LATTICE QCD AND THE CKM MATRIX

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These lectures provide an introduction to lattice methods for nonperturbative studies of Quantum Chromodynamics. Lecture 1 (Ch. 2) is a very vanilla introduction to lattice QCD. Lecture 2 (Ch. 3) describes examples of recent lattice calculations relevant to fixing the parameters of the CKM matrix.

1 Introduction

The lattice regularization of QCD has been a fruitful source of qualitative and quantitative information about QCD for many years, especially when combined with Monte Carlo simulation. Lattice methods are presently the only way we know how to compute masses and matrix elements in the strong interactions beginning with the Lagrangian of QCD. My goal in these lectures is to give enough of an overview of the subject that you will be able to make an intelligent appraisal of a lattice calculation.

The first lecture will describe how to put QCD on a lattice. This is a long story with a lot of parts. Lattice QCD is full of technicalities, but I will try to make the discussion physical. In Lecture Two I will discuss lattice calculations of matrix elements which are needed to convert experimental numbers to predictions for the CKM matrix. These calculations have a lot of ingredients: a typical one starts with a particular choice of discretization and simulation algorithm, and a choice of operators whose matrix elements are appropriate for one’s measurement. After the lattice number is computed, it may have to be converted into a number in a continuum regularization scheme (like $\overline{MS}$), which will involve some kind of perturbative or nonperturbative matching calculation. Finally, it might have to be extrapolated in quark mass, to some physical quark mass value or the the chiral limit. None of these parts are simple or obvious (or more precisely, most of the time the simple and obvious idea doesn’t work very well). Hopefully you will find the physics in the calculations more interesting than the tables of numbers which result.

2 Basics of Lattice QCD
2.1 Lattice Variables and Actions

All quantum field theories must be regulated in order to control their ultraviolet divergences while calculations are performed. The lattice is a space-time cutoff which eliminates all degrees of freedom from distances shorter than the lattice spacing $a$. As with any regulator, it must be removed after renormalization. Contact with experiment only exists in the continuum limit, when the lattice spacing is taken to zero. The lattice is a unique regulator compared to the ones you might already know. Other regularization schemes are tied closely to perturbative expansions: one calculates a process to some order in a coupling constant; divergences are removed order by order in perturbation theory. The lattice, however, is a nonperturbative cutoff. Before a calculation begins, all wavelengths less than a lattice spacing are removed.

All regulators have a price. On the lattice we sacrifice all continuous space-time symmetries but preserve all internal symmetries, including local gauge invariance. This preservation is important for nonperturbative physics. For example, gauge invariance is a property of the continuum theory which is nonperturbative, so maintaining it as we pass to the lattice means that all of its consequences (including current conservation and renormalizability) will be preserved. The bill is paid when we take the lattice spacing to zero and try to recover what we have left out.

Let’s begin by thinking about a lattice version of scalar field theory. One just replaces the space-time coordinate $x_{\mu}$ by a set of integers $n_{\mu}$ ($x_{\mu} = a n_{\mu}$, where $a$ is the lattice spacing). Field variables $\phi(x)$ are defined on sites $\phi(x_{n}) \equiv \phi_{n}$. The action, an integral over the Lagrangian, is replaced by a sum over sites

$$S = \int d^{4}x L \to a^{4} \sum_{n} L(\phi_{n}).$$

and the generating functional for Euclidean Green’s functions is replaced by an ordinary integral over the lattice fields

$$Z = \int (\prod_{n} d\phi_{n}) e^{S}.$$  

Gauge fields are a little more complicated. They carry a space-time index $\mu$ in addition to an internal symmetry index $a$ ($A_{\mu}^{a}(x)$) and are associated with a path in space $x_{\mu}(s)$: a particle traversing a contour in space picks up a phase factor

$$\psi \to P(\exp i g \int_{s} dx_{\mu} A_{\mu}) \psi \equiv U(s) \psi(x).$$
$P$ is a path-ordering factor analogous to the time-ordering operator in ordinary quantum mechanics. Under a gauge transformation $g$, $U(s)$ is rotated at each end:

$$U(s) \rightarrow g^{-1}(x_\mu(s))U(s)g(x_\mu(0)). \quad (4)$$

These considerations led Wilson to formulate gauge fields on a space-time lattice, in terms of a set of fundamental variables which are elements of the gauge group $G$ living on the links of a four-dimensional lattice, connecting neighboring sites $x$ and $x + a\mu$: $U_\mu(x)$, with $U_\mu(x + \mu) = U_\mu(x)$

$$U_\mu(n) = \exp(igaT^aA_\mu^a(n)) \quad (5)$$

for $SU(N)$. ($g$ is the coupling, $A_\mu$ the vector potential, and $T^a$ is a group generator).

Under a gauge transformation link variables transform as

$$U_\mu(x) \rightarrow V(x)U_\mu(x)V(x + \hat{\mu}) \quad (6)$$

and site variables as

$$\psi(x) \rightarrow V(x)\psi(x) \quad (7)$$

so the only gauge invariant operators we can use as order parameters are matter fields connected by oriented “strings” of $U$’s

$$\bar{\psi}(x_1)U_\mu(x_1)U_\mu(x_1 + \hat{\mu}) \ldots \psi(x_2) \quad (8)$$

or closed oriented loops of $U$’s

$$\text{Tr} \ldots U_\mu(x)U_\mu(x + \hat{\mu}) \ldots \rightarrow \text{Tr} \ldots U_\mu(x)V(x + \hat{\mu})V(x + \hat{\mu})U_\mu(x + \hat{\mu}) \ldots \quad (9)$$

An action is specified by recalling that the classical Yang-Mills action involves the curl of $A_\mu$, $F_{\mu\nu}$. Thus a lattice action ought to involve a product of $U_\mu$’s around some closed contour. Gauge invariance will automatically be satisfied for actions built of powers of traces of $U$’s around arbitrary closed loops, with arbitrary coupling constants. If we assume that the gauge fields are smooth, we can expand the link variables in a power series in $gaA_\mu^a$. For almost any closed loop, the leading term in the expansion will be proportional to $F^{2}_{\mu\nu}$. This is not a bug, it is a feature. All lattice actions are just bare actions characterized by many bare parameters (coefficients of loops). In the continuum (scaling) limit all these actions are in the same universality class, which is (presumably) the same universality class as QCD with any regularization scheme, and there will be cutoff-independent predictions from any lattice actions which are simply predictions of QCD.
Let’s hold that thought while we do an example:
The simplest contour has a perimeter of four links. In $SU(N)$
\[
S = \frac{2}{g^2} \sum_n \sum_{\mu > \nu} \text{Re} \Tr \left(1 - U_\mu(n)U_\nu(n + \hat{\mu})U_\mu^\dagger(n + \hat{\nu})U_\nu^\dagger(n)\right).
\] (10)
This action is called the “plaquette action” or the “Wilson action” after its
inventor. $g^2$ is the bare lattice coupling, whose associated cutoff is $a$. The
lattice parameter $\beta = 2N/g^2$ is often written instead of $g^2 = 4\pi\alpha_s$.
Let us see how this action reduces to the standard continuum action. Specializing to the $U(1)$ gauge group, and slightly redefining the coupling,
\[
S = \frac{1}{g^2} \sum_n \sum_{\mu > \nu} \text{Re} \left(1 - \exp(iga[A_\mu(n) + A_\nu(n + \hat{\mu}) - A_\mu(x + \hat{\nu}) - A_\nu(n)])\right). \tag{11}
\]
The naive continuum limit is taken by assuming that the lattice spacing $a$ is
small, and Taylor expanding
\[
A_\mu(n + \hat{\nu}) = A_\mu(n) + a\partial_\nu A_\mu(n) + \ldots \tag{12}
\]
so the action becomes
\[
\beta S = \frac{1}{g^2} \sum_n \sum_{\mu > \nu} 1 - \text{Re} \left(\exp(iga[a(\partial_\nu A_\mu - \partial_\mu A_\nu) + O(a^2)])\right) \tag{13}
\]
\[
= \frac{1}{4g^2} a^4 \sum_n \sum_{\mu\nu} g^2 F_{\mu\nu}^2 + \ldots \tag{14}
\]
\[
= \frac{1}{4} \int d^4x F_{\mu\nu}^2 \tag{15}
\]
transforming the sum on sites back to an integral.

2.2 Numerical Simulations
In a lattice calculation, like any other calculation in quantum field theory,
we compute an expectation value of any observable $\Gamma$ as an average over a
ensemble of field configurations:
\[
\langle \Gamma \rangle = \frac{1}{Z} \int [d\phi] \exp(-S)\Gamma(\phi). \tag{16}
\]
We do this by Monte Carlo simulation: we construct an ensemble of states
(collection of field variables), where the probability of finding a particular config-
uration in the ensemble is given by Boltzmann weighting (i. e. proportional
to \exp(-S)$. Then the expectation value of any observable $\Gamma$ is given simply by an average over the ensemble:

$$\langle \Gamma \rangle \simeq \bar{\Gamma} = \frac{1}{N} \sum_{i=1}^{N} \Gamma[\phi(i)].$$

(17)

As the number of measurements $N$ becomes large the quantity $\bar{\Gamma}$ will become a Gaussian distribution about a mean value, our desired expectation value. The idea of essentially all simulation algorithms is to construct a new configuration of field variables from an old one. One begins with some initial field configuration and monitors observables while the algorithm steps along. After some number of steps, the value of observables will appear to become independent of the starting configuration. At that point the system is said to be “in equilibrium” and Eq. (17) can be used to make measurements.

Dynamical fermions are a complication for QCD. The fermion path integral is not a number and a computer can’t simulate fermions directly. However, one can formally integrate out the fermion fields. For $n_f$ degenerate fermion flavors

$$Z = \int [dU][d\psi][d\bar{\psi}] \exp(-\beta S_G(U) - \sum_{i=1}^{n_f} \bar{\psi}M(U)\psi)$$

(18)

$$= \int [dU](\det M(U))^{n_f} \exp(-\beta S(U)).$$

(19)

The determinant introduces a nonlocal interaction among the $U$’s:

$$Z = \int [dU] \exp(-\beta S(U) - n_f \text{Tr} \ln(M(U))).$$

(20)

Generating configurations of the $U$’s involves computing how the action changes when the set of $U$’s are varied. Typically, this involves inverting the fermion matrix $M(U)$ ($d \log M / dM = M^{-1}$). This is the major computational problem dynamical fermion simulations face. $M$ has eigenvalues with a very large range— from $2\pi$ down to $m_q a$— and in the physically interesting limit of small $m_q$ the matrix becomes ill-conditioned. At present it is necessary to compute at unphysically heavy values of the quark mass and to extrapolate to $m_q = 0$. (The standard inversion technique today is one of the variants of the conjugate gradient algorithm.) This tremendous expense is responsible for one of the “standard” lattice approximations, the “quenched” approximation. In this approximation the back-reaction of the fermions on the gauge fields is neglected, by setting $n_f = 0$ in Eq. (19). Valence quarks, or quarks which
appear in observables, are kept, but no sea quarks. No one knows how good an approximation this is, in principle. In practice it works very well for spectroscopy. The only way we know how to test it is to compare simulations in the quenched approximation with those from full QCD.

2.3 Spectroscopy Calculations

Masses are computed in lattice simulations from the asymptotic behavior of Euclidean-time correlation functions. A typical (diagonal) correlator can be written as

\[ C(t) = \langle 0 | O(t) O(0) | 0 \rangle. \] (21)

Making the replacement

\[ O(t) = e^{Ht} O e^{-Ht} \] (22)

and inserting a complete set of energy eigenstates, Eq. 21 becomes

\[ C(t) = \sum_n |\langle 0 | O | n \rangle|^2 e^{-E_n t}. \] (23)

At large separation the correlation function is approximately

\[ C(t) \approx |\langle 0 | O | 1 \rangle|^2 e^{-E_1 t} \] (24)

where \( E_1 \) is the energy of the lightest state which the operator \( O \) can create from the vacuum. Fig. 1 shows an example of this. If the operator does not couple to the vacuum, then in the limit of large \( t \) one hopes to to find the mass \( E_1 \) by measuring the leading exponential falloff of the correlation function. If the operator \( O \) has poor overlap with the lightest state, a reliable value for the mass can be extracted only at a large time \( t \). In some cases that state is the vacuum itself, in which \( E_1 = 0 \). Then one looks for the next higher state—a signal which disappears into the constant background. This is hard to do.

Most of the observables we are interested in will involve valence fermions. Let’s suppose we wanted to measure the mass of a meson. Then we might take

\[ C(t) = \sum_x \langle J(x, t) J(0, 0) \rangle \] (25)

where

\[ J(x, t) = \bar{\psi}(x, t) \Gamma \psi(x, t) \] (26)

and \( \Gamma \) is a Dirac matrix. The intermediate states \( |n\rangle \) which saturate \( C(x, t) \) are the hadrons which the current \( J \) can create from the vacuum: the pion,
for a pseudoscalar current, the rho, for a vector current, and so on. Now we write out the correlator in terms of fermion fields

\[ C(t) = \sum_x \langle 0 | \bar{\psi}_i(x,t)^\alpha \Gamma_{ij}(x,t)^\alpha \bar{\psi}_k(0,0)^\beta \Gamma_{kl} \psi_l(0,0)^\beta | 0 \rangle \] (27)

with a Roman index for spin and a Greek index for color. We contract creation and annihilation operators into quark propagators

\[ \langle 0 | T(\bar{\psi}_j(x,t)^\alpha \bar{\psi}_k(0,0)^\beta) | 0 \rangle = G^\alpha^\beta_{jk}(x,t;0,0) \] (28)

so

\[ C(t) = \sum_x \text{Tr}G(x,t;0,0)\Gamma G(0,0;x,t)\Gamma \] (29)

where the trace runs over spin and color indices. Baryons are constructed similarly. A good way to think about these correlators is by using a sort of Feynman-diagram language which keeps track of the valence quark lines but ignores all the gluons and sea quarks.

2.4 The Continuum Limit

When we define a theory on a lattice the lattice spacing \( a \) is an ultraviolet cutoff and all the coupling constants in the action are the bare couplings defined with
respect it. When we take $a$ to zero we must also specify how the couplings
behave. The proper continuum limit comes when we take $a$ to zero holding
physical quantities fixed, not when we take $a$ to zero fixing the couplings.

On the lattice, if all quark masses are set to zero, the only dimensionful
parameter is the lattice spacing, so all masses scale like $1/a$. Said differently, a
lattice calculation produces the dimensionless combination $am(a)$. One can
determine the lattice spacing by fixing one mass from experiment. Then all other
dimensionful quantities can be predicted. Imagine computing some masses at
several values of the lattice spacing. (Pick several values of the bare parameters
and calculate masses for each set of couplings.) Our calculated mass ratios
will depend on the lattice cutoff. If the lattice spacing is small enough, the
typical behavior will look like

$$(am_1(a))/(am_2(a)) = m_1(0)/m_2(0) + O(m_1a) + O((m_1a)^2) + \ldots \quad (30)$$

The leading term does not depend on the value of the UV cutoff, while the
other terms do. The goal of a lattice calculation is to discover the value of
some physical observable as the UV cutoff is taken to be very large, so the
physics is in the first term. Everything else is an artifact of the calculation.
We say that a calculation “scales” if the $a$-dependent terms in Eq. (30)
are zero or small enough that one can extrapolate to $a = 0$, and generically refer to all
the $a$-dependent terms as “scale violations.”

We can imagine expressing each dimensionless combination $am(a)$ as some
function of the bare coupling(s) $\{g(a)\}$, $am = f(\{g(a)\})$. As $a \to 0$ we must
tune the set of couplings $\{g(a)\}$ so

$$\lim_{a \to 0} \frac{1}{a} f(\{g(a)\}) \to \text{constant}. \quad (31)$$

From the point of view of the lattice theory, we must tune $\{g\}$ so that correlation
lengths $1/ma$ diverge. This will occur only at the locations of second (or
higher) order phase transitions. In QCD the fixed point is $g_c = 0$ so we must
tune the coupling to vanish as $a$ goes to zero.

One needs to set the scale by taking one experimental number as input. A
complication that you may not have thought of is that the theory we simulate
on the computer is different from the real world. For example, the quenched
approximation, or for that matter QCD with two flavors of degenerate quarks,
almost certainly does not have the same spectrum as QCD with six flavors
of dynamical quarks with their appropriate masses. Using one mass to set
the scale from one of these approximations to the real world might not give a
prediction for another mass which agrees with experiment.
(The glass is always half empty... In the strong coupling limit, lattice regularized QCD automatically confines and chiral symmetry is spontaneously broken. So unless there is some kind of phase transition as the bare couplings are tuned to take the cutoff away, which probably doesn’t happen, we are working with a confining theory without doing anything special.)

Today’s QCD simulations range from $16^3 \times 32$ to $32^3 \times 100$ points and run from hundreds (quenched) to thousands (full QCD) of hours on the fastest supercomputers in the world. The cost of a Monte Carlo simulation in a box of physical size $L$ with lattice spacing $a$ and quark mass $m_q$ scales roughly as

$$\left(\frac{L}{a}\right)^4 \left(\frac{1}{a}\right)^{1-2} \left(\frac{1}{m_q}\right)^{2-3}$$

where the 4 is just the number of sites, the 1-2 is the cost of “critical slowing down”—the extent to which successive configurations are correlated, and the 2-3 is the cost of inverting the fermion propagator, plus critical slowing down from the nearly massless pions. Thus it is worthwhile to think about how to do the discretization, to maximize the value of the lattice spacing. The thing to keep in mind is that the lattice action is just a bare action defined with a cutoff. No lattice discretization is any better or worse (in principle) than any other. Any bare action which is in the same universality class as QCD will produce universal numbers in the scaling limit. However, by clever engineering, it might be possible to devise actions whose scaling behavior is better, and which can be used at bigger lattice spacing.

An example of a test of scale violations is shown in Fig. 2. The x axis is the lattice spacing, in units of a quantity $r_1$, which is defined through the heavy quark potential: $r_1^2 dV(r)/dr|_{r_1} = 1.0$, about 0.4 fm. The plotting symbols are for different kinds of discretizations. The flatter the curve, the smaller the scale violations.

The simplest organizing principle for “improvement” is to use the canonical dimensionality of operators as a guide. Consider the gauge action as an example. If we perform a naive Taylor expansion of a lattice operator like the plaquette, we find that it can be written as

$$1 - \frac{1}{3} \text{Re} \text{ Tr}U_{\text{plaqt}} = r_0 \text{ Tr} F_{\mu\nu}^2 + a^2 \left[ r_1 \sum_{\mu\nu} \text{ Tr} D_\mu F_{\mu\nu} D_\mu F_{\mu\nu} + r_2 \sum_{\mu\nu\sigma} \text{ Tr} D_\mu F_{\nu\sigma} D_\mu F_{\nu\sigma} + r_3 \sum_{\mu\nu\sigma} \text{ Tr} D_\mu F_{\mu\sigma} D_\nu F_{\nu\sigma} \right] + O(a^4)$$

The expansion coefficients have a power series expansion in the coupling, $r_j = A_j + g^2 B_j + \ldots$ and the expectation value of any operator $T$ computed using
the plaquette action will have an expansion
\[ \langle T(a) \rangle = \langle T(0) \rangle + O(a) + O(g^2 a) + \ldots \] (34)

Other loops have a similar expansion, with different coefficients. Now the idea
is to take the lattice action to be a minimal subset of loops and systemati-
cally remove the \( a^n \) terms for physical observables order by order in \( n \) by taking
the right linear combination of loops in the action, \( \tilde{S} = \sum c_j O_j \) with \( c_j = c_j^0 + g^2 c_j^1 + \ldots \). This method was developed by Symanzik and co-workers \cite{8,9,10}
in the mid-80’s.

Ordinary perturbation theory (expansions in the bare lattice coupling \( g \))
are not very convergent, but clever prescriptions for definitions of couplings\cite{11}
or nonperturbative tuning methods\cite{12} have been quite successful in developing
improved lattice actions.

2.5 Relativistic Fermions on the Lattice

Defining fermions on the lattice involves yet another problem: doubling. Let’s
illustrate this with free field theory. The continuum free action is
\[ S = \int d^4 x [\bar{\psi}(x)\gamma_\mu \partial_\mu \psi(x) + m \bar{\psi}(x) \psi(x)] . \] (35)
One obtains the so-called naive lattice formulation by replacing the derivatives by symmetric differences:

\[ S_{\text{naive}}^L = \sum_{n,\mu} \bar{\psi}_n \frac{\gamma_\mu}{2a} (\psi_{n+\mu} - \psi_{n-\mu}) + m \sum_n \bar{\psi}_n \psi_n. \]  

(36)

The propagator is:

\[ G(p) = (i\gamma_\mu \sin p_\mu a + ma)^{-1} = \frac{-i\gamma_\mu \sin p_\mu a + ma}{\sum_\mu \sin^2 p_\mu a + m^2 a^2} \]  

(37)

We identify the physical spectrum through the poles in the propagator, at \( p_0 = iE \):

\[ \sinh^2 Ea = \sum_j \sin^2 p_j a + m^2 a^2 \]  

(38)

The lowest energy solutions are the expected ones at \( p = (0, 0, 0), E \simeq \pm m \), but there are other degenerate ones, at \( p = (\pi, 0, 0), (0, \pi, 0), \ldots (\pi, \pi, \pi) \). As \( a \) goes to zero, the lightest excitations of the spectrum, the ones whose energy is \( O(1) \), not \( O(1/a) \), are the relevant ones, and there are sixteen of these, in all the corners of the Brillouin zone. Thus our action is a model for sixteen light fermions, not one. This is the famous “doubling problem.”

In fact, associated with the “doubling problem” is the Nielsen-Ninomaya theorem, which says that no lattice action can be undoubled, chiral, and have couplings which extend over a finite number of lattice spacings (ultralocality). However, there are three ways to get two out of three. They are

(a) Wilson Fermions (undoubled, nonchiral, ultralocal)

We can alter the dispersion relation so that it has only one low energy solution. The other solutions are forced to \( E \simeq 1/a \) and become very heavy as \( a \) is taken to zero. The simplest version of this solution, called a Wilson fermion, adds an irrelevant operator, a second-derivative-like term

\[ S^W = -\frac{r}{2a} \sum_{n,\mu} \bar{\psi}_n (\psi_{n+\mu} - 2\psi_n + \psi_{n-\mu}) \simeq ar\bar{\psi}D^2\psi \]  

(39)

to \( S_{\text{naive}}^L \). The parameter \( r = 1 \) is almost always used and is implied when one speaks of using “Wilson fermions.”

There are two dimension-five operators which can be added to a fermion action. The Wilson term is just one of them. The other dimension-five term is a magnetic moment term

\[ S_{SW} = -\frac{iaq}{4} \bar{\psi}(x)\sigma_{\mu\nu} F_{\mu\nu} \psi(x) \]  

(40)
and if both terms are included, their coefficients can be tuned so that there are no $O(a^2g^2)$ lattice artifacts. This action is called the “Sheikholeslami-Wohlert” or “clover” action because the lattice version of $F_{\mu\nu}$ is the sum of paths shown in Fig. 3.

Wilson-type fermions contain an explicit chiral-symmetry breaking term. This causes a lot of bad things to happen. The most obvious is that the zero bare quark mass limit is not respected by interactions; the quark mass is additively renormalized. The value of bare quark mass $m_q$ which the pion mass vanishes, is not known a priori before beginning a simulation; it must be computed. This is done in a simulation involving Wilson fermions by varying $m_q$ and watching the pion mass extrapolate quadratically to zero as $m_{\pi}^2 \simeq m_q - m_q^c$. It actually turns out that this is a worse problem than you would think: the Dirac operator $D$ on a gauge configuration could develop a real eigenmode $\lambda$ at minus the bare quark mass you dialed into the program. Then $D + m$ would be non-invertible! Other nasty things happen (operator mixing, see the next section) and people argue about how serious they are in practice.

(b) Staggered or Kogut-Susskind Fermions (chiral, doubled, ultralocal)

In this formulation one reduces the number of fermion flavors by using one component “staggered” fermion fields rather than four component Dirac spinors. The Dirac spinors are constructed by combining staggered fields on
Figure 4: An example of flavor symmetry breaking in an improved staggered action. The different $\gamma$'s are a code for the various pseudoscalar states. Data are from Ref. 17. For an explanation of the splitting, see Ref. 18.

different lattice sites. Staggered fermions preserve an explicit chiral symmetry as $m_q \rightarrow 0$ even for finite lattice spacing, as long as all four flavors are degenerate, although it is not the $SU(N_f) \times SU(N_f)$ of the continuum, it is a $U(1)$. Thus there is only one Goldstone pion at finite $a$, plus other non-degenerate pseudoscalar states whose mass goes to zero in the continuum limit (See Fig. 4 for an example of this.) They are preferred over Wilson fermions in situations in which the chiral properties of the fermions dominate the dynamics. They also cheaper to simulate than Wilson fermions, because there are less variables. However, flavor and translational symmetry are all mixed together.

(c) Chiral, undoubled, but not ultralocal

These actions implement a modified version $\delta \psi = \gamma_5 (1 - \frac{1}{2}aD) \psi$; $\delta \bar{\psi} = \bar{\psi} (1 - \frac{1}{2}aD) \gamma_5$ (41)

which is sufficient to preserve all the interesting features of continuum chiral symmetry. An example of such an action is the “domain wall fermion”. It is a variation on the idea that if you have a fermion coupled to a scalar field, and the scalar field interpolates between two minima (forms a soliton), the fermion will develop a zero-energy chiral mode bound to the center of the soliton. Now we go into brane world, extend QCD into five dimensions, and put ourselves
and our four dimensional world on the kink. There is an anti-kink out there in the fifth dimension, and as long as it is far away the mode on the kink doesn’t see the anti-kink and the 4-d theory on the kink is chiral. But if the anti-kink is too close (fifth dimension too small) the modes mix and chiral symmetry is broken. How close is “too close” is (yet) another engineering question. There are four dimensional analogs of this—think of integrating out the modes in the fifth dimension in favor of a tower of massive fermions, and get “overlap fermions $^{21}$,” or construct a low energy Wilsonian effective action from an underlying chiral theory and get “fixed point fermions $^{22}$.” The bad feature is that these actions have couplings which reach out to many neighboring sites. Their strength drops exponentially with distance, so they are true local actions in the continuum limit, but they are very expensive to simulate. But stay tuned...

3 Hadronic Matrix Elements from the Lattice

One of the major goals of lattice calculations is to provide hadronic matrix elements which either test QCD or can be used as inputs to test the standard model.

3.1 Generic Matrix Element Calculations

Most of the matrix elements measured on the lattice are extracted from expectation values of local operators $J(x)$ composed of quark and gluon fields. For example, if one wanted $\langle 0 | J(x) | h \rangle$ one could look at the two-point function

$$C_{JO}(t) = \sum_x \langle 0 | J(x, t) O(0, 0) | 0 \rangle.$$ (42)

Inserting a complete set of correctly normalized momentum eigenstates

$$1 = \frac{1}{L^3} \sum_{A, \vec{p}} |A, \vec{p}\rangle \langle A, \vec{p}|$$ (43)

and using translational invariance and going to large $t$ gives

$$C_{JO}(t) = e^{-m_A t} \frac{\langle 0 | J | A \rangle \langle A | O | 0 \rangle}{2m_A}.$$ (44)

A second calculation of

$$C_{OO}(t) = \sum_x \langle 0 | O(x, t) O(0, 0) | 0 \rangle \rightarrow e^{-m_A t} \frac{|\langle 0 | O | A \rangle|^2}{2m_A}$$ (45)
is needed to extract $\langle 0|J|A \rangle$ by fitting two correlators with three parameters.

Similarly, a matrix element $\langle h|J|h' \rangle$ can be gotten from

$$C_{AB}(t, t') = \sum_x \langle 0|O_A(t)J(x, t')O_B(0)|0 \rangle.$$ (46)

by stretching the source and sink operators $O_A$ and $O_B$ far apart on the lattice, letting the lattice project out the lightest states, and then measuring and dividing out $\langle 0|O_A|h \rangle$ and $\langle 0|O_B|h \rangle$.

These lattice matrix elements are not yet the continuum matrix elements. Typically, one is interested in some matrix element defined with a particular regularization scheme. It is a generic feature of quantum field theory that an operator defined in one scheme ($\overline{\text{MS}}$) will be a superposition of operators in another scheme (lattice). In principle, the superposition could be all possible operators. So generically an operator of dimension $D$ will mix like

$$\langle f|O^{\text{cont}}(\mu)|i \rangle_{\overline{\text{MS}}} = a^D \sum_m Z_{nm} \langle f|O^{\text{latt}}(a)_m|i \rangle_{\overline{\text{MS}}}.$$ (47)

The only restriction are symmetries: in a theory where parity is conserved a vector operator and an axial vector operator can’t mix. This is relevant for lattice calculations because the symmetries of the lattice action are in general different from continuum symmetries. For example, the space-time symmetry of the lattice is given by the group of discrete rotations. A more serious source of mixing for light quark operators is the way lattice fermions treat chiral symmetry. Wilson-type fermions break chiral symmetry (even massless ones do so off-shell) and so nothing prevents mixing into “wrong chirality” operators.

In Eq. 47 the “diagonal” term will contain the anomalous dimension of the continuum operator

$$Z_{nn} = 1 + \frac{g^2}{16\pi^2}(\gamma_n \log a\mu + A) + \ldots$$ (48)

(which cancels the $\mu$-dependence of the coefficient function $C(\mu)\langle f|O^{\text{cont}}(\mu)|i \rangle_\mu$ is independent of the renormalization point). In principle the leading log could be summed, but in practice we don’t know how much of the constant term $A$ should be absorbed into a change of scale of $g$, so they are just left there. The mixing terms to other dimension $D$ operators die out in the continuum so they don’t have any logs. There are also terms for mixing with higher dimensional operators, which give contributions proportional to positive powers of $a$. (These are usually benign.) One can also have mixing with lower dimensional operators, with contributions involving negative powers of $a$. (Four fermion
operators for $B_K$ could mix with $s\bar{d}$.) These are deadly. They must drop out in the continuum but it is a delicate business, since they look like they are growing as an inverse power of $a$.

This is probably more than you wanted to know, but you need the $Z_{nm}$’s to produce numbers. People get them in a number of ways. Most straightforward is to compute them in perturbation theory, but lattice perturbation theory in terms of the bare coupling $g(a)$ is not very convergent, and it is a long tricky story to do better. The culprit is the “tadpole graph.” The lattice fermion-gauge field interaction is generically $\bar{\psi}(x)U_\mu(x)\psi(x+\hat{\mu}a)$ and $U \approx 1 + i g a A_\mu - g^2 a^2/2A_\mu^2 + \ldots$. The $\bar{\psi}A_\mu^2\psi$ vertex, not present in any sensible continuum regularization, causes problems when the gluon forms a loop: the quadratic divergence from the loop integral combines with the $a^2$ to give a finite contribution—in fact, it is often the dominant contribution. In perturbation theory one must also choose the momentum scale in the running coupling constant. There are reasonable choices for how to do that.

Often one can find $Z_{nm}$’s by forcing lattice observables to obey Ward identities. One can also play this game with quark propagators and vertices, by computing analogs of quark vertices on the lattice and matching ones results to a continuum calculation.

Besides, the $Z$’s, there are other things that can go wrong. Most lattice actions break down when the quark mass gets heavy. The dispersion relation for Wilson or clover actions is $E(p) = m_1 + p^2/(2m_2)$ and the quark magnetic moment is $\mu = 1/m_3$ with $m_1 \neq m_2 \neq m_3$. The residue of the quark propagator at its pole is not $1/(2E)$ as in the continuum. What to do then is not obvious (meaning that lattice people fight over what to do).

3.2 Heavy quark operators

There are many lattice calculations of $f_B$, $f_D$, $B_B$, and form factors for semileptonic decay. $\bar{B}-B$ mixing is parameterized by the ratio $x_d = (\Delta M)_{b\bar{d}}/\Gamma_{b\bar{d}}$

$$x_d = \tau_{bd} \frac{G_F}{6\pi^2} \eta_{QCD} F\left(\frac{m_B^2}{m_W^2}\right)|V_{tb}V_{td}|^2 b(\mu) \left\{ \frac{3}{8} \langle \bar{B} | \bar{b} \gamma_\mu (1 - \gamma_5) d \bar{d} \gamma_\mu (1 - \gamma_5) d | B \rangle \right\}$$

Experiment is on the left; theory on the right. Moving into the long equation from the left, we see many known (more or less) parameters from phase space integrals or perturbative QCD calculations, then a combination of CKM matrix elements, followed by a four quark hadronic matrix element. We would like to extract the CKM matrix element from the measurement of $x_d$ (and its strange partner $x_s$). To do so we need to know the value of the object in the curly brackets, defined as $3/8M_{bd}$ and parameterized as $m_B^2 f_B^2 B_{bd}$.
where $B_{bd}$ is the so-called B-parameter, and $f_B$ is the B-meson decay constant, $\langle 0 | \bar{b} \gamma_\mu \gamma_5 d | B \rangle = f_B m_B$. Vacuum saturation suggests that $B_B = 1$. From the lattice one can try to get a real value.

In Eq. (49) $b(\mu)$, the coefficient which runs the effective interaction down from the W-boson scale to the QCD scale $\mu$, and the matrix element $M(\mu)$ both depend on the QCD scale. One often sees the renormalization group invariant quantities $\hat{M}_{bd} = b(\mu) M_{bd}(\mu)$ or $\hat{B}_{bd} = b(\mu) B_{bd}(\mu)$ quoted in the literature.

Decay constants probe very simple properties of the wave function: in the nonrelativistic quark model $f_M = \psi(0)/\sqrt{m_M}$, where $\psi(0)$ is the $\bar{q}q$ wave function at the origin. For a heavy quark ($Q$) light quark ($q$) system $\psi(0)$ should become independent of the heavy quark’s mass as the $Q$ mass goes to infinity, and in that limit one can show in QCD that $\sqrt{m_M} f_M$ approaches a constant.

The decay constant is computed by combining a heavy quark and a light antiquark propagator into Eq. (42). You might think it would be difficult to calculate $f_B$ directly on present day lattices with relativistic lattice fermions because the lattice spacing is much greater than the $b$ quark’s Compton wavelength (or the UV cutoff is below $m_b$). But it is better to think of the lattice theory as an effective field theory for the low-momentum excitations in the presence of additional high energy scales—the cutoff (inverse lattice spacing) and the heavy quark mass. As in any effective field theory, the effects of the short distance are lumped into coefficients of the effective theory. As a practical matter, one can use the good old clover action to do the calculations—it contains all the necessary operators. The bare mass has nothing direct to do with the results; one tunes it, monitoring the kinetic energy $E(p) = m_1 + p^2/(2m_2) + \ldots$, and takes the hadron mass to be $m_2$.

Nonrelativistic QCD has also been discretized and used to make very precise calculations of the properties of quarkonia. This formalism can also be used for the heavy quark (again as long as its momentum is small.) The “static” limit (infinite $b$-quark mass) is often used as an additional point on the curve. Then one can try to extrapolate all the way from light quarks to heavies and get all the decay constants at once.

I will show some pictures from the lattice decay constant of Ref. 30. These authors (my name is on it but I didn’t do anything) did careful quenched simulations at many values of the lattice spacing, which allows one to extrapolate to the continuum limit by brute force. They have also done a set of simulations which include light dynamical quarks, which should give some idea of the accuracy of the quenched approximation.

Examples of results of Ref. 30 are shown in Figs. 5 and 6. The simulations
with dynamical fermions are not as good quality as the quenched simulations: the lattice spacings are generally larger, the simulations all have two degenerate flavors (what about the strange quark), and the dynamical quark masses are still a bit large. We think that the Wilson results (crosses in Fig. 3b) overestimate the continuum result, and the clover action we are using underestimates it, but we also suspect that quenched $f_B$ is a bit too low.

![Figure 5: Pseudoscalar meson decay constant vs $1/M$, from Ref. 30.](image)

Soni has presented a summary of data from various collaborations, as of last winter. Again, there is a hint that the $N_f=2$ results may be about 30 MeV above the quenched results.

Lattice calculations have been predicting quenched $f_{D_s} \simeq 200$ MeV for about twelve years. The central values have changed very little, while the uncertainties have decreased. Experimental determinations of $f_{D_s}$ all come in higher than the lattice results, though with large error bars. We need to do a good quality unquenched lattice calculation.

Now back to the $B$ parameter. On the lattice, one could measure the decay
Table 1: Heavy-light decay constants and their ratios.

| Quantity     | Quenched ($N_f = 0$) | Partially Unquenched ($N_f = 2$) |
|--------------|----------------------|-----------------------------------|
| $f_B$/MeV    | 170 ± 20             | 200 ± 30                          |
| $f_{B_S}$/MeV| 190 ± 20             | 220 ± 30                          |
| $f_D$/MeV    | 205 ± 20             | 225 ± 30                          |
| $f_{D_S}$/MeV| 225 ± 20             | 245 ± 30                          |
| $f_B/f_B$    | 1.14 ± .06           | 1.14 ± .06                        |
| $f_{D_S}/f_D$| 1.10 ± .06           | 1.10 ± .06                        |

constants and $B$ parameter separately and combine them after extrapolation, or measure $M$ directly. In principle the numbers should be the same, but in practice the first technique has produced better numbers so far. That is because the $B$ parameter is measured as the ratio of a correlator with a four-fermion vertex to a product of two current-current correlators (see Fig. 7). A lot of systematics cancel in the ratio.

Many groups have visited this problem. Reviews by Draper and Soni quote a world summary, which I copy into Table 2.

Semileptonic decays involve processes like Eqn. 46. On the lattice, one just measures the matrix element of a current and fits it to the expected set of form factors—for $B \rightarrow \pi\ell\nu$, for example,

$$\langle \pi(p)|V_\mu|B(p')\rangle = f^+(q^2)[p' + p - \frac{m_B^2 - m_\pi^2}{q^2}q_\mu] + f^0(q^2)\frac{m_B^2 - m_\pi^2}{q^2}q_\mu \tag{50}$$

The best signals come when the momenta of the initial and final hadron are
small. Then the large $B$ mass forces $q^2$ ($q =$ lepton 4-momentum $= p_B - p_\pi$) to be large. If the form factor is needed at $q^2 \sim 0$, a large extrapolation is needed, and there will be additional errors and model dependence in the answer. (Lattice people have no advantage over anyone else at guessing at functional forms.) However, finding $V_{ub}$ from experimental data only requires knowing the form factor at one value of $q^2$. This should work so long as the experiment has enough data to measure the differential rate around that region of $q^2$. Two recent approaches try to do this: UKQCD focussed on near the end-point or the zero-recoil region where the lattice data tends to be cleanest and heavy quark symmetry can be used. The FNAL group has measured $B \to D\ell\nu$ form factors at zero recoil\cite{34}. They have a clever technique from removing much of the lattice-to-continuum $Z$-factors by computing ratios of matrix elements, such as

$$\frac{(D|\bar{c}\gamma_0 b|\bar{B})(\bar{B}|\bar{b}\gamma_0 c|D)}{(D|\bar{c}\gamma_0 c|D)(\bar{B}|\bar{b}\gamma_0 b|\bar{B})} = |h_+(v \cdot v' = 1)|^2 \quad (51)$$

The denominators are just diagonal matrix elements of the charge density,
and they can easily be normalized. They are also computing semi-leptonic form factors for $B \rightarrow \pi \ell \nu$ and $D \rightarrow \pi(K) \ell \nu$, by concentrating directly on the differential decay spectrum in an interval with $0.4 \lesssim \bar{p}_\pi/\text{GeV} \lesssim 0.8$ thus avoiding the need for large extrapolation in $q^2$.

### 3.3 Kaon Matrix Elements

Lattice calculations of kaon weak interaction matrix elements begin with the full Standard Model at high energies and use the operator product expansion, combined with the renormalization group, to construct a low-energy effective field theory valid at scales $\mu$ of a few GeV. The effective Hamiltonian basically reduces to a sum of four-fermion interactions

$$H_{4f}^{\text{eff}} = \frac{G_F}{\sqrt{2}} \sum_{i=0}^{10} c_i(\mu)O_i(\mu)$$

People have expended the most effort on, and have the best results for, $B_K$; there are some results on the $\Delta I = 1/2$ rule; and last, there is $\epsilon'/\epsilon$, with unreliable results so far.

$B_K$

The JLQCD collaboration has the best results on $B_K$, from a calculation using staggered fermions. They have data from many lattice spacings and several choices for the lattice discretization of the operator. (See Fig. 8.) They find quenched $B_K(MS, \mu = 2 \text{ GeV}) = 0.616(5)$. The main limitations of this result are quenching, plus the fact that the lattice calculations are actually done without $SU(3)$ flavor breaking (the lattice “kaon” is a pseudoscalar made of degenerate quarks). These effects are believed to be 5-10 per cent corrections.

JLQCD has also done a calculation with Wilson fermions. This was done not so much to get a number itself but to check the staggered result. The systematics are very different and the operator mixing is fierce due to the loss of chiral symmetry inherent in Wilson fermions. For example, $\bar{s}\gamma_\mu(1 - \gamma_5)d \cdot \bar{s}\gamma_\mu(1 - \gamma_5)d$ mixes with $\bar{s}\gamma_5d \cdot \bar{s}\gamma_5d$ and that operator has a $\bar{K} - K$ matrix element ten times greater.

$\Delta I = 1/2$ Rule

Can the lattice reproduce the experimentally observed factor of 22 between $K^0 \rightarrow (\pi\pi)_{I=0}$ and $K^0 \rightarrow (\pi\pi)_{I=2}$ amplitudes? The lattice calculations are difficult. In addition to graphs of Fig. 7, which are reasonably straightforward to compute, there are a host of other topologies, some of which involve computing propagators from many points on the lattice to many other points. But I think the reason there are so few lattice results is because all of the quantities of interest are scheme dependent and one must compute a lattice-to-continuum
matching factor. In addition, people don’t calculate $K \rightarrow \pi\pi$ directly on the lattice; it is difficult to extract the phase shifts from the $\pi\pi$ final state interactions from lattice data (never mind trying to separate the two pions to asymptotically great distances). Instead, they use chiral perturbation theory to relate $K \rightarrow \pi\pi$ amplitudes to $K \rightarrow \pi$. In the case of the $\Delta I = 3/2$ amplitude there is a factor of two change in the lattice result depending on whether tree level or one loop chiral perturbation theory is used. This is shown in Fig. 9.

The only recent work I am aware of is by Pekurovsky and Kilcup. The calculation is hard. The biggest operators $O_6$ and $O_8$ in the nomenclature have opposite signs and nearly cancel. But the big problem is the scheme matching. In a perturbative calculation, we saw that $\langle O \rangle_{\overline{MS}} \simeq Z \langle O \rangle_{\text{latt}}$ and $Z = 1 + \alpha_s C + \ldots$. But in this equation, what scheme is used to compute $\alpha_s$, and what is the scale $q^*$ at which $\alpha_s$ is evaluated? Pekurovsky and Kilcup found that their numbers for one operator, $O_6$, shifted by a factor of 4 when they were converted into $\overline{MS}$, and the factor of 4 could become a factor of 30.
Figure 9: $\Delta I = 3/2 \ K \rightarrow \pi\pi$ amplitude with (fancy symbols) and without (plain symbols) one-loop corrections of quenched chiral perturbation theory. Data are crosses and fancy crosses, $40$; diamonds and fancy diamonds, $41$. Data are plotted as a function of lattice meson mass. This figure (and much else) is from $42$.

(or worse) as $q^*$ was varied from $\pi/a$ to $1/a$. They attempt to guesstimate numbers but since they say plainly that they should be used “with extreme caution” I won’t quote them. A nonperturbative approach to matching is clearly needed but does not exist yet.

4 Conclusions

What about the future? Matrix elements are at the end of a long chain involving a large set of both simulation and physics issues. They are the most complicated corner of the lattice game. If all you want are the numbers, Moore’s law says that computer speed doubles every eighteen months, and statistics is
\[ \sqrt{N}, \] so error bars will fall by a factor of 2 every three years for everything we know how to do today and will learn nothing new about how to do better in the future. And there are many projects and proposals to build clusters or dedicated supercomputers at a cost which is “chicken feed” compared to the experimental program. This will enable us to begin to chip away at the biggest systematic in all the calculations I have shown here—the neglect of the quenched approximation.

But new hardware is not really where the action is. It is merely “enabling technology,” so we can make mistakes faster, learn more about the physics, and test new ideas.

The main bottleneck to progress on hadronic matrix elements is just that these calculations are complex and have many parts. Some of us (me, let’s not be shy) think that better discretization algorithms will help. The problem with that approach is that many pieces of the puzzle have to be determined from scratch: learning how to optimize the new algorithm, testing spectroscopy, computing the Z’s. This takes a couple of years, if the inventor of the algorithm doesn’t get tired first. Others of us prefer to live with poorer algorithms (which have already been well calibrated) and try to tweak the parts of them which work the worst. The simulations still take a couple of years. Believe it or not, even though lattice QCD is a mature field, there are still many questions about QCD which lattice people do not know how to answer, and an outsider might. Maybe you would enjoy thinking about them.

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