Strong Interactions on the Computer: Gauge Theory on the Lattice.

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Abstract

In this work, we investigate the Wilson gauge action of lattice QCD by simulating a pure gauge theory on a four-dimensional lattice of size $6^3 \times 4$, using $SU(2)$ as the gauge group. Gauge-field configurations, represented by the link variables $U_\mu(n)$, are generated via Monte Carlo simulations employing the Metropolis algorithm. After achieving thermalization, we compute the expectation value of the plaquette, $\langle E_p \rangle$, and the specific heat, χ_p. These observables provide insight into the thermodynamic properties of the theory.

1 Introduction

Quantum Chromodynamics (QCD) constitutes one of the fundamental pillars of the Standard Model. However, making reliable predictions for observables associated with particle processes, particularly within the energy ranges accessible to current particle colliders, and even beyond, requires performing highly nontrivial and computationally demanding calculations. In this context, Lattice Gauge Theory provides a powerful framework in which such complex computations become tractable by discretizing spacetime into a finite lattice, effectively replacing the continuum with a computationally manageable approximation. This formalism reaches its full potential when combined with advanced numerical techniques, most notably Monte Carlo methods. These stochastic algorithms allow for the efficient evaluation of path integrals, enabling the extraction of physical quantities such as particle masses, correlation functions, and signatures of phase transitions from non-perturbative numerical methods.

1.1 Short review of QCD

Quantum chromodynamics (QCD) is the theory of strongly interacting particles and fields, i.e., the theory of quarks and gluons which are described by quantum fields following the rules of Quantum Field Theory,

$$\Psi^{(f)}(x)_{\substack{\alpha \\ c}}, \quad \bar{\Psi}^{(f)}(x)_{\substack{\alpha \\ c}} \tag{1}$$

These quark fields carry several indices and arguments. The space–time position is denoted by x, the Dirac index by $\alpha = 1, 2, 3, 4$, and the color index by $c = 1, 2, 3$. Each field $\Psi(f)(x)$ thus has 12 independent components. In addition, the quarks come in several flavors called up, down, strange, charm, bottom, and top, which we indicate by a flavor index $f = 1, 2, ..., 6$. In addition to the quarks, QCD contains gauge fields describing the gluons,

$$A_\mu(x)_{cd} \tag{2}$$

This gluon field carries color indices $c, d = 1, 2, 3$. For given x and μ, the field $A_\mu(x)$ is a traceless, hermitian 3×3 matrix at each space–time point x. With these elements, we can construct the fermionic part $S_F[\Psi, \bar{\Psi}, A]$ of the QCD action as a bilinear functional in the fields Ψ and Ψ. For a single flavor, the contribution to the action is given by (we drop the flavor index and use matrix/vector notation for the color and Dirac indices),

$$S_F[\Psi, \bar{\Psi}, A] = \int d^4x \bar{\Psi}(x)(\gamma_\mu(\partial_\mu + iA_\mu(x)) + m)\Psi(x) \tag{3}$$

In addition, QCD is a gauge invariant theory, since the action above is invariant under the following transformations of the fields:

$$\begin{aligned} \Psi(x) &\to \Psi'(x) = \Omega(x)\Psi(x), \\ \bar{\Psi}(x) &\to \bar{\Psi}'(x) = \bar{\Psi}(x)\Omega(x)^\dagger \end{aligned} \tag{4}$$

similarly for de gluon field

$$A_\mu(x) \to A'_\mu(x) = \Omega(x)A_\mu(x)\Omega(x)^\dagger + i(\partial_\mu\Omega(x))(\Omega(x))^\dagger \tag{5}$$

Which allows us to define the covariant derivative $D_\mu(x) = \partial_\mu + iA\mu$ and its transformation

$$D_\mu(x) \to D'_\mu(x) = \partial_\mu + iA'\mu(x) = \Omega(x)D_\mu(x)\Omega(x)^\dagger \tag{6}$$

The matrices $\Omega(x)$ are required to be unitary, and to have $\det[\Omega(x)] = 1$. Such matrices are the defining representation of the special unitary group, denoted by $SU(3)$ for the case of 3×3 matrices.
The action for the gluon fields $A_\mu(x)$, $S_G[A]$ is a functional of only the gauge fields. In this case we define the field strength tensor $F_{\mu\nu}(x)$ as the commutator

$$F_{\mu\nu}(x) = -i[D_\mu(x), D_\nu(x)] \tag{7}$$

So, the action for the gluon fields reads as follows

$$S_G[A] = \frac{1}{2g^2}\int d^4x \,\mathrm{tr}[F_{\mu\nu}F_{\mu\nu}] \tag{8}$$

where the factor $\frac{1}{g^2}$ counts for the coupling strength of the gauge fields to the quarks.

1.2 Fermión and Gluon action on the Lattice

The first step on the lattice formulation is the introduction of the $4D$ lattice Λ,

$$\Lambda = \{n = (n_1, n_2, n_3, n_4) | n_1, n_2, n_3 = 0, 1, \cdots, N-1; \; n_4 = 0, 1, \cdots, N_T - 1\} \tag{9}$$

The vectors $n \in \Lambda$ label points in space–time separated by a lattice constant a. In our lattice discretization of QCD, we now place spinors at the lattice points only, i.e., our fermionic degrees of freedom are $\Psi(n)$, $\bar{\Psi}(n)$, $n \in \Lambda$. In the lattice, we implement the same transformation $\Omega(n)$ for each lattice side n and transform the fermion fields according to

$$\Psi(n) \to \Psi'(n) = \Omega(n)\Psi(n)\,, \qquad \bar{\Psi}(n) \to \bar{\Psi}'(n) = \bar{\Psi}(n)\Omega(n)^\dagger \tag{10}$$

Thus, for example, the free fermion action reads (setting $A_\mu = 0$ in (3)),

$$S_F^0[\Psi, \bar{\Psi}] = a^4 \sum_{n\in\Lambda} \bar{\Psi}(n) \left(\sum_{\mu=1}^{4} \gamma_\mu \frac{\Psi(n+\hat{\mu}) - \Psi(n-\hat{\mu})}{2a} + m\Psi(n) \right) \tag{11}$$

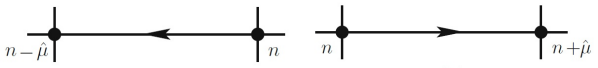
where the gauge invariance is satisfied if we introduce the field $U_\mu(n)$, then

$$\Psi'(n)U'_\mu(n)\Psi'(n+\hat{\mu}) = \bar{\Psi}(n)\Omega(n)^\dagger U'_\mu(n) \times \Omega(n+\hat{\mu})\Psi(n+\hat{\mu}) \tag{12}$$

and the gauge transformation for the new field es defined by

$$U_\mu(n) \to U'_\mu(n) = \Omega(n)U_\mu(n)\Omega(n+\hat{\mu})^\dagger \tag{13}$$

The gauge fields $U_\mu(n)$ are elements of the gauge group $SU(3)$, these matrix-valued variables have a defined orientation and are attached to the links of the lattice, thus they are often referred to as link variables. $U_\mu(n)$ lives on the link which connects the sites n and $n + \hat{\nu}$. Since the link variables are oriented, we can also define link variables that point in the negative μ direction, $U_{-\mu}(n) = U_\mu(n - \hat{\mu})^\dagger$.



(a) $U_{-\mu}(n) \equiv U_\mu(n-\hat{\mu})^\dagger$ (b) $U_\mu(n)$

Figure 1: Link variables $U_\mu(n)$ and $U_{-\mu}(n)$ [1].

Having introduced the link variables and their properties under gauge transformations, we can now generalize the free fermion action (11) to the so-called naive fermion action for fermions in an external gauge field U:

$$S_F^0[\Psi,\bar{\Psi}] = a^4 \sum_{n\in\Lambda} \bar{\Psi}(n) \left(\sum_{\mu=1}^{4} \gamma_\mu \left(\frac{U_\mu(n)\Psi(n+\hat{\mu})}{2a} - \frac{U_{-\mu}(n)\Psi(n-\hat{\mu})}{2a} \right) + m\Psi(n) \right) \tag{14}$$

Let us now discuss the link variables in more detail. In the continuum an object with such transformation properties is known: It is the path-ordered exponential integral of the gauge field A_μ along some curve C_{xy} connecting two points x and y, the so-called *gauge transporter*

$$G(x,y) = P \exp\left(i \int_{C_{xy}} A \cdot ds \right) \tag{15}$$

It is possible to show that $G(x,y)$ follows the same transformations properties as the link variables $U_\mu(n)$ when n and $n+\hat{\mu}$ are considered as end points of a path. Based on these transformation properties, we interpret the link variable $U_\mu(n)$ as a lattice version of the gauge transporter that connects the points n and $n+\hat{\mu}$. For this reason, we introduce algebra-valued lattice gauge fields $A_\mu(n)$ and write

$$U_\mu(n) = \exp(i\, a A_\mu(n)) \tag{16}$$

The lattice action approaches the continuum form in the limit $a \to 0$. So, for small a

$$\begin{aligned} U_\mu(n) &= \mathbb{1} + iaA_\mu(n) + \mathcal{O}(a^2) \\ U_{-\mu}(n) &= \mathbb{1} - iaA_\mu(n-\hat{\mu}) + \mathcal{O}(a^2) \end{aligned} \tag{17}$$

In this way the interaction part of the fermion action reads

$$S_F^I[\Psi,\bar{\Psi},A] = ia^4 \sum_{n\in\Lambda} \sum_{\mu=1}^{4} \bar{\Psi}(n)\gamma_\mu A_\mu(n)\Psi + \mathcal{O}(a) \tag{18}$$

Using (14) and (18) the complete fermion action on the lattice is

$$S_F[\Psi,\bar{\Psi},U] = S_F^0[\Psi,\bar{\Psi}] + S_F^I[\Psi,\bar{\Psi},A] \tag{19}$$

For the gluon action, it is sufficient to use the shortest, nontrivial closed loop on the lattice, the so-called plaquette. The plaquette variable is defined $U_{\mu\nu}(n)$ as a product of only four link variables as follows,

$$\begin{aligned} U_{\mu\nu} &= U_\mu(n) U_\nu(n+\hat{\mu}) U_{-\mu}(n+\hat{\mu}+\hat{\nu}) U{-}\nu(n+\hat{\nu}) \\ &= U_\mu(n) U_\nu(n+\hat{\mu}) U_\mu(n+\hat{\nu})^\dagger U\nu(n)^\dagger \end{aligned} \tag{20}$$

Using the Baker–Campbell–Hausdorff formula to compute the plaquette and the Taylor expansion for $A_\mu(n)$ it is possible to show that

$$U_{\mu\nu} = \exp(ia^2 F_{\mu\nu}(n) + \mathcal{O}(a^3)) \tag{21}$$

Expanding the exponential (21) for small a we can find the expression for the gluon action (8) on the lattice:

$$S_G[U] = \frac{\beta}{N} \sum_{n\in\Lambda} \sum_{\mu<\nu} \mathrm{Re}\,\mathrm{tr}[\mathbb{1} - U_{\mu\nu}(n)] \tag{22}$$

Equation (22) shows the well known Wilson's action, where $\beta = \frac{2N}{g^2}$, for the group $SU(N)$. The Wilson gauge action is a sum over all plaquettes, with each plaquette counted with only one orientation. This sum can be realized by a sum over all lattice points n where the plaquettes are located, combined with a sum over the Lorentz indices $1 \le \mu \le \nu \le 4$.

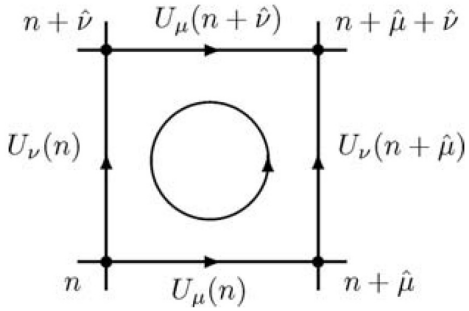


Figure 2: The four link variables which build up the plaquette $U_{\mu\nu}(n)$. The circle indicates the order that the links are run through in the plaquette [1].

1.3 Numerical Simulation of pure Gauge Theory

The vacuum expectation value of an observable in the quantized Euclidean gauge field theory on a lattice is formally given by the functional integral

$$\begin{aligned}\langle O\rangle &= \frac{1}{Z}\int \mathcal{D}[U]\, e^{-S_G[U]}\, O[U] \\ \text{with}\quad Z &= \int \mathcal{D}[U]\, e^{-S_G[U]}\end{aligned} \tag{23}$$

However, this expression cannot be evaluated analytically except for very small lattice volumes. To address this, a Monte Carlo simulation approximates the path integral by averaging the observable over N sampled gauge field configurations U_n, each generated with a probability proportional to $\exp(-S[U_n])$:

$$\langle O\rangle \approx \frac{1}{N}\sum_{n=1}^{N} O[U_n]\,. \tag{24}$$

For a sufficiently large number of configurations, this average provides a reliable estimate of the expectation value. The sequence of configurations is generated via a Markov chain, beginning from an arbitrary initial configuration and evolving through a stochastic process until it samples from the equilibrium distribution $P(U) \propto \exp(-S[U])$. This evolution is realized through a homogeneous Markov process:

$$U_0 \to U_1 \to U_2 \to \cdots$$

In this work, we employ the Metropolis algorithm to construct such a chain and generate new configurations U'. Specifically, we implement this approach for the four-dimensional $SU(2)$ Wilson gauge action. Starting from a given configuration U, a proposed configuration U' differs from U by the update of a single link variable $U_\mu(n) \to U'_\mu(n)$. The Metropolis algorithm then determines whether this new configuration is accepted based on the change in action, ensuring detailed balance and convergence to the correct equilibrium distribution. In four dimensions, this link is shared by six plaquettes, and only these six plaquettes are affected when changing one link variable. Thus, the action changes locally by the amount

$$S[U_\mu(n)']_{loc} = \frac{\beta}{N}\text{Re tr}[6\mathbb{1} - U_\mu(n)'A]\ , \tag{25}$$

where A is given by

$$\begin{aligned}A = \sum_{\nu\neq\mu} &(U_\nu(n+\hat{\mu})U_{-\mu}(n+\hat{\mu}+\hat{\nu})U_{-\nu}(n+\hat{\nu}) \\ &+ U_{-\nu}(n+\hat{\mu})U_{-\mu}(n+\hat{\mu}-\hat{\nu})U_\nu(n-\hat{\nu}))\end{aligned} \tag{26}$$

So, the global change in the action is

$$\begin{aligned}\Delta S =& S[U_\mu(n)']_{loc} - S[U_\mu(n)]_{loc} \\ =& \frac{\beta}{N}\text{Re tr}[(U_\mu(n)' - U_\mu(n))A]\end{aligned} \tag{27}$$

Based on equations (27), we can perform the Metropolis algorithm with single link variable updates and symmetric selection probability as follows,

- Given some gauge field configuration, we choose a site n and direction μ and a candidate value $U_\mu(n)'$.
- Next, we compute the sum over the staples and from this the change in the action ΔS according to (27). If $\Delta S \leq 0$ then the new variable $U_\mu(n)'$ is accepted. In other case, we compute a random number r uniformly distributed in the interval $[0, 1)$ and the new variable is accepted if $r \leq \exp(-\Delta S)$.
- Finally, we repeat these steps from the beginning

This process would lead to a minimum of the action in the configuration space, corresponding to a solution of the classical field equations. However, due to the random variable r also configurations with increased action will be accepted every now and then, which reproduces the quantum fluctuations of the system.

Since a numerical simulation works on a finite lattice, boundary conditions have to be implemented. For gauge fields, one usually uses periodic boundary conditions

$$\begin{aligned}U_\mu(N, n_2, n_3, n_4) &= U_\mu(0, n_2, n_3, n_4) \\ U_\mu(n_1, N, n_3, n_4) &= U_\mu(n_1, 0, n_3, n_4) \\ U_\mu(n_1, n_2, N, n_4) &= U_\mu(n_1, n_2, 0, n_4) \\ U_\mu(n_1, n_2, n_3, N_T) &= U_\mu(n_1, n_2, n_3, 0)\end{aligned} \tag{28}$$

For the present work, we studied link variables, which are elements of the SU(2) group. This group is of interest since it is simpler than SU(3) and is also a subgroup of SU(3). Important ideas, such as topological charge and instantons, which are solutions of the classical equations of motion for the gauge field, can also be formulated in SU(2).
In addition, we start the initial configuration in what is called a *hot start*, which consists of setting the

link variables on the lattice as random elements of the $SU(2)$ (using the Haar measure) gauge group and then proceeding to perform the Metropolis algorithm.

2 Results

The Monte Carlo simulation, along with the Metropolis algorithm for the Wilson action, was performed in Fortran. We employed a lattice volume of $n_i = 6$, $i = 1, 2, 3$ and $N_T = 4$, and we vary the value of the gauge coupling β in intervals, $\beta = 0, 0.05, 0.1, \ldots, 4$. The evolution of the Wilson action was also measured to track the thermalization of the system, as shown in Figure 3. The thermalization is reached after approximately 3000 sweeps for different β values, where a sweep consists of visiting every point of the lattice once. To generate significant statistical results, we performed 10^5 sweeps for each β.

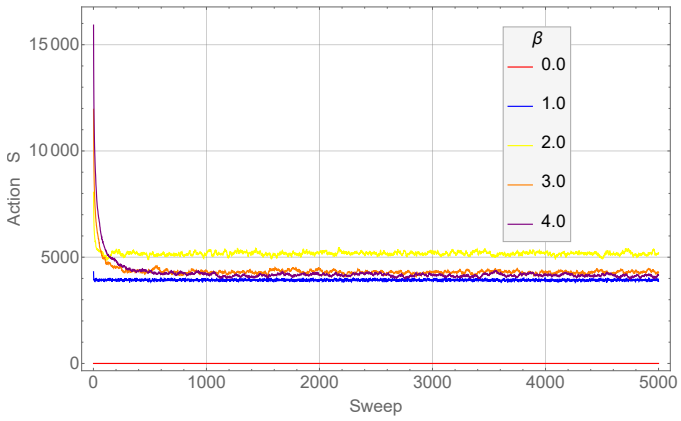


Figure 3: Evolution of Wilson's action (22) within the thermalization range for different values of β.

Within the plateau region of the action (Figure 3), we take measurements of the plaquette value, which is defined as follows

$$S_p[U] = \frac{1}{2}\sum_p \text{Re tr}[U_p] \tag{29}$$

where the sum runs over all plaquettes. We define the plaquette expectation value E_p as

$$E_p = \frac{\langle S_p \rangle}{6 \text{ VOL}} \tag{30}$$

The plaquette expectation value E_p is shown in figure (4), which is consistent with previous findings [5,6]. For small couplings, we observe a linear growth of E_P while for larger couplings, E_P approaches asymptotically to 1. We can also define the specific heat of the system as

$$\chi_p = 6 \text{ VOL} \left(\langle S_p^2 \rangle - \langle S_p \rangle^2\right) \tag{31}$$

Figure 5 shows the measurements of χ_p, where we observe that the specific heat has a maximum at an intermediate coupling value $\beta \sim 2.15$.

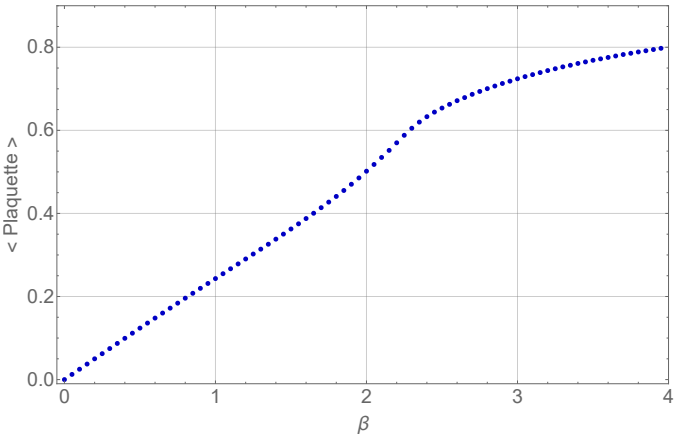


Figure 4: E_p within the thermalization range for different values of β.

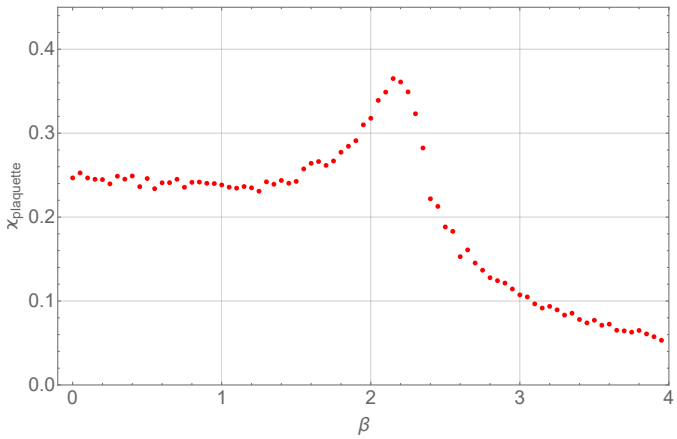


Figure 5: χ_p for different coupling values β.

Conclusions

In this work, we have implemented a lattice simulation of a pure gauge theory using Wilson's action for the gauge group $SU(2)$ on a finite four-dimensional hypercubic lattice. The Monte Carlo algorithm with Metropolis updating allowed us to explore the configuration space and compute relevant observables, in particular the average energy and specific heat, across a range of β values.

These findings demonstrate the capacity of lattice gauge theory and Monte Carlo methods to capture essential non-perturbative aspects of strong interactions. Future work could extend this study by increasing the lattice size to reduce finite-size effects, incorporating dynamical fermions to simulate full QCD, or analyzing additional observables such as Wilson loops or Polyakov lines to further characterize the phase structure.

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