Lattice gauge notes V

We have now covered the basic canonical path to lattice gauge simulations with the hybrid Monte Carlo proceedure. A few steps and branches were skipped along the way:

- duality – insight into toy models
- staggered fermions – alternative to the Wilson $1+\gamma_\mu$ approach
- mean field theory
- the Hamiltonian formulation
- finite temperature and the quark-gluon plasma

I hope to come back to at least the last three subjects later. First I want to get more involved with chiral symmetry and some recent lattice developments. Here I will review some introductory material to set the stage for later issues.

Goldstone bosons

Let me briefly review effective potentials. In generic continuum field theory language, consider

$$Z = \int d\phi e^{-S(\phi)}$$

Adding in some external sources

$$Z(J) = \int d\phi e^{-S(\phi)+J\phi}$$

general correlation functions can be found by differentiating with respect to J. Here I shorthand notate $J\phi = \int dx J(x)\phi(x)$ in the continuum, or $J\phi = \sum_i J_i\phi_i$ on the lattice. Think of J as an external force pulling on the field. Such a force will give the field an expectation value

$$\langle\phi\rangle_J = -\frac{\partial F}{\partial J}$$

where I define the free energy $F(J) = -\log(Z(J))$. Now imagine inverting this to find what force $J(\Phi)$ gives some desired expectation value, *i.e.* solve

$$\Phi(J) = \langle\phi\rangle_{J(\Phi)} = -\frac{\partial F}{\partial J}$$

In terms of this formal solution, construct the "Legendre transform"

$$V(\Phi) = F(J(\Phi)) + \Phi J(\Phi)$$

and look at

$$\frac{\partial V}{\partial \Phi} = -\Phi\frac{\partial J}{\partial \Phi} + J + \Phi\frac{\partial J}{\partial \Phi} = J$$

If I turn off the sources, this derivative vanishes. Thus the minimum of V tells us the expectation value of the field. This quantity V is the "effective potential."

But now let me confuse you by looking at the second derivative of V

$$\frac{\partial^2 V}{\partial \Phi^2} = \frac{\partial J}{\partial \Phi}$$

Actually, it is easier to look at the inverse

$$\frac{\partial \Phi}{\partial J} = -\frac{\partial^2 F}{\partial J^2} = \langle \phi^2 \rangle - \langle \phi \rangle^2 = \langle (\phi - \langle \phi \rangle)^2 \rangle \geq 0.$$

Thus this second derivative has a single sign! This shows we are actually looking for a minimum and not a maximum of V, but in addition it implies that V can only have ONE minimum!

So what is going on? Are phase transitions impossible? The more you pull, the larger the expectation of Φ should be. It won't go back. Physically, we must do Maxwell's construction. If we force the expectation of ϕ to lie between two distinct stable phases, the system phase separates into a mixture of the two. Note that there is no large volume limit in the above discussion. However other definitions of V can allow a small barrier at finite volume due to surface tension effects. A mixed phase must contain interfaces, and their energy represents a barrier.

The pion is much lighter than the rho, which contains the same quarks, but in a different spin state. The standard picture is that pions are approximate Goldstone bosons from a spontaneous breaking of chiral symmetry. The standard picture considers an effective potential constructed for the fields

$$\sigma = c\overline{\psi}\psi$$
$$\vec{\pi} = ic\overline{\psi}\gamma_5\vec{\tau}\psi$$

The Fermion ψ has two isospin components, for which $\vec{\tau}$ represents the standard Pauli matrices. The factor c is inserted to give the fields their usual dimensions. Its value is not particularly relevant to the qualitative discussion that follows, but one convention is take $c = F_\pi/|\langle\overline{\psi}\psi\rangle|$ where F_π is the pion decay constant and the condensate is in the standard æther.

For the massless theory many of the chiral symmetries become exact. Because of the anomaly, the chiral transformation which mixes the σ and η fields, is not a good symmetry. I will come back to this extensively later. However flavored axial rotations should be valid. For example, the rotation

$$\psi \longrightarrow e^{i\gamma_5\tau_3\phi/2}\psi$$

which mixes σ with π_3

$$\sigma \longrightarrow \cos(\phi)\sigma + \sin(\phi)\pi_3$$
$$\pi_3 \longrightarrow \cos(\phi)\pi_3 - \sin(\phi)\sigma$$

should be a good symmetry.

I now use the experimental fact that chiral symmetry is spontaneously broken. The minimum of the effective potential should not occur for all fields having vanishing expectation. Assuming that parity and flavor are good symmetries of the strong interactions, the expectation value of the fields can be chosen in the σ direction. The potential should have the canonical "sombrero" shape, as stereotyped by the form

$$V = \lambda(\sigma^2 + \vec{\pi}^2 - v^2)^2.$$

Here v is the magnitude of the æther expectation value for σ, and λ is a coupling strength related to the σ mass. The normalization convention mentioned above would have $v = F_\pi/2$. This gives the standard picture of pions as Goldstone Bosons associated with fields oscillating along degenerate minima.

Next I turn on the Fermion masses. I consider small masses, and assume they appear as a linear perturbation of the effective potential

$$V \longrightarrow V - m\sigma/c.$$

This tilts the sombrero, picking the vacuum at positive sigma, and generates a mass for the pions. The square of the pion mass is linearly proportional to the quark mass.

Now for a brief discussion on some formal aspects of Goldstone Bosons. Suppose I have a conserved current

$$\partial_\mu j_\mu = 0$$

so the corresponding charge $Q = \int d^3x j_0(x)$ is a constant

$$\frac{dQ}{dt} = -i[H, Q] = 0.$$

Suppose, however, that the vacuum is not a singlet under this charge

$$Q|0\rangle \neq 0$$

Then there cannot be a mass gap in the theory. Consider the state

$$\exp(i\theta \int d^3x j_0(x) e^{-\epsilon x^2})|0\rangle$$

where ϵ is a convenient cutoff and θ some parameter. As epsilon goes to zero this state by assumption is not the vacuum, but the expectation value of the Hamiltonian goes to zero (normalize so the ground state energy is zero). Thus "spontaneously broken symmetries" have no mass gap, *i.e.* the theory contains states of arbitrarily low energy. These are manifested as massless particles called Goldstone bosons.

Free massless field theory is a marvelous example of all this where everything can be worked out. The massless equation of motion

$$\partial_\mu \partial_\mu \phi = 0$$

can be written in the form

$$\partial_\mu j_\mu = 0$$

where

$$j_\mu = \partial_\mu \phi.$$

The broken symmetry is the invariance of the Lagrangian $L = \int d^4x (\partial_\mu \phi)^2$ under shifts of the field

$$\phi \to \phi + c$$

Note that $j_0 = \partial_0 \phi = \pi$, the conjugate variable to ϕ. One can work out explicitly

$$\langle 0| \exp(i\theta \int d^3x j_0(x) e^{-\epsilon x^2/2})|0\rangle.$$

but we can save ourselves the work using dimensional analysis. The field ϕ has dimensions of inverse length, while j_0 goes as inverse length squared. Thus θ above has units of inverse length. These are the same dimensions as ϵ^2. Now for a free theory by Wick's theorem the answer must be Gaussian in θ, so we conclude that the above overlap must go as

$$\exp(-C\theta^2/\epsilon^4)$$

where C is some non-vanishing dimensionless number. This expression rapidly goes to zero as epsilon becomes small, showing that the vacuum is indeed not invariant under the symmetry. As ϵ goes to zero, we obtain a new vacuum that is not even in the same Hilbert space. Its overlap with any polynomial of fields on the original vacuum vanishes.

Two dimensions give some interesting twists on this argument. Now the scalar field is dimensionless, and the current has dimensions of inverse length. Thus theta is dimensionless and we expect

$$\langle 0| \exp(i\theta \int dx j_0(x) e^{-\epsilon x^2/2})|0\rangle \sim \exp(-C\theta^2)$$

There can be no $\log(\epsilon)$ since there is nothing to set the scale. Thus the vacuum is not invariant, but the symmetry relation does not give you a fully independent state. This is clearly a borderline case, and for an interacting theory the massless particles can be lost.

This is tied in with the propagator in two dimensions not being a distribution. Put in a small mass cutoff. Then

$$\Delta(x) = \int \frac{d^2p}{(2\pi)^2} \frac{e^{-ipx}}{p^2 + m^2}$$

gets very singular as m goes to zero. Consider the simple test function $e^{-x^2/2}$. This is infinitely differentiable and well behaved at infinity. Now integrate this test function with the free particle propagator

$$\int d^2x\Delta(x)e^{-x^2/2} \sim \int \frac{d^2p}{(2\pi)^2}\frac{e^{-p^2/2}}{p^2+m^2} \sim \log(1/m) \Longrightarrow_{m\to 0} \infty$$

Thus $\Delta(x)$ is not a tempered distribution, contrary to the basic assumptions of quantum field theory. However Green's functions of j_0 are tempered distributions since they involve derivatives that kill the divergent part. In most cases Goldstone bosons are lost in two dimensions, however, if they are free, as in the above case, they can exist. The X-Y model, with spins in $U(1)$, has a massless phase, but no long range order. Lore is that higher symmetries only have massive phases, but Seiler and Patrascioiu have argued that this may be wrong.

Strong CP violation

As discussed earlier, scale anomalies reduce the number of physically independent dimensionless parameters in the quark confining dynamics of quarks and gluons. For massless quarks, dimensional transmutation leaves no undetermined continuous parameters; the theory only depends the gauge group and the number of Fermion flavors.

With masses for the quarks, the number of parameters increases. Naively there is one additional mass parameter for each quark. However, due to chiral anomalies, one more parameter, usually called Θ, is hidden in the phases in these quark masses. If non-zero, this parameter gives rise to CP violating processes in the strong interactions. Such appear to be extremely small in nature, suggesting that this parameter may vanish. In a grand unified context this raises puzzles since CP violation is present in the weak interactions and has no particular reason to be small.

For the lattice it is crucial that any Fermion formulation be able to account for this parameter. To define a phase for a single Fermion mass, break the naive mass term into two parts

$$\overline{\psi}\psi = \overline{\psi}_L\psi_R + \overline{\psi}_R\psi_L$$

where the left and right parts are eigenstates of γ_5

$$\psi_{R,L} = \frac{1}{2}(1 \pm \gamma_5)\psi_{R,L}.$$

Then a generic complex mass term has the form

$$\overline{\psi}_L M\psi_R + \overline{\psi}_R M^*\psi_L$$

with M a complex number, i.e. of form $M = me^{i\theta}$. Another convenient form for the mass term is

$$m_1\overline{\psi}\psi + im_2\overline{\psi}\gamma_5\psi$$

so that $M = m_1\cos(\theta) + im_2\sin(\theta)$.

At the classical level the phase of the quark mass is easily removed by a chiral rotation. The change of variables

$$\psi \to e^{i\theta\gamma_5/2}\psi$$
$$\overline{\psi} \to \overline{\psi}e^{i\theta\gamma_5/2}$$

takes

$$M \to e^{i\theta}M.$$

Since this is just a redefinition, if the path integral measure is invariant under the same phase change, theta can be rotated away. However, here the chiral anomalies come into play. Flavor non-singlet axial symmetries are believed to be preserved; so, one can eliminate any non-singlet phases in the mass. However one overall phase always remains. Using the anomaly, this can be moved from the quark masses into pure gauge terms of the action; indeed, the latter form is the starting point for most conventional discussions of Θ in terms of topological structures in the gauge sector.

How this physics manifests itself in a theoretical formalism depends on approach. With a Pauli-Villars regulator, the heavy auxiliary field has a phase in its mass; the theta parameter is the relative phase between the regulator mass and that of the physical Fermion. In other continuum schemes the phase is often pushed into the path integral measure.

In usual lattice approaches, the Fermion measure is a direct product of discrete Grassmann integrals, leaving no room in the measure for forbidding the change of variables alluded to above. However with Wilson fermions we have the added Wilson term, which is itself of a mass like form. Theta then becomes a relative phase between the Wilson term and the explicit mass.

For another angle on the meaning of theta, it is useful to think in terms of effective chiral Lagrangians. This temporarily leads away from the lattice, but gives insight into the expected structure of Wilson Fermions with complex mass. Also, the chiral Lagrangian approach will be useful in later sections for understanding other phenomena of direct relevance to the lattice, such as the Aoki phase and the Wess-Zumino motivation for exploring higher dimensions.

I begin with a lightning summary of effective theories of Goldstone Bosons. Suppressing other indices, consider left and right handed quark fields ψ_L^a, ψ_R^a with a flavor index a running from one to three. Spontaneous chiral symmetry breaking appears in a non-vanishing expectation

$$\langle\overline{\psi}_L^a\psi_R^b\rangle = vg^{ab}.$$

The vacuum is not unique, and is labeled by g^{ab}, an element of $SU(3)$. The basic $SU(3)_L \otimes SU(3)_R$ chiral symmetry is realized via the global transformation

$$g \to g_L^\dagger g g_R.$$

Picking $g = I$ for a standard vacuum, the 8 fields π^α which excite the Goldstone modes are nicely parametrized by

$$g = e^{i\lambda^\alpha \pi^\alpha / F_\pi}$$

where the matrices λ^α are a set of generators for the group $SU(3)$ and are normalized $\mathrm{Tr}\lambda^\alpha\lambda^\beta = 2\delta^{\alpha\beta}$

Effective Lagrangians start from the assumption that in the low energy limit only the Goldstone excitations are important; one considers an effective theory depending on g alone. For low momenta, this theory is expanded in terms of increasing numbers of derivatives. To lowest order the effective Lagrangian is

$$L = \frac{F_\pi^2}{4}\mathrm{Tr}(\partial_\mu g^\dagger \partial_\mu g).$$

This is invariant under the global chiral symmetry. The parameter F_π is related to the pion decay, which occurs through the axial vector coupling to the intermediate weak Boson. The phenomenological value is $F_\pi = 93$ MeV.

To give the quarks masses, add an explicit symmetry-breaking term. For degenerate quarks the simplest possibility adds to L a potential term

$$V = -\frac{m}{v}\mathrm{ReTr}g.$$

Minimizing V for positive m selects the standard $g = I$ to represent the vacuum. The pions are no longer massless, but acquire a mass proportional to the square root of the quark mass. For $SU(2)$, $-I$ is an element of the group, so changing the sign of the mass simply induces a rotation to a new vacuum represented by $g = -I$. However $-I$ is not an element of $SU(3)$, requiring a somewhat more detailed analysis.

This leads me to a digression on some details of the $SU(N)$ group manifold. In particular, where is $\mathrm{ReTr}(g)$ extremal? At such a point, first order changes in g must vanish; in particular

$$0 = \frac{d}{d\epsilon^\alpha}\mathrm{ReTr}(g e^{i\lambda^\beta \epsilon^\beta})|_{\epsilon=0} = i\mathrm{Tr}(g - g^\dagger)\lambda^\alpha.$$

The λ matrices are almost a complete set, only the identity is missing. This indicates that $g - g^\dagger$ is proportional to the identity; thus I write

$$g - g^\dagger = isI$$

where the constant s is yet to be determined.

Since Trg is a class function, the extrema being discussed are by definition classes in the group. Given some extremal point g, all elements of form $h^\dagger g h$, with h an arbitrary group element, are in the same equivalence class. Using this freedom, define a standard member of the class by diagonalizing g and ordering the diagonal elements by increasing magnitude of the real part. After doing this, the diagonal elements are phases, and all have the same imaginary part. The diagonals must all be taken from the two numbers $c + is$ or $-c + is$ with $c = \sqrt{1 - s^2}$.

In general there are a variety of such extremal elements, some of which are maxima, some minima, and some saddle points of ReTrg. To distinguish them, look at the second variation

$$\frac{d^2}{d\epsilon^2}\mathrm{ReTr}(ge^{i\lambda\epsilon})|_{\epsilon=0} = -\mathrm{Tr}((g + g^\dagger)\lambda^2)$$

with λ a generator of the group. Using diagonal generators, it is a straightforward exercise to see that for a maximum (minimum), the real parts of g must all be positive (negative). All other solutions are saddle points. Thus all the maxima and minima are elements of the group center.

Specializing to $SU(3)$, there are four extremal classes. The single maximum of ReTrg occurs at the identity, two degenerate minima occur at the other two center elements $g = e^{\pm 2\pi i/3}$, and a class of saddle point elements is represented by

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

A complex curve that passes through all these extrema and encloses all values of Trg is given by

$$z = \mathrm{Tr}\exp(i\theta\lambda)$$

with

$$\lambda = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

as theta runs from 0 to 2π.

Using this basic structure of the $SU(3)$ group, it is now straightforward to see how the picture of first order phase transitions in the phase of the mass arises. For $m > 0$ the vacuum is the usual one with $g = I$. For a real but negative mass, the vacuum should lie at a minimum of ReTrg, which occur in a degenerate pair at $g = e^{\pm 2\pi i/3}$. Adding a small imaginary piece to m breaks this degeneracy, showing the first order nature of the transition along the negative m axis.

With a diagonal mass term $m = |m|e^{i\Theta/3}$ with a general phase, the vacuum is always represented by one of these three extremal classes. For $\Theta = \pi$ there is a discontinuity,

with the system jumping discontinuously from $g = I$ to $g = Ie^{2\pi i/3}$. This is exactly the first order transition alluded to in the previous section. The three transition lines in the (m_1, m_2) plane are physically equivalent since a phase change $m \to me^{2\pi i/3}$ can be absorbed by taking $g \to ge^{-2\pi i/3}$. Later I will extend the above discussion to non-degenerate masses, providing a nice route between various numbers of flavors.

One flavor

The one flavor situation, while not phenomenologically particularly relevant, is fascinating in its own right. In this case anomalies remove all chiral symmetries from the problem. No massless Goldstone Bosons are expected, and there is nothing to protect the quark mass from additive renormalization. Nevertheless, I have argued previously that there should be a non-trivial dependence on the phase of the mass. A large negative mass should be accompanied by a spontaneous breakdown of parity.

A quick but dirty argument gives the expected picture. With only one flavor, there is only one light pseudo-scalar meson, which I call the η. Were it not for anomalies, conventional chiral symmetry arguments suggest the mass squared of this particle would go to zero linearly with the quark mass,

$$m_\eta^2 \sim m_q.$$

But, just as the $\eta\prime$ gets mass from anomalies, a similar contribution should appear here; assume it is simply an additive constant

$$m_\eta^2 \sim m_q + C.$$

Try to describe this model by an effective potential for the η field. This should include the possibility for these particles to interact, suggesting something like

$$V(\eta) = \frac{am_q + C}{2}\eta^2 + \lambda\eta^4.$$

At $m_q = -C/a$ the effective mass of the eta goes negative. This should give a spontaneous breaking in the canonical manner, with the field acquiring an expectation value

$$\langle\eta\rangle \sim \langle\overline{\psi}\gamma_5\psi\rangle \neq 0.$$

As this is an odd parity field, parity is spontaneously broken. In particular, odd numbers of physical mesons can be created, unlike in the unbroken theory where the number of mesons is preserved modulo 2.

Note that this transition occurs at a negative quark mass, and nothing special happens at $m_q = 0$. Of course the bare quark mass is a divergent quantity in need of renormalization. Without chiral symmetry, there is nothing to prevent an additive shift in this parameter.

Nevertheless, with a cutoff in place, these qualitative arguments suggest it is only for negative quark mass that this parity violating phase transition will take place.

The anomaly involves processes that mix left and right handed quarks. This is exactly the role of a mass term, and thus the quark-antiquark pseudo-scalar bound state, the analogue of the η' meson, gains a mass. Now imagine making the quark masses slightly negative. This can cancel some of the mass generated by the anomaly and should reduce the mass of the meson. If the quarks become sufficiently negative in mass, one might decrease the bare mass of the meson to negative values. This gives the classic situation of spontaneous symmetry breaking and the meson field acquires an expectation value.

This argument is not at all rigorous. To lend more credence to this qualitative picture, note that a similar phenomenon occurs in two dimensional electrodynamics. The Schwinger model is exactly solvable at zero bare mass, with the spectrum being a free massive Boson. However for negative bare mass qualitative semi-classical arguments indicate the same structure as discussed in the previous paragraph, with a spontaneous generation of a parity violating background electric field. Under the Bosonizaton process, the quark mass term corresponds to a sinusoidal term in the effective potential for the scalar field

$$m\overline{\psi}\psi \leftrightarrow m\cos(2\sqrt{\pi}\eta).$$

Regularization and normal ordering are required for a proper definition but are not important here (Coleman, 1976). Combining this with the photon mass from the anomaly suggests an effective potential for the η field of form

$$V(\eta) \sim \frac{e^2}{2\pi}\eta^2 - m\cos(2\sqrt{\pi}\eta).$$

For small positive m, the second term shifts the Boson mass and introduces a four meson coupling, making the theory no longer free. If the mass is negative and large enough, the cosine term can dominate the behavior around small η, making the perturbative vacuum unstable. The Bosonization process relates $\overline{\psi}\gamma_5\psi$ with $\sin(2\sqrt{\pi}\eta)$; thus, when η gains an expectation value, so does the the pseudo-scalar density. Since the scalar field represents the electric field, this symmetry breaking represents the spontaneous generation of a background field. As discussed by Coleman, this corresponds to a non-trivial topological term in the action, usually referred to as Θ.

A third way to understand the one flavor behavior is to consider a larger number of flavors and give all but one large masses. Starting with two flavors. requires some additional assumptions regarding the spectrum; these assumptions become less important for larger symmetry groups. Thus I consider the three flavor case, and give two quarks a larger mass than the third.

I begin with the effective three flavor Lagrangian of the previous section. With two quarks

of mass M and one of mass m, consider the potential

$$V(g) \propto -\mathrm{ReTr}\left\{ g \begin{pmatrix} m & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & M \end{pmatrix} \right\}.$$

It is convenient to break this into two terms

$$V(g) \propto -\frac{M+m}{2}\,\mathrm{ReTr}(g) + \frac{M-m}{2}\,\mathrm{ReTr}(gh)$$

where

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

The minimum of the first term was worked out in the previous section; when $M+m$ is positive this occurs at the identity element. For the second term, note that I have written the factor of g as an $SU(3)$ group element. Via the previous discussions, the extrema of this term occur when the product gh is in the group center. For the case $M-m$ positive, there is a degenerate pair of minima occurring at

$$g = e^{\pm 2\pi i/3} h.$$

We have two competing terms, one having a unique minimum and the other having two degenerate ground states. For the degenerate case with $M = m$, only the first term is present and the vacuum is unique. However when $m = -M$ only the second term is present with its corresponding pair of degenerate vacuua. Between these points there is a critical value m_c where the situation shifts between a unique and a doubly degenerate vacuum.

To determine the critical mass, consider matrices of form

$$g = \exp\left\{ i\phi \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\}.$$

For these the potential is

$$V(\phi) \propto -m\cos(2\phi) - 2M\cos(\phi).$$

The extremum at $\phi = 0$ changes from a minimum to a maximum at $m = -M/2$, the desired critical point. As discussed at the beginning of this section, it occurs at a negative value of m. The only dimensional scale present is M, to which the result must be proportional. This analysis immediately generalizes to larger groups: for N_f flavors $m_c = \frac{-1}{N_f - 1}$. b This discussion suggests that a similar phenomenon should occur with one flavor of Wilson Fermion. Here the bare mass is controlled by the hopping parameter. As the hopping parameter increases, the Fermion mass decreases. In the plane of the gauge coupling and hopping parameter, a critical line should mark where the above parity breaking begins.