

High-precision scale setting in lattice QCD

Budapest-Marseille-Wuppertal collaboration

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ABSTRACT: Scale setting is of central importance in lattice QCD. It is required to predict dimensional quantities in physical units. Moreover, it determines the relative lattice spacings of computations performed at different values of the bare coupling, and this is needed for extrapolating results into the continuum. Thus, we calculate a new quantity, w_0 , for setting the scale in lattice QCD, which is based on the Wilson flow like the scale t_0 (M. Luscher, *JHEP* **08** (2010) 071). It is cheap and straightforward to implement and compute. In particular, it does not involve the delicate fitting of correlation functions at asymptotic times. It typically can be determined on the few per-mil level. We compute its continuum extrapolated value in 2 + 1-flavor QCD for physical and non-physical pion and kaon masses, to allow for mass-independent scale setting even away from the physical mass point. We demonstrate its robustness by computing it with two very different actions (one of them with staggered, the other with Wilson fermions) and by showing that the results agree for physical quark masses in the continuum limit.

KEYWORDS: Lattice QCD, Lattice Gauge Field Theories

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1 Introduction

Quantum chromodynamics (QCD) is a theory with few parameters: the quark masses and an overall scale. To determine the latter, one has to compute a dimensionful quantity or an observable at a known energy, and adjust the overall scale of the theory to reproduce the corresponding experimental measurement. In lattice calculations this is equivalent to fixing the lattice spacing a . The lattice spacing is determined by calculating a dimensionful quantity Q — for definiteness, Q is chosen to be of mass dimension one here — such as the mass of the Omega baryon, M_Ω , or the pion decay constant, F_π , and by relating its lattice value to its experimental value through $a = (aQ)^{\text{latt}}/Q^{\text{expt}}$. In principle any dimensionful quantity can be used. However, it is clear that the quality of any dimensionful prediction from the lattice can only be as good as the quality of the determination of the overall scale. This statement is particularly relevant now that lattice QCD results with errors below 2% are beginning to be reported.

Besides the overall scale in physical units, it is also important to accurately determine the relative lattice spacings of simulations performed at different values of the bare coupling in order to carry out a continuum extrapolation. Independent calculations can be compared too, if dimensionful quantities are expressed in units of a well measured quantity. For this purpose it may be useful to consider an observable which is not directly measured in experiment, but which is particularly simple to compute with high accuracy. Moreover, if this observable is computed accurately in physical units once, its value can be used in all subsequent lattice calculations to fix their overall scales.

One popular observable of this type is the Sommer scale, r_0 , introduced nearly two decades ago [1]. More recently, MILC has found it more convenient to consider the related scale r_1 [2]. One of the advantages of these scales is that they are based on the calculation of the static potential from gauge fields: they do not require the costly computation of quark propagators, as do observables such as M_Ω or F_π . However, the determination of

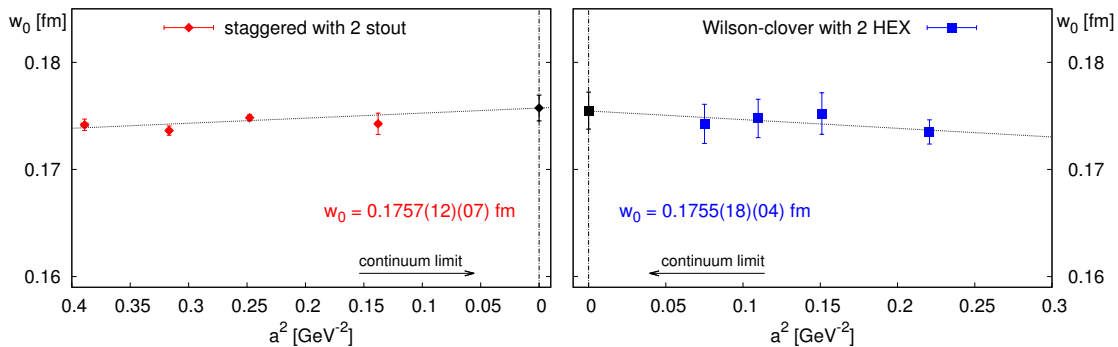


Figure 1. Representative continuum extrapolations of the w_0 scale, at the physical mass point. The values at different lattice spacings are obtained by using the Wilson flow described below. The continuum limit values on the plots are results from our final, full analyses. The results obtained with 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.

the potential requires a delicate study of the asymptotic time behavior of Wilson loops and the calculation of r_0 or r_1 from the potential is a much more complicated analysis (see [3] for a recent example) than, say, fitting the mass of a particle, such as the pion, from a measured correlator. The introduction of HYP smearing [4] on the gauge links has reduced the problem of the poor signal-to-noise ratio of Wilson loops, but the calculation of r_0 or r_1 remains non-trivial. These subtleties might be at least partially responsible for the tension within present determinations of the Sommer scale between [5] and [6, 7], and for a similar tension between recent and present determinations [7, 8]. While these differences are only on the two standard deviation level they have an important impact on the search for new physics in the leptonic decays of the D_s meson, as discussed in [9].

In this paper we propose an alternative to the r_0 scale: the w_0 scale. The method is based on the Wilson flow. The Wilson flow was considered in the context of trivializing maps by Luscher [10]. It was studied earlier by Narayanan and Neuberger [11] in a different context, too. Its important renormalization properties were clarified in [12, 13]. Its application to scale setting, which we build upon, was suggested recently in [12].

The w_0 scale keeps the advantages of the Sommer scale (i.e. no expensive fermion inversion is needed). However, it is easier to determine with high precision, since it requires neither a fitting of the asymptotic time behavior of correlation functions nor fighting signal-to-noise issues.

Before discussing the method in detail (see section 2), we present our results for the w_0 scale in physical units. These values can henceforth be used to determine the lattice spacing in physical units in $N_f = 2+1$ lattice QCD calculations. (The dependence of w_0 on N_f should be studied before it is used to set the scale in simulations with $N_f \neq 2+1$.) We performed two independent calculations of w_0 , both based on simulations with pion masses all the way down to its physical value and below. The first uses our 2HEX smeared Wilson fermion ensembles [14–16] and the second, 2-stout smeared staggered simulations [17–23]. 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 [24, 25]). Representative continuum limits (see below) are displayed in figure 1, 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:

$$w_0 = 0.1755(18)(04) \text{ fm}, \tag{1.1}$$

where the first error is statistical and the second is systematic. Note that the overall uncertainty is 1%, most of which is statistical. Furthermore, the statistical error in the dimensionless quantity $w_0 M_\Omega$ comes dominantly from $a M_\Omega$. 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. Another interesting application is the determination of the ratio of the lattice spacings for anisotropic actions [26]. As a side product we also compute a related quantity $(t_0)^{1/2}$ suggested in [12] (though on the same set of configurations its *relative* systematic error is four times larger than that of w_0).

This paper is organized as follows. After this introductory section we discuss the scale setting method based on the Wilson (and Symanzik) flow in section 2. The next two sections (3), (4) deal with our results obtained with Wilson and with staggered fermions, respectively. Section 5 discusses two possible problems, namely finite volume effects and autocorrelations for the flow. Section 6 presents the final results and concludes. In order to make the practical application of the scale setting procedure presented here easier, the method is implemented in the CHROMA software system [27]. In addition, along with this paper we submit two codes to the arXiv, both written in C, as ancillary files. The first (`wilson_flow.c`) determines the Wilson (and Symanzik) flow. It was written emphasizing readability over speed. It works both for isotropic and anisotropic [26] lattice actions. The second one (`w0_scale.c`) uses the output of `wilson_flow.c` or that of CHROMA to determine the scale w_0/a and its statistical uncertainty.

2 The scales $(t_0)^{1/2}$ and w_0

The scale setting method can be summarized as follows. Following the strategy of ref. [12] we calculate the Wilson flow, that is we integrate infinitesimal gauge-field 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 [11, 12]:

$$\dot{V}_t = Z(V_t)V_t, \quad V_0 = U \tag{2.1}$$

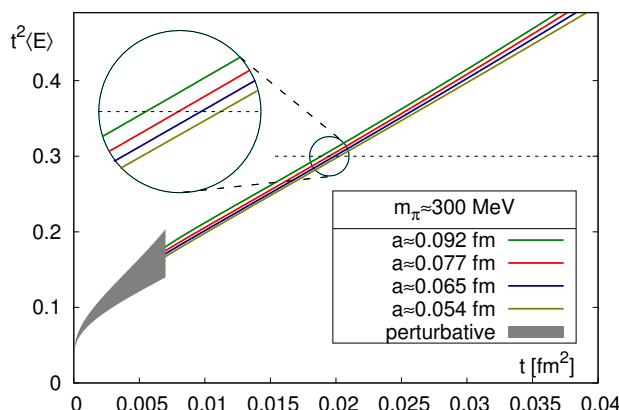


Figure 2. Analogously to the Wilson flow in figure 2 of [12] here we show the Symanzik flow, which can be used to define the w_0 scale and the $t_0^{1/2}$ scale proposed by [12]. These flows are obtained using our $N_f=2+1$ Wilson fermion simulations. For our four lattice spacings we have runs close to $M_\pi \approx 300$ MeV (the individual pion masses are somewhat different). The perturbative expectation is shown by the gray band. Its width indicates the uncertainty in Λ_{QCD} using two representative values from the literature (c.f. refs. [28, 29]).

where V_t are the gauge links at flow time t and U are the original gauge links. In [12, 13], 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. As it can be seen from eq. (2.1) an infinitesimal change of the link variable is obtained by the product of the link variable itself and the sum of the staples around it. Thus, for the present case the flow is generated by infinitesimal stout-smearing steps. As a consequence the action decreases and the gauge field is getting smoother. 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 [12] 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 $G_{\mu\nu}^a(t)G_{\mu\nu}^a(t)/4$, where $G_{\mu\nu}^a(t)$ is a lattice version of the chromoelectric field-strength tensor at flow time t . Here we use the usual clover-leaf definition for this tensor. Note that $t^2 \langle E \rangle$ turned out to be approximately proportional to t for large flow times, a similar observation was made for the pure gauge theory in ref. [12].

Here we propose to use another, related observable, namely

$$W(t) \equiv t \frac{d}{dt} \{ t^2 \langle E(t) \rangle \} \tag{2.2}$$

and define the w_0 scale, via the condition

$$W(t)|_{t=w_0^2} = 0.3 . \tag{2.3}$$

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

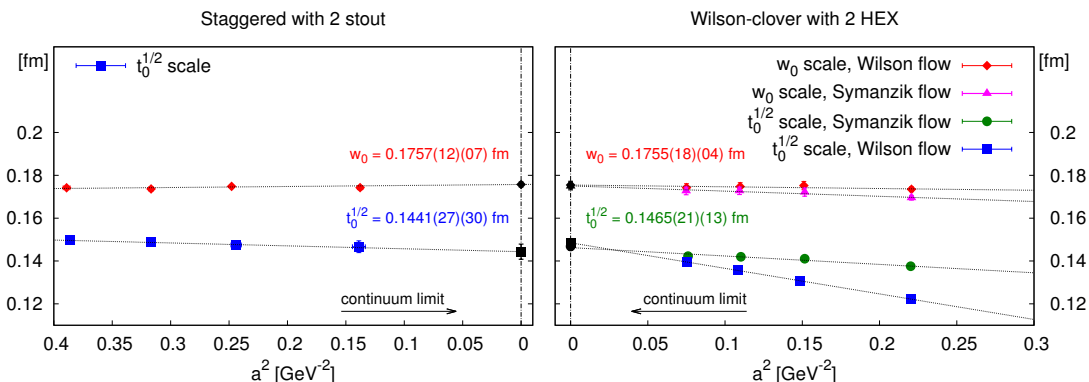


Figure 3. Representative continuum extrapolations of two different scale observables ($t_0^{1/2}$ and w_0) at physical quark masses, using our $N_f = 2 + 1$ staggered (left panel) and Wilson (right panel) simulation data. An illustration of the different cutoff effects is also shown. We determined $t_0^{1/2}$ and w_0 with Wilson fermions using two different flow equations (Wilson and Symanzik flow). The results based on the different flow equations show different discretization effects. For the two very different actions the final results are in good agreement and the overall uncertainties on the continuum values are very small.

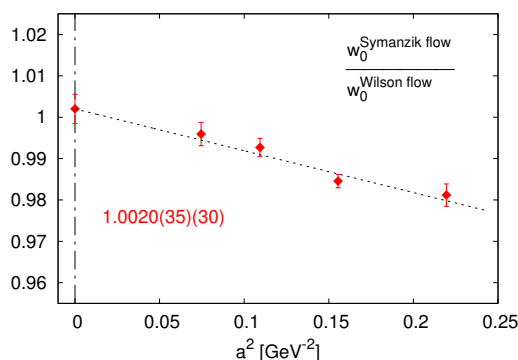


Figure 4. Ratio of the w_0 scales obtained by Symanzik and Wilson flows for physical pion and kaon masses.

than $\mathcal{O}(1/\sqrt{t})$ (thus including scales also around the cutoff), $W(t)$ mostly depends on scales around $\mathcal{O}(1/\sqrt{t})$. This is an advantage, because the behavior of the flow at small $t \sim a^2$ is subject to discretization effects. Let us illustrate these cutoff effects by one example. The flow $t^2\langle E(t) \rangle$ starts vertically at the origin in the continuum, while it must start horizontally for any lattice spacing and for any lattice action. The value of $t^2\langle E(t) \rangle$ at t is influenced by this cutoff effect appearing at small t , whereas the derivative $W(t)$ is less affected. In the original approach, the flow times t corresponding to different values of $t^2\langle E(t) \rangle$ yield different relative scales. Contrary to that, $W(t)$ yields very similar scales when different values are considered on the r.h.s. of (2.2). Furthermore, the perturbative calculation of [12] provides strong evidence that t_0 , and also w_0 , does not require renormalization.

Of course one is free to modify the lattice observable used or the flow equation (2.1) by terms which vanish in the continuum limit. For instance, as section 3 of [12] discusses,

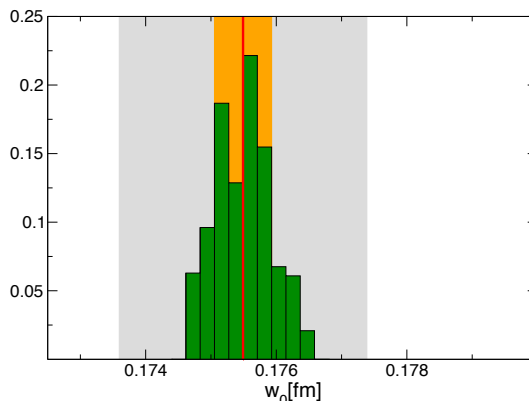


Figure 5. Final histogram for the different analyses used to compute w_0 with our Wilson fermion simulations. Each entry is weighted by its corresponding fit quality. The orange (thinner) band denotes the systematic and the gray (thicker) one the combined (systematic and statistical) uncertainties. The vertical line depicts the central value. Due to the small width of the distribution (note the scale), our final result (1.1) is very precise.

$\langle E(t) \rangle$ can be obtained directly from the sum of the plaquettes or from the more symmetric clover definition of $G_{\mu\nu}^a(t)$. Both definitions are acceptable and lead to results which must converge to the same continuum limit. One can look at the pure SU(3) gauge theory with no quarks and study the flow in units of r_0 . The symmetric definition turns out to be advantageous [12], since it results in negligible cutoff effects, whereas the non-symmetric definition leads to approximately 5% cutoff effects at a lattice spacing of 0.1 fm [12]. The choice of $Z(V_t)$ in (2.1) is also only fixed up to discretization corrections. The natural choice is to consider the algebra-valued derivative of the gauge action used in the simulation (c.f. section 6 of [10]). In our case this is a tree-level Symanzik improved action [30] and we call the corresponding flow, the Symanzik flow (c.f. figure 2). However, the use of the Wilson flow is also correct and should give the same continuum limit. This is illustrated in figure 3, with 2HEX Wilson fermions. As can be seen, $t_0^{1/2}$ obtained by the Wilson flow has larger cutoff effects than the one coming from the Symanzik flow. For w_0 , both choices are good and cutoff effects are around or less than two percent, in the range of lattice spacings considered. This is confirmed by looking at the ratio of the w_0 scales obtained from the Symanzik and the Wilson flows as a function of lattice spacing. Figure 4 shows that the ratio approaches 1 in the continuum limit, as it should. Here the pion and kaon masses are tuned to their physical values (this tuning leads to systematic uncertainties included on the points and discussed below). For our staggered action both $t_0^{1/2}$ and w_0 can be obtained with small cutoff effects using the Wilson flow. Note that in our case it is consistent to use one action for generating the fields and another one in the gauge flow. The two actions differ only in higher order in the lattice spacing, thus the derivative of the action with respect to the link variable will have the same order cutoff effect. Since in our setup the fermionic sector has already a^2 cutoff effects — at least — using the Wilson flow instead of the Symanzik flow does not deteriorate the continuum extrapolation. Obviously, one should use the same definition for different lattice spacings, if a continuum extrapolation is carried out.

In fact the w_0 scale determined with the Wilson flow has tiny cutoff effects for both our Wilson and staggered actions. Since integrating the Wilson flow is several times faster than working with the Symanzik flow, the former provides a quick and straightforward determination of the lattice spacing through the w_0 scale.

On a practical level, the flow equation (2.1) can be efficiently integrated by using the explicit fourth-order Runge-Kutta scheme proposed in [12]. The links at flow time $t + \epsilon$ are obtained from those at flow time t via

$$\begin{aligned}
 X_0 &= V_t, \\
 X_1 &= \exp\left(\frac{1}{4}Z_0\right) X_0, \\
 X_2 &= \exp\left(\frac{8}{9}Z_1 - \frac{17}{36}Z_0\right) X_1, \\
 V_{t+\epsilon} &= \exp\left(\frac{3}{4}Z_2 - \frac{8}{9}Z_1 + \frac{17}{36}Z_0\right) X_2,
 \end{aligned}
 \tag{2.4}$$

where $Z_i \equiv \epsilon Z(X_i)$. It turns out that the step size ϵ can be chosen rather coarse, since the total integration error associated with the finite step size scales like ϵ^3 [12]. Indeed we find that a value of $\epsilon = 0.01$ yields finite-step-size errors far below the per-mil level, which is negligible for our purposes. These findings are in agreement with those of [12].

3 $N_f = 2 + 1$ Wilson fermion computation

We compute the w_0 scale (and also the $t_0^{1/2}$ scale) using our 2HEX smeared [31] Wilson fermion ensembles [14–16], dropping the coarsest lattice with $\beta = 3.31$, as it appears to be less suited for studying various options for flows and/or scale setting procedures. Note that we are still left with four lattice spacings, which provide a safe continuum extrapolation, and pion masses down to, or even below, the physical value.

As discussed above, the Symanzik or the Wilson flows are equally valid for determining scale observables. Our continuum results for these observables agree within systematic errors. In order to reduce the uncertainties coming from the continuum extrapolation, one should favor the flow which has small cutoff effects. As we illustrated in figure 3 the continuum extrapolation of the w_0 scale with the Symanzik and the Wilson flows are almost equally good (the Wilson flow is slightly better). For the $t_0^{1/2}$ scale the Symanzik flow gives smaller cutoff effects than the Wilson flow, resulting in a factor of two smaller systematic error. Thus, for our results (c.f. figure 3) we used the flows with the smaller cutoff effects. Even with this favourable choice the *relative* systematic error of the $t_0^{1/2}$ scale is still about four times larger than that of the w_0 scale. This huge difference in accuracy justifies our preference for the w_0 scale (for the w_0 scale Symanzik or Wilson flows are similarly good). Moreover, since integrating the Wilson flow is several times faster than integrating the Symanzik flow, the best way to set the scale is to use w_0 determined from the Wilson flow.

As discussed above, we use the Ω baryon mass to express w_0 in physical units. Thus, the scale is extracted from aM_Ω at the point where the ratios $(M_\pi/M_\Omega, M_K/M_\Omega)$ acquire their physical values, as described in [14]. We then compute $w_0(M_\pi, M_K, a)$ in physical

Source	Relative error [%]
Physical point interpolation	15
M_π -cut	40
Continuum limit	55
Spectrum	55
Scale	45

Table 1. Contributions to the systematic uncertainty on w_0 , as fractions of the total systematic error in % (rounded to the closest 5%). The various uncertainties are explained in the main text and they are listed in the same order here. Note that the fractions must be added in quadrature and do not sum up exactly to 100% due to correlations and rounding.

units for each ensemble and perform a combined quark-mass interpolation and continuum extrapolation to obtain the physical value of w_0 .

Four different fit functions are used to interpolate to the physical mass point in the M_π - M_K plane. They have the form $w_0 = a_0 + a_1 M_\pi^2 + a_2 M_K^2 + d(a) + \text{hoc.}$, where *hoc.* stands for higher order contributions in M_π^2 and/or M_K^2 . Because our fermion action is tree-level improved, the discretization corrections, $d(a)$, are chosen to be either proportional to $\alpha_s a$ or a^2 (since the continuum extrapolation of w_0/M_Ω is practically constant, essentially no difference is observed between these two choices).

The various strategies that we apply for the mass extractions, to interpolate to the physical point and to extrapolate to the continuum limit are all combined to estimate the systematic uncertainties. To that end we use 64 different analyses, i.e. the 4 different fit forms in the M_π - M_K plane, 2 pion mass cuts for these fits ($M_\pi < 300$ MeV, 350 MeV), 2 different scaling assumptions in the lattice spacings, 2 fit ranges for extracting M_K , M_π and M_Ω as well as 2 methods for setting the scale (corresponding to different pion mass cuts in the M_Ω -fits, i.e. $M_\pi < 380$ MeV, 480 MeV). Each of these analyses can be fully justified and can be considered “the” final analysis. Thus, according to our standard procedure [14, 16, 25, 32], we construct a histogram out of the values obtained for w_0 , where each one is weighted by the corresponding fit quality. We compute the median and the central 68% confidence interval of the resulting distribution and take these values to be our central value and systematic error, respectively (c.f. figure 5). A detailed error budget is given in table 1. The same set of analyses has been repeated for the observable based on the Symanzik flow. We found an agreement within error (see figure 3).

The statistical error is computed by repeating the analysis on 2000 bootstrap samples. Note that the statistical error is much larger than the systematic. The statistical error of w_0/a is much smaller than that of aM_Ω . Therefore, the error of our w_0 in physical units is dominated by the statistical uncertainties in aM_Ω . In that way, we obtain the result with its systematic and statistical errors given in eq. (1.1).

4 $N_f = 2 + 1$ staggered fermion computation

An interesting test is a comparison of continuum results obtained with Wilson and staggered fermions. Therefore, we perform a fully independent determination of w_0 . We consider the

β , scale	am_s	m_s/m_u
3.7500	0.050254	28,14,10
$a^{-1} = 1.605(6)(3)$ GeV	0.048	27.9,20,10
	0.040	10
3.7920	0.05	20
$a^{-1} = 1.778(7)(1)$ GeV	0.045	28,20,14,10
	0.040	20,10
3.8500	0.0395	27.3,20,14,10
$a^{-1} = 2.024(18)(7)$ GeV	0.0388	20,14,10
	0.037	10
3.9900	0.0283	28.15,10,6
$a^{-1} = 2.684(58)(7)$ GeV	0.0277	14,10,6

Table 2. Staggered ensembles used in this analysis.

2-step stout-smearred staggered fermion action [33] used in our thermodynamics studies [17–21, 34]. The parameters of the ensembles used here are summarized in table 2. Note that the pion masses either straddle the physical value (obtained from M_π/M_Ω) or even touch it within errors. We express all quantities as functions of the bare masses for fixed gauge coupling. The w_0 scale in lattice units, $w_0/a(am_{ud}, am_s)$, is then computed for each simulation point as described before. These results are then interpolated to the physical point. This interpolation is done for every lattice spacing separately. Again, we use four functional forms as in the Wilson case. Since there is no additive mass renormalization for staggered fermions and the bare quark masses are known exactly, in the interpolating fits we use these masses. Thus, instead of M_π^2 we use $2m_{ud}$ and instead of M_K^2 we use $m_{ud} + m_s$ in the fit functions. For both the kaon and pion mass, we use three polynomial fit formulae to describe their quark mass dependence. Finally, we perform a linear continuum extrapolation in a^2 . In order to estimate the cutoff effects we use the four or the three finest lattice spacings. We end up with 72 different continuum values for w_0 , where each one can be weighted by the combined goodness of fit. Note that we have a much larger statistics for our staggered action than for the Wilson one.

On a subset of the ensembles used here we have already carried out a scaling study for r_0 in ref. [19]. We found that for the same action and lattice spacing range one observes about 10% cutoff effect for r_0 (see the right panel of figure 4 in ref. [19], where the scale was set by f_K). We also gave a scaling plot for M_Ω in the same paper.

5 Finite volume effects and autocorrelations

At fixed physical volume, finite-volume effects on the Wilson or Symanzik flow increase as the flow time increases. It is, therefore, important to check that these effects remain small for our choice of w_0 scale. Figure 6 displays the volume dependence of w_0/a on the second finest staggered lattice at physical quark masses. (For this test we used a couple of thousand trajectories for each volume.) It shows that finite-volume effects only become relevant for

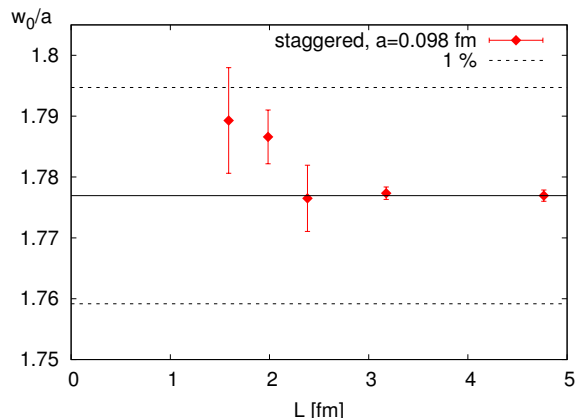


Figure 6. Finite-volume effects in the w_0 scale. Here we plot the measured values of w_0/a as a function of L , obtained with fixed bare quark masses corresponding to the physical point. Notice that it is perfectly feasible to determine w_0/a to per-mil precision on the 164 configurations we have on our $48^3 \times 64$ lattice. Even for boxes of size slightly below 2 fm, deviations from the large-volume value never exceed 1%.

box sizes $\lesssim 2$ fm. For lattices larger than that, finite volume effects are essentially absent. Note that for a lattice of 2 fm one has $M_\pi L = 1.35$, which is far smaller than the spatial size suggested by the rule of thumb $M_\pi L \gtrsim 4$. These tiny finite volume effects and the smallness of the error on w_0/a make the w_0 scale a very attractive intermediate quantity to determine the lattice spacing.

Since the Wilson/Symanzik flow incorporates more and more information from the whole lattice as t increases, it is important to study autocorrelations. Thus, we compute the integrated autocorrelation time of the flow as a function of t , using the standard methodology described in [35]. We do so by looking at several long (5000 trajectories) parallel HMC streams on our finest staggered lattices or simply analyzing a long HMC stream on one of our finest Wilson ensembles [14]. We find that for lattice spacings down to about $a = 0.54$ fm, the integrated autocorrelation time of $E(t = w_0^2)$ is around or below 50 unit-length trajectories. These autocorrelations are taken into account by appropriate binning.

6 Results and conclusions

We presented a new quantity for setting the scale in lattice QCD calculations. Precise determinations of this new w_0 scale were obtained using Wilson and staggered fermion simulations with lattice spacings down to 0.054 fm and average up and down quark masses all the way down to, and even below, its physical value. Therefore, we showed that the w_0 scale can be used to reliably determine the lattice spacing in physical units in upcoming lattice calculations. Moreover, the good agreement between the Wilson and staggered determinations illustrates the robustness of this scale-setting method (c.f. figure 1).

In eq. (2.2) we define the w_0 scale as the square root of the “time” at which the logarithmic derivative of $t^2 \langle E(t) \rangle$ reaches 0.3. A larger value, say 0.5, increases the cost of integrating the flow, as well as the size of statistical and finite-volume errors. A smaller

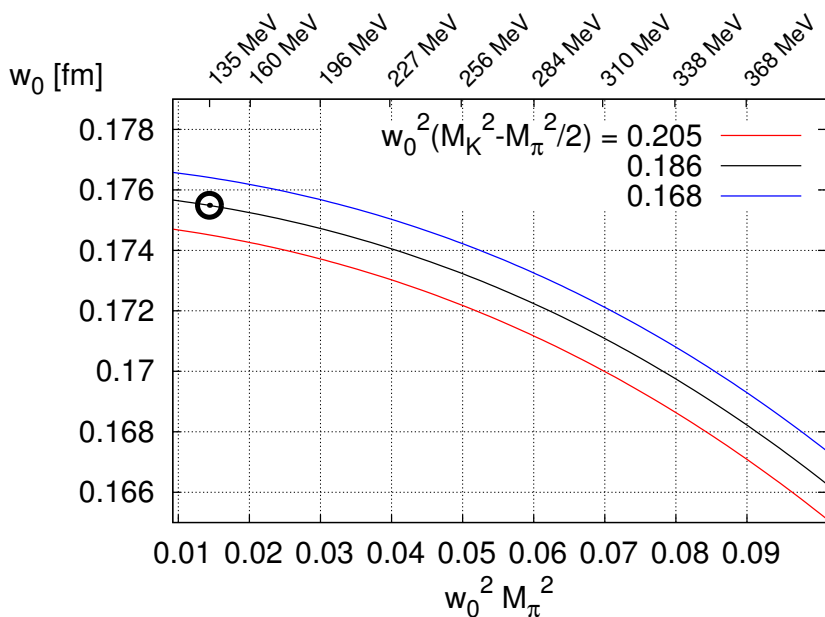


Figure 7. The value of the w_0 scale at various pion and kaon masses in the continuum limit. The results are based on our Wilson simulations. The black dot represents the physical point. To use the figures one should compute aM_π , aM_K and w_0/a . Then one reads off the value of w_0 in physical units corresponding to the combinations $w_0^2 M_\pi^2$ and $w_0^2(M_K^2 - M_\pi^2/2)$. The black curve in the middle corresponds to the physical $M_K^2 - M_\pi^2/2$ (used to fix m_s), whereas the lines below/above correspond to a 10% smaller/larger value of this quantity. As it can be seen the change in w_0 is small. Changing the pion mass from its physical value to a three times larger value (thus, almost an order of magnitude larger quark mass) results in about 5% change in w_0 . Changing the strange quark mass by 10% means changing w_0 on the 0.5% level. The mass independent scale setting prescription is used here.

value would probe short-distance physics which is more strongly affected by discretization errors. For values below 0.1, this becomes a serious concern for coarser lattices. The value 0.3 is chosen to be safely away from these two extremes and is optimal for modern day simulations, performed with lattice spacings in the range $0.05 \text{ fm} \lesssim a \lesssim 0.1 \text{ fm}$ and lattice sizes larger than 2 fm.

The continuum extrapolated value of w_0 for the physical point is given in eq. (1.1):

$$w_0 = 0.1755(18)(04) \text{ fm.}$$

For non-physical pion and/or kaon masses the pion and kaon mass dependence of w_0 is displayed in figure 7. This figure allows to determine the lattice spacing and its uncertainty as follows. One measures $M_\pi a$, $M_K a$ and w_0/a . Using these three quantities one then determines the dimensionless combinations $x = w_0^2 M_\pi^2$ and $y = w_0^2(M_K^2 - M_\pi^2/2)$. These two quantities define a point in figure 7. Reading off the value of w_0 in physical units and combining it with the computed value of w_0/a gives the lattice spacing in fm. For pion and kaon masses covered by this figure the uncertainty of the w_0 scale is essentially mass independent and its value is 1% (fully dominated by the statistical error of M_Ω). The same

result for w_0 and the lattice spacing can be obtained by using the following formula:

$$w_0 = 0.18515 - 0.5885x^2 - 0.0497y - 0.11xy - 1.476x^3 \pm 18 \cdot 10^{-3}(\text{stat}) \pm 4 \cdot 10^{-3}(\text{sys}) \quad (6.1)$$

which is valid for $0.01 \lesssim x \lesssim 0.1$ and $0.165 \lesssim y \lesssim 0.205$.

In this paper we have shown that the w_0 scale has several advantages over other scale setting procedures (most of which are also shared by t_0 , though the latter is more sensitive to cut-off effects). The most important are:

- w_0 is cheap and easy to implement and compute (note that our reference implementations are publicly available); in particular:
 - w_0 does not require the computation of quark propagators;
 - w_0 does not involve the delicate fitting of correlation functions at asymptotic times.
- the determination of w_0 is not only cheap but it can be done precisely and reliably; typically one obtains results with an accuracy on the few per mil level;
- the value of w_0 in physical units is known for physical and non-physical quark masses (for mass independent scale setting);
- our results suggest that w_0 depends weakly on quark masses; in particular, unlike scale setting with M_Ω , even a 10% deviation in m_s from its physical value only translates into a $\lesssim 0.5\%$ change in the w_0 scale;
- in the present investigation the most precise and fastest method to determine the scale was w_0 based on the Wilson flow: independently of the type of the flow w_0 has quite small cutoff effects and consequently small systematic uncertainties, whereas integrating the Wilson flow is the fastest among all flow choices.

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References

- [1] R. Sommer, *A new way to set the energy scale in lattice gauge theories and its applications to the static force and α_s in SU(2) Yang-Mills theory*, *Nucl. Phys. B* **411** (1994) 839 [[hep-lat/9310022](#)] [[INSPIRE](#)].
- [2] C.W. Bernard et al., *The static quark potential in three flavor QCD*, *Phys. Rev. D* **62** (2000) 034503 [[hep-lat/0002028](#)] [[INSPIRE](#)].
- [3] M. Donnellan, F. Knechtli, B. Leder and R. Sommer, *Determination of the static potential with dynamical fermions*, *Nucl. Phys. B* **849** (2011) 45 [[arXiv:1012.3037](#)] [[INSPIRE](#)].
- [4] A. Hasenfratz and F. Knechtli, *Flavor symmetry and the static potential with hypercubic blocking*, *Phys. Rev. D* **64** (2001) 034504 [[hep-lat/0103029](#)] [[INSPIRE](#)].
- [5] RBC, UKQCD collaboration, Y. Aoki et al., *Continuum limit physics from 2 + 1 flavor domain wall QCD*, *Phys. Rev. D* **83** (2011) 074508 [[arXiv:1011.0892](#)] [[INSPIRE](#)].
- [6] HPQCD collaboration, C. Davies, E. Follana, I. Kendall, G.P. Lepage and C. McNeile, *Precise determination of the lattice spacing in full lattice QCD*, *Phys. Rev. D* **81** (2010) 034506 [[arXiv:0910.1229](#)] [[INSPIRE](#)].
- [7] FERMILAB LATTICE AND MILC collaboration, A. Bazavov et al., *B- and D-meson decay constants from three-flavor lattice QCD*, *Phys. Rev. D* **85** (2012) 114506 [[arXiv:1112.3051](#)] [[INSPIRE](#)].
- [8] HPQCD COLLABORATION, UKQCD collaboration, E. Follana, C. Davies, G. Lepage and J. Shigemitsu, *High precision determination of the π , K, D and D_s decay constants from lattice QCD*, *Phys. Rev. Lett.* **100** (2008) 062002 [[arXiv:0706.1726](#)] [[INSPIRE](#)].
- [9] A.S. Kronfeld, *The $f(D_s)$ puzzle*, [arXiv:0912.0543](#) [[INSPIRE](#)].
- [10] M. Lüscher, *Trivializing maps, the Wilson flow and the HMC algorithm*, *Commun. Math. Phys.* **293** (2010) 899 [[arXiv:0907.5491](#)] [[INSPIRE](#)].
- [11] R. Narayanan and H. Neuberger, *Infinite N phase transitions in continuum Wilson loop operators*, *JHEP* **03** (2006) 064 [[hep-th/0601210](#)] [[INSPIRE](#)].
- [12] M. Lüscher, *Properties and uses of the Wilson flow in lattice QCD*, *JHEP* **08** (2010) 071 [[arXiv:1006.4518](#)] [[INSPIRE](#)].
- [13] M. Lüscher and P. Weisz, *Perturbative analysis of the gradient flow in non-abelian gauge theories*, *JHEP* **02** (2011) 051 [[arXiv:1101.0963](#)] [[INSPIRE](#)].
- [14] S. Dürr et al., *Lattice QCD at the physical point: simulation and analysis details*, *JHEP* **08** (2011) 148 [[arXiv:1011.2711](#)] [[INSPIRE](#)].
- [15] S. Dürr et al., *Lattice QCD at the physical point: light quark masses*, *Phys. Lett. B* **701** (2011) 265 [[arXiv:1011.2403](#)] [[INSPIRE](#)].
- [16] S. Dürr et al., *Precision computation of the kaon bag parameter*, *Phys. Lett. B* **705** (2011) 477 [[arXiv:1106.3230](#)] [[INSPIRE](#)].
- [17] Y. Aoki, G. Endrodi, Z. Fodor, S. Katz and K. Szabo, *The order of the quantum chromodynamics transition predicted by the standard model of particle physics*, *Nature* **443** (2006) 675 [[hep-lat/0611014](#)] [[INSPIRE](#)].
- [18] Y. Aoki, Z. Fodor, S. Katz and K. Szabo, *The QCD transition temperature: results with physical masses in the continuum limit*, *Phys. Lett. B* **643** (2006) 46 [[hep-lat/0609068](#)] [[INSPIRE](#)].

- [19] Y. Aoki et al., *The QCD transition temperature: results with physical masses in the continuum limit II*, *JHEP* **06** (2009) 088 [[arXiv:0903.4155](#)] [[INSPIRE](#)].
- [20] WUPPERTAL-BUDAPEST collaboration, S. Borsányi et al., *Is there still any T_c mystery in lattice QCD? Results with physical masses in the continuum limit III*, *JHEP* **09** (2010) 073 [[arXiv:1005.3508](#)] [[INSPIRE](#)].
- [21] S. Borsányi et al., *The QCD equation of state with dynamical quarks*, *JHEP* **11** (2010) 077 [[arXiv:1007.2580](#)] [[INSPIRE](#)].
- [22] G. Endrodi, Z. Fodor, S. Katz and K. Szabo, *The QCD phase diagram at nonzero quark density*, *JHEP* **04** (2011) 001 [[arXiv:1102.1356](#)] [[INSPIRE](#)].
- [23] S. Borsányi et al., *Fluctuations of conserved charges at finite temperature from lattice QCD*, *JHEP* **01** (2012) 138 [[arXiv:1112.4416](#)] [[INSPIRE](#)].
- [24] S. Dürr et al., *Scaling study of dynamical smeared-link clover fermions*, *Phys. Rev. D* **79** (2009) 014501 [[arXiv:0802.2706](#)] [[INSPIRE](#)].
- [25] S. Dürr et al., *Ab-initio determination of light hadron masses*, *Science* **322** (2008) 1224 [[arXiv:0906.3599](#)] [[INSPIRE](#)].
- [26] S. Borsanyi et al., *Anisotropic lattices without tears*, WUB/12-03 (2012).
- [27] SCIDAC, LHPC, UKQCD collaboration, R.G. Edwards and B. Joo, *The Chroma software system for lattice QCD*, *Nucl. Phys. Proc. Suppl.* **140** (2005) 832 [[hep-lat/0409003](#)] [[INSPIRE](#)].
- [28] E. Shintani et al., *Strong coupling constant from vacuum polarization functions in three-flavor lattice QCD with dynamical overlap fermions*, *Phys. Rev. D* **82** (2010) 074505 [[arXiv:1002.0371](#)] [[INSPIRE](#)].
- [29] C. McNeile, C. Davies, E. Follana, K. Hornbostel and G. Lepage, *High-precision c and b masses and QCD coupling from current-current correlators in lattice and continuum QCD*, *Phys. Rev. D* **82** (2010) 034512 [[arXiv:1004.4285](#)] [[INSPIRE](#)].
- [30] M. Luscher and P. Weisz, *On-shell improved lattice gauge theories*, *Commun. Math. Phys.* **97** (1985) 59.
- [31] S. Capitani, S. Dürr and C. Hölbling, *Rationale for UV-filtered clover fermions*, *JHEP* **11** (2006) 028 [[hep-lat/0607006](#)] [[INSPIRE](#)].
- [32] S. Dürr et al., *The ratio $FK/F\pi$ in QCD*, *Phys. Rev. D* **81** (2010) 054507 [[arXiv:1001.4692](#)] [[INSPIRE](#)].
- [33] C. Morningstar and M.J. Peardon, *Analytic smearing of SU(3) link variables in lattice QCD*, *Phys. Rev. D* **69** (2004) 054501 [[hep-lat/0311018](#)] [[INSPIRE](#)].
- [34] S. Borsányi et al., *QCD equation of state from the lattice*, *AIP Conf. Proc.* **1343** (2011) 519 [[INSPIRE](#)].
- [35] ALPHA collaboration, U. Wolff, *Monte Carlo errors with less errors*, *Comput. Phys. Commun.* **156** (2004) 143 [*Erratum ibid.* **176** (2007) 383] [[hep-lat/0306017](#)] [[INSPIRE](#)].
- [36] G.I. Egri et al., *Lattice QCD as a video game*, *Comput. Phys. Commun.* **177** (2007) 631 [[hep-lat/0611022](#)] [[INSPIRE](#)].