

Properties of light quarks from lattice QCD simulations¹

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Abstract. By numerical study of the simple bound states of light quarks, in particular the π and K mesons, we are able to deduce fundamental quark properties. Using the “improved staggered” discretization of QCD, the MILC Collaboration has performed a series of simulations of these bound states, including the effects of virtual quark-antiquark pairs (“sea” quarks). From these simulations, we have determined the masses of the up, down, and strange quarks. We find that the up quark mass is not zero (at the 10 sigma level), putting to rest a twenty-year-old suggestion that the up quark could be massless. Further, by studying the decays of the π and K mesons, we are able to determine the “CKM matrix element” V_{us} of the Weak Interactions. The errors on our result for V_{us} are comparable to the best previous determinations using alternative theoretical approaches, and are likely to be significantly reduced by simulations now in progress.

1. Introduction

Quantum Chromodynamics (QCD) is the theory of the Strong Interactions, which are responsible for binding quarks into protons and neutrons and holding them together in the atomic nucleus. QCD describes quarks interacting through the exchange of gluons. At high energy or short distances (much less than the radius of a proton), QCD becomes weakly coupled: The coupling constant (the QCD analogue of electric charge) becomes small. This property of QCD is called “asymptotic freedom.” Gross, Politzer, and Wilczek received the 2004 Nobel Prize in Physics for its discovery. Short distance QCD is well described by a perturbative expansion in the small coupling constant.

The flip side of asymptotic freedom is that QCD becomes strongly coupled at long distances (or low energy). This is responsible for the property called “confinement”: Quarks cannot be observed separately from their low energy bound states (hadrons). The large coupling constant also implies that the properties of quarks in bound states cannot be studied by perturbative

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methods. Nonperturbative, numerical simulations by the methods of lattice gauge theory are needed. Such simulations can determine the fundamental parameters of QCD (quark masses and the coupling constant) and then predict the properties of hadrons.

The basic steps in the numerical simulations are:

1. Replace continuous space and time by a discrete set of points (the lattice), separated by lattice spacing a .
2. Discretize the field equations of quarks and gluons on the lattice. The number of degrees of freedom of the fields are then finite (in a finite volume).
3. Generate “typical” lattices (configurations) of gluon fields using Monte Carlo methods. The back-effect of quarks on the gluons is included. Numerical limitations imply that the masses of the lightest (up and down) quarks in this step (and next one) must be taken to be heavier than in the real world.
4. Compute the quark propagators through background gluon lattices (requires a sparse matrix inversion). A “propagator” is the amplitude for a quark to move between space-time points.
5. Combine the quark propagators to find bound-state (hadron) propagators.
6. Analyze the hadron propagators to find the properties (*e.g.*, masses) of the hadrons.
7. Extrapolate the hadronic properties to the physical regime:
 - (a) Extrapolate to lower masses of the up and down quarks: the “chiral extrapolation.”
 - (b) Extrapolate the volume of space-time $\rightarrow \infty$: the “infinite volume extrapolation.”
 - (c) Extrapolate the lattice spacing $a \rightarrow 0$: the “continuum extrapolation.”
8. Comparing some computed hadron masses to experimentally known masses determines the physical values of the quark masses and the strong coupling constant. Once quark masses and coupling constant are known, we can make predictions for hadronic properties such as decay amplitudes or masses of other hadrons.

As an example, consider a π^+ meson, which is made up an up (u) and an anti-down (\bar{d}) quark. These two quarks are called the “valence quarks” in the π^+ ; it is their propagators that we calculate in step 4 above. Putting the two valence quark propagators together and averaging over gluon backgrounds computes the effects of gluon exchange between the quarks. The exchanged gluons, in turn, can interact with virtual quark-antiquark pairs, which, by the laws of quantum mechanics, are always popping in and out of existence in the vacuum. Such quark-antiquark pairs are known as “sea quarks,” and they are responsible for the back-effect of quarks on gluons mentioned in step 3 above.

Including the sea-quark effects is the step that is the most demanding of computer resources. It requires computing the determinant (or at least the change of the determinant) of a large matrix. For many years, the determinant was so computationally daunting that it was simply left out: a brutalization of the theory known as the “quenched approximation.”

This stumbling block has now been overcome: The solution we implement involves a discretization of the quark field equations that is very fast (“staggered quarks” [1]), the addition of terms to the equations to reduce discretization artifacts on gluons and quarks [2] (“improved staggered quarks”), and an efficient algorithm for computing sea-quarks effects [3].

Improved staggered quarks allow one to include sea-quark effects without losing control of the systematic errors due to the chiral, infinite volume, and continuum extrapolations. Using these quarks, the MILC Collaboration [4, 5] has been generating lattices including the effects of the three relevant sea-quark “flavors”: u, d, s (up, down, strange). The project began in 1999, but the pace of these simulations has been sped up greatly by application of SciDAC resources. MILC makes its lattices publicly available: <http://qcd.nersc.gov/>

In 2003 a lattice QCD milestone was reached. MILC joined with the Fermilab, HPQCD, and UKQCD groups to show that a wide range of simple quantities could be computed with high accuracy (1–3% errors) in lattice QCD using the MILC lattices [6].

2. Details of the Calculation

The computation described here is based on two sets of MILC lattices:

- “coarse” runs with lattice spacing $a \approx 0.125$ fm and a wide range of sea-quark masses, with lowest average up and down quark mass $\hat{m}' \sim 10$ MeV, about 3 times the physical value.
- “fine” runs with $a \approx 0.09$ fm, and lowest $\hat{m}' \sim 15$ MeV, about 5 times the physical value.

Extensions in progress include a fine run with $\hat{m}' \sim 10$ MeV, which is nearly half finished, and a “super fine” set with $a \approx 0.06$ fm, and lowest $\hat{m}' \sim 10$ MeV. The super fine run will begin in earnest once the DOE QCDOC comes on line. All the above lattices have volume $\geq (2.5 \text{ fm})^3$

We compute valence-quark propagators with many different quark mass values for every sea-quark mass choice. This procedure allows us to get the maximum amount of information out of the gluon lattices, which are so expensive to generate when sea-quark back-effects are included. At the end of the calculation, we set valence and sea mass values equal and recover the true theory, namely “full QCD.” The valence-quark masses are called m_x and m_y . We take the masses of the u and d sea quarks equal, which is a good approximation; the sea-quark masses in the simulation are called $\hat{m}' \equiv m'_u = m'_d$ and m'_s . After the simulations are performed, we interpolate m'_s to its physical value m_s ; while we extrapolate \hat{m}' to its physical value $\hat{m} = (m_u + m_d)/2$.

For the valence-quark masses, the extrapolation/interpolation depends on which bound state we are studying. For the π^+ , we could extrapolate $m_x \rightarrow m_u$ and $m_y \rightarrow m_d$; in practice, however, taking both m_x and m_y to \hat{m} gives an “average” π meson, called $\hat{\pi}$, whose mass is very close to the π^+ mass (up to electromagnetic corrections). For a K^+ (K^0) meson, a bound state of a u (d) and an \bar{s} , we extrapolate $m_x \rightarrow m_u$ (m_d) and interpolate $m_y \rightarrow m_s$. In the K system, it is convenient to look first at an fictitious “average” K meson, called \hat{K} , with mass squared equal the average mass squared of K^+ and K^0 . For a \hat{K} , we extrapolate $m_x \rightarrow \hat{m}$ and interpolate $m_y \rightarrow m_s$.

The errors in the chiral extrapolations/interpolations can be controlled if we know the functional form of the mass dependence. In the continuum, the functional form is given by an effective field theory, called “chiral perturbation theory” (χ Pt). The form of the mass dependence of many interesting quantities has been calculated; see, *e.g.*, Ref [7].

On the lattice, the errors introduced by discretization modify the formulas of χ Pt. For staggered quarks, the modified form of χ Pt has been worked out [8]: It is called “staggered chiral perturbation theory” (S χ Pt). S χ Pt also gives the leading corrections from finite volume. Further, since S χ Pt includes discretization errors, it helps control the extrapolation to the continuum. We use S χ Pt for our fits to lattice data. All data shown below have already been corrected for finite volume effects with S χ Pt.

Figures 1 and 2 present the analysis that determines the quark masses. The symbols \times , \diamond , \circ , and \square show a small subset of our lattice data, with errors too small to be visible. The \diamond and \square are $\hat{\pi}$ points, with valence masses $m_y = m_x$; while the \times and \circ are \hat{K} points, with m_y held fixed to one of three different values, giving three sets of points for each symbol.

In Fig. 1, the dark solid lines are the result of a single S χ Pt fit to all the data, with confidence level CL = 0.28. Setting valence and sea quark masses equal and extrapolating to the continuum gives the lighter solid lines. We then adjust m'_s , the simulated mass of the strange quark, until both the \hat{K} and the $\hat{\pi}$ hit their physical masses at the same value of m_x . This gives the two dotted lines, and from them we get a determination of m_s and the average u, d mass, \hat{m} .

To obtain m_u and m_d separately, we continue the upper dotted line in Fig. 1 until the mass of the K^+ is reached. The region of the continuation is magnified in Fig. 2. This is an extrapolation in the valence mass m_x , with the other masses (sea masses \hat{m}, m_s and valence mass $m_y = m_s$) fixed at their physical values. The up quark mass, m_u is the value of m_x that gives the K^+ its experimental mass. In principle, the up and down sea quark masses should also be adjusted away from their average, \hat{m} , but we cannot do this since all our simulations have $m'_u = m'_d = \hat{m}'$. However, the error introduced can be shown to be negligible.

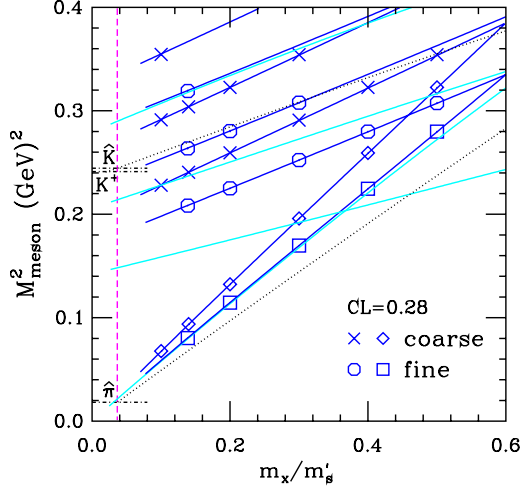


Figure 1. Extrapolation/interpolation of π and K meson squared masses as a function of valence quark mass m_x divided by the strange sea quark mass in the simulation, m'_s .

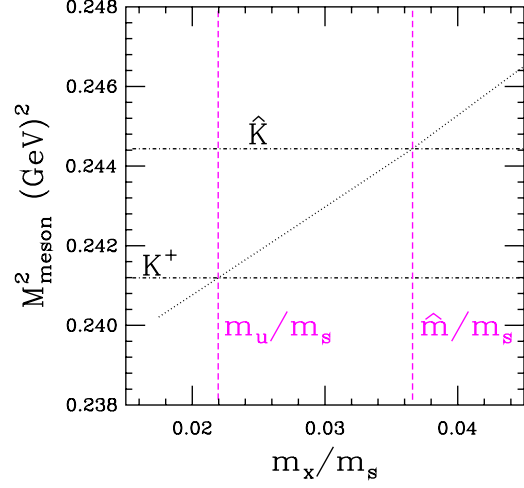


Figure 2. Blow-up of region at left center of Fig. 1.

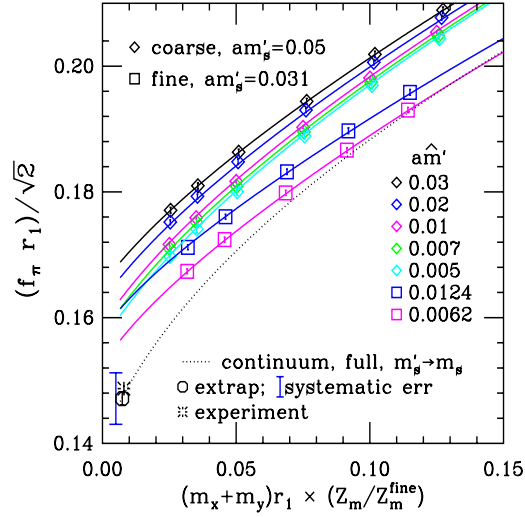


Figure 3. Fit and extrapolation of f_π data

The “decay constant” of the K or π meson, f_K or f_π , is the “wave function at the origin”: It determines the probability that the two quarks in the bound state are close. When they are close, the quarks can annihilate by the Weak Interactions, ultimately producing a muon (μ) (or electron) and a neutrino (ν). If f_K and f_π are computed in QCD, then the experimentally measured decay rates for $K \rightarrow \mu\nu$ and $\pi \rightarrow \mu\nu$ determine parameters of the Weak Interactions: “CKM matrix elements” V_{us} and V_{ud} . Knowing V_{us} , V_{ud} and other CKM matrix elements is crucial to testing the Standard Model of particle physics and searching for new physics.

Figure 3 shows f_π vs. the sum of valence masses $m_x + m_y$, in units of r_1 , a known length scale. Coarse lattice values of the quark masses have been adjusted by a calculated renormalization constant, Z_m , to correspond to those of the the fine lattices. The five sets of \diamond 's are all coarse lattice points with different sea quark mass \hat{m}' ; the two sets of \square 's are fine lattice points with different \hat{m}' . The lines through the points are the results of the same SXPT fit that was shown in Fig. 1. Data for masses and decay constants are fit simultaneously to give better numerical

control. The dotted line is the result after extrapolating to the continuum, setting valence and sea quark masses equal (“full QCD”) and adjusting m'_s to its physical value m_s . The \circ shows our result for f_π after extrapolation to $2\hat{m}$, the physical value of $m_x + m_y$ for a π meson. The experimental point shown assumes an alternative determination of V_{ud} ; the agreement of our lattice result with experiment is excellent.

3. Results and Outlook

Our results for quark masses [9, 5] (in $\overline{\text{MS}}$ scheme at scale 2 GeV) and decay constants [5] are:

$$\begin{aligned} m_s &= 76(0)(3)(7)(0) \text{ MeV} , & m_u &= 1.6(0)(1)(2)(1) \text{ MeV} , & f_\pi &= 129.5 \pm 0.9 \pm 3.6 \text{ MeV} \\ \hat{m} &= 2.8(0)(1)(3)(0) \text{ MeV} , & m_d &= 3.9(0)(1)(4)(1) \text{ MeV} , & f_K &= 156.6 \pm 1.0 \pm 3.8 \text{ MeV} \\ m_s/\hat{m} &= 27.4(1)(4)(0)(1) , & m_u/m_d &= 0.41(0)(1)(0)(4) , & f_K/f_\pi &= 1.210(4)(13) . \end{aligned}$$

The first two errors in each case are from statistics and lattice systematics; while the additional errors on the masses are from perturbation theory and electromagnetic effects, respectively. The result for m_u/m_d rules out, at the 10σ level, the possibility of $m_u = 0$. This puts to rest a longstanding proposal [10] that the up quark could be massless. A massless up quark could have solved the “Strong CP Puzzle” [11]. Alternative solutions are now more likely: *e.g.*, the “axion” [12], a possible component of Dark Matter.

Our result for f_K/f_π implies $|V_{us}| = 0.2219(26)$, which is consistent with the world average value $|V_{us}| = 0.2200(26)$ [13] from alternative methods. Runs planned for the near future, as well as those now in progress, should reduce the error on our result for $|V_{us}|$, making it significantly more precise than the current world-average determination. Similar methods can be used to study mesons with one heavy (charm or bottom) and one light quark. Such studies, now in progress in collaboration with the Fermilab and HPQCD groups, promise to give a wealth of information about other crucial CKM matrix elements.

Finally, we note that there is still a theoretical issue with the use of staggered quarks in this context. However, the agreement of existing results with experiment, as well as a growing body of direct studies of the issue [14], give us confidence that no fundamental problem exists. Further studies, by us and others, are in progress.

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