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Lattice results: continuum extrapolation with physical quark masses

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In this talk some illustrative lattice results are presented. It is shown that lattice QCD reached a new era: today several continuum extrapolated results, all the way down to physical light quark masses are available. In particular, the hadron spectrum, F_K/F_π, the quark masses and a new way to set the scale are discussed. Some QCD thermodynamics results, such as the equation of state and fluctuations are briefly listed, too.

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1. Introduction

Lattice quantum chromodynamics (QCD) is the most systematic tool to understand the nonperturbative regime of strong interactions. It has a long history going back to the early 1970s. Lattice gauge theory was introduced in Ref. [1]. After almost forty years, lattice QCD entered a new era. Today, we have several full results for various physical questions. These answers represent findings with fully controlled systematic uncertainties at physical quark masses (directly simulating at them or extrapolating from pion masses, e.g. below 200 MeV to the physical pion mass value of 135 MeV) with controlled continuum extrapolation (at least three lattice spacings in the scaling region).

Since it is hard for non-lattice theorists to judge if and how these procedures were carried out there is a growing interest for summary papers, which carefully analyze these issues. As an illustration for such a summary Table 1 is shown. It is depicting the upper part of Table 2. of Ref. [2] with the most recent results on the light and strange quark masses. For clarity they used a color coding with red, orange or green, respectively. The colored symbols illustrate that the various sources of systematics were controlled in an unsatisfactory (red), reasonable (orange) or convincing (gree) way. Clearly, the goal is to have everywhere "green stars". However, as it can be seen, it is very difficult to simulataneously fulfill the above two conditions (thus, controlled chiral –more precisely physical mass– and continuum extrapolations). It is important to note, that today all of the listed works have one or several "green stars" (for some of them all of the ingredients are at that level, which we call *full result*). Similarly instructive is to recognize that the first "green star" in the full table [2] appears as late as 2007. The main motivation for the above discussion was to emphasize that lattice results may still have uncontrolled systematic uncertainties. Findings should not always be taken at face value but more care is needed when one interprets them. The good news is, however, that more and more full results will appear in the literature, that is why it is legitimate to speak about a new era.

In this proceedings, several full results from the Budapest–Marseille–Wuppertal Collaboration are summarized. We used both staggered and Wilson fermions. Staggered fermions were used mostly for thermodynamics and Wilson fermions mostly for T=0 physics. Since QCD thermodynamics is related to the restoration of the chiral symmetry, it is important to apply a fermion formulation with such a symmetry. Note, that staggered fermions are (in some sense) not as clean theoretically as Wilson fermions, that is the reason why we applied Wilson fermions in our T=0 studies, for which no symmetry restoration is needed.

This summary is structured as follows. In Sect. 2, T=0 physics is discussed. The advantage of smearing is illustrated. A fully controlled determination of the light hadron spectrum is presented. The light and strange quark masses are calculated. The usefulness of a new scale definition is illustrated. In Sect. 3, QCD at nonvanishing temperatures is studied. The equation of state is presented. Results at non-vanishing chemical potentials and on fluctuations are briefly discussed.

2. QCD at vanishing temperatures

This section of the report presents some selected T=0 lattice QCD results of the Budapest–Marseille–Wuppertal Collaboration. The vast majority of our T=0 results were obtained using smeared Wilson fermions. We utilized two types of very similar smearing. For the spectrum calculation, for F_K/F_π (and for the nucleon

Collaboration	publication status	chiral extrapolation	continuum extrapolation	finite volume	renormalization	running	m_{ud}	m_s
PACS-CS 10	P	★	■	■	★	*a*	2.78(27)	86.7(2.3)
MILC 10A	C	●	★	★	●	–	3.19(4)(5)(16)	–
HPQCD 10	A	●	★	★	★	–	3.39(6)*	92.2(1.3)
BMW 10AB	P	★	★	★	★	*b*	3.469(47)(48)	95.5(1.1)(1.5)
RBC/UKQCD	P	●	●	★	★	*c*	3.59(13)(14)(8)	96.2(1.6)(0.2)(2.1)
Blum et al. 10	P	●	■	●	★	–	3.44(12)(22)	97.6(2.9)(5.5)

Table 1: Results of various groups for the light and strange quark masses. The colored symbols indicate how well the individual systematic uncertainties were controlled (see text).

sigma term, which we do not discuss here) we applied six steps of stout smearing at three lattice spacings down to 0.065 fm and pion masses down to 190 MeV (we call this our 2008 data set). For the quark mass determination (and also [3] for B_K, which is not discussed here) two steps of HEX [4] smearing were applied. We call this our 2010 data set, which covers five lattice spacings down to 0.054 fm and pion masses down to 120 MeV. These pion masses enabled an interpolation to the physical mass point. In both data sets the strange quark mass was set to its approximate physical value. When discussing the spectrum, our general strategy to control all systematics is discussed in some detail. For the F_K/F_π determination our error analysis by using the hystogram method is illustrated. For all of the works listed here a similar strategy to control all systematics and hystogram analysis to determine the errors were carried out.

2.1 Light hadron spectrum

This part summarizes our light hadron spectrum analysis[5] (for a recent review on the topic see Ref.[6]).

We aimed at a full calculation controlling all the systematic uncertainties. To that end we set up five conditions (these conditions are accepted by a large fraction of the community as reliable; of course one can choose other conditions and can focus on other points of interest). These conditions are listed below and a few of them are briefly commented on in parenthesis concerning our analysis.

I. 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. For the light hadron spectrum, the effects of the heavier charm, bottom and top quarks are included in the coupling constant and light quark masses.

II. A complete determination of the masses of the light ground-state, flavor nonsinglet mesons and octet and decuplet baryons. Three of these are used to fix the masses of the isospin averaged light (m_{ud}) and strange (m_s) quark masses and the overall scale in physical units. (We set the overall scale by using one of the two most precise hadron masses of our analysis: in one case it was the Ξ in the other case it was the Ω baryon.)

III. Large volumes to guarantee small finite-size effects and at least one data point at a significantly larger volume to confirm the smallness of these effects. In large volumes, finite-size corrections to the spectrum are exponentially small [7, 8]. As a conservative rule of thumb $M_\pi L \gtrsim 4$, with M_π the pion mass and

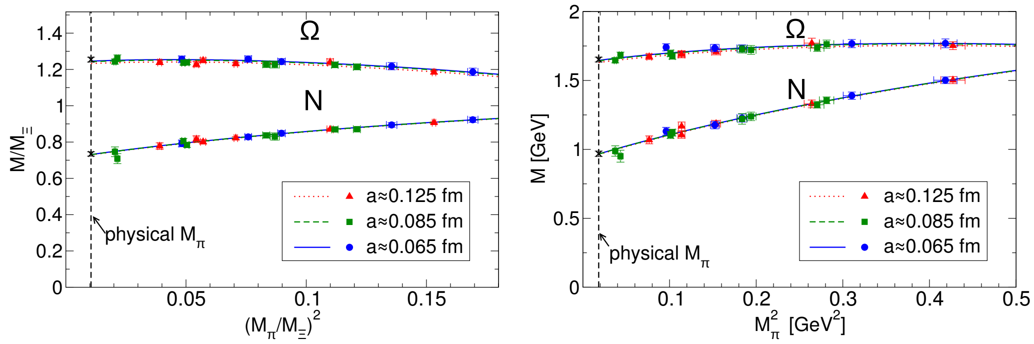

Figure 1: Pion mass dependence of the nucleon (N) and Ω for all three values of the lattice spacing. Left panel: masses normalized by M_Ξ, evaluated at the corresponding simulation points. Right panel: masses in physical units. The scale in this case is set by M_Ξ at the physical point. Triangles on dotted lines correspond to $a{\approx}0.125$ fm, squares on dashed lines to $a{\approx}0.085$ fm and circles on solid lines to $a{\approx}0.065$ fm. The points were obtained by interpolating the lattice results to the physical m_s (defined by setting $2M_K^2$-M_π^2 to its physical value). The curves are the corresponding fits. The crosses are the continuum extrapolated values in the physical pion mass limit. The lattice-spacing dependence of the results is barely significant statistically despite the factor of 3.7 separating the squares of the largest ($a{\approx}0.125$ fm) and smallest ($a{\approx}0.065$ fm) lattice spacings. The χ^2/degrees of freedom values of the fits in the left panel are 9.46/14 (Ω) and 7.10/14 (N), whereas those of the fits in the right panel are 10.6/14 (Ω) and 9.33/14 (N), respectively.

L the lattice size, guarantees that finite-volume errors in the spectrum are around or below the percent level. Resonances require special care. Their finite volume behavior is more involved. The literature provides a conceptually satisfactory framework for these effects [9, 10] which should be included in the analysis. (For one of our simulation points we used several volumes and determined the volume dependence, which was in good agreement with Ref.[11]. This was included as a negligible correction at all points. We also calculated the corrections necessary to reconstruct the resonance masses from the finite volume ground-state energy and included them.)

IV. Controlled interpolations and extrapolations of the results to physical m_{ud} and m_s (or eventually directly simulating at these mass values). Although interpolations to physical m_s, corresponding to $M_K{\simeq}495$ MeV, are straightforward, the extrapolations to the physical value of m_{ud}, corresponding to a pion mass of $M_\pi{\simeq}135$ MeV, are difficult. They need computationally intensive calculations with M_π reaching down to 200 MeV or less. (We used chiral perturbation theory and Taylor expansion to reach the physical value of the pion mass from our 190 MeV pion mass point.)

V. Controlled extrapolations to the continuum limit, requiring that the calculations be performed at no less than three values of the lattice spacing, in order to guarantee that the scaling region is reached. (Our three-flavor scaling study [12] showed that hadron masses deviate from their continuum values by less than approximately 1% for lattice spacings up to $a{\approx}0.125$ fm. This observation was confirmed by the present analysis.)

Our analysis includes all five ingredients listed above. The combined extrapolation to the physical mass point and to the continuum limit is shown in Fig. 1. As an illustration we show a comparison with other lattice results, too [13].

2.2 The ratio of F_K/F_π

We used the same 2008 data set (which was used to determine the light hadron spectrum) to determine F_K/F_π in the physical limit (extrapolated to physical quark masses and to the continuum limit). The details

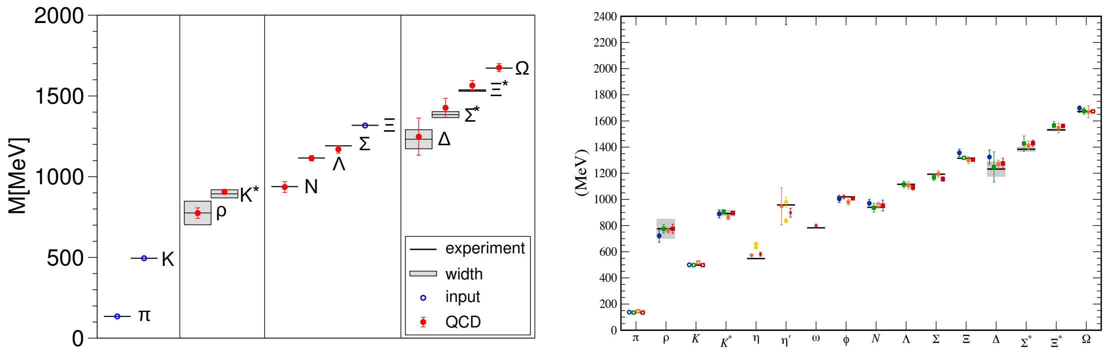

Figure 2: Left panel: the light hadron spectrum of QCD obtained by the Budapest-Marseille-Wuppertal Collaboration. Horizontal lines and bands are the experimental values with their decay widths. Our results are shown by solid circles. Vertical error bars represent our combined statistical and systematic error estimates. π, K and Ξ have no error bars, because they are used to set the light quark mass, the strange quark mass and the overall scale, respectively. Right panel: various results for the hadrons spectrum as shown in Ref. [13] (only light and strange quarks)

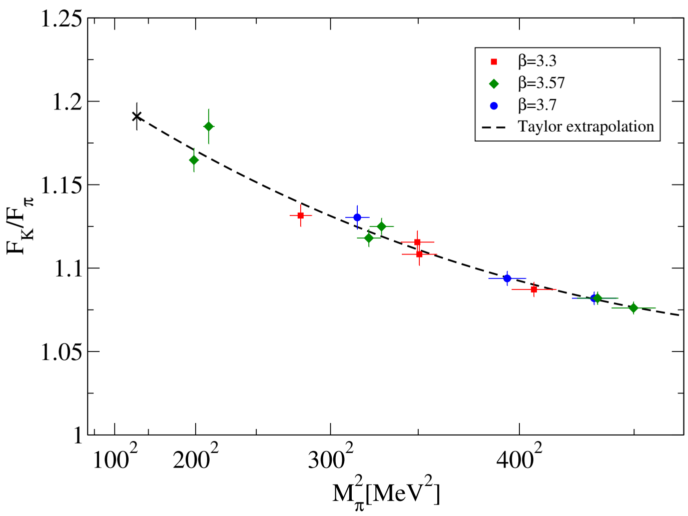

Figure 3: *Extrapolation of the lattice data for F_K/F_π to the physical point for a particular choice of two-point function fits ($t_{min}/a = 6,8,11$ for $\beta = 3.3, 3.57, 3.7$, respectively), mass cut (M_π<460 MeV) and using the Ξ to set the scale. The plot shows one (of the 21) fits used to estimate the uncertainty associated with the functional form used for the mass extrapolation. The data have been slightly adjusted to the physical strange quark mass, as well as corrected for tiny finite-volume effects.*

of the calculation can be found in Ref. [14]. We followed a proposal by Marciano [15] to derive $|V_{us}|$ from $|V_{ud}|$, using a lattice determination of the ratio F_K/F_π of leptonic decay constants.

The following discussion illustrates our generic strategy to estimate errors. Our results for F_K/F_π display a small dependence on lattice spacing. To estimate the systematic error associated with the continuum extrapolation we consider fits with and without $O(a^2)$ and $O(a)$ Symanzik factors. These choices, with seven choices for the fitting strategies to the physical mass point, 18 different fitting intervals for the individual correlators, two scale-setting procedures and two cuts for the pion mass range (350 and 460 MeV) provided us with $3\cdot 7\cdot 18\cdot 2\cdot 2 = 1512$ alternative analyses. The central value obtained from each procedure is weighted with the quality of the (correlated) fit to construct a distribution. The median and the 16th/84th

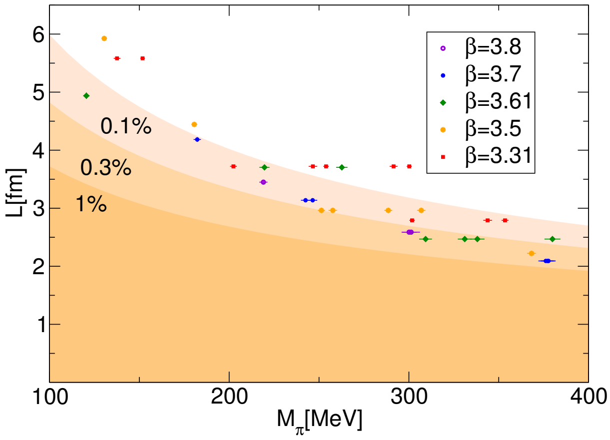

Figure 4: Summary of our simulation points. The pion masses and the spatial sizes of the lattices are shown for our five lattice spacings. The percentage labels indicate regions, in which the expected finite volume effect [11] on M_π is larger than 1%, 0.3% and 0.1%, respectively. This effect is smaller than about 0.5% for all of our runs and, as described, we corrected for it. Error bars are statistical.

percentiles yield the final central value and the systematic error associated with possible excited state contributions, scale setting, and the chiral and continuum extrapolations. To determine the statistical error, the whole procedure is bootstrapped (with 2000 samples) and the variance of the resulting medians is computed.

A "snapshot" fit using our data set (with a specific choice for the time intervals used in fitting the correlators, scale setting, and pion mass range) can be seen in Fig. 3. To avoid the complications of a multi-dimensional plot, the extrapolation is shown as a function of the pion mass only.

Following the procedure outlined above, our final result is

$$\left.\frac{F_K}{F_\pi}\right|_{phys} = 1.192(7)_{stat}(6)_{syst} \qquad \text{or} \qquad \left.\frac{F_\pi}{F_K}\right|_{phys} = 0.839(5)_{stat}(4)_{syst} \tag{2.1}$$

at the physical point. This can be transformed to $|V_{us}|/|V_{ud}| = 0.2315(19)$. Using the most precise information on the first CKM matrix element available today, $|V_{ud}| = 0.97425(22)$ [16], we obtain $|V_{us}| = 0.2256(18)$.

The same 2008 data set was used to determine the nucleon's sigma term [17]. Without going into details the final result reads $\sigma_{\pi N} = 39(4)^{+18}_{-7}$ (the first error is the statistical the second one is the systematic).

2.3 Light and strange quark masses.

In the two previous subsections two illustrative works were presented, which used our 2008 data set. The present (and also the next) subsection deals with the 2010 data set. This data set contains 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 for the quark masses (the topic of this subsection) between the results obtained on the finest lattice and those in the continuum limit was $\sim$3%, whereas between those of the coarsest lattice and the continuum limit was $\sim$10%. Our data set contains physical or smaller than physical quark masses for three of the lattice spacings. The data set is well illustrated on a plot showing the pion mass and the spatial extension (Fig. 4). The details of the quark mass determination can be found in Refs.[18, 19].

In the present analysis (determination of the light and strange quark masses) essentially the same conditions should be applied as for the case of the light hadron spectrum. In addition to the hadron masses, the unrenormalized partially conserved axial current (PCAC) quark masses are determined.

Since the quark masses depend on the renormalization scheme we need in addition a fully nonperturbative renormalization procedure. While the PCAC masses renormalize multiplicatively, the bare La-

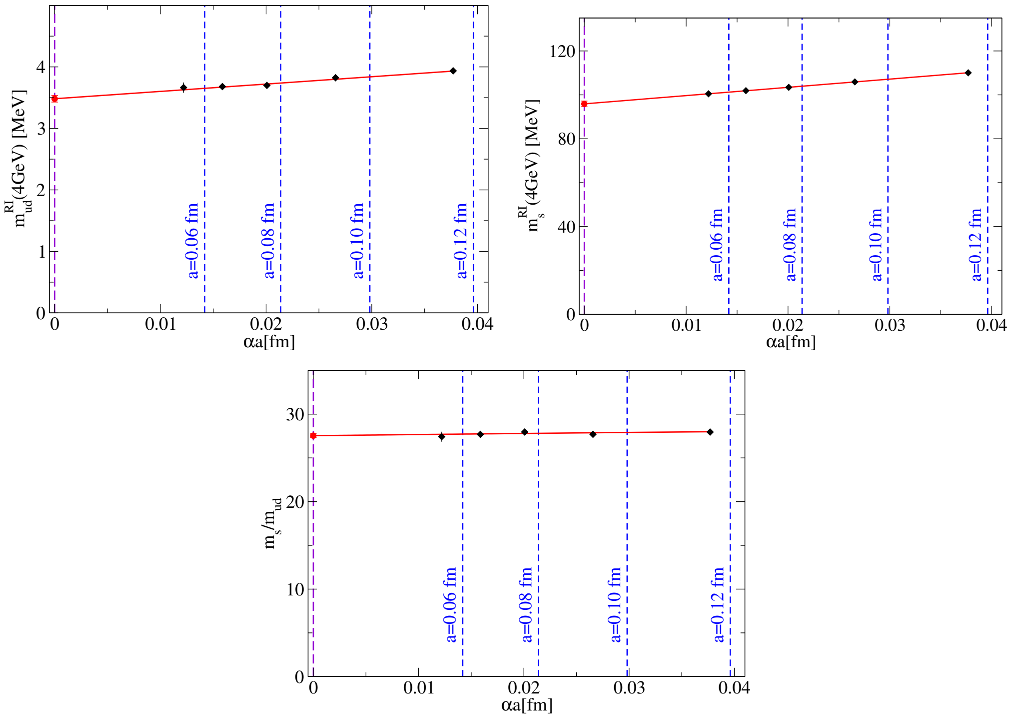

Figure 5: Continuum extrapolation of the average up/down quark mass, of the strange quark mass and of the ratio of the two. The errors of the individual points, which are statistical only here, are smaller than the symbols in most of the cases. The only exceptions are the light quark mass and its ratio 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.

grangian masses require an additional additive renormalization. In the difference $d \equiv m_s^{\text{bare}} - m_{ud}^{\text{bare}}$, this additive renormalization is eliminated. Moreover, the multiplicative renormalization factors cancel in the ratio $r \equiv m_s^{\text{PCAC}}/m_{ud}^{\text{PCAC}}$. 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 $m_{ud}^{\text{ren}} = (d/Z_S)/(r-1)$ and $m_s^{\text{ren}} = (rd/Z_S)/(r-1)$ in the unimproved case. Our final analysis is tree-level $\mathcal{O}(a)$ improved with slightly more complicated formulae (see Sect. 11.2 of Ref. [19]).

The strange and average up-down quark masses renormalized in the RI (regularization-independent) scheme (Rome-Southampton method, see Ref. [20]) at 4 GeV are extrapolated to the continuum and interpolated to the physical mass point. In these fits, we include terms to correct linear ($\alpha_s a$) or quadratic (a^2) cutoff 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 Fig. 5. In order to control the systematic uncertainties we carry out 288 such analyses [19]. The figure depicts results from one analysis with one of the best fit qualities.

Since all the systematic uncertainties have been controlled the result can be considered as a full result. This is illustrated by the fact that in Table 1 this result received overall "green stars".

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 may include the electromagnetic U(1) gauge field in the lattice framework, as was done recently e.g. in Ref. [21, 22]. We have not carried out such a calculation (yet). Nevertheless our precise m_s and m_{ud} values can be combined [19] with model-independent results based on dispersive studies of $\eta \to 3\pi$ decays to derive the individual up and down quark masses (see

	RI (4 GeV)	RGI	$\overline{MS}$ (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 2: Renormalized quark masses in the RI scheme at 4 GeV, and after conversion to RGI and the $\overline{MS}$ 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.

Table 2). 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} (for details see Ref.[19]).

2.4 Scale setting.

Our method [23] is based on the Wilson flow. The Wilson flow was considered in the context of trivializing maps by Luscher [24]. It was studied earlier by Narayanan and Neuberger [25] in a different context, too. Its important renormalization properties were clarified in [26, 27]. Its application to scale setting was suggested recently in [26]. The method can be summarized as follows. On each original configuration we integrate infinitesimal smearing steps up to a scale t, whose units are inverse mass-squared. The smearing is performed until a well-chosen dimensionless observable reaches a specified value. The universal "flow time," $t = t_0$, at which this happens can then be used to set the scale on the original lattices.

Integrating the infinitesimal smearing steps is equivalent to finding the solution to the flow equation [25, 26]: $\dot{V}_t = Z(V_t)V_t, \quad V_0 = U$ where V_t are the gauge links at flow time t and U are the original gauge links. (In [26, 27], where the Wilson action is used, $Z(V_t)$ is the derivative of the plaquette action and the corresponding flow is called the Wilson flow. For improved gauge actions, one can take $Z(V_t)$ to be the algebra-valued derivative of the gauge action.) To obtain the scale t_0, it is suggested in [26] to integrate the flow and to compute $t^2\langle E(t)\rangle$ as a function of t, t_0 being the flow time where $t^2\langle E(t)\rangle$ reaches 0.3. Here $\langle E(t)\rangle$ is the expectation value of the continuum-like action density $G^a_{\mu\nu}(t)G^a_{\mu\nu}(t)/4$. We proposed another quantity, namely w_0 being the flow time where $t\cdot(d/dt)t^2\langle E(t)\rangle$ reaches 0.3. The most important reasons for this choice can be summarized as follows. While $t^2\langle E(t)\rangle$ incorporates information about the gauge configurations from all scales larger than $\mathscr{O}(1/\sqrt{t})$ (thus including scales also around the cutoff), $W(t)$ mostly depends on scales around $\mathscr{O}(1/\sqrt{t})$. This is an advantage, because the behavior of the flow at small $t \sim a^2$ is subject to discretization effects.

In order to determine the scale we used our 2010 data set with two steps of HEX smearing (Wilson fermions) and compared it with the results obtained on our T=0 subset of the thermodynamics runs (see next section). In both cases w_0 is interpolated to the physical quark masses as well as extrapolated into the continuum. The Ω mass is used to convert these scales to physical units (with our smeared actions hadron mass ratios show very small cutoff effects [12, 5]). Representative continuum limits (see below) are displayed in Fig. 6, where the staggered and Wilson results are shown on the l.h.s. and r.h.s., respectively. The plot indicates that w_0 has cutoff effects similar to M_Ω, resulting in a very mild continuum scaling, and that the uncertainties on the extrapolated value are very small. Moreover, the staggered and Wilson results are in good agreement and the precisions reached with the two actions are on the same level. We quote the Wilson result, which does not rely on the "rooting" of the fermion determinant, as our final result: w_0=0.1755(18)(04) fm, where the first error is statistical and the second is systematic. Note that the overall uncertainty is 1%, most of which is statistical. Furthemore, the statistical error in the dimensionless quantity w_0M_Ω comes dominantly from aM_Ω. Thus, the error on w_0/a itself is subdominant, typically on the level of a few per mil or less. This fact makes w_0/a a particularly attractive candidate to set the relative scale between simulations for continuum extrapolations and for comparing calculations from different groups.

3. Results at non-vanishing temperatures and/or chemical potentials

At this conference the most important thermodynamics results were summarized by P. Petreczky [28]. Here only a few illustrative results are presented.

3.1 Status of the equation of state.

The QCD transition at non-vanishing temperatures and at zero chemical potential is an analytic cross-over [29]. The first step to obtain any trustworthy result in QCD thermodynamics is to determine the overall scale of this analytic QCD transition. Its value was disputed for some years, but it is a great succes of lattice QCD that the field has reached now a point at which the results from different groups completely agree [30, 31, 32, 33]. The next important step is the determination of the equation of state. There are various calculations with different fermion formulations. So far the most precise results have been obtained by staggered quarks. In these calculations the quark masses (light and strange) take their physical (or approximately physical) values. There is still a discrepancy for the equation of state in the literature. The Wuppertal-Budapest group obtained in 2005 [34] a value around 4 for the peak height of the trace anomaly (ε–3p), which was confirmed in 2010 [35] (at three characteristic temperatures the continuum result was given; it pinned down the result for the equation of state, which is also given as a simple parametrization). The hotQCD collaboration typically receives higher values for the peak height of the trace anomaly (for a recent summary see e.g. Ref. [36]). The left panel of Fig. 7 shows the comparison of the results of the two groups. Obviously, more work is needed to clarify the source of the difference.

Far less is known about the transition at non-vanishing chemical potentials. About a decade ago [37] a renewed interest resulted in many interesting results (for a recent review see e.g. [38] or [39]), though only very few with continuum extrapolations and physical quark masses. One of them is the curvature of the phase diagram [40], the other is the equation of state for small non-vanishing chemical potentials [41].

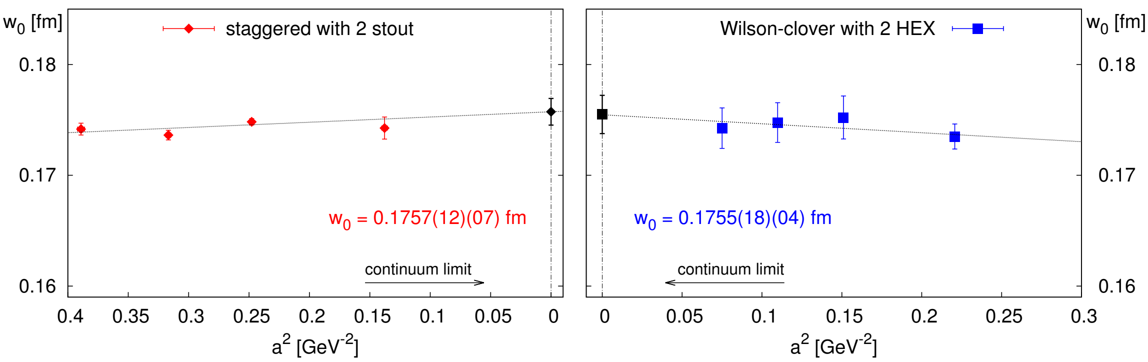

Figure 6: Representative continuum extrapolations of the w_0 scale, at the physical mass point. The values at different lattice spacings are obtaind by using the Wilson flow described below. The continuum limit values on the plots are results from our final, full analyses. The results obtained with the two very different actions (staggered fermions on the left and Wilson fermions on the right panel) are in good agreement and the overall uncertainties are very small.

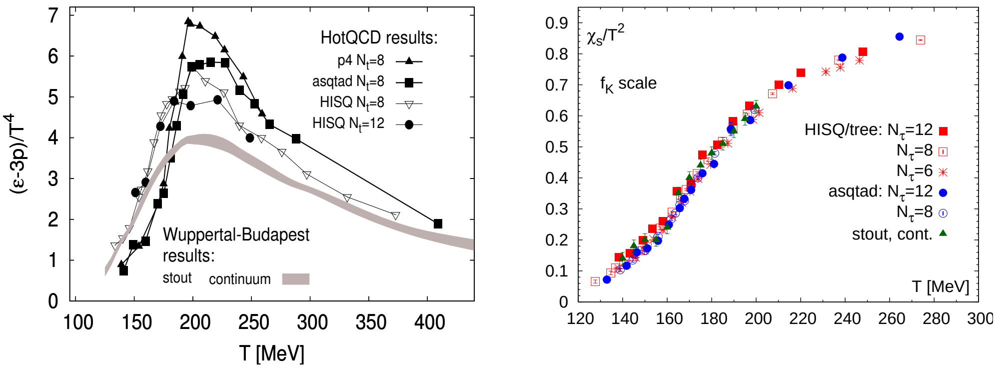

Figure 7: Comparison of the equation of states obtained by the Wuppertal-Budapest group (stout action) and the hotQCD Collaboration. There is still a sizable discrepancy (left panel). Comparison of the strange susceptibilities. In the continuum limit the two results agree (right panel).

3.2 Susceptibilities from lattice.

Fluctuations and correlations of conserved charges are important probes of various aspects of deconfinement. This is because fluctuation of conserved charges are sensitive to the underlying degrees of freedom which could be hadronic (in the low temperature phase) or partonic (in the high temperature phase). Fluctuations of conserved charges have been studied using different staggered actions (though some results with Wilson fermions are also available). The two most complete calculations have been carried out by the Wuppertal-Budapest group and by the hotQCD Collaboration [42, 43]. As an illustration the right panel of Fig. 7 shows the comparison of the results of the two groups for the strange quark number susceptibility. Fluctuations are small at low temperatures because strangness is carried by massive strange hadrons (in this case mostly by kaons). This part of the figure is well described by the Hadron Resonance Gas (HRG) model. Strangeness fluctuations sharply rise in the transition region, in which quarks get more and more free. The susceptibility approaches the value one for infinitely large temperatures. Note that the strange susceptibility is the quantity, which was determined with a high precision. Other quantities and particularly higher cumulants are under investigation by many lattice groups and high quality results are expected in the near future.

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