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The asymptotic approach to the continuum of lattice QCD spectral observables

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Abstract

We consider spectral quantities in lattice QCD and determine the asymptotic behavior of their discretization errors. Wilson fermion with O(a)-improvement, (Möbius) Domain wall fermion (DWF), and overlap Dirac operators are considered in combination with the commonly used gauge actions. Wilson fermions and DWF with domain wall height $M_5 = 1 + O(g_0^2)$ have the same, approximate, form of the asymptotic cutoff effects: $K a^2 \left[\bar{g}^2 (a^{-1}) \right]^{0.760}$. A domain wall height $M_5 = 1.8$, as often used, introduces large mass-dependent $K'(m) a^2 \left[\bar{g}^2 (a^{-1}) \right]^{0.518}$ effects. Massless twisted mass fermions have the same form as Wilson fermions when the Sheikholeslami-Wohlert term [1] is included. For their mass-dependent cutoff effects we have information on the exponents $\hat{\Gamma}_i$ of $\bar{g}^2(a^{-1})$ but not for the pre-factors. For staggered fermions there is only partial information on the exponents.

We propose that tree-level $O(a^2)$ improvement, which is easy to do [2], should be used in the future – both for the fermion and the gauge action. It improves the asymptotic behavior in all cases.

Keywords:

Lattice QCD, Perturbation Theory, Discretisation effects, Effective Field Theory

1. Introduction

Quantum Chromo Dynamics (QCD), the fundamental theory of hadrons and nuclei can be treated perturbatively at small distances (or large momentum transfers, μ), where the running coupling $\alpha_s(\mu)$ is small (asymptotic freedom). Discretizing the theory on a regular space-time lattice with spacing *a* provides further a rigorous definition of QCD in the limit $a \rightarrow 0$. This lattice approach has been developed in the last decades and for many observables \mathcal{P} a numerical "computation" by Monte Carlo simulations yields rather precise results (in large volume) for lattice spacings of $a \approx 0.1 \text{ fm} \dots 0.04 \text{ fm}$. Since these spacings are not orders of magnitude smaller than the typical QCD scales of order 1 fm, care has to be taken to understand the discretisation errors

$$\Delta_{\mathcal{P}}(a) = \mathcal{P}(a) - \mathcal{P}(0), \qquad (1)$$

and remove them by an extrapolation $\mathcal{P}(0) = \lim_{a \to 0} \mathcal{P}(a)$.

So far these extrapolations of numerical data have used the form of the discretisation errors of the classical theory. Results obtained by different discretizations and different collaborations do not always agree at the level of the quoted uncertainties. For example we may look at a presently much discussed

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observable, the hadronic vacuum polarization contribution to the anomalous magnetic moment of the muon [3, 4] The contribution from intermediate distances displayed in figure 4 of ref. [4] differs from computation to computation by much more than the error bars. More cases can be found in the FLAG report on phenomenology-related lattice results [5]. Even if $\Delta_{\mathcal{P}}$ is not the only difficult-to-control uncertainty it is certainly a very important one.

In particular, work by Balog, Niedermayer & Weisz [6, 7] in the also asymptotically free two-dimensional O(3) sigma model has shown that continuum extrapolations can be *very* difficult. A purely classical form of discretisation effects $\Delta_{\mathcal{P}}(a) = ka^2 + O(a^4)$ is completely off in this model. At the same time this work has realized how to use asymptotic freedom to systematically derive the leading asymptotic behavior.

It should not come as a surprise that the asymptotics can be obtained analytically because of the vanishing of the coupling for $\mu = a^{-1} \rightarrow \infty$. The steps to derive the analytic form are 1) formulate an effective field theory for the *a*-expansion. It is Symanzik's effective theory, SymEFT [8, 9, 10, 11, 12], given by insertions of dimension six local operators (we assume O(*a*)improved QCD throughout) into the continuum path integral 2) obtain the coefficients of these operators by matching effective theory and continuum theory at the renormalization scale $\mu = a^{-1}$, and 3) rewrite the result in terms of (in general non-perturbative) renormalization group invariants and coefficient functions which run with the scale a^{-1} .

We have explained these steps in detail in [13] for the example of the Yang-Mills theory. Here we define the ingredients in the final formula, ¹

$$\Delta_{\mathcal{P}} \sim a^2 \sum_i \hat{c}_i \left[2b_0 \bar{g}^2 (a^{-1}) \right]^{\hat{\Gamma}_i} \mathcal{M}_{\mathcal{P},i}^{\text{RGI}}, \qquad (2)$$

give numerical results and discuss them for relevant discretizations.

Observables \mathcal{P} are given by (functions of) correlation functions $\langle O \rangle$, where O may be a combination of local fields and $\langle . \rangle$ denotes the Euclidean lattice path integral. The SymEFT local continuum Lagrangian,

$$\mathcal{L}_{\text{Sym}} = \mathcal{L}_{\text{cont}} + a^2 \sum_{i} \bar{c}_i(g^2) \mathcal{B}_i(x) + \dots$$
(3)

describes the *a*-dependence of a scale independent $\langle O \rangle$ through local operators. First order corrections in a^2 are given by the insertions,

$$\mathcal{M}_{O,i}(\mu) = -\int \mathrm{d}^4 y \, \langle O \, \mathcal{B}_i(y;\mu) \rangle_{\mathrm{cont}} \,, \tag{4}$$

of the dimension six operators \mathcal{B}_i renormalized at a scale μ . These and therefore also $\mathcal{M}_{\mathcal{P},i}(\mu)$ are turned into scale-independent ones by

$$\mathcal{M}_{\mathcal{P},i}^{\mathrm{RGI}} = \left[2b_0 \bar{g}^2(\mu) \right]^{-\hat{\gamma}_i} \mathcal{M}_{\mathcal{P},i}(\mu) \times \left[1 + \mathrm{O}(\bar{g}^2(\mu)) \right]$$
(5)

where $\hat{\gamma}_i$ are the leading anomalous dimensions,

$$\mu \frac{\mathrm{d}}{\mathrm{d}\mu} \mathcal{B}_i(y;\mu) = 2b_0 \,\bar{g}^2(\mu) \,\hat{\gamma}_i \,\mathcal{B}_i(y;\mu) + \mathcal{O}(\bar{g}^4(\mu)) \,. \tag{6}$$

The final ingredient in eq. (2) is

$$\hat{\Gamma}_i = \hat{\gamma}_i + n_i^{\rm I},\tag{7}$$

where $n_i^{\rm I}$ give the leading perturbative behavior of

$$\bar{c}_i(g^2) = \hat{c}_i g^{2n_i^1} \times (1 + \mathcal{O}(g^2)).$$
 (8)

For example in a tree-level improved theory we have $n_i^{I} > 0$ for all *i*.

The one-loop anomalous dimensions do not depend on the renormalization scheme. We obtained them from the divergences in dimensional regularization, following the strategy described in [13]. Details as well as analytic expressions are given in [14], results for Gradient Flow obervables [15] in the pure gauge theory in [16].

2. Common Lattice discretisations and Symanzik effective Lagrangian

We start the discussion of a few commonly used formulations from the discretized actions,

$$S_{\text{lat}} = S_{\text{G}} + S_{\text{F}}, \ S_{\text{F}} = \sum_{x} \overline{\psi}(x) \mathcal{D}_{\text{lat}} \psi(x),$$
 (9)

of massless QCD. The gauge action, S_G , is a sum of the trace of parallel transporters around the plaquettes of the lattice for the original Wilson action [17]. Other pure gauge actions are listed e.g. in [13], where also the *a*-expansion has been discussed in detail for the pure gauge theory. The classical *a*-expansion of S_G reads [18],

$$S_{\rm G} = \int d^4 x \left\{ -\frac{1}{2g_0^2} \operatorname{tr} F^2 + a^2 \sum_{i=1}^2 \omega_i O_i + \dots \right\}, \qquad (10)$$

where the ellipsis contains terms which can be eliminated by the equations of motion of the continuum theory as well as $O(a^4)$ terms or total divergences.² The expansion coefficients of the operators

$$O_1 = \frac{1}{g_0^2} \sum_{\mu,\nu,\rho} \operatorname{tr} \left(D_{\mu} F_{\nu\rho} D_{\mu} F_{\nu\rho} \right), \tag{11}$$

$$O_2 = \frac{1}{g_0^2} \sum_{\mu,\nu} \operatorname{tr} \left(D_{\mu} F_{\mu\nu} D_{\mu} F_{\mu\nu} \right)$$
(12)

are denoted by ω_i . The operator O_2 breaks continuum O(4) symmetry down to the lattice group H(4).

For a number of current large scale simulations of QCD, e.g. by MILC [19], CLS [20] and KEK [21], Symanzik tree-level improved gauge actions are used where $\omega_1 = \omega_2 = 0$ by construction [18]. Instead, RBC/UKQCD [22] and ETMc [23] use the Iwasaki gauge action with

$$\omega_1 = 0, \ \omega_2 = -0.248, \tag{13}$$

while the Wilson plaquette action with

$$\omega_1 = 0, \ \omega_2 = 1/12, \tag{14}$$

is hardly used any more. See also the discussion in [13].

The set $\{O_1, O_2\}$ not only appears in the classical expansion, but it is also the complete set of dimension six pure gauge operators in SymEFT. They are invariant under the symmetries of the lattice theory and exclude total divergence operators. Furthermore operators related to fermion ones by the equations of motion² are dropped since they do not contribute to on-shell matrix elements eq. (4) [18]. The relevant lattice symmetries are Euclidean reflections, charge conjugation, H(4) and gauge transformations. The coefficients of O_i in the effective Lagrangian are $\bar{\omega}_i = \omega_i + O(g_0^2)$. The leading ω_i are sufficient to determine the coefficients \hat{c}_i when $n_i^{I} = 0$, see below.

We turn to $S_{\rm F}$ and include in our discussion the most commonly used discretizations $\mathcal{D}_{\rm lat}$ of the Dirac operator. These have the same space-time symmetries as $S_{\rm G}$ but depending on

¹We denote by $b_0 = (11 - 2N_{\rm f}/3)/(4\pi)^2$ the lowest order coefficient of the β function.

Table 1: Fermion discretizations and symmetries of the mass-less Dirac operators. The $U(1)_{\bar{A}}$ symmetry of staggered fermions [24] is not to be mixed up with the continuum (broken) $U(1)_{A}$.

description	$\mathcal{D}_{ ext{lat}}$	flavor symmetries
chiral	\mathcal{D}_{χ}	$SU(N_f)_L \times SU(N_f)_R \times U(1)_V$
Wilson	\mathcal{D}_{W}	$\mathrm{U}(N_\mathrm{f})_\mathrm{V}$
staggered	$\mathcal{D}_{\mathrm{st}}$	$U(1)_B \times U(1)_{\tilde{A}}$

 \mathcal{D}_{lat} we have different flavor (vector and chiral) symmetries as listed in Tab. 1.

"Chiral" actions are invariant under SU(N_f)_L × SU(N_f)_R × U(1)_V for vanishing quark masses. The symmetry transformation has a special form on the lattice [25], but SymEFT is invariant under the standard continuum transformations. All actions satisfying the Ginsparg-Wilson (GW) relation [26] fall into this category, and Domain wall fermion discretizations (DWF) [27, 28, 29] can be included approximately – usually to a very good approximation. We need again the classical *a*-expansion ($\sigma_{\mu\nu} = \frac{i}{2} [\gamma_{\mu}, \gamma_{\nu}]$)

$$\mathcal{D}_{\text{lat}} = D_{\mu}\gamma_{\mu} - a\,\omega_{\text{sw}}\frac{i}{4}\sigma_{\mu\nu}F_{\mu\nu} + a^{2}\omega_{3}\sum_{\mu}\gamma_{\mu}D_{\mu}^{3} + \dots, \quad \omega_{3} = 1/6, \qquad (15)$$

of the Dirac operators given explicitly in 6.1. The meaning of the ellipsis is as above. The above simple structure is due to the form of the Wilson Dirac operator which also underlies the considered solutions of the GW relation. At this level, only the coefficient ω_{sw} of the Pauli-term can be different. For chiral actions, it vanishes due to the GW relation and for Wilson we assume that O(a) improvement has been taken care of and $\omega_{sw} = 0$. Later we will remark on the Pauli term in connection with twisted mass fermions. Note that $\sum_{\mu} \gamma_{\mu} D_{\mu}^{3}$ is a further source of O(4) violations.

Even though only one operator of dimension six appears in the classical expansion, it mixes with all other operators of dimension six under renormalization. Apart from the purely gluonic ones from above, they are given by 4-fermion operators of the form

$$O_i = g_0^2 (\overline{\psi} \Sigma_i \psi)^2, \qquad (16)$$

$$\Sigma_{4\dots7} = \gamma_{\mu}, \gamma_{\mu}\gamma_{5}, \gamma_{\mu}T^{a}, \gamma_{\mu}\gamma_{5}T^{a}, \qquad (17)$$

$$\Sigma_{8...13} = 1, \gamma_5, \sigma_{\mu\nu}, T^a, \gamma_5 T^a, \sigma_{\mu\nu} T^a, \qquad (18)$$

with the standard summation convention (e.g. $O_{13} = \sum_{\mu,\nu,a} g_0^2 (\overline{\psi} \sigma_{\mu\nu} T^a \psi)^2$). The fields eq. (18) are present only for Wilson fermions because they are neither invariant under $SU(N_f)_L \times SU(N_f)_R$ nor under $U(1)_{\tilde{A}}$ transformations. Note that their tree-level coefficients vanish,

$$\omega_i = 0, \quad i = 8 \dots 13,$$
 (19)

for an action of the form eq. (9).

We now turn to the effects of quark masses. Already the continuum mass term

$$\mathcal{L}_{\rm m}^{\rm cont} = \overline{\psi} m \psi \,, \quad m = {\rm diag}(m_1, \dots, m_{N_{\rm f}}) \tag{20}$$

breaks the flavor symmetries down to $U(1)^{N_f}$. The same is true for chiral and Wilson fermions and therefore SymEFT contains all additional dimension six operators invariant under this reduced symmetry. These eleven operators, listed in 6.2, contain up to the third power of the mass matrix.

For Wilson fermions, the mass-term is form-identical to the continuum one and also the use of the equations of motion of the massive continuum theory does not introduce any new massive operators:

$$\omega_i^{\mathsf{W}} = 0, \quad i \ge 14. \tag{21}$$

In contrast, the classical expansion of actions (45) with lattice chiral symmetry yields

$$\mathcal{L}_{m}^{\chi} = \mathcal{L}_{m}^{\text{cont}} + a^{2} [\omega_{14}^{\chi} O_{14} + \omega_{18}^{\chi} O_{18}] + \dots, \qquad (22)$$

$$O_{14} = \frac{\iota}{4} \overline{\psi} \, m \, \sigma_{\mu\nu} F_{\mu\nu} \psi \,, \quad O_{18} = \overline{\psi} \, m^3 \psi \,, \quad (23)$$

after using the continuum equations of motion. The coefficients are

$$\omega_{14}^{\text{ov}} = 1, \qquad \omega_{14}^{\text{DWF}} = \frac{-2(M_5 - 1)}{M_5(2 - M_5)}$$
 (24)

$$\omega_{18}^{\text{ov}} = 1/4, \qquad \omega_{18}^{\text{DWF}} = \frac{(M_5 - 1)(M_5^2 - 3M_5 + 1)}{M_5^2(2 - M_5)^2}, \qquad (25)$$

where M_5 is the dimensionless domain wall height for $g_0 = 0$, see (44). All coefficients of massive operators vanish when M_5 is set to one or approaches one as $g_0^2 \rightarrow 0$. We include $M_5 \neq 0$ because it has been used in large-scale simulations.

3. Exponents $\hat{\Gamma}$ and coefficients \hat{c}

The operators O_i discussed in the previous section mix under renormalization. For the central eq. (2) we need the coefficients of operators \mathcal{B}_i , which do not mix at one-loop and therefore have a unique power $\hat{\Gamma}_i$. The renormalization of dimension six operators has been considered before, see e.g. [30, 31, 32]. Here we have to take into account a larger set including the O(4) noninvariant operators. The computation of their one-loop anomalous dimensions was done along the lines of [13] and is described in detail in [14]. Here we summarize the results and provide suggestions how to use them.

We temporarily order the operators such that the massive ones come first, $Q_i = O_{r(i)}$, r(i) = i + 13, i = 1...11, r(i) = i - 11, i = 12...24. Then the one-loop anomalous dimension matrix η , defined by

$$\mu \frac{d}{d\mu} Q_i(\mu) = 2b_0 \,\bar{g}^2(\mu) \,\sum_j \eta_{ij} \,Q_j(\mu) + \mathcal{O}(\bar{g}^4(\mu)) \,, \qquad (26)$$

has the block structure

$$\eta = \begin{pmatrix} \eta_{\rm mm} & 0 & 0\\ \eta_{\chi m} & \eta_{\chi \chi} & 0\\ \eta_{\rm wm} & \eta_{\rm w \chi} & \eta_{\rm ww} \end{pmatrix}.$$
 (27)

²For example the operator $\frac{1}{g_0^2} \operatorname{tr} (D_{\mu} F_{\mu\nu} D_{\rho} F_{\rho\nu})$ can be replaced by a fermionic one using the equation of motion.



Figure 1: Coefficients \hat{c}_i . Gray entries just indicate the position of the unknown \hat{c}_i with $n_i = 1$.

Blocks are vanishing because massless operators do not mix into massive ones and chirally non-invariant operators do not mix into chirally invariant ones. We diagonalize η in the form

$$V \eta V^{-1} = \operatorname{diag}(\lambda_1, \dots, \lambda_{24}), \qquad (28)$$

with a lower triangular block matrix V. It is composed of the left eigenvectors of η and lets us rewrite the full d = 6 Lagrangian at leading order in the coupling as

$$\mathcal{L}_{d=6} = \sum_{i} \omega_i \mathcal{Q}_i = \sum_{i} \bar{c}'_i \mathcal{B}'_i, \quad \bar{c}'_i = \sum_{j} \omega_{r(j)} (V^{-1})_{ji}.$$
(29)

Somewhat arbitrarily we normalize

$$\mathcal{B}'_i = V_{ij} Q_j \tag{30}$$

to the leading Q_j : for each *i* the largest absolute value of V_{ij} is set to one.

In the massive theory, there are degeneracies $\lambda_i = \lambda_{j\neq i}$. Such terms contribute with the same power $\bar{g}^{2\hat{\Gamma}_i}$ in eq. (2). We thus add them up and order the eigen-values at the same time,

$$\hat{\gamma}_{p(i)} = \lambda_i < \hat{\gamma}_{p(i)+1}. \tag{31}$$

$$\mathcal{B}_j = \bar{c}_j^{-1} \sum_{\{i|p(i)=j\}} \bar{c}_i' \mathcal{B}_i', \qquad (32)$$

with the factor \bar{c}_j chosen again to normalize to the leading Q_j . Note that the case $\bar{c}'_i = 0 \forall i | p(i) = j$ occurs only for nondegenerate eigen-values. In that case we have no contribution from \mathcal{B}_j at leading order in g^2 , which means that $n^I_j \ge 1$ in eq. (8) and we assume $n^I_j = 1$. The coefficient \hat{c}_j is then not known. Otherwise, we have $\hat{c}_j = \bar{c}_j(0)$ and arrive at the ingredients \hat{c}_j , $\hat{\Gamma}_j$ of eq. (2).

Numerical results for $N_f = 3, 4$ are compiled in table 2 and illustrated in figure 1. Additionally we give the massive \mathcal{B}_i , i = 1, 3, 7 in table 3. They contribute only when quark masses are non-zero and are marked by b=m in table 2 and by blue entries in figure 1. Large values are encountered for \hat{c}_i^G and the massive $\hat{c}_{1,3,7}^{OWF}$ if $M_5 = 1.8$:

$$\hat{c}_{1,3,7}^{\text{DWF}} = \begin{cases} (-0.814, -5.533, -1.686) \text{ for } N_{\text{f}} = 3\\ (-0.922, -5.533, -1.692) \text{ for } N_{\text{f}} = 4 \end{cases}$$
(33)

3.1. Renormalisation schemes and a^2m^n effects

Apart from O_{14} and O_{15} the massive O_i are either of the form

$$O_i = \frac{f_i(m)}{2g_0^2} \operatorname{tr} F^2, \quad i = 16, 17,$$
 (34)

$$O_i = \overline{\psi} h_i(m) \psi, \quad i \ge 18, \qquad (35)$$

with $f_i(m)$, $h_i(m)$ functions of the quark mass matrix m. For continuum extrapolations in a massive hadronic renormalisation scheme³, such terms are just absorbed into the renormalisation of the theory and do not contribute to cutoff effects. In

particular, this is so when one extrapolates to the continuum at the physical point or in the chiral limit. We keep those terms because in practice one often uses mass-independent renormalisation schemes (see the discussion in [33] at the level of O(a)) or performs combined extrapolations to the physical point and the continuum limit (see e.g. [34]). Then different values of the renormalized masses enter in one extrapolation formula and all massive terms contribute to the a^2 effects unless their coefficients vanish.

A look at table 3 shows that O_{15} does not contribute at all and only \mathcal{B}_3 contains O_{14} .

3.2. Numerically dominant contributions

The general form of lattice artifacts is complicated because several terms with similar $\hat{\Gamma}_i$ contribute. Fortunately numerically small suppression factors are present which may be taken into account. Indeed, a look at figure 1 shows that the coefficients \hat{c}_i differ drastically in magnitude. We have no reason to expect such variations also for the unknown $\mathcal{M}_{\mathcal{P},i}^{\text{RGI}}$. Despite their somewhat arbitrary normalization we assume that they are comparable. Another significant suppression factor is given by the light quark masses, where we assume $am_k \leq am_{\text{strange}} \lesssim$ 1/20, which holds for reasonable lattice spacings and for the physical strange quark mass m_{strange} .⁴

Two more restrictions need to be taken into account. First, each term in eq. (2) receives corrections of order $\bar{g}^{2\hat{\Gamma}_i+2}$ with unknown coefficients. Not accounting for the quark mass suppression, we should therefore restrict the discussion to $\hat{\Gamma}_i < \hat{\Gamma}_1 + 1$. That border is marked by " χ " in tables and figures. With the quark mass suppression we may further ignore i = 1 and use $\hat{\Gamma}_i < \hat{\Gamma}_2 + 1$ as the effective boundary. It is marked by "massless χ ". Second, the coefficients of the chiral symmetry violating four-fermion operators which contribute only for Wilson fermions are unknown. For strict statements we therefore remain below $\hat{\Gamma}_6$ (border "w") for Wilson fermions.

Let us now enter a more detailed discussion of the numbers.

$$N_{f} = 2 + 1$$

First we consider a tree-level improved gauge action ($\omega_1 = \omega_2 = 0$) and O(*a*) improved **Wilson fermions**. Within a precision of 10^{-2} , we then have a dominance of i = 5, $\hat{c}_5^W = 0.16$, $\hat{\Gamma}_5 = 0.76$ while $\hat{c}_{2,4}^W$ are a factor 1/10 smaller in magnitude and others are even smaller or suppressed by the quark masses. This simple structure arises because only ω_3 is nonvanishing and mixing effects are relatively small. The latter means that also $\mathcal{B}_5 \approx O_3$ is not such a bad approximation. The first term with unknown coefficient has $\hat{\Gamma}_6 = 0.795$. Since it is very close to $\hat{\Gamma}_5 = 0.760$, it can effectively be absorbed into the i = 5 term. This leaves further corrections with $\hat{\Gamma}_9 = 1.11$ and others not far above.

Next we consider actions with **exact lattice chiral symmetry**. Since ω_3 is unchanged, the situation for m = 0 is the same, except that the border for corrections with unknown coefficients is pushed to $\hat{\Gamma}_{10} = 1.126$ and the spectrum above is less dense.

³In a hadronic scheme, the theory is renormalised by specifying $N_{\rm f}$ ratios of hadron masses (or other dimensionfull hadronic parameters). Keeping those fixed when taking the continuum limit, the quark mass matrix is eliminated.

⁴Exceptions are simulations using deliberately heavy quarks as a tool [35].

Table 2: Numerical results for \hat{c} at one-loop ordered according to $\hat{\Gamma}_i$. We label by "b=m" the massive terms where all components $V_{ij} = 0$, j > 11. The coefficients \hat{c}^W or \hat{c}^{ov} assume $\omega_1 = \omega_2 = 0$ and \hat{c}^G is for $\omega_i = -0.248 \, \delta_{i2}$, i.e. the pure contribution of the Iwasaki gauge action. Entries "x" are unknown because the tree-level matching vanishes. The tree-level coefficients at i = 8 ($N_f = 3$) and i = 10 ($N_f = 4$) vanish if $\omega_2 = 0$. In this case, they contribute one power in the coupling further suppressed with unknown coefficients. These contributions are listed with i = 15 and i = 16 respectively. Note that $\hat{c}_i^{\chi} = \hat{c}_i^{ov}$ for all non-massive operators and any of the chiral actions considered. For $\chi = DWF$ and $M_5 = 1$ the coefficients of the massive operators equal the Wilson ones. For $M_5 = 1.8$ [22] we have given them in eq. (33).

	$N_{\rm f} = 3$					$N_{\rm f} = 4$						
i	$\hat{\gamma}_i$	$\hat{\Gamma}_i$	b	\hat{c}^{W}_i	\hat{c}_i^{ov}	$\hat{c}^{ ext{G}}_i$	$\hat{\gamma}_i$	$\hat{\Gamma}_i$	b	\hat{c}^{W}_i	\hat{c}_i^{ov}	$\hat{c}_i^{ m G}$
1	-0.11111	-0.11111	m	-0.02941	0.14706	0.01969	-0.04000	-0.04000	m	-0.03333	0.16667	0.02232
2	0.24731	0.24731		-0.01593	-0.01593	0.09482	0.20902	0.20902		-0.01189	-0.01189	0.07077
3	0.51852	0.51852	m	-0.20000	1.00000	0.30905	0.56000	0.56000	m	-0.20000	1.00000	0.26784
4	0.66790	0.66790		-0.01502	-0.01502	0.08937	0.69814	0.69814		-0.01624	-0.01624	0.09665
							w					
5	0.75991	0.75991		0.16374	0.16374	-0.01535	-0.30097	0.69903		х	_	_
	w											
6	-0.20460	0.79540		Х	_	-	0.81699	0.81699		0.16339	0.16339	-0.01405
	····· <i>X</i> ······						····· X ······					
7	0.88889	0.88889	m	0.14136	-0.80864	-1.48616	0.96000	0.96000	m	0.13551	-0.81449	-0.91566
8	1.00000	1.00000		0	0	1.03015	0.04000	1.04000		Х	-	_
9	0.11111	1.11111		х	-	-	1.13963	1.13963		0.00085	0.00085	-0.00505
10	1.12600	1.12600		-0.00071	-0.00071	0.00422	1.16000	1.16000		0	0	0.53568
	\ldots massless χ \ldots					\ldots massless χ \ldots						
11	1.37854	1.37854		-0.00605	-0.00605	0.03604	0.41903	1.41903		Х	-	_
12	0.46207	1.46207		х	-	_	1.48654	1.48654		0.00844	0.00844	-0.05023
13	1.63762	1.63762		-0.04642	-0.04642	-0.24365	1.85235	1.85235		-0.05666	-0.05666	-0.24313
14	0.94534	1.94534		х	-	-	0.94097	1.94097		Х	-	_
15	1.00000	2.00000		Х	х	Х	1.12000	2.12000		Х	-	-
16	1.11111	2.11111		Х	-	-	1.16000	2.16000		Х	Х	Х
17	1.61201	2.61201		Х	_	-	1.66097	2.66097		Х	_	_

On the other hand, the m_{strange} contributions to $\mathcal{B}_{1,3,7}$ may not be entirely negligible. For DWFs with $M_5 = 1$ they are just due to ω_3 , i.e. identical to those of Wilson fermions – very small. For overlap fermions with the Wilson kernel, the two coefficients $\hat{c}_{3,7}^{\text{ov}}$ are of order one, which may make up for the mass-suppression. For $M_5 = 1.8$, as used in [22], these two coefficients are even much larger (see table 3) and it seems like mass-dependent cutoff effects are very relevant.

Without tree-level improvement in the gauge sector, also the contribution from the gauge action needs to be considered, in particular due to a rather strong mixing from the massive operators. The coefficients \hat{c}^{G} listed in the last column have to be added to \hat{c}^{ov} or \hat{c}^{w} or \hat{c}^{DWF} when the Iwasaki gauge action is used. For other commonly used gauge actions they are not relevant.

$N_{\rm f} = 2 + 1 + 1$

There are no large changes in the numerical values of $\hat{\Gamma}_i$, \hat{c}_i when the charm quark is added. For Wilson fermions, the border where coefficients \hat{c}_i are known is shifted down a little. Below it, the coefficient of a massive operator is largest and it comes with an enhancement by the charm quark mass. The dominant term is therefore expected to be $\hat{c}_3^W = -0.20$, $\hat{\Gamma}_3 =$ 0.56 and a number of terms with $\hat{\Gamma} \ge 0.699$ follow. The first one is generated by chirally non-invariant four-fermion operators with unknown \hat{c}_5 and the following two have relatively large coefficients $\hat{c}_{6,7} \gtrsim 0.14$.

For actions with chiral symmetry, the statements about the massive operators made for $N_{\rm f} = 2 + 1$ remain, except that there is a large enhancement by $m_{\rm charm}/m_{\rm strange} \approx 10$.

4. Practical consequences

What are the consequences of our results for recent and future large scale simulations which achieve precision results?

First we emphasize that the knowledge gained is far from complete. In particular in most applications one has matrix elements of local operators or integrated correlation functions thereof. The logarithmic corrections which arise from the a^2 corrections to these operators have not yet been studied. Similarly, we here do not discuss mixed actions and one has to keep in mind that there are $O(a^3)$ corrections for Wilson fermions and $O(a^4)$ otherwise. Still, all these limitations are no reason to ignore what is known so far.

For staggered fermions we unfortunately have only limited information at present. Since the chiral invariant operators contribute, the range of eigenvalues $\hat{\gamma}_i$ covers at least the range given for them in table 1. Whether particular terms are suppressed by small \hat{c}_i or whether eigenvalues significantly outside the chiral range appear cannot be said at the moment. However, we note that MILC has been using tree-level $O(a^2)$ improved actions [36] for a while. This suppresses all terms by one power of $\bar{g}^2(a^{-1})$. It therefore appears advisable to test a few extrapolations, e.g. with plain a^2 and $a^2\bar{g}^2(a^{-1})$ or even $a^2\bar{g}^4(a^{-1})$ until the anomalous dimension matrix exists including taste-violating operators.

Next, consider the DWF simulations at KEK [21] and the improved Wilson fermion simulations of CLS [20] for $N_f = 2 + 1$. Neglecting the terms proportional to the small quark masses, their asymptotic behavior is given by $\hat{\Gamma}_i$, i = 2, 4, 5, but since \hat{c}_2, \hat{c}_4 are very small it is expected that to a good approximation i = 5 dominates at small but still realistic *a*. This yields

$$\Delta_{\mathcal{P}} \approx K \left[2b_0 \bar{g}^2(a^{-1}) \right]^{0.760} a^2 \times \left[1 + \mathcal{O}(\bar{g}^2(a^{-1})^{0.351}) \right] (36)$$

For DWF, $K = -0.164 \mathcal{M}_{\mathcal{P},5}^{\text{RGI}}$ is given by a single number $\mathcal{M}_{\mathcal{P},5}^{\text{RGI}} \sim \Lambda^2$ for each observable, while for Wilson fermions $\hat{\Gamma}_6 \approx \hat{\Gamma}_5$ such that we can combine both contributions $K = \hat{c}_6 \mathcal{M}_{\mathcal{P},6}^{\text{RGI}} - 0.164 \mathcal{M}_{\mathcal{P},5}^{\text{RGI}}$ from i = 5 and i = 6. Recall that \hat{c}_6 is an unknown one-loop coefficient which is present only when chiral symmetry is violated.

The DWF simulations of RBC/UKQCD are different both because they use the Iwasaki gauge action and because they have $M_5 = 1.8$. This yields $\hat{c}_i = \hat{c}_i^{\text{DWF}} \Big|_{M_5=1.8} + \hat{c}_i^{\text{G}}$ and

$$\Delta_{\mathcal{P}} \approx -0.079 \left[2b_0 \bar{g}^2 (a^{-1}) \right]^{0.247} a^2 \mathcal{M}_{\mathcal{P},2}^{\text{RGI}} -0.074 \left[2b_0 \bar{g}^2 (a^{-1}) \right]^{0.668} a^2 \mathcal{M}_{\mathcal{P},4}^{\text{RGI}}$$
(37)

$$\Delta_{\varphi}^{\text{massive}} \approx -0.147 \left[2b_0 \bar{g}^2 (a^{-1}) \right]^{0.760} a^2 \mathcal{M}_{\varphi,5}^{\text{RGI}} + \Delta_{\varphi}^{\text{massive}}$$
$$\Delta_{\varphi}^{\text{massive}} \approx -0.794 \left[2b_0 \bar{g}^2 (a^{-1}) \right]^{-0.111} a^2 \mathcal{M}_{\varphi,1}^{\text{RGI}}$$
$$-5.22 \left[2b_0 \bar{g}^2 (a^{-1}) \right]^{0.519} a^2 \mathcal{M}_{\varphi,3}^{\text{RGI}}.$$
(38)

It is unclear which terms will be dominant. The *am*_{strange} suppression is not large enough to compensate the large pre-factors of the massive terms. When continuum extrapolations are carried out at fixed renormalized masses, the effects of $\mathcal{M}_{\mathcal{P},1}^{\text{RGI}}$ are absorbed into the renormalisation of quark masses and coupling constant. In such a situation, the dominance of the $\mathcal{M}_{\mathcal{P},3}^{\text{RGI}}$ term may be a reasonable assumption.

 $N_{\rm f} = 2+1+1$ simulations with twisted mass Wilson fermions at maximum twist have been carried out by ETMc [23]. In contrast to earlier $N_{\rm f} = 2$ twisted mass simulations, they include the Pauli-term with a tad-pole improved tree-level coefficient. For our purpose this means that not only O(*a*) effects are absent (which is guaranteed in any case by automatic O(*a*) improvement at maximal twist [37, 38]), but also double insertions of the Pauli term contribute only at higher order in perturbation theory. Thus, apart from the mass-terms, the asymptotic behavior is similar to RBC/UKQCD, but for $N_{\rm f} = 4$. It is

$$\begin{split} \Delta_{\mathcal{P}} &\sim -0.059 \left[2b_0 \bar{g}^2 (a^{-1}) \right]^{0.209} a^2 \mathcal{M}_{\mathcal{P},2}^{\text{RGI}} \\ &- 0.080 \left[2b_0 \bar{g}^2 (a^{-1}) \right]^{0.698} a^2 \mathcal{M}_{\mathcal{P},4}^{\text{RGI}} \qquad (39) \\ &- 0.150 \left[2b_0 \bar{g}^2 (a^{-1}) \right]^{0.817} a^2 \mathcal{M}_{\mathcal{P},6}^{\text{RGI}} + \Delta_{\mathcal{P}}^{\text{massive}} \,. \end{split}$$

Here the structure of the mass-terms is not known. The anomalous dimensions are as before, but the coefficients $\hat{c}_{1,3,7}$ are not

known, because the full mixing matrix has not yet been evaluated in the theory with the symmetry of the twisted mass term. For more details see [14].

 $N_{\rm f} = 2 + 1 + 1$ simulations with standard Wilson fermions have their own challenges. In particular one should carefully make use of a massive renormalisation and O(*a*) improvement scheme [39]. Beyond that, our results do not show enhanced cutoff effects of O(*a*²). Coefficients $\hat{c}_{1,3,7}^{\rm W}$ of the massive operators are small.

For new simulations with Wilson fermions, or DWFs whether 2+1 or 2+1+1, we suggest to remove ω_3 by complete a^2 improvement at tree-level via [2]

$$\mathcal{D}_{\mathrm{W}} \to \mathcal{D}_{\mathrm{W}} - \frac{a^2}{12} \sum_{\mu} (\nabla_{\mu} + \nabla^*_{\mu}) \nabla^*_{\mu} \nabla_{\mu} \gamma_{\mu} , \qquad (40)$$

where ∇_{μ} , ∇^*_{μ} are the standard gauge covariant forward and backward lattice derivatives. Then all coefficients $\bar{c}_i(0)$ vanish at tree level and we have $n_i^{\rm I} = 1$ for all *i*. For Domain wall fermions it is enough to use this improvement in the kernel operator.⁵

5. Conclusions

In summary, our most robust conclusions are:

1) There is no significantly negative $\hat{\Gamma}_i$ known so far. This is good news since strongly negative $\hat{\Gamma}_i$ slow down the approach to the continuum limit and can have drastic consequences [6]. For staggered fermions, $\hat{\Gamma}_1 < -1$, say, cannot be excluded. However, tree-level O(a^2) improved actions are often used which already ensures $\hat{\Gamma}_i \ge \hat{\gamma}_i + 1$.

2) It is advisable to include tree-level $O(a^2)$ improvement also for Wilson fermion and DWF simulations in the future. For the latter and for twisted mass fermions, one should search for alternatives to the Iwasaki gauge action.

3) For Wilson fermions or DWF with $M_5 = 1 + O(g_0^2)$ with an improved gauge action there is a clear dominance of the asymptotic cutoff-effects by the simple form eq. (36).

For 2+1 DWF with $M_5 = 1.8$ and Iwasaki gauge action the prediction is (37). It is not so obvious how to truncate it to a form with sufficiently few parameters to be used in practice. We argued that the $\mathcal{M}_{\mathcal{P},3}^{\text{RGI}}$ term in (38) dominates due to its large prefactor, but the influence of other powers of \bar{g}^2 may need to be investigated as well.

In general, care should be taken with continuum extrapolations; given the difficulties (higher powers in \bar{g}^2 and in *a*) a verification of the universality of the continuum limit appears more important than ever.

A number of generalizations remain to be investigated: Gradient Flow observables [15, 40], matrix elements of electromagnetic and weak currents, Heavy Quark Effective Theory and staggered quarks. For all of these, the asymptotic a^2 -effects

⁵It may suffice to have the sum over μ extend over $\mu = 1...4$ and leave the extra dimensional couplings of the 5 – *d* operator untouched.

Table 3: Massive basis, \mathcal{B}_i , i = 1, 3, 7 in the form $\mathcal{B}_i = W_{ij}O_j$. Only non-vanishing elements are listed. The complete basis can be reconstructed from the matrix V provided in the files V_Nf3.txt, V_Nf4.txt.

		$N_{\rm f}=3$			$N_{\rm f}=4$		
j	W_{1j}	W_{3j}	W_{7j}	W_{1j}	W_{3j}	W_{7j}	O_j
14	0	0.8333	0	0	0.8333	0	$\frac{i}{4}\bar{\psi}m\sigma_{\mu\nu}F_{\mu\nu}\psi,$
16	1.0000	-0.1471	0	1.0000	-0.1667	0	$\frac{\mathrm{tr}(m^2)}{N_{\mathrm{f}}} \frac{1}{g_{\mathrm{o}}^2} \mathrm{tr}(F_{\mu\nu}F_{\mu\nu})$
18	0	1.0000	1.0000	0	1.0000	1.0000	$\frac{\mathrm{tr}(m)^3}{N\epsilon^3}\bar{\psi}\psi$
20	-0.8889	0.3529	0.3144	-0.9600	0.4000	0.3542	$\frac{\operatorname{tr}(m^2)}{N_{\rm f}}\bar{\psi}m\psi$

have not yet been determined. Part of the necessary preparations and perturbative computations are in progress, but a lot remains to be done.

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6. Appendix

6.1. Lattice Dirac operators

The standard, O(a)-improved, Wilson Dirac operator is [1, 17]

$$\mathcal{D}_{\mathrm{W}} = \frac{1}{2} (\nabla_{\mu} + \nabla^{*}_{\mu}) \gamma_{\mu} - \frac{a}{2} \nabla^{*}_{\mu} \nabla_{\mu} + a \frac{i}{4} c_{\mathrm{sw}} \sigma_{\mu\nu} \hat{F}_{\mu\nu}, \qquad (41)$$

with forward and backward covariant derivatives ∇_{μ} , ∇^*_{μ} , and a discretisation of the field strength tensor, $\hat{F}_{\mu\nu}(x) = F_{\mu\nu}(x) + O(a^2)$. The improvement coefficient $c_{sw} = 1 + O(g_0^2)$ achieves $\omega_{sw} = O(g^2)$ in SymEFT.

We further consider Dirac operators with exact on-shell lattice chiral symmetry [25] based on the GW relation [26]. The massless operators are

$$\mathcal{D}_{\chi}(0) = \frac{k_{\chi}}{a} \left[1 + \gamma_5 H_{\chi}(H_{\chi}^2)^{-1/2} \right].$$
(42)

For the original overlap fermions [41] one needs to insert

$$H_{\rm ov} = \gamma_5 (a \mathcal{D}_{\rm W} - 1), \quad k_{\rm ov} = 1, \quad c_{\rm sw} = 0.$$
 (43)

For Möbius domain wall fermions [28, 29, 42] the kernel operator is given by $(c_{sw} = 0)$

$$H_{\rm DWF} = \gamma_5 \frac{-M_5 + a\mathcal{D}_{\rm W}}{2 - M_5 + a\mathcal{D}_{\rm W}}, \quad k_{\rm DWF} = \frac{M_5(2 - M_5)}{2}.$$
 (44)

up to exponentially small corrections in the extent of the fifth dimension. The dimensionless domain wall height $M_5 \in (0, 2)$ was taken to $M_5 = 1$ [21] and $M_5 = 1.8$ [22] in recent large-scale lattice simulations.

The massive Dirac operators are

$$\mathcal{D}_{\chi}(m) = \mathcal{D}_{\chi}(0) + m\left(1 - \frac{a}{2}\mathcal{D}_{\chi}(0)\right).$$
(45)

We note that only the tree-level value of M_5 enters our considerations. Since besides $M_5 = 1$ also $M_5 = 1.8$ (independent of g_0) has been used, we consider general M_5 , while for overlap fermions we assume that deviations from (43) vanish as $g_0 \rightarrow 0$ (in possible future simulations).

Violations of lattice chiral symmetry, i.e. violations of (42), due to a finite extent of the fifth dimension of DWFs are assumed to be small compared to the discussed cutoff effects. They are beyond the scope of our approach and are hopefully monitored in an independent way.

6.2. Massive operators of SymEFT

The complete massive basis of operators $O_{i\geq 14}$ reads

$$\begin{aligned} O_{14} &= \frac{i}{4} \bar{\psi} m \sigma_{\mu\nu} F_{\mu\nu} \psi, & O_{15} &= \frac{\mathrm{tr}\,(m)}{N_{\mathrm{f}}} \frac{i}{4} \bar{\psi} \sigma_{\mu\nu} F_{\mu\nu} \psi, \\ O_{16} &= \frac{\mathrm{tr}\,(m^2)}{N_{\mathrm{f}}\,g_0^2} \,\mathrm{tr}\,(F_{\mu\nu} F_{\mu\nu}), & O_{17} &= \frac{\mathrm{tr}\,(m)^2}{N_{\mathrm{f}}^2\,g_0^2} \,\mathrm{tr}\,(F_{\mu\nu} F_{\mu\nu}), \\ O_{18} &= \bar{\psi} m^3 \psi, & O_{19} &= \frac{\mathrm{tr}\,(m)}{N_{\mathrm{f}}} \bar{\psi} m^2 \psi, \\ O_{20} &= \frac{\mathrm{tr}\,(m^2)}{N_{\mathrm{f}}} \bar{\psi} m \psi, & O_{21} &= \frac{\mathrm{tr}\,(m)^2}{N_{\mathrm{f}}^2} \bar{\psi} m \psi, \\ O_{22} &= \frac{\mathrm{tr}\,(m^3)}{N_{\mathrm{f}}} \bar{\psi} \psi, & O_{23} &= \frac{\mathrm{tr}\,(m^2) \,\mathrm{tr}\,(m)}{N_{\mathrm{f}}^2} \bar{\psi} \psi, \\ O_{24} &= \frac{\mathrm{tr}\,(m)^3}{N_{\mathrm{f}}^3} \bar{\psi} \psi. \end{aligned}$$

6.3. Additional files with results

The matrices V for the cases $N_f = 3,4$ are given in the included files V_Nf3.txt, V_Nf4.txt. They also contain the eigenvalues $\hat{\gamma}_i$ with more digits than given in the text.

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