

A novel method for the physical scale setting on the lattice and its application to $N_f=4$ simulations

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This letter reports on a new procedure for the lattice spacing setting that takes advantage of the very precise determination of the strong coupling in Taylor scheme. Although it can be applied for the physical scale setting with the experimental value of $\Lambda_{\overline{MS}}$ as an input, the procedure is particularly appropriate for relative “calibrations”. The method is here applied for simulations with four degenerate light quarks in the sea and leads to prove that their physical scale is compatible with the same one for simulations with two light and two heavy flavours.

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INTRODUCTION

The field theory of the strong interactions, QCD, is essentially nonperturbative in its low energy domain. There, its asymptotic states differ from the non-interacting elementary fields and it should properly account for the main features of the strong phenomenology: chiral symmetry breaking and confinement. One of the most fruitful nonperturbative approaches to the QCD low-energy phenomenology is the lattice field theory [1] which, more and more in the last few years, is providing with accurate numerical results to account for the rich phenomenology of QCD [27]. To this goal, a key role is played by the physical scale setting or lattice “calibration”: the adjustment of the lattice spacing to reproduce properly a low-energy experimental value: masses, decay constants, etc.

The purpose of this letter is to present a novel technique to perform this scale setting, which is based on the direct computation of the strong coupling constant from the gauge and ghost propagators. In the past, gluonic quantities, as the string tension for the linear static interquark potential [2–5], has been used to perform a relative calibration: to fix the lattice spacing for one simulation from that known from another different simulation. The method presented here avails for a relative calibration from gluonic quantities but, the strong coupling being directly accessible from experiments, also for an absolute lattice calibration with Λ_{QCD} as an input. This is particularly useful for simulations with many degenerate light flavours, as those to compute renormalization constants in the flavour massless limit [6] or motivated

by the expected similarities of many-light-flavours QCD with Walking models for technicolor [7] as Refs. [8–12]. In those cases, there is no physical quantity to compare with for the scale setting, but Λ_{QCD} can be well defined by assuming the strong coupling running not to depend on the quark masses, at least far away from the flavour thresholds. Furthermore, for more than 2 light degenerate flavours and 3 Goldstone bosons, the standard chiral behaviour cannot be reliably applied to guide the chiral fits of masses or decay constants. On the other hand, Λ_{QCD} being the fundamental scale of QCD, to which many different experiments refer, to use it for the scale setting could be taken as a theoretical “*ace*”. Last but not least, the strong coupling running being obtained from data for different simulations, the results can be compared to each other and directly confronted to analytical QCD predictions. This provides with a very valuable crosscheck for the scale setting reliability and ensures the best accuracy.

THE MATCHING BY THE TAYLOR COUPLING

The strategy is to get the ratios of lattice spacings from different simulations by the intercomparison of a renormalization-group invariant (RGI) quantity, as the one defining a coupling, computed with the lattice gauge field configurations obtained from the simulations.

Let’s call Q this quantity that could be computed from lattice QCD such that one would have

$$Q_{\text{phys}}(p) = Q_{\text{Latt}}(p_L) + \mathcal{O}(a), \quad (1)$$

where the physical and the lattice momenta are related

such that $p_L = a(\beta, \mu)p$, where $a(\beta, \mu)$ stands for the lattice spacing. We consider a particular simulation in a $N^3 \times N_t$ lattice with β , for the bare lattice coupling, and μ , standing for any other relevant set-up parameter (in our next application, the twisted mass of the light [28] degenerated quarks [13, 14]). After the appropriate Fourier transform of data in configuration space from the simulations, one would be left with

$$p_L^2 = \left(\frac{2\pi}{N}\right)^2 \left(n_x^2 + n_y^2 + n_z^2 + \frac{N^2}{N_t^2} n_t^2\right), \quad (2)$$

defined by the four integers n_x, n_y, n_z and n_t . In Eq. (1)'s r.h.s., we included terms of the order a to account for the lattice artefacts that should tend to disappear when approaching the continuum limit. Q_{phys} will be now supposed not to depend on the lattice set-up parameters at sufficiently high energy where the matching is possible, such that, for two different simulations with parameters (β_1, μ_1) and (β_2, μ_2) , after neglecting (or properly correcting) the lattice artefacts, we can write:

$$Q_{\text{Latt}}^{(\beta_1, \mu_1)}(p_L) \equiv Q_{\text{phys}}(p) \equiv Q_{\text{Latt}}^{(\beta_2, \mu_2)}(p'_L), \quad (3)$$

where: $p'_L/a(\beta_2, \mu_2) = p_L/a(\beta_1, \mu_1) = p$. Then, the ratio of lattice spacings, $a(\beta_2, \mu_2)/a(\beta_1, \mu_1)$ is to be obtained by computing Q from the two different simulations and impose the results to match as Eq. (3) requires. The latter implies that, where the matching is required, any dependence of Q on β and μ has been supposed to be captured by the lattice spacing through the scale setting. This will be confirmed, in our procedure, by the comparison of the running of Q with the momentum for the different simulations, after the scale setting.

In order to apply the matching procedure above described, we will choose for Q the Taylor coupling [15–18],

$$Q_{\text{Latt}}(p_L) \equiv \alpha_T^{\text{Latt}}(p_L) = \frac{g_0^2(a)}{4\pi} \tilde{Z}_3^2(p_L, a) Z_3(p_L, a), \quad (4)$$

estimated from different lattice simulations, where \tilde{Z}_3 and Z_3 are the ghost and gluon propagator renormalization constants in MOM scheme. Then, we will first apply the so-called $H(4)$ -extrapolation procedure [19–21], that exploits the remaining symmetry which is restricted to the $H(4)$ isometry group for the elimination of $O(4)$ -breaking lattice artefacts,

$$\alpha_T^{\text{Latt}}(p_L) \Rightarrow \alpha_T^{H(4)}(p_L). \quad (5)$$

We will next correct for the $O(4)$ -invariant lattice artefacts as shown in Refs. [22, 23],

$$\alpha_T^{H(4)}(p_L) = \alpha_T^{\text{phys}}(a^{-1}p_L) + c_{a^2 p^2} p_L^2, \quad (6)$$

and will finally be left with the “continuum” Taylor coupling that have been shown to be, in practice, very well described by

$$\alpha_T^{\text{phys}}(p) = \alpha_T(p^2) + \frac{d_x}{p^x}, \quad (7)$$

with

$$\alpha_T(p^2) = \alpha_T^{\text{pert}}(p^2) \left(1 + \frac{9}{p^2} R(\alpha_T^{\text{pert}}(p^2), \alpha_T^{\text{pert}}(q_0^2)) \times \left(\frac{\alpha_T^{\text{pert}}(p^2)}{\alpha_T^{\text{pert}}(q_0^2)}\right)^{1-\gamma_0^{A^2}/\beta_0} \frac{g_T^2(q_0^2) \langle A^2 \rangle_{R, q_0^2}}{4(N_C^2 - 1)}\right), \quad (8)$$

derived from the OPE description of ghost and gluon dressing functions in terms of the dimension-two gluon condensate, $R(\alpha, \alpha_0)$ including higher-order corrections to the Wilson coefficient beyond the leading logarithm. The purely perturbative running is given by α_T^{pert} up to four-loops through the integration of the β -function [24], in terms of $\ln(p/\Lambda_T)$ where $\Lambda_T/\Lambda_{\overline{\text{MS}}} = 0.5608$ for $N_f=4$. In ref. [23], Eqs. (6-8) have been successfully applied to fit the running of the Taylor coupling obtained from unquenched lattice simulations with two light degenerate quark flavours and two heavier non-degenerate ones ($N_f=2+1+1$). The results, recently updated in ref. [25], for the best-fit parameters are: $\Lambda_{\overline{\text{MS}}}\bar{a}(1.90, 0) = 0.1413(32)$, $g^2 \langle A^2 \rangle \bar{a}^2(1.90, 0) = 0.76(11)$, $x = 5.73(27)$ and $d_x \bar{a}^x(1.90, 0) = -0.157(10)$; expressed in units of $\bar{a}(1.90, 0)$ (we used here \bar{a} for simulations with $N_f=2+1+1$ and keep a for $N_f=4$ degenerate flavours).

Then, for any simulation with set-up parameters (β, μ) , according to Eqs. (3-6), one can write

$$\alpha_{T,(\beta,\mu)}^{H(4)}(p_L) = \alpha_T^{\text{phys}}\left(\frac{p'_L}{\bar{a}(1.90, 0)}\right) + c_{a^2 p^2} p_L^2, \quad (9)$$

where $p'_L = p_L \bar{a}(1.90, 0)/a(\beta, \mu)$, p_L being the lattice momentum for the simulation, Eq. (2), and the running of α_T^{phys} given by Eqs. (7-8) and expressed in units of $\bar{a}(1.90, 0)$,

$$\alpha_T^{\text{phys}}\left(\frac{p'_L}{\bar{a}(1.90, 0)}\right) = \alpha_T\left(\frac{p_L'^2}{\bar{a}^2(1.90, 0)}\right) + \frac{d_x \bar{a}^x(1.90, 0)}{p_L'^x}, \quad (10)$$

with $x = 5.73$ and the central value for the parameters $\Lambda_{\overline{\text{MS}}}\bar{a}(1.90, 0)$, $g^2 \langle A^2 \rangle \bar{a}^2(1.90, 0)$ and $d_x \bar{a}^x(1.90, 0)$ above presented. The latter is a consequence of our main assumption: $\Lambda_{\overline{\text{MS}}}$ and the nonperturbative corrections, coded by $g^2 \langle A^2 \rangle$ and d_x , are supposed to depend only on the number of active quarks and, far above the quark mass thresholds, their masses should not matter so much. As the matching of coupling data for simulations with μ and μ' set-up parameters naturally implies [29]

$$\frac{\Lambda_{\overline{\text{MS}}}^{\mu'}}{\Lambda_{\overline{\text{MS}}}^{\mu}} \simeq \left(\frac{g^2 \langle A^2 \rangle^{\mu'}}{g^2 \langle A^2 \rangle^{\mu}}\right)^{1/2} \simeq \left(\frac{d_x^{\mu'}}{d_x^{\mu}}\right)^{1/x} \simeq 1, \quad (11)$$

this main assumption will appear supported “*a posteriori*” (see next Fig. 2). Thus, taking the ratios in Eq. (11) to be exactly 1, the ratio of lattice spacings, $\bar{a}(1.90, 0)/a(\beta, \mu)$, and the coefficient $c_{a^2 p^2}$ are the two only free parameters to be determined by the best fit of Eqs. (9,10) to the Taylor coupling lattice data.

RELATIVE CALIBRATION

In the following, the above-described procedure will be applied to estimate the lattice spacing for simulations with $N_f=4$ degenerate twisted-mass flavours [6] (Tab. I gathers their set-up parameters), produced by ETMC to apply the massless renormalization. To our knowledge, no other method allows for such a reliable scale setting in this case, as the Taylor coupling can be properly taken not to depend very much [30] on the set-up parameters for $N_f=4$ and $N_f=2+1+1$ simulations.

β	$a\mu$	am_{PCAC}	aM_0	confs.
1.90	0.0080	-0.0390(01)	0.0285(01)	130
1.90	0.0080	0.0398(01)	0.0290(01)	130
1.90	0.0080	-0.0358(02)	0.0263(01)	200
1.90	0.0080	0.0356(01)	0.0262(01)	200
1.90	0.0080	-0.0318(01)	0.0237(01)	200
1.90	0.0080	0.0310(02)	0.0231(01)	200
1.90	0.0080	-0.0273(02)	0.0207(01)	130
1.90	0.0080	0.0275(04)	0.0209(01)	130
1.95	0.0085	-0.0413(02)	0.0329(01)	130
1.95	0.0085	0.0425(02)	0.0338(01)	130
1.95	0.0085	-0.0353(01)	0.0285(01)	130
1.95	0.0085	0.0361(01)	0.0285(01)	130
1.95	0.0020	-0.0363(01)	0.0280(01)	120
1.95	0.0020	0.0363(01)	0.0274(01)	120
1.95	0.0180	-0.0160(02)	0.0218(01)	130
1.95	0.0180	0.0163(02)	0.0219(01)	130
1.95	0.0085	-0.0209(02)	0.0182(01)	130
1.95	0.0085	0.0191(02)	0.0170(01)	130
1.95	0.0085	-0.0146(02)	0.0141(01)	130
1.95	0.0085	0.0151(02)	0.0144(01)	130
2.10	0.0078	-0.00821(11)	0.0102(01)	180
2.10	0.0078	0.00823(08)	0.0102(01)	180
2.10	0.0064	-0.000682(13)	0.0084(01)	180
2.10	0.0064	0.00685(12)	0.0084(01)	180
2.10	0.0046	-0.00585(08)	0.0066(01)	120
2.10	0.0046	0.00559(14)	0.0064(01)	120
2.10	0.0030	-0.00403(14)	0.0044(01)	240
2.10	0.0030	0.00421(13)	0.0045(01)	240

TABLE I: Set-up parameters, m_{PCAC} and the bare polar mass for the ensembles here exploited. Borrowed from ref. [6].

We will take the lattice spacing to depend on the bare gauge coupling, β , and on the dynamical degenerate-flavour mass only through the bare polar mass, M_0 (see Tab. I and Ref. [6]). Then, we compute the Taylor coupling, α_T^{Latt} , given by Eq. (4) for each lattice ensemble. Next, we average for the two ensembles with roughly the same m_{PCAC} but opposite sign, as explained in ref. [6], in order to achieve approximatively the $O(a)$ improvement though working out of the maximal twist. We apply the $H4$ extrapolation procedure to remove the hypercubic artefacts and, finally, the cured results for the coupling is fitted with Eqs. (9,10), as explained in the previous section. Thus, we obtain the ratios of lattice spacings, $\bar{a}(1.90, 0)/a(\beta, aM_0)$, and $c_{a^2 p^2}$ as the best-fit parameters gathered in Tab. II. The results appear also plotted in Fig. 1, where a linear extrapolation on M_0^2 , as the use of a $\mathcal{O}(a)$ -improved lattice action suggests, down to the chiral limit is also shown. It should be noticed that the fitted parameters for the coefficient correcting the $O(4)$ -invariant lattice artefacts, $c_{a^2 p^2}$, shows no important dependence on the light quark mass, as expected, and fairly well agree with the same parameter obtained for our previous analysis with simulations for $N_f=2+1+1$ [23, 25].

β	aM_0	$\bar{a}(1.90, 0)/a(\beta, aM_0)$	$c_{a^2 p^2}$	$\chi^2/\text{d.o.f.}$
1.90	0.0288	0.932(18)	-0.0074(14)	5.6/44
1.90	0.0263	0.969(17)	-0.0067(5)	3.3/45
1.90	0.0234	0.969(11)	-0.0080(10)	7.6/45
1.90	0.0208	1.004(25)	-0.0056(12)	2.4/46
1.90	0	1.049(46)		
1.95	0.0334	1.024(12)	-0.0079(8)	4.4/46
1.95	0.0285	1.059(12)	-0.0088(9)	10.2/49
1.95	0.0277	1.019(20)	-0.0099(9)	5.6/46
1.95	0.0219	1.086(20)	-0.0069(9)	3.4/47
1.95	0.0176	1.105(11)	-0.0066(11)	19.8/48
1.95	0.0143	1.115(18)	-0.0054(7)	9.9/50
1.95	0	1.134(18)		
2.10	0.0102	1.530(15)	-0.0053(4)	142./93
2.10	0.0084	1.518(15)	-0.0048(5)	90.3/93
2.10	0.0065	1.533(19)	-0.0049(5)	161./93
2.10	0.0045	1.578(42)	-0.0055(10)	240./94
2.10	0	1.533(35)		

TABLE II: ratios of lattice spacings obtained as explained in the text. The values obtained by performing a chiral extrapolation down to a zero light quark mass is also shown. The quality of the fits is characterized by the $\chi^2/\text{d.o.f.}$. All the errors have been derived by applying the Jackknife’s method.

In Tab. III, the ratios of $N_f=4$ lattice spacings over that at $\beta = 1.90$ for $N_f=2+1+1$ from Tab. II, after the chiral extrapolation, are shown in comparison with ratios of the same lattice spacings for $N_f=2+1+1$, borrowed

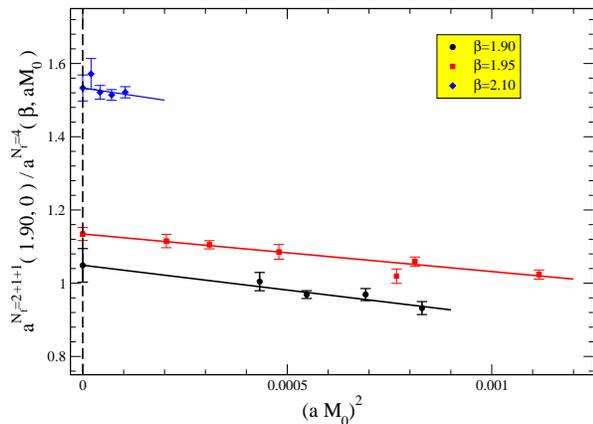


FIG. 1: ratios of lattice spacings (see tab. II) obtained by the matching procedure of the Taylor coupling and the corresponding chiral extrapolation in solid line.

from Refs. [25, 26]. They all agree within the errors, although the lattice spacings for $N_f=4$ appear to be systematically larger ($\sim 5\%$) than those for $N_f=2+1+1$.

β	$\bar{a}(1.90, 0)/a(\beta, 0)$	$a(1.90, 0)/a(\beta, 0)$	$\bar{a}(1.90, 0)/\bar{a}(\beta, 0)$
1.90	1.049(46)	1	1
1.95	1.134(18)	1.081(50)	[26]: 1.085(59)
2.10	1.533(35)	1.461(72)	[25]: 1.477(28) [26]: 1.429(71)

TABLE III: Comparison of the ratios of lattice spacings for $N_f=4$ (noted as a) obtained here and those for $N_f=2+1+1$ simulations (noted as \bar{a}) from Refs. [25, 26].

ABSOLUTE CALIBRATION FROM $\Lambda_{\overline{\text{MS}}}$

In the previous section, the matching of the Taylor coupling led to a relative scale setting for the analysed simulations, *i.e.* in terms of a given lattice spacing for another simulation ($\beta = 1.90$ and $N_f=2+1+1$, with chiral light flavours). Then, the “absolute” calibration of the former, in physical units, requires from the latter’s knowledge. On the other hand, the Taylor coupling from lattice data confronted to Eqs. (6,8) provided with an estimate for $\Lambda_{\overline{\text{MS}}}$ in terms of the lattice spacing. Such an estimate was used in Refs. [22, 23, 25] to compute, after the scale setting from ETMC, $\Lambda_{\overline{\text{MS}}}$ in physical units and hence $\alpha_{\overline{\text{MS}}}(m_Z^2)$. Alternatively, one can also take the experimental value for $\Lambda_{\overline{\text{MS}}}$ and use it to estimate the lattice spacing. We have $\bar{a}(1.90, 0)\Lambda_{\overline{\text{MS}}} = 0.1413(32)$, from lattice data with $N_f=2+1+1$ unquenched flavours, as mentioned above, and $\Lambda_{\overline{\text{MS}}}^{N_f=4} = 296(10)$ MeV from PDG [24]. Then, for $N_f=2+1+1$, one would have $\bar{a}(1.90, 0) = 0.0940(38)$ fm, which compares fairly well to the very recent ETMC result: $\bar{a}(1.90, 0) = 0.0885(36)$ fm [26]. It

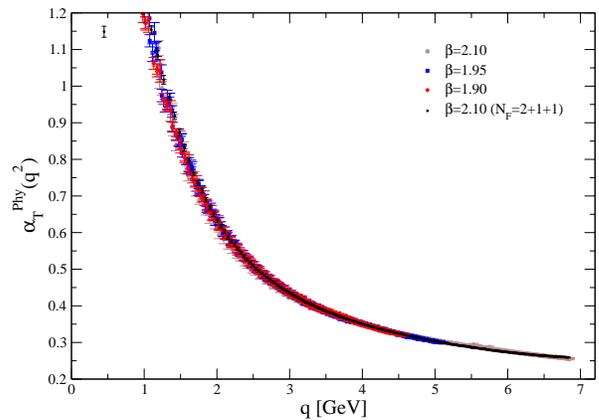


FIG. 2: The physical running of the Taylor coupling, defined by Eq. (6), for all the properly calibrated lattices from Tab. I. $N_f=2+1+1$ data from [25] are included for comparison.

should be furthermore noticed that the determination of $\bar{a}(1.90, 0)\Lambda_{\overline{\text{MS}}}$ in ref. [25] takes into account systematic uncertainties we do not include in the present calibration. These uncertainties could be drastically reduced by performing a simulation at as larger a β parameter as possible, to reach larger physical momenta but keeping the higher-order hypercubic artefacts under control.

Thus, we can take our estimate for the lattice spacing and set the physical scale for all the lattices in Tab. I, with the help of the ratios from Tab. II. Then, we verify that the running of α_T^{phys} , defined by Eq. (6), is the same for all of them and the same as for $N_f=2+1+1$, as can be seen in Fig. 2. In particular, in the chiral limit, we obtain

$$\frac{a(\beta, 0)}{1\text{fm}} = \begin{cases} 0.0896(53) & \beta = 1.90 \\ 0.0829(36) & \beta = 1.95 \\ 0.0613(29) & \beta = 2.10 \end{cases}, \quad (12)$$

for the $N_f = 4$ simulations.

CONCLUSIONS

We have proposed a novel method for the scale setting on lattice simulations that only needs the evaluation of gauge and ghost propagators to determine the strong coupling running and requires for it, after the appropriate removal of lattice artefacts, to be the same for different simulations, when the scale is properly fixed. The method allows for a relative calibration of lattices, the lattice spacing for them being expressed in terms of the one in another given simulation, but also for an absolute calibration with $\Lambda_{\overline{\text{MS}}}$ as an input. The method has been successfully applied to perform the scale setting for unquenched simulations including four degenerate light flavours. Thus, we have also concluded that, within our statistical uncertainties, the lattice spacings for $N_f=4$ and $N_f=2+1+1$ simulations appear to be compatible.

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 [27] See the lattice review of [24] or the contributions in PoS(Lattice 2012).
 [28] The dependence in the heavy masses will be dealt with at length in this paper.
 [29] Deviations from Eq. (11) should be included in the procedure's systematic uncertainties.
 [30] This is the case, as the matching we reach shows, at least for quark masses varying not too much, as happens for our simulations.