

Scale Setting from a Mixed Action with Twisted Mass Valence Quarks

Alejandro Saez,^{a,*} Alessandro Conigli,^a Julien Frison,^b Gregorio Herdoiza,^a Carlos Pena^a and Javier Ugarrio^a

^a*Department of Theoretical Physics, Universidad Autónoma de Madrid, 28049 Madrid, Spain
and Instituto de Física Teórica UAM-CSIC, c/ Nicolás Cabrera 13-15
Universidad Autónoma de Madrid, 28049 Madrid, Spain*

^b*ZPPT/NIC, DESY Zeuthen, Platanenallee 6, 15738 Zeuthen, Germany*

E-mail: alejandrosaezg@uam.es

We present preliminary results for a scale setting procedure based on a mixed action strategy consisting of Wilson twisted mass valence fermions at maximal twist on CLS ensembles with $N_f = 2 + 1$ flavours of $O(a)$ -improved Wilson sea quarks. Once the matching of valence and sea quark masses is performed, universality tests are carried out by comparing the continuum-limit results of the mixed action setup to those of the regularisation based solely on $O(a)$ -improved Wilson fermions. The scale setting uses the pion and kaon decay constants, in units of the gradient flow scale t_0 , obtained from combining computations with the unitary Wilson action and the mixed action. The proper isolation of ground states as well as the continuum-chiral extrapolations are evaluated through model variation techniques. An update on the determination of t_0 will be presented.

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*Speaker

1. Introduction

Most of the fundamental parameters of the Standard Model (SM) belong to Flavor physics, making the field one of the central topics of particle physics. In particular, flavor physics within the quark sector poses a theoretical challenge, since strong interactions happening at low-energies cannot be studied perturbatively. Thus, robust computations of amplitudes of relevant processes for the SM rely heavily on lattice QCD simulations. The same is true for extensions beyond the Standard Model.

We consider a setup [1–5] whose objective is the control of large cutoff effects in heavy quark observables. To achieve this, lattice artifacts are reduced by the use of a mixed-action regularization consisting in twisted mass fermions in the valence and CLS ensembles with $O(a)$ -improved fermions in the sea [10, 14]. In addition, topology freezing at fine lattice spacings is avoided through the use of open boundary conditions in time [9] in the CLS ensembles.

One feature of this lattice regularization is that when valence twisted mass fermions are tuned to maximal twist, automatic $O(a)$ improvement is achieved [2, 11] (up to residual effects coming from the sea). This is of particular relevance when working with heavy quarks. In this work we present an update of the use of this lattice formulation in the light (up/down) and strange quark sectors. This is a necessary step before studying heavy quark physics, since a matching between the valence quark masses and the $N_f = 2 + 1$ flavors in the sea is needed. In addition to this, we will describe the tuning of the valence fermions to maximal twist. Finally, we can carry out an independent computation of light-quark observables such as the pion and kaon decay constants and perform the scale setting using the gradient flow scale t_0 . For a study of the light-quark masses, we report [6].

Throughout the analysis, finite volume effects are corrected using LO χ PT [19]. The corrections are found to be smaller than the statistical uncertainty in all the observables considered for each gauge configuration ensemble studied. Also, in order to get the ground state signal of lattice observables, the method proposed in [16] is used, in which several fit intervals are considered for each observable and a weight is assigned to each choice, penalizing fits with a large number of cut points.

2. Sea sector: CLS ensembles

The CLS gauge ensembles [14] used for the sea sector of our mixed action are given in Table 1. These ensembles use the Lüscher-Weisz gauge action and $N_f = 2 + 1$ $O(a)$ non-perturbatively improved Wilson fermions. Open boundary conditions in time are chosen in order to avoid topology freezing at fine lattice spacings.

These ensembles are generated along a chiral trajectory, characterized by

$$\text{Tr}(M_q) = m_u + m_d + m_s = \text{cnst}, \quad (1)$$

(where M_q is the bare quark mass matrix), which ensures that the improved bare coupling \tilde{g}_0 is constant up to cutoff effects of $O(a^2)$ for a given lattice spacing when varying the quark masses. However, in practice it is convenient to work with a renormalized chiral trajectory. In order to do

β	a [fm]	id	m_π [MeV]	m_K [MeV]
3.40	0.086	H101	420	420
		H102	350	440
		H105	280	460
3.46	0.076	H400	420	420
3.55	0.064	N202	420	420
		N203	340	440
		N200	280	460
		D200	200	480
3.70	0.050	N300	420	420
		J303	260	470

Table 1: $N_f = 2 + 1$ CLS ensembles [14] used in this work. The ensembles use non-perturbatively $O(a)$ -improved Wilson fermions.

this, we need to impose that all ensembles have a constant value of ϕ_4

$$\phi_4 = 8t_0 \left(m_K^2 + \frac{1}{2} m_\pi^2 \right) = 8t_0 m_K^2 + \frac{1}{2} \phi_2, \quad (2)$$

since according to LO χ PT

$$\phi_4 \propto m_{u,R} + m_{d,R} + m_{s,R}. \quad (3)$$

To impose a lines of constant ϕ_4 , a mass-shift in the simulated quark masses is required, consisting of Taylor expanding all observables in the bare quark masses

$$\langle O(m'_u, m'_d, m'_s) \rangle = \langle O(m_u, m_d, m_s) \rangle + \sum_q (m'_q - m_q) \frac{d \langle O \rangle}{dm_q}. \quad (4)$$

For the value of ϕ_4 to which observables are mass-shifted, an educated guess of the physical value t_0^{ph} is initially chosen as

$$\sqrt{t_0^{\text{guess}}} = 0.1451(9) \text{ fm}, \quad (5)$$

which together with the pion and kaon meson masses in the QCD isospin symmetry limit (isoQCD) [20]

$$m_\pi^{isoQCD} = m_{\pi^0}^{exp} = 134.9768(5) \text{ MeV}, \quad (6)$$

$$m_K^{isoQCD} = m_{K^0}^{exp} = 497.611(13) \text{ MeV}, \quad (7)$$

lead to a value for ϕ_4^{guess} . The value for the educated guess t_0^{guess} together with its error comes from a preliminary analysis. Thus, all the correlations are preserved in this error.

The mass-shift can be performed in the up/down and strange quarks, or only in the strange quark. Following [18], the latter case is chosen.

3. Valence sector: twisted mass fermions

For the valence sector, twisted mass fermions on the CLS ensembles in the sea are used. Wilson twisted mass fermions add a chirally rotated mass term to the standard Wilson fermion operator

$$D_W + m_q \rightarrow D_{tm} = D_W + m_q + i\gamma_5\mu_q . \quad (8)$$

Twisted mass fermions, when tuned to maximal twist, ensure automatic $O(a)$ improvement up to residual effects coming from the sea. In particular, the same valence standard quark mass m_q for the up/down and strange quarks is used, while the twisted quark mass μ_q for the up/down and strange quarks is different, $\mu_q = \{\mu_l, \mu_l, \mu_s\}$. This means that it is enough for the up/down PCAC quark mass m_{ud}^{val} to vanish in order to impose maximal twist, since up to cutoff effects this condition will also hold for the strange quark mass,

$$m_{ud}^{val} \equiv m_{12}^{val} \equiv \frac{m_u^{val} + m_d^{val}}{2} \equiv 0. \quad (9)$$

In order to impose this maximal twist condition a grid of values for the valence parameters $(\kappa^{val}, \mu_l, \mu_s)$ is used, allowing to compute m_{12}^{val} as a function of those parameters and then interpolate to the condition in eq. (9).

4. Matching sea and valence sectors

In any mixed action setup, it is needed to perform a matching between the sea and valence sectors, in order to recover unitarity of the theory at the continuum limit. This matching consists in imposing that the physical quark masses are the same in both the sea and valence sectors. To achieve this, ϕ_2 and ϕ_4 defined in eq. (2) are used, which to LO χ PT are proportional to the strange and light (up/down) quark masses. Analyzing the CLS ensembles in the sea, the values of ϕ_2^{sea} and ϕ_4^{sea} are obtained, and then an small interpolation along the grid in the valence is needed in order to impose

$$\phi_2^{\text{val}} \equiv \phi_2^{\text{sea}}, \quad \phi_4^{\text{val}} \equiv \phi_4^{\text{sea}}. \quad (10)$$

The interpolation fit functions used for this are based in LO χ PT. The matching is shown in Fig. 1.

Once the values of the valence parameters at which maximal twist and the matching conditions are satisfied are determined, $(\tilde{\kappa}_{cr}^{val}, \mu_l^{*val}, \mu_s^{*val})$, the pion and kaon decay constants in the valence need to be interpolated to those valence parameters, getting the mixed action results for those observables, which are used to perform the scale setting.

5. Continuum limit and chiral extrapolation: t_0^{ph}

In order to obtain a new physical determination of the flow scale t_0 , the pion and kaon decay constants are used in the combination [15]

$$\sqrt{8t_0}f_{\pi K} = \sqrt{8t_0} \times \frac{2}{3} \left(f_K + \frac{1}{2}f_\pi \right), \quad (11)$$

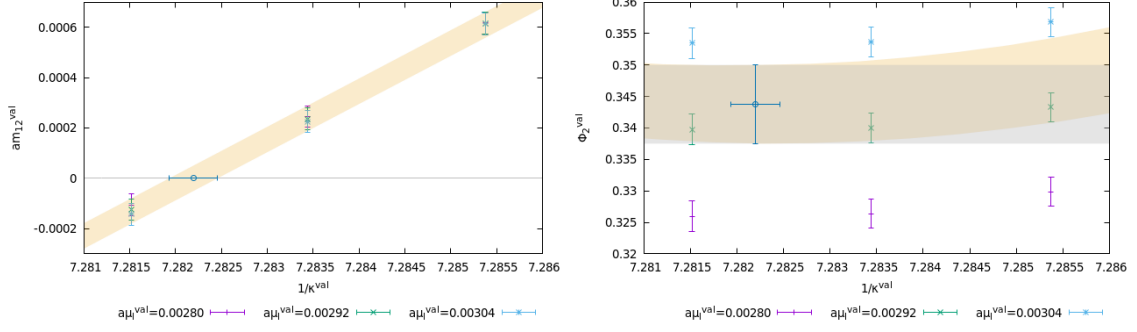


Figure 1: Left: Up/down PCAC valence quark mass along the valence grid, interpolated to $m_{12}^{\text{val}} = 0$ to impose maximal twist. Right: ϕ_2^{val} along the valence grid, interpolated to the sea value ϕ_2^{sea} . The sea sector parameters correspond to those of Table 1 for ensemble H105. The orange band in both figures represents the interpolation along the grid of valence parameters, while the horizontal gray line and band represent the target value to which we want to interpolate both observables. In the case of am_{12}^{val} , it is set to zero, and for ϕ_2^{val} to ϕ_2^{sea} .

since at NLO in SU(3) χ PT, this quantity remains constant along the renormalized chiral trajectory up to logarithmic terms.

In total, three sets of data are available: the results coming from the sea analysis, which are called ‘‘Wilson’’ data; those coming from the mixed action after the matching, called ‘‘Wtm’’; and a combined set of data, in which the two previous sets are analyzed simultaneously by imposing a common continuum limit. More specifically, the Wilson and Wtm results can be analyzed independently, thus extracting two different values of t_0^{ph} . For the combined case, a combined fit is done, fitting both data sets simultaneously to the same continuum dependence, but independent cutoff effects.

The lattice data are parametrized as

$$\left(\sqrt{8t_0}f_{\pi K}\right)^{\text{latt}} = \left(\sqrt{8t_0}f_{\pi K}\right)^{\text{cont}} + c(a, \phi_2), \quad (12)$$

with $c(a, \phi_2)$ parametrizing the cutoff effects. Several possible choices for the continuum behaviour and the cutoff effects are explored.

For the continuum behaviour, using SU(3) NLO χ PT [18]

$$\left(\sqrt{8t_0}f_{\pi K}\right)^{\text{cont}} = \frac{p_1}{8\pi\sqrt{2}} \left[1 - \frac{7}{6}L\left(\frac{\phi_2}{p_1^2}\right) - \frac{4}{3}L\left(\frac{\phi_4 - \phi_2/2}{p_1^2}\right) - \frac{1}{2}L\left(\frac{4\phi_4/3 - \phi_2}{p_1^2}\right) + p_2\phi_4 \right], \quad (13)$$

$$(14)$$

$$L(x) = x \log(x). \quad (15)$$

Taking this functional form for the continuum behaviour and eq. (12) with cutoff effects $c(a, \phi_2)$ of order $O(a^2)$, we get the fit results in Fig. 2.

Another choice is to take a Taylor expansion on ϕ_2 around the symmetric point value ϕ_2^{sym}

$$\left(\sqrt{8t_0}f_{\pi K}\right)^{\text{cont}} = p_1 + p_2(\phi_2 - \phi_2^{\text{sym}})^2. \quad (16)$$

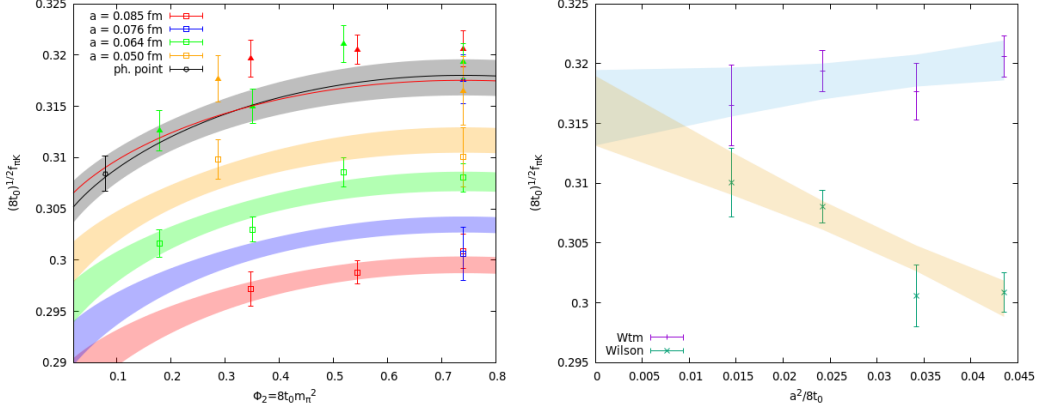


Figure 2: Left: chiral and continuum limit of the decay constants for Wilson (empty points), Wtm (filled points) and combined sets. No cuts in the data were made, using eq. (13) for the continuum behaviour. Points with the same color represent the same lattice spacing. The black curve represents the continuum limit of Wilson data, and the red curve the Wtm data. The grey band represents the continuum limit for the combined set of data. Right: Continuum limit of $\phi_2 = 0.740(9)$ ensembles, which correspond to the symmetric point $m_\pi = m_K$.

For the cutoff effects $c(a, \phi_2)$, we vary over $O(a^2)$, $O(\phi_2 a^2)$ or $O(a^2 \alpha_s^{\hat{\Gamma}})$. The $O(a^2 \alpha_s^{\hat{\Gamma}})$ cutoff dependence comes from [21], in which the contribution of the anomalous dimensions $\hat{\Gamma}_i$ of the relevant physical observables to the cutoff effects were considered. We choose to take the smallest value of $\hat{\Gamma} = -0.111$, which is the same for the Wilson and mixed action regularization. For an estimation of $\alpha_s(a^{-1})$, it can be used that $\alpha_s(a^{-1}) \propto -1/\ln(a\Lambda_{\text{QCD}})$ and take the value of Λ_{QCD} from [20].

We observe the quality of fit for with $O(\phi_2 a^2)$ cutoff effects to be poor for the Wilson data but not for the Wtm. Since in both data sets the cutoff effects are independent, in the combined data set fits we also consider the case of using $O(a^2)$ cutoff effects for the Wilson data and $O(\phi_2 a^2)$ for the Wtm. Following this we could explore all other possible combinations of cutoff effects for Wilson and Wtm data sets in the combined fits, but since the $O(a^2)$ and $O(a^2 \alpha_s^{\hat{\Gamma}})$ cutoff effects give very similar fits (choosing $\hat{\Gamma} = -0.111$), these combinations do not explore much the model space.

In addition to a variation of the functional forms, an exploration of the cuts in the data is done. We consider the possibility of removing $\beta = 3.40$ or removing $m_\pi = 420$ MeV. Since the Wilson and Wtm data have independent cutoff effects, in principle one could cut $\beta = 3.40$ from the Wilson data set but not from the Wtm, or the reverse. However, these models are ruled out by poor fit qualities.

To study the systematic associated with model variation in the chiral and continuum extrapolation, we use the bayesian model averaging method [16], which penalizes fits with a large number of parameters k and large number of cut points N_{cut} . Each fit model is assigned a weight

$$W \propto \exp\left(-\frac{1}{2}(\chi^2 + 2k + 2N_{\text{cut}})\right), \quad (17)$$

which allows to compute a weighted average for $\sqrt{t_0} f_{\pi K}$. The method also assigns a systematic uncertainty coming from the model variation. The fits performed are uncorrelated, while χ^2 in eq. (17) must be the correlated χ^2 , which for good fits equals the number of degrees of freedom (dof).

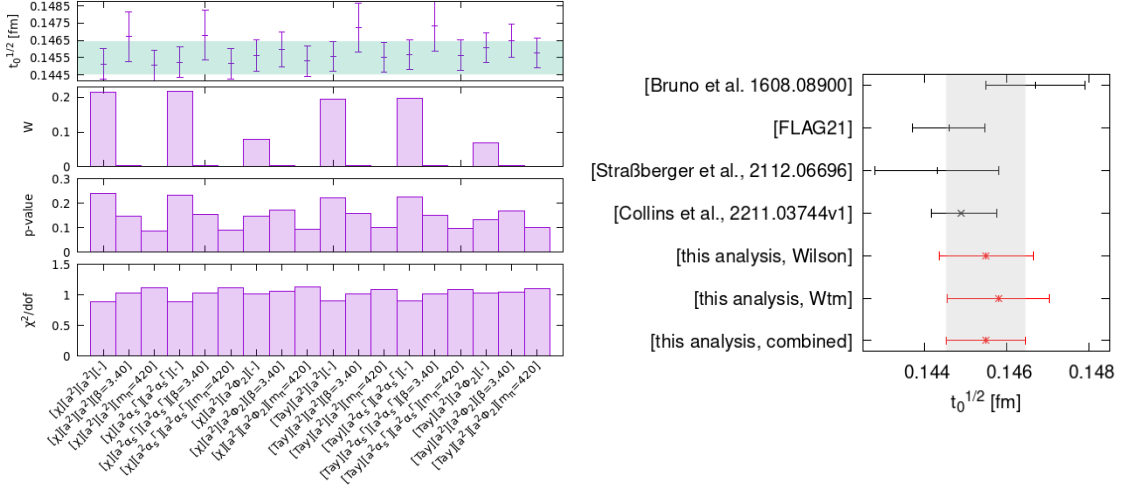


Figure 3: Left: results for the combined set of data of t_0 in physical units for each model considered. The fits are uncorrelated, the p-values and χ^2_{exp} being computed following [22]. The green band represents the Bayesian model average following [16], with the systematic contribution coming from the model variation added. The x-axis represents the model considered. The first model in the list corresponds to that of Fig. 2. The horizontal axis represents the models explored: the first tag ($[X]$ or $[Tay]$) represents the continuum parametrization according to eq. (13) or eq. (16) respectively; the second and third tags represent the cutoff effects of the Wilson and Wtm subsets of data respectively ($[a^2]$, $[a^2\alpha_s^{\hat{r}}]$ or $[\phi_2 a^2]$); and the fourth tag ($[\beta = 3.40]$ or $[m_\pi = 420]$) represent the cuts performed in both Wilson and Wtm data for the fit. Right: results of t_0 in physical units after the Bayesian model average, for the three sets of data analyzed, Wilson, Wtm and combined.

However, in Fig. 3 we show that our results for the uncorrelated χ^2 are close to the number of degrees of freedom, so we can approximate our uncorrelated values of χ^2 to the correlated ones, using eq. (17) with the uncorrelated χ^2 . The results of the model average can be seen in Fig. 3.

Once $\sqrt{8t_0}f_{\pi K}$ is found at the physical point (physical pion mass and continuum limit), using as physical input the values for the decay constants f_π and f_K in eq. (18), one can extract the flow scale t_0 in physical units at the physical point.

The physical inputs used are [20]

$$f_\pi^{isoQCD} = 130.56(13) \text{ MeV}, \quad f_K^{isoQCD} = 157.2(5) \text{ MeV}. \quad (18)$$

Preliminary results for the three sets of data are presented in Fig. 3.

Once the physical value of t_0 has been determined, following [18] the value of the lattice spacing a in fm can be extracted.

6. Conclusions

We have presented an update on the scale setting based on physical inputs for the pion and kaon decay constants, using a mixed action consisting of twisted mass valence quarks on CLS $O(a)$ -improved sea quarks. We have explored the systematic assigned to model variation in the chiral and continuum limits needed for the scale setting, and shown the effectiveness of combining

the Wilson and mixed action (Wtm) data for reducing the uncertainty in t_0^{ph} . We refer to [6] for a study of the light quark masses using this mixed action, and to [8], [7] for an update on the study of the charm quark mass and leptonic and semileptonic decays involving a charm quark using this mixed action.

7. Acknowledgements

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References

- [1] G. Herdoíza, C. Pena, D. Preti, J. Á. Romero and J. Ugarrío, “A tmQCD mixed-action approach to flavour physics”, EPJ Web Conf. 175 (2018), 13018, [arXiv:1711.06017 [hep-lat]].
- [2] A. Bussone et al. [ALPHA], “Heavy-quark physics with a tmQCD valence action”, PoS LATTICE2018 (2019), 270, [arXiv:1812.01474 [hep-lat]].
- [3] J. Ugarrío et al. [Alpha], “First results for charm physics with a tmQCD valence action”, PoS LATTICE2018 (2018), 271, [arXiv:1812.05458 [hep-lat]].
- [4] A. Bussone et al. [ALPHA], “Matching of $N_f = 2 + 1$ CLS ensembles to a tmQCD valence sector”, PoS LATTICE2018 (2019), 318, [arXiv:1903.00286 [hep-lat]].
- [5] J. Frison et al., “Heavy semileptonics with a fully relativistic mixed action”, PoS LATTICE2019 (2019), 234, [arXiv:1911.02412 [hep-lat]].
- [6] G. Herdoiza et al., PoS LATTICE2022 (2022), 268.
- [7] J. Frison et al., PoS LATTICE2022 (2022), 378.
- [8] A. Conigli et al., PoS LATTICE2022 (2022), 235.
- [9] M. Lüscher and S. Schaefer, “Lattice QCD without topology barriers”, JHEP 07 (2011), 036, [arXiv:1105.4749 [hep-lat]].
- [10] M. Bruno et al., “Simulation of QCD with $N_f = 2 + 1$ flavors of non-perturbatively improved Wilson fermions”, JHEP 02 (2015), 043, [arXiv:1411.3982 [hep-lat]].
- [11] R. Frezzotti and G. C. Rossi, JHEP 08 (2004), 007, doi:10.1088/1126-6708/2004/08/007, [arXiv:hep-lat/0306014 [hep-lat]].

- [12] R. Frezzotti et al. [Alpha], “Lattice QCD with a chirally twisted mass term”, JHEP 08 (2001), 058, [arXiv:hep-lat/0101001 [hep-lat]].
- [13] C. Pena, S. Sint and A. Vladikas, “Twisted mass QCD and lattice approaches to the Delta I=1/2 rule”, JHEP 09 (2004), 069, [arXiv:hep-lat/0405028 [hep-lat]].
- [14] D. Mohler, S. Schaefer and J. Simeth, “CLS 2+1 flavor simulations at physical light- and strange-quark masses”, EPJ Web Conf. 175 (2018) 02010, [1712.04884].
- [15] M. Bruno, T. Korzec and S. Schaefer, “Setting the scale for the CLS 2 + 1 flavor ensembles,” Phys. Rev. D **95** (2017) no.7, 074504, doi:10.1103/PhysRevD.95.074504, [arXiv:1608.08900 [hep-lat]].
- [16] William I. Jay and Ethan T. Neil, “Bayesian model averaging for analysis of lattice field theory results”, Phys. Rev. D **103**, 114502 (2021), doi:10.1103/PhysRevD.103.114502, [arXiv:2008.01069].
- [17] Jochen Heitger, Fabian Joswig, Simon Kuberski, “Determination of the charm quark mass in lattice QCD with 2+1 flavours on fine lattices”, JHEP 2021, 288 (2021), [arXiv:2101.02694].
- [18] Straßberger *et. al.*, “Scale Setting for CLS 2+1 Simulations”, [arXiv:2112.06696].
- [19] Gilberto Colangelo and Stephan Durr and Christoph Haefeli, “Finite volume effects for meson masses and decay constants”, [arXiv:hep-lat/0503014].
- [20] Y. Aoki *et. al.*, “FLAG Review 2021”, Eur.Phys.J.C 82 (2022) 10, 869, doi:10.1140/epjc/s10052-022-10536-1, [arXiv:hep-lat/2111.09849].
- [21] Nikolai Husung, “Logarithmic corrections to $O(a)$ and $O(a^2)$ effects in lattice QCD with Wilson or Ginsparg-Wilson quarks”, [arXiv:hep-lat/2206.03536].
- [22] Mattia Bruno and Rainer Sommer, “On fits to correlated and auto-correlated data”, [arXiv:2209.14188].