Further precise determinations of α_s from lattice QCD

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We present a new determination of the strong coupling constant from lattice QCD simulations. We use four different short-distance quantities to obtain the coupling, three different (infrared) meson splittings to tune the simulation parameters, and a wide range of lattice spacings, quark masses, and lattice volumes to test for systematic errors. Our final result consists of ten different determinations of $\alpha_P^{(3)}(8.2\ \mathrm{GeV})$, which agree well with each other and with our previous results. The most accurate of these, when evolved perturbatively to the Z^0 mass, gives $\alpha_{\overline{\mathrm{MS}}}^{(5)}(M_Z)=0.1174(24)$. We compare our results with those obtained from other recent lattice simulations. [S0556-2821(97)01117-X]

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I. INTRODUCTION

Precise measurements of the strong coupling constant α_s are important not only for strong-interaction phenomenology, but also in the search for new physics. Any discrepancy between low-energy and high-energy determinations of this coupling could signal the existence of supersymmetry or other phenomena beyond the standard model. No significant discrepancies have yet been observed [1]; more stringent tests of the standard model require further improvements in precision. In an earlier paper [2] we showed that lattice simulations of quantum chromodynamics (QCD), when combined with the very accurate experimental data on the Υ meson spectrum, provide among the most accurate and reliable determinations of α_s. Υ's probe the strong interactions at the relatively low energies of 500–1000 MeV, where supersymmetry or other new physics has little effect. Thus it is important to compare the couplings obtained from lattice QCD with those obtained from high-energy accelerator experiments, where effects due to a more fundamental underlying theory would be much more important. And it is essential that these couplings be measured as accurately as possible, with realistic estimates of the uncertainties involved. In this paper we review our earlier determination of the coupling, and update it to take advantage of new results from third-order perturbation theory, as well as new simulations which substantially reduce some of our Monte Carlo errors. We also report on several new simulations that further bound our systematic errors, particularly with respect to contributions from quark vacuum polarization.

As discussed in [2], there are two steps in our determination of the coupling constant. The first is to create a numerical simulation that accurately mimics QCD dynamics. We do this by tuning the bare masses and coupling in a lattice QCD simulation until it reproduces experimental results for the orbital and radial excitations of Υ mesons. We use the Υ family because it is one of the few systems for which both accurate simulations and accurate experimental data are available.

Having tuned our simulation, the second step in our determination of the coupling is to use the simulation to generate nonperturbative Monte Carlo ''data'' for a variety of short-distance quantities. Comparison with the perturbative expansions for the same quantities then fixes the value of the QCD coupling constant. We use the expectation values of small Wilson loops as our short-distance quantities. These are very easy to compute in simulations. They are also completely Euclidean and very ultraviolet, and therefore largely free of hadronization or other nonperturbative corrections. Finally, small Wilson loops have very convergent perturbative expansions that are known through second order for arbitrary n_f, the number of light-quark flavors, and through third order for $n_f=0$.

In this paper we examine each of these steps in detail. We begin in Sec. II by describing how we tune the simulation parameters. The most important of these for our analysis is the bare coupling constant, or equivalently the lattice spacing, used in the lattice QCD Lagrangian. The number and masses of light quarks entering through vacuum polarization is also important; we present new simulation results that bear on these parameters. In Sec. III we describe several different determinations of $\alpha_{\overline{\mathrm{MS}}}$ using different Wilson loops. Each of these sections deals extensively with potential systematic errors. Finally, in Sec. IV we summarize our results and discuss future directions.

II. TUNING OF THE SIMULATION

A. Procedure

Given a lattice spacing a, the QCD parameters that determine Υ properties are the bare coupling constant g_{lat} in the lattice Lagrangian, the bare mass M^0 of the constituent b quarks, and the bare masses m_q^0 of the light quarks that enter through quark vacuum polarization. Only the u, d, and s quarks are light enough to contribute to vacuum polarization appreciably. These parameters all vary with the lattice spacing. In a simulation, they must be tuned so that physical

quantities computed in the simulation agree with the corresponding experimental values. The tuning procedure is much simpler, and therefore more reliable, if one uses physical quantities that are very sensitive to one of the parameters and insensitive to the others.

Our main interest in this paper is the coupling constant, and so we are particularly careful in tuning the bare coupling. We use the mass splittings between radial and orbital excitations of the Υ for this purpose. These splittings are ideal since they are almost completely insensitive to the b-quark mass. The spin-averaged mass splittings between $1P$ and $1S$ levels, and $2S$ and $1S$ levels are observed experimentally to vary by only a few percent between the Υ and ψ systems, even though b quarks are roughly three times heavier than c quarks. This striking insensitivity to the mass of the constituents is an accident, but is confirmed by simulations for a range of masses near the b mass.

These splittings are also quite insensitive to the masses of the light quarks. These contribute through vacuum polarization, and affect hadronic masses in two ways. First, they allow decays to multihadronic final states; mixing with these states shifts the masses of the original hadrons. Υ decay rates are typically 0.1% or less of the mass splittings, and the states we examine are all far below the BB threshold. Thus we may ignore such effects in our analysis. The second effect of vacuum polarization is to renormalize the gluonic interactions between the constituents of the hadron. The typical momentum q_Υ exchanged between the b quarks in an Υ is from 0.5 to 1 GeV. This is small compared to the c, b, and t quark masses, and we may ignore their contribution to vacuum polarization. In contrast, the u, d, and s quarks are effectively almost massless at these energies and must be included in a realistic simulation. At the same time, because their masses are small relative to q_Υ, our simulation results depend only weakly on their exact values.

For sufficiently small masses, the dependence of an Υ mass splitting should be linear [3]:

$$\Delta M \approx \Delta M^0 \left\{ 1 + \text{const} \times \sum_{u,d,s} \frac{m_q^0}{q_\Upsilon} + \cdots \right\}, \qquad (1)$$

where the renormalized s mass is 50–100 MeV [4], and the u and d masses are 20 or 30 times smaller and therefore negligible. It is very costly to simulate lattice QCD with realistic u and d masses. Here that is unnecessary. The simple dependence of ΔM on m_q^0 means that we obtain realistic results if we set all three light-quark masses equal to $m_{\text{eff}}^0 \equiv m_s^0/3$, which generates the same correction to ΔM as two massless quarks and a strange quark. Thus $m_{\text{eff}} = 15-30$ MeV, and Eq. (1) suggests that the dependence on light-quark masses is a few percent or less of the total mass splitting, comparable to the Monte Carlo statistical errors in our analysis.[1]

[1]It is conceivable that the linear term in Eq. (1), which is due to chiral symmetry breaking, is strongly suppressed for tiny mesons such as the Υ, and becomes nonleading. Then the dependence on m_{eff} would be quadratic, with the correct value for $m_{\text{eff}} = m_s^0/\sqrt{3}$. The sensitivity to m_{eff} would then be far smaller and probably negligible for our analysis.

There are several other properties of the Υ system that make it ideal for tuning the bare coupling. These mesons are essentially nonrelativistic; the use of a nonrelativistic effective action [5] to exploit this allows a large portion of the spectrum to be computed efficiently and precisely [6,7]. They are physically small—three or four times smaller than light-quark hadrons—and so do not suffer from finite-volume errors even on modestly sized lattices. Finally, we have detailed phenomenological quark models that are well-founded theoretically and that give us unprecedented control over systematic errors.

In addition to the bare coupling constant, we must also tune the bare masses of the b quark and of the light quarks. We tune the bare b-quark mass M^0 by requiring that the Υ mass in the simulation has its correct value of 9.46 GeV. Reference [8] presents a detailed discussion. The light-quark masses are tuned until the pion and kaon masses are correct. As discussed, we need only the s-quark mass, as we set all $n_f = 3$ light-quark masses to $m_s^0/3$.

Finally we note that it is customary in tuning lattice simulations to switch the roles of the lattice spacing and the bare coupling constant. Rather than choose a lattice spacing and then tune the bare coupling constant to its correct value, it is far simpler to choose a value for the bare coupling constant g_{lat}, and then *compute* the corresponding lattice spacing a using simulation results. All explicit dependence on the spacing can be removed from the simulation code by expressing dimensionful quantities in units of a or a^{-1}. The spacing is then not needed as an input to the code, but is specified implicitly through the input value for g_{lat}, or equivalently through $\beta \equiv 6/g_{\text{lat}}^2$. We determine a from the Υ mass splittings ΔM. The simulation produces these in the dimensionless combination $a\Delta M$; to obtain a, we divide by the experimentally measured values for ΔM.

The lattice spacing is a crucial ingredient in our determination of the renormalized coupling α_s. As we discuss in Sec. III, the short-distance quantities we study specify $\alpha_s(q^*)$ for a specific value of aq^*. The expectation value of the $a \times a$ Wilson loop, for example, gives $\alpha_s(q^*)$ for $q^* = 3.4/a$. For this to be useful, we need to know q^*, and therefore a^{-1}, in physical units such as GeV. Consequently, the next section focuses on how precisely we are able to determine the lattice spacing corresponding to a given value of β.

B. Results: a^{-1} determination

Our lattice simulations used the standard Wilson action for the gluons, and the staggered-quark action and the hybrid molecular dynamics algorithm for the light quarks. We employed a nonrelativistic formulation of quark dynamics (NRQCD) for the b quarks [5–7]. The $n_f = 0$ gauge-field configurations used in our Monte Carlo calculations were provided by Kilcup and his collaborators ($\beta = 6, 6.4$) [9], Kogut ($\beta = 6$) [10], and by the UKQCD Collaboration ($\beta = 5.7, 6.2$)[11]. The $n_f = 2$ configurations are from the SCRI Lattice Gauge Theory Group and their colleagues in the HEMCGC Collaboration ($\beta = 5.6$) [12], and from the MILC Collaboration ($\beta = 5.415, 5.47$) [13]. Unfortunately, we were unable to obtain configurations with $n_f = 3$ light-quark flavors, which is the correct number for Υ physics.

TABLE I. Simulation results for meson mass splittings $a\Delta M$ and inverse lattice spacings a^{-1}, in GeV, for a range of couplings β, light-quark masses m_q^0 and heavy-quark masses M_q^0. The gluonic a^2 corrections $a\Delta M_g$ shown are added to $a\Delta M$ to obtain the corrected splitting. The error estimates for a^{-1} are for statistical errors, a^2 and v^4 errors, and errors in the light-quark mass, respectively. Experimental values for ΔM are 0.563 GeV for $\Upsilon'-\Upsilon$, 0.440 GeV for $\chi_b-\Upsilon$, and 0.458 GeV for $\chi_c-\psi/\eta_c$.

β	n_f	$am_{\rm eff}^0$	aM_q^0	Splitting	$a\Delta M$	$a\Delta M_g$	a^{-1} (GeV)
6.0	0	-	1.71	$\chi_b-\Upsilon$	0.174 (3)	−0.004	2.59 (4)(4)(0)
			1.80		0.174 (12)		
			2.00		0.173 (10)		
6.0	0	-	1.71	$\Upsilon'-\Upsilon$	0.232 (5)	−0.001	2.44 (5)(3)(0)
			1.80		0.239 (11)		
			2.00		0.235 (11)		
5.6	2	0.010	1.80	$\chi_b-\Upsilon$	0.185 (5)	−0.005	2.44 (7)(4)(7)
		0.025			0.200 (12)		
5.6	2	0.010	1.80	$\Upsilon'-\Upsilon$	0.239 (10)	−0.002	2.38 (10)(3)(10)
		0.025			0.262 (13)		
5.7	0	-	0.80	$\chi_c-\psi/\eta_c$	0.383 (10)	−0.009	1.22 (3)(18)(0)
			3.15	$\chi_b-\Upsilon$	0.326 (6)	−0.015	1.41 (4)(4)(0)
5.415	2	0.0125	0.80	$\chi_c-\psi/\eta_c$	0.359 (14)	−0.008	1.30 (5)(20)(5)
			2.80	$\chi_b-\Upsilon$	0.323 (10)	−0.017	1.44 (6)(4)(6)
5.47	2	0.05	0.80	$\chi_c-\psi/\eta_c$	0.335 (15)		
			2.8	$\chi_b-\Upsilon$	0.307 (12)		
6.2	0	-	1.22	$\chi_b-\Upsilon$	0.127 (5)	−0.002	3.52 (14)(5)(0)
				$\Upsilon'-\Upsilon$	0.175 (8)	−0.0003	3.22 (15)(5)(0)
6.4	0	-	1.00	$\chi_b-\Upsilon$	0.107 (16)	−0.002	4.19 (63)(6)(0)

Consequently, we performed complete analyses for $n_f=0$ and $n_f=2$ and extrapolated our results to $n_f=3$. The extrapolation was the last step of our analysis, and is described in Sec. III.

As discussed above, we use mass splittings in the Υ system to determine the lattice spacing. Specifically, we use two different mass splittings to make two independent determinations of the lattice spacing. One is the splitting $\Delta M(\Upsilon'-\Upsilon)$ between the Υ' and the Υ, and the other is the splitting $\Delta M(\chi_b-\Upsilon)$ between the spin average of the χ_b mesons and the Υ. These can be measured accurately in a simulation [6,7], and are known very accurately from experiments. Table I summarizes the parameters used in our main simulations and the results for these two splittings. Our most reliable results are based on the $\beta=6$ and 5.6 simulations. We use results from the other simulations, including those for the splitting between the spin-averaged χ_c mesons and the spin average of the J/ψ and η_c mesons, to calibrate systematic errors. Our $\beta=6.2$ result agrees with that in [14].

Several factors contribute to the uncertainty in our determination of the lattice spacing. We used the lattice NRQCD formalism to simulate heavy-quark dynamics [5], and included all relativistic corrections through $O(v^2)$ and all finite lattice-spacing corrections through $O(a^2)$. The leading finite-a error is due to $O(a^2)$ errors in the gluon dynamics. We estimate this effect using perturbation theory [2], which indicates that only S states are affected and that our measured S-state energies should be shifted by

$$a\Delta M_g=\frac{3}{40}\,(aM_q)^2 a\Delta M_{\rm HFS}, \qquad (2)$$

where $\Delta M_{\rm HFS}$ is the hyperfine spin splitting of the state and M_q is the heavy-quark mass. We assume 1.5 GeV and 5 GeV for c and b quarks, respectively. The corrections we used are listed in Table I, as are our final values for the inverse lattice spacing a^{-1}. We allow for a systematic error of $\pm\Delta M_g/2$ in ΔM when computing the error in a^{-1}, although our analysis in [2] suggests a much smaller uncertainty. Note that $\Delta M(\Upsilon'-\Upsilon)$ is almost unaffected by this correction. Relativistic corrections of order v^4 are most likely negligible for the Υ since the v^2 corrections, which we include, shift our mass splittings by less than 10%; we include a systematic uncertainty of $\pm 1\%$ for this. The v^4 corrections are certainly larger for ψ's, where, for example, the $J/\psi-\eta_c$ splitting is a v^2 effect and 25% of the $\chi_c-\psi/\eta_c$ splitting. This suggests v^4 errors could be of order $\pm 6\%$ for ψ's. Recent simulations [15] indicate that certain spin-dependent v^4 terms can shift levels by as much as 60 MeV, which is 15% of the splitting. We include a systematic uncertainty of $\pm 15\%$ for v^4 errors in the ψ splitting.

Our simulations confirm that the b-quark mass has very little effect on either of the Υ splittings. The $\beta=6$ results show that a 17% change in M^0 leads to changes of only a few percent in the Υ'-Υ and χ_b-Υ splittings. (Note that the statistical errors in the splittings for different M^0's are correlated. Consequently, the statistical errors in the differences between the splittings are somewhat smaller than those for any individual splitting.) Since we determine M^0 to within 6% [8], the resulting uncertainty in the determination of the lattice spacing is probably no more than a percent, which is much smaller than the statistical errors.

Uncertainties in the light-quark mass can also affect our lattice spacing determination. In our $\beta=5.6$ simulations we expect am_s^0 to be somewhere in the range 0.01–0.02. This

can be inferred from the dependence of the pion mass on m_q^0, and allows for uncertainties due to quenching and finite-a errors. Thus we want light-quark masses $am_q^0 = am_{\rm eff}^0$ in the range 0.003–0.006. We have simulation results for $am_{\rm eff}^0 = 0.01$ and 0.025. By fitting formula (1) to these results we find that $am_q^0 = 0.01$ should give the correct result to within 4%, which equals our statistical error. The correct range of light-quark masses in our $\beta = 5.415, 5.47$ simulations is roughly $am_{\rm eff}^0 = 0.005 - 0.015$. We have simulation results for $am_{\rm eff}^0 = 0.0125$ and 0.050, and again the 6–7% shift caused by changing $m_{\rm eff}$ is roughly the same as our statistical errors for both ψ and Υ splittings.[2] Note that ψ's should be more sensitive to small quark masses than Υ's since they are roughly twice as large; we saw no evidence for this in our simulations. These results all indicate that the $m_{\rm eff}$ dependence is too small compared to our statistical errors to allow an accurate measurement.[3] This also means that the tuning errors associated with $am_{\rm eff}$ are no larger than our statistical errors, and so we take our statistical errors as a measure of the uncertainty due to this parameter.

We checked for finite-volume errors by computing the charmonium splittings using lattices that are 1.5 fm and 3.0 fm per side. We observed no difference, indicating that these errors are smaller than the 2% statistical errors in these tests. The lattices we used at $\beta = 6$ and 5.6 are both $16a \approx 1.35$ fm per side; the Υ's are half the size of the ψ's, with a radius of about 0.2 fm. We therefore expect finite volume errors in our mass splittings that are substantially less than 2%.

We estimated the electromagnetic shifts of the Υ masses using a potential model. For individual mesons, we found mass shifts of approximately 1 MeV, with smaller shifts for the splittings between them. These are too small to affect our result.

Our final values for a^{-1}'s are listed in Table I, obtained by dividing the experimental values for the splittings ΔM by the corrected Monte Carlo simulation results $a\Delta M + a\Delta M_g$. The error estimates for the a^{-1}'s include statistical errors in $a\Delta M$, as well as systematic errors associated with the finite-a correction $a\Delta M_g$, v^4 corrections, and the light-quark mass m_q^0. Other systematic errors are negligible.

A striking feature of these simulation results is the disagreement at $\beta = 6$ between a^{-1} computed using the Υ'-Υ splitting and that computed using the χ_b-Υ splitting. Taking proper account of correlations, this disagreement is three standard deviations: our simulation gives 1.36(3) for the ratio of these splittings, rather than the experimental value of 1.28.

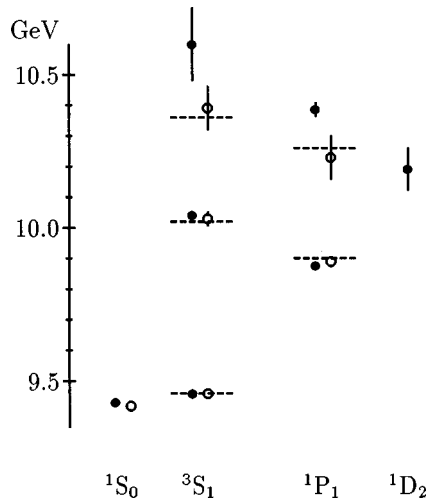

FIG. 1. NRQCD simulation results for the spectrum of the Υ system, including radial excitations. Dashed lines indicate experimental values for the triplet S states and for the spin average of the triplet P states. The energy zero from simulation results is adjusted to give the correct mass to the $\Upsilon(1^3S_1)$. Results are from a simulation with $n_f = 0$ (filled circles) and from one with $n_f = 2$ (open circles), using $a^{-1} = 2.4$ GeV for both. The errors shown are statistical; systematic errors are of order 20 MeV or less.

Thus the $\beta = 6$ simulation is inconsistent with experiment. This is because in this simulation, in contrast to nature, $n_f = 0$; there is no light-quark vacuum polarization. The disagreement is smaller when $n_f = 2$, as is apparent in the $\beta = 5.6$ data. And, as we will demonstrate, it disappears completely when we extrapolate n_f to three.

As expected, using an incorrect value for n_f leads to inconsistencies such as the one found in our $\beta = 6$ simulation. Perturbation theory, though not justified at the momenta relevant for these systems, provides a qualitative explanation for this discrepancy. The centrifugal barrier makes the average separation between the quarks in the P state χ_b larger than for the S state Υ or Υ', as is familiar from hydrogen or positronium. As a result, the typical exchanged momentum for χ_b quarks, q_{χ_b}, is smaller than $q_{\Upsilon'}$. The perturbative binding energy is given by $\alpha_s^2(q) C_F^2 M_b/16$, with $q = q_{\Upsilon'}$ for Υ' and q_{χ_b} for χ_b. Since $q_{\chi_b} < q_{\Upsilon'}$, the χ_b is more tightly bound. However, for $n_f = 0$, this effect is exaggerated, as $\alpha_s^{(0)}(q)$ increases more quickly than $\alpha_s^{(3)}(q)$ with decreasing q. Thus, for $n_f < 3$, $\Delta M(\chi_b - \Upsilon)$ should be underestimated relative to $\Delta M(\Upsilon' - \Upsilon)$, as is observed. Fitting to data would then require a larger a^{-1} for $\Delta M(\chi_b - \Upsilon)$ than for $\Delta M(\Upsilon' - \Upsilon)$.

We end this section by displaying in Figs. 1 and 2 results from the $\beta = 6$ and 5.6 simulations for several of the low-lying excitations and spin splittings, compared with experimental values. The agreement is excellent and supports the reliability of our simulations. We emphasize that these are calculations from first principles; our approximations can be systematically improved. The only inputs are the Lagrangians describing gluons and quarks, and the only parameters are the bare coupling constant and quark masses. In particular, these simulations are *not* based on a phenomenological quark potential model.

[2]To compare mass splittings at $\beta = 5.415$ with those at $\beta = 5.47$ one needs the expectation value of the plaquette at each beta; see the following section. From the plaquette values one finds that the lattice spacing at the larger β is about 12% smaller. Since the $a\Delta M$'s are only 5–6% smaller at the larger beta, the splittings ΔM themselves are actually about 6–7% larger for the larger mass.

[3]This insensitivity to $m_{\rm eff}$ is because $m_{\rm eff}$ is so small in our simulations. Our $n_f = 0$ simulations are equivalent to $m_{\rm eff} = \infty$ and give results that are quite different from $n_f = 2$. So shifts would become apparent, even with our statistics, for sufficiently large $m_{\rm eff}$.

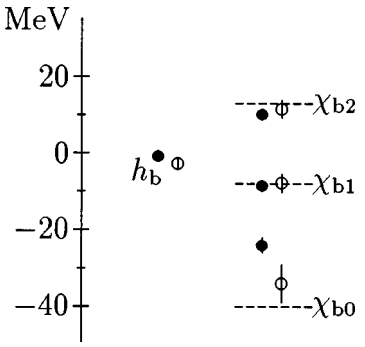

FIG. 2. NRQCD simulation results for the spin structure of the lowest-lying P states. Dashed lines indicate experimental values for the triplet P states. Masses are relative to the spin-averaged state. Results are from a simulation with $n_f=0$ (filled circles) and from one with $n_f=2$ (open circles), using $a^{-1}=2.4$ GeV for both. The errors shown are statistical; systematic errors are within about 5 MeV.

III. DETERMINATION OF THE RENORMALIZED COUPLING

A. The coupling constant from Wilson loops

Having tuned the simulation, we performed Monte Carlo simulations to generate ''data'' for a variety of short-distance quantities. We determined the coupling by matching the perturbative expansions for these quantities to the nonperturbative Monte Carlo results. For short-distance quantities we chose the expectation values $W_{m,n}$ of Wilson loop operators. In the continuum,

$$W_{m,n}\equiv\frac{1}{3}\left\langle \mathrm{Re\ Tr}\ \ P\exp\left(-ig\oint_{n,m}A\cdot dx\right)\right\rangle, \qquad (3)$$

where P denotes path ordering, A_μ is the QCD vector potential, and the integral is over a closed $ma\times na$ rectangular path. Loop operators for small paths are among the most ultraviolet, and therefore most perturbative, objects that can be studied in lattice QCD simulations. Unlike most other quantities used to determine the QCD coupling, the loop operators are truly short-distance quantities in Euclidean space. There are no corrections for hadronization, and nonperturbative effects are expected to be very small. For example, the leading nonperturbative contribution to $W_{m,n}$ due to condensates is probably from the gluon condensate, with

$$\delta W_{m,n}=-\frac{\pi a^4(mn)^2}{36}\langle\alpha_s F^2\rangle. \qquad (4)$$

Most studies find that $\langle\alpha_s F^2\rangle$ is of order 0.042 GeV^4 [16]. Since a^{-1} ranges from 1.2 to 4.2 GeV in our simulations, we expect condensate contributions to $-\ln W_{1,1}$, for example, to be in the range of 0.2–0.01 %, much too small to be important here. When $n_f\neq 0$ there are also contributions from quark condensates, but these are suppressed by α_s^2 and so are probably even smaller. The tiny size of such effects make the $W_{m,n}$ for small m and n ideal quantities for determining the coupling in lattice QCD, particularly given the ease with which they can be computed in simulations.

To obtain four independent determinations of the coupling, we used expectation values for the four smallest loops on the lattice: the plaquette $W_{1,1}$, $W_{1,2}$, $W_{1,3}$, and $W_{2,2}$. Each of these loop operators is very different from the others; as different, for example, as various moments of a structure function. Each is affected differently by nonperturbative effects and higher-order uncalculated perturbative corrections. The contribution of the gluon condensate, for example, is 16 times larger for $W_{2,2}$ than for $W_{1,1}$. By comparing results obtained from different loop operators we can bound such systematic errors.

TABLE II. Coefficients for the perturbative expansions, in powers of $\alpha_P(q_{m,n})$, of small Wilson loops. Scale $q_{m,n}$ is the average momentum carried by the gluon in the first-order correction.

		c_2		c_3	
Loop	c_1	$n_f=0$	$n_f=2$	$n_f=0$	$aq_{m,n}$
$-\ln W_{1,1}$	4.19	−4.98	−5.57	0	3.40
$-\ln W_{1,2}$	7.22	−7.57	−8.51	2.6	3.07
$-\ln W_{1,3}$	10.07	−9.60	−10.89	5.3	3.01
$-\ln W_{2,2}$	11.47	−10.58	−11.84	11.1	2.65

Each of our expectation values has a perturbative expansion of the form

$$-\ln W_{m,n}^{(n_f)}=\sum_{i=1}c_i^{(n_f)}(m,n)[\alpha_P^{(n_f)}(q_{m,n})]^i, \qquad (5)$$

where α_P is a new nonperturbative definition for the coupling constant introduced in our earlier paper [2] to facilitate lattice calculations. The scale $q_{m,n}$ is the average gluon momentum in the first-order contribution to $W_{m,n}$, computed directly from the Feynman diagrams as described in [17,18].

In Table II we list the perturbative coefficients through third order for $n_f=0$, and through second order for $n_f=2$ [19]. Unfortunately, the n_f dependence of the third-order coefficients has not yet been computed. Given that the second-order coefficients depend only weakly on n_f by design [17,18], it is likely that the $n_f=0$ third-order coefficients are also good approximations when $n_f=2$. We assume this in our analysis, but when estimating errors at $n_f=2$ we take the size of the entire $n_f=0$ third-order contribution as an estimate of the uncertainty due to n_f dependence. When $n_f=0$, we estimate the truncation error in perturbation theory to be of order $\alpha_P^3(q_{m,n})$ times the leading order contribution.

Note that the plaquette $W_{1,1}$ has no third-order contribution. This is because the coupling α_P is defined in terms of the plaquette [2]; the absence of third- and higher-order corrections is merely a consequence of our conventions. Truncation errors in the plaquette's expansion reappear when our coupling is converted to more standard couplings, such as $\alpha_{\overline{\mathrm{MS}}}$:

$$\alpha_{\overline{\mathrm{MS}}}^{(n_f)}(Q)=\alpha_P^{(n_f)}(e^{5/6}Q)\{1+2\alpha_P^{(n_f)}/\pi+X_{\overline{\mathrm{MS}}}(\alpha_P^{(n_f)})^2 + O((\alpha_P^{(n_f)})^3)\}. \qquad (6)$$

Here the third-order coefficient $X_{\overline{\mathrm{MS}}}\approx 0.95$ for $n_f=0$ [20]. The third-order coefficient is new since our first paper. Unfortunately, the n_f dependence of this coefficient is not known. However, the variation of this coefficient as n_f goes

TABLE III. Expectation values of Wilson loop operators for small loops, and the corresponding α_P's for a variety of lattice QCD parameters. The uncertainties listed for the expectation values are Monte Carlo (MC) statistical errors. Those listed for the α_P's are estimates of the truncation errors in perturbation theory.

β	n_f	$am^0_{\rm eff}$	Loop	MC value	$\alpha_P^{(n_f)}(q_{m,n})$
6.0	0	-	$-\ln W_{1,1}$	0.5214 (0)	0.1519 (0)
			$-\ln W_{1,2}$	0.9582 (1)	0.1571 (6)
			$-\ln W_{1,3}$	1.3757 (2)	0.1584 (6)
			$-\ln W_{2,2}$	1.6605 (3)	0.1657 (8)
5.6	2	0.025	$-\ln W_{1,1}$	0.5719 (0)	0.1792 (0)
		0.010	$-\ln W_{1,1}$	0.5709 (0)	0.1788 (0)
		0.010	$-\ln W_{1,2}$	1.0522 (1)	0.1828 (30)
		0.010	$-\ln W_{1,3}$	1.5123 (2)	0.1832 (40)
		0.010	$-\ln W_{2,2}$	1.8337 (3)	0.1907 (80)
5.7	0	-	$-\ln W_{1,1}$	0.5995 (0)	0.1829 (0)
5.415	2	0.0125	$-\ln W_{1,1}$	0.6294 (0)	0.2075 (0)
5.47	2	0.050	$-\ln W_{1,1}$	0.6134 (0)	0.1993 (0)
6.2	0	-	$-\ln W_{1,1}$	0.4884 (0)	0.1398 (0)
6.4	0	-	$-\ln W_{1,1}$	0.4610 (0)	0.1302 (0)

to two or three is unlikely to be large. The factor $e^{5/6}$ in the scale is chosen to eliminate n_f dependence in the second-order coefficient of the expansion [18], and therefore also removes much of the n_f dependence in third order. As above, we use the $n_f=0$ value for $X_{\overline{\rm MS}}$ throughout our analysis, but when $n_f=2$ we take the size of the entire third-order term as our estimate of the uncertainty due to n_f dependence.

The coupling α_P was defined to coincide through second order with the continuum coupling α_V defined in [18,17] from the static-quark potential. The third-order correction to the static-quark potential has recently been computed [21], leading to

$$\alpha_V^{(n_f)}(Q)=\alpha_P^{(n_f)}(Q)\{1+X_V(\alpha_P^{(n_f)})^2+\cdots\}, \qquad (7)$$

where $X_V=1.86-0.14n_f+X_{\overline{\rm MS}}$, which is 2.81 for $n_f=0$. Note that this expansion has infrared divergences in fourth-order and beyond, due to residual retardation effects in the static quark potential [22].

B. Results: α_P determinations

Monte Carlo simulation results for the expectation values of the Wilson loop operators are summarized in Table III [23]. We also tabulate the values of $\alpha_P(q_{m,n})$ obtained by matching perturbation theory to Monte Carlo simulation results. The uncertainties quoted are our estimates of the potential truncation errors in perturbation theory; see Sec. III A. The only other potential sources of error are nonperturbative effects, and as discussed, these are almost certainly negligible compared to truncation errors. Finite-volume errors are much less than 1% for such small loops.

The values for the various coupling constants in this table are all different. This is because the coupling-constant scales $q_{m,n}$ are different for each operator and for each parameter set. To compare these results we must first evolve the running coupling constants to a common scale. In Table IV we present the couplings evolved to 8.2 GeV, which is the scale we chose in [2]. To generate these values, we converted the corresponding $q_{m,n}$'s from units of a^{-1} to GeV using the lattice spacings inferred from each of the Υ or ψ mass splittings for which we have simulation results. We then evolved the couplings to 8.2 GeV by numerically integrating the evolution equation for α_P. We used the universal second-order β function together with the $n_f=0$ third-order term for α_P. The n_f dependence of the third-order β function is unknown, but the entire third-order term generally has negligible effect. This is especially true for our most important results at $\beta=6$ and 5.6, since 8.2 GeV was chosen to be very close to the $q_{m,n}$'s and very little evolution is required.

If one groups the various couplings in this table according to the splitting used to tune the simulation and the number of light-quark flavors n_f, one finds that the values within a single group are completely consistent. In particular, results obtained using different loops are in excellent agreement, which shows that our estimates of the errors caused by truncating perturbation theory are reasonable. Also, the coupling constants obtained from the plaquette using β's ranging from 5.7 to 6.4, corresponding to scales $q_{1,1}$ ranging from 4.8 GeV to 14.2 GeV, agree well. This demonstrates that the evolution of our coupling constant α_P is well described by the perturbative β function; no lattice artifacts are apparent. This is also illustrated by Fig. 3, where we plot the coupling constant $\alpha_P(q_{1,1})$, obtained from the plaquette, versus the effective momentum scale $q_{1,1}=3.4/a$ at which the coupling is measured on each lattice. The simulation results for the running of α_P agree well with the prediction of third-order perturbation theory [24].

C. Extrapolation to $n_f=3$

The coupling constants in Table IV from simulations with different n_f's are significantly different, as are the couplings from simulations tuned using different meson mass splittings. Our final step is to extrapolate to $n_f=3$, which is the correct number of light-quark flavors for Υ and ψ physics. The extrapolated results, which are shown in Table V, should all agree, and do. To make the extrapolation, we paired $n_f=0$ and $n_f=2$ simulations as indicated in the table. For

TABLE IV. Values of $\alpha_P(8.2\,\mathrm{GeV})$ from several operators $W_{m,n}$ and a variety of tunings for QCD simulations, with different β's, n_f's, and meson mass splittings used to fix a^{-1}. The two uncertainties listed are due to uncertainties in the inverse lattice spacing, and to truncation errors in the extraction of α_P using perturbation theory.

				$\alpha_P^{(n_f)}(8.2\,\mathrm{GeV})$		
β	n_f	am_{eff}^0	Loop	$\chi_b-\Upsilon$	$\Upsilon'-\Upsilon$	$\chi_c-\psi/\eta_c$
6.0	0	-	$-\ln W_{1,1}$	0.1552 (10)(0)	0.1525 (11)(0)	
			$-\ln W_{1,2}$	0.1556 (10)(6)	0.1528 (11)(6)	
			$-\ln W_{1,3}$	0.1560 (11)(6)	0.1531 (11)(6)	
			$-\ln W_{2,2}$	0.1565 (11)(8)	0.1537 (12)(7)	
5.7	0	-	$-\ln W_{1,1}$	0.1528 (18)(0)		0.1465 (61)(0)
6.2	0	-	$-\ln W_{1,1}$	0.1561 (21)(0)	0.1519 (23)(0)	
6.4	0	-	$-\ln W_{1,1}$	0.1515 (67)(0)		
5.6	2	0.010	$-\ln W_{1,1}$	0.1794 (24)(0)	0.1781 (33)(0)	
		0.010	$-\ln W_{1,2}$	0.1777 (24)(30)	0.1764 (32)(30)	
		0.010	$-\ln W_{1,3}$	0.1770 (24)(40)	0.1757 (32)(40)	
		0.010	$-\ln W_{2,2}$	0.1767 (23)(71)	0.1754 (32)(71)	
5.415	2	0.0125	$-\ln W_{1,1}$	0.1748 (34)(0)		0.1696 (78)(0)

each separate combination of Wilson loop and meson mass splitting, we extrapolated $1/\alpha_P$ using the corresponding α_P's from the two simulations.

We chose to extrapolate $1/\alpha_P$ rather than α_P because numerical experiments using third-order perturbation theory suggest that $1/\alpha_P$ is significantly more linear in n_f. To see how the couplings from our simulations might depend on n_f, note that the Υ splittings that we use to determine the lattice spacing probe QCD at momentum scales q_Υ of the order 0.5–1 GeV. Thus when we choose a lattice spacing that gives these splittings their correct physical values, we are in effect tuning the QCD coupling constant in our simulation to have its correct value at the scale q_Υ. (If $n_f \neq 3$, the simulation's coupling will have the correct value *only* at q_Υ.) This means that the couplings in our $n_f=0$ and 2 simulations agree with the correct $n_f=3$ coupling at q_Υ:

$$\alpha_P^{(0)}(q_\Upsilon)=\alpha_P^{(2)}(q_\Upsilon)=\alpha_P^{(3)}(q_\Upsilon). \tag{8}$$

This equation specifies the dependence of the couplings obtained in our simulations on n_f, but we are unable to use it directly since perturbation theory is not particularly reliable at q_Υ. Nevertheless, we can use this relation to test different schemes to extrapolate n_f as follows. Taking $q_\Upsilon=1$ GeV, we set all the couplings at that scale equal to some large value, say 0.65. We then evolve all three to 8.2 GeV using the three-loop β function. Finally, we compare the 8.2 GeV coupling extrapolated from $n_f=0$ and 2 with the $n_f=3$ coupling obtained by evolving from q_Υ. Extrapolating α_P gives results that are ''correct'' to within 1.4%, while extrapolating $1/\alpha_P$ is correct to within 0.3%. This exercise indicates that we should extrapolate the inverse coupling and that the extrapolation errors are probably less than 1%. Such errors are negligible relative to the other systematic and statistical errors. Nevertheless, it would be desirable to repeat our analysis using simulations with $n_f=3$ or even $n_f=4$.

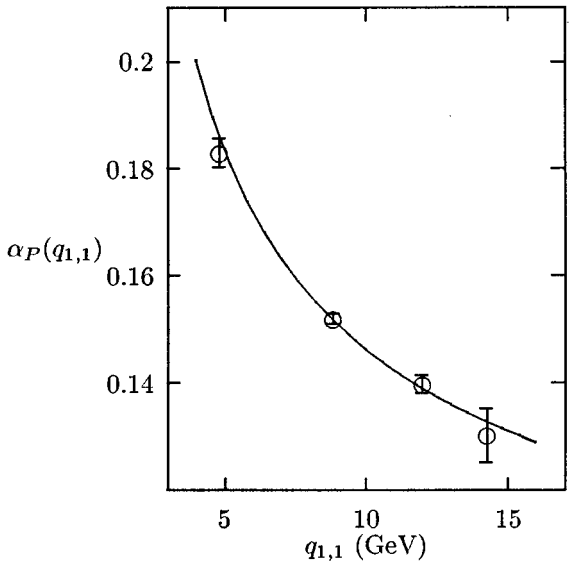

FIG. 3. Values of the QCD coupling constant α_P determined from the plaquette in simulations with differing lattice spacings corresponding to $\beta=5.7$, 6, 6.2, and 6.4, all with $n_f=0$. The coupling constant is plotted vs the average momentum $q_{1,1}$ carried by gluons in the plaquette at the various lattice spacings, with $q_{1,1}=3.4/a$. The line shows the coupling constant evolution predicted by third-order perturbation theory.

Equation (8) played a key role in the earliest determinations of the running coupling constant using lattice QCD [25]. These studies used only $n_f=0$ simulations. As can be seen from our results, the coupling at $n_f=0$ is 25% smaller than the correct $n_f=3$ coupling. This correction was estimated in these earlier papers by perturbatively evolving the $n_f=0$ coupling down to q_Υ, changing n_f to three, and then evolving back up to the original large scale, which is 8.2 GeV in the present analysis. This procedure suggests a correction of 15–20%, which our simulations show to be an underestimate but within the error range quoted in the earlier papers. We emphasize that there is no inconsistency between these earlier analyses and ours. Our simulations with $n_f=0$ give results that are identical with the earlier work. What is different here is that we have actual simulation results at $n_f \neq 0$ and so get to $n_f=3$ using extrapolation, rather than a

TABLE V. Values of $\alpha_P^{(3)}(8.2\ \mathrm{GeV})$ from different operators and different tunings of the QCD simulation. The two uncertainties listed are due to uncertainties in the inverse lattice spacing, and to truncation errors in the extraction of α_P using perturbation theory.

		$\alpha_P^{(3)}(8.2\ \mathrm{GeV})$		
β	Loop	$\chi_b-\Upsilon$	$\Upsilon'-\Upsilon$	$\chi_c-\psi/\eta_c$
6.0,5.6	$-\ln W_{1,1}$	0.1946 (41)(0)	0.1944 (60)(0)	
	$-\ln W_{1,2}$	0.1913 (42)(52)	0.1912 (57)(53)	
	$-\ln W_{1,3}$	0.1897 (42)(69)	0.1897 (57)(70)	
	$-\ln W_{2,2}$	0.1889 (40)(120)	0.1887 (56)(123)	
5.7,5.415	$-\ln W_{1,1}$	0.1884 (57)(0)		0.1841 (146)(0)

perturbative analysis that is well motivated but only partly justified. That the sizable correction due to light-quark vacuum polarization was so accurately predicted using perturbation theory strengthens our confidence that our nonperturbative treatment of vacuum polarization is correct. Note that if we use the perturbative analysis to correct just our $n_f=2$ couplings, ignoring our $n_f=0$ couplings, we obtain results that are in excellent agreement with the extrapolated coupling [26].

Our final results for α_P in Table V agree well with each other and with our earlier results [2]. In particular, the 3σ discrepancy between results using different Υ splittings at $n_f=0$ disappears completely at $n_f=3$. This is highly nontrivial; we are in effect counting the number of light-quark flavors that affect real upsilons. It provides confirmation that the quark vacuum polarization is correctly included in our simulations and extrapolation.

D. Conversion to $\alpha_{\overline{\mathrm{MS}}}$

To compare with nonlattice determinations of the coupling constant, we have converted our results to the modified minimal subtraction scheme ($\overline{\mathrm{MS}}$) definition of the coupling, using Eq. (6) with $X_{\overline{\mathrm{MS}}}=0.95\pm0.95$. Our results are listed in Table VI, and together with our α_P's in Table V, are the main result of this paper. The $\overline{\mathrm{MS}}$ results are somewhat larger than in our earlier paper because we now use the $n_f=0$ value for $X_{\overline{\mathrm{MS}}}$, rather than setting it to zero as before. Our estimate in the earlier paper for the size of this term was correct and was included as an error. Consequently, our old results are consistent with our new results within errors.

To further facilitate comparisons with other analyses, we have numerically integrated the third-order perturbative evolution equation for $\alpha_{\overline{\mathrm{MS}}}$ and applied appropriate matching conditions at quark thresholds [27] to evolve it to the mass of the Z^0. The results for our ten determinations are shown in Table VII. For matching we assumed $\overline{\mathrm{MS}}$ masses of 1.3(3) GeV and 4.1(1) GeV for the c and b quarks, respectively [27,28]. The uncertainties in these masses can shift the final coupling constant by less than half a percent; we ignore them.

IV. DISCUSSION AND CONCLUSIONS

In this paper we have demonstrated that lattice simulations provide among the simplest, most accurate, and most reliable determinations of the strong coupling constant. Our ten different results, tabulated in Tables V–VII, are in excellent agreement with each other. Indeed, all but one of them agree with our best determination to within *its* uncertainty; that is, to within the smallest error bars. Our best result implies

$$\alpha_{\overline{\mathrm{MS}}}^{(n_f)}(Q) = \begin{cases} 0.3706(288) & \text{for } Q=1.3\ \mathrm{GeV}\approx M_c \text{ and } n_f=3, \\ 0.3701(288) & \text{for } Q=1.3\ \mathrm{GeV}\approx M_c \text{ and } n_f=4, \\ 0.2234(93) & \text{for } Q=4.1\ \mathrm{GeV}\approx M_b \text{ and } n_f=4, \\ 0.2233(93) & \text{for } Q=4.1\ \mathrm{GeV}\approx M_b \text{ and } n_f=5, \\ 0.1174(24) & \text{for } Q=91.2\ \mathrm{GeV}=M_Z \text{ and } n_f=5, \end{cases} \tag{9}$$

with errors due to lattice-spacing and perturbation-theory uncertainties combined in quadrature. These results are about 1σ higher than our previous results [2]. The shift is entirely

TABLE VI. Values of $\alpha_{\overline{\mathrm{MS}}}^{(3)}(3.56\ \mathrm{GeV})$ from different operators and different tunings of the QCD simulation. The two uncertainties listed are due to uncertainties in the inverse lattice spacing, and to truncation errors in the extraction of α_P and conversion to $\alpha_{\overline{\mathrm{MS}}}$ using perturbation theory.

		$\alpha_{\overline{\mathrm{MS}}}^{(3)}(3.56\ \mathrm{GeV})$		
β	Loop	$\chi_b-\Upsilon$	$\Upsilon'-\Upsilon$	$\chi_c-\psi/\eta_c$
6.0,5.6	$-\ln W_{1,1}$	0.2258 (56)(74)	0.2254 (81)(70)	
	$-\ln W_{1,2}$	0.2213 (56)(99)	0.2211 (77)(98)	
	$-\ln W_{1,3}$	0.2192 (57)(116)	0.2191 (77)(114)	
	$-\ln W_{2,2}$	0.2181 (54)(176)	0.2178 (75)(177)	
5.7,5.415	$-\ln W_{1,1}$	0.2174 (76)(67)		0.2117 (197)(62)

TABLE VII. Values of $\alpha_{\overline{\rm MS}}^{(5)}(M_Z)$ from several operators and various tunings of the QCD simulation. The two uncertainties listed are due to uncertainties in the inverse lattice spacing, and to truncation errors in perturbative expansions.

		$\alpha_{\overline{\rm MS}}^{(5)}(M_Z)$		
β	Loop	$\chi_b-\Upsilon$	$\Upsilon'-\Upsilon$	$\chi_c-\psi/\eta_c$
6.0,5.6	$-\ln W_{1,1}$	0.1174 (15)(19)	0.1173 (21)(18)	
	$-\ln W_{1,2}$	0.1163 (15)(26)	0.1161 (21)(26)	
	$-\ln W_{1,3}$	0.1157 (15)(31)	0.1156 (21)(31)	
	$-\ln W_{2,2}$	0.1154 (14)(46)	0.1152 (20)(48)	
5.7,5.415	$-\ln W_{1,1}$	0.1152 (20)(18)		0.1136 (52)(16)

due to the new third-order term in the perturbative formula, Eq. (6), relating the lattice coupling α_P to $\alpha_{\overline{\rm MS}}$. Our Monte Carlo simulation results are essentially identical to those in our earlier paper. The shift relative to our earlier result is only 1σ because we previously estimated the size of this third-order term accurately.

The bulk of our effort in this analysis was devoted to understanding and estimating the systematic errors. We varied every parameter in the simulation. We used four different short-distance quantities to extract the coupling, and three different (infrared) meson splittings, in two different meson families, to tune the bare coupling or lattice spacing. We demonstrated that the gross features of Υ and ψ physics are accurately described by our simulations. We explored the role of light-quark vacuum polarization for a range of light-quark masses. Our simulations were sufficiently accurate to show that $n_f=0$ is the wrong number of light-quark flavors for Υ's. Only when we extrapolated to $n_f=3$, the correct value, did our simulation results agree with experiment. To see how robust our results are, we redid the analysis but with various ingredients missing. The corresponding shifts in $\alpha_{\overline{\rm MS}}^{(5)}(M_Z)$ are listed in Table VIII; omitting the n_f extrapolation led to the only appreciable difference.

The various parts of our analysis agree well with the results of other groups. The α_P's that we extract from Wilson loop operators agree to within statistical and truncation errors with those obtained by very different techniques [29]. This is the easy part of the analysis. The remainder, involving the determination of lattice spacings, has now also been duplicated. A recent analysis of simulation results from the Fermilab and SCRI groups, both of which employ a totally different formalism for b-quark dynamics, gives $\alpha_{\overline{\rm MS}}^{(5)}(M_Z)=0.116(3)$, in complete agreement with our results [30].

TABLE VIII. Changes in the coupling constant at M_Z when different parts of our simulation or analysis are omitted.

	$\Delta\alpha_{\overline{\rm MS}}^{(5)}(M_Z)$
Omit $O(a^2)$ gluonic corrections	-0.6%
Omit tadpole improvement of NRQCD	-0.5%
Omit $O(v^2,a,a^2)$ corrections in NRQCD	$+0.9\%$
Omit extrapolation (use $n_f=2$)	-4.7%

Lattice coupling constant determinations such as ours enjoy a fundamental advantage over traditional methods based on perturbative high-energy processes, allowing significantly greater accuracy. The systematic uncertainties in the perturbative parts of the analyses are similar in both approaches, but the nonperturbative elements differ substantially. When we tune our simulation to reproduce the Υ spectrum, we are in effect directly tuning the QCD scale parameter $\Lambda_{\overline{\rm MS}}$. Consequently, a 5% simulation error in a mass splitting results in a 5% error in $\Lambda_{\overline{\rm MS}}$, which implies only a 1% error in $\alpha_{\overline{\rm MS}}(M_Z)$. In high-energy determinations, however, one measures the coupling constant rather than the scale parameter, and usually only through small radiative corrections to an electroweak process. Measuring $\Lambda_{\overline{\rm MS}}$ is intrinsically much more accurate than measuring $\alpha_{\overline{\rm MS}}$.

There are prospects for substantially improving the accuracy of our result fairly soon. We list sources of error in our value for $\alpha_{\overline{\rm MS}}^{(5)}(M_Z)$ in Table IX. The dominant error is due to truncation in perturbative expansions, specifically because the n_f dependent parts of our third-order coefficients have not yet been calculated. The agreement we observe between couplings from different loop operators, each with its own perturbative series, suggests that our estimates of this systematic error are realistic or even pessimistic. Nevertheless, our total error could be cut in half by computing this n_f dependence, particularly for Eq. (6). This is a straightforward perturbative calculation. For this paper, we halved our statistical errors for our $n_f=0$ simulations; the same should be done for $n_f\neq 0$. Use of an improved gluon action would remove the need for the a^2 correction in the $\chi_b-\Upsilon$ analysis, while it already has negligible effect on $\Upsilon'-\Upsilon$. The addi-

TABLE IX. Sources of error in our best determination of $\alpha_{\overline{\rm MS}}^{(5)}(M_Z)$.

Source	Uncertainty
Unknown n_f dependence in third-order perturbation theory	1.9%
Statistical error in determination of a^{-1}	0.9%
Light-quark masses	0.9%
Extrapolation in n_f	0.3%
Finite a and $O(v^4)$ errors	0.2%
Fourth-order evolution of $\alpha_{\overline{\rm MS}}$	0.01%

tional cost would be small [31]. Using a relativistic formulation of c-quark dynamics, rather than NRQCD, might allow accurate results from the charmonium spectrum. A simulation with either $n_f=3$ or 4 light quarks would eliminate the extrapolation error and would require perhaps only twice the computational effort needed for $n_f=2$. Finally, simulations with *larger* light-quark masses $m_{\rm eff}$ would allow us to pin down more accurately the dependence on this parameter.

Our lattice determinations of the strong coupling constant agree well with most determinations based on perturbative high-energy processes. This fact provides striking evidence that the nonperturbative QCD of hadronic confinement and the perturbative QCD of high-energy jets are the same theory.

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