LGT unit 3 lecture 1

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1 Introduction

In this unit we discuss fermions on the lattice. This first lecture will be about discretizing the continuum QCD action, and showing the need for different fermion formulations due to the appearance of doublers in the naive lattice quark propagator.

The main references used were Christoph Lehner's lecture notes, chapter 10 and 11, Gattringer and Lang section 2.2, chapter 5, and Montvay and Munster section 4.2

2 Continuum QCD

We begin by quickly looking at QCD in the continuum, to familiarize ourselves with a few concepts that we will need once we go to the lattice.

First, our fermion fields, denoted by ψ and $\overline{\psi}$, are Dirac 4-spinors that carry a Dirac index, a color index, a flavor index, and a spacetime argument. Conventionally we separate the action into fermionic parts and gluonic parts, where the fermionic parts depends on all fields, and the gluonic part is a pure gauge action.

We can write the free fermion action as

$$S_F^0[\psi,\overline{\psi}] = \int d^4x\overline{\psi}(x)\left(\gamma_\mu\partial_\mu + m\right)\psi(x) \tag{1}$$

This is not gauge invariant - this has nontrivial transformation properties under a local SU(3) transformation $\Omega(x)$. This is because the fields transform as

$$\psi(x) \to \psi'(x) = \Omega(x)\psi(x), \quad \overline{\psi}(x) \to \overline{\psi}'(x) = \overline{\psi}(x)\Omega^\dagger(x) \tag{2}$$

The action becomes

$$S_F^0[\psi',\overline{\psi}'] = \int d^4x\overline{\psi}\Omega(x)^\dagger(x)\left(\gamma_\mu\partial_\mu + m\right)\Omega(x)\psi(x) \tag{3}$$

This becomes gauge invariant if we introduce the gauge field with transformation properties

$$A_\mu(x) \to A'_\mu(x) = \Omega(x)A_\mu\Omega(x)^\dagger + i(\partial_\mu\Omega(x))\Omega(x)^\dagger \tag{4}$$

such that the extra term from the derivative with respect to the gauge transformation cancels. This introduces the covariant derivative

$$D_\mu = (\partial_\mu + iA_\mu) \tag{5}$$

$D_\mu \psi$ transforms like ψ under gauge transformations, so a bilinear with the covariant derivative is invariant under gauge transformations.

Now we can write the full fermionic continuum QCD action,

$$S_f[\psi, \overline{\psi}, A] = \sum_{f=1}^{N_f} \int d^4x \overline{\psi}^{(f)}(x) \left(\gamma_\mu (\partial_\mu + iA_\mu(x)) + m^{(f)} \right) \psi^{(f)}(x) \tag{6}$$

Where we use vector or matrix notation for the flavor, Dirac, and color indices. We have written a gauge invariant action for fermions at the cost of introducing a term that couples the gauge field to the fermion fields. This is the key point here, because we will see a similar thing in the lattice theory.

3 Naive discretization

Let's make an attempt at discretizing the free fermion action first. We introduce the lattice Λ where a site $n \in \Lambda$ is a four component vector, $n = (n_1, n_2, n_3, n_4)$, in $[0, N-1]$ for the spatial components, and in $[0, N_t - 1]$ for the time extent. Lattice spacing is a. We have toroidal boundary conditions $f(n + \hat{\mu} N_\mu) = e^{i2\pi\theta_\mu} f(n)$, for each direction. We place spinors at the lattice points, so we write the spacetime argument of our fermion fields as $\psi(n)$, where the physical spacetime point is $x = an$.

We want to discretize the free fermion action first. This requires two things, writing the integral as a sum, and writing the derivative as a finite difference.

$$\int d^4x \to a^4 \sum_{n\in\Lambda}, \quad \partial_\mu \psi(n) \to \frac{1}{2a}(\psi(n + \hat{\mu}) - \psi(n - \hat{\mu})$$

$$S_F^0[\psi, \overline{\psi}] = a^4 \sum_{n\in\Lambda} \overline{\psi}(n) \left(\sum_{\mu=1}^{4} \frac{\psi(n + \hat{\mu}) - \psi(n - \hat{\mu})}{2a} + m\psi(n) \right) \tag{7}$$

Once again, we see this form of the action is not gauge invariant. Similarly to the continuum case we need to introduce the gauge field, or in the lattice theory the gauge links, to make this invariant under local SU(3) transformations.

On the lattice, we implement a gauge transformation by choosing $\Omega(n) \in$ SU(3) for each lattice site, where the fields transform the same way that they do in the continuum. In particular though, we are interested in the transformation of the bilinear

$$\overline{\psi}(n)\psi(n + \hat{\mu}) \to \overline{\psi}'(n)\psi'(n + \hat{\mu}) = \overline{\psi}(n)\Omega(n)^\dagger \Omega(n + \hat{\mu})\psi(n + \hat{\mu}) \tag{8}$$

Clearly this isn't gauge invariant. However, if we introduce the gauge links, which transform like

$$U_\mu(n) \to U'_\mu(n) = \Omega(n) U_\mu(n) \Omega(n+\hat{\mu})^\dagger \tag{9}$$

in between the fermion fields in this bilinear form,

$$\overline{\psi}'(n) U'_\mu(n) \psi'(n+\hat{\mu}) = \overline{\psi}(n) \Omega(n)^\dagger U'_\mu(n) \Omega(n+\hat{\mu}) \psi(n+\hat{\mu}) \tag{10}$$

we find that it is gauge invariant. Once again, in the discretized theory, we are required to introduce the gauge links to ensure gauge invariance of the fermion action. Similar to the covariant derivative in the continuum, these are called covariant shifts, and they are denoted by $C^{\pm}_\mu$. Explicitly they are defined as

$$C^{+}_\mu \psi(x) = U_\mu(x) \psi(n+\hat{\mu}), \quad C^{-}_\mu \psi(n) = U^\dagger_\mu(n-\hat{\mu}) \psi(n-\hat{\mu}). \tag{11}$$

Finally we can write the naive lattice fermion action as

$$S_F[\psi, \overline{\psi}, U] = a^4 \sum_{n\in\Lambda} \overline{\psi}(n) \left(\sum_{\mu=1}^{4} \gamma_\mu \frac{U_\mu(n)\psi(n+\hat{\mu}) - U_{-\mu}(n)\psi(n-\hat{\mu})}{2a} + m\psi(n) \right) \tag{12}$$

where $U_{-\mu} = U_\mu(n-\hat{\mu})^\dagger$.

4 The appearance of doublers

With this naively discretized quark action in hand, we can define the lattice Dirac operator. We first rewrite the action (restricting ourselves to one flavor for now)

$$S_F[\psi, \overline{\psi}, U] = a^4 \sum_{n,m\in\Lambda} \sum_{a,b,\alpha,\beta} \overline{\psi}(n)_{\alpha,a,i} D_{i,n;j,m}(U)_{\alpha,a;\beta,b} \psi(m)_{\beta,b,j} \tag{13}$$

where we explicitly write the naive Dirac operator as

$$D_{i,n;j,m}(U)_{\alpha,a;\beta,b} = \sum_{\mu=1}^{4} (\gamma_\mu)_{\alpha\beta} \frac{U_\mu(n)_{ab}\delta_{n+\hat{\mu},m} - U_{-\mu}(n)_{ab}\delta_{n-\hat{\mu},m}}{2a} + m\delta_{\alpha\beta}\delta_{ab}\delta_{n,m} \tag{14}$$

Next what we want to do is calculate the quark propagator for free lattice fermions. We set $U_\mu = \mathbb{I}$, and we use a discrete Fourier transform on the above form of the naive lattice Dirac operator. Fourier transforms on the lattice look like

$$\tilde{f}(p) = \frac{1}{\sqrt{|\Lambda|}} \sum_{n\in\Lambda} f(n) \exp(-ip\cdot na) \tag{15}$$

Where we can define the lattice in momentum space $\tilde{\Lambda}$, The momenta $p \in \tilde{\Lambda}$ are defined in each direction by $p_\mu = \frac{2\pi}{aN_\mu}(k_\mu + \theta_\mu$ where $k_\mu = -\frac{N_\mu}{2} + 1, ..., \frac{N_\mu}{2}$, where θ_μ is a boundary phase, 0 for periodic BC's and 1/2 for anti-periodic BC's. For fermions we generally take periodic BC's in space and antiperiodic BC's in time, due to the negative sign appearing in the expression of a trace as a Grassmann integral. Thus the lattice momenta takes values in the periodic Brillouin zone $p_\mu \in (-\pi/a, \pi/a]$.

We must Fourier transform the two spacetime arguments independently,

$$\begin{aligned}\tilde{D}(p|q) &= \frac{1}{|\Lambda|}\sum_{n,m\in\Lambda} e^{-ip\cdot na} D(n|m) e^{iq\cdot ma} \\ &= \frac{1}{|\Lambda|}\sum_{n\in\Lambda}\left(\sum_{\mu=1}^{4}\gamma_\mu \frac{e^{+iq_\mu a} - e^{-iq_\mu a}}{2a} + m\mathbb{I}\right) \\ &= \delta(p-q)\tilde{D}(p)\end{aligned} \tag{16}$$

Where

$$\tilde{D}(p) = m\mathbb{I} + \frac{i}{a}\sum_{\mu=1}^{4}\gamma_\mu \sin(p_\mu a) \tag{17}$$

We can see that the Dirac operator is diagonal in momentum space, thus to calculate the quark propagator, the inverse of the position space Dirac operator, we simply need to invert the 4×4 matrix $\tilde{D}(p)$, and then do an inverse Fourier transform.

Using the formula for inverting a linear combination of gamma matrices,

$$\left(a\mathbb{I} + i\sum_{\mu=1}^{4}\gamma_\mu b_\mu\right)^{-1} = \frac{a\mathbb{I} - i\sum_{\mu=1}^{4}\gamma_\mu b_\mu}{a^2 + \sum_{\mu=1}^{4} b_\mu^2} \tag{18}$$

we can write

$$\tilde{D}(p)^{-1} = \frac{m\mathbb{I} - ia^{-1}\sum_\mu \gamma_\mu \sin(p_\mu a)}{m^2 + a^{-2}\sum_\mu \sin(p_\mu a)^2} \tag{19}$$

Then we do an inverse Fourier transform

$$D^{-1}(n|m) = \frac{1}{|\Lambda|}\sum_{p\in\tilde{\Lambda}} \tilde{D}(p)^{-1} e^{ip\cdot(n-m)a} \tag{20}$$

We eliminate the second momentum sum with the delta function. The sum is over all momenta sites in momenta space, where the lattice in momentum space is defined by sites $p_\mu = \frac{2\pi}{aN_\mu k_\mu}$.

The quark propagator is quite the important object, and it will come up in our study of fermionic correlation functions later. For free fermions we will analyze the quark propagator in momentum space, $\tilde{D}(p)^{-1}$. Let's look at the massless fermion case,

$$\tilde{D}(p)^{-1}\Big|_{m=0} = \frac{-ia^{-1}\sum_\mu \gamma_\mu \sin(p_\mu a)}{a^{-2}\sum_\mu \sin(p_\mu a)^2} \to \frac{-i\sum_\mu \gamma_\mu p_\mu}{p^2} \tag{21}$$

Where the right arrow indicates the continuum limit here.

The last expression is the continuum limit massless quark propagator, and it clearly has a pole at $p = (0, 0, 0, 0)$. This corresponds to a single fermion described by the continuum Dirac operator. On the lattice, as we can see, the denominator of the massless free quark propagator has a sine squared, we have additional poles. Whenever all components are either $p_\mu = 0$ or $p_\mu = \pi/a$, we have a pole. Momentum space contains all momenta $p_\mu \in (-\pi/a, \pi/a]$ with the boundaries identified, so we cannot simply exclude these extra poles. Therefore, this naive propagator has $2^4 = 16$ poles, the one at $p = (0, 0, 0, 0)$ and 15 other poles, $p = (\pi/a, 0, 0, 0), (0, \pi/a, 0, 0), ..., (\pi/a, \pi/a, \pi/a, \pi/a)$. We have a quark propagator that describes the massless mode we are interested in, along with 15 other unwanted poles, which we call doublers. Each doubler is at a corner of the Brillouin zone. With free fermions, we might be able to tolerate an increase in the degrees of freedom, but in the interacting theory, these extra fermions can be pair-produced through interactions of the fermion field, so they affect the physics in a non-trivial way. Even if the external particles are the physical states at the $p = (0, 0, 0, 0)$ corner of the Brillouin zone, the states at the other corners, the doublers, appear in virtual loops. How do we fix this issue?

5 Wilson fermions

The first fermion formulation we discuss that fixes these doubler solutions is Wilson fermions. In this framework we add a higher order term in our Dirac operator to remove only the unwanted poles. Let's see how that works.

We want to identify spurious poles and remove them. Wilson's solution was to add a term to the action such that in the Dirac operator we get

$$\tilde{D}(p) = m\mathbb{I} + \frac{1}{a}\sum_\mu \gamma_\mu \sin(p_\mu a) + \mathbb{I}\frac{1}{a}\sum_\mu (1 - \cos(p_\mu a)) \tag{22}$$

This cosine, the Wilson term, removes the doublers. for $p_\mu = 0$, the entire term vanishes. For each component with $p_\mu = \pi/a$, we get an extra contribution of $2/a$. This acts like an additional mass term, and the total mass of the doublers is $m + \frac{2l}{a}$ where l is the number of momentum components with π/a. In the continuum limit, these doubler modes become very heavy and they decouple from the theory.

We can use the same trick to write the Wilson quark propagator, where we see the doubler poles are gone and we only have the physical pole we are interested in remains (exercise?)

We can inverse Fourier transform the Wilson term in the momentum space Wilson Dirac operator to write it in position space,

$$-a\sum_{\mu=1}^{4} \frac{U_\mu(n)_{ab}\delta_{n+\hat{\mu},m} - 2\delta_{ab}\delta_{n,m} + U_{-\mu}(n)_{ab}\delta_{n-\hat{\mu},m}}{2a^2} \tag{23}$$

This is a discretization of a second derivative, $-(a/2)\partial_\mu\partial_\mu$. We combine this with the naive discretized Dirac operator to get the complete Wilson Dirac operator.

$$D^{(f)}(n|m)_{\alpha,a;\beta,b} = \left(m^{(f)} + \frac{4}{a}\right)\delta_{\alpha\beta}\delta_{ab}\delta_{n,m} - \frac{1}{2a}\sum_{\mu=\pm1}^{\pm4}(\mathbb{I}-\gamma_\mu)_{\alpha\beta}U_\mu(n)_{ab}\delta_{n+\hat{mu},m} \tag{24}$$

We can write this in a more compact notation using the covariant shift operators,

$$D(U) = \sum_\mu \gamma_\mu D_\mu + m - \frac{1}{2}\sum_\mu (C_\mu^+ + C_\mu^- - 2) \tag{25}$$

And we have fixed the doubler issue by adding the Wilson term to our naive discretization. The main drawback of this fermion formulation is how the Wilson term explicitly breaks chiral symmetry, which, in the interacting theory, will then allow certain explicit chiral symmetry breaking terms, such as mass terms and 5D operators, which must be fine tuned away via the bare quark mass.

6 Symmetries of the Wilson Dirac operator

Lattice discretization certainly breaks many of the continuum symmetries we enjoy, such as rotational or translation invariance. On the lattice we do have some symmetries, specifically discrete translations and rotations. more specifically, the Wilson Dirac operator is invariant under the full hypercubic group, along with charge conjugation and γ_5-hermiticity.

We write out the full Wilson action,

$$S = \sum_n \overline{\psi}(n)\left(\sum_\mu \gamma_\mu D_\mu + m - \frac{1}{2}\sum_\mu D_{\mu,L}D_{\mu,R}\right)\psi(n) + \beta\sum_n\sum_{\mu<\nu}(1 - P_{\mu\nu}(n)) \tag{26}$$

6.1 Charge conjugation

The first symmetry we will examine is charge conjugation. Under C in Minkowski space, $\psi \to \psi^C = -i\gamma^2\gamma^0\overline{\psi}^T$. Thus the Euclidean space transformation, $\psi \to \psi^C = C^{-1}\overline{\psi}^T$ where we define the charge conjugation operator as $C^{-1} = i\gamma^2\gamma^4$ such that $C^{-1} = C = C^\dagger = -C^T$. We can show that $C\gamma^\mu C = -(\gamma_\mu)^T$. For the free theory this gives us a symmetry of the action under $\psi \to C\overline{\psi}^T$ such that

$$\overline{\psi} \to (C\overline{\psi}^T)^\dagger\gamma^4 = (\overline{\psi}^T)^\dagger C\gamma^4 = -(\gamma^4\overline{\psi}^\dagger)^T C = -\psi^T C \tag{27}$$

With these transformations we can transform the free action,

$$S^C = -\sum_n \psi(n)^T C\left(\sum_\mu \gamma_\mu\partial_\mu + m - \frac{1}{2}\sum_\mu \partial_\mu\partial_\mu\right)C\overline{\psi}(n)^T \tag{28}$$

The fields are Grassmannian, so they anticommute. The charge conjugation operators act only on the gamma, and we use integration by parts of the form

$$\sum_n f(x)g(x+\hat{\mu}) = \sum_n g(x)f(x-\hat{\mu}) \tag{29}$$

on the second derivative, this gives us two minus signs, and on the first derivative term we pick up a single minus sign. We also use $v^T X^T w^T = wXv$ This leaves us with

$$\begin{aligned} S^C &= -\sum_n \psi(n)^T \left(\sum_\mu (-\gamma_\mu)^T \partial_\mu + m - \frac{1}{2}\sum_\mu \partial_\mu \partial_\mu \right) \overline{\psi}(n)^T \\ &= \sum_n \overline{\psi}(n) \left(\sum_\mu \gamma_\mu \partial_\mu + m - \frac{1}{2}\sum_\mu \partial_\mu \partial_\mu \right) \psi(n) = S \end{aligned} \tag{30}$$

And we see the free Wilson fermion action is invariant under charge conjugation. To preserve this symmetry in the interacting case, we need the covariant shifts to transform like

$$\sum_n f(x) C_\mu^{\pm} g(x) \to \sum_n g(x)^T C_\mu^{\mp} f(x)^T \tag{31}$$

thus the gauge links in the covariant shifts need to ober

$$\begin{aligned} \sum_n f(n) U_\mu^C(n) g(n+\hat{\mu}) &= \sum_n g(n)^T U_\mu^\dagger(n-\hat{\mu}) f(n-\hat{\mu})^T \\ &= \sum_n g(n+\hat{\mu})^T U_\mu^\dagger(n) f(n)^T = \sum_n f(n) U_\mu^*(n) g(n+\hat{\mu}) \end{aligned} \tag{32}$$

Then under the action of charge conjugation, the gauge field transforms like $U_\mu^C = U_\mu^*$ With this in mind we can check the gauge part of the action

$$U_{\mu\nu}(n) \to (U_\mu^\dagger(n))^T (U_\nu^\dagger(n+\hat{\mu}))^T U_\mu(n+\hat{\nu})^T U_\nu^T = U_{\nu\mu}(n)^T \tag{33}$$

such that $\mathrm{Tr} U_{\mu\nu}(n) \to \mathrm{Tr} U_{\nu\mu}(n)$, and since $U_{\mu\nu}^\dagger = U_{\nu\mu}(n)$ such that due to the real part $P_{\mu\nu}$ and therefore the full Wilson action is invariant under charge conjugation.

6.2 γ_5-Hermiticity

Now we prove the γ_5 Hermiticity of the Wilson Dirac operator. We first note that $(C_\mu^+)^\dagger = (U_\mu S_\mu^+)^\dagger = (S_\mu^+)^\dagger U_\mu^\dagger = S_\mu^- U_\mu^\dagger = C_\mu^-$ Where these $S^\pm$ are shift operators, which only shift the spacetime argument the a fermion field it is applied to. These shifts behave under hermitian conjugate

$$\begin{aligned} \sum_n f(x)^\dagger (S_\mu^+)^\dagger g(x) &= \sum_n g(x)^\dagger (S_\mu^+)^\dagger f(x))^\dagger = \sum_n (g(x)^\dagger f(n+\hat{\mu}))^\dagger \\ &= \sum_n f(n+\hat{\mu})^\dagger g(x) = \sum_n f(x)^\dagger g(n-\hat{\mu}) = \sum_n f(x)^\dagger S_\mu^- g(x) \end{aligned} \tag{34}$$

With these we can now show the invariance of the Wilson Dirac operator under the following transformation

$$
\begin{aligned}
\gamma_5 D(U)^\dagger \gamma_5 &= \gamma_5 \left(\sum_\mu \gamma_\mu (D_\mu)^\dagger + m - \frac{1}{2} \sum_\mu (D_{\mu,L} D_{\mu,R})^\dagger \right) \gamma_5 \\
&= \left(-\sum_\mu \gamma_\mu (D_\mu)^\dagger + m - \frac{1}{2} \sum_\mu (D_{\mu,L} D_{\mu,R})^\dagger \right) \qquad (35) \\
&= \left(\sum_\mu \gamma_\mu (D_\mu) + m - \frac{1}{2} \sum_\mu (D_{\mu,L} D_{\mu,R}) \right) = D(U)
\end{aligned}
$$

This is equivalent to $(\gamma_5 D(U))^\dagger = \gamma_5 D(U)$

6.3 Space time symmetries

We consider an n-dimensional lattice $\Lambda = \{\vec{n} \in \mathbb{Z}^n\}$ and operations $g : \Lambda \to \Lambda$ that can be expressed as a sequence of axis exchange operations and reflection operations,

$$
\begin{aligned}
(A_{\mu\nu}\vec{n})_\rho &= \begin{cases} \vec{n}_\rho & \text{if} \quad \rho \neq \mu \wedge \rho \neq \nu \\ \vec{n}_\mu & \text{if} \quad \rho = \nu \\ \vec{n}_\nu & \text{if} \quad \rho = \mu \end{cases} \\
(R_\mu \vec{n})_\rho &= \begin{cases} \vec{n}_\rho & \text{if} \quad \rho \neq \mu \\ -\vec{n}_\rho & \text{if} \quad \rho = \mu \end{cases}
\end{aligned}
\qquad (36)
$$

We can construct rotations out of strings of transformations from the above set of reflections and axis exchange operations. For example, the rotation about the z axis of a three dimensional vector, $(x, y, z) \to (y, -x, z)$ can be written as a product $R_1 \circ A_{01}$. In n dimensions we have $n!2^n$ unique space time symmetries on a lattice. If we want to consider the symmetries of the Hamiltonian, we take $n = 3$, and we have 48 unique operations, whose corresponding group is the full cubic group O_h. For the action we take $n = 4$, and we have 384 unique operations, whose group is called the hypercubic group.

Axis exchange on the gauge links changes the Lorentz index of the link accordingly, and operates the axis exchange operator on the spacetime argument of the link. For fermions, we find axis exchange symmetry of the entire action if we transform the fermion fields such that $\overline{\psi}\gamma_\rho\psi = \overline{\psi}\gamma_{\rho'}\psi$ where the index on the gamma changes according to the axis exchange prescription above.

These symmetries apply to a lattice of finite spatial sites in each direction. For reflection symmetry it is convinient to consider lattice sites in $[-N_\mu/2, N_\mu/2]$. In this convention the action also exhibits reflection symmetry. We can also write the set of reflections in Euclidean space as a product of three reflection operations, for example time reversal in Euclidean space can be written $P_0 = R_1 R_2 R_3$. The action can be shown to be invariant under all P_μ where these are defined by a product of three reflection operators orthogonal to direction μ, if

$$\begin{aligned} \psi(x) &\to \gamma_\mu \psi(P_\mu x), \\ \overline{\psi} &\to \overline{\psi}(P_\mu x)\gamma_\mu, \\ U_\mu(x) &\to U_\mu(P_\mu x), \\ U_\nu(x) &\to U_\nu(P_\mu x - a\hat{\nu})^\dagger \end{aligned} \tag{37}$$

7 Exercises

- Calculate $\tilde{D}(p)^{-1}$ with the new Wilson term included
- Show the Wilson Dirac operator is invariant under parity, $P_0 = R_1 R_2 R_3$
- Implement the Wilson Dirac operator in python and show that it is γ_5-Hermitian (template on the github page)