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Lattice QCD at the physical point: light quark masses

S. Durr,[1,2] Z. Fodor,[1,2,3] C. Hoelbling,[1] S.D. Katz,[1,3] S. Krieg,[1,2]
T. Kurth,[1] L. Lellouch,[4] T. Lippert,[1,2] K.K. Szabo,[1] and G. Vulvert[4]

(Budapest-Marseille-Wuppertal Collaboration)

[1] *Bergische Universität Wuppertal, Gaussstr. 20, D-42119 Wuppertal, Germany.*
[2] *Jülich Supercomputing Centre, Forschungszentrum Jülich, D-52425 Jülich, Germany.*
[3] *Institute for Theoretical Physics, Eötvös University, H-1117 Budapest, Hungary.*
[4] *Centre de Physique Théorique*[†]*, Case 907,*
Campus de Luminy, F-13288 Marseille, France.

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Abstract

Ordinary matter is described by six fundamental parameters: three couplings (gravitational, electromagnetic and strong) and three masses: the electron's (m_e) and those of the up (m_u) and down (m_d) quarks. An additional mass enters through quantum fluctuations: the strange quark mass (m_s). The three couplings and m_e are known with an accuracy of better than a few per mil. Despite their importance, m_u, m_d (their average m_{ud}) and m_s are relatively poorly known: e.g. the Particle Data Group quotes them with conservative errors close to 25%. Here we determine these quantities with a precision below 2% by performing ab initio lattice quantum chromodynamics (QCD) calculations, in which all systematics are controlled. We use pion and quark masses down to (and even below) their physical values, lattice sizes of up to 6 fm, and five lattice spacings to extrapolate to continuum spacetime. All necessary renormalizations are performed nonperturbatively.

The masses of the up, down and strange quarks cannot be measured using standard experimental methods. The strong interaction confines quarks within hadrons (e.g. protons) in such a way that a single quark cannot be isolated. Moreover, the strength of the interaction is such that the mass of a hadron is not the simple sum of the masses of the quarks it contains. Rather it is provided by complicated nonperturbative dynamics (e.g. [2]). This confinement mechanism is the low energy counterpart of the strong interaction's asymptotic freedom [3, 4], by which the interactions between quarks and gluons weaken as their relative momenta are increased.

Interestingly enough, the experimental data for m_u, m_d and m_s has been available for about sixty years (the pion and kaon were discovered in the late 1940's and the proton already 30 years before). Even the theory of the strong interaction, QCD, which–in principle–completely describes bound states of light quarks, has been known for almost four decades [5]. The fact that such a fundamental question has remained poorly answered despite the available experimental and theoretical knowledge is related to the computational difficulties one encounters when trying to solve the underlying equations in the domain of interest. The only known systematic technique to solve them is lattice QCD [6, 7]. Several decades of theoretical, algorithmic and hardware development have been necessary to reach the level at which the light quark masses can be determined reliably. This determination is the goal of the present paper.

For many years calculations were done in the quenched approximation. Although this approach omits the most computationally demanding part of a full QCD calculation –the quark determinant obtained after integrating over the fermion fields– a controlled determination of the strange quark mass in this approximation (with m_u=m_d=m_s equal to about half the physical m_s) took about 20 years [8]. Moreover, the physics of the u and d quarks remained inaccessible, because the quenched approximation, an uncontrolled truncation of QCD, distorts the small quark mass behavior [9, 10].

A very important step was made with the inclusion of u and d sea quark effects (N_f=2) [11–15]. But even there, physical m_{ud} remained elusive, this time for algorithmic reasons. A first breakthrough was made by the MILC collaboration [16], which used an N_f=2+1 staggered fermion formulation to include strange sea quark effects, pushing calculations to smaller light quark masses, finer lattices and larger volumes. Updates from calculations with root-mean-squared masses of the pion taste partners down to 258 MeV and on even finer lattices are presented in [17, 18]. On a subset of the MILC configurations, an attempt has also been made by the HPQCD collaboration to indirectly obtain m_s and m_{ud} via the m_c/m_s ratio [19]. Due to their use of quenched and partially quenched charmed and strange quarks with a non-unitary staggered formalism and their aggressive error estimates on the derived input quantities that they use (m_c and r_1), this work does not fulfill the conditions which are necessary for a controlled ab initio calculation (see below). Recently, also ETMC (N_f=2) [20] and RBC-UKQCD (N_f=2+1) [21] have presented results with $M_\pi \gtrsim 270$ MeV and significantly larger error bars.

The second breakthrough came recently when it was shown that improvements in algorithms [22, 23] allowed the use of theoretically sound Wilson and domain wall fermions for ab initio calculations (e.g. [2, 24]) and even for reaching for the first time physically light m_{ud}, albeit in small volumes and at a single lattice spacing [25].

All previous lattice results on m_{ud} and m_s have neglected one or more of the ingredients required for a full and controlled calculation. The six most important of those are:

1. The inclusion of the up (u), down (d) and strange (s) quarks in the fermion determinant with an exact algorithm and with an action whose universality class is QCD. Rooted staggered fermions provide a numerically efficient way to investigate nonperturbative QCD. However, this discretization is neither local nor unitary for $a>0$, making it difficult to show that it leads to QCD in the continuum limit [17]. While such a partially quenched approach is useful, it is debated whether it can lead to a fully controlled ab initio calculation. Here we use, instead, N_f=2+1 Wilson fermions with local improvement terms which do not affect the continuum limit.

2. Controlled interpolations and extrapolations of the results to physical quark masses. Practically, it means reaching pion masses as small as 200 MeV (clearly the value depends on the problem and on the required accuracy) or most preferably simulating at the physical mass point itself. At three of our lattice spacings we use physical (or even smaller) light quark masses.

3. Large volumes to guarantee small finite-size effects. Our finite volume corrections are tiny (we use volumes up to 6 fm). Nevertheless they are included in the analysis.

4. Controlled extrapolations to the continuum limit. This requires that calculations be performed at no less than three values of the lattice spacing, to check whether the scaling region is reached. We use five lattice spacings between 0.116 and 0.054 fm, thereby gaining full control on the continuum extrapolation.

5. Nonperturbative treatment in all steps. We obtain our primary results (m_{ud} and m_s in the RI scheme at 4 GeV) in a completely nonperturbative manner. In particular, we eliminate all truncation errors associated with the often used perturbative renormalization.

6. Input parameters. The parameters of the theory (scale and quark masses) should be fixed with well measured observables whose error bars are undisputed and whose connection to experiment is transparent and contains no hidden assumptions. To that end we use M_π, M_K and M_Ω exclusively. The influence of their error bars is negligible on our final uncertainties. Taking instead derived quantities, like m_c and r_1 as is done in [19], can be problematic. The error assigned to the input quantity m_c in [19] is smaller by a factor 13 than that of the established Particle Data Group value [26]. Similarly, due to the difficulties in estimating its systematic uncertainty, the continuum value of r_1 (and the related r_0) is disputed.

In this paper we determine m_{ud} and m_s, while fulfilling all of the above conditions. This determination requires two, apparently straightforward, calculations. First we compute hadron masses for tuning the quark masses to their physical values. Then we determine the renormalization constant to convert the bare quark masses to finite quantities in the continuum limit.

We now list the most important steps of our work:

(i) Production of the N_f=2+1 gauge field ensembles. We use a Symanzik improved gauge action and 2-level HEX (hypercubic stout-smearing [29–31]) smeared clover fermions, with m_s held close to its physical value, and use $M_\pi \simeq 135\,\mathrm{MeV}$, $M_K \simeq 495\,\mathrm{MeV}$ and $M_\Omega \simeq 1672\,\mathrm{MeV}$ as input parameters [32]. Gauge field configurations for 47 different values of the parameters ($\beta = 6/g^2$, am_{ud} and am_s) were produced (c.f. Fig. 1 for our $M_\pi < 400\,\mathrm{MeV}$ $N_f = 2+1$ data).

We used five lattice spacings ($a \approx 0.116$, 0.093, 0.077, 0.065 and 0.054 fm), which are the basis for the continuum extrapolation. As we will see, the difference between the results obtained on the finest lattice and those in the continuum limit is $\sim 3\%$, whereas between those of the coarsest lattice and the continuum limit is $\sim 10\%$.

At two pion mass points we carried out detailed finite V analyses, which give us a full understanding of the finite V corrections, as well as their M_π dependence. In all of our calculations which enter the quark mass determination, we have taken $M_\pi L \gtrsim 4$ and/or $L \gtrsim 5\,\mathrm{fm}$, so that the limit $V \to \infty$ can be taken safely. The difference between the results obtained

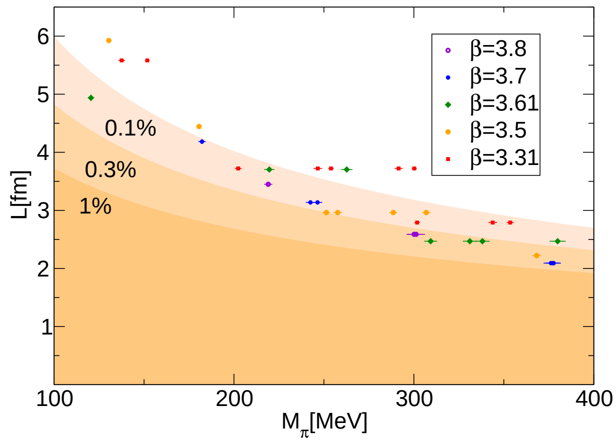

FIG. 1. Summary of our simulation points. The pion masses and the spatial sizes of the lattices are shown for our five lattice spacings. The percentage labels indicate regions, in which the expected finite volume effect [28] on M_π is larger than 1%, 0.3% and 0.1%, respectively. This effect is smaller than about 0.5% for all of our runs and, as described, we corrected for it. Error bars are statistical.

directly on our large lattices and those in the $V\to\infty$ limit is below the five per mil level. Furthermore, for $M_\pi<200$ MeV (which is most relevant for our final result) these corrections are even smaller, namely on the one per mil level.

In our calculations M_π ranges from $\approx$380 down to $\approx$120 MeV (for three of the five lattice spacings we tuned M_π to the vicinity of 135 MeV and for the two finest lattices, the smallest M_π are around 180 and 220 MeV, respectively). Bracketing the physical mass point allows us to circumvent potentially troublesome chiral extrapolations. We perform calculations with m_s values slightly below and above the physical mass, allowing a straightforward interpolation.

(ii) Hadron and bare quark mass calculations. The pion and kaon masses are used to fix m_{ud} and m_s respectively, with M_Ω providing the overall scale. The calculation of hadron masses and the "mass independent scale setting" follows that of [2]. All three hadron masses receive finite volume corrections, falling off exponentially with $M_\pi L$ [33]. Even though these corrections are tiny, they are included. In addition to the hadron masses, the unrenormalized partially conserved axial current (PCAC) quark masses are determined.

(iii) Renormalization of the bare quark masses. In addition to the PCAC masses discussed above, the bare m_{ud} and m_s in the Lagrangian also provide a measure of the quark masses used in our simulations. Once suitably renormalized, these two definitions yield quark masses

which agree in the continuum limit.

While the PCAC masses renormalize multiplicatively, the bare Lagrangian masses require an additional additive renormalization. In the difference $d{\equiv}m_s^{\rm bare}-m_{ud}^{\rm bare}$, this additive renormalization is eliminated. Moreover, the multiplicative renormalization factors cancel in the ratio $r{\equiv}m_s^{\rm PCAC}/m_{ud}^{\rm PCAC}$. To obtain fully renormalized quantities, we must still multiply d by $1/Z_S$, the inverse of the scalar density renormalization factor. From the renormalized mass difference d/Z_S and the renormalization independent ratio r we obtain $m_{ud}^{\rm ren}=(d/Z_S)/(r{-}1)$ and $m_s^{\rm ren}=(rd/Z_S)/(r-1)$ in the unimproved case. Our final analysis is tree-level $\mathcal{O}(a)$ improved with slightly more complicated formulae (see [32]).

To compute Z_S nonperturbatively (RI scheme), we apply the Rome-Southampton method [34] with tree-level improvement, augmented with nonperturbative running.

Our procedure eliminates the possible difficulties of the Rome-Southampton method on coarser lattices. Since the RI scheme is defined in the $N_f{=}3$ chiral limit, we generate additional sets of $N_f{=}3$ configurations at our five lattice spacings and, for each β, at four or more values of m_q that allow an extrapolation to the massless limit. For each of these simulations, we fix gluon configurations to Landau gauge and compute numerically the normalized spin-color trace, $\Gamma_S(\beta,p,m_q)$, of the amputated forward vertex function of the scalar density between quark states. Here $p{=}\sqrt{p^2}$ is the momentum imparted to the ingoing and the outgoing quark. The RI renormalization constant $Z_S^{\rm RI}(\beta,\mu)$, at renormalization scale $\mu{=}p$, is defined to be $\lim_{m_q\to 0}\Gamma_{V_C}(\beta,\mu,m_q)/\Gamma_S(\beta,\mu,m_q)$. $\Gamma_{V_C}(\beta,\mu,m_q)$ is the vertex function of the conserved vector current, which we introduce to eliminate wavefunction renormalization factors. This defines a valid renormalization scheme as long as $p{\ll}\pi/a$. However, only if $p{\gg}\Lambda_{\rm QCD}$ can the results be converted perturbatively to other schemes (including instrinsically perturbative schemes such as $\overline{\rm MS}$) or be used in a perturbative context. On coarser lattices, it is difficult to simultaneously satisfy both constraints on p. To solve this difficulty we first determine the quark masses at $\mu=1.3$ and $2.1\,{\rm GeV}$, then apply the continuum extrapolated nonperturbative running to $\mu'=4\,{\rm GeV}$.

(iv) Combined analysis of mass and lattice spacing dependence. For the masses, two strategies, called “Taylor fit” and “chiral fit” [2] are applied. Clearly, the results of these fits are dominated by the results at the physical point. In the analysis, two different pion mass ranges are used, namely $M_\pi{<}340, 380\,{\rm MeV}$.

The strange and average up-down quark masses renormalized in the RI scheme at 4 GeV

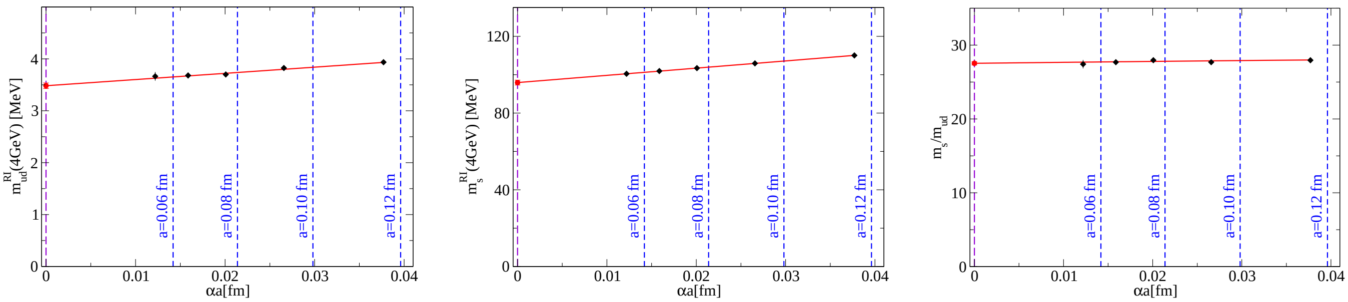

FIG. 2. Continuum extrapolation of the average up/down quark mass, of the strange quark mass and of the ratio of the two. The errors of the individual points, which are statistical only here, are smaller than the symbols in most of the cases. The only exceptions are the light quark mass and its ratio to the strange quark mass at the two finest lattice spacings. These exceptions underline the importance of using physical quark masses to reach a high accuracy.

are extrapolated to the continuum and interpolated to the physical mass point. In these fits, we include terms to correct linear (g^2a) or quadratic (a^2) effects. A combined mass and lattice spacing fit is carried out. We show the continuum extrapolation for m_{ud} and m_s in the RI scheme at 4 GeV, as well as their ratio, in Figure 2. In order to control the systematic uncertainties we carry out 288 such analyses. The figure depicts results from one analysis with one of the best fit qualities.

Our procedure yields the RI quark masses m_{ud} and m_s, with statistical and fully controlled systematic errors. These results do not rely on perturbation theory and from them it is straightforward to obtain the quark masses in other commonly used frameworks such as renormalization group invariant (RGI) and $\overline{\text{MS}}$ [35] ones.

The determination of the individual up and down quark masses at the physical point is in principle possible using exclusively lattice simulations. To that end one should include the electromagnetic U(1) gauge field into the lattice framework. Such a project goes beyond the scope of the present paper, which deals with QCD only. Nevertheless our precise m_s and m_{ud} values can be combined with model-independent results based on dispersive studies of $\eta{\to}3\pi$ decays to derive the individual up and down quark masses (c.f. Tab. I). In this approach the relationship between the input parameters and experiments is not as transparent as for the determination of m_s and m_{ud} (see condition 6 above).

Our results provide precise and reliable input for phenomenological calculations which require light quark mass values. They highlight the progress that has been achieved in the

	RI(4 GeV)	RGI	$\overline{\text{MS}}$(2 GeV)
m_s	96.4(1.1)(1.5)	127.3(1.5)(1.9)	95.5(1.1)(1.5)
m_{ud}	3.503(48)(49)	4.624(63)(64)	3.469(47)(48)
m_u	2.17(04)(10)	2.86(05)(13)	2.15(03)(10)
m_d	4.84(07)(12)	6.39(09)(15)	4.79(07)(12)

TABLE I. Renormalized quark masses in the RI scheme at 4 GeV, and after conversion to RGI and the $\overline{\text{MS}}$ scheme at 2 GeV. The RI values are fully nonperturbative, so the first column is our main result. The first two rows emerge directly from our lattice calculation. The last two include additional dispersive information. The precision of m_s and m_{ud} is somewhat below the 2% level, for m_u and m_d it is about 5% and 3%, respectively. The ratio m_s/m_{ud}=27.53(20)(08) is independent of the scheme and accurate to better than 1%.

last 30 years [36] by showing that phenomenologically relevant lattice QCD calculations can now be carried out bracketing the physical values of the light quark masses.

The details of this work can be found in [32].

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