on the lattice with the gauge-fixed Monte-Carlo simulations via the proposed MLLG [35].

Solving the lattice Landau gauge fixing equations for higher dimensional lattices is essential to studying Gribov copies and the Neuberger 0/0 problem in both the SLLG and the MLLG. Moreover, the SLLG is studied extensively as a spin-glass system in statistical mechanics and condensed matter theory, where Gribov copies are the extrema and saddle points of the classical Hamiltonian of the corresponding spin-glass system. In principle, the Groebner basis technique and the NPHC method can solve the corresponding polynomial equations, and efforts are currently underway to do this. Most importantly, it will clarify if the gauge fixing partition function (i.e., N_{GC} in this case) for the MLLG is orbit-independent.

It is highly desirable to solve the problems translated to the systems of polynomial equations in Appendix C via these methods. Most importantly, the classical equations of motion for a pure gauge theory on the lattice can in principle be written in terms of polynomial equations and then we can get all solutions numerically using the NPHC method. Note that since for compact U(1) and SU(2) group parameterizations are available, converting the corresponding equations of motion to polynomial ones is straightforward. For the SU(3) case, firstly, to obtain a suitable parameterization of the group matrices is required. We have already stated and discussed this problem in Appendix C in context of both the Groebner basis technique and the NPHC method, though further work is required to get the corresponding parametrization. It should then be possible to write down the corresponding equations of motion for the SU(3) case too.

Our findings in Chapter 6 generalizes the results obtained for SU(2) in Ref. [51], and will, most importantly, allow us to calculate the non-perturbative quantum mass of 't Hooft-Polyakov monopoles for SU(N) theories on the lattice, with even N.

Appendix A

No Neuberger 0/0 **Problem in Higher Dimensional Lattices**

Theorem: There is no Neuberger Zero problem in the MLLG for any dimension with anti-periodic boundary conditions.

With anti-periodic boundary conditions, the Faddeev-Popov operator for the MLLG can be decomposed, in the same way as the one-dimensional case, as

$$M_{FP}^{s} = \sum_{\mu=1}^{d} (M_{\mu} D_{\mu}^{s} M_{\mu}^{T}), \qquad (A.1)$$

where D^s_{μ} 's are diagonal matrices with the diagonal entries $\sec^2((\phi_{i,\mu}+\theta_{i+\hat{\mu}}-\theta_i)/2)$ with *i* running over all lattice sites and μ running over the lattice dimension *d*.

Now, it can be shown that the non-singular matrices M_1, \ldots, M_d are permutations of each other. That is, $M_2 = P_2 M_1 P_2^T, \ldots, M_d = P_d M_1 P_d^T$, where P_{μ} 's are the permutation matrices containing exactly single entry 1 and all other entries 0 in any given row or column, i.e., they only *reorder* the corresponding matrices M_{μ} 's. Moreover, their determinants are ± 1 , and so

$$M_{FP}^{s} = \sum_{\mu=1}^{d} ((P_{\mu}M_{1}P_{\mu}^{T})^{T} D_{\mu}^{s} (P_{\mu}M_{1}P_{\mu}^{T})), \qquad (A.2)$$

where we have taken P_1 as the identity matrix to be consistent with the notations. Now, since the diagonal entries of all D^s_{μ} are positive definite real numbers for $\phi^{\theta}_{i,\mu} = \phi_{i,\mu} + \theta_{i+\hat{\mu}} - \theta_{\mu} \mod 2\pi \in (-\pi,\pi)$, all D^s_{μ} are positive definite matrices. Moreover, since M_{μ} are non-singular matrices, all $M_{\mu}D^s_{\mu}M^T_{\mu}$ are positive definite matrices for all $\mu = 1, \ldots, d$, according to Sylvester's law of inertia. Because the sum of positive definite matrices is also a positive definite matrix, M^s_{FP} in this case is strictly a positive definite matrix. So, for all solutions (though they are not known yet), there is no cancellation of signs of the corresponding Faddeev-Popov determinants, i.e., no Neuberger zero. We can use the same arguments for the Faddeev-Popov operator in Eq. (E.3) for the modification via orbifolding case where the diagonal entries of the diagonal matrices D^{abs}_{μ} are $|\cos \phi^{\theta}_{i,\mu}|$ which are always positive definite numbers for $\phi^{\theta}_{i,\mu} \in (-\pi, \pi]$. So again there is no Neuberger zero.

Theorem: There is no Neuberger Zero problem in the MLLG for any dimension with periodic boundary conditions.

With periodic boundary conditions, a decomposition of the corresponding M_{FP}^s is not available so far and so we use another method here. We first separate M_{FP}^s for different μ in Eq. (3.6), i.e., $M_{FP}^s = \sum_{\mu} (M_{FP}^s)_{\mu}$ for a *d*-dimensional square lattice. Now, we consider the quadratic form for the symmetric matrices $(M_{FP}^s)_{\mu}$ with an $n^d \times 1$ vector $\vec{y} \neq \vec{0}$ whose elements are y_i where now $i = (i_1, \ldots, i_d)$ with i_1, \ldots, i_d running over $1, \ldots, n$ for the square lattice. Thus, it is easy to check that for any μ ,

$$\vec{y}^T (M^s_{FP})_\mu \ \vec{y} = \sum_i \sec^2 \frac{\phi^\theta_{i,\mu}}{2} (y_{i+\hat{\mu}} - y_i)^2,$$
 (A.3)

which is 0 only if all y_i are equal, which is the constant zero mode and is strictly positive for all other cases. Also, these y_i are taken to be following the periodic boundary conditions, in this expression. Thus, the matrix $(M_{FP}^s)_{\mu}$ is positive semi-definite for all $\mu = 1, \ldots, d$. Since the sum of positive semi-definite matrices is a positive semi-definite matrix, M_{FP}^s is also a positive semi-definite matrix. Thus there is no Neuberger zero since there exists no cancellations among the Faddeev-Popov determinants.

Appendix B

One-dimensional Periodic Boundary conditions

Here, we deal with the gauge-fixing conditions with periodic boundary conditions for both the SLLG and the MLLG.

B.1 SLLG

Since with periodic boundary conditions there is one free variable, the system of gauge-fixing equations for the SLLG is

$$\sin \phi_1^{\theta} = \sin \phi_n^{\theta}
\dots
\sin \phi_n^{\theta} = \sin \phi_{n-1}^{\theta}.$$
(B.1)

Out of these n equations n-1 are linearly independent. To eliminate it, without loss of generality, we can set $\theta_n = 0$ so that there are n-1 independent variables in the system. Also notice that then nth equation can safely be removed from the system since it is a linearly dependent equation. Thus, we are left with n-1equations in n-1 variables θ_i . The new system, with $\theta_n = 0$, is

$$\sin \phi_1^{\theta} = \sin \phi_n^{\theta}
 \dots
 \sin \phi_{n-1}^{\theta} = \sin \phi_{n-2}^{\theta},$$
(B.2)

which in turn gives

$$\phi_1^{\theta} + 2\pi k_1 = \phi_n^{\theta} \text{ or } \pi - \phi_n^{\theta}$$

$$\dots$$

$$\phi_{n-1}^{\theta} + 2\pi k_{n-1} = \phi_{n-2}^{\theta} \text{ or } \pi - \phi_{n-2}^{\theta}.$$
(B.3)

Now, instead of n-1 variables k_i , we take n variables p_i as $2k_i\pi = p_i - p_{i-1}$ with constraints $\sum_{i=1}^{n} p_i = 0$, and with the periodic boundary conditions, i.e., as $p_0 = p_n$. Thus, we get

$$\phi_{1}^{\theta} + p_{1} = \phi_{n}^{\theta} + p_{n} \text{ or } \pi - (\phi_{n}^{\theta} + p_{n})$$
...
$$\phi_{n-1}^{\theta} + p_{n-1} = \phi_{n-2}^{\theta} + p_{n-2} \text{ or } \pi - (\phi_{n}^{\theta} + p_{n-2}). \quad (B.4)$$

Here, p_i is always an integer multiples of 2π up to a constant contribution which is an integer multiple of $\frac{2\pi}{n}$, say $\frac{2\pi}{n}r$. Thus, for fixed $r = 0, 1, \ldots, n-1$, and for integers l_i ,

$$p_i = 2\pi l_i + \frac{2\pi}{n}r,\tag{B.5}$$

with i = 1, ..., n. Also using $\sum_{i=1}^{n} p_i = 0$ we get

$$\sum_{i=1}^{n} l_i = -r, \quad -\sum_{i=1}^{n-1} l_i - r = l_n.$$
(B.6)

The original n-1 independent k_i each runs over all integers when n constrained integers l_i do. After relabelling $\tilde{\phi}_i^{\theta} := \phi_i^{\theta} + 2\pi l_i = \tilde{\phi}_i + \theta_{i+1} - \theta_i$, Eq. (B.4), for a fixed $r = 0, \ldots, n-1$, becomes

$$\tilde{\phi}_{1}^{\theta} = \tilde{\phi}_{n}^{\theta} \text{ or } \pi - \tilde{\phi}_{n}^{\theta}$$
...
$$\tilde{\phi}_{n-1}^{\theta} = \tilde{\phi}_{n-2}^{\theta} \text{ or } \pi - \tilde{\phi}_{n-2}^{\theta}.$$
(B.7)

We should instead choose to write it as

$$\tilde{\phi}_{1}^{\theta} = (-1)^{q_{n}} \tilde{\phi}_{n}^{\theta} + q_{n} \pi$$
...
$$\tilde{\phi}_{n-1}^{\theta} = (-1)^{q_{n-2}} \tilde{\phi}_{n-2}^{\theta} + q_{n-2} \pi,$$
(B.8)

where all $q_i \in \{0, 1\}$ with $q_0 = q_n$ (we choose to leave q_{n-1} to be 1 here but our results are independent of it). In terms of ϕ_i^{θ} variables, there are still *n* variables in n-1 equations and so it would be better to transform the $\tilde{\phi}_i^{\theta}$ of Eq. (B.8) in terms of $\tilde{\phi}_n^{\theta}$ on the right hand side. This can be done by substituting the first equation in the second and the resulting second equation to the third and so on in Eq. (B.8), and finally we get

$$\tilde{\phi}_{i}^{\theta} = (q_{i-1} + \sum_{l=0}^{i-2} q_{l} (\prod_{k=l}^{i-2} (-1)^{q_{k+1}}))\pi + \tilde{\phi}_{n}^{\theta} \prod_{l=0}^{i-1} (-1)^{q_{l}},$$
(B.9)

for $i = 1, \ldots, n-1$. Now, summing over Eq. (B.9) for all $i = 1, \ldots, n-1$, we get

$$\sum_{i=1}^{n-1} \tilde{\phi}_{i}^{\theta} = \sum_{i=1}^{n-1} \left(\left(q_{i-1} + \sum_{l=0}^{i-2} q_{l} \left(\prod_{k=l}^{i-2} (-1)^{q_{k+1}} \right) \right) \pi + \tilde{\phi}_{n}^{\theta} \prod_{l=0}^{i-1} (-1)^{q_{l}} \right)$$

$$= \sum_{i=1}^{n-1} \left(q_{i-1} + \sum_{l=0}^{i-2} q_{l} \left(\prod_{k=l}^{i-2} (-1)^{q_{k+1}} \right) \right) \pi + \tilde{\phi}_{n}^{\theta} \sum_{i=1}^{n-1} \left(\prod_{l=0}^{i-1} (-1)^{q_{l}} \right)$$

$$= \sum_{i=1}^{n-1} \left(q_{i-1} + \sum_{l=0}^{i-2} q_{l} \left(\prod_{k=l}^{i-2} (-1)^{q_{k+1}} \right) \right) \pi + \left(\tilde{\phi}_{n} + \theta_{1} \right) \sum_{i=1}^{n-1} \left(\prod_{l=0}^{i-1} (-1)^{q_{l}} \right)$$
(B.10)

where in the last equality we have used $\tilde{\phi}_n^{\theta} = \tilde{\phi}_n + \theta_1$ with $\tilde{\phi}_n = \phi_n + 2\pi l_i$. Now, using $\tilde{\phi}_i^{\theta} = \tilde{\phi}_i + \theta_{i+1} - \theta_i$ for $i = 1, \ldots, n-1$,

$$\sum_{i=1}^{n-1} \tilde{\phi}_i^{\theta} = \sum_{i=1}^{n-1} (\tilde{\phi}_i + \theta_{i+1} - \theta_i) = \sum_{i=1}^{n-1} (\tilde{\phi}_i) - \theta_1.$$
(B.11)

Using this in Eq. (B.10) and adding $\tilde{\phi}_n$ on both sides, we get

$$\sum_{i=1}^{n} \tilde{\phi}_{i} = \sum_{i=1}^{n-1} \left(q_{i-1} + \sum_{l=0}^{i-2} q_{l} (\prod_{k=l}^{i-2} (-1)^{q_{k+1}}) \right) \pi + \tilde{\phi}_{n}^{\theta} \left(\sum_{i=1}^{n-1} (\prod_{l=0}^{i-1} (-1)^{q_{l}}) + 1 \right)$$
$$\therefore n(\overline{\phi} - \frac{2\pi r}{n}) = \sum_{i=1}^{n-1} \left(q_{i-1} + \sum_{l=0}^{i-2} q_{l} (\prod_{k=l}^{i-2} (-1)^{q_{k+1}}) \right) \pi + \tilde{\phi}_{n}^{\theta} \left(\sum_{i=1}^{n-1} (\prod_{l=0}^{i-1} (-1)^{q_{l}}) + 1 \right)$$
$$\therefore \tilde{\phi}_{n}^{\theta} = \frac{n(\overline{\phi} - \frac{2\pi r}{n}) - \left(\sum_{i=1}^{n-1} (q_{i-1} + \sum_{l=0}^{i-2} q_{l} (\prod_{k=l}^{i-2} (-1)^{q_{k+1}})) \right) \pi}{(\sum_{i=1}^{n-1} (\prod_{l=0}^{i-1} (-1)^{q_{l}}) + 1)}$$
(B.12)

where, we have defined $\overline{\phi} := \frac{1}{n} \sum_{i=1}^{n} \phi_i$. Thus, we finally have an expression for $\tilde{\phi}_n^{\theta}$ which appears on RHS of all the equations in Eq. (B.9). Together with (B.12) we get all the $\tilde{\phi}_i^{\theta}$ for $i = 1, \ldots, n$, in terms of single variable, namely average of links angles before gauge-fixing, $\overline{\phi}$. Here, different values of positive integers q_i give different solutions. Since the term in Eq. (B.9) multiplied with π can take only integer values, it can only be either 0 or 2π modulo 2π .

After straight-forward though tedious combinatorics we find that for odd n

$$N_{GC} = \sum_{i=0}^{\frac{n-1}{2}} (n-2i) \binom{n}{i},$$
 (B.13)

and for even n

$$N_{GC} = \sum_{i=0}^{\frac{n-2}{2}} (n-2i) \binom{n}{i}.$$
 (B.14)

Thus, N_{GC} in this case exponentially grows with the number of lattice sites.

B.1.1 Classification Of Gribov Copies of The SLLG

For the one-dimensional lattice with periodic boundary conditions, we should classify all the Gribov copies presented in the appendix B according to the number of eigenvalues of the Faddeev-Popov operator. For the anti-periodic boundary conditions case, this was relatively straight-forward with the help of Sylvester's law of inertia. However, the decomposition of the Faddeev-Popov operator in Eq. (3.28) is much difficult. Instead, we use another trick here. Consider an arbitrary vector $\vec{y} = (y_1, \ldots, y_n) \neq \vec{0}$. Now, we use the Faddeev-Popov operator including the constant zero mode that is given in Eq. (3.5) for $\mu = 1$ and

$$\vec{y}^T M_{FP} \vec{y} = \sum_{i=1}^n c_i (y_i - y_{i+1})^2$$
$$= c_n \sum_{i=1}^n (-1)^{q_i} (y_i - y_{i+1})^2, \qquad (B.15)$$

where $c_i = \cos \phi_i^{\theta}$ and $q_n = 0$. In the second equality we have used the fact that for the gauge-fixed configurations $\sin \phi_i^{\theta} = \sin \phi_n^{\theta}$ for all $i = 1, \ldots, n-1$ and so $\cos \phi_i^{\theta} = (-1)^{q_i} \cos \phi_n^{\theta}$ for all $i = 1, \ldots, n-1$ with $q_i \in \{0, 1\}$ and $q_n = 1$. The case where $y_1 = \cdots = y_n$ represents the constant zero mode and we disregard this in our discussion and the case $c_n = 0$ at which M_{FP} is a matrix with all entries zero. At all other solutions, M_{FP} is a non-singular matrix. Now, the number of negative (positive/zero) eigenvalues of M_{FP} is the same as the number of negative (positive/zero) signs of the above quadratic form, according to Sylvester's law of inertia (see Ref. [76] for more details on the quadratic form version of Sylvester's law of inertia).

Now, for the class of solutions with all $(-1)^{q_i} = 1$, all n-1 non-zero eigenvalues are positive definite numbers when c_n is positive, and negative definite numbers when c_n is negative. There are total n Gribov copies for this class in terms of ϕ_n^{θ} labelled by $r = 0, \ldots, n-1$ as shown above. These are the maxima and minima (both global and local) of the SLLG functional. With some combinatorics, we can deduce that in the class of solutions for which there are exactly i negative eigenvalues there are $\frac{n(\frac{n}{2}-i)}{n-i}$ Gribov copies for $i = 0, \ldots, \frac{(n-2)}{2}$ (corresponding to c_n being a positive number, formally) and $\frac{n(i-\frac{n-2}{2})}{i+1} \binom{n-1}{i}$ Gribov copies for $i = \frac{(n)}{2} \binom{n-1}{i}, \ldots, n-1$ (corresponding to c_n being a negative number, formally) for even n. Similarly, there are $\frac{n(\frac{n+1}{2}-i)}{n-i} \binom{n-1}{i}$ Gribov copies for $i = 0, \ldots, \frac{(n-1)}{2}$ and $\frac{n(i-\frac{n-1}{2})}{i+1}$ Gribov copies for $i = \frac{(n+1)}{2}, \ldots, n-1$ for odd n, with i negative eigenvalues for odd n. Thus, we have classified Gribov copies in terms of Gribov regions here.

B.2 MLLG

In this case, analogous to Eq. (B.4) we have, after eliminating the global gauge freedom,

$$\tan \frac{\phi_1^{\theta}}{2} = \tan \frac{\phi_n^{\theta}}{2}$$

$$\dots$$

$$\tan \frac{\phi_{n-1}^{\theta}}{2} = \tan \frac{\phi_{n-2}^{\theta}}{2},$$
(B.16)

i.e.,

$$\tilde{\phi}_{1}^{\theta} = \tilde{\phi}_{n}^{\theta} \\
\dots \\
\tilde{\phi}_{n-1}^{\theta} = \tilde{\phi}_{n-2}^{\theta},$$
(B.17)

where we follow exactly the same steps that lead to Eq. (B.8) in the SLLG above except in the last step where we use the fact that the tangent function is strictly monotonous for the $(-\pi, \pi)$ range. Thus there is no q_i variables unlike the SLLG. In Eq. (B.12), the denominator is now n and in the numerator the π term turns out to be 0 mod 2π for the MLLG. So, we are left with

$$\tilde{\phi}_n^\theta = \overline{\phi} - \frac{2\pi r}{n},\tag{B.18}$$

for $r = 0, \ldots, n-1$ which gives all $\tilde{\phi}_i^{\theta}$ as

$$\widetilde{\phi}_{i}^{\theta} = \overline{\phi} - \frac{2\pi}{n}r,$$
i.e.,
$$\phi_{i}^{\theta} = \overline{\phi} - \frac{2\pi}{n}r + 2\pi l_{i}.$$
(B.19)

Thus, for the MLLG in the one-dimensional lattice with periodic boundary conditions there are n Gribov copies

Let us now write Eq. (B.17) now as,

$$\theta_2 - \theta_1 = \overline{\phi} - \tilde{\phi}_1, \theta_3 - \theta_2 = \overline{\phi} - \tilde{\phi}_2 \dots, -\theta_{n-1} = \overline{\phi} - \tilde{\phi}_{n-1}, \tag{B.20}$$

Now, there are n-1 variables θ_i and n-1 linear equations. Writing these equations in matrix form and solving them finally gives, for $i = 1, \ldots, n-1$,

$$\theta_i = \sum_{j=i}^{n-1} (\phi_j - \overline{\phi}) + 2\pi \sum_{j=i}^{n-1} l_j + \frac{2\pi}{n} r(n-i),$$
(B.21)

for each $r = 0, \ldots, n - 1$. To write this in more convenient form, we define

$$\theta_i^{(0)} := \sum_{k=i}^{n-1} (\phi_k - \overline{\phi}), \qquad (B.22)$$

then

$$\theta_i = \theta_i^{(0)} + 2\pi m_i - \frac{2\pi}{n} ir , \qquad (B.23)$$

for each $r = 0, \ldots, n-1$ and integers

$$m_i = \sum_{j=i}^{n-1} l_j + r$$
, (B.24)

with r = 0, ..., n-1 labelling the *n* Gribov copies. Thus solutions (B.21) can be written as,

$$\theta_i = \theta_i^{(0)} + 2\pi m_i - \frac{2\pi}{n} ir,$$
(B.25)

again for each $r = 0, \ldots, n - 1$.

The integers m guarantee that for each r, there is precisely one solution with all θ_i in the range $[0, 2\pi)$. All n Gribov copies here are related to one another by gauge transformation of the form,

$$\theta_k = \frac{2\pi}{n} rk \mod 2\pi, \ k = 1, \dots, n-1.$$
(B.26)

This changes all link angles by $\frac{2\pi r}{n}$ modulo 2π , i.e.,

$$\phi_{i}^{\theta} = \phi_{i} + \frac{2\pi}{n} r \mod 2\pi, \text{ for } i = 1, \dots, n-2,$$

$$\phi_{n-1}^{\theta} = \phi_{n-1} - \frac{2\pi}{n} r(n-1) = \phi_{n-1} + \frac{2\pi}{n} r \mod 2\pi,$$

$$\phi_{n}^{\theta} = \phi_{n} + \theta_{1} = \phi_{n} + \frac{2\pi}{n} r.$$
(B.27)

The average link angle, $\overline{\phi}$, changes from one copy to the next by the same amount

$$\overline{\phi} = \frac{1}{n} \sum_{i=1}^{n} \phi_i \mapsto \overline{\phi} + \frac{2\pi}{n} r \tag{B.28}$$

This means that n-1 independent gauge angles θ_i just can rotate every link angle ϕ_i along the chain to equal one of the *n* copies of $\overline{\phi}$, i.e., $\overline{\phi}_r = \overline{\phi} - \frac{2\pi}{n}r \mod 2\pi$. This fixes the one dimensional gauge freedom up to the constant gauge rotations which remains unconstrained.

Appendix C

Miscellaneous: Algebraic Geometry

C.1 Transforming Problems To Algebraic Geometry

Here, we transform several theoretical physics problems to polynomial systems in order to be able to use computational and numerical Algebraic Geometry to solve them.

Ising Model

The classical Ising model Hamiltonian is,

$$H = -\sum_{i,\mu} J_{i,\hat{\mu}} \sigma_{i+\hat{\mu}} \sigma_i \tag{C.1}$$

where for $J_{i,\hat{\mu}} > 0$ the interaction is called ferromagnetic, for $J_{i,\hat{\mu}} < 0$ the interaction is called antiferromagnetic and for $J_{i,\hat{\mu}} = 0$ it is called non-interacting. Moreover, σ_i 's can be ± 1 .

To transform it to polynomial form, we use the Lagrange multipliers trick and set the Hamiltonion as

$$H = -\sum_{i,\mu} J_{i,\hat{\mu}} \sigma_{i+\hat{\mu}} \sigma_i + \sum_i \lambda_i (\sigma_i^2 - 1)$$
(C.2)

To obtain all extrema of this Hamiltonion, we equate first derivatives of H with respect to all σ_i 's to zero, i.e.,

$$\frac{\partial H}{\partial \sigma_i} = 0$$

$$\frac{\partial H}{\partial \lambda_i} = 0.$$
(C.3)

These will give equations at each site, i, as

$$2\lambda_{i}\sigma_{i} + \sum_{\mu} (J_{i,\hat{\mu}}\sigma_{i-\hat{\mu}} + J_{i+\hat{\mu},\hat{\mu}}\sigma_{i+\hat{\mu}}) = 0$$

$$\sigma_{i}^{2} - 1 = 0, \qquad (C.4)$$

which ensures the combined system is a system of polynomial equations. It must be noted that $J_{i,\mu}$ can be treated even as algebraic coefficients and the Comprehensive Groebner Basis can be calculated in theory or the polynomial homotopy continuation methods can be very useful here.

Adding the magnetic field term, the Hamiltonion is now,

$$H = -\sum_{i,\mu} J_{i+\hat{\mu},i}\sigma_{i+\hat{\mu}}\sigma_i + \sum_i h_i\sigma_i, \qquad (C.5)$$

and the corresponding equations are modified to:

$$2\lambda_{i}\sigma_{i} + \sum_{\mu} (J_{i,\hat{\mu}}\sigma_{i-\hat{\mu}} + J_{i+\hat{\mu},\hat{\mu}}\sigma_{i+\hat{\mu}} + h_{i}) = 0$$

$$\sigma_{i}^{2} - 1 = 0.$$
(C.6)

This is again a polynomial system with all variables and parameters taking values from the real field. It should be noted here that the periodic and anti-periodic boundary conditions can be used in all or some variables and coefficients here.

Compact QED and Instantons

The standard plaquette-action for compact QED [161] on lattice is¹

$$S = \beta \sum_{i,\mu < \nu} \cos(\phi_{i,\mu} + \phi_{i+\hat{\mu},\nu} - \phi_{i+\hat{\nu},\mu} - \phi_{i,\nu}), \qquad (C.7)$$

where μ and ν are directional indices and *i* is site index. β is the lattice coupling constant. To get all extrema of this action, we take first derivatives of it with respect to all $\phi_{i,\mu}$'s

$$f_{i,\mu} = \frac{\partial S}{\partial \phi_{i,\mu}} = 0. \tag{C.8}$$

Here, there are always dn^d equations and dn^d variables. Again by expanding all the trigonometric terms, writing $\sin \phi_{i,\mu} = s_{i,\mu}$ and $\cos \phi_{i,\mu} = c_{i,\mu}$ and adding constraint equations we get $2dn^d$ equations and $2dn^d$ variables and hence we obtain the corresponding ideal, *I*. β can be treated as a parameter of the system. Now, what we are interested in addition to several other things, is to get all

 $^{^1\}mathrm{I}$ am thankful to Peter Moran for explaining this problem to me.

instanton solutions, i.e., those solutions of these equations at which $S = \frac{8k\pi^2}{g}$. These are called instanton solutions. By using the Groebner Basis method or Polynomial Homotopy method which is introduced in Chapter 5, we can get all solutions of the above mentioned equations and then it will be trivial to check at which solutions the action satisfies this instanton condition.

We may also use another trick to get exactly those solutions for which, say $S = \frac{8\pi^2}{g}, \frac{16\pi^2}{g}$ etc. In the above mentioned $2dn^d$ equations, add one more equation $S - \frac{8\pi^2}{g} = 0$ with S as in Eq. (C.7) in terms of $s_{i,\mu}$ and $c_{i,\mu}$. Here, dim $R[\{c_{i,\mu}, s_{i,\mu}\}]/I$ will give the number of instanton solutions with instanton charge $\frac{8\pi^2}{a}$ etc.

Abelian Higgs Model On The Lattice

The classical action for the Abelian Higgs model [161] on lattice is

$$S = \beta_{1} \sum_{i,\mu < \nu} \cos(\phi_{i,\mu} + \phi_{i+\hat{\mu},\nu} - \phi_{i+\hat{\nu},\mu} - \phi_{i,\nu}) + \beta_{2} \sum_{i,\mu} (R_{i}^{2} + R_{i+\hat{\mu}}^{2} - 2R_{i}^{2}R_{i+\hat{\mu}}\cos(\phi_{i,\mu} + \theta_{i+\hat{\mu}} - \theta_{i})) + \beta_{3} \sum_{i} (R_{i}^{2} - f^{2})^{2},$$
(C.9)

where $R_i e^{i\theta_i}$'s are Higgs fields and $\phi_{i,\mu}$ are gauge fields. The β_j , for j = 1, 2, 3, are coupling constants. To obtain instanton solutions of this model, we again take first derivatives of this action with respect to all variables, i.e.,

$$\frac{\partial S}{\partial \theta_i} = \frac{\partial S}{\partial \phi_{i,\mu}} = \frac{\partial S}{\partial R_i} = 0.$$
(C.10)

Here, again after expanding them in trigonometric functions, it becomes a system of polynomial equations in variables $c_{i,\mu}^{\phi}, s_{i,\mu}^{\phi}, c_i, s_i$ and R_i , with the R_i 's already being algebraic variables. And

$$\beta_1 = \frac{1}{a^2 g^2}, \beta_2 = 1, \beta_3 = \lambda a^2,$$
 (C.11)

after appropriate renormalization.

SU(2)

SU(2) group is a set of complex matrices U such that det U = 1 and $U^{\dagger}U = I$. The Groebner basis technique can be used to solve these two constraints and to obtain a general form of an SU(2) matrix. Let U be any 2×2 complex matrix,

$$U = \begin{pmatrix} a+ib & c+id \\ e+if & g+ih \end{pmatrix},$$
 (C.12)

with $a, b, c, d \in R$. Now,

$$\det U = -ce - ide - icf + df + ag + ibg + iah - bh = 1$$

$$1 = -ce + df + ag - bh$$

$$0 = -de - cf + bg + ah = 0.$$
 (C.13)

The second constraint $UU^{\dagger} = I$ finally giving equations to be solved after comparing real and imaginary parts as,

$$-ce + df + ag - bh - 1 = 0$$

$$-de - cf + bg + ah = 0$$

$$a^{2} + b^{2} + c^{2} + d^{2} - 1 = 0$$

$$ae + bf + cg + dh = 0$$

$$ae + bf + cg + dh = 0$$

$$e^{2} + f^{2} + g^{2} + h^{2} - 1 = 0$$

$$be - af + dg - ch = 0$$

$$-be + af - dg + ch = 0.$$

A Groebner Basis for lexicographic ordering $a \ b \ c \ d \ e \ f \ g \ h$ is

$$G_{SU2} = \langle e^2 + f^2 + g^2 + h^2 - 1, d - f, c + e, b + h, a - g \rangle$$
(C.14)

whose solutions are,

$$d = f$$

$$c = -e$$

$$b = -h$$

$$a = g$$

$$e^{2} + f^{2} + g^{2} + h^{2} - 1 = 0.$$
(C.15)

So any SU(2) matrix U is now, for $e = \sqrt{-f^2 - g^2 - h^2 + 1}$,

$$U = \begin{pmatrix} g - ih & if - \sqrt{-f^2 - g^2 - h^2 + 1} \\ if + \sqrt{-f^2 - g^2 - h^2 + 1} & g + ih. \end{pmatrix}$$
(C.16)

Thus this group can be parameterized by three real numbers.

SU(2): Another Approach

A more useful way for solving constraints on SU(N) is by treating complex conjugate variables as independent variables and we show this trick at work in the SU(2) case. Let us take an arbitrary matrix U as

$$U = \left(\begin{array}{cc} a & b \\ c & d \end{array}\right) \tag{C.17}$$

where now a, b, c, d are complex variables, unlike the above mentioned case where they were real variables. Now, the constraint equation det $U = 1 = \det U^{\dagger}$ gives,

$$ad - bc - 1 = 0$$

 $a^*d^* - b^*c^* - 1 = 0$ (C.18)

and $UU^{\dagger} = I$ gives

$$aa^{*} + bb^{*} - 1 = 0$$

$$ac^{*} + bd^{*} = 0$$

$$ca^{*} + db^{*} = 0$$

$$cc^{*} + dd^{*} - 1 = 0,$$

(C.19)

and $U^{\dagger}U = I$ gives

$$aa^{*} + cc^{*} - 1 = 0$$

$$ba^{*} + dc^{*} = 0$$

$$ab^{*} + cd^{*} = 0$$

$$bb^{*} + dd^{*} - 1 = 0.$$
 (C.20)

Now, computing a Groebner basis for $a \succ b \succ c \succ d \succ a^* \succ b^* \succ c^* \succ d^*$ lexicographic ordering, we get

$$< -b^*c^* + a^*d^* - 1, d - a^*, c + b^*, b + c^*, a - d^* >$$
 (C.21)

and so we finally get

$$d = a^*$$

$$c = -b^* \tag{C.22}$$

giving,

$$U = \begin{pmatrix} a & b \\ -b^* & a^*, \end{pmatrix}$$
(C.23)

as is well known.

SO(2, *R***)**

SO(2, R) group is a set of matrices U with det U = 1 and $UU^T = I$ with real entries in it. Let

$$U = \left(\begin{array}{cc} a & b \\ c & d \end{array}\right). \tag{C.24}$$

Then the constraints give equations as

$$\begin{array}{rcl}
-bc + ad - 1 &= 0 \\
a^2 + b^2 - 1 &= 0 \\
ac + bd &= 0 \\
ac + bd &= 0 \\
c^2 + d^2 - 1 &= 0.
\end{array}$$
(C.25)

A Groebner basis with respect to lexicographic ordering $a \ b \ c \ d$ is

$$G_{SO(2,R)} = \langle c^2 + d^2 - 1, b + c, a - d \rangle.$$
 (C.26)

After solving these simple equations, we obtain a general form of an SO(2, R) matrix as

$$\left(\begin{array}{cc} d & -\sqrt{1-d^2} \\ \sqrt{1-d^2} & d \end{array}\right),\tag{C.27}$$

which is parameterized by a single parameter.

SO(3)

For higher gauge groups, we have more free parameters and so we may not have such a simple final matrix expression in the end. However we work out the case for SO(3) which consists of 3×3 matrices U with det U = 1 and $UU^T = I$. Let

$$U = \begin{pmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{pmatrix}.$$
 (C.28)

The two constraints give equations,

$$\begin{array}{rcl}
0 &=& -1 + a_1^2 + a_2^2 + a_3^2 \\
0 &=& a_1 * b_1 + a_2 * b_2 + a_3 b_3 \\
0 &=& -1 + b_1^2 + b_2^2 + b_3^2 \\
0 &=& a_1 c_1 + a_2 c_2 + a_3 c_3 \\
0 &=& -1 - a_3 b_2 c_1 + a_2 b_3 c_1 + a_3 b_1 c_2 - a_1 b_3 c_2 \\
&& -a_2 b_1 c_3 + a_1 b_2 c_3 \\
0 &=& b_1 c_1 + b_2 c_2 + b_3 c_3 \\
0 &=& -1 + c_1^2 + c_2^2 + c_3^2.
\end{array}$$
(C.29)

A Groebner basis with respect to $a_1 \succ a_2 \succ a_3 \succ b_1 \succ b_2 \succ b_3 \succ c_1 \succ c_2 \succ c_3$, with lexicographic ordering

$$G_{SO(3,R)} = \langle -1 + c_1^2 + c_2^2 + c_3^2, 1 - b_2^2 - b_3^2 - c_2^2 + b_3^2 c_2^2 - 2b_2 b_3 c_2 c_3 - c_3^2 + b_2^2 c_3^2, -b_1 - b_2 c_1 c_2 + b_1 c_2^2 - b_3 c_1 c_3 + b_1 c_3^2, b_1 c_1 + b_2 c_2 + b_3 c_3, -(b_1 b_2) - c_1 c_2 + b_3^2 c_1 c_2 - b_2 b_3 c_1 c_3 -b_1 b_3 c_2 c_3 + b_1 b_2 c_3^2, c_1 - b_2^2 c_1 - b_3^2 c_1 + b_1 b_2 c_2 + b_1 b_3 c_3, -1 + b_1^2 + b_2^2 + b_3^2, a_3 + b_2 c_1 - b_1 c_2, a_2 - b_3 c_1 + b_1 c_3, a_1 + b_3 c_2 - b_2 c_3 > .$$
 (C.30)

Eliminating b_2, b_3, c_1, c_2, c_3 and getting all equations in the rest of the variables we get,

$$a_{1} = b_{2}c_{3} - b_{3}c_{2}$$

$$a_{2} = b_{3}c_{1} - \frac{c_{1}c_{3}(b_{2}c_{2} + b_{3}c_{3})}{c_{2}^{2} + c_{3}^{2} - 1}$$

$$a_{3} = \frac{-b_{2}c_{1}c_{3}^{2} + b_{3}c_{1}c_{2}c_{3} + b_{2}c_{1}}{c_{2}^{2} + c_{3}^{2} - 1}$$

$$b_{1} = \frac{c_{1}(b_{2}c_{2} + b_{3}c_{3})}{c_{2}^{2} + c_{3}^{2} - 1}.$$
(C.31)

SU(3)

Let us take an arbitrary 3×3 matrix with complex entries a, b, c, d, e, f, g, h, k as

$$U = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & k \end{pmatrix}.$$
 (C.32)

Now, this matrix to be an SU(3) matrix should satisfy $\det U=I=\det U^*$ and $UU^\dagger=I=U^\dagger U,$ i.e.,

$$-ceg + bfg + cdh - afh - bdk + aek - 1 = 0$$

$$-c^*e^*g^* + b^*f^*g^* + c^*d^*h^* - a^*f^*$$

$$h^* - b^*d^*k^* + a^*e^*k^* = 0$$
(C.33)

and

$$aa^{*} + bb^{*} + cc^{*} - 1 = 0$$

$$ad^{*} + be^{*} + cf^{*} = 0$$

$$ag^{*} + bh^{*} + ck^{*} = 0$$

$$da^{*} + eb^{*} + fc^{*} = 0$$

$$dd^{*} + ee^{*} + ff^{*} - 1 = 0$$

$$dg^{*} + eh^{*} + kf^{*} = 0$$

$$ga^{*} + hb^{*} + kc^{*} = 0$$

$$gd^{*} + he^{*} + kf^{*} = 0$$

$$gg^{*} + hh^{*} + kk^{*} - 1 = 0$$

$$aa^{*} + dd^{*} + gg^{*} - 1 = 0$$

$$ba^{*} + ed^{*} + hg^{*} = 0$$

$$ca^{*} + fd^{*} + kg^{*} = 0$$

$$ab^{*} + de^{*} + gh^{*} = 0$$

$$bb^{*} + ee^{*} + hh^{*} - 1 = 0$$

$$cb^{*} + fe^{*} + kh^{*} = 0$$

$$ac^{*} + df^{*} + gk^{*} = 0$$

$$bc^{*} + ef^{*} + hk^{*} = 0$$

$$cc^{*} + ff^{*} + kk^{*} - 1 = 0.$$
 (C.34)

Now, a Groebner basis for $a \succ b \succ ... \succ h^* \succ k^*$ lexicographic ordering is

$$< -c^{*}e^{*}g^{*} + b^{*}f^{*}g^{*} + c^{*}d^{*}h^{*} - a^{*}f^{*}h^{*} - b^{*}d^{*}k^{*} + a^{*}e^{*}k^{*} - 1,$$

$$b^{*}d^{*} - a^{*}e^{*} + k, -c^{*}d^{*} + a^{*}f^{*} + h, c^{*}e^{*} - b^{*}f^{*} + g,$$

$$-b^{*}g^{*} + a^{*}h^{*} + f, c^{*}g^{*} - a^{*}k^{*} + e, -c^{*}h^{*} + b^{*}k^{*} + d,$$

$$c + e^{*}g^{*} - d^{*}h^{*},$$

$$b - f^{*}g^{*} + d^{*}k^{*}, a + f^{*}h^{*} - e^{*}k^{*} > .$$

(C.35)

One can now solve this new set of equations in terms of the independent variables. However, since there are 8 free parameters, it is still cumbersome to write down all equations in terms of these free parameters unlike the SU(2) case.

SU(4)

Consider an arbitrary 4×4 matrix with complex entries a, \ldots, r . Imposing constraints det $U = \det U^* = 1$ and $UU^{\dagger} = U^{\dagger}U = I$,

$$\begin{split} dglo - chlo - dfmo + bhmo + cfno - bgno - dgkp \\ + chkp + demp - ahmp - cenp + agnp + dfkq - bhkq - delq + ahlq \\ + benq - afnq - cfkr + bgkr + celr - aglr - bemr + afmr - 1 &= 0 \\ aa^* + bb^* + cc^* + d^*d - 1 &= 0, a^*e + b^*f + c^*g + d^*h &= 0 \\ a^*k + b^*l + c^*m + d^*n, a^*o + b^*p + c^*q + d^*r &= 0 \\ ae^* + bf^* + cg^* + h^*d &= 0 \\ e^*e + f^*f + g^*g + h^*h - 1 &= 0, e^*k + f^*l + g^*m + h^*n &= 0 \\ e^*o + f^*p + g^*q + h^*r = 0, ak^* + bl^* + cm^* + n^*d &= 0 \\ k^*e + l^*f + m^*g + n^*h = 0, k^*k + l^*l + m^*m + n^*n - 1 &= 0 \\ k^*e + l^*f + m^*q + n^*r &= 0, aa^* + e^*e + k^*k + o^*o - 1 &= 0 \\ ba^* + e^*f + k^*l + o^*p = 0, ca^* + e^*g + k^*m + o^*q &= 0 \\ a^*d + e^*h + k^*n + o^*r &= 0, ab^* + f^*e + l^*k + p^*o &= 0 \\ bb^* + f^*f + l^*l + p^*p - 1 &= 0, cb^* + f^*g + l^*m + p^*q &= 0 \\ b^*d + f^*h + l^*n + p^*r &= 0, ac^* + g^*e + m^*k + q^*o &= 0 \\ bc^* + g^*f + m^*l + q^*p = 0, cc^* + g^*g + m^*m + q^*q - 1 &= 0 \\ c^*d + g^*h + m^*n + q^*r &= 0, ao^* + bp^* + cq^* + r^*d &= 0 \\ o^*e + p^*f + q^*g + r^*h &= 0, o^*k + p^*l + q^*m + r^*n &= 0 \\ ad^* + h^*e + n^*k + r^*o &= 0, bd^* + h^*f + n^*l + r^*p &= 0 \\ cd^* + h^*g + n^*m + r^*q &= 0, d^*d + h^*h + n^*n + r^*r - 1 &= 0 \\ d^*g^{l^*o^*} - c^*h^{l^*o^*} - d^*f^*m^*o^* + b^*h^*m^*o^* \\ + c^*f^*n^*o^* - b^*g^*n^*o^* - d^*g^*k^*p^* + c^*h^*k^*p^* \\ + d^*e^*m^*p^* - a^*h^*m^*p^* - c^*e^*n^*p^* + a^*g^*n^*p^* \\ + d^*e^*n^*q^* - a^*f^*n^*q^* - c^*f^*k^*r^* + b^*g^*k^*r^* \\ + c^*e^{l}l^*r^* - a^*g^{l^*}r^* - b^*e^*m^*r^* + a^*f^*m^*r^* - 1 &= 0 \\ (C.36) \end{split}$$

we get and with lexicographic ordering $a \succ b \succ ...q^* \succ r^*$, a Groebner basis is

Again we can solve these equations for few of the independent variables.

C.2 Special Appearance: Numerical Algebraic Geometry

In Chapters 4 and 5, we have been working on systems which have isolated solutions (zero-dimensional varieties). For positive dimensional varieties, since there are infinitely many solutions, one needs a proper representation of the solutions. The important first question to be asked is how we need to represent the solutions. For a 0-dimensional variety, the solutions are just a finite set of points, so they can be represented by complex numbers. For positive dimensional varieties the situation is more involved. The solutions in this case form curves or hypersurfaces. For nonlinear algebraic equations such parameterizations are rare [162]. A way to represent the solutions is to use the defining equations for the solutions. However, this is also computationally expensive. The reader can find a nice discussion about it in Ref. [92].

Numerical Algebraic Geometry (NAG) cleverly uses another approach² in which the solutions are represented as Witness Sets. We start with the fact that the number of points at which a curve or a hypersurface defined by an irreducible component, say of dimension d[i] in *m*-dimensional affine complex space, of a system of polynomial equations intersects with a random hyperplane of dimension c[i] = m - d[i] is equal to the degree of the hypersurface. For example, a cubic curve in 3 dimensions intersects with a two-dimensional random hyperplane at exactly three points. These intersection points are called Witness points. Here, a *random* hyperplane means a hyperplane defined by c[i] linear equations with random coefficients. After computing the Witness points, one needs to slide this random hyperplane around to obtain as many points on the hypersurface as needed. This is now a *parameterization* of the hypersurface, called the Witness sets representation.

Often the varieties have several irreducible components of different dimensions, i.e., the solution space is made of more than one hypersurface with different dimensions. Witness sets representation can be easily carried forward in such cases as well, by first obtaining intersection points of the whole variety with a dimensional line. This will give the Witness points on an n-1 dimensional component of the variety. Then we obtain intersection points of the variety with a two-dimensional plane and get Witness points on a n-2 dimensional component of the variety and so on.

One of the most interesting starting examples [94] for particle physics is that of the constraint equations for an SO(3) matrix, say A, i.e., det A = 1 and $AA^T = I$ as listed in Eq. (C.29). Here there are 7 equations in 9 variables. We used a NAG package called Bertini for this purpose. Of course, all other packages mentioned above also deal with the positive dimensional components, however Bertini is distinguished in the sense that it gives full classification of all positive dimensional components according to their degree as shown in the Table (C.1).

Dim.	Degree	Components
3	8	1

Table C.1: Summary of the solutions for SO(3).

Thus, solution-space of these constraint equations is a curve in three dimensions of degree 8. This is expected for SO(3) because there are three independent variables. Bertini also gives the random complex hyperplane of dimension 3 and a point intersecting with the 3 dimensional degree 8 solution curve. Then, Bertini can give as many points on this three-dimensional curve as one wants, by *sliding*

 $^{^{2}}$ I am very grateful to Daniel Bates, Jonathan Hauenstein and the whole Bertini group for very useful comments on the NAG and help on various related issues.

the complex hyperplane through the curve. In other words, one can get as many SO(3) matrices as needed once the constraint equations are solved. We also solve the SU(2) case below.

C.2.1 SLLG and NAG

For the one-dimensional, n = 3, trivial orbit, periodic boundary conditions, SLLG case *without* eliminating the global zero mode, we end up having a onedimensional variety. NAG can deal with such systems (see Table (C.2)).

Dim.	Degree	Components
1	2	6

Table C.2: Summary of the solutions for the SLLG with periodic boundary conditions for the one-dimensional n = 3 lattice, from NAG. Note that this summary remains valid for both the trivial orbit and random orbit cases.

For the 3×3 lattice with periodic boundary conditions and the trivial orbit, the stable mixed volume is of course the same as the anti-periodic boundary conditions trivial orbit case since they have the same monomials, i.e., 148480. The number of actual solutions are 8428. However, to get the actual information about the solution space, we need to know the dimensions and degree of individual components and a complete classification is underway.

C.2.2 Discussion

Having briefly explained NAG, we should mention that these results are not very helpful for our purposes. Since our original system is made of trigonometric functions for both the SLLG and the MLLG, we are only interested in the real solutions of the corresponding polynomial system. For systems having only isolated solutions, the PHC method can give all complex and real solutions. But for the positive dimensional varieties, the Witness sets are obtained by intersecting complex planes of respective codimension and the probability of getting real intersection points is practically zero. In other words, using NAG one can obtain complex solution curves of positive dimension but not real curves in general. Moreover, finding real components from the complex curves is an extremely difficult task. This is a very important problem and a lot of research is underway. Some useful results have already arisen via [145] but the practical implementation is still in progress.

Numerical Algebraic Geometry For SU(2)

We here solve the positive dimensional ideal made of Eqs. (C.18) and (C.19) using NAG with Bertini. The variables involved are $a, b, c, d, a^*, b^*, c^*, d^*$ and all

of them are treated as independent variables. Solving them using Bertini gives the following summary:

- 1. The solution curve is a 3-dimensional curve in 8 dimensional complex space. Moreover, the degree of this curve is 2 as expected for a three dimensional sphere in complex space.
- 2. Bertini gives a complex hyperplane of codimension 5 which intersects the solution curve at 2 points generically.
- 3. After obtaining this information, Bertini can also be used to obtain as many sample points as required out of this solution curve, e.g.,
 - (0.5546545584451108253732531, -0.67600440845477946280)a= $(0.9123189562160420763443641, 0.583475112027970414594 \times 10^{-2})$ b =(0.1221371509751447876319489, 0.426812269970270574382)c= $= (0.115166043074885518857118 \times 10^{1}, 0.702872152644067855306)$ d $= (0.115166043074885518857118 \times 10^{1}, 0.702872152644067855)$ a^* = (-0.1221371509751447876319489, 0.42681226997027057) b^* $= (-0.912318956216042076344364, 0.5834751120279704 \times 10^{-2})$ c^* = (0.5546545584451108253732531, -0.6760044084547794628) d^* (C.38)

Here, the known results such as $a = d^*$ and $b = -c^*$ are apparent.

Appendix D

Mixed Boundary Conditions and Magnetic Monopole Charge

D.1 Mixed boundary conditions

D.1.1 z Direction C-periodic and x, y Directions Periodic

Suppose that we employ boundary conditions with a single C-periodic direction, chosen to be the z direction. These boundary conditions can be written as

$$\begin{split} \Phi(\vec{x} + n\hat{1}) &= \Omega_{1}^{\dagger} \Phi(\vec{x}) \Omega_{1}, \qquad U_{\mu}(\vec{x} + n\hat{1}) = \Omega_{1}^{\dagger} U_{\mu}(\vec{x}) \Omega_{1} \\ \Phi(\vec{x} + n\hat{2}) &= \Omega_{2}^{\dagger} \Phi(\vec{x}) \Omega_{2}, \qquad U_{\mu}(\vec{x} + n\hat{2}) = \Omega_{2}^{\dagger} U_{\mu}(\vec{x}) \Omega_{2} \\ \Phi(\vec{x} + n\hat{3}) &= \Omega_{3}^{\dagger} \Phi^{*}(\vec{x}) \Omega_{3}, \qquad U_{\mu}(\vec{x} + n\hat{3}) = \Omega_{3}^{\dagger} U_{\mu}^{*}(\vec{x}) \Omega_{3}. \end{split}$$
(D.1)

Consistency of the boundary conditions requires

$$\Omega_1 \Omega_2 = z_{12} \Omega_2 \Omega_1,$$

$$\Omega_1^* \Omega_3 = z_{13} \Omega_3 \Omega_1,$$

$$\Omega_2^* \Omega_3 = z_{32} \Omega_3 \Omega_2,$$
(D.2)

where the $z_{ij} = e^{i\theta_{ij}} \in Z_N$ are center elements as always. Note that charge conjugation only ever happens on one side of the equation.

It is straightforward to derive the corresponding boundary conditions for the Abelian projected fields (6.27),



Figure D.1: Integration curves for one and two C-periodic directions.

except for the special cases

$$\begin{aligned} &\alpha_1^a(\vec{x} + (n-1)\hat{1} + n\hat{2}) &= \theta_{12} + \alpha_1^a(\vec{x} + (n-1)\hat{1}) \\ &\alpha_1^a(\vec{x} + (n-1)\hat{1} + n\hat{3}) &= -\theta_{13} - \alpha_1^a(\vec{x} + (n-1)\hat{1}) \\ &\alpha_2^a(\vec{x} + (n-1)\hat{2} + n\hat{3}) &= -\theta_{23} - \alpha_2^a(\vec{x} + (n-1)\hat{2}). \end{aligned}$$

As expected, it follows that, that the Abelian field strength tensors $\alpha_{ij}^a(\vec{x})$ in Eq. (6.29) are periodic in the x and y directions, but anti-periodic in the z direction. Therefore, we only have net flux through the faces of the lattice perpendicular to the z direction.

The contribution to the total magnetic charge from the x and y directions cancels, and the both ends of the lattice in the z direction give equal contributions. The total charge charge is therefore given by

$$Q = 2\Phi_+, \tag{D.4}$$

where Φ_+ is the flux through the curve shown in the left panel of Fig. D.1. To calculate it, we need to integrate $\alpha_i^a(\vec{x})$ around the curve. Applying the boundary conditions, we find that all of the links $\alpha_i^a(\vec{x})$ cancel with those on the opposite side of the boundary, except for the far corner, which gives

$$\Phi_{+} = \frac{\alpha_{1}^{a}(\vec{x} + (n-1)\hat{1}) - \alpha_{1}^{a}(\vec{x} + (n-1)\hat{1} + n\hat{2})}{g} = \frac{\theta_{12}}{g}.$$
 (D.5)

The total charge is therefore

$$Q = \frac{2\theta_{12}}{g}.\tag{D.6}$$

It would be interesting if the twist angle in the mixed plane θ_{12} were permitted to be a phase other than 0 or π , though unfortunately this is not the case. The proof of this involves permutations of the twist matrices as before. Comparison of

$$\Omega_{1}^{*}(\vec{x})\Omega_{2}^{*}(\vec{x}+n\hat{1})\Omega_{3}(\vec{x}+n\hat{1}+n\hat{2})$$

$$= z_{23}\Omega_{1}^{*}(\vec{x})\Omega_{3}(\vec{x}+n\hat{1})\Omega_{2}(\vec{x}+n\hat{1}+n\hat{3})$$

$$= z_{23}z_{13}\Omega_{3}(\vec{x})\Omega_{1}(\vec{x}+n\hat{3})\Omega_{2}(\vec{x}+n\hat{1}+n\hat{3})$$

$$= z_{23}z_{13}z_{12}\Omega_{3}(\vec{x})\Omega_{2}(\vec{x}+n\hat{3})\Omega_{1}(\vec{x}+n\hat{2}+n\hat{3})$$
(D.7)

with

$$\Omega_{1}^{*}(\vec{x})\Omega_{2}^{*}(\vec{x}+n\hat{1})\Omega_{3}(\vec{x}+n\hat{1}+n\hat{2})$$

$$= z_{21}\Omega_{2}^{*}(\vec{x})\Omega_{1}^{*}(\vec{x}+n\hat{2})\Omega_{3}(\vec{x}+n\hat{1}+n\hat{2})$$

$$= z_{21}z_{13}\Omega_{2}^{*}(\vec{x})\Omega_{3}(\vec{x}+n\hat{2})\Omega_{1}(\vec{x}+n\hat{3}+n\hat{2})$$

$$= z_{21}z_{13}z_{23}\Omega_{3}(\vec{x})\Omega_{2}(\vec{x}+n\hat{3})\Omega_{1}(\vec{x}+n\hat{2}+n\hat{3})$$
(D.8)

yields

$$z_{12}^2 = 1.$$
 (D.9)

Therefore

$$\theta_{12} = \begin{cases} 0 & \text{for N odd} \\ 0 \text{ or } \pi & \text{for N even.} \end{cases}$$
(D.10)

It follows that the allowed charges are exactly those we found for fully C-periodic boundary conditions.

D.1.2 y, z Directions C-periodic and x Direction Periodic

We can also consider boundary conditions with two C-periodic directions, chosen to be the y and z directions. Then the consistency conditions are modified to

$$\Omega_{1}^{*}\Omega_{2} = z_{12}\Omega_{2}\Omega_{1},
\Omega_{1}^{*}\Omega_{3} = z_{13}\Omega_{3}\Omega_{1},
\Omega_{2}^{*}\Omega_{3} = z_{23}\Omega_{3}^{*}\Omega_{2},$$
(D.11)

with $z_{ij} = e^{i\theta_{ij}} \in Z_N$. The Abelian projected fields inherit boundary conditions with anti-periodicity in both C-periodic directions,

$$\begin{aligned}
\alpha_{i}(\vec{x} + n\hat{1}) &= \alpha_{i}(\vec{x}), \\
\alpha_{i}(\vec{x} + n\hat{2}) &= -\alpha_{i}(\vec{x}), \\
\alpha_{i}(\vec{x} + n\hat{3}) &= -\alpha_{i}(\vec{x}),
\end{aligned}$$
(D.12)

except for the special cases

$$\begin{aligned} \alpha_1(\vec{x} + (n-1)\hat{1} + N\hat{2}) &= -\theta_{12} - \alpha_1(\vec{x} + (n-1)\hat{1}) \\ \alpha_1(\vec{x} + (n-1)\hat{1} + N\hat{3}) &= -\theta_{13} - \alpha_1(\vec{x} + (n-1)\hat{1}) \\ \alpha_2(\vec{x} + (n-1)\hat{2} + N\hat{3}) &= \theta_{23} - \alpha_2(\vec{x} + (n-1)\hat{2}). \end{aligned}$$
(D.13)

To find the total flux we now need to integrate $\alpha_i^a(\vec{x})$ around the boundary of two of the faces orthogonal to the y and z directions and double the result. Contributions from the sides related by periodicity in the x direction automatically cancel. We are left with

$$Q = \frac{2}{g} \left(\sum_{n=0}^{n-1} \alpha_1^a (n\hat{1} + n\hat{3}) - \alpha_1^a (n\hat{1} + n\hat{2}) \right)$$

= $\frac{2}{g} (\alpha_1 ((n-1)\hat{1} + n\hat{3}) - \alpha_1 ((n-1)\hat{1} + n\hat{2}))$
= $\frac{2}{g} (-\theta_{12} + \theta_{13}),$

where we have applied the boundary conditions (D.12) in the second line and (D.13) in the third line.

Again, we find that the twist angles in the mixed planes are restricted. Comparison of

$$\Omega_{1}^{*}(\vec{x})\Omega_{2}(\vec{x}+n\hat{1})\Omega_{3}^{*}(\vec{x}+n\hat{1}+n\hat{2})
= z_{32}\Omega_{1}^{*}(\vec{x})\Omega_{3}(\vec{x}+n\hat{1})\Omega_{2}^{*}(\vec{x}+n\hat{1}+n\hat{3})
= z_{32}z_{13}\Omega_{3}(\vec{x})\Omega_{1}(\vec{x}+n\hat{3})\Omega_{2}^{*}(\vec{x}+n\hat{1}+n\hat{3})
= z_{32}z_{13}z_{21}\Omega_{3}(\vec{x})\Omega_{2}^{*}(\vec{x}+n\hat{3})\Omega_{1}^{*}(\vec{x}+n\hat{2}+n\hat{3})$$
(D.14)

with

$$\Omega_{1}^{*}(\vec{x})\Omega_{2}(\vec{x}+n\hat{1})\Omega_{3}^{*}(\vec{x}+n\hat{1}+n\hat{2})$$

$$= z_{12}\Omega_{2}(\vec{x})\Omega_{1}(\vec{x}+n\hat{2})\Omega_{3}^{*}(\vec{x}+n\hat{1}+n\hat{2})$$

$$= z_{12}z_{31}\Omega_{2}(\vec{x})\Omega_{3}^{*}(\vec{x}+n\hat{2})\Omega_{1}^{*}(\vec{x}+n\hat{3}+n\hat{2})$$

$$= z_{12}z_{31}z_{32}\Omega_{3}(\vec{x})\Omega_{2}^{*}(\vec{x}+n\hat{3})\Omega_{1}^{*}(\vec{x}+n\hat{2}+n\hat{3})$$
(D.15)

yields

$$z_{21}^2 z_{13}^2 = 1. (D.16)$$

 So

$$-\theta_{12} + \theta_{13} = \begin{cases} 0 & \text{for N odd} \\ 0 \text{ or } \pi & \text{for N even.} \end{cases}$$
(D.17)

Once more, we are left with the same possibilities for the Abelian magnetic charges. We conclude that the allowed charges are identical whether we have one, two, or all three directions charge conjugated.

Appendix E

Another Approach To Modify Lattice Landau Gauge

Instead of stereographic projection, we can also modify lattice Landau gauge by modifying *orbifolding* (S^1/Z_2) at each link, i.e., by identifying all the points of the lower half of S^1 circle to those of the upper half of it. The corresponding gauge fixing functional, following the discussion in section 2.3.2, is

$$F_{\phi}^{\text{abs}}(\theta) = \sum_{i,\mu} |\cos(\phi_{i,\mu} + \theta_{i+\hat{\mu}} - \theta_i)|, \qquad (E.1)$$

where $\phi_{i,\mu} \in (-\pi,\pi]$ and $\theta_i \in (-\pi,\pi]$.

The corresponding gauge fixing conditions are

$$f_{i}^{abs}(\theta) = \sum_{i,\mu} |\cos(\phi_{i,\mu} + \theta_{i+\hat{\mu}} - \theta_{i})| \tan(\phi_{i,\mu} + \theta_{i+\hat{\mu}} - \theta_{i}) - |\cos(\phi_{i-\hat{\mu},\mu} + \theta_{i} - \theta_{i-\hat{\mu}})| \tan(\phi_{i-\hat{\mu},\mu} + \theta_{i} - \theta_{i-\hat{\mu}}) = 0,$$
(E.2)

where *i* runs over all lattice sites and $\mu = 1, ..., d$ with *d* being the lattice dimension.

The Faddeev-Popov operator is then

$$(M_{FP}^{abs})_{i,j} = -\sum_{\mu} (|\cos(\phi_{i,\mu}^{\theta})| (\delta_{i+\hat{\mu},j} - \delta_{i,j}) + |\cos(\phi_{i-\hat{\mu},\mu}^{\theta})| (\delta_{i,j} - \delta_{i-\hat{\mu},j})) \quad (E.3)$$

and with anti-periodic boundary conditions it can be decomposed as

$$M_{FP}^{\rm abs} = \sum_{\mu=1}^{d} (M_{\mu} D_{\mu}^{\rm abs} M_{\mu}^{T}), \qquad (E.4)$$

where the non-singular matrices M_{μ} 's are the same as the standard case, and the diagonal matrices D_{μ}^{abs} 's contain the diagonal elements $|\cos(\phi_{i,\mu} + \theta_{i+\hat{\mu}} - \theta_{\mu})|$'s which are always positive definite numbers for $\phi_{i,\mu}^{\theta} = \phi_{i,\mu} + \theta_{i+\hat{\mu}} - \theta_{\mu} \in (-\pi, \pi]$.

In one dimension, after changing the variables to s_i with anti-periodic boundary conditions, same as in Chapter 3, these equations can be written in matrix form as

$$M\vec{S}^{\rm abs} = \vec{0},\tag{E.5}$$

where

$$\vec{S}^{\text{abs}} = (|\cos(s_1)|\tan(s_1), |\cos(s_2)|\tan(s_2), ..., |\cos(s_n)|\tan(s_n))^T.$$
(E.6)

Due to the non-singularity of M, only trivial solution exist, i.e., $|\cos(s_i)| \tan(s_i) = 0$ and so all $s_i \in (-\pi, \pi]$ are 0 or π . But since π is identified with 0, there is only one gauge-fixed configuration, i.e., $\vec{s} = \vec{0}$ and all remaining combinations of 0's and π 's are just the *trivial copies* of this configuration, leaving no Gribov copy.

Thus,

$$M_{FP}^{\rm abs} = M^T D^{\rm abs} M, \tag{E.7}$$

where

$$D^{\rm abs} = D(|c_1|, |c_2|, |c_3|, ..., |c_n|), \tag{E.8}$$

with $c_i = \cos s_i$ for i = 1, ..., n. The determinant M_{FP}^{abs} is $4 \prod_{i=1}^{n} |c_i|$ and so for the gauge-fixed configuration, it is 4. Thus, M_{FP}^{abs} is positive definite and there is no Neuberger zero nor any Gribov copies.

An important remark: Although this modification works well too, the Euler characteristic of an orbifold is a more involved issue [163, 164]. It still needs to be verified explicitly if the straightforward application of Poincaré-Hopf theorem calculates the actual orbifold Euler characteristic or some another topological invariant. So, we only concentrate on the modification via stereographic projection and we refer as the modified lattice Landau gauge (MLLG) to the same.

Appendix F

Published Articles of Author

- Lattice Landau gauge via Stereographic Projection, L von Smekal, A Jorkowski, D Mehta, and A Sternbeck, Talk presented at the 8th Conference Quark Confinement and the Hadron Spectrum September 1-6, 2008, Mainz, Germany. e-Print: arxiv: 0812.2992 [hep-lat] [165].
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