Lattice gauge notes, part II
Fermions

Here I will approach Wilson fermions in three different ways. First as a simple hamiltonian system, then from a path integral approach, and finally as a Dirac operator in the path integral.

The essence of the lattice doubling problem already appears with the simplest Fermion Hamiltonian in one space dimension

$$H = iK \sum_j a_{j+1}^\dagger a_j - a_j^\dagger a_{j+1}.$$

Here j is an integer labeling the sites of an infinite chain and the a_j are Fermion annihilation operators satisfying standard anticommutation relations

$$\left[a_j, a_k^\dagger\right]_+ \equiv a_j a_k^\dagger + a_k^\dagger a_j = \delta_{j,k}.$$

The bare vacuum $|0\rangle$ satisfies $a_j|0\rangle = 0$. This vacuum is not the physical one, which contains a filled Dirac sea. We refer to K as the hopping parameter. Energy eigenstates in the single Fermion sector

$$|\chi\rangle = \sum_j \chi_j a_j^\dagger |0\rangle$$

can be easily found in momentum space

$$\chi_j = e^{iqj}\chi_0.$$

where $0 \leq q < 2\pi$. The result is

$$E(q) = 2K\sin(q).$$

The physical vacuum has the negative energy states filled to form a Dirac sea.

- H.W.: show that the i in our Hamiltonian is just a convention. find a change of variables that would reduce the Hamiltonian to $H = K\sum_j a_{j+1}^\dagger a_j + a_j^\dagger a_{j+1}$

If we consider a Fermionic wave packet produced from small momentum q, then since the group velocity dE/dq is positive in this region, it will move to the right. On the other hand, a wave packet produced from momenta in the vicinity of $q \sim \pi$ will be left moving. The essence of the Nielsen Ninomiya theorem is that we must have both types of excitation. The periodicity in q requires the dispersion relation to have an equal number of zeros with positive and negative slopes.

Here I will concentrate on a Hamiltonian version of Wilson approach to remove the doubles. Work in one dimension with a two component spinor

$$\psi = \begin{pmatrix} a \\ b \end{pmatrix}.$$

The most naive lattice Hamiltonian begins with the simple hopping case of above and adds in the lower components and a mass term to mix the upper and lower components

$$\begin{aligned} H = iK \sum_j & a_{j+1}^\dagger a_j - a_j^\dagger a_{j+1} - b_{j+1}^\dagger b_j + b_j^\dagger b_{j+1} \\ & + M \sum_j a_j^\dagger b_j + b_j^\dagger a_j. \end{aligned}$$

Introducing Dirac matrices

$$\gamma_0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \gamma_1 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

and defining $\overline{\psi} = \psi^\dagger \gamma_0$, we write the Hamiltonian more compactly as

$$H = \sum_j iK(\overline{\psi}_{j+1}\gamma_1\psi_j - \overline{\psi}_j\gamma_1\psi_{j+1}) + M\sum_j \overline{\psi}_j\psi_j.$$

As before, the single particle states are easily found by Fourier transformation and satisfy

$$E^2 = 4K^2\sin^2(q) + M^2$$

Again, we are to fill the negative energy sea.

Naive chiral symmetry is implemented through distinct phase rotations for the upper and lower components of ψ. The mass term mixes these components and opens up a gap in the spectrum. The doublers at $q \sim \pi$, however, are still with us.

To remove the degenerate doublers, we make the mixing of the upper and lower components momentum dependent. A simple way of doing this was proposed by Wilson. In our language, we add one more term to the Hamiltonian

$$\begin{aligned} H = iK \sum_j & a_{j+1}^\dagger a_j - a_j^\dagger a_{j+1} - b_{j+1}^\dagger b_j + b_j^\dagger b_{j+1} \\ & + M \sum_j a_j^\dagger b_j + b_j^\dagger a_j \\ & - rK \sum_j a_j^\dagger b_{j+1} + b_j^\dagger a_{j+1} + b_{j+1}^\dagger a_j + a_{j+1}^\dagger b_j \\ & = \sum_j K(\overline{\psi}_{j+1}(i\gamma_1 - r)\psi_j - \overline{\psi}_j(i\gamma_1 + r)\psi_{j+1}) + \sum_j M\overline{\psi}_j\psi_j. \end{aligned}$$

Now the spectrum satisfies

$$E^2 = 4K^2 \sin^2(q) + (M - 2rK\cos(q))^2.$$

Note how the doublers at $q \sim \pi$ are increased in energy relative to the states at $q \sim 0$. The physical particle mass is now $m = M - 2rK$ while the doubler is at $M + 2rK$.

When r becomes large, the dip in the spectrum of near $q = \pi$ actually becomes a maximum. This is irrelevant for our discussion, although we note that the case $r = 1$ is somewhat special. For this value, the matrices $i\gamma_1 \pm r$, which determine how the Fermions hop along the lattice, are proportional to projection operators. In a sense, the doubler is removed because only one component can hop. This choice for r has been the most popular in practice, but we remain more general.

The hopping parameter has a critical value at

$$K_{crit} = \frac{M}{2r}$$

At this point the gap in the spectrum closes and one species of Fermion becomes massless. The Wilson term, proportional to r, still mixes the a and b type particles; so, there is no exact chiral symmetry. Nevertheless, in the continuum limit this represents a candidate for a chirally symmetric theory. Beforehand, chiral symmetry does not provide a good order parameter.

A difficulty with this approach is that gauge interactions will renormalize the parameters. To obtain massless pions one must finely tune K to K_{crit}, an *a priori* unknown function of the gauge coupling. Despite the awkwardness of such tuning, this is how numerical simulations with Wilson quarks generally proceed. The hopping parameter is adjusted to get the pion mass right, and one hopes for the remaining predictions of current algebra to reappear in the continuum limit.

Fermionic transfer matrices

Anticommutation is at the heart of fermionic behavior. This is true in both Hamiltonian operator formalisms and Lagrangian path integral approaches, but in rather complementary ways. If an operator $a^\dagger$ creates a fermion in some normalized state on the lattice or the continuum, it satisfies the basic relation

$$[a, a^\dagger]_+ \equiv aa^\dagger + a^\dagger a = 1.$$

This contrasts sharply with the fields in a path integral, which all anticommute

$$[\chi, \chi^\dagger]_+ = 0.$$

The connection between the Hilbert space approach and the path integral appear through the transfer matrix formalism. For bosonic fields this is straightforward, but for fermions certain subtlies arise, related to the so called "doubling problem." Ref: hep-lat/9905024

To be more precise, consider a single fermion state created by the operator $a^\dagger$, and an antiparticle state created by another operator $b^\dagger$. For an extremely simple model, consider the Hamiltonian

$$H = m(a^\dagger a + b^\dagger b) + \mu(a^\dagger a - b^\dagger b).$$

Here m can be thought of as a "mass" for the particle, and μ represents a chemical potential. What I want is an exact path integral expression for the partition function

$$Z = \mathrm{Tr} e^{-\beta H}.$$

Of course, since my Hilbert space has only four states, this is trivial to work out: $Z = 1 + e^{m+\mu} + e^{m-\mu} + e^{2m}$. However, I want this in a form that easily generalizes to many variables, makes the connection with the Wilson projection operator clear, and illustrates how the chemical potential is properly inserted into a path integral.

A path integral for fermions uses Grassmann variables. I introduce a pair of such, χ and $\chi^\dagger$, which will be connected to the operator pair a and $a^\dagger$, and another pair, ξ and $\xi^\dagger$, for b, $b^\dagger$. All the Grassmann variables anticommute. Integration over any of them is determined by the simple formulas

$$\int d\chi \; 1 = 0 \; ; \qquad \int d\chi \; \chi = 1.$$

This determines my phase conventions. For notational simplicity I join individual Grassmann variables into spinors

$$\psi = \begin{pmatrix} \chi \\ \xi^\dagger \end{pmatrix} ; \quad \psi^\dagger = \begin{pmatrix} \chi^\dagger & \xi \end{pmatrix} .$$

To make things appear still more familiar, introduce a "Dirac matrix"

$$\gamma_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and the usual

$$\overline{\psi} = \psi^\dagger \gamma_0.$$

Then we have

$$\overline{\psi}\psi = \chi^\dagger \chi + \xi^\dagger \xi.$$

The temporal Wilson projection operators

$$P_\pm = \frac{1}{2}(1 \pm \gamma_0)$$

arise when one considers the fields at two different locations

$$\chi_i^\dagger \chi_j + \xi_i^\dagger \xi_j = \overline{\psi}_i P_+ \psi_j + \overline{\psi}_j P_- \psi_i.$$

The indices i and j will soon label the ends of a temporal hopping term; this formula is the basic transfer matrix justification for the projection operator formalism.

For a moment I ignore the antiparticles and consider some general operator $f(a, a^\dagger)$ in my Hilbert space. How is this related to an integration in Grassmann space? To proceed I need a convention for ordering the operators in f. I adopt the usual normal ordering definition with the notation $: f(a, a^\dagger) :$ meaning that creation operators are placed to the left of destruction operators, with a minus sign inserted for each exchange. In this case a rather simple formula gives the trace of the operator as a Grassmann integration

$$\mathrm{Tr}\ : f(a, a^\dagger) : = \int d\chi d\chi^\dagger e^{2\chi^\dagger \chi} f(\chi, \chi^\dagger).$$

To verify, just check that all elements of the complete set of operators $\{1, a, a^\dagger, a^\dagger a\}$ work. However, this formula is actually much more general; with a set of Grassmann variables $\{\chi, \chi^\dagger\}$, one pair for each fermion state, this immediately generalizes to the trace of any normal ordered operator acting in a many fermion Hilbert space.

What about a product of several normal ordered operators? This leads to the introduction of multiple sets of Grassmann variables and the general formula

$$\begin{aligned}
&\mathrm{Tr}\ : f_1(a^\dagger, a) : : f_2(a^\dagger, a) : \ldots : f_n(a^\dagger, a) : = \\
&\int d\chi_1\ d\chi_1^* \ldots d\chi_n\ d\chi_n^* \\
&e^{\chi_1^*(\chi_1 + \chi_n)} e^{\chi_2^*(\chi_2 - \chi_1)} \ldots e^{\chi_n^*(\chi_n - \chi_{n-1})} \\
&f_1(\chi_1^*, \chi_1) f_2(\chi_2^*, \chi_2) \ldots f_n(\chi_n^*, \chi_n).
\end{aligned}$$

The positive sign on χ_n in the first exponential factor indicates the natural occurance of antiperiodic boundary conditions. With just one factor, this formula reduces to the

previous relation. Note how the "time derivative" terms are "one sided;" this is how doubling is eluded.

This exact relationship provides the starting place for converting our partition function into a path integral. The simplicity of the Hamiltonian allows this to be done exactly at every stage. First I break "time" into a number N of "slices"

$$Z = \mathrm{Tr}\left(e^{-\beta H/N}\right)^N .$$

Now I need normal ordered factors for the above formula. For this I use

$$e^{\alpha a^\dagger a} = 1 + (e^\alpha - 1)a^\dagger a = :e^{(e^\alpha - 1)a^\dagger a}: ,$$

true for arbitrary parameter α. Combining the particles and antiparticles into one matrix equation gives

$$\exp((\alpha+\rho)a^\dagger a + (\alpha-\rho)b^\dagger b) = :\exp\left(\begin{pmatrix} a^\dagger & b^\dagger \end{pmatrix}\left(e^{\alpha+\rho\gamma_0} - 1\right)\begin{pmatrix} a \\ b \end{pmatrix}\right): ,$$

This is all the machinery I need to write

$$Z = \int (d\psi d\psi^\dagger) e^S$$

where

$$S = \sum_{i=1}^{n} \overline{\psi}_n e^{-\beta m/N} e^{-\beta\mu\gamma_0/N}\psi_n - \overline{\psi}_n P_+ \psi_{n-1} - \overline{\psi}_{n-1} P_- \psi_n .$$

Note how the Wilson projection factors of $P_\pm$ automatically appear to handle the reverse convention of χ versus ξ in our field ψ. The projection operator formalism is a natural consequence of an exact transfer matrix.

The chemical potential appears simply as an inserted factor of $e^{-\beta\mu\gamma_0/N}$ in the "mass" term. This is not quite in the conventional form since the chemical potential piece is temporally diagonal. However this is actually only a convention, as the factor can be moved to temporal links with a change of variable

$$\Psi \equiv e^{\frac{-\beta\mu\gamma_0}{2N}}\psi .$$

With this substitution, we have

$$S = \sum_{i=1}^{n} \overline{\Psi}_n e^{-\beta m/N}\Psi_n - \overline{\Psi}_n P_+ e^{\beta\mu/N}\Psi_{n-1} - \overline{\Psi}_{n-1} P_- e^{-\beta\mu/N}\Psi_n .$$

If μ were imaginary, this would be precisely the form of a $U(1)$ gauge field on the timelike bonds.

In this discussion I have ignored spatial hoppings. Terms in the action of the form

$$\overline{\psi}\vec{D}\cdot\vec{\gamma}\psi$$

are invariant under this change of variables since γ_0 anticommutes with $\vec{\gamma}$. However, more complicated terms, such as spatial Wilson hoppings, are generally not invariant under this change. This would be a modification of higher order in the lattice spacing for Wilson fermions. These are lattice artifacts, presumably irrelevant to the continuum limit. Thus, it is only a convention whether the chemical potiential is inserted as a matrix valued mass as or as a direction dependent link term.

If we consider the action as a generalized matrix connecting fermionic variables

$$S = \overline{\psi}M\psi,$$

the matrix M is not symmetric. The upper components propagate forward in time, and the lower components backward. Even though our Hamiltonian was Hermitian, the matrix appearing in the corresponding action is not. With further interactions, such as gauge field effects, the intermediate fermion contributions to a general path integral are generally not positive, or even real. Of course the final partition function, being a trace of a positive definite operator, is positive. However, depending on the order of operations, there can be negative intermediate results. With Monte Carlo methods, this can lead to uncontrollable fluctuations. This is the primary unsolved problem in lattice gauge theory. With no chemical potential term, symmetry between particles and antiparticles results in a real fermion determinant, which in turn is positive for an even number of flavors.

For our simple Hamiltonian, this discussion has been exact. The discretization of time adds no approximations since we could do the normal ordering by hand. In general with spatial hopping or more complex interactions, the normal ordering can produce extra terms going as $O(1/N^2)$. In this case exact results require a limit of a large number of time slices.

More on Wilson fermions

In the continuum, we usually write for the free fermion action density

$$\overline{\psi} D \psi = \overline{\psi}(\not{\partial} + m)\psi$$

or in momentum space

$$\overline{\psi}(i\not{p} + m)\psi$$

My convention is hermitan gamma matrices. Note that D is the sum of hermitian and antihermitian parts. In the continuum the former is just a constant, the mass. A hermitian operator appears in the combination $\gamma_5 D$, but we don't need that just now.

A matrix can be diagonalized when it commutes with its adjoint; then it is called "normal." For this continuum operator this is the case, and we see that all eigenvalues lie along a line parallel to the imaginary axis intersecting the real axis at m.

As discussed earlier, a naive transcription of derivatives onto the lattice replaces factors of p with trig functions. Thus the naive lattice action is

$$\overline{\psi}(1/a \sum_\mu i\gamma_\mu \sin(p_\mu a) + m)\psi$$

For small momentum this agrees with the continuum result. Now let one component of p get large and be near π/a. Then we again have small eigenvalues and a nearby pole in the propagator.

The Wilson solution adds a momentum dependent mass. Since it also involves only nearest neighbor terms, it also involves trig functions. Explicitly for free fields

$$\overline{\psi} D_W \psi = \overline{\psi}\left(1/a \sum_\mu (i\gamma_\mu \sin(p_\mu a) + 1 - \cos(p_\mu a)) + m\right)\psi$$

Now at momentum π_a the roots are of order $1/a$ in size. Note that the lattice artifacts in the propagator start at order $p^2 a$, rather than $O(a^2)$ as for the bosonic case or for naive fermions.

The eigenvalue structure of D_W is rather interesting. For the free theory the hermitian and antihermitian parts still commute; this is not true in the interacting case. The eigenvalues occur at

$$\lambda = \pm\frac{i}{a}\sqrt{\sum_\mu \sin^2(p_\mu a)} + m + \frac{1}{a}\sum_\mu 1 - \cos(p_\mu a)$$

Note that for real eigenvalues each component of the momentum must be a multiple of π. In the complex plane the spectrum fills a set of overlapping elipses.

Note that $m \leftrightarrow -m$ is not a symmetry. Naively it would be in the continuum, but as we will extensively discuss later, it cannot be in the quantum theory. This is a hint of anomalies and things to come.

For $m = 0, 2, 4, 6, 8$ we have $1, 4, 6, 4, 1$ massless species. When interactions are present these values of m will be renormalized.