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Quantum Field Theory on a Highly Symmetric Lattice

Tesi di Laurea Magistrale

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Abstract

The regularization on a Euclidean lattice, first proposed by Kenneth G. Wilson in 1974, remains the only approach to study strongly coupled, non-supersymmetric non-Abelian gauge theories (including, in particular, quantum chromodynamics: the fundamental theory of the strong nuclear interaction in the Standard Model of elementary-particle physics) from first principles.
While normally the theory is discretized on a four-dimensional hypercubic grid, this is not the only possible choice, and the fact that the explicit breaking of Lorentz-Poincaré symmetries due to the discretization has an impact on the approach to the continuum limit is a motivation to consider the regularization also on other, more symmetric, lattices.
The goal of this thesis project consists in studying Yang-Mills theories based on local SU(N) invariance on the lattice of the roots of the exceptional simple Lie group F_4, which is a four-dimensional body-centered cubic lattice, and the most symmetric regular lattice that exists in four dimensions.

Contents

Yang-Mills Theories on the Lattice

1.1 The Yang-Mills Continuum Action

The aim of this chapter is to discretize the Yang-Mills action on a hypercubic lattice in 4 dimensions. In order to do so, the action is obtained firstly in the continuum, beginning from the simplest case, Quantum Electrodynamics.
This first section is based on material that can be found in standard textbooks on quantum field theory [1–5], personal notes and computations.

1.1.1 Scalar Fields

In quantum field theory, a real scalar massive field is described, in a 4-dimensional space-time with metric $\eta_{\mu\nu} = \text{diag}(-1, 1, 1, 1)$, by the following Lorentz-covariant action (in natural units, where $c = \hbar = 1$):

$$S[\phi] = \int \mathrm{d}^4x \left(-\frac{1}{2}\partial^\mu\phi\partial_\mu\phi - \frac{1}{2}m^2\phi^2 + V(\phi) \right) \tag{1.1.1}$$

where $V(\phi)$ is any potential, such as $\frac{g}{6}\phi^3$ or $\frac{g}{4!}\phi^4$. Real scalar fields do not describe any real-world elementary particle, though they are useful to learn basic principles of quantum field theory, as they are the simplest fields that can be written.

1.1.2 Dirac Spinor Fields

Let us now take into consideration a (free) quantum field theory describing a fermion, such as a quark or a lepton. Its action can be written as:

$$S_\psi[\psi(x), \overline{\psi}(x)] = \int \mathrm{d}^4x \left(\mathrm{i}\overline{\psi}\partial\!\!\!/\psi - m\overline{\psi}\psi\right) \tag{1.1.2}$$

from which, upon the application of the variational principle, the Dirac equation follows:

$$\left(\mathrm{i}\partial\!\!\!/ - m\right)\psi(x) = 0 \tag{1.1.3}$$

It can now be easily checked by direct computation that this action is invariant under a rigid (global) phase transformation, also called a global $U(1)$ transformation:

$$\begin{aligned} \psi(x) &\to \psi'(x) = e^{-\mathrm{i}\alpha}\psi(x) \\ \overline{\psi}(x) &\to \overline{\psi}'(x) = \overline{\psi}(x)e^{\mathrm{i}\alpha} \end{aligned} \tag{1.1.4}$$

where α is a constant that does not depend on the spacetime coordinate x, because if α was a function of x, the kinetic term of the action (1.1.2) would not be invariant under such transformation.

1.1.3 Quantum Electrodynamics

As the free field theory itself is non interacting, it does not provide any real-world prediction, so it is useful to write an interacting action where the spinor field is coupled, for instance, to a vector field A_μ, i.e., the photon. One way to implement this interaction is to ask for local, instead of global, invariance of the action (1.1.2) under the phase transformation (1.1.4), where now $\alpha = \alpha(x)$. In order to do so, the covariant derivative has to be defined as follows:

$$D_\mu \equiv \partial_\mu + \mathrm{i}gA_\mu \tag{1.1.5}$$

where g is the couplig constant.[1]
The vector field's kinetic term is written in terms of its field-strength, namely:

$$\begin{aligned} F_{\mu\nu} \equiv& -\frac{\mathrm{i}}{g}\left[D_\mu, D_\nu\right] = \\ =& -\frac{\mathrm{i}}{g}\left(D_\mu\left(\partial_\nu + \mathrm{i}gA_\nu\right) - D_\nu\left(\partial_\mu + \mathrm{i}gA_\mu\right)\right) = \\ =& -\frac{\mathrm{i}}{g}\left(\cancel{\partial_\mu\partial_\nu} + \mathrm{i}g\partial_\mu A_\nu - g^2A_\mu A_\nu - \cancel{\partial_\nu\partial_\mu} - \mathrm{i}g\partial_\nu A_\mu + g^2A_\nu A_\mu\right) = \\ =& \partial_\mu A_\nu - \partial_\nu A_\mu + \mathrm{i}g[A_\mu, A_\nu] = \\ =& \partial_\mu A_\nu - \partial_\nu A_\mu \end{aligned} \tag{1.1.6}$$

where $[A_\mu, A_\nu] = A_\mu A_\nu - A_\nu A_\mu = 0$ in the abelian theory.
Two different fields A_μ and A'_μ describe the same physics if one can be obtained from

[1] Usually, in QED, g is called e, the electron charge, though g will be used in analogy to nonabelian gauge theories.

another through a gauge transformation:

$$\begin{aligned} A'_\mu(x) =& A_\mu(x) + \frac{1}{g}\partial_\mu\alpha(x) \\ F'_{\mu\nu} =& F_{\mu\nu} + \frac{1}{g}\left(\partial_\mu\partial_\nu - \partial_\nu\partial_\mu\right)\alpha(x) = F_{\mu\nu} \end{aligned} \tag{1.1.7}$$

Thus, the free action for the vector field is:

$$S_{EM} = -\frac{1}{4}\int \mathrm{d}^4x F_{\mu\nu}F^{\mu\nu} \tag{1.1.8}$$

That is also gauge invariant, i.e. invariant under (1.1.7), as $F_{\mu\nu}$ is gauge invariant.
The term that broke the local phase invariance of the action (1.1.2) can now be "absorbed" by A_μ through a gauge transformation (1.1.7), thus making the full action gauge invariant:

$$\begin{aligned} S_{QED} =& \int \mathrm{d}^4x \left(\mathrm{i}\overline{\psi}\not{D}\psi - m\overline{\psi}\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}\right) = \\ =& \int \mathrm{d}^4x \left(\mathrm{i}\overline{\psi}\not{\partial}\psi - m\overline{\psi}\psi - g\overline{\psi}\not{A}\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}\right) \\ S_{QED} \to S'_{QED} =& \int \mathrm{d}^4x \left(\mathrm{i}\overline{\psi}\not{\partial}\psi + \cancel{\overline{\psi}\not{\partial}\alpha\psi} - m\overline{\psi}\psi - g\overline{\psi}\not{A}\psi - \cancel{\overline{\psi}\not{\partial}\alpha\psi} - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}\right) = \\ =& \int \mathrm{d}^4x \left(\mathrm{i}\overline{\psi}\not{\partial}\psi - m\overline{\psi}\psi - g\overline{\psi}\not{A}\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}\right) = S_{QED} \end{aligned} \tag{1.1.9}$$

1.1.4 Non-Abelian Gauge Theories

Let us now consider a theory with N fermions, all with the same mass m, described by the spinorial fields $\psi_i(x)$ with $i = 1, \ldots, N$. These N fermions represent the N possible charges of the same particle[2] and are not to be confused with, for instance, the different possible flavors of the quarks, that describe different particles with different masses.
Its free action is:

$$S_\psi[\psi_i(x), \overline{\psi}_i(x)] = \sum_{i=1}^{N}\int \mathrm{d}^4x \left(\mathrm{i}\overline{\psi}_i\not{\partial}\psi_i - m\overline{\psi}_i\psi_i\right) \tag{1.1.10}$$

From now on, the sum over i (and all other repeated latin indexes) will be omitted, unless differently specified. This action is invariant under the global transformation:

$$\begin{aligned} \psi_i(x) \to \psi'_i(x) &= U_{ij}\psi_j(x) \\ \overline{\psi}_i(x) \to \overline{\psi}'_i(x) &= \overline{\psi}_j(x)U^\dagger_{ji} \end{aligned} \tag{1.1.11}$$

if U is any (constant) $N \times N$ matrix such that $UU^\dagger = U^\dagger U = \mathbb{1} \Leftrightarrow U^\dagger = U^{-1}$, or in other words, if $U \in U(N)$. For this reason, this transformation is also called a global $U(N)$ transformation. The phase transformation (1.1.4) is the particular case where $U = e^{-\mathrm{i}\alpha} \in U(1)$, that is the only Abelian (commutative) unitary group.
As $U(N) = SU(N) \otimes U(1)\ \forall N > 1$, $U \in SU(N)$ instead of $U \in U(N)$ can be imposed,

[2] For example, if $N = 3$ the 3 possible charges are the color charges of QCD, as will be shown later.

and will be from now on, without loss of generality.
In an analogous way to what has been done in Section 1.1.3 , this invariance can be made local by implementing a proper covariant derivative, similar to (1.1.5). In order to do so, the infinitesimal $SU(N)$ transformation has to be considered:

$$U_{ij}(x) = \delta_{ij} + \mathrm{i}\theta^a(x)\,(T^a)_{ij} + O(\theta^2) \tag{1.1.12}$$

where the indices i and j run from 1 to N (as before) and the index a runs from 1 to N^2-1 (the dimension of the group $SU(N)$). The matrixes T^a are the N^2-1 generators of $\mathfrak{su}(N)$ (the Lie algebra of $SU(N)$), thus they are $N\times N$ hermitean and traceless, which obey the commutation relations:

$$\left[T^a, T^b\right] = \mathrm{i} f^{abc} T^c \tag{1.1.13}$$

where f^{abc} are called *structure constants* of $\mathfrak{su}(N)$. The normalization of these matrices can be chosen such that they obey the condition:

$$\mathrm{Tr}\left(T^a T^b\right) = \frac{1}{2}\delta^{ab} \tag{1.1.14}$$

some examples are:

- $N=2$, $T^a = \frac{\sigma^a}{2}$, with σ^a the Pauli matrices and $f^{abc} = \varepsilon^{abc}$;
- $N=3$, $T^a = \frac{\lambda^a}{2}$, with λ^a the Gell-Mann matrices.

where ε^{abc} is the completely antisymmetric Levi-Civita symbol.
The covariant derivative, therefore, is written as:

$$D_\mu \equiv \partial_\mu + \mathrm{i}g\mathbf{A}_\mu(x) \tag{1.1.15}$$

where an $N\times N$ identity matrix $\mathbb{1}$ multiplying ∂_μ has to be understood, and $\mathbf{A}_\mu(x)$ is a gauge field of $SU(N)$, i.e., a traceless, hermitean $N\times N$ matrix, or, in other words, $\mathbf{A}_\mu(x) \in \mathfrak{su}(N)$.
The covariant derivative can be written more explicitly acting on the set of spinors ψ_i:

$$\left(D_\mu\right)_{ij}\psi_j = \partial_\mu \mathbb{1}_{ij}\psi_j + \mathrm{i}g\left(\mathbf{A}_\mu(x)\right)_{ij}\psi_j$$

In order for the action to be gauge invariant, the field $\mathbf{A}_\mu$ must satisfy the gauge transformation property

$$\mathbf{A}_\mu(x) \to \mathbf{A}'_\mu(x) = U(x)\mathbf{A}_\mu(x)U^\dagger(x) - \frac{\mathrm{i}}{g}U(x)\partial_\mu U^\dagger(x) \tag{1.1.16}$$

This expression is a little more complicated than (1.1.7), due to the fact that $\mathbf{A}_\mu$ is now a non-commuting matrix. However if the Abelian case $U(1)$ is taken into consideration, where $U(x) = e^{-\mathrm{i}\alpha(x)}$, (1.1.7) follows directly from (1.1.16).
Now, it can be easily checked that the kinetic term of the Lagrangian

$$\mathcal{L}_K = \mathrm{i}\overline{\psi}_i \not{D}\psi_i = \mathrm{i}\overline{\psi}_i \not{\partial}\psi_i - g\overline{\psi}_i \not{\mathbf{A}}\psi_i$$

is gauge invariant (i.e., invariant under (1.1.11) and (1.1.16)) through direct computation:

$$\begin{aligned}\mathcal{L}_K \to \mathcal{L}'_K =& \mathrm{i}\overline{\psi}_i U^\dagger \not{\partial}\left(U\psi_i\right) - g\overline{\psi}_i \underbrace{U^\dagger U}_{\mathbb{1}} \not{\mathbf{A}} \underbrace{U^\dagger U}_{\mathbb{1}} \psi_i + \mathrm{i}\overline{\psi}_i \underbrace{U^\dagger U}_{\mathbb{1}} \left(\not{\partial} U^\dagger\right) U\psi_i = \\ =& \mathrm{i}\overline{\psi}_i U^\dagger \left(\not{\partial} U\right)\psi_i + \underbrace{\mathrm{i}\overline{\psi}_i \not{\partial}\psi_i - g\overline{\psi}_i \not{\mathbf{A}}\psi_i}_{\mathcal{L}_K} + \mathrm{i}\overline{\psi}_i \left(\not{\partial} U^\dagger\right) U\psi_i = \\ =& \mathcal{L}_K + \mathrm{i}\overline{\psi}_i \gamma^\mu \left(U^\dagger \partial_\mu U + \partial_\mu U^\dagger U\right)\psi_i = \\ =& \mathcal{L}_K + \mathrm{i}\overline{\psi}_i \gamma^\mu \partial_\mu \left(U^\dagger U\right)\psi_i = \\ =& \mathcal{L}_K + \mathrm{i}\overline{\psi}_i \gamma^\mu \underbrace{\partial_\mu\left(\mathbb{1}\right)}_{=0}\psi_i = \mathcal{L}_K\end{aligned}$$

Because of this fact, it is directly implied that the covariant derivative (1.1.15) must transform, under a gauge transformation, in the adjoint representation:

$$D_\mu \to D'_\mu = U D_\mu U^\dagger \tag{1.1.17}$$

The field-strength for the field $\mathbf{A}_\mu$ is obtained, as for the Abelian case, through the commutator of two covariant derivatives. The computation is the same as (1.1.6), but this time the commutator term is non-vanishing:

$$F_{\mu\nu} \equiv -\frac{\mathrm{i}}{g}[D_\mu, D_\nu] = \partial_\mu \mathbf{A}_\nu - \partial_\nu \mathbf{A}_\mu + \mathrm{i}g[\mathbf{A}_\mu, \mathbf{A}_\nu] \tag{1.1.18}$$

This expression can be simplified a little by considering that $\mathbf{A}_\mu$ and $F_{\mu\nu}$ are elements of $\mathfrak{su}(N)$, thus writing them in terms of their components w.r.t. the basis T^a:

$$\mathbf{A}_\mu(x) = A^a_\mu(x) T^a \tag{1.1.19}$$

$$F_{\mu\nu}(x) = F^a_{\mu\nu}(x) T^a \tag{1.1.20}$$

and by considering the relation (1.1.13):

$$\begin{aligned}F^a_{\mu\nu} T^a =& \left(\partial_\mu A^a_\nu - \partial_\nu A^a_\mu\right) T^a + \mathrm{i}g\left[A^b_\mu T^b, A^c_\nu T^c\right] = \\ =& \left(\partial_\mu A^a_\nu - \partial_\nu A^a_\mu\right) T^a + \mathrm{i}g A^b_\mu A^c_\nu \underbrace{\left[T^b, T^c\right]}_{if^{bca}T^a} = \\ =& \left(\partial_\mu A^a_\nu - \partial_\nu A^a_\mu - g f^{abc} A^b_\mu A^c_\nu\right) T^a \\ F^a_{\mu\nu} =& \partial_\mu A^a_\nu - \partial_\nu A^a_\mu - g f^{abc} A^b_\mu A^c_\nu\end{aligned} \tag{1.1.21}$$

In order to write a kinetic action for the field $\mathbf{A}_\mu$, a term proportional to $F_{\mu\nu}F^{\mu\nu}$, like in (1.1.8), is not enough: because of (1.1.17) and the definition (1.1.18), it must transform as $F_{\mu\nu}F^{\mu\nu} \to U F_{\mu\nu}F^{\mu\nu}U^\dagger$, therefore it would not be gauge invariant. In fact a gauge invariant action, called Yang-Mills action, is:

$$S_{YM} = -\frac{1}{2}\int \mathrm{d}^4x \,\mathrm{Tr}\left(F_{\mu\nu}F^{\mu\nu}\right) \tag{1.1.22}$$

because of the ciclic property of the trace.[3] This action can be written in components, using (1.1.20) and the trace property (1.1.14):

$$S_{YM} = -\frac{1}{2}\int \mathrm{d}^4x \,\mathrm{Tr}\left(F^a_{\mu\nu}F^{b\mu\nu}T^aT^b\right) = -\frac{1}{4}\int \mathrm{d}^4x F^a_{\mu\nu}F^{a\mu\nu} \tag{1.1.23}$$

[3] Actually, a term proportional to $\det\left(F^a_{\mu\nu}F^{a\mu\nu}\right)$ would be gauge invariant as well, but it would not be a suitable kinetic term as it would involve terms of higher order than 2 in the components $F^a_{\mu\nu}$

Here, there are two remarks that need to be done. The first one is that, if the gauge group is taken to be $U(1)$, the action (1.1.23) reduces to (1.1.8), as $a = 1$ because the group $U(1)$ has only 1 generator. The second one is that, if non-Abelian gauge groups are taken into consideration, this action naturally introduces self-interacting cubic and quartic terms, because the structure constants f^{abc} are non-vanishing. This is, for example, the case for the group $SU(3)$, that is used to describe gluon interaction, i.e., Quantum Chromodynamics (QCD). These self-interactions make the the Yang-Mills action interesting to be studied even alone, without any other fermionic or bosonic interacting field, as it will be shown later.

1.1.5 Wick Rotation

Up to now, actions were written in Minkowskian spacetime, where $\eta_{\mu\nu} = \text{diag}(-1, 1, 1, 1)$. In order to have a positive-defined metric $\eta_{\mu\nu} = \delta_{\mu\nu}$ a Wick rotation can be performed by re-defining the time coordinate to be $\tau = \mathrm{i}t = \mathrm{i}x^0$, as is rigorously proven in [6]. The principle behind Wick rotation is that the time coordinate is promoted to be a complex number and the integration (in the action) from $-\infty$ to ∞ is made to be from $-\mathrm{i}\infty$ to $+\mathrm{i}\infty$ through a rotation of $\frac{\pi}{2}$ in the complex plane, assuming that correlators and other physical quantities do not present singularities in the first and third quadrant of the complex plane of t. This rotation is not only a matter of convenience, in fact it is needed in perturbative QFT for the computation of (otherwise oscillating) functional integrals and in lattice field theory because a Minkowskian lattice cannot be rigorously defined.
The relation between the Minkowski actions written before and the Euclidean actions is $S^M = \mathrm{i}S^E$, because $\mathrm{d}^4x^E = \mathrm{i}\mathrm{d}^4x^M$.
Thus, the Euclidean actions are[4]:

$$S^E[\phi] = \int \mathrm{d}^4x \left(\frac{1}{2}\partial^\mu\phi\partial_\mu\phi + \frac{1}{2}m^2\phi^2 + V(\phi)\right) \tag{1.1.24}$$

$$S_F^E = \int \mathrm{d}^4x\overline{\psi}\left(\gamma^\mu\left(\partial_\mu + \mathrm{i}g\mathbf{A}_\mu\right) + m\right)\psi \tag{1.1.25}$$

$$S_{YM}^E = \frac{1}{4}\int \mathrm{d}^4x F^a_{\mu\nu}F^{a\mu\nu} \tag{1.1.26}$$

where the superscript E, meaning that the action is written in the Euclidean spacetime, will be omitted from now on.

1.2 Lattice Field Theory

1.2.1 Why Lattice Field Theory

After the Wick rotation, quantum field theory can be studied perturbatively through the saddle-point evaluation of the path integral, where the partition function

$$Z = \int \mathcal{D}\varphi e^{\mathrm{i}S^M[\varphi]} = \int \mathcal{D}\varphi e^{-S^E[\varphi]}$$

[4]Note that they are not the same as their Minkowskian counterpart, as some redefinitions of the fields and the γ matrices have been implicitly made, in order to have the respective theories non ill-defined.

has become non-oscillating. This approach, however, works well only if the coupling constants are *small enough* and does not allow to obtain non-perturbative results, i.e., physical quantities that depend on essential singularities in the coupling constant, like glueballs for Yang-Mills theories.
For this reason, a non-perturbative approach has to be taken into consideration and one possibility is Lattice Field Theory: the spacetime is discretized to a lattice, with lattice spacing a, and the fields can assume different values only on particular parts of the lattice. More in detail, a scalar field lives on lattice sites, a vector field lives on links between sites and objects with k indices live on k-simplexes.
If the limit $a \to 0$ is taken, the theory must reproduce results obtained in the continuum, like the ones obtained in perturbation theory in the regime where it can be applied, however the presence of a discrete spacetime provides a natural cutoff for the momenta, allowing ultraviolet divergencies to be kept under control, although they need to be taken into consideration when approaching the continuum limit.
In this section, based on standard quantum field theory textbooks cited before and lattice field theory textbooks [7–9], the regularization of the previous quantum field theories on a Simple Hypercubic (SH) lattice is presented. A more detailed description of the geometric properties of the figures mentioned below can be found in [10].

1.2.2 Lattice

A lattice Λ in $\mathbb{R}^D$ is defined as the set of all possible linear combinations with integer coefficients of the vectors $\{v_i\}$, which form a basis of $\mathbb{R}^D$. Formally:

$$\Lambda = \left\{ \sum_{i=1}^{D} c_i v_i \;\middle|\; c_i \in \mathbb{Z} \right\} \tag{1.2.1}$$

1.2.2.1 Simple Hypercubic Lattice

If the basis $\{v_i\}$ is taken to be orthonormal, the lattice is called *Simple Hypercubic*[5].
In Figure (1.2.1) is represented a portion of a Simple Hypercubic lattice in $D = 3$.

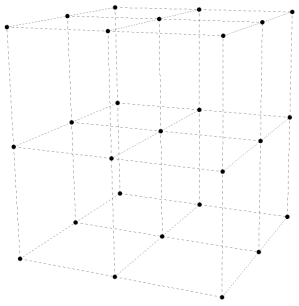
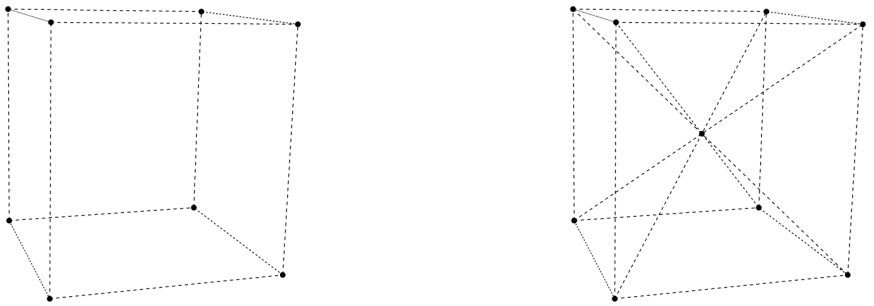


Figure 1.2.1: A cubic lattice.

For the SH lattice in $D = 4$, the fundamental region (the smallest D-dimensional polyhedron) is a 4-dimensional hypercube, also called a tesseract. This means that a SH lattice

[5]The word *simple* is used to make a distinction with the Body-Centered Hypercubic lattice.

can be seen as a tassellation of the spacetime with tesseracts as elementary cells. Each point of the lattice has 8 nearest neighbours that are identified by the vectors obtained through all possible permutations of position and sign of $(\pm 1, 0, 0, 0)$.
The plaquette (the simplest bidimensional figure) is a square. This will be important when implementing gauge theories on the lattice.



(a) Simple cube. (b) Body-centered cube.

Figure 1.2.2: Tridimensional representation of a simple cubic cell (1.2.2a) and a body-centered one (1.2.2b).

1.2.2.2 Body-Centered Tesseract

The SH lattice is not, of course, the only possible choice of a lattice in 4 spacetime dimensions. Another common choice, already used to simulate gauge theories [11], is the Body-Centered Tesseract (BCT). It consists of packing the spacetime with tesseracts, as the name suggests, but considering both the corners and the centers of every hypercube as lattice sites. Every site has, therefore, 24 nearest neighbours: 16 are identified by all possible sign permutations of $\left(\pm\frac{1}{2}, \pm\frac{1}{2}, \pm\frac{1}{2}, \pm\frac{1}{2}\right)$, the 8 remaining are the ones of the SH lattice. The cell of this lattice is known as 24-cell, shown in Figure (1.2.3), and the plaquettes are triangular.

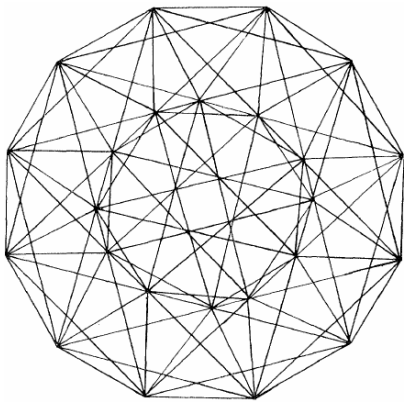


Figure 1.2.3: Bidimensional projection of the 24-cell.

1.2.3 Scalar Fields on the Simple Hypercubic Lattice

Let us consider a simple hypercubic lattice Λ_{SH} extending over $L = L_1 = L_2 = L_3$ lattice spacings in the spatial directions and over $T = L_0$ lattice spacings in the temporal direction. Let us also consider a scalar field $\phi(x)$, in order to introduce some useful tools that will be needed later. As anticipated in the beginning of this section, a scalar field can only assume values on the sites of the lattice, therefore $x \in \Lambda_{SH}$, and let us assume, for simplicity, periodic boundary conditions on the fields, therefore $\phi(x + a\hat{\mu}L_\mu) = \phi(x)$. The Fourier transform of the field becomes

$$\tilde{\phi}(p) = \sum_x a^4 e^{-ip\cdot x}\phi(x) \tag{1.2.2}$$

and the allowed momenta are given by

$$p_\mu = \frac{2\pi}{aL_\mu} n_\mu, \qquad n_\mu = 0, \dots, L_\mu \tag{1.2.3}$$

This ensures that the momenta can take only the assigned values of the Brillouin zone (1.2.3) and therefore cannot go to infinity, providing a natural cutoff given by the lattice spacing a.
The discretization also implies that derivatives of the fields cannot be computed, therefore the lattice forward derivative is used:[6]

$$\partial_\mu\phi(x) \to \nabla_\mu\phi(x) = \frac{\phi(x + a\hat{\mu}) - \phi(x)}{a} \tag{1.2.4}$$

Assuming a self-interaction potential $V(\phi) = \frac{\lambda}{4!}\phi^4$, the action (1.1.1) can be written in terms of the lattice in the following way:

$$S = a^4 \sum_x \left(\frac{1}{2a^2} \left[\phi(x + a\hat{\mu}) - \phi(x)\right]^2 + \frac{1}{2}m^2\phi^2(x) + \frac{\lambda}{4!}\phi^4(x) \right) \tag{1.2.5}$$

A similar approach will be used in the following section to obtain the action for Yang-Mills theories.

1.2.4 Gauge Fields on the Simple Hypercubic Lattice

Let us now take into consideration a Yang-Mills theory, as in Section 1.1.4 , with gauge group $SU(N)$. As anticipated before, gauge fields, being vector fields, can assume value only on links between sites of the lattice.
One could naively think that putting gauge vectors $A_\mu(x)$ on the links is enough, but this would explicitly break gauge invariance. For this reason, Wilson's idea was to put the gauge group (and not algebra) elements, namely $U_\mu(x) = e^{iagA_\mu(x)}$, on the links.
The field $U_\mu(x)$ lives on the link connecting the site x with the site $x + a\hat{\mu}$, therefore the link is oriented and link variables in negative directions can also be defined:
$U_{-\mu}(x) \equiv U_\mu^\dagger(x - a\hat{\mu})$.

[6] Note that, in the continuum limit, the two derivatives coincide.

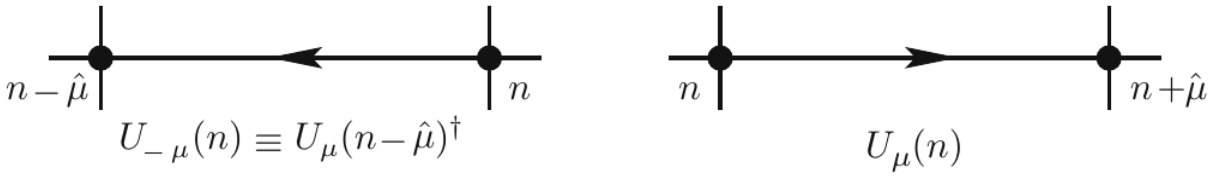


Figure 1.2.4: Schematic visualization of link variables.

Under a gauge transformation, the fields U_μ transform according to the following relation:

$$U_\mu(x) \to \Omega(x) U_\mu(x) \Omega^\dagger(x + a\hat{\mu}) \tag{1.2.6}$$

where $\Omega(x)$ is any $SU(N)$ matrix at the point x on the lattice. As a consequence of this relation, the trace of any product of links forming a closed path is a gauge-invariant quantity, thanks to the cyclic property of the trace.
With this in mind, Wilson's idea was to choose the simplest closed path possible: the plaquette, that in the simple hypercubic lattice is a square. The product of link variables along a square plaquette is defined in the following way (the lattice spacing a is set $= 1$ for brevity of notation):

$$\begin{aligned} U_{\mu\nu}(x) \equiv & U_\mu(x) U_\nu(x+\hat{\mu}) U_{-\mu}(x+\hat{\mu}+\hat{\nu}) U_{-\nu}(x+\hat{\nu}) = \\ = & U_\mu(x) U_\nu(x+\hat{\mu}) U_\mu^\dagger(x+\hat{\nu}) U_\nu^\dagger(x) \end{aligned} \tag{1.2.7}$$

Thus a gauge-invariant action, called Wilson action, can be written as follows:

$$S_W[U] = \frac{\beta}{2N} \sum_{x \in \Lambda} \sum_{\mu < \nu} \mathrm{Re}\,\mathrm{Tr}[\mathbb{1} - U_{\mu\nu}(x)] \tag{1.2.8}$$

where β is a parameter that is going to be set in the following passages, N the number of colors (the same N in $SU(N)$), the real part is needed to preserve unitarity and $U_{\mu\nu}$ is the plaquette of (1.2.7).

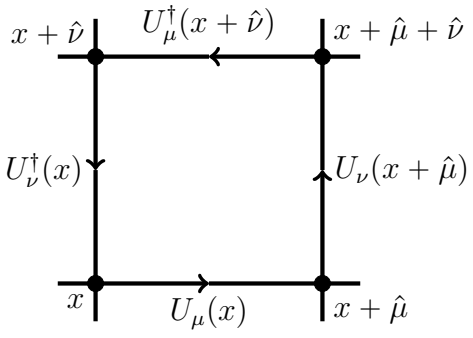


Figure 1.2.5: Link variables building a plaquette $U_{\mu\nu}(x)$.

In the following part, the naive continuum limit is taken, showing that Wilson action reproduces Yang-Mills action of (1.1.26) when $a \to 0$. Let us start by defining an auxiliary field $B_\mu(x)$:

$$B_\mu(x) = agA_\mu^a(x) T^a \tag{1.2.9}$$

thus the gauge group element becomes $U_\mu(x) = e^{\mathrm{i}B_\mu(x)}$.
The expansion for small a of the plaquette $U_{\mu\nu}$ is:

$$\begin{aligned}
U_{\mu\nu} =& U_\mu(x)U_\nu(x+\hat{\mu})U_\mu^\dagger(x+\hat{\nu})U_\nu^\dagger(x) = \\
=& e^{\mathrm{i}B_\mu(x)}e^{\mathrm{i}B_\nu(x+\hat{\mu})}e^{-\mathrm{i}B_\mu(x+\hat{\nu})}e^{-\mathrm{i}B_\nu(x)} = \\
& \text{applying (1.2.4), } B_\mu(x+\hat{\nu}) = a\nabla_\nu B_\mu(x) \\
=& e^{\mathrm{i}B_\mu(x)}e^{\mathrm{i}B_\nu(x)+a\nabla_\mu B_\nu(x)}e^{-\mathrm{i}B_\mu(x)-a\nabla_\nu B_\mu(x)}e^{-\mathrm{i}B_\nu(x)} \simeq \\
& \text{From now on, the dependance from } x \text{ will be omitted.} \\
& \text{Using BCH formula, } e^Xe^Y = e^{X+Y+\frac{1}{2}[X,Y]}, \text{ up to } O(a^2): \\
\simeq& \exp\Big\{\cancel{\mathrm{i}B_\mu} + \cancel{\mathrm{i}B_\nu} + \mathrm{i}a\nabla_\mu B_\nu - \cancel{\mathrm{i}B_\mu} - \mathrm{i}a\nabla_\nu B_\mu - \cancel{\mathrm{i}B_\nu} + \\
& + \frac{1}{2}\left(-[B_\mu, B_\nu] + \cancel{[B_\mu, B_\nu]} + \cancel{[B_\nu, B_\mu]} - [B_\mu, B_\nu]\right)\Big\} = \\
=& \exp\{\mathrm{i}a\left(\nabla_\mu B_\nu - \nabla_\nu B_\mu\right) - [B_\mu, B_\nu]\}
\end{aligned}$$

Now, substituting back (1.2.9), the discretized electromagnetic tensor can be found:

$$\begin{aligned}
U_{\mu\nu} \simeq& \exp\left\{\mathrm{i}a^2 g\left(\nabla_\mu \mathbf{A}_\nu - \nabla_\nu \mathbf{A}_\mu + \mathrm{i}g[\mathbf{A}_\mu, \mathbf{A}_\nu]\right)\right\} = \exp\left\{\mathrm{i}a^2 g F_{\mu\nu}\right\} \simeq \\
\simeq& \mathbb{1} + \mathrm{i}a^2 g F_{\mu\nu} - \frac{1}{2}a^4 g^2 F_{\mu\nu}F^{\mu\nu} + O(a^6)
\end{aligned} \tag{1.2.10}$$

Finally, the small-a approximation for the Wilson action (1.2.8) can be obtained:

$$\begin{aligned}
S_W \simeq& \frac{\beta}{2N}\sum_{x\in\Lambda}\sum_{\mu<\nu}\mathrm{Re}\,\mathrm{Tr}\left(\cancel{\mathbb{1}} - \cancel{\mathbb{1}} - \mathrm{i}a^2 g F^i_{\mu\nu}T^i + \frac{1}{2}a^4 g^2 F^i_{\mu\nu}F^{j\mu\nu}T^iT^j\right) = \\
=& \underbrace{-i\frac{a^2\beta}{2N}\sum_{x\in\Lambda}\sum_{\mu<\nu}\mathrm{Re}(F^i_{\mu\nu}\,\mathrm{Tr}\big(T^i\big))}_{=0 \text{ for (1.1.12)}} + \frac{g^2a^4\beta}{4N}\sum_{x\in\Lambda}\sum_{\mu<\nu}\mathrm{Re}(\underbrace{F^i_{\mu\nu}F^{j\mu\nu}\,\mathrm{Tr}\big(T^iT^j\big)}_{=\frac{1}{2}F^i_{\mu\nu}F^{i\mu\nu} \text{ for (1.1.14)}}) = \\
=& \frac{g^2\beta}{8N}a^4\sum_{x,\mu,\nu}F^i_{\mu\nu}F^{i\mu\nu} \xrightarrow[a\to 0]{} \frac{g^2\beta}{8N}\int \mathrm{d}^4x F^i_{\mu\nu}F^{i\mu\nu}
\end{aligned} \tag{1.2.11}$$

where the Yang-Mills action (1.1.26) can be recognized if $\beta = \frac{2N}{g^2}$.

1.2.4.1 Wilson Loops

Now that the lattice action has been defined, observables need to be taken into account. As mentioned below equation (1.2.6), the trace of the product of link variables along any closed path is a gauge-invariant quantity. This means that any quantity of the sort is a good candidate for an observable and, in fact, given any closed path γ on the lattice, the Wilson loop is defined as follows:

$$W[\gamma] \equiv \mathrm{Tr}\left[\prod_{(x,\mu)\in\gamma}U_\mu(x)\right] \tag{1.2.12}$$

It is worthwile to mention that this definition is does not depend on the type of lattice and of boundary conditions chosen for such lattice. If the path γ does not include any

temporal link, the loop is called *spacelike Wilson loop*, otherwise it is called *timelike Wilson loop*. If all the links in γ lie on the same plane, the Wilson loop is *planar*, otherwise it is *nonplanar*.

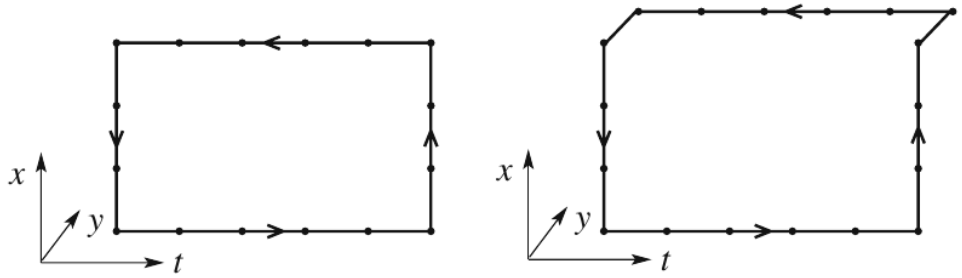


Figure 1.2.6: Example of a planar (left) and nonplanar (right) Wilson loop.

Wilson loops are important for a variety of reasons, that will not be elaborated further as this is not the focus of this project, however it is worth knowing that they can be used as operators for purely gluonic bound states, the so-called *glueballs*: the mass spectrum of these states can be obtained through the exponential decay of Wilson loops' correlation functions.

1.2.4.2 Polyakov Loops

Another important observable can be defined in lattices where periodic boundary conditions in the time direction are assumed. Thanks to periodicity, a whole new class of closed paths arises: all paths that wind around the time direction. A Polyakov loop is thus defined as a line at a fixed spatial position $\vec{x} = (x^1, x^2, x^3)$ that runs along the whole time direction:

$$P(\vec{x}) \equiv \mathrm{Tr}\left[\prod_{t=0}^{T-1} U_0(t, \vec{x})\right] \tag{1.2.13}$$

The Polyakov loop has a lot of interesting properties: its physical interpretation is the world-line of a single static quark, therefore its expectation value is an order parameter of the deconfinement transition, as well as of a new global symmetry, called *center symmetry*, arising from the periodicity of the time direction.
This means that, if the system is confined (quarks and gluons cannot move around freely), its expectation value is 0, while if the system is deconfined, $\langle P(\vec{x})\rangle \neq 0$.
Another property, that will be used in the simulations, is that the expectation value of the product of two Polyakov loops at distance $r = a|\vec{x} - \vec{y}|$ is a function of the static quark-antiquark potential $V(r)$, as indicated below:

$$\left\langle P(\vec{x})P^\dagger(\vec{y})\right\rangle \propto e^{-TaV(r)}\left(1 + O(e^{-Ta\Delta E})\right) \tag{1.2.14}$$

where ΔE is the difference between $V(r)$ and the first excited energy level of the quark-antiquark pair.
The value of the potential $V(r)$ will be used, in this project, to study the recovery of rotational invariance when approaching the continuum limit.
Various methods of performing computer simulations of lattice field theory and how to obtain these quantities, such as plauette values, Wilson and Polyakov loops, is shown in the following chapter.

Computer Simulation of Pure Gauge Theories

2.1 Introduction

Monte Carlo simulations are a powerful tool that can be used to evaluate observables in lattice field theory. Given an observable O (such as a plaquette, a Wilson or Polyakov loop, etc.), its vacuum expectation value is formally given by the functional integral

$$\langle O \rangle = \frac{1}{Z} \int \mathcal{D}[U] e^{-S[U]} O[U] \qquad \text{with} \qquad Z = \int \mathcal{D}[U] e^{-S[U]} O[U] \tag{2.1.1}$$

where $\mathcal{D}[U]$ is to be intended as a Haar measure.
This expression, however, cannot be evalued analytically except for very small lattices, therefore (2.1.1) is approximated by an average of the observable evaluated on N sample gauge field configurations $\{U_n\}$[1], distributed according a probability density $\propto e^{-S[U_n]}$.

[1] Here the subscript n distinguishes the different configurations.

The expectation value is then obtained by computing the following sum for a sufficient number of configurations generated by the proper Monte Carlo algorithm(s):

$$\langle O \rangle \simeq \frac{1}{N} \sum_{\{U_n\}} O[U_n] \tag{2.1.2}$$

Because of the probability density $\propto e^{-S[U_n]}$, only configurations $\{U_n\}$ that minimize the action are *good configurations*, as all other configurations are exponentially suppressed. For this reason, generating totally random gauge fields on the lattice links is not an efficient way to evaluate (2.1.2), as most of the $\{U_n\}$ will have a very small Boltzmann factor (the $e^{-S[U_n]}$) and expression (2.1.2) will give incorrect results unless a huge number (orders of magnitude higher than what is reasonably possible) of different configurations is tried.
In order to avoid the evaluation of a great number of configurations that would contribute little-to-nothing to the observables' values, a sequence of configurations $\{U_n\}$ is generated through a Markov chain process, built such that its stationary distribution minimizes the action $S[U]$. This process is usually called *thermalization*.
Every process of this type must begin from a starting configuration, usually chosen by the user. The starting configurations usually used are two: if the simulation begins with the fields in an ordered way (for example, all the gauge links set to the identity), the initial configuration is called *cold start*, if the simulation begins with random gauge fields in every link, the initial configuration is called *hot start*. Of course, the Markov chain must have the same stationary distribution if the hot or cold start is chosen.
In this chapter the main Monte Carlo algorithms used to thermalize the starting configuration are presented, then the method for evaluating some observables of interest, such as plaquettes and Polyakov loops is explained.

2.2 Markov Processes

As anticipated before, a Markov chain is needed to evolve an arbitrary starting configuration U_0 up to a region of the configuration space with a relatively large Boltzmann factor e^{-S}, therefore with high probability. A Markov process is charaterized by a probability of transitioning from a configuration α to another configuration β depending only on α and β and not on the history of the process, namely the previous transitions that already occourred. In formulae, this is expressed as

$$P(U_n = \beta | U_{n-1} = \alpha) = T(\beta|\alpha) \tag{2.2.1}$$

That is to say that the transition matrix T does not depend on the index n, representing the computer time.
Being a transition probability, the matrix T must obey the following equations

$$0 \leqslant T(\beta|\alpha) \leqslant 1 \qquad \forall \alpha, \beta \tag{2.2.2}$$

$$\sum_{\beta} T(\beta|\alpha) = 1 \qquad \forall \alpha \tag{2.2.3}$$

where (2.2.2) is a consequence of $T(\beta|\alpha)$ representing a probability, and (2.2.3) means that the probability of transitioning to any configuration must be 1 (of course, the case when $\alpha = \beta$ is included as well).
In order for the stochastic process to not have any sink or source of probability, the following balance equation must be satisfied:

$$\sum_{\alpha} T(\beta|\alpha)P(\alpha) = \sum_{\alpha} T(\alpha|\beta)P(\beta) \tag{2.2.4}$$

This equation states that the probability of transitioning to the configuration β, written in the l.h.s. as the sum of the transition probability from the configuration α weighted by the probability $P(\alpha)$ that the system is actually in that configuration, must be equal to the probability of transitioning out of the configuration β, given by the probability of finding the system in the configuration β times the transition probability $T(\alpha|\beta)$ over all the final configurations, in the right-hand side. Thanks to (2.2.3), the r.h.s. is easily proven to be equal to $P(\beta)$.
A sufficient (but not necessary) condition to obey the balance equation (2.2.4) is obtained by requiring that it holds true term-by-term, thus obtaining the detailed balance condition:

$$T(\beta|\alpha)P(\alpha) = T(\alpha|\beta)P(\beta) \tag{2.2.5}$$

Although it is not a necessary condition, most algorithms, including the ones discussed in the following section, satisfy it.

2.3 Monte Carlo Algorithms

Monte Carlo algorithms are a class of algorithms that, singularly or combined together, allow to advance the Markov chain, while satisfying the condition presented in the previous section. Each algorithm, if applied once, allows the transition from a configuration U_{n-1} to a configuration U_n (eventually the same as U_{n-1}). The repeated application of the algorithm allows to advance through the Markov chain.

2.3.1 Metropolis Algorithm

The first algorithm presented is the Metropolis algorithm. It is not very much efficient and usually it is not used in simulations, however it contains the fundamental steps that are present in some of the more advanced algorithms and it is quite easy to understand. For this reasons it is usually viewed as the *"ancestor"* of all Monte Carlo algorithms and it is present in every textbook on the subject.
This algorithm consists in two steps that implement in one of the most simple ways the detailed balance condition (2.2.5):

1) A candidate configuration β is chosen, according to some *a priori* selection probability $T_0(\beta|\alpha)$, where $\alpha = U_{n-1}$.

2) The candidate configuration β is accepted as the new configuration U_n with the acceptance probability

$$T_A(\beta|\alpha) = \min\left(1, \frac{T_0(\alpha|\beta)\exp(-S[\beta])}{T_0(\beta|\alpha)\exp(-S[\alpha])}\right) \tag{2.3.1}$$

If it is not accepted, the unchanged configuration is considered again ($U_n = \alpha$) and the measurements are eventually made again.

These two steps are repeated a sufficient amount of times up unitl the needed measurements are taken.
Note that the fact that $P(\alpha) = \frac{e^{-S[\alpha]}}{Z} \propto e^{-S[\alpha]}$ has been used.
The total transition probability T is obtained through the product $T = T_0 T_A$, as the two steps are independant from each other, and it is straightforward to see that it satisfies the detailed balance condition (2.2.5):

$$\begin{aligned} T(\beta|\alpha)P(\alpha) =& \frac{1}{Z} T_0(\beta|\alpha) T_A(\beta|\alpha) \exp(-S[\alpha]) = \\ =& \frac{1}{Z} T_0(\beta|\alpha) \min\left(1, \frac{T_0(\alpha|\beta)\exp(-S[\beta])}{T_0(\beta|\alpha)\exp(-S[\alpha])}\right) \exp(-S[\alpha]) = \\ =& \frac{1}{Z} \min\left(T_0(\beta|\alpha)\exp(-S[\alpha]), T_0(\alpha|\beta)\exp(-S[\beta])\right) = \\ =& \frac{1}{Z} T(\alpha|\beta)\exp(-S[\beta]) = \\ =& T(\alpha|\beta)P(\beta) \end{aligned}$$

□

In many cases a symmetric selection probability is used $T_0(\alpha|\beta) = T_0(\beta|\alpha)$, thus (2.3.1) simpliefies to:

$$T_A(\beta|\alpha) = \min\left(1, e^{-\Delta S}\right) \quad \text{with} \quad \Delta S = S[\beta] - S[\alpha] \tag{2.3.2}$$

That means that if the new configuration lowers the action, the change is accepted with probability 1 (as $e^{-\Delta S} > 1$), otherwise it is accepted with a certain probability that decays exponentially as the difference in the action of the two configurations becomes greater. This ensures that the algorithm *moves across* the configuration space towards the minimums of the action, while allowing quantum fluctuations in order to not *"get stuck"* on a local minimum.
If the change in the action is local (it involves a single link variable), ΔS can be computed using only the field values in the local neighbour. This will be the case for $SU(N)$ gauge theories.

2.3.1.1 Application to SU(N) Gauge Theories

For a $SU(N)$ gauge theory, the algorithm is implemented in the following way. For each iteration, a single link is changed, then the acceptance probability is computed, a random number is extracted and, if it is less than the acceptance probability the change is accepted, otherwise it is rejceted. The algorithm is then iterated a certain number of times and measures are taken.
The candidate link $U'_\mu(x)$ for step 1 is generated in the vicinity of the old value $U_\mu(x)$, in order to not have a too great ΔS that would lead to too low accentance rates. This can be done by exploiting the property that the product of any two elements of $SU(N)$

is still an element of $SU(N)$, therefore extracting a matrix $X \in SU(N)$ near the identity allows to write the candidate link as:

$$U'_\mu(x) = XU_\mu(x) \tag{2.3.3}$$

The matrix X is chosen such that it has the same probability as X^{-1}, this way the selection probability T_0 is symmetric and the computation of the acceptance probability T_A becomes easier.
For this reason, only the variation of the action ΔS must be computed, where of course the action is the Wilson action (1.2.8). In particular, only the plaquettes containing the candidate link must be evaluated: the change in the action is local, so all the other plaquettes will have the same value both before and after the change of the link. Hence $\Delta S = S[U'_\mu(x)]_{loc} - S[U_\mu(x)]_{loc}$.
In a SH lattice, each link is shared between 6 plaquettes. For each plaquette the change of the action is given by the change of the link, while the product of the other three gauge links, that is called *staple* and will be indicated as P_i, remains unchanged. Therefore, the local contribution to the action can be computed as:

$$S[U_\mu(x)]_{loc} = \frac{\beta}{2N} \sum_{i=1}^{6} \mathrm{Re}\,\mathrm{Tr}\,[\mathbb{1} - U_\mu(x)P_i] = \frac{\beta}{2N}\,\mathrm{Re}\,\mathrm{Tr}\left[6\mathbb{1} - U_\mu(x)\sum_{i=1}^{6} P_i\right]$$

where the sum over all the staples is:

$$A = \sum_{i=1}^{6} P_i = \sum_{\nu\neq\mu} \left(U_\nu(x+\hat{\mu})U^\dagger_\mu(x+\hat{\nu})U^\dagger_\nu(x) + U^\dagger_\nu(x+\hat{\mu})U^\dagger_\mu(x-\hat{\nu})U_\nu(x-\hat{\nu})\right) \tag{2.3.4}$$

The change of the action can now be computed as

$$\Delta S = S[U'_\mu(x)]_{loc} - S[U_\mu(x)]_{loc} = \frac{\beta}{2N}\,\mathrm{Re}\,\mathrm{Tr}\left[\left(U_\mu(x) - U'_\mu(x)\right)A\right] \tag{2.3.5}$$

where A is not affected by the change of $U_\mu(x)$.

2.3.2 Heat Bath Algorithm

The heat bath algorithm is an *enhanced* version of the Metropolis algorithm, that combines the two steps into a single one and chooses the new candidate according to the probability distribution obtained by the computing the surrounding staples:

$$\mathrm{d}P(U) = \mathrm{d}U \exp\left(\frac{\beta}{2N}\,\mathrm{Re}\,\mathrm{Tr}[UA]\right) \tag{2.3.6}$$

where $\mathrm{d}U$ denotes the Haar integration measure of the gauge group and A is computed according to (2.3.4). This probability distribution can be computationally quite demanding, but has the advantage that, unlike the Metropolis algorithm, the link variable always changes.
The implementation details depend on the gauge group, for this reason, the heat bath

method for the gauge group $SU(2)$ will be now explained[2]. Since the sum of any two $SU(2)$ elements is proportional to another $SU(2)$ element, the sum of all staples A (2.3.4) can be written in the form

$$A = V\sqrt{\det(A)} \qquad \text{with} \qquad V \in SU(2) \tag{2.3.7}$$

where it can be proven that $\det(A) \geqslant 0$. Plugging into (2.3.6) and using the invariance of the Haar measure under trasformation of the origin of the group space ($\mathrm{d}U = \mathrm{d}(UV) = \mathrm{d}X$), the distribution probability of the matrix $X = UV$ is

$$\mathrm{d}P(X) = \mathrm{d}X \exp\left(\frac{\beta}{2N}\sqrt{\det(A)}\,\mathrm{Re}\,\mathrm{Tr}[X]\right) \tag{2.3.8}$$

If a matrix X distributed according to (2.3.8) is generated, then the new candidate link, distributed according to (2.3.6), is obtained as $U'_\mu(x) = XV^\dagger = \frac{1}{\sqrt{\det(A)}} X A^\dagger$.
Any $U \in SU(2)$ matrix can be written in the following representation, using 4 real numbers:

$$U = x_0 \mathbb{1} + \mathrm{i}\boldsymbol{x}\cdot\boldsymbol{\sigma} \qquad \text{with} \qquad \det(U) = |x|^2 = \sum_{i=0}^{3} x_i^2 = 1 \tag{2.3.9}$$

where $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is a vector built using the Pauli matrices and $x = (x_0, \boldsymbol{x})$ can be seen as a normalized 4-compnents vector. Using this representation, the Haar measure in (2.3.8) can be written as:

$$\begin{aligned}\mathrm{d}X =& \frac{1}{\pi^2}\mathrm{d}^4x\,\delta\left(x_0^2 + \boldsymbol{x} - 1\right) = \\ =& \frac{1}{\pi^2}\mathrm{d}^4x \frac{1}{2\sqrt{1-x_0^2}}\left(\delta\left(|\boldsymbol{x}| - \sqrt{1-x_0^2}\right) + \delta\left(|\boldsymbol{x}| + \sqrt{1-x_0^2}\right)\right)\end{aligned} \tag{2.3.10}$$

where a well known property of the Dirac delta function has been used.
The volume element can be rewritten in terms of the components of the vector x:

$$\mathrm{d}^4x = \mathrm{d}x_0 \mathrm{d}|x||x|^2 \underbrace{\mathrm{d}(\cos\theta)\,\mathrm{d}\varphi}_{\mathrm{d}^2\Omega} \tag{2.3.11}$$

Plugging back into (2.3.10) and integrating out the $|\boldsymbol{x}|$ thanks to the delta functions (actually, only the first one contributes, as $x_i^2 \leqslant 1\ \forall i$), the Haar measure takes the form:

$$\mathrm{d}X = \frac{1}{\pi^2}\mathrm{d}x_0\mathrm{d}^2\Omega\frac{1-x_0^2}{2\sqrt{1-x_0^2}} = \frac{1}{2\pi^2}\mathrm{d}x_0\mathrm{d}^2\Omega\sqrt{1-x_0^2} \tag{2.3.12}$$

Then, in terms of the variables, the probability distribution becomes:

$$\mathrm{d}P(X) = \frac{1}{2\pi^2}\mathrm{d}x_0\mathrm{d}\cos\theta\mathrm{d}\varphi\sqrt{1-x_0^2}\exp\left(\frac{\beta}{2}\sqrt{\det(A)}x_0\right) \tag{2.3.13}$$

with $x_0 \in [-1,1]$, $\cos\theta \in [-1,1]$, $\varphi \in [0, 2\pi)$, where $\mathrm{Tr}(X) = 2x_0$ has been used.
Thus, the problem of generating a matrix X distributed according to (2.3.8) has been

[2] As matrixes of $SU(N)$ can be built using $SU(2)$ matrixes, the general case is just a little more complicated, but it follows the same principles.

reduced to the determination of three random variables x_0, θ, φ, whose distribution factorizes, so they can be determined independetly from each other. The random variable x_0, being distributed according to $\sqrt{1-x_0^2}\exp\left(\frac{\beta}{2}\sqrt{\det(A)}x_0\right)$, is determined through the auxiliary variable $\lambda \in [0,1]$ such that $x_0 = 1-2\lambda^2$, therefore

$$\mathrm{d}x_0\sqrt{1-x_0^2}\exp\left(\frac{\beta}{2}\sqrt{\det(A)}x_0\right) \propto \mathrm{d}\lambda\lambda^2\sqrt{1-\lambda^2}\exp\left(-\beta\sqrt{\det(A)}\lambda^2\right) \tag{2.3.14}$$

The variable λ is generated with the polynomially modified Gaussian distribution density

$$p_1(\lambda) = \lambda^2 e^{-\beta\sqrt{\det(A)}\lambda^2} \tag{2.3.15}$$

and accepted with an accept/reject step using the square root function

$$p_2(\lambda) = \sqrt{1-\lambda^2} \tag{2.3.16}$$

There are several algorithms that can perform this computation in an efficient way [12, 13].
After this, the length $|x| = \sqrt{1-x_0^2}$ is computed, in order to determine the remaining variables.
The variables $\cos\theta$ and φ are uniformely distributed, therefore a possible way of proceeding is by generating three random uniformely distributed numbers r_1, r_2 and r_3 in the interval $[-1,1)$ and accepting them only if $r_1^2+r_2^2+r_3^2 \leqslant 1$. Then, the 3-vector (r_1,r_2,r_3) is normalized to length $|x|$ computed before, obtaining $\boldsymbol{x} = (x_1,x_2,x_3)$.
After these steps, the vector $x = (x_0,\boldsymbol{x})$ can be used to generate the matrix X according to (2.3.8), using representation (2.3.9), thus the new link variable can be obtained.
This algorithm rapidly leads the Markov process to a minimum of the action, however the risk of "getting stuck" on a local minimum is present. For this reason, it is usually combined with the overrelaxation algorithm discussed below.

2.3.3 Overrelaxation Algorithm

The overrelaxation algorithm tries to change the variables as much as possible, exploiting the property that new configuration are always accepted if they do not change the action, as can be seen in (2.3.2). The case with gauge group $U(1)$ is the simplest one: the group element can be written as $U = e^{\mathrm{i}\varphi}$, the sum of staples becomes $A = \rho e^{\mathrm{i}\alpha}$ and the local action can be wirtten as:

$$S[U]_{loc} = \frac{\beta}{2}\,\mathrm{Re}(UA) = \frac{\beta}{2}\rho\,\mathrm{Re}(e^{\mathrm{i}\varphi}e^{\mathrm{i}\alpha}) = \frac{\beta}{2}\rho\cos(\varphi+\alpha) \tag{2.3.17}$$

The reflection $\varphi+\alpha \to -\varphi-\alpha$ or the change $\varphi+\alpha \to 2\pi-\varphi-2\alpha$ leave the local action invariant, thus a change of this type is always accepted. For a non-Abelian group, this change is performed through the ansatz:

$$U \to U' = V^\dagger U^\dagger V^\dagger \tag{2.3.18}$$

where V is a gauge group element chosen such that the local action is invariant. The selection probability for a transformation of this kind is symmetric, as can be easily

proven by inverting (2.3.18), obtaining $U = V^\dagger U'^\dagger V^\dagger$.
For the gauge group $SU(2)$, the matrix V is chosen proportional to the sum of staples: $V = \frac{A}{\sqrt{\det(A)}}$, like in (2.3.7). Because of this,

$$\mathrm{Tr}(U'A) = \mathrm{Tr}\Big(V^\dagger U^\dagger V^\dagger \sqrt{\det(A)} V\Big) = \sqrt{\det(A)}\,\mathrm{Tr}\big(V^\dagger U^\dagger\big) = \mathrm{Tr}\big(A^\dagger U^\dagger\big) = \mathrm{Tr}(UA) \tag{2.3.19}$$

therefore the choice for U' leaves the action invariant. In case $\det(A) = 0$, any random link variable is accepted.
As the overrelaxation algorithm leaves the action invariant, it moves the Markov chain in the subspace of constant action, called *micro-canonical* ensemble, thus it is not ergodic: it does not visit every possible point in the configuration space if given enough time. For this reason, it needs to be used in combination with other updating algorithms, such as some steps of the Metropolis or heat bath algorithm.

2.4 Measurements

In this section, the techiniques used to compute the value of some observables are explained. After the proper Monte Carlo algorithms have been iterated a sufficient number of times, the lattice is *thermalized* and measures can be taken. The observables presented below are the plaquettes and Polyakov loops, because they are the ones that will be evaluated in the simulation in the fourth chapter.

2.4.1 Plaquettes

The mean value of the plaquette, indicated as $\langle \square \rangle$, is obtained by evaluating expression (1.2.7) for all possible plaquette in the lattice, summing all the results and taking the trace of the result, divided by the total number of plaquettes present in the lattice. In formulae:

$$\langle \square \rangle = \frac{1}{12 N n_s} \sum_{x \in \Lambda} \sum_{\mu=0}^{3} \sum_{\substack{\nu=0 \\ \nu \neq \mu}}^{3} \mathrm{Re}\,\mathrm{Tr}\, U_{\mu\nu}(x) \tag{2.4.1}$$

where N is the number of color charges (the same N in $SU(N)$), $12 = 4 \cdot 3$ is the total number of ways of choosing the first direction μ times the number of possible ways of choosing the second direction ν, and $n_s = TL_1L_2L_3$ is the total number of sites of the lattice.
The expectation value of the plaquette is important because it is directly linked to the Wilson action, thus it gives an intuition of the thermalization of the lattice.

2.4.2 Polyakov Loops

Polyakov loops are another important observable that will be evaluated in the simulations. In particular, the product of two Polyakov loops will be considered, in order to obtain the static quark potential, as explained in (1.2.14).
In order to achieve better statistics, the discrete translational invariance of the lattice is exploited, by computing the so-called *nonzero momentum Polyakov correlators*: because

of this invariance, the quantity $\langle P(0)P^\dagger(x)\rangle$, with $x \in \Lambda$ is the same as $\langle P(y)P^\dagger(x+y)\rangle$ $\forall y \in \Lambda$, therefore the expectation value is obtained as

$$\langle P(0)P^\dagger(x)\rangle = \frac{1}{n_s}\sum_{y\in\Lambda}\langle P(y)P^\dagger(x+y)\rangle \tag{2.4.2}$$

In this way, from the same configuration, more smaples of the same quantity can be obtained, making the average more statistically accurate.

2.5 Summary of a Simulation

Now that the Monte Carlo algorithms and the way observables are "read" from the lattice have been described, a brief explanation on how a full simulation works is presented.

2.5.1 Initialization

The first step is the initialization: the program reads from a file the size of the lattice (the number of sites in each direction: t, x, y, z), the parameter β (that is the same in the Wilson action (1.2.8)), the thermalization time t_{TH}, the reunitarization period t_U, the number of measurements to be made n_M, the number of updates to be done between each measurement n_{BM} and the start type, either fully ordered (cold start) or totally random (hot start). The number of color charges and other parameters, like the type of measurements that have to be made are set in the source code of the program. Then, according to these parameters, the variables are initialized to the proper value and the simulation can begin.

2.5.2 Thermalization

The thermalization step is needed, as anticipated before, to advance the Markov process up to equilibrium configurations. This is done by updating the configuration with the Monte Carlo algorithms until the number of updates equals the thermalization time t_{TH} indicated in the input file. Every update step consists of a certain number of heat bath steps followed by another number of overrelaxation iterations. Both these numbers are set in the source code and for these simulations 1 iteration of heat bath and 3 of overrelaxation have been used.
The thermalization time is determined by looking, in other simulations, at the behaviour of some observables in different types of start: for instance, when some observable from a cold start assumes a mean value compatible to the one obtained from a hot start, the system is assumed as thermalized.
The thermalization time t_{TH} is then set as 2 or 3 times the number of steps needed to achieve thermalization, in order to keep a certain margin of confidence.
Additionally, every t_U iterations, all the lattice link variables are *reunitarized*, that means that each one matrix is checked, and eventually corrected, that it still is unitary (i.e., $U^\dagger = U^{-1}$), because unitarity can be lost due to computer roundig errors. After each update step, the mean value of the plaquette is written to a file.

2.5.3 Measurements

After the lattice has achieved thermalization, observables can finally be measured. Each observable is computed once, according to the methods illustrated in the previous section, and written to a file, then the system is updated a number of times equal to n_{BM}, with a reunitarization process every t_U updates, in the same way as the thermalization step. This process is iterated until the observables are measured n_M times.
After that, the simulation is concluded.

2.6 Statistical Analysis

In this final section, an overview on the analysis of the data collected from the simulations is given. After a run of the program is finished, usually one has a few thousands expectation values of each observable, obtained in different configurations of the fields. The average of these values is used as an indicator for each observable, with its own statistical error. Let us assume that the values $(o_1, \dots, o_N)$ of some observable O have been computed from a Markov sequence of Monte Carlo generated configurations in equilibrium. The expectation value and variance of these variables are the same:

$$\langle o_i \rangle = \langle O \rangle \qquad \sigma^2_{o_i} = \left\langle (o_i - \langle o_i \rangle)^2 \right\rangle = \sigma^2_O \tag{2.6.1}$$

whose estimators can be:

$$\hat{O} = \frac{1}{N} \sum_{i=1}^{N} o_i \tag{2.6.2}$$

$$\hat{\sigma}^2_O = \frac{1}{N-1} \sum_{i=1}^{N} \left(o_i - \hat{O} \right)^2 \tag{2.6.3}$$

If the values are uncorrelated,

$$\langle o_i o_j \rangle = \langle o_i \rangle \langle o_j \rangle = \langle O \rangle^2 \qquad \forall i \neq j \tag{2.6.4}$$

and the variance $\hat{\sigma}^2_O$ allows to determine the statistical error of $\hat{O}$. In fact, the sample mean value (2.6.2) is itself a random variable, since its value may change from one set of N configurations to another. Its variance is:

$$\begin{aligned}
\sigma^2_{\hat{O}} =& \left\langle \left(\hat{O} - \langle O \rangle \right)^2 \right\rangle = \left\langle \left(\frac{1}{N} \sum_{i+1}^{N} (o_i - \langle O \rangle) \right)^2 \right\rangle = \\
=& \frac{1}{N^2} \left\langle \sum_{i,j=1}^{N} (o_i - \langle O \rangle)(o_j - \langle O \rangle) \right\rangle = \\
=& \frac{1}{N^2} \left\langle \sum_{i=1}^{N} o_i^2 \right\rangle + \frac{1}{N^2} \left\langle \sum_{i \neq j} o_i o_j \right\rangle - \frac{2}{N} \langle O \rangle \sum_{i=1}^{N} o_i + \frac{1}{N^2} \left\langle \sum_{i,j=1}^{N} \langle O \rangle^2 \right\rangle = \\
=& \frac{1}{N} \langle O^2 \rangle + \frac{1}{N^2} \sum_{i \neq j} \langle o_i o_j \rangle - 2 \langle O \rangle^2 + \langle O \rangle^2 = \\
\sigma^2_{\hat{O}} =& \frac{1}{N} \langle O^2 \rangle - \langle O \rangle^2 + \frac{1}{N^2} \sum_{i \neq j} \langle o_i o_j \rangle
\end{aligned} \tag{2.6.5}$$

For uncorrelated o_i, the last two terms cancel each other because of (2.6.4) and

$$\sigma_{\hat{O}}^2 = \frac{1}{N}\sigma_O^2 \tag{2.6.6}$$

Therefore, for N uncorrelated measurements, the standard deviation σ, i.e., the statistical error, is $\sigma_{\hat{O}}$ and the final result is

$$\hat{O} \pm \sigma \quad \text{with} \quad \sigma = \frac{\hat{\sigma}_O}{\sqrt{N}} \tag{2.6.7}$$

As can be easily seen, the statistical error decreases $\propto 1/\sqrt{N}$ with the number of uncorrelated configurations N.

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