

## High-Precision Lattice QCD Confronts Experiment

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The recently developed Symanzik-improved staggered-quark discretization allows unquenched lattice-QCD simulations with much smaller (and more realistic) quark masses than previously possible. To test this formalism, we compare experiment with a variety of nonperturbative calculations in QCD drawn from a restricted set of “gold-plated” quantities. We find agreement to within statistical and systematic errors of 3% or less. We discuss the implications for phenomenology and, in particular, for heavy-quark physics.

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For almost 30 years, precise numerical studies of non-perturbative QCD, formulated on a space-time lattice, have been stymied by our inability to include the effects of realistic quark vacuum polarization. In this Letter, we present evidence that a milestone has been reached: Simulations that include vacuum-polarization effects for three light quarks are now possible. This implies that accurate nonperturbative QCD calculations for a restricted (“gold-plated”) set of quantities are achievable. The set includes, for example,  $B$  and  $D$  meson decay constants, mixing amplitudes, and semileptonic form factors—all quantities of great importance in current experimental studies of heavy quarks. The key to our work is the use of the Symanzik-improved staggered-

quark formalism for the light quarks [1–3], which allows us to include three dynamical light quarks in simulations, with a physical strange quark mass, and  $u$  and  $d$  quark masses that are 3–5 times smaller than in previous studies.

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 uncontrolled systematic errors that can be as large as

30%. The Symanzik-improved staggered-quark formalism is among the most accurate discretizations, and it is much faster in simulations than current alternatives of comparable accuracy. Furthermore, an exact chiral symmetry of the formalism permits efficient simulations with small quark masses. Consequently, realistic simulations are possible now, with all three light-quark flavors. The smallest  $u$  and  $d$  masses we use are still 3 times too large, but they are now small enough that chiral perturbation theory is a reliable tool for extrapolating to the correct masses, at least for the quantities we study.

In this Letter, we show that LQCD simulations, with improved staggered quarks, 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 are expected *a priori* to have small systematic errors in LQCD calculations 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, such as the  $\rho$  and the  $\phi$ , 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 ( $\pi$ ,  $K$ ,  $B_s$ ,  $J/\psi$ ,  $Y$ , ...); 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 masses and matrix elements can be called “gold-plated”: LQCD calculations of them 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 4 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 it is the price paid for speed. Much is known that is reassuring: For example, no problems result from fractional roots of the fermion determinant in any order of continuum QCD perturbation theory [4]; phenomena, such as  $\pi^0 \rightarrow 2\gamma$ , connected with chiral anomalies are correctly handled [because the relevant (taste-singlet) currents are only approximately conserved [5]]; 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 except for taste-changing interactions. Taste-changing interactions are short dis-

tance, so they can be removed with perturbation theory [6]—at present to order  $a^2\alpha_s$ . They may also be removed after the simulation with modified chiral perturbation theory [7]. To press further requires nonperturbative studies. The tests we present here are among the most stringent nonperturbative tests ever of staggered quarks (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 [2], a “tadpole-improved”  $\mathcal{O}(a^2\alpha_s)$  accurate discretization of the gluon action [8], an  $\mathcal{O}(a^2, v^4)$  improved lattice version of nonrelativistic QCD (NRQCD) for  $b$  quarks [9], and the Fermilab action for  $c$  quarks [10]. 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 experimentally measured values of  $m_\pi^2$ ,  $2m_K^2 - m_\pi^2$ ,  $m_{D_s}$ , and  $m_Y$ , respectively. In each case, the experimental quantity is approximately proportional to the corresponding parameter, approximately independent of the other parameters, and gold plated.

Rather than tune the bare coupling, one normally sets it to a particular value, and determines the lattice spacing  $a$  in its place (*after* the simulation). We adjusted the lattice spacing to make the  $Y$ - $Y'$  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 [11].

Having tuned all free parameters in the simulation, we then computed a variety of gold-plated 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:  $\pi$  and  $K$  decay constants, a baryon mass splitting, a  $B_s$ - $Y$  splitting, and mass differences between various  $J/\psi$  and  $Y$  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

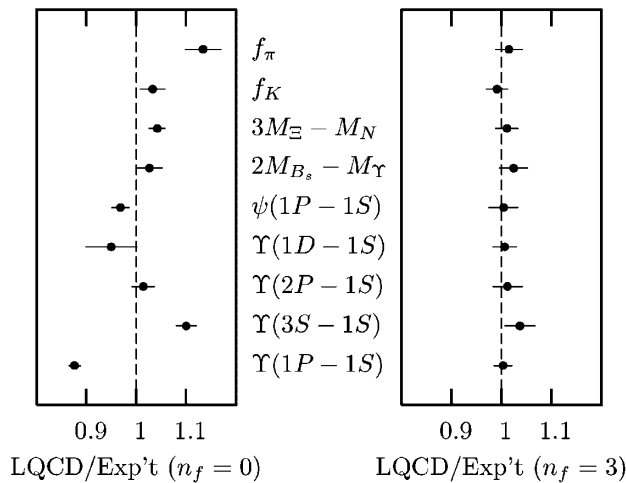


FIG. 1. LQCD results divided by experimental results for nine different quantities, without and with quark vacuum polarization (left and right panels, respectively). The top three results are from our  $a = 1/11$  and  $1/8$  fm simulations; all others are from  $a = 1/8$  fm simulations.

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 quantities used in this plot were chosen to test several different aspects of LQCD. Our results for  $f_\pi$  and  $f_K$  are sensitive to light-quark masses; they test our ability to extrapolate these masses to their correct values using chiral perturbation theory. Accurate simulations for a wide range of small quark masses were essential here. The remaining quantities are much less sensitive to the valence  $u/d$  mass, and therefore are more stringent tests of LQCD since discrepancies cannot be due to tuning errors in the  $u/d$  mass. The  $\Xi$  mass tests our ability to analyze (strange) baryons, while the  $B_s$  mass tests our formalism for heavy quarks. The  $b$  rest mass cancels in  $2M_{B_s} - M_Y$ , making this a particularly clean and sensitive test. The same is true of all the  $Y$  splittings, and our simulations confirm that these are also independent ( $\leq 1\%$ – $2\%$ ) of the sea-quark masses for our smallest masses, and of the lattice spacing (by comparing with  $r_0$  and  $r_1$  computed from the static-quark potential) [12]. The  $Y(P)$  masses are averages over the known spin states; the  $Y(1D)$  is the  $1^3D_2$  state recently discovered by CLEO [13].

Note 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 heavy-quark effective theory (HQET),  $Y$  physics in LQCD is inextricably linked to  $B$  physics, through the  $b$ -quark action. Our results confirm that effective field theories, such as NRQCD and the Fermilab

formalism, are reliable and accurate tools for analyzing heavy-quark dynamics.

A serious problem in the previous work was the inconsistency between light-hadron,  $B/D$ , and  $Y/\psi$  quantities. Heavy-quark masses and inverse lattice spacings, for example, were routinely retuned by 10%–20% when going from an  $Y$  analysis to a  $B$  analysis in the *same* quenched simulation [14]. Such discrepancies lead to the results shown in the left panel of Fig. 1. The results in the right panel for  $\pi$ ,  $K$ ,  $\Xi$ ,  $D_s$ ,  $J/\psi$ ,  $B_s$ , and  $Y$  physics mark the first time that agreement has been achieved among such diverse physical quantities using the same QCD parameters throughout.

The dominant uncertainty in our light-quark quantities comes from our 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  $f_\pi$  and  $f_K$ . The  $s$ -quark mass required only a small shift; we estimated corrections due to this shift by interpolation (for valence  $s$  quarks) or from the sea  $u/d$  mass dependence (for sea  $s$  quarks). We 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 [15], 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 [7] that remain after linear extrapolation in  $a^2$ , were estimated as 2% for  $f_\pi$  and 1% for  $f_K$ . Perturbative matching was unnecessary for the decay constants since they were extracted from partially conserved currents. Our final results 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 corrected for discretization errors by assuming these are the same as in our  $n_f = 3$  analysis.

Figure 2, which shows our fits for  $f_\pi$  and  $f_K$  as functions of the valence  $u/d$  mass, 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 particular simulations; and the sea  $u/d$  masses were too large— $m_s/2.3$  and  $m_s/4.5$  for the top and bottom results in each pair (fit simultaneously by a single fit function). The dashed lines show the fit functions with corrected valence  $s$  and sea  $u/d/s$  quark masses; these lines extrapolate to our final fit results. The bursts mark the experimental values. Our extrapolations are not large—only 4%–9%. Indeed the masses are sufficiently small that simple linear extrapolations give the same results as our

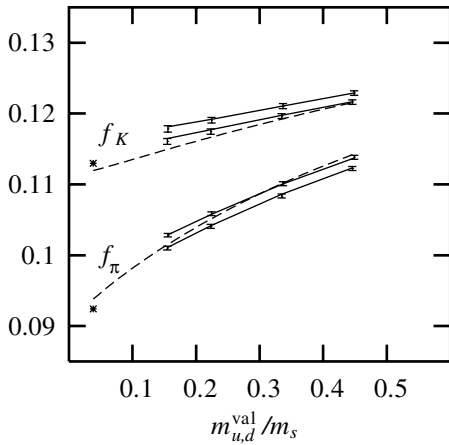


FIG. 2. Chiral fits to LQCD determinations of  $f_\pi$  and  $f_K$  (in GeV) for different values of the valence  $u/d$ -quark mass at  $a = 1/11$  fm.

fits, within few percent errors. These decay constants represent the current state of an ongoing project; a more thorough analysis will be published soon [16].

As a final test of high-precision LQCD, we examine the applicability of perturbation theory, which is essential for connecting most interesting 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 second-order perturbation theory for the expectation value of a  $1 \times 1$  Wilson loop with (exact) values from the simulations [11,17]. 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 particularly sensitive to the tuning of the lattice spacing. We show results for two different tunings: one using the  $Y(1P - 1S)$  splitting, and the other using  $Y(2S - 1S)$ . The two tunings give couplings that are ten statistical standard deviations apart (systematic errors correlate) and 25% too small when sea-quark masses are infinite.

TABLE I. The QCD coupling  $\alpha_V(6.3 \text{ GeV})$  from  $1 \times 1$  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 which we take to be  $\mathcal{O}(1\alpha_V^3)$  [11].

$a$ (fm)	$m_{u,d}$	$m_s$	$1P - 1S$	$2S - 1S$
1/8	$\infty$	$\infty$	0.177 (1)(5)	0.168 (0)(4)
1/8	0.5	$\infty$	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)

With smaller, more realistic sea-quark masses, the two tunings agree to within 1% (as expected from Fig. 1), and the coupling becomes mass independent. Our results, converted to the modified minimal subtraction scheme ( $\overline{\text{MS}}$ ) and evolved perturbatively to scale  $M_Z$ , imply  $\alpha_{\overline{\text{MS}}}^{(5)}(M_Z) = 0.121(3)$ , which agrees with the current world average of  $0.117(2)$  [18]. Unlike previous determinations, ours includes realistic quark vacuum polarization,  $\mathcal{O}(a^2)$  improved actions, and a thorough study of the quark mass dependence (or independence); it is further supported by a wide range of heavy-quark and light-quark calculations. A more detailed discussion, with results from other short-distance quantities (they agree), will be presented elsewhere.

Our results suggest that light improved staggered quarks, with NRQCD or Fermilab heavy quarks, enable accurate nonperturbative calculations for gold-plated quantities. Further work is required, however. Chiral extrapolations for nonstrange baryons, for example, are expected to be larger than for pions and kaons, as are finite volume and statistical errors; computations with these hadrons are not yet under control. Also, there are many gold-plated quantities that we have not yet fully analyzed. Heavy-quark mixing amplitudes, and semileptonic decay form factors, for example, are essential to high-precision experiments at CLEO-c and the  $B$  factories; our lattice techniques for these require independent tests.

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 Cabibbo-Kobayashi-Maskawa (CKM) matrix element except  $V_{tb}$  (Fig. 3). An immediate challenge is to predict the  $D/D_s$  leptonic and semileptonic decay rates to within a few percent before CLEO-c measures them.

$$\left( \begin{array}{ccc} V_{ud} & V_{us} & V_{ub} \\ \pi \rightarrow l\nu & K \rightarrow l\nu & B \rightarrow \pi l\nu \\ & K \rightarrow \pi l\nu & \\ V_{cd} & V_{cs} & V_{cb} \\ D \rightarrow l\nu & D_s \rightarrow l\nu & B \rightarrow D l\nu \\ D \rightarrow \pi l\nu & D \rightarrow K l\nu & \\ V_{td} & V_{ts} & V_{tb} \\ \langle B_d | \bar{B}_d \rangle & \langle B_s | \bar{B}_s \rangle & \end{array} \right)$$

FIG. 3. Gold-plated LQCD processes that bear on CKM matrix elements.  $\epsilon_K$  is another gold-plated quantity.

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- [1] C.W. Bernard *et al.*, Nucl. Phys. (Proc. Suppl.) **B60**, 297 (1998); G. P. Lepage, Nucl. Phys. (Proc. Suppl.) **B60**, 267 (1998); MILC Collaboration, C.W. Bernard *et al.*, Phys. Rev. D **58**, 014503 (1998).
  - [2] G. P. Lepage, Phys. Rev. D **59**, 074502 (1999).
  - [3] MILC Collaboration, K. Orginos *et al.*, Phys. Rev. D **59**, 014501 (1999); MILC Collaboration, K. Orginos *et al.*, Nucl. Phys. (Proc. Suppl.) **B73**, 909 (1999); MILC Collaboration, K. Orginos *et al.*, Phys. Rev. D **60**, 054503 (1999); MILC Collaboration, C.W. Bernard *et al.*, Phys. Rev. D **61**, 111502 (2000).
  - [4] G. G. Batrouni *et al.*, Phys. Rev. D **32**, 2736 (1985).
  - [5] H. S. Sharatchandra, H. J. Thun, and P. Weisz, Nucl. Phys. **B192**, 205 (1981); J. Smit and J. C. Vink, Nucl. Phys. **B298**, 557 (1988).
  - [6] HPQCD Collaboration, Q. Mason *et al.*, Nucl. Phys. (Proc. Suppl.) **B119**, 446 (2003).
  - [7] MILC Collaboration, C. Bernard, Phys. Rev. D **65**, 054031 (2002); C. Aubin *et al.*, Nucl. Phys. (Proc. Suppl.) **B119**, 233 (2003); C. Aubin and C. Bernard, Phys. Rev. D **68**, 034014 (2003); **68**, 074011 (2003).
  - [8] M. G. Alford, W. Dimm, G. P. Lepage, G. Hockney, and P. B. Mackenzie, Phys. Lett. B **361**, 87 (1995).
  - [9] C. T. H. Davies *et al.*, Phys. Rev. D **52**, 6519 (1995).
  - [10] A. X. El-Khadra, A. S. Kronfeld, and P. B. Mackenzie, Phys. Rev. D **55**, 3933 (1997).
  - [11] C. T. H. Davies *et al.*, Phys. Rev. D **56**, 2755 (1997).
  - [12] C. T. H. Davies *et al.*, Phys. Rev. D **58**, 054505 (1998).
  - [13] CLEO Collaboration, S. E. Csorna *et al.*, hep-ex/0207060.
  - [14] A. Ali Khan *et al.*, Phys. Rev. D **53**, 6433 (1996).
  - [15] S. R. Sharpe and N. Shores, Phys. Rev. D **62**, 094503 (2000).
  - [16] S. Gottlieb, hep-lat/0310041.
  - [17] C. T. H. Davies *et al.*, Nucl. Phys. (Proc. Suppl.) **B119**, 595 (2003).
  - [18] K. Hagiwara *et al.*, Phys. Rev. D **66**, 010001 (2002).