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 $\alpha_s(M_Z^2)$; 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.

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 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
deck threshold or have negligible widths (J/ψ, Ψ′, . . . );
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 import-
ant with staggered quarks. These discretizations have
the unusual property that a single quark field ψ(x) cre-
ates 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 determi-
nant in the path integral is replaced by its fourth root.
This construction introduces nonlocalities that are po-
etially 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 π 0 → 2γ, connected with chi-
ral anomalies are correctly handled (because the
relevant (taste-singlet) currents are only approxi-
ately 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 cor-
rect up to short-distance taste-changing interac-
tions, which are perturbative; these interactions
are suppressed by a^2 α_s and can be systematically
removed \[ \frac{\alpha_s}{\pi} \]
or they can be removed after the simulation using modified chiral perturbation
theory \[ \frac{\alpha_s}{\pi} \].

To press further requires nonperturbative studies. The
tests we present here are among the most stringent non-
perturbative 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 pro-
duced by the MILC collaboration; heavy-quark propa-
gators 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 O(a^2) im-
proved staggered-quark discretization of the light-quark
action \[ \frac{\alpha_s}{\pi} \], a “tadpole-improved” O(a^2 α_s) accurate
discretization of the gluon action \[ \frac{\alpha_s}{\pi} \], an O(a^2, v^4) improved

lattice version of NRQCD for b quarks \[ \frac{\alpha_s}{\pi} \] and the Fer-
milab action for c quarks \[ \frac{\alpha_s}{\pi} \]. Several valence u/d quark
masses, ranging from m_s/2 to m_s/8, were needed for ac-
curate 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 mea-
sured values of m_c^2, 2m_b^2 − m_c^2, m_d^2, and m_t, re-
spectively. In each case the experimental quantity is ap-
proximately 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 deter-
nines the lattice spacing a in its place (after the simu-
lation). 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 \[ \frac{\alpha_s}{\pi} \]. 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

\[ \begin{array}{c|c|c}
\hline
| & f_\pi & f_K \\
\hline
3M_\Xi - M_N & 2M_{\phi} - M_T & \psi(1P - 1S) \\
\hline
\end{array} \]

FIG. 1: LQCD results divided by experimental results for
different quantities, without and with quark vacuum pola-
rization (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.
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.

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 $B_s$-$\Upsilon$ splitting, and mass differences between various $J/\psi$ and $\Upsilon$ 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 $f_{\pi}$ 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 $\pi$ 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 were estimated as 1.9% 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 for $f_{\pi}$ and $f_K$ agree with experiment to within systematic and statistical uncertainties of 2.8%. For the $n_f = 0$ case we analyzed only $a \approx 1/8$ fm, but extrapolated to the continuum in an approximate way based upon our $n_f = 3$ analysis.

Fig. 4 which shows our fits for $f_{\pi}$ 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. 3 are much less sensitive to the valence $u/d$ mass and soft-pion effects. Consequently, they are more stringent tests of LQCD. The combinations $3M_{B_b} - M_{\Upsilon}$ 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 $\Upsilon$ splittings, and our simulations confirm that these are also independent ($\lesssim 1–2\%$) of the sea quark masses for our smallest masses. The $\Upsilon(1D)$ 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, $\Upsilon$ 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, $\alpha_s(6.3$ GeV), by comparing $2^{\text{nd}}$-order perturbation theory for the expectation value of a $1 \times 1$ Wilson loop with (exact) values from the simulations [16, 18]. Results for several sea-quark masses are shown in Table 1; 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 $\alpha_s (6.3 \text{ GeV})$ 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 ($\mathcal{O}(\alpha_s^3)$).

<table>
<thead>
<tr>
<th>$a$ (fm)</th>
<th>$m_{u,d}$</th>
<th>$m_s$</th>
<th>$1P - 1S$</th>
<th>$2S - 1S$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/8</td>
<td>$\infty$</td>
<td>$\infty$</td>
<td>0.177 (1) (5)</td>
<td>0.168 (6) (4)</td>
</tr>
<tr>
<td>1/8</td>
<td>0.5</td>
<td>$\infty$</td>
<td>0.211 (1) (9)</td>
<td>0.206 (1) (8)</td>
</tr>
<tr>
<td>1/8</td>
<td>0.5</td>
<td>1.3</td>
<td>0.231 (2)(12)</td>
<td>0.226 (2)(11)</td>
</tr>
<tr>
<td>1/8</td>
<td>1.3</td>
<td>1.3</td>
<td>0.234 (2)(12)</td>
<td>0.233 (1)(12)</td>
</tr>
<tr>
<td>1/11</td>
<td>0.2</td>
<td>1.1</td>
<td>0.238 (1)(13)</td>
<td>0.236 (1)(13)</td>
</tr>
</tbody>
</table>

We show results for two different tunings: one using the $T(1P - 1S)$ splitting, and the other using $T(2S - 1S)$. 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 MS and evolved perturbatively to scale $M_Z$, imply

$$\frac{\alpha_s^{(5)}(M_Z)}{\alpha_s^{(5)}} = 0.121 (3),$$

(1)

which agrees well with the current world average of 0.117 (2).

Ours is the first determination from lattice QCD simulations with realistic quark vacuum polarization, the first with $\mathcal{O}(\alpha_s^3)$ 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-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 $V_{ub}$ (Fig 1). An immediate challenge is to predict the $D/D_s$ leptonic and semi-leptonic decay rates to within a few percent before CLEO-c measures them.

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$$\begin{pmatrix}
V_{ud} & V_{us} & V_{ub} \\
\bar{V}_{ut} & V_{ts} & V_{tb} \\
\bar{V}_{et} & \bar{V}_{es} & \bar{V}_{eb} \\
\bar{V}_{dt} & \bar{V}_{ds} & \bar{V}_{db} \\
\bar{V}_{dt} & \bar{V}_{ds} & \bar{V}_{db} \\
\end{pmatrix}
$$

FIG. 3: Gold-plated LQCD processes that bear on CKM matrix elements. $\epsilon_1^1$ is another gold-plated quantity.