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First determination of the strange and light quark masses from full lattice QCD

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We compute the strange quark mass m_s and the average of the u and d quark masses $\hat{m}$ using full lattice QCD with three dynamical quarks combined with the experimental values for the π and K masses. The simulations have degenerate u and d quarks with masses $m_u = m_d \equiv \hat{m}$ as low as $m_s/8$, and two different values of the lattice spacing. The bare lattice quark masses obtained are converted to the $\overline{\mathrm{MS}}$ scheme using perturbation theory at $\mathcal{O}(\alpha_S)$. Our results are $m_s^{\overline{\mathrm{MS}}}(2\ \mathrm{GeV}) = 76(0)(3)(7)(0)$ MeV, $\hat{m}^{\overline{\mathrm{MS}}}(2\ \mathrm{GeV}) = 2.8(0)(1)(3)(0)$ MeV, and $m_s/\hat{m} = 27.4(1)(4)(0)(1)$, where the errors are from statistics, simulation, perturbation theory, and electromagnetic effects, respectively.

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I. INTRODUCTION

The masses of the strange and light quarks are fundamental parameters of the standard model that are *a priori* unknown and must be determined from experiment. This is complicated, however, by confinement in QCD, so that quarks cannot be observed as isolated particles. We can only determine their masses by solving QCD for observable quantities, such as hadron masses, as a function of the quark mass. This can be accomplished with the numerical techniques of lattice QCD. Precise knowledge of quark masses constrains beyond the standard model scenarios as well as providing input for phenomenological calculations of standard model physics. The strange quark mass, in particular, is needed for various phenomenological studies, including the important *CP*-violating quantity ϵ'/ϵ [1], where its uncertainty severely limits the theoretical precision.

Previously, shortcomings in the formulation of QCD on the lattice and limitations in computing power have meant that lattice calculations were forced to work with an unrealistic QCD vacuum that either ignored dynamical (sea) quarks or included only u and d quarks with masses much heavier than in Nature. This condemned determinations of the quark masses to rather large systematic errors (10–20 %) arising from the inconsistency of comparing such a theory with experiment. The determination presented here uses simulations with the improved staggered quark formalism that have a much more realistic QCD vacuum with two light dynamical quarks and one strange dynamical quark. We describe how the bare quark masses in the lattice QCD Lagrangian can be fixed using chiral perturbation theory to extrapolate lattice results to the physical point, and how the lattice quark masses obtained can be transformed to a continuum scheme ($\overline{\mathrm{MS}}$) using lattice perturbation theory. Working in the region of dynamical u/d quark masses below $m_s/2$ and down to $m_s/8$ gives us control of chiral extrapolations and avoids the large systematic errors from dynamical quark mass and unquenching effects that previous calculations have had.

Staggered quarks are fast to simulate. They keep a remnant of chiral symmetry on the lattice, and therefore give a Goldstone pion mass which vanishes with the bare quark mass. This allows the relatively simple determination of the quark mass described here, which is not available, for example, in the Wilson quark formalism.

The staggered quark formalism does have several unwanted features, however. With the naive staggered action, large discretization errors appear, although they are formally only $\mathcal{O}(a^2)$ or higher (a is the lattice spacing). The renormalization of operators to match a continuum scheme can also be large and badly behaved in perturbation theory. This is true, for example, for the mass renormalization that is needed here. It turns out that both problems have the same

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source, a particular form of discretization error in the action, called ''taste violation,'' and both are ameliorated by use of the improved staggered formalism [2]. The perturbation theory then shows small renormalizations [3–5] and discretization errors are much reduced [6–8]. Empirically, taste violation remains the most important discretization error in the improved theory, despite being subleading to ''generic'' discretization errors. The Goldstone meson masses we will discuss here are affected by this at one loop in the chiral expansion. Staggered chiral perturbation theory (SχPT) [9–12] allows us to control these effects and reduce discretization errors significantly.

A more fundamental concern about staggered fermions is based on the need to take the fourth root of the quark determinant to convert the fourfold duplication of ''tastes'' into one quark flavor. It is possible that there are nonlocalities in the continuum limit that would spoil the description of QCD at some level. Checks of the formalism against experimental results [12–16], make this unlikely, we believe, but further work along these lines is crucial and continuing.

II. LATTICE DATA

The simulation data of the MILC collaboration [14,17] are analyzed; staggered quarks with leading errors at $\mathcal{O}(\alpha_S a^2, a^4)$ [2] and one-loop Symanzik improved gluons with tadpole improvement [18,19]. Two sets of configurations are used: a ''coarse'' set at lattice spacing $a \approx 1/8$ fm and sea quark masses of $am'_u = am'_d \equiv a\hat{m}' = 0.005$, 0.007, 0.01, 0.02, 0.03 with $am'_s = 0.05$, and a ''fine'' set at $a \approx 1/11$ fm with sea quark masses of $a\hat{m}' = 0.0062$, 0.0124 and $am'_s = 0.031$. Here we use primes on the sea quark masses to emphasize that these are the nominal quark masses used in the simulation, not the physical masses m_s or $\hat{m} \equiv (m_u + m_d)/2$. The simulations are ''partially quenched,'' with a range of valence masses from m'_s down to $m'_s/10$ (coarse) and $m'_s/5$ (fine), not necessarily equal to the sea quark masses, simulated on each lattice. It should be noted that the quark masses in lattice units quoted here contain a factor of u_{0P}, the tadpole-improvement factor determined from the fourth root of the average plaquette, compared with a more conventional definition of quark mass [2]. This is taken care of nonperturbatively before our renormalization below.

The lattice spacing a is determined ultimately from the Υ'-Υ mass difference [20], a useful quantity because it is approximately independent of quark masses, including the b mass. An analysis of a wide range of other ''gold-plated'' hadron masses and decay constants on these configurations shows agreement with experiment at the 2–3 % level [13]. Gold-plated hadrons are stable (in QCD), with masses at least 100 MeV below decay thresholds, so their masses are well-defined both experimentally and theoretically, important for fixing the parameters of QCD. The only gold-plated light mesons available to fix $\hat{m}$ and m_s are the π and K. There is none with only s valence quarks because the ϕ is unstable and the pseudoscalar is strongly mixed. Baryons can provide an alternative, the nucleon for $\hat{m}$ and the Ω for m_s, but their statistical errors are large, and they are not very sensitive to the quark masses.

Our analysis uses SχPT [11] to fit the dependence of the results on the quark masses. This dependence can then be extrapolated/interpolated to the point where the (Goldstone) π and K have their physical masses, thereby determining the bare lattice $\hat{m}$ and m_s. At the level of precision at which we are working, and because we take $m_u = m_d$, we must be careful about electromagnetic (EM) and isospin-violating effects. At lowest nontrivial order in e^2 and the quark masses, Dashen's theorem [21] states that $m^2_{\pi^+}$ and $m^2_{K^+}$ receive equal EM contributions; while the π^0 and K^0 masses are unaffected. However, at next order, there can be large and different contributions to $m^2_{\pi^+}$ and $m^2_{K^+}$ of order $e^2 m^2_K$ [22–24]. Let Δ_E [25] parameterize violations of Dashen's theorem: $(m^2_{K^+} - m^2_{K^0})_{\rm EM} = (1+\Delta_E)(m^2_{\pi^+} - m^2_{\pi^0})_{\rm EM}$. Then Refs. [22–24] suggest $\Delta_E \approx 1$.

Including EM and isospin effects, the physical values of $\hat{m}$ and m_s can then be determined by extrapolating the lattice squared meson masses to $m^2_{\hat{\pi}} \equiv m^2_{\pi^0}$ and $m^2_{\hat{K}} \equiv [m^2_{K^0} + m^2_{K^+} - (1+\Delta_E)(m^2_{\pi^+} - m^2_{\pi^0})]/2$, using experimental values on the right hand side of these expressions. We are neglecting $\mathcal{O}((m_u - m_d)^2)$ corrections, which should be tiny [26]. EM contributions to the neutral particle masses are also neglected, and we take account of this in our error. For the π^0 the violation of Dashen's theorem is $\mathcal{O}(e^2 m^2_\pi/(8\pi^2 f^2_\pi))$ and negligible. For $m^2_{K^0}$ the violation is in principle the same order as for $m^2_{K^+}$ [23], but in model calculations [24] it appears to be very small. To be conservative, we consider EM contributions to $m^2_{K^0}$ of order of half the violations of Dashen's theorem, with unknown sign. Effectively, this replaces $\Delta_E \approx 1$ in the formula for $m^2_{\hat{K}}$ above with the range 0–2, which we take as the EM systematic error.

III. CHIRAL FITS AND SYSTEMATIC ERRORS

Here we briefly describe the fits to SχPT theory forms and the estimate of the associated errors [12,15]. Because the squared meson masses ($M^2_{\rm meson}$) are nearly linear in the valence quark masses, the final values of the quark masses are quite insensitive to details of the chiral fits. Chiral logs and analytic terms at next-to-leading order (NLO) and higher only affect the results at the $\approx 5\%$ level.

SχPT is a joint expansion in x_q and x_{a^2}, which are dimensionless measures of the size of quark mass and lattice spacing effects, respectively:

$$x_q \equiv \frac{2\mu m_q}{8\pi^2 f^2_\pi}; \quad x_{a^2} \equiv \frac{a^2\overline{\Delta}}{8\pi^2 f^2_\pi}. \qquad (1)$$

m_q is the quark mass, $2\mu m_q$ is the tree-level mass of a $q\overline{q}$ meson, and $f_\pi \approx 131$ MeV. $a^2\overline{\Delta}$ is an average meson splitting between different tastes. On the coarse lattices $x_{a^2} \approx 0.09$; on the fine, $x_{a^2} \approx 0.03$.

For physical kaons, the relevant expansion parameter is $x_{ud,s} \equiv (x_{ud} + x_s)/2 \approx 0.18$. Since our lattice data is very precise (0.1 to 0.7% on M^2_{meson}), it is clear that we cannot expect NLO or even NNLO χPT to work well up to the kaon mass. If however the valence quark masses are limited by $m_x+m_y \lesssim 0.75 m_s'$, we obtain good fits including NNLO analytic terms. Such fits are consistent with χPT expectations: the coefficients of NLO and NNLO terms are $\mathcal{O}(1)$ when these terms are expressed as functions of x_q and x_{a^2}. When fitting up to the strange mass we include NNNLO as well as NNLO terms, but satisfy the chiral constraints by fixing the NLO terms from lower mass fits. Since the s quark mass can be reached in simulations, the form of the NNLO and NNNLO terms is not important; such terms simply allow for a reasonable interpolation to the physical m_s.

Both decay constant and M^2_{meson} data and both coarse and fine ensembles are fit simultaneously. Although NLO taste violations are explicitly included, we allow for "generic" discretization errors by using a Bayesian fit [27] that permits physical parameters to change by order $\alpha_S a^2 \Lambda^2_{QCD} \sim 2\%$ in going from the coarse to the fine configurations.

The Υ system provides an absolute lattice scale, but it is convenient to use the relative scale determined from r_1, a parameter derived from the heavy quark potential [28,29], to compare accurately the scale for different sea quark masses within the coarse or fine set. Υ splittings give $r_1 = 0.317(7)(3)$ fm [14]. Using the volume dependence calculated in NLO SχPT [10,11], (and tested against results on different volumes [14]) the small finite-volume effects ($<0.75\%$ in M^2_{meson}) can be removed from our data with negligible residual error.

Figure 1 compares our fit with our partially quenched data for M^2_{meson}. The data appear quite linear to the eye. Indeed, linear fits change our result for the quark masses by only 2% to 7%, depending on the fit range chosen and whether or not the correlated decay constants are fit simultaneously. However, since the statistical errors in our data are so small, the nonlinearities from chiral logs and higher order analytic terms are crucial for obtaining good fits: linear fits have $\chi^2/(\text{degrees of freedom}) \sim 20$. Nonlinear fits have a confidence level of 0.28, are crucial to obtaining Gasser-Leutwyler parameters and affect the decay constants by ~ 4–12%.

We extrapolate/interpolate in mass on the coarse and fine lattices separately to find the lattice values of the light and strange masses that give $m^2_{\hat\pi}$ and $m^2_{\hat K}$. We get $am_s = 0.0390(1)(20)$, $a\hat m = 0.00141(1)(8)$ on the coarse lattices and 0.0272(1)(12) and 0.000989(3)(40) on the fine, where errors are statistical and systematic. The systematic errors are dominated by the chiral extrapolation/interpolation, estimated by varying the fits, and the scale uncertainty (EM effects account for the slight difference with [14]). Alternatively one can extrapolate the chiral fit parameters to the continuum, setting taste-violating parameters zero, and then perform the chiral extrapolation/interpolation to the physical masses. This is shown as the dashed green lines in Fig. 1. The methods give final $\overline{\mathrm{MS}}$ masses that differ by less than 2%. We choose the first method for the central values and include the variation with method in the systematic error.

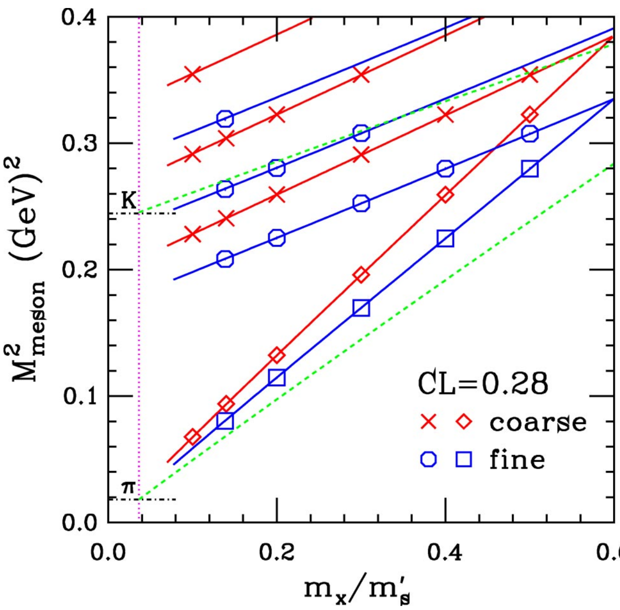

FIG. 1. Partially quenched data for squared meson masses made out of valence quarks x and y as a function of m_x/m_s'. We show results from two lattices: a coarse lattice with sea quark masses $a\hat m' = 0.01$, $am_s' = 0.05$, and a fine lattice with $a\hat m' = 0.0062$, $am_s' = 0.031$. Three sets of "kaon" points with $m_y = m_s', 0.8 m_s', 0.6 m_s'$, are plotted for each lattice. "Pion" points have $m_x = m_y$. The solid lines come from a fit to all the data (not just that plotted). The statistical errors in the points, as well as the variation in the data with sea quark masses are not visible on this scale. The green dashed lines give the continuum fit described in the text, and the magenta vertical dotted line gives the physical $\hat m/m_s$ obtained.

The same SχPT fits that produce the quark masses above give Gasser-Leutwyler parameters in reasonable agreement with phenomenological values [12] and f_π and f_K in agreement with experiment [12,13]. Final results and all details of the fits will be described in Ref. [15].

It is important to provide further checks of m_s and $\hat m$ using other gold-plated masses and mass differences. We focus on m_s because it has smaller statistical error and less dependence on chiral extrapolations. From the heavy hadron sector $2m_{B_{av},s} - m_\Upsilon$ is sensitive to m_s but not to other masses. Here $2m_{B_{av},s}$ is the B_s, B_s^* spin-averaged mass, used to reduce dependence on the coefficients of relativistic corrections in the b-quark action. Note, however, that the B_s^* is close to decay threshold and may not be gold-plated. Figure 2 shows coarse-lattice data for this splitting. The results are 2% high, but this is also our estimate of discretisation errors in the calculation (we do not expect sensitivity to taste violation [30]). This quantity then provides a check of our m_s determination at the 20% level because the experimental splitting varies only by $\approx 15\%$ in changing from $\hat m$ to m_s. Figure 2 also shows results for the Ω baryon mass, on both coarse and fine ensembles. Although statistical errors are large there is a trend downwards on the finer lattices and signs that a continuum extrapolated result will agree with experiment. An expected 2% error on the final value for m_Ω would lead to a 6% determination of m_s.

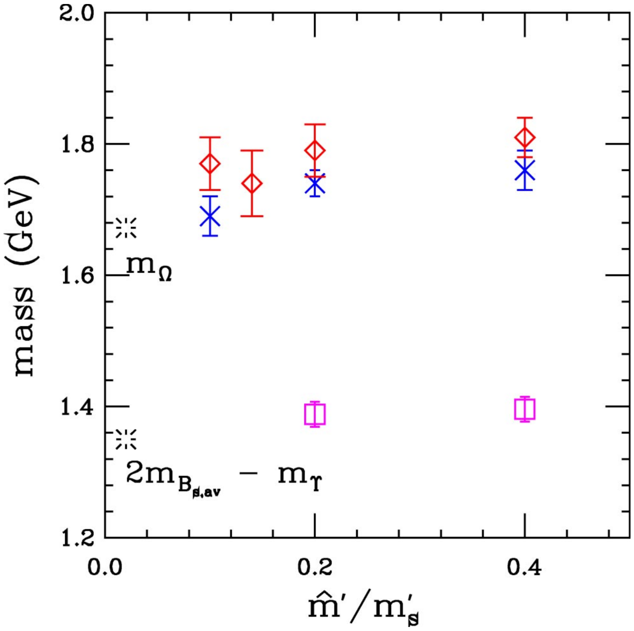

FIG. 2. Lattice results for two masses which show sensitivity to m_s, plotted against $\hat{m}'/m_s'$. The valence s masses are taken at the m_s values determined here. The bursts give the corresponding experimental result. The squares are $2m_{B_{s,av}} - m_\Upsilon$ for two of the coarse ensembles. The upper results are for the mass of the Ω (sss) baryon, on both coarse (diamonds) and fine (crosses) ensembles.

IV. CONNECTING $m^{lattice}$ WITH $m^{\overline{MS}}$

The continuum quark mass in the conventional modified Minimal Subtraction scheme is determined from

$$m^{\overline{\rm MS}}(\mu) = \frac{(am)_0}{a}[1 + \alpha_V(q^*)Z_m^{(2)}(a\mu,(am)_0) + \mathcal{O}(\alpha^2)], \tag{2}$$

where $(am)_0$ is the *a posteriori* tuned bare mass in lattice units obtained above, converted from the MILC convention by dividing by u_{0P}. Z_m is the mass renormalization that connects the bare lattice mass and the $\overline{\rm MS}$ mass. The strong coupling constant in the V scheme is set using third order perturbative expressions for the logarithms of small Wilson loops [31,32] compared with lattice results on these configurations. The value obtained is run to an optimal scale q^*, chosen as described below.

Z_m is calculated by connecting the bare quark-mass to the pole-mass in lattice perturbation theory [3], and using the pole mass to $\overline{\rm MS}$ mass relation [33] at one loop. The lattice calculation was done both by hand and using automated methods [34,35], which become increasingly important for improved actions. The evaluation has been checked to lower precision via a completely different method [36]. Integrals were evaluated here using the numerical integration package, VEGAS [37]. We find

$$Z_m^{(2)}(a\mu,am_0) = \left(b(am_0) - \frac{4}{3\pi} - \frac{2}{\pi}\ln(a\mu) \right), \tag{3}$$

where $b(am) \approx 0.5432 - 0.46(am)^2$, correct to 0.1% up to $(am) = 0.1$. $\gamma_0 = 2/\pi$ is the universal one-loop anomalous mass dimension. Naive staggered quarks have a poorly convergent Z_m with $b(0) \approx 3.6$ as a result of taste-violations. It is clear that the improved staggered quark result is much better. Tadpole-improvement is also important, because of the long paths of gluon fields required to suppress taste-violations. Without tadpole-improvement $b(0) = 2.27$.

We match our lattice to the $\overline{\rm MS}$ scheme at the target scale of 2 GeV, though the results and errors are not sensitive to this choice. Because the mass renormalization has an anomalous dimension, the optimal q^* value for α_V at this scale is dependent on a. q^* is set by a second order BLM method [38]. On the fine lattices, q^* is $1.80/a$ [20] and $\alpha_V(q^*) = 0.247(4)$ in Z_m. On the coarse lattices, $q^* = 2.335/a$, giving $\alpha_V(q^*) = 0.252(5)$. A conservative estimate of the perturbative error in Z_m, informed by the chiral fits, is $1.5 \times \alpha_V^2 \approx 9\%$.

This gives $m_s^{\overline{\rm MS}}$ values of 74.3 MeV on the fine lattices and 72.3 MeV on the coarse lattices. Our central values are obtained by extrapolating linearly in $\alpha_S a^2$, the size of the leading discretization errors. Alternatives, such as a linear extrapolation in $\alpha_S^2 a^2$, the size of taste-violations, or a continuum-extrapolated chiral fit, give results that vary by less than 1 MeV, which we take as the extrapolation error and fold into the total systematic error. Our final quark masses are:

$$m_s^{\overline{\rm MS}}(2\ \text{GeV}) = 76(0)(3)(7)(0)\ \text{MeV}, \tag{4}$$

$$\hat{m}^{\overline{\rm MS}}(2\ \text{GeV}) = 2.8(0)(1)(3)(0)\ \text{MeV}, \tag{5}$$

$$m_s/\hat{m} = 27.4(1)(4)(0)(1), \tag{6}$$

where the errors come from statistics, simulation systematics, perturbation theory, and electromagnetic effects, respectively. The systematic error includes the scale error in quadrature with the chiral and continuum extrapolation errors. The ratio $m_s/\hat{m}$ in Eq. (6) is almost independent of the perturbation theory. It is also strongly constrained by the fact that $2m_K^2 - m_\pi^2$ is almost independent of light quark mass over a large range. For our coarse lattices it increases by 2% as $\hat{m}'$ changes from $m_s'/5$ to m_s'; for the fine lattices by 4%.

V. COMPARISON WITH PREVIOUS DETERMINATIONS

There is a long history of sum rule determinations of the strange quark mass, with the general trend of decreasing values. The current status [39–41] is broad agreement between results from scalar and pseudoscalar spectral functions and from SU(3) breaking in τ hadronic decays, with m_s around 100(20) MeV. The latter method, however, is sensitive to the value of $|V_{us}|$. Lattice results in the quenched approximation give values around 100 MeV but more recent results with two flavors of rather heavy dynamical quarks give a smaller value around 90 MeV [42]. Both quenched and $n_f = 2$ results suffer from the inherent systematic error of comparing an unphysical theory with experiment: results depend on what hadronic masses are used. Some determinations also do not use gold-plated quantities. The JLQCD Collaboration [43] quotes a preliminary $n_f = 3$ result of 75.6(3.4) MeV, not yet including discretization and finite volume errors. They use clover quarks with $\hat{m}' \gtrsim m_s/2$, setting a with the ρ mass.

Here we give results from $n_f = 3$ simulations in the chiral regime. Using gold-plated quantities to fix the QCD parameters means that there is no remaining ambiguity in the match between QCD and experiment. The value we obtain for m_s is lower than previous results, but we maintain that it is based on a firmer footing. It violates some quoted bounds from sum rules [44], but these are open to question [41]. Our result for $m_s/\hat{m}$ is significantly larger than that determined from NLO χPT phenomenology [45], but is compatible with a NNLO analysis [46]. We believe that existing staggered-quark results [12–15] make it unlikely that there are fundamental problems with the formalism we are using.

VI. CONCLUSIONS

Lattice QCD simulations with improved staggered quarks have allowed a new determination of the strange and light quark masses with much reduced systematic error: our final values are $m_s^{\overline{\rm MS}}(2\ \text{GeV}) = 76(8)$ MeV; $\hat{m}^{\overline{\rm MS}}(2\ \text{GeV}) = 2.8(3)$ MeV (adding errors in quadrature). The current lattice simulation error can be reduced still further by generating ensembles with a second (lower) value of the sea strange quark mass and is already underway. The limiting factor for this determination is no longer unquenching but the unknown higher order terms in the perturbative mass renormalization. The two-loop calculation is clearly needed to improve our result significantly and is also underway. The three-loop errors on masses that would then remain would be only $\mathcal{O}(2\%)$, putting the determination into a new region of precision.

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