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Lattice QCD with Chiral Quarks: Using Symmetry to Explore Symmetry Breaking

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Abstract.
Over the last 15 years, lattice discretizations of quarks that preserve chiral symmetry have progressed from beautiful theoretical ideas to practical simulation tools. With control over chiral symmetry, lattice calculations of more of the matrix elements relevant to the violation of charge-conjugation and parity (CP) symmetry in the Standard Model can be done. The progression to practical simulation tool has been aided by the continued growth in computing power, as well as marked advances in algorithms. The status of simulations with chiral quarks will be reviewed, emphasizing the physics of CP violation that is currently being done. The prospects for future simulations with physical values for the light quarks will also be discussed.

1. Introduction
Quantum Chromodynamics (QCD) is the name for the theory of the strong nuclear force. This force, which acts on spin 1/2 particles called quarks and is mediated by spin-1 particles called gluons, produces bound states of quarks, called hadrons, which include the familiar proton and neutron of the atomic nucleus. Adding to QCD theories of the weak nuclear force and electromagnetism, which are built on the same principle of gauge invariance that underlies QCD, yields the Standard Model of particle physics, an extraordinarily precise description of all non-gravitational interactions. Tremendous theoretical and experimental effort is being expended to probe the standard model, for example in the search for the Higgs particle, and to seek physics that is outside its scope. Current numerical simulations of QCD are playing an ever larger role in constraining parameters that enter the Standard Model and this report will detail progress in numerical simulations of QCD that have been made possible through the development of better lattice discretizations of the Dirac equation, improved algorithms and faster computers.

2. Defining QCD
Before discussing the broader issues of QCD and particle physics, we will first introduce the important components of numerical QCD simulations. The QCD interactions between the spin-1 force-carrying particles, called gluons, and quarks are very similar to those between the photons and electrons of QED, Quantum Electrodynamics - the quantum theory of electromagnetic phenomena. Before quantization, electromagnetic phenomena are described by Maxwell’s equations coupled to charged matter fields - a complicated system in its own right, particularly
when macroscopic media are present. Even if one neglects bulk material, the classical interaction of electromagnetic fields and charged particles has internal inconsistencies. Maxwell’s equations
\[
\begin{align*}
\nabla \cdot \vec{E} &= 4\pi \rho \\
\nabla \cdot \vec{B} &= 0 \\
\nabla \times \vec{B} &= \frac{4\pi}{c} \vec{J} + \frac{1}{c} \frac{\partial \vec{E}}{\partial t} \\
\nabla \times \vec{E} &= -\frac{1}{c} \frac{\partial \vec{B}}{\partial t}
\end{align*}
\]
yield solutions for the fields when the motion of the charged particles is given, or allow particle motions to be determined when the fields are given, through the solutions of
\[
\dot{\vec{p}}_i = \vec{F}_{\text{external}}(1)
\]
When both field and particle motion are to be determined, the basic formalism becomes problematic since the external force \(\vec{F}_{\text{external}}\) is poorly defined in the classical context. There is no appropriate separation between the self-field and external fields that a particle sees.

The quantum version of electrodynamics, QED, solves these problems and produces a theory which is perturbatively free of ambiguities and inconsistencies. A remnant of the self/external field problem is the need to renormalize the theory, where renormalization refers to the detailed division of forces into self and external field contributions. In particular, the parameters that enter the fundamental Lagrangian of the system are not directly the physically observed particle masses and couplings - these physical quantities are the renormalized versions of the Lagrangian parameters. There is substantial arbitrariness in the division into self and external fields, but this arbitrariness is not present in any physical predictions. Renormalization is a well understood subject in analytic work and it is important to retain the ability to do accurate renormalizations when numerical techniques are employed.

A powerful description of QED, and also QCD, comes via the Feynman path integral, where the quantum system is represented as a sum (integral) over all classical configurations of the system. The path integral takes the general form
\[
Z = \int [dA] [d\psi] [d\bar{\psi}] \exp \left\{ -\frac{i}{4} \left( \partial_\mu A_\nu - \partial_\nu A_\mu \right)^2 + \bar{\psi} \left[ i \gamma^\mu \left( \partial_\mu - ie_0 A_\mu \right) - m_0 \right] \psi \right\}
\]
Here \(A_\mu \equiv (\Phi, \vec{A})\) is the four-vector potential made of the scalar potential and three-vector potential of Maxwell electromagnetism and \([dA]\) is a product measure representing the integral over all values of the fields at all four-dimensional space-time points. The fields \(\psi\) are four-component Dirac fields representing the spin 1/2 electrons, \(\gamma^\mu\) are four, 4 \(\times\) 4 matrices in the internal spin space of the Dirac field (the Dirac matrices) and variation of the action in braces in equation 2 yields the Dirac equation
\[
D(A, m_0, e_0) \psi \equiv [i \gamma^\mu \left( \partial_\mu - ie_0 A_\mu \right) - m_0] \psi = 0
\]
The parameter \(m_0\) is the bare electron mass and \(e_0\) is the bare charge of the theory. The physical values of the mass and the charge are functions of these bare parameters.

The fields \(\psi\) that enter in the path integral are Grassman (anti-commuting) fields, which are required by the Fermi statistics of the spin 1/2 electron. Since non-commuting numbers are not directly representable in a computer, we anticipate numerical simulations by doing the fermionic part of the path integral analytically to arrive at
\[
Z = \int [dA] \det[D(A, m_0, e_0)] \exp \left\{ -\frac{i}{4} \left( \partial_\mu A_\nu - \partial_\nu A_\mu \right)^2 \right\}
\]
QED and, as we will see, QCD, have an important symmetry if the bare mass is zero - a chiral symmetry. For massless spin 1/2 particles, the Dirac equation splits into two equations, the Weyl equations.

\[ i\gamma^\mu(\partial_\mu - ieA_\mu) - m \psi = 0 \]

Here \( \psi_L = (1 + \gamma_5)/2 \) and \( \psi_R = (1 - \gamma_5)/2 \) The theory is classically invariant under separate rotations of the left- and right-handed electron fields. Chiral symmetry simplifies the renormalization of the theory and preserving this symmetry in numerical simulations is one of the major advances in this field in recent years.

For QCD, the one electron field of QED is replaced by one quark field for each of the six flavors of quarks (the quark flavors are up, down, strange, charm, bottom and top) and the photon field is replaced by the 8 gluon fields. The Feynman path integral for QCD is quite similar to equation 4 and is given by

\[
Z = \int [dA] \prod_{i=1}^{6} (\det[D(A, m_0^i, g_0)]) \exp \left\{ -\frac{i}{4} (\partial_\mu A_\nu - \partial_\nu A_\mu + g_0 f^{abc} A^b_\mu A^c_\nu) \right\} \]

where the Dirac operator is modified by the inclusion of the \( 3 \times 3 \) matrices \( t^a \) (the generators of the SU(3) gauge group) to become \( D_\mu(A, m_0^i, g_0) \equiv it^a(\partial_\mu - ig_0 A^a_\mu t^a / 2) - m_0^i \). The QCD path integral includes the vitally important gluon interaction term \( g_0 f^{abc} A^a_\mu A^b_\nu \), where \( g_0 \) is the bare QCD coupling constant, which is responsible for the dramatically different features of QCD as compared to QED. One consequence of the gluon self-interaction is the increasing strength of the color force at large distances, which leads to the confinement of quarks into hadrons, such as the proton.

The QCD path integral in equation 5 can evaluated via perturbation theory, where the value of \( g \) is presumed small. This is the case at high enough energy scales, since the effective strength of the coupling at an energy scale \( \mu \), \( g(\mu) \), decreases with increasing \( \mu \). For energy scales below a few GeV, the convergence of perturbation theory is not good and non-perturbative techniques are required. Numerical simulations are a first principles technique for dealing with the QCD path integral and we now turn to them.

3. Discretizing QCD

Numerical simulations of the QCD path integral, equation 5 are relevant for QCD phenomena at energy scales below a few GeV. For such studies, the effects of the determinant factors from heavy quarks in equation 5 can be neglected, so one generally includes the effects of the up, down and strange quarks in the path integral. To use Monte Carlo methods for the path integral, we analytically continue from Minkowski space to Euclidean space by setting \( t \rightarrow -it \). This yields a path integral with positive definite measure, which for three light quarks we write as integral

\[
Z = \int [dA] \prod_{i=u,d,s} (\det[D(A, m_0^i, g_0)]) \exp \{-S_g(A)\} \]

where \( S_g(A) \) is the gluon contribution to the action. Evaluation of this path integral via Monte Carlo would seem completely straightforward; the system is discretized by replacing derivatives with finite differences and importance sampling is used to sample the phase space of the gluon fields. In truth, the discretization of the Dirac operator has been highly problematic and the presence of the determinants makes the Monte Carlo sampling difficult. Fortunately, there has been substantial progress on both of this issues in recent years, which we now describe.
3.1. Discretizing the Dirac operator

In Wilson’s original formulation of discretized QCD, problems with the Dirac operator were discussed. A naive finite difference version of the continuum Dirac operator yields more fermion modes than desired. This is known as the fermion doubling problem, since the number of additional modes is $2^d$, where $d$ is the dimensionality of space-time. Various methods have been proposed to remove the unwanted doubler degrees of freedom, with Wilson and staggered fermions being two of the most commonly used methods. Both of these approaches break some of the important symmetries of QCD, in particular the chiral symmetries.

Kaplan [1] proposed a method for preserving chiral symmetry for discretized fermions that makes four-dimensional chiral fermions come from a five-dimensional theory with a carefully chosen mass term. In particular, he started with the five-dimensional Euclidean Dirac equation

$$\left(\gamma_\mu \partial^\mu + \gamma_5 \partial_s + M(s)\right) \Psi(x, s) = 0$$

(7)

where $\Psi(x, s)$ is a four-component Dirac spinor, $\gamma_5$ is the conventional $4 \times 4$ matrix proportional to $\gamma^1 \gamma^2 \gamma^3 \gamma^4$, $x$ labels four-dimensional space-time and $s$ labels a new fifth-dimensional coordinate. By choosing $M(s) = M_5^+$ positive and constant for $s > 0$ and negative and constant for $s < 0$, he showed that there are solutions to the five-dimensional equation with

$$\Psi(x, s) = \begin{cases} \exp(-M_5 s) \psi_R(x) & s > 0 \\ \exp(+M_5 s) \psi_R(x) & s < 0 \end{cases}$$

(8)

where $\psi_R$ satisfies the massless four-dimensional Dirac equation. If $M(s)$ has the opposite overall sign, a left-handed light fermion state appears at the defect. Thus one sees that a step-function defect in the five-dimensional quark masses produces light chiral fermions in a lower dimension.

Kaplan’s idea has provided a solution to the problem of coupling chiral fermions to a gauge field, provided both the left and right handed fermions couple to the same gauge field. (The general case of a chiral fermion, say left-handed, coupled to a gauge field has been studied, without a completely satisfactory conclusion.) Following Kaplan’s idea, Shamir [2], Furman and Shamir [3] and Narayanan and Neuberger [4] further developed the lattice discretization for chiral fermions. Shamir’s variant, commonly know as domain wall fermions, maintains a finite extent for the fifth dimension, while in the Narayanan and Neuberger approach, the infinite fifth dimensional limit is taken analytically, yielding a lattice fermion operator, known as the Neuberger operator, appropriate for chiral fermions. For numerical work, the approximations needed to manipulate the Neuberger operator make it conceptually very similar to the approach of Shamir. We will concentrate on the Shamir version of domain wall fermions in the remainder of this paper, since they have been used most extensively in numerical simulations.

The domain wall fermion Dirac operator, $D_{\text{dwf}}(A, m_f, g_0, M_5)$, is a $12V L_s \times 12V L_s$ matrix, where $V$ is the four-dimensional space-time volume and $L_s$ is the length of the fifth dimension. It depends on two mass parameters: the five dimensional mass (or domain wall height) $M_5$ and the light quark mass $m_f$. It produces light, chiral quark states bound to the ends of the fifth dimension, as shown in Figure 1. The light left-handed chiral modes are bound to the left boundary and the right-handed chiral modes are bound to the right boundary. These bound modes can overlap in the interior of the fifth dimension, and this produces a small residual chiral symmetry breaking, which to leading order in the discretization scale is an additive contribution to the quark mass, $m_f$. The size of this extra contribution to the quark mass is controlled by the length of the fifth dimension, so one can get arbitrarily light quarks even when the lattice spacing is non-zero. It is important to note that the desired chiral symmetry is only a feature of the eigenvectors near zero and these eigenvalues constitute $O(1/L_s)$ of the eigenvalues on the operator.
Figure 1. Schematic behavior of domain wall fermion eigenvectors with small eigenvalues. The overlap in the interior between the left-handed modes bound to the left boundary and the right-handed modes bound to the right boundary produces an additive contribution to the input quark mass.

3.2. The Rational Hybrid Monte Carlo Algorithm

With domain wall fermions providing suitable discretization of the Dirac operator, we now discuss a recently developed Monte Carlo algorithm for QCD, the Rational Hybrid Monte Carlo of Clark and Kennedy [5] that provides an exact method to handle the fermionic determinants appearing in the path integral. We will be concentrating on the domain wall fermion Dirac operator, so in this section \( D(m_i) \equiv D_{\text{dwf}}(A, m_i, g_0, M_5) \). Since the domain wall fermion Dirac operator has many eigenvectors that do not correspond to the light quark modes of QCD, these must be removed from the path integral measure so that in the large \( L_s \) limit they do not dominate the system. This is accomplished by dividing each determinant factor in equation 6 by a determinant with a large, \( \mathcal{O}(1) \) quark mass, which cancels the contribution of heavy modes to the path integral measure. Finally, we note that while the determinant factors in the path integral are positive definite, the individual eigenvalues are not. In preparation for writing the determinants as integrals over pseudofermions (4 component fields which are not Grassman valued), we replace the determinant of the domain wall fermion operators, \( \det D(m_i) \), by \( \left( \det[D^\dagger(m_i)D(m_i)] \right)^{1/2} \). We can then write the path integral as

\[
Z = \int [dA] \prod_{i=u,d,s} \left( \frac{\det[D^\dagger(m_i)D(m_i)]}{\det[D^\dagger(1)D(1)]} \right)^{1/2} \exp \{-S_g(A)\}
\]

\[
= \int [dA][d\Phi_i][d\Phi_i] \exp \left\{ -S_g(A) - \sum_{i=u,d,s} \Phi_i^\dagger[D(1)D^\dagger(m_i)^{-1}D(m_i)^{-1}D^\dagger(1)]^{1/2}\Phi_i \right\}
\]

Note that the exponential weight term involves the square root of the domain wall fermion Dirac operator. The Rational Hybrid Monte Carlo uses a rational function approximation to
the square root of the Dirac operator, \( i.e. \) for some matrix \( M \) acting on a vector \( \Phi \), we have

\[
M^{1/2} \Phi = \left( \alpha_0 + \sum_{k=1}^{n} \frac{\alpha_k}{M + \beta_k} \right) \Phi
\]

where \( \alpha_i \) and \( \beta_i \) are found by the Remez algorithm.

Monte Carlo sampling of the path integral in equation 3.2 proceeds by 1) introducing a conjugate momentum Gaussian integral into the partition function, \( \int [d\pi^*][d\pi] \exp(-\pi * \pi) \), 2) choosing a value for \( \Phi \) from a heatbath. Adding in a starting configuration for the gauge fields \( A \), we then use molecular dynamics to move from \( (A, \Phi, \pi)_{\text{initial}} \) to \( (A, \Phi, \pi)_{\text{final}} \). A Monte Carlo accept/reject step is then applied to correct for any finite time step errors in the molecular dynamics integration. The result is an exact algorithm for simulating QCD with three light quarks, using an action that preserves the desired symmetries of QCD to any desired approximation.

4. 2+1 flavor Domain Wall Quark QCD

We can now describe some of the algorithmic optimizations that the RBC and UKQCD collaborations have incorporated in our current simulations of QCD with domain wall fermions. Since the physical up and down quarks have very similar masses, we set them equal and therefore have 3 unknown input parameters in our calculations: the light quark mass common to the up and down quarks, the strange quark mass and the input QCD coupling constant, \( g \), which is also commonly describe by \( \beta \sim \frac{1}{g^2} \).

For our current 2+1 flavor simulations, we have found it optimal to rewrite the path integral as

\[
Z = \int [dA] \left( \frac{\det[D^\dagger(m_1)D(m_1)]}{\det[D^\dagger(m_s)D(m_s)]} \right)^3 \prod_{i=1}^{3} \left( \frac{\det[D^\dagger(m_s)D(m_s)]}{\det[D^\dagger(1)D(1)]} \right)^{1/2} \exp \{-S_g(A)\}
\]

where \( m_l = m_u = m_d \). During our molecular dynamics integration, we must solve the Dirac equation for each step of the integration. This generally dominates the calculational time, so we have chosen the ratios of the determinants in equation 10 to do the fewest number of Dirac equation solves for the lightest quarks.

We employ a multiple time-step integrator. The first determinant ratio, involving the light quarks, is expensive to calculate. However, the force produced by this term in the molecular dynamics integration is small, so it is integrated on the coarsest molecular dynamics time scale. The three, 1/2 powers of the strange quark determinant are integrated on a coarser time scale and the gauge fields on the finest time scale. Using this three time-scale scheme, we see only a modest 30 - 40 % increase in time as we take the light quarks from \( m_s/2 \) down to \( m_s/5 \). This has had a dramatic effect on current simulations, since with previous algorithms, approaching the light quark limit has made the calculation markedly more expensive. For moderately light quarks, our current scheme is about six times faster than our previous algorithm and we are currently simulating at light quark masses that would not have been possible with previous algorithms and current machines.

5. Symmetries in QCD and the Standard Model

The discrete symmetry known as parity (\( P \)), which takes a physical process into its mirror image, was long thought a fundamental symmetry of nature. Lee and Yang pointed out that experimental evidence was lacking and parity violation was subsequently measured. The combination of charge conjugation and parity symmetry (\( CP \) symmetry), which takes a particle to its antiparticle, was shown by Cronin and Fitch to be violated in 1964. In the modern
standard model, parity violation is built in, since the weak interactions only couple to left-handed particles. CP violation comes about through a single non-zero parameter in the quark sector, and a likely similar parameter in the neutrino sector. The parameter in the quark sector, known as the $\eta$ parameter of the Cabbibo-Kobayashi-Maskawa (CKM) matrix, should relate all measured CP violation, provided the standard model is correct. Some experiments determine $\eta$ directly, with minimal theoretical input, but for kaon systems, the determination of $\eta$ requires detailed knowledge of the quark distributions of the kaon. This is only accessible via lattice QCD and we now describe a calculation of this parameter in 2+1 flavor QCD using domain wall fermions. This calculation has been done by the RBC and UKQCD collaborations.

Figure 2 shows the standard model diagram that is responsible for indirect CP violation. A kaon mixes with its antiparticle through intermediate virtual particles. The heavy quarks and $W$ bosons in the top part of the figure have masses much too heavy to include in current QCD simulations. Fortunately, these virtual particle effects can be accurately handled with analytic techniques and they result in a single, four-quark operator that needs to be evaluated in lattice QCD. This operator is represented by the black dot in the lower part of the figure. The matrix element of this operator is parameterized by $B_K$, which is given by

$$\langle \bar{K}^0 | Q^{(\Delta S=2)} | K^0 \rangle \equiv \frac{8}{3} B_K (\mu) f_K^2 m_K^2$$  \hspace{1cm} (11)$$

where $f_K$ is the kaon decay constant and $m_K$ is the kaon mass. $B_K$ should be a number of order one and its precise value is needed to relate the experimental measurement of indirect CP violation in kaons, given by $\epsilon$, to standard model parameters. The relation is

$$\epsilon = B_K \Im \lambda_\eta \frac{G_F^2 f_K^2 m_K M_w^2}{12 \sqrt{2} \pi^2 \Delta M_K} \{ \Re \lambda_c [\eta_1 S_0(x_c) - \eta_3 S_0(x_c, x_t)] - \Re \lambda_t \eta_2 S_0(x_t) \} \exp(i \pi/4)$$  \hspace{1cm} (12)$$

Given $\epsilon$, a determination of $B_K$ and standard model parameters for masses and decay constants, the CKM parameter $\eta$ can be determined. $B_K$ is analytically related to $B_K$ and $\eta$ is contained in the $\lambda_t$ term in this equation.

In equation 11 the matrix element of the operator needed for determining $B_K$ needs to be renormalized to the same conventions that are present in equation 12. With current numerical capability, this renormalization is only possible with a fermion discretization that has control over chiral symmetry breaking, which the domain wall formulation does. In addition, with domain wall fermions, the renormalization can be done numerically so that there is no reliance on analytic methods which may converge poorly in this region [6, 7].

Using the QCDOC [8] computers at Brookhaven National Laboratory, Columbia University and the University of Edinburgh, we have recently completed a first calculation of $B_K$ with 2+1 flavors of domain wall fermions [9]. We have used non-perturbative renormalization to renormalize our result and, working at a single lattice spacing, we find $B_K^{\text{MS}} = 0.557(12)(16)$. Estimating the effects of taking the lattice spacing to zero gives $B_K^{\text{MS}} = 0.557(12)(29)$. Our results are shown in Figure 3 along with a sampling of other results. Many of the other results [10, 11] are in the quenched approximation, where the fermion determinants are simply left out of the path integral. The accuracy of this uncontrolled truncation of the theory is not known a priori. The other 2+1 flavor result [12] shown in Figure 3 has a large error from renormalization. This is done with ASQTAD fermions, where non-perturbative renormalization is not possible currently. This brings out the utility of domain wall fermions for these calculations.

Our result achieves a total error of about 5% for $B_K$, which translates into a constraint on the $\eta$ parameter of the CKM matrix which is competitive with constraints from other measurements. The other measurements which contain $\eta$ are coming primarily from $b$ quark systems. Thus to see that the CP violation measured in $b$ quark systems and kaons has a common origin, lattice QCD determinations of $B_K$ are vital.
Figure 2. The standard model diagram, involving the W boson and heavy quarks, that produces kaon, anti-kaon mixing.

6. Conclusions
The last few years have seen important progress in the numerical simulation of QCD with fermions which preserve the symmetries of QCD at finite lattice spacing. New algorithms have allowed us to run many times faster and tackle simulations that were not possible previously. We have generally used three 4,096 node QCDOC partitions for these simulations and a 4,096 node QCDOC provides over a sustained Teraflop for our codes. The simulations presented here required a few sustained Teraflops-years to complete.

Other fermion discretizations are in active use and results from these simulations are being presented at this conference. Domain wall fermions are more expensive to simulate than other formulations, given that a fifth dimension is introduced for domain wall fermions, but there are many quantities, such as $B_K$, for which the presence of chiral symmetry is important for accurate results. Additionally, at fixed lattice spacing, we can use domain wall fermions to simulate at arbitrarily light quark masses, provided the fifth dimension is large enough. The full chiral symmetry of domain wall fermions means that one does not have to first take the lattice spacing to zero and then take the quark mass small. Physically light quark simulations at finite lattice spacing are within reach in a few years with our current algorithms, assuming a normal evolution of computer power.

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Figure 3. Some of the available lattice QCD results for $B_K$. Our 2+1 flavor domain wall fermion calculation (red diamond) was done at a single lattice spacing, with $a^2 \approx 0.015$. Estimating the $a \rightarrow 0$ errors yields the red diamond at $a = 0$. 

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