High-Precision Lattice QCD Confronts Experiment

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We argue that high-precision lattice QCD is now possible, for the first time, because of a new improved staggered quark discretization. We compare a wide variety of nonperturbative calculations in QCD with experiment, and find agreement to within statistical and systematic errors of 3% or less. We also present a new determination of $\alpha_{\overline{\text{MS}}}^{(5)}(M_Z)$; we obtain 0.121(3). We discuss the implications of this breakthrough for phenomenology and, in particular, for heavy-quark physics.

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For almost thirty years precise numerical studies of nonperturbative QCD, formulated on a space-time lattice, have been stymied by our inability to include the effects of realistic quark vacuum polarization. In this paper we present detailed evidence of a breakthrough that may now permit a wide variety of nonperturbative QCD calculations including, for example, high-precision B and D meson decay constants, mixing amplitudes, and semi-leptonic form factors—all quantities of great importance in current experimental work on heavy-quark physics. The breakthrough comes from a new discretization for light quarks: Symanzik-improved staggered quarks [1, 2, 3, 4, 5, 6, 7, 8].

Quark vacuum polarization is by far the most expensive ingredient in a QCD simulation. It is particularly difficult to simulate with small quark masses, such as u and d masses. Consequently, most lattice QCD (LQCD) simulations in the past have either omitted quark vacuum polarization ("quenched QCD"), or they have included effects for only u and d quarks, with masses 10–20 times larger than the correct values. This results in uncon-

trolled systematic errors that can be as large as 30%. The Symanzik-improved staggered-quark formalism is among the most accurate discretizations, and it is 50–1000 times more efficient in simulations than current alternatives of comparable accuracy. Consequently realistic simulations are possible now, with all three flavors of light quark. An exact chiral symmetry of the formalism permits efficient simulations with small quark masses. The smallest u and d masses we use are still three times too large, but they are now small enough that chiral perturbation theory is a reliable tool for extrapolating to the correct masses.

In this paper we demonstrate that LQCD simulations, with this new light-quark discretization, can deliver nonperturbative results that are accurate to within a few percent. We do this by comparing LQCD results with experimental measurements. In making this comparison, we restrict ourselves to quantities that are accurately measured ($< 1\%$ errors), and that can be simulated reliably with existing techniques. The latter restriction excludes unstable hadrons and multihadron states (e.g., in nonleptonic decays); both of these are strongly affected by

the finite volume of our lattice (2.5 fm across). Unstable hadrons, like the ρ and the ϕ, are constantly fluctuating into on-shell or nearly on-shell decay products that can easily propagate to the boundaries of the lattice; similar problems afflict multihadron states. Consequently we focus here on hadrons that are at least 100 MeV below decay threshold or have negligible widths (J/ψ, Υ...); and we restrict our attention to hadronic masses, and to hadronic matrix elements that have at most one hadron in the initial and final states. These are the "gold-plated" calculations of LQCD — calculations that must work if LQCD is to be trusted at all.

Unambiguous tests of LQCD are particularly important with staggered quarks. These discretizations have the unusual property that a single quark field $\psi(x)$ creates four equivalent species or "tastes" of quark. "Taste" is used to distinguish this property, a lattice artifact, from true quark flavor. A quark vacuum polarization loop in such formalisms contributes four times what it should. To remove the duplication, the quark determinant in the path integral is replaced by its fourth root. This construction introduces nonlocalities that are potentially worrisome, but much is known about the formalism that is reassuring: for example,

- perturbation theory, which governs the theory's short-distance behavior, is correct to all orders;

- phenomena, such as $\pi^0 \to 2\gamma$, connected with chiral anomalies are correctly handled (because the relevant (taste-singlet) currents are only approximately conserved);

- the CP violating phase transition that occurs when $m_u + m_d < 0$ does *not* occur in this formalism, but the real world is neither in this phase nor near it;

- the nonperturbative quark loop structure is correct up to short-distance taste-changing interactions, which are perturbative; these interactions are suppressed by $a^2\alpha_s$ and can be systematically removed [9]; or they can be removed after the simulation using modified chiral perturbation theory [10, 11].

To press further requires nonperturbative studies. The tests we present here are among the most stringent nonperturbative tests ever of a staggered quark formalism (and indeed of LQCD).

The gluon configurations that we used, together with the raw simulation data for pions and kaons, were produced by the MILC collaboration; heavy-quark propagators came from the HPQCD collaboration. The lattices have lattice spacings of approximately $a = 1/8$ fm and $a = 1/11$ fm. The simulations employed an $\mathcal{O}(a^2)$ improved staggered-quark discretization of the light-quark action [4], a "tadpole-improved" $\mathcal{O}(a^2\alpha_s)$ accurate discretization of the gluon action [12], an $\mathcal{O}(a^2, v^4)$ improved
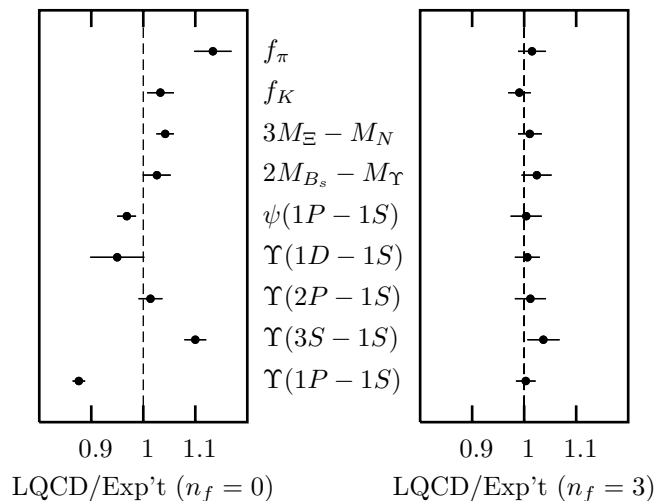

FIG. 1: LQCD results divided by experimental results for nine different quantities, without and with quark vacuum polarization (left and right panels, respectively). The top three results are from our $a = 1/11$ and $1/8$ fm simulations; all others are from $a = 1/8$ fm simulations.

lattice version of NRQCD for b quarks [13], and the Fermilab action for c quarks [14]. Several valence u/d quark masses, ranging from $m_s/2$ to $m_s/8$, were needed for accurate extrapolations, as were sea u/d masses ranging between $m_s/2$ and $m_s/6$. Only u, d and s quark vacuum polarization was included; effects from c, b and t quarks are negligible ($< 1\%$) here.

To test LQCD, we first tuned its five parameters to make the simulation reproduce experiment for five well-measured quantities. The five parameters are the bare u and d quark masses, which we set equal, the bare s, c and b masses, and the bare QCD coupling. There are no further free parameters once these are tuned.

Setting $m_u = m_d$ simplifies our analysis, and has a negligible effect ($< 1\%$) on isospin-averaged quantities. We tuned the u/d, s, c, and b masses to reproduce measured values of m_π^2, $2m_K^2 - m_\pi^2$, m_{D_s}, and m_Υ, respectively. In each case the experimental quantity is approximately proportional to the corresponding parameter, and approximately independent of the other parameters.

Rather than tune the bare coupling, one normally sets the coupling in LQCD to a particular value, and determines the lattice spacing a in its place (*after* the simulation). We adjusted the lattice spacing to make the Υ-Υ' mass difference agree with experiment. We chose this mass difference since it is almost independent of all quark masses, including, in fact, the b mass [15]. We could equally well have chosen, instead, any of the nine test quantities discussed below, with similar results.

Having tuned all free parameters in the simulation, we then computed a variety of experimentally accessible
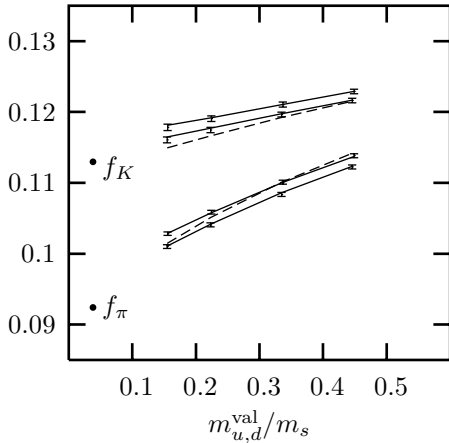
FIG. 2: Chiral fits to LQCD determinations of f_π and f_K (in GeV) for different values of the valence u/d-quark mass at $a = 1/11$ fm.

quantities (in addition to the five used for tuning). Our results are summarized in Fig. 1 where we plot the ratio of LQCD results to experimental results for nine quantities: π and K decay constants, a baryon mass splitting, a B_s–Υ splitting, and mass differences between various J/ψ and Υ states. On the left we show ratios from QCD simulations without quark vacuum polarization ($n_f = 0$). These results deviate from experiment by as much as 10–15%; the deviations can be made as large as 20–30% by tuning QCD's input parameters against different physical quantities. The right panel shows results from QCD simulations that include realistic vacuum polarization. These nine results agree with experiment to within systematic and statistical errors of 3% or less — with no free parameters.

The dominant uncertainty in the light-quark quantities in this plot (the top four) comes from extrapolations in the sea and valence light-quark masses. We used partially quenched chiral perturbation theory to extrapolate pion and kaon masses, and the weak decay constants f_π and f_K. Chiral perturbation theory was unnecessary for correcting the s-quark mass; simple linear *interpolation* is adequate, and preferable since chiral perturbation theory converges slowly for masses as large as m_s. We also kept u/d masses smaller than $m_s/2$ in our fits, so that low-order chiral perturbation theory was sufficient. Our chiral expansions included the full first-order contribution [16], and also approximate second-order terms, which are essential given our quark masses. We corrected for errors caused by the finite volume of our lattice (1% errors or less), and by the finite lattice spacing (2–3% errors). The former corrections were determined from chiral perturbation theory; the latter by comparing results from the coarse and fine lattices. Residual discretization errors, due to nonanalytic taste-violations [10, 11], were estimated as 1.9% for f_π and 1% for f_K. Perturbative

matching was unnecessary for the decay constants since they were extracted from partially conserved currents. Our final results for f_K and f_π agree with experiment to within systematic and statistical uncertainties of 2.8%. For the $n_f = 0$ case we analyzed only $a = 1/8$ fm, but extrapolated to the continuum in an approximate way based upon our $n_f = 3$ analysis.

Fig. 2, which shows our fits for f_π and f_K, demonstrates that the u/d masses currently accessible with improved staggered quarks are small enough for reliable and accurate chiral extrapolations, at least for pions and kaons. The valence and sea s-quark masses were 14% too high in these simulations; and the sea u/d masses were $m_s/2.3$ and $m_s/4.5$ for the top and bottom results in each pair. The dashed lines show the fit function with corrected s and sea-quark masses; these lines extrapolate to the final fit results. The extrapolations are not large — only 4–9%. Indeed the masses are sufficiently small that simple linear extrapolations give the same results as our fits, within few percent errors. These decay constants represent the current state of an ongoing project; a more thorough analysis will be published soon.

The other quantities in the ratio plot, Fig. 1, are much less sensitive to the valence u/d mass and soft-pion effects. Consequently, they are more stringent tests of LQCD. The combinations $3M_\Xi - M_N$ and $2M_{B_s} - M_\Upsilon$ depend upon the valence s mass, but the s masses we used in our simulations are off by only 10–20% and easily corrected. The b's rest mass cancels in $2M_{B_s} - M_\Upsilon$, making this a particularly clean and sensitive test. The same is true of all the Υ splittings, and our simulations confirm that these are also independent ($\leq$ 1–2%) of the sea quark masses for our smallest masses. The $\Upsilon(P)$ masses are averages over the known spin states; the $\Upsilon(1D)$ is the 1^3D_2 state recently discovered by CLEO [17].

It is important to appreciate that our heavy-quark results come directly from the QCD path integral, with only bare masses and a coupling as inputs — five numbers. Furthermore, unlike in quark models or HQET, Υ physics in LQCD is inextricably linked to B physics, through the b-quark action. Our results strongly suggest that effective field theories, like NRQCD, are reliable and accurate tools for analyzing heavy-quark dynamics.

Another important ingredient in high-precision LQCD is perturbation theory, which connects lattice results to the continuum. We tested perturbation theory by extracting values of the coupling from our simulations and comparing them with non-LQCD results. We determined the renormalized coupling, $\alpha_V(6.3\,\text{GeV})$, by comparing 2nd-order perturbation theory for the expectation value of a 1×1 Wilson loop with (exact) values from the simulations [15, 18]. Results for several sea-quark masses are shown in Table I; the masses become more realistic as one moves down the table.

The QCD coupling is sensitive to the tuning of the lattice spacing, since this in effect tunes the bare coupling.

TABLE I: The QCD coupling $\alpha_V(6.3\,\text{GeV})$ from 1×1 Wilson loops in simulations with different u/d and s sea-quark masses (in units of the physical s mass), and using two different tunings for the lattice spacing. The first error shown is statistical, and the second is truncation error ($\mathcal{O}(\alpha_V^3)$).

a (fm)	$m_{u,d}$	m_s	$1P - 1S$	$2S - 1S$
1/8	∞	∞	0.177 (1)(5)	0.168 (0)(4)
1/8	0.5	∞	0.211 (1)(9)	0.206 (1)(8)
1/8	1.3	1.3	0.231 (2)(12)	0.226 (2)(11)
1/8	0.5	1.3	0.234 (2)(12)	0.233 (1)(12)
1/8	0.2	1.3	0.234 (1)(12)	0.234 (1)(12)
1/11	0.2	1.1	0.238 (1)(13)	0.236 (1)(13)

We show results for two different tunings: one using the $\Upsilon(1P - 1S)$ splitting, and the other using $\Upsilon(2S - 1S)$. The two tunings give couplings that are ten standard deviations apart and 25% smaller than the physical coupling when the sea-quark masses are infinite.

With smaller, more realistic sea-quark masses, the two tunings agree to within 1%, and the coupling becomes mass independent. Our results, converted to $\overline{\text{MS}}$ and evolved perturbatively to scale M_Z, imply

$$\alpha_{\overline{\text{MS}}}^{(5)}(M_Z) = 0.121\,(3), \tag{1}$$

which agrees well with the current world average of 0.117 (2) [19]. Ours is the first determination from lattice QCD simulations with realistic quark vacuum polarization, the first with $\mathcal{O}(a^2)$ improved actions, and the first that is verified by a wide range of heavy-quark *and* light-quark calculations; and it is by far the most thorough study of the light-quark mass dependence (or independence) of lattice QCD determinations. A more detailed discussion will be presented elsewhere.

The results presented here suggest that we now have a reasonably generic and accurate tool for solving a real-life, strongly coupled, quantum field theory — for the first time in the history of particle physics. Much is required to complete the argument. Chiral extrapolations for non-strange baryons, for example, are expected to be much larger than for pions and kaons, as are finite-

$$\begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ \pi \to l\nu & K \to \pi l\nu & B \to \pi l\nu \\ V_{cd} & V_{cs} & V_{cb} \\ D \to l\nu & D_s \to l\nu & B \to Dl\nu \\ D \to \pi l\nu & D \to K l\nu & \\ V_{td} & V_{ts} & V_{tb} \\ \langle B_d|\overline{B}_d\rangle & \langle B_s|\overline{B}_s\rangle & \end{pmatrix}$$

FIG. 3: Gold-plated LQCD processes that bear on CKM matrix elements. ϵ_K is another gold-plated quantity.

volume errors; computations with these hadrons are not yet under control. Also a wider variety of tests is important. Heavy-quark mixing amplitudes, and semileptonic decay form factors, for example, are essential to the high-precision experiments at B factories; our lattice techniques for these require independent tests. The new CLEO-c program will be particularly useful for this.

The larger challenge facing LQCD is to exploit these new techniques in the discovery of new physics. Again, B and D physics offer extraordinary opportunities for new physics from LQCD. There are, for example, gold-plated lattice quantities for every CKM matrix element except V_{tb} (Fig. 3). An immediate challenge is to *predict* the D/D_s leptonic and semi-leptonic decays rates to within a few percent *before* CLEO-c measures them.

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