An Introduction to Lattice Quantum Chromodynamics

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Abstract

When $\alpha_s \simeq 1$, such as for low-energy hadronic interactions, perturbation theory fails, so spacetime is discretized into a lattice of points in Lattice Quantum Chromodynamics (LQCD). This makes the path integrals integrate over only finitely many degrees of freedom, so they can be integrated by traditional means. In this paper, we show how this discretization recovers continuum QCD in the limit as lattice spacing goes to zero for a free scalar field and gauge fields, which naturally live on the links between lattice points. Treating fermions the same way leads to an unphysical doubling of fermions, so extra terms are introduced that either damp out the unphysical modes at the cost of breaking chiral symmetry, or damp out the unphysical modes while keeping an alternative form of chiral symmetry at great computational cost. We then review a common Monte Carlo method for carrying out LQCD calculations.

1 Introduction

The fundamental tool behind most calculations for high-energy particle physics (anything to do with Feynman diagram) is perturbation theory, calculating terms proportional to increasing powers of some coupling constant that describes the strength of the force being studied. For electricity and magnetism, this coupling constant is approximately $\alpha_{\text{EM}} \approx \frac{1}{137}$ at energy scales of 511 KeV (the mass of the electron), so perturbation theory becomes very accurate with only a few terms.

However, these “constants” must always be renormalized at each new energy scale, making them slowly-changing functions of the energy scale in question. The coupling constant governing quantum chromodynamics $\alpha_s$ behaves differently from those governing the electroweak interaction - it decreases with energy scale. Only at energies on the order of 10 GeV does it become small enough, $\alpha_s \simeq 0.1$, for perturbation to be effective. We call this behavior asymptotic freedom [7].

On the other hand, at lower energies, the constant grows, so at energy scales corresponding to length scales of 0.1 fm (about the width of a proton), we have $\alpha_s \simeq 1$. When the coupling constant is greater than or equal to one, higher-order terms in perturbation theory matter just as much, if not more than, lower-order terms, so perturbative techniques completely fail. Using perturbative quantum chromodynamics to explain low-energy quark phenomena like quark confinement or nuclear structure is impossible [5].
For low-energy nonperturbative quantum chromodynamics, we need a new theory. Instead of approximating the path integral by expanding it in a series in $\alpha_s$, we make it tractable by discretizing our space. Instead of a continuum of spacetime, we have a lattice of finitely many points with a constant spacing $a$ between them, in a theory called **lattice quantum chromodynamics (LQCD)**. This accomplishes two major tasks: it reduces the path integral to have finitely many degrees of freedom (one for each field at each spacetime point), and it imposes a natural regularization scheme for the theory. Instead of imposing an ultraviolet cutoff by hand, such as in Pauli-Villars regularization, waves with wavelength smaller than $\pi/a$ cannot exist in this discrete space, providing an automatic ultraviolet cutoff [8].

The path integral, while mathematically tractable, is still huge. Standard LQCD simulations use a grid of $64^3 \times 128$ spactime points, with the time dimension twice as long as the other two. For a single field, this is over $3.3 \times 10^7$ degrees of freedom, and calculating this many Gaussian-like integrals using standard numerical techniques is far too computationally expensive to be feasible. Instead, we’ll need to use statistical techniques and **Monte Carlo integration** in any LQCD calculations of this scale.

Now, instead of uncertainties in calculations coming from neglected higher-order terms in perturbation theory, they come from two other sources: the statistical uncertainty from Monte Carlo integration of the path integral, and the systematic uncertainty of discretizing our space and introducing a new dimensionful parameter $a$ [5].

However, LQCD calculations are not so simple as computing correlation functions with path integrals and minimizing error. Discretizing space can violate many important symmetries or introduce nonphysical particles, so studying a variety of ways to represent particles on a lattice is critical for finding a way to preserve all the symmetries relevant to a given problem. Poincare symmetry is easily restored in the continuum limit, and parity symmetries are easy to keep on the lattice. However, chiral symmetry is broken by terms needed to deal with unphysical lattice artifacts, so a major challenge of LQCD is choosing which symmetries to preserve and how, judging between theoretical and computational tradeoffs [2].

### 2 Scalar Field Theory on the Lattice

When constructing a field theory on a lattice, we’ll first need to understand the Fourier transform of our functions so we can work with them in momentum space, as we do in the continuum version. For 1D functions, when they can only take values on $x = na$ for $n \in \mathbb{Z}$, the Fourier transform (1) and inverse Fourier transform (2) are

\[
\begin{align*}
  f(na) &= \int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi} \tilde{f}_a(k) e^{i k a} \quad \text{(1)} \\
  \tilde{f}_a(k) &= a \sum_{n=-\infty}^{\infty} f(na) e^{-i k a} \quad \text{(2)}
\end{align*}
\]

Momentum integration only happens over the region $[-\pi/a, \pi/a]$, called the **Brillouin zone**.
As \( a \to 0 \), the limits of this zone go to infinity, as they should. This idea extends to multiple dimensions, as fields over \( 3 + 1 \)-dimensional spacetime will have momenta over \([-\pi/a, \pi/a]^4\).

It will later be useful to have the delta function in this Fourier transform, but because of the periodicity of the space, we only need to integrate over one segment of the Brillouin zone, not all of \([-\infty, \infty]\). So, if we want to integrate over the delta function and have it normalized, the peak needs to be \( f(na) = \frac{1}{2\pi} \), not \( f(na) = \infty \). Now, we find a periodic kind of delta function when we plug this into (2) to find its Fourier transform,

\[
\delta_P(k) = \frac{a}{2\pi} \sum_n e^{-ina}.
\]  

(3)

This delta function \( \delta_P(k) \), rather than just being nonzero at \( k = 0 \), is nonzero at \( k = 0 \mod 2\pi n \).

To calculate correlation functions for scalar fields, we need to compute

\[
\langle \phi(x)\phi(y)\cdots \rangle = \frac{\int \mathcal{D}\phi(\phi(x)\phi(y)\cdots)e^{-S_E[\phi]} \int \mathcal{D}\phi e^{-S_E[\phi]}}{\int \mathcal{D}\phi e^{-S_E[\phi]}},
\]

where we use the Euclidean action for the scalar field,

\[
S_E[\phi] = \frac{1}{2} \int d^4x \phi(x)(-\Box + m^2)\phi(x).
\]  

(4)

(5)

In the Euclidean metric, the d’Alembertian operator is the usual Laplacian, \( \Box = \sum_{\mu=1}^4 \partial_\mu \partial_\mu \) (indices are only written lowered since raising an index would not create any sign changes in the Euclidean metric).

Now, we can begin discretizing this. We make the obvious coordinate replacements \( x \to na \) (where \( x \) and \( n \) are four-vectors of reals and integers, respectively), \( \phi(x) \to \phi(na) \), and \( \int d^4x \to a^4 \sum_n \) (including the factors of \( a \) to preserve the proper dimension). Discretizing the derivative is a little trickier, since we can no longer take infinitesimal limits. Instead, we’ll make them the smallest finite differences possible. Since the d’Alembertian is a second derivative, we want to compare two derivatives at \( na \) that are as close by as possible. One will need to be the difference between \( \phi \) at \( na \) and \( na + \hat{\mu}a \) (where \( \hat{\mu} \) is the unit vector pointing along the \( \mu \) direction), and the other will need to be the difference between \( \phi \) at \( na \) and \( na - \hat{\mu}a \). Each finite derivative will need to be divided by \( a \), the distance between the adjacent points, and then the differences between these two derivatives needs to be divided by \( a \) again. Summing over all \( \mu \) to calculate the Laplacian, we get

\[
\Box \phi(na) = \sum_\mu \frac{1}{a} \left( \frac{\phi(na + \hat{\mu}a) - \phi(na)}{a} - \frac{\phi(na) - \phi(na - \hat{\mu}a)}{a} \right)
\]

(6)

\[
= \frac{1}{a^2} \sum_\mu (\phi(na + \hat{\mu}a) + \phi(na - \hat{\mu}a) - 2\phi(na)).
\]

(7)

In order to work with dimensionless quantities, which will be more convenient, we’ll define \( \Box \) as (7) without the factor \( 1/a^2 \), so we have to make the replacement \( \Box \phi(x) \to \frac{1}{a} \Box \phi(na) \). Similarly, we can rewrite the other dimensionful quantities with
the natural length scale of the problem, $\hat{\phi}_n \rightarrow a\hat{\phi}(na)$ and $\hat{M} \rightarrow aM$. The correlation function and action (in terms of an operator that will be useful later) for these dimensionless quantities is now

$$<\hat{\phi}_n\hat{\phi}_m\ldots> = \frac{\int (\Pi_id\hat{\phi}_l)(\hat{\phi}_n\hat{\phi}_m\ldots)e^{-S_E[\hat{\phi}]}}{\int (\Pi_id\hat{\phi}_l)e^{-S_E[\hat{\phi}]}}$$

(8)

$$S_E = \frac{1}{2} \sum_{n,m} \hat{\phi}_n K_{nm} \hat{\phi}_m$$

(9)

$$K_{nm} = -\sum_{\mu>0} (\delta_{n+\mu,m} + \delta_{n-\mu,m} - 2\delta_{nm} + \hat{m}^2\delta_{nm}) + \hat{m}^2\delta_{nm}.$$  

(10)

Using the standard result, the generating functional with source functions is

$$Z_0[J] = \frac{1}{\sqrt{\text{det} K}} e^{\frac{1}{2} \sum_{n,m} J_n K_{nm}^{-1} J_m}$$

(11)

so the propagator for dimensionless scalar fields is

$$<\hat{\phi}_n\hat{\phi}_m> = K_{nm}^{-1}.$$  

(12)

To invert this matrix, we can sum it over its inverse, component by component, and set it equal to the Kronecker delta, which we can write in dimensionless momentum space as a Fourier transform across the momentum space $[-\pi, \pi]$.

$$\sum_l K_{nl} K_{lm}^{-1} = \delta_{nm} = \frac{d^4\hat{k}}{(2\pi)^4} e^{ik(n-m)}.$$  

(13)

This will be most natural to solve in momentum space, so if we take the Fourier transform of $K$ and an ansatz for $K^{-1}$,

$$K_{nm} = \int_{-\pi}^{\pi} \frac{d^4\hat{k}}{(2\pi)^4} (4 \sum_{\mu} \sin^2(\frac{\hat{k}_{\mu}}{2}) + \hat{m}^2) e^{ik(n-m)}$$

(14)

$$K_{nm}^{-1} = \int_{-\pi}^{\pi} \frac{d\hat{k}}{(2\pi)^4} G(\hat{k}) e^{ik(n-m)}.$$  

(15)

Solving these in (13), we get

$$K_{nm}^{-1} = \int_{-\pi}^{\pi} \frac{d\hat{k}}{(2\pi)^4} \frac{e^{ik(n-m)}}{4 \sum_{\mu} \sin^2(\frac{\hat{k}_{\mu}}{2}) + \hat{m}^2}$$

(16)

$$= a^2 \int_{-\pi/a}^{\pi/a} \frac{d^4\hat{k}}{(2\pi)^4} \frac{e^{ik(x-y)}}{\sum_{\mu} \hat{k}_{\mu}^2 + m^2}.$$  

(17)
where $\tilde{k}_\mu = \frac{2}{a} \sin(k_\mu a/2)$. We also write it in the dimensionful form (after a change of variables) so we can check the limit as $a \to 0$. Giving the propagator $K_{nm}^{-1}$ the proper dimensions as the continuum propagator through extra factors of $a$, we get

$$\lim_{a \to 0} \frac{1}{a^2} K_{nm}^{-1}(x/a, y/a, ma) = \int_{-\infty}^{\infty} \frac{d^4 k}{(2\pi)^4} \frac{e^{ik(x-y)}}{k^2 + m^2},$$

which is exactly the continuum propagator $\langle \phi(x)\phi(y) \rangle$, just as it should be. This lattice model of free scalar fields gives us the continuum model in the limit $a \to 0$, so we can be confident that we are constructing a physically meaningful theory [8].

(In (18), $k_{nm}^{-1}$ is written with $ma$ dependence since that quantity also changes with the $a$ limit, and we use the limit identity $\lim_{x \to 0} \sin(x)/x = 1$ to simplify them momentum in the denominator.)

If we are to extract physically meaningful results from this lattice theory, there is one more step we need to do. The theory is naturally regularized through the lattice cutoff on momentum, but it is not yet renormalized - the $m$ given in (5) is not yet the mass of the free scalar particle at a given energy. If we can calculate dimensionless results that have no dependence on the discretization of the model, then we can compare these to known continuum results and tune our parameters, such as $m$, accordingly. Since the propagator has units of mass squared, we make it dimensionless by dividing by $m$. Then, in the continuum limit, we ought to have

$$\lim_{a \to 0} \frac{\langle \hat{\phi}_n \hat{\phi}_m \rangle}{\hat{m}} = \frac{\langle \phi(x)\phi(y) \rangle}{m},$$

where $n$ and $m$ refer to points corresponding to $x$ and $y$. If we calculate the left-hand side with increasingly small values of $a$ and find it approaching a constant, we can then tune $\hat{m}$ to a renormalized value that corresponds to the continuum $m$ \footnote{Sometimes, physical values are too computationally expensive, such as light quark masses, so masses can instead be adjusted to computationally lighter values. Several calculations with different parameter values can be used to extrapolate to the calculation at the physical parameter value [5].} [8].

### 3 Fermions on the Lattice and Fermion Doubling

We can begin treating free fermions on a lattice in the same way as we did for the scalar field, but the end result will introduce unphysical fermions, called fermion doubling, unless chiral symmetry can be sacrificed. Wilson fermions are the simplest way to define lattice fermions that match continuum physics in the limit $a \to 0$, but they no longer have chiral symmetry for massless fermions. Other schemes, such as Ginsparg-Wilson fermions, preserve a modified form of chiral symmetry but are significantly more computationally expensive.

Henceforth, when writing the spatial input of a lattice field, it will only be written as $n$, representing a vector of integers, with the spacing $a$ left implicit.

#### 3.1 Free Fermions

We’ll define the fermion action in the Euclidean metric as
\[ S_F = \int d^4x \overline{\psi}(x)(\gamma^E_\mu \partial_\mu + M)\psi(x) \] (20)

where the Euclidean gamma matrices are \( \gamma^E_4 = \gamma^0 \) and \( \gamma^E_i = -i\gamma^i \). We discretize the path integrals and rewrite all the quantities to be dimensionless like before, with the only key difference being that the first derivative is symmetric about \( n \), comparing the points \( n + \hat{\mu} \) and \( n - \hat{\mu} \). The distance between them is \( 2a \), but we will drop the \( a \) so the derivative \( \hat{\partial}_\mu \) can be defined to be dimensionless.

\[ \hat{\partial}_\mu \hat{\psi}_\alpha(n) = \frac{1}{2}(\hat{\psi}_\alpha(n + \hat{\mu}) - \hat{\psi}_\alpha(n - \hat{\mu})) \] (21)

where \( \alpha \) is the spinor index. Now, our fermion action is

\[ S_F = \sum_{n,m,\alpha,\beta} \overline{\psi}_\alpha(n)K_{\alpha\beta}(n,m)\hat{\psi}_\beta(m) \] (22)

\[ K_{\alpha\beta}(n, m) = \sum_\mu \frac{1}{2}(\gamma_\mu)_{\alpha\beta}(\delta_{m,n+\hat{\mu}} - \delta_{m,n-\hat{\mu}}) - \hat{M}\delta_{mn}\delta_{\alpha\beta}. \] (23)

Then, through usual continuum path integral methods [7], we know that \( K_{\alpha\beta}^{-1} \) is the propagator for \( \langle \hat{\psi}_\alpha(n)\overline{\psi}_\beta(m) \rangle \). Solving for it using the same techniques from Section II, we get

\[ K_{\alpha\beta}^{-1}(n, m) = a^2 \int_{-\pi/a}^{\pi/a} d^4p \frac{(-i\sum \gamma_\mu \vec{p}_\mu + M)_{\alpha\beta} e^{ip(x-y)}}{(2\pi)^4 \sum_\mu \vec{p}_\mu^2 + M^2} \] (24)

where \( \vec{p}_\mu = \frac{a}{2} \sin(p_\mu a) \). If we take the \( a \to 0 \) limit like in the scalar field case, it seems like we should get the continuum result for the fermion propagator, but the lack of a factor of \( \frac{1}{2} \) in the period for \( \vec{p}_\mu \) makes a critical difference [8].

As the momentum ranges over the Brillouin zone, a value at a corner of the zone, such as \( p_\mu = (\pm \pi/a, 0, 0, 0) \), gives the same value for \( \vec{p}_\mu \) as the momentum \( p_\mu = (0, 0, 0, 0) \). As we take the \( a \to 0 \) limit, these other momentum modes are also valid solutions to the fermion propagator (which would not have been the case in the free scalar propagator, since the factor of \( 1/2 \) in (17) prevents any other momentum in the Brillouin zone from reaching another zero of sine). There are a total of sixteen such modes that fulfill the propagator, since we can choose for each momentum coordinate whether it lies in the center (0) or the edge (\( \pm \pi/2 \)) of the zone, giving us \( 2^d \) fermion modes. Each of these is a valid fermion particle, so where we ought to have one fermion in the continuum limit, we have sixteen. We call these excess fermions **doubler fermions** [3].

This is a fundamental problem, not just because of this particular approach to discretization. According to the **Nielsen-Ninomiya theorem**, one cannot define lattice fermions having exact, continuum-like chiral symmetry without introducing doubler fermions [3]. In figuring out how to deal with the doubler fermions, we will explore a few approaches that make different tradeoffs with sacrificing symmetries and computational efficiency.
3.2 Fermion Doubling and Wilson Fermions

Since we already have nonphysical results from our lattice fermion action, we can add other nonphysical terms to potentially dampen these effects. Any artificial terms we add to the action to cancel out doubled fermions needs to have at least one factor of \(a\), so that when we take the continuum limit, the nonphysical term vanishes. The simplest such term, for Wilson fermions, is

\[ S_W = -\frac{r}{2} \sum_n \bar{\psi}(n) \hat{\Box} \psi(n), \]  

(25)

where \(r\) is the Wilson parameter, a dimensionless coefficient that determines the strength of the term. If we rewrite this in terms of dimensionful fields to take the continuum limit, each \(\hat{\psi}\) contributes \(a^{3/2}\) and the \(\hat{\Box}\) contributes \(a^2\), for a total of \(a^5\). As we take the sum to an integral over \(d^4\hat{x}\), each \(\hat{x}\) contributes \(1/a\), so the expression we use for the continuum limit is proportional to \(a^5\). Thus, it vanishes in the continuum limit, exactly what we need it to do.

The Wilson term modifies the free Fermion action so it becomes

\[ S_{F,W} = \sum_{n,m} \bar{\psi}_\alpha K_{W,\alpha\beta}(n,m) \psi_\beta(m) \]  

(26)

\[ K_{W,\alpha\beta}(n,m) = (\hat{M} + 4r) \delta_{nm} \delta_{\alpha\beta} - \frac{1}{2} \sum_\mu ((r - \gamma_\mu)_{\alpha\beta} \delta_{m,n+\hat{\mu}} + (r + \gamma_\mu)_{\alpha\beta} \delta_{m,n-\hat{\mu}})[8]. \]  

(27)

There are two important features. First, it is normally the mass term in the fermion Lagrangian that breaks chiral symmetry [7]. Now that there is a nonzero term \(4r\) along with the mass that doesn’t vanish as \(\hat{M} \to 0\), that chiral symmetry-breaking term will always be present. Any interactions that depend on chiral symmetry, such as \(K \to \pi\pi\) decays [5], will need to use another fermion scheme.

However, the other feature is that, when we calculate the new fermion propagator, the primary change is that the mass is now dependent on momentum,

\[ M(p) = M + \frac{2r}{a} \sum_\mu \sin^2 \left( \frac{P_\mu a}{2} \right). \]  

(28)

This has a term dependent on sine of the momentum, like the momentum in (24) which leads to the doubler fermions with momenta on the corners of the Brillouin zone. So, when a doubler fermion has such a momentum mode, it gets a new contribution to its mass that was not present for the original fermion [3]. As we take the limit \(a \to 0\), the doubler fermions become infinitely massive and lose any dynamics, giving us the proper physical continuum limit.

3.3 Ginsparg-Wilson Fermions and Preserving Chiral Symmetry

Now that we understand gauge fields on the lattice, we can define a new kind of fermion that prevents the doubling problem but also preserves a kind of chiral symmetry on the lattice.
Let $K$ be our Dirac operator, the operator which gives us the fermion action (in examples like (23) and (27)). If $K$ obeys the anticommutation relation

$$\{K, \gamma_5\} = aK\gamma_5K$$

(29)

then we can define a new kind of chiral symmetry that applies to the lattice. If we transform our fermion fields as

$$\delta \hat{\psi} = \epsilon \gamma_5 (1 - \frac{a}{2}K) \hat{\psi}$$

(30)

$$\delta \overline{\psi} = \epsilon \overline{\psi} (1 - \frac{a}{2}K) \gamma_5,$$

(31)

then the fermion action is invariant [1].

There are potentially many operators that satisfy (29), but one of the most commonly-used ones is the given $K$, defined as

$$A = 1 - aK_W$$

(32)

$$K = \frac{1}{a}(1 - \frac{A}{\sqrt{AA^\dagger}})[6].$$

(33)

This operator gives us the proper continuum limit. As $a \to 0$, $\sqrt{AA^\dagger} \to 1$, so the $1/a$ and $1/(a\sqrt{AA^\dagger})$ terms cancel. Then, the factors of $1/a$ and $a$ in the $K_W/\sqrt{AA^\dagger}$ term cancel, and we get the operator from (27), which we already showed has the proper continuum limit.

While this operator preserves a kind of chiral symmetry while also eliminating doubler fermions (a property it inherits from $K_W$), there are immense computational costs to using this operator, chiefly because of calculating and then inverting $\sqrt{AA^\dagger}$ [5]. If a calculation is not dependent on chiral symmetry, sacrificing it for greater computational speed may be desirable.

4 Gauge Fields on the Lattice

We are using almost exclusively the lattice fields in the next section, so I will drop the hats from the notation and assume that all fields are lattice fields. For theoretical ease, we will also assume that all fermions are Wilson fermions, using the Dirac operator (27).

Now that we have a notion of fermions on the lattice, we want to make these fermions gauge invariant under an $SU(N)$ group, and in the process, create a lattice equivalent of the gauge fields that should (hopefully) reproduce gauge bosons in the continuum limit.

Our lattice fermions transform under local gauge transformations $G(n) \in SU(N)$ just as they do in the continuum,

$$\psi(n) \to G(n)\psi(n)$$

(34)

$$\overline{\psi}(n) \to \overline{\psi}(n)G^{-1}(n),$$

(35)
and like in the continuum, these local gauge transformations need to be mediated by some other factor when the interacting fields are at two different spacetime points. This \( U_{n,m} \) needs to transform like an element of \( SU(N) \), making it an element of \( SU(N) \) itself.

\[
U_{n,m} \to G(n)U_{n,m}G^{-1}(m). \tag{36}
\]

Now, whenever our lattice Fermion Lagrangian has terms with fields at different spacetime points, we need to insert this gauge field to maintain local gauge invariance,

\[
\bar{\psi}(n)(r - \gamma_\mu)\psi(n + \hat{\mu}) \to \bar{\psi}(n)(r - \gamma_\mu)U_{n,n+\hat{\mu}}\psi(n + \hat{\mu}) \tag{37}
\]

\[
\bar{\psi}(n + \hat{\mu})(r + \gamma_\mu)\psi(n) \to \bar{\psi}(n + \hat{\mu})(r + \gamma_\mu)U_{n+\hat{\mu},n}\psi(n). \tag{38}
\]

For hermiticity, we need \( U_{n+\hat{\mu},n} = U_{n,n+\hat{\mu}}^\dagger \).

Since \( U_{n,n+\hat{\mu}} \) is defined in terms of a single point \( n \) and a direction from that point \( \hat{\mu} \), we can think of it as lying on the link between the two lattice points \( n \) and \( n + \hat{\mu} \). Even more, because \( \hat{\mu} \) is directed, this “link field” is also directed.

Since this \( U_\mu(n) \), as we will now write it to express its position and direction as a link, is in \( SU(N) \), we can write it as an exponentiated element of the Lie algebra,

\[
U_\mu(n) = e^{i\phi_\mu(n)}. \tag{39}
\]

The field \( \phi_\mu \) is dimensionless, but we can relate it to the more physically meaningful dimensionful gauge field \( A_\mu \) in the Lie algebra for \( SU(N) \) (where \( A_\mu = A_\mu^a t^a \) in terms of the generators \( t^a \) of \( SU(N) \)).

\[
\phi_\mu(n) = g_0 a A_\mu(n). \tag{40}
\]

Note that the coupling constant, \( g_0 \), is an unphysical bare parameter and pertains only to physics on the lattice.

To find an analog of \( F_{\mu\nu} \) for lattice gauge fields, it helps to think of \( F_{\mu\nu} \) geometrically, as the measurement of the infinitesimal curvature of the space. We’ll need a product of gauge fields about a two-dimensional loop (but since “loop” already means something else important, I will call these “plaquettes”). Going first in the \( \mu \) direction then in the \( \nu \) direction, and using \( \dagger \) to write the fields in terms of simpler base points if it is more useful to reverse the direction, we have, as the curvature at one point \( n \) measured in the \( \mu \) and \( \nu \) directions (Fig. 1),

\[
U_{\mu\nu}(n) = U_\mu(n)U_\nu(n + \hat{\mu})U_\mu^\dagger(n + \hat{\nu})U_\nu^\dagger(n) \tag{41}
\]

\[
\equiv e^{ig_0 a^2 F_{\mu\nu}(n)}. \tag{42}
\]

We define the curvature tensor so the lattice version of \( F_{\mu\nu} \) (conceptually, the infinitesimal curvature) is in the field exponentiated to get the larger curvature, with the appropriate coupling constant and factors of \( a \) to make the exponent dimensionless.

By expressing each field in the product in (41) in terms of (39) and (40), with \( A_\mu \) and \( A_\nu \) Lie algebra fields, we can use the Baker-Campbell-Hausdorff identity to relate the two in a series. Taking the continuum limit \( a \to 0 \), we will find, for continuum fields,
Figure 1: The product of gauge field links at a point \( n \) in the \( \mu \), then \( \nu \) directions. This is the lattice equivalent of the infinitesimal curvature at \( n \) and gives us the field \( e^{ig_0 a^2 F_{\mu\nu}} \).

\[
F_{\mu\nu} = \partial_\mu A_\nu \partial_\nu A_\mu + ig_0 [A_\mu, A_\nu],
\]

(43)

just as we should.

Now that we have a lattice analog of the fields \( F_{\mu\nu} \), we would like to get a term like the one for the continuum gauge field action,

\[
S_{\text{Gauge}}^\text{cont.} = \frac{1}{2} \text{Tr} \int d^4 x F_{\mu\nu} F_{\mu\nu}.
\]

(44)

We can recover this in the limit for small \( a \) (as we would do when taking the continuum limit) in terms of the gauge links with the action

\[
S_{\text{Gauge}} = c \text{Tr} \sum_{n,\mu<\nu} \left( 1 - \frac{1}{2} (U_{\mu\nu}(n) + U_{\mu\nu}^\dagger(n)) \right),
\]

(45)

where we only sum over \( \mu < \nu \) to make sure not to double-count the same plaquettes, and \( c \) is an undetermined coefficient. If we take the continuum limit, we’ll find

\[
S_G \to c \frac{g_0^2}{2} S_{\text{Gauge}}^\text{cont.},
\]

(46)

so we need \( c = \frac{2}{g_0^2} \) in order to make the proper limit. This makes the lattice gauge action

\[
S_{\text{Gauge}}^\text{lattice} = \beta \sum_{\text{loops } P} \left( 1 - \frac{1}{2N} \text{Tr}(U_P + U_P^\dagger) \right)
\]

(47)

where \( \beta = \frac{2N}{g_0^2} \) \cite{3}.

5 Monte Carlo Calculations on the Lattice

Now that we know how to describe fermion fields and gauge fields on a lattice, as well as add other terms that keep important symmetries or suppress nonphysical artifacts, we can calculate the path integrals numerically. However, even though we now have finitely many
degrees of freedom (making the path integrals make perfect mathematical sense) to integrate over, we need to use statistical Monte Carlo methods to evaluate such an integral.

However, there is one more detail about fermions that needs to be addressed before they can be properly numerically simulated. While there are many well-developed numerical techniques for simulating integrals with numbers that behave like normal numbers (such as for bosonic fields), these generally do not apply to integrals of Grassmann numbers. In order to compute fermionic fields as bosonic fields, we integrate out the fermion fields so their path integrals are expressed in terms of bosonic fields. When $K$ is the Dirac operator for the fermions, we treat the fermionic integral as a continuous limit of Gaussian integrals so we can express it as a determinant, which we can then in turn express with bosonic fields ("ghosts"), $\chi$ and $\chi^\dagger$.

$$\frac{1}{Z} \int [d\bar{\psi}] [d\psi] e^{-S(\phi) - \bar{\psi}K\psi} = \frac{1}{Z'} \det(K) e^{-S(\phi)} = \frac{1}{Z''} \int [d\chi^\dagger][d\chi] e^{-S(\phi) - \chi^\dagger(K^\dagger K)^{-1}\chi},$$

where $S(\phi)$ represents the action of the bosonic fields and $Z, Z', Z''$ are constants which absorb unimportant normalizations. Now, we can integrate over all fields using standard numerical techniques.

Rather than integrate over every possible field configuration, we need to generate a random sampling of them, weighted by $e^{-S(\phi)}$ where $S(\phi)$ is the action of a given bosonic field. After calculating the path integral for some operator $\Omega$, we average over $N$ path integrals to get $\langle \Omega \rangle$, with the usual counting uncertainty $1/\sqrt{N}$.

To get these field configurations, we can start with a simple field configuration and then generate new ones through an iterative process, where the new configuration is constructed from the previous ones. Ideally, we should minimize the correlation between successive field configurations so we get a random sampling of the phase space of field configurations. If the process is ergodic (eventually moves through all of phase space) and obeys the probability relationship of detailed balance, a condition about its reversibility, then we know it will eventually converge to a fixed-point distribution of the probabilities of the configurations it generates. If this is true, then the process is "memoryless" with respect to whatever field configuration seeds the process, as it should be for a random distribution.

If $P(\phi_i \to \phi_j)$ is the probability of the process producing field configuration $\phi_j$ from field configuration $\phi_i$, and $\rho(\phi_i)$ is the probability density of $\phi_i$ in the space of configurations generated by the Markov process after it has reached equilibrium (become independent of its initial conditions), the detailed balance condition is

$$\rho(\phi_i)P(\phi_i \to \phi_j) = \rho(\phi_j)P(\phi_j \to \phi_i).$$

A commonly-used method for generating field configurations in this way for LQCD calculations is to introduce a new nonphysical Hamiltonian to evolve the fields. For the action $S(\phi)$ of whatever bosonic fields are involved and a nonphysical momentum $\pi$, where the initial momentum $\pi$ is chosen from a Gaussian distribution of momenta centered at 0, the Hamiltonian and initial momenta distribution are
Then, we evolve a given field configuration and its momentum for a fixed time $\tau_0$, a nonphysical “time” applying only to this momentum. After solving Hamilton’s equations numerically to evolve it, we have a new field configuration. Generating field configurations in this way, the probability of any given field configuration is $\rho(\phi) = e^{-S(\phi)}$.

To see if this process satisfies detailed balance, we first need to use that, for field configurations $(\phi_i, \pi_i)$ and $(\phi_j, \pi_j) = (\phi_i(\tau_0), \pi_i(\tau_0))$,

\[
\rho(\phi_i)\rho_P(\pi_i) \propto e^{-\pi_i^2/2 - S(\phi_i)} = e^{-H(\phi_i, \pi_i)} \tag{52}
\]

\[
\rho(\phi_j)\rho_P(\pi_j) \propto e^{-\pi_j^2/2 - S(\phi_j)} = e^{-H(\phi_j, \pi_j)}. \tag{53}
\]

Since $H$ is conserved across any field configurations it evolves, the product of these two probability distributions are equal.

To get the total probability of our process transitioning between configurations $\phi_i \to \phi_j$, we need to integrate over all possible momenta configurations they could have. Where $P_H((\phi_i, \pi_i) \to (\phi_j, \pi_j))$ is the probability of our Hamiltonian evolving from the first state to the second, this total probability is

\[
P(\phi_i \to \phi_j) = \int [d\pi_i][d\pi_j]\rho_P(\pi)P_H((\phi_i, \pi_i) \to (\phi_j, \pi_j)). \tag{54}
\]

This $P_H$ is just a delta function for $(\phi_i(\tau_0), \pi_i(\tau_0))$ and $(\phi_j, \pi_j)$ since the Hamiltonian is deterministic. Since a Hamiltonian is also time-reversible, we also have $P_H((\phi_i, \pi_i) \to (\phi_j, -\pi_j)) = P_H((\phi_j, -\pi_j) \to (\phi_i, -\pi_i))$, and since $P_P$ is symmetric under $\pi_i \to -\pi_i$, we can integrate over this reverse process for $P_{\phi_j \to \phi_i}$. This gives us

\[
\int [d\pi_i][d\pi_j]\rho(\phi_i)\rho_P(\pi_i)P_H((\phi_i, \pi_i) \to (\phi_j, \pi_j)) = \int [d\pi_i][d\pi_j]\rho(\phi_j)\rho_P(-\pi_i)P_H((\phi_j, -\pi_j) \to (\phi_i, -\pi_i))
\]

which integrates out with (54) to give us the detailed balance condition [4].

References


