Determination of c_{sw} in $N_f = 3+1$ Lattice QCD with massive Wilson fermions

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We develop a strategy for the non-perturbative determination of the $O(a)$-improvement coefficient c_{sw} for Wilson fermions with massive sea quarks. The improvement condition is defined via the PCAC relation in the Schrödinger functional. It is imposed along a line of constant physics designed to be close to the correct mass of the charm quark. The numerical work uses the tree-level improved Lüscher-Weisz gauge action in $N_f = 3+1$ Lattice QCD.

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1. Introduction

In Lattice QCD, the Wilson discretization of the fermion action introduces $O(a)$ cutoff effects, which may be systematically reduced by the well-established Symanzik improvement programme [1]. In the case of massless fermions, only the clover term with the Sheikholeslami-Wohlert coefficient c_{sw} [2] needs to be added to the action, but composite fields require additional improvement terms [3].

The function $c_{sw}(g_0^2)$ has been determined for various numbers of massless, dynamical quark flavours and different actions [4, 5, 6, 7, 8, 9, 10]. It has found successful application in simulations with *massless* quarks (e.g. [11] with $N_f = 4$) or *light* quarks (e.g. [12, 13] with $N_f = 3$). In the latter case, in addition to the clover term there exist *mass-dependent* improvement terms of order $O(am_{q,\text{light}})$, which can usually be treated perturbatively or even be neglected if $am_{q,\text{light}}$ is small.

The present work aims at improvement of the general, non-degenerate four flavor Wilson fermion action with a *massive* charm quark. In that case, an incomplete knowledge of the coefficients of the mass-dependent improvement terms introduces large cutoff effects, see below. We want to avoid both these large effects and the non-perturbative determination of a large number of improvement coefficients. This is possible by switching to a *massive* improvement and renormalization scheme, in which the improvement condition for c_{sw} is formulated at *finite* charm quark mass along a line of constant physics (LCP).

2. Symanzik improvement with four non-degenerate quark flavors

We are interested in lattice QCD simulations with four flavors of Wilson quarks ψ,

$$\mathscr{L} = \mathscr{L}_G + \mathscr{L}_F \,, \qquad\qquad \mathscr{L}_F = \bar{\psi}(D_W + M + m_{\text{crit}})\psi \,, \qquad (2.1)$$

$$\mathscr{L}_{I,0} = \mathscr{L} + a\mathscr{L}_{sw} \,, \qquad\qquad \mathscr{L}_{sw} = c_{sw}(g_0^2)\bar{\psi}\tfrac{i}{4}\sigma_{\mu\nu}F_{\mu\nu}\psi \,, \qquad (2.2)$$

and consider a non-degenerate matrix of bare subtracted quark masses

$$M = \text{diag}(m_{q,u}, m_{q,d}, m_{q,s}, m_{q,c}) \,, \qquad\qquad m_{q,i} = m_{i,0} - m_{\text{crit}} \,. \qquad (2.3)$$

The particular choice of a lattice gauge action $\mathscr{L}_G$ is irrelevant for the present discussion, but will be the tree-level improved Lüscher-Weisz gauge action in section 5. While $\mathscr{L}_{I,0}$ is the correct on-shell $O(a)$ improved action density for simulations at the critical line ($m_{q,i} = 0$), additional mass-dependent $O(a)$ terms arise for non-vanishing quark masses. They read

$$\mathscr{L}_{aM} = \sigma_1\bar{\psi}M^2\psi + \sigma_2\text{Tr}(M)\bar{\psi}M\psi + \left(\sigma_3\text{Tr}(M^2) + \sigma_4\text{Tr}(M)^2\right)\bar{\psi}\psi + \sigma_5\text{Tr}(M)\text{Tr}(F_{\mu\nu}F_{\mu\nu}) \quad (2.4)$$

and should be included in the simulation ($\mathscr{L}_{I,M} = \mathscr{L}_{I,0} + a\mathscr{L}_{aM}$) with suitably chosen coefficients $\sigma_i(g_0^2)$. One may absorb the above improvement terms into a redefinition of the bare parameters of the theory,

$$g_0^2 \rightarrow \tilde{g}_0^2 = g_0^2(1 + ab_g(g_0^2)\text{Tr}[M]/N_f) \,, \qquad m_{q,i} \rightarrow \tilde{m}_{q,i} = m_{q,i}f_i(g_0^2, \{aM\}) \,, \qquad (2.5)$$

where f is a non-trivial function of the bare subtracted quark masses in aM [3, 14] and a number of improvement coefficients related to those in (2.4).

For full $O(a)$ improvement of the action at finite quark mass, a non-perturbative determination of the numerous improvement coefficients is in principle necessary. However, this is clearly out of reach for any number of flavors. In the past, without a charm quark, one could circumvent the problem due to the smallness of the mass-dependent improvement terms. For typical lattice spacings $a \leq 0.1$ fm, assuming $m_{q,s} \approx 100$ MeV and $m_{q,c} \approx 1$ GeV, they are roughly of sizes

$$am_{q,s} \lesssim 0.05 , \qquad am_{q,c} \lesssim 0.5 . \tag{2.6}$$

Hence, a viable way for small lattice spacings and quark masses, i.e. simulations with $N_f \leq 3$, has been to treat the terms appearing in $\mathscr{L}_{aM}$ as small and account for them approximately.

Regarding (2.6), the effects of the charm mass in the improved theory are numerically much more important, which makes the non-perturbative treatment of all improvement coefficients unavoidable. Even if such a treatment was feasible, any uncertainties in the improvement coefficients would be amplified by the large charm mass, leading to a significant uncertainty in the improved theory. Note that the same issue concerns the renormalization constants, for which it arises already at the $O(a^0)$ level,

$$m_{R,i} = Z_m \left[m_{q,i} + (r_m - 1) \frac{\text{Tr}[M]}{N_f} \right] + O(a) . \tag{2.7}$$

In particular for observables in the light sector (no charm valence quarks involved), the large charm mass cutoff and renormalization effects and assigned uncertainties would be likely to surpass the small physical effects of a massive dynamical charm quark [15] that one is interested in.

3. Massive renormalization and improvement scheme

For the reasons discussed in the previous section, the massless renormalization and improvement scheme is impractical and unstable if a physical charm quark is to be included in the sea. Instead, we choose a massive scheme, in which the mass dependent improvement terms are absorbed in the bare parameters Eq. (2.5), which are tuned such that a LCP is followed. Accordingly, the renormalization and improvement conditions are imposed at finite quark masses, and the coefficients become mass-dependent:

$$Z(g_0^2, a\mu) \to Z(g_0^2, aM, a\mu), \quad c(g_0^2) \to c(g_0^2, aM) . \tag{3.1}$$

Here, Z and c are renormalization constants (depending in general on a renormalization scale μ) and improvement coefficients, respectively, and we recall that aM is the bare subtracted mass matrix. The action in the massive scheme then simply reads

$$\mathscr{L}_{I,M} = \mathscr{L} + ac_{sw}(g_0^2, aM) \bar{\psi} \frac{i}{4} \sigma_{\mu\nu} F_{\mu\nu} \psi . \tag{3.2}$$

This scheme dispenses with the need for the non-perturbative determination of a large number of improvement coefficients at the cost of a more complicated renormalization pattern. Note that the mass-dependence of the improvement coefficients, Eq. (3.1), is not a necessity for $O(a)$ improvement, as the difference is of $O(a^2)$ in the action. However, we will use this form both for consistency and in the hope of reducing the overall $O(a^2)$ cutoff effects.

4. Determination of c_{sw} in $N_f = 3+1$

There are two qualifications to be added to the determination of c_{sw} in the massive scheme. First, the major effect of the non-vanishing masses on c_{sw} stems from the charm quark. In order to substantially reduce the effort, it is therefore reasonable to treat the up, down, and strange quark as mass-degenerate light quarks with mass $am_{q,l}$, i.e. to determine c_{sw} in $N_f = 3+1$.

Second, it is not practicable to vary all the bare parameters $(g_0^2, am_{q,l}, am_{q,c})$ and find an interpolating formula for c_{sw} in this 3-dimensional space. Hence, we will fix the masses to approximately physical values, indicated by an asterisk. These two approximations,

$$c_{\text{sw}}(g_0^2, aM) \xrightarrow{N_f=3+1} c_{\text{sw}}(g_0^2, am_{q,l}, am_{q,c}) \xrightarrow[\text{masses}]{\text{fix ren.}} c_{\text{sw}}(g_0^2, am_{q,l}^\star, am_{q,c}^\star) , \qquad (4.1)$$

together explicitly introduce $O(a^2)$ effects proportional to

$$m_{q,u} - m_{q,l}^\star, \quad m_{q,d} - m_{q,l}^\star, \quad m_{q,s} - m_{q,l}^\star, \qquad m_{q,c} - m_{q,c}^\star , \qquad (4.2)$$

which modify the already existing cutoff effects of this order. These modifications are small if the mass differences are small. The relevant point obviously is to ensure that the last difference is not too large.

4.1 Line of constant physics

The improvement condition on c_{sw} will be imposed with the help of Schrödinger functional correlation functions (sec. 4.2). The relevant physical scales of the $N_f = 3+1$ theory in such a finite volume are the size L of the box and the renormalization group invariant masses M_l and M_c (not to be confused with the mass matrix M) of the light and charm quark, respectively. The bare masses are fixed to $m_{q,l}^\star$ and $m_{q,c}^\star$ (cf. Eq. (4.1)) by requiring the RGI masses to assume their physical values, $M_l^\star$ and $M_c^\star$. In order to fix these in physical units, a scale is needed. The obvious choice is L, which we keep constant as well, at a value $L^\star$ to be specified:

$$L = L^\star, \quad LM_l = L^\star M_l^\star, \quad LM_c = L^\star M_c^\star . \qquad (4.3)$$

Not only is the approach to keep all physical scales fixed convenient, it also has the advantage of avoiding possibly large $O(a)$ ambiguities in c_{sw}, by forcing these to vanish proportional to a in the limit $g_0^2 \to 0$. A discussion can for instance be found in section I.2.4.1 of [16]. The conditions (4.3) define a line of constant physics (LCP), i.e. they determine the bare parameters $(g_0^2, am_{q,l}^\star, am_{q,c}^\star)$ for a given lattice resolution L/a.

In order to realize the LCP on the lattice, it is reformulated in terms of three more easily accessible quantities,

$$\Phi_1 = \bar{g}_{GF}^2(L) \qquad (4.4)$$

$$\Phi_2 = L \cdot \Gamma_{ud} \qquad (4.5)$$

$$\Phi_3 = L \cdot \left(\Gamma_{uc} - \frac{1}{2}\Gamma_{ud} \right) . \qquad (4.6)$$

Here, $\bar{g}_{GF}^2$ is the gradient flow coupling [17] as defined in [18] for Schrödinger functional boundary conditions with $c = 0.3$ by means of the Wilson flow. The functions

$$\Gamma_{ij} = -\tilde{\partial}_0 \log \left(f_{A,I}^{ij}(x_0) \right) \big|_{x_0 = T/2} \, , \tag{4.7}$$

are effective pseudoscalar meson masses with quark flavors i, j defined in terms of the Schrödinger functional correlation function f_A (see e.g. Eq. (6.11) in [3] for its definition). All Φ_i are associated with $T = L$ and vanishing boundary gauge fields. While each of them is a function of all three physical scales (or equivalently all bare parameters), they were chosen such that each of them dominantly depends on a single parameter. In terms of the Φ_i, Eq. (4.3) gets replaced by

$$\Phi_i = \Phi_i^\star \, , \qquad i = 1, 2, 3 \, , \tag{4.8}$$

where the (continuum) values $\Phi_i^\star$ correspond to the scales $L^\star, M_l^\star$ and $M_c^\star$. In order to do the translation between the two sets of quantities, one needs scale setting, mass renormalization and the input parameters $M_l^\star$ and $M_c^\star$. Since this is not available in $N_f = 3 + 1$, we resort to $N_f = 2$ results. While this alters the particular LCP that is established, it again only concerns the explicitly introduced $O(a^2)$ effects in (4.2) via the values with asterisk. In $N_f = 2$, the setting of the scale is available from [19], and the hopping parameters which correspond to the input parameters $M_l^\star$ [19] and $M_c^\star$ [20] can be derived under use of mass renormalization constants [19, 21], the improvement coefficient b_m [21] and the critical hopping parameter κ_{crit} [22]. We then reused the ensembles produced in the course of [22] with

$$L^\star \approx 0.8 \, \text{fm} \tag{4.9}$$

and $L^\star/a = 12, 16, 20, 24, 32$ in order to evaluate $\Phi_i^\star(a/L^\star)$. The results which we employ to define the LCP in its form (4.8) are the continuum extrapolated values. We find

$$\Phi_1^\star = 7.31, \quad \Phi_2^\star = 0.59, \quad \Phi_3^\star = 5.96 \, , \tag{4.10}$$

from $L^\star \approx 0.8 \, \text{fm}$, $M_l^\star \approx M_s^{(N_f=2)}/3 = 138/3 \, \text{MeV}$ [19], and $M_c^\star \approx M_c^{(N_f=2)} = 1.51 \, \text{GeV}$ [20].

4.2 Improvement condition

Along the LCP, we impose the improvement condition for c_{sw} in the Schrödinger functional. As this follows a standard procedure, we will not cover it here and refer to the original literature [3] instead. Concerning the choice of Schrödinger functional parameters, we follow [10], with only a few exceptions. First, with respect to the LCP, $T = L^\star$ is kept, while L is reduced by a factor 2, $L = L^\star/2$. This in particular implies that we use an even number of lattice sites in the temporal direction, in contrast to [10]. Furthermore, the improvement condition in our case is

$$\Delta M^{ud} = 0 \, . \tag{4.11}$$

The quantity ΔM^{ud} corresponds to ΔM (cf. Eq. (3.10) in [10]) in the previous determinations of c_{sw} at vanishing quark masses. However, in contrast to these, we have to specify the quark flavors (u,d) which enter, due to the different masses involved in our case. We thus use the PCAC relation in the light sector, as we are mainly interested in improving light quark physics. Moreover, we do not use a tree-level value $\Delta M^{(0)}$ on the right hand side of (4.11), since this is not needed when one performs the improvement on a line of constant physics, $L = L^\star$.

c_{sw}	g_0^2	κ_l	κ_c	Φ_1	Φ_2	Φ_3	$L^\star \Delta M^{ud}$
1.6	1.7188	0.1403	0.1222	7.10(4)	0.56(2)	5.94(1)	0.133(7)
1.9	1.7847	0.1374	0.1203	7.18(2)	0.59(2)	5.96(1)	0.046(8)
1.95	1.7969	0.1369	0.1199	7.21(4)	0.60(2)	6.00(1)	0.040(8)
2.1	1.8340	0.1356	0.1190	7.36(5)	0.61(3)	6.02(1)	0.013(8)
2.2	1.8534	0.1345	0.1182	7.17(5)	0.60(3)	6.03(1)	0.002(8)
2.3	1.8825	0.13369	0.1180	7.33(6)	0.60(3)	5.96(1)	0.006(10)
2.4	1.9069	0.13278	0.1175	7.34(6)	0.58(4)	5.94(1)	$-0.018(9)$

Table 1: Preliminary results for $L/a = 8$. At the bare parameters given in columns 2-4, the values Φ_i sufficiently close to the LCP were found in $T = L = L^\star$ simulations with vanishing boundary fields. At the very same bare parameters, the quantity in the last column was obtained in simulations with half the spatial size and non-vanishing boundary fields. The simulations were performed with the HMC of the openQCD package [23] and error estimates have been obtained under use of the Γ-method [24].
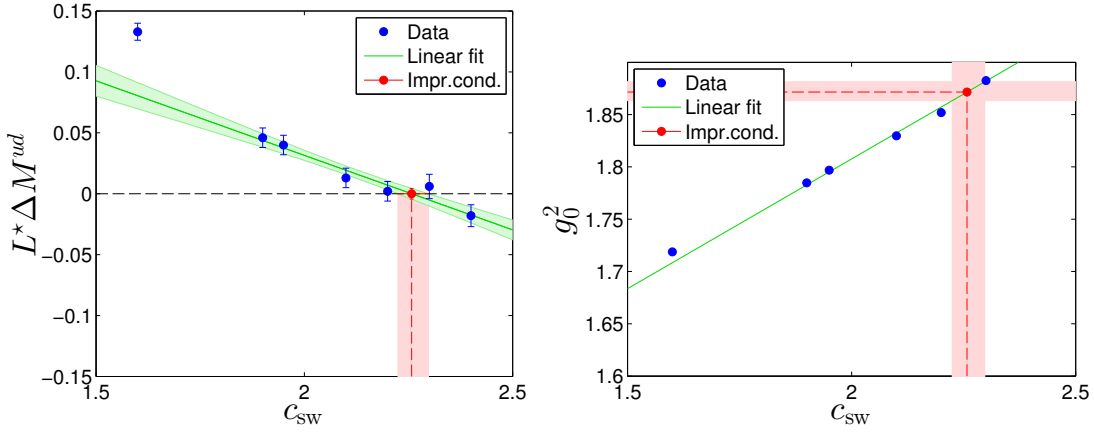

Figure 1: $L^\star \Delta M^{ud}$ (left panel) and g_0^2 (right panel) for $L/a = 8$ as a function of c_{sw} and their linear interpolation (green) to the improvement point (red). The data point at $c_{sw} = 1.6$ is excluded from the fits as it is clearly outside the range of linear behaviour.

5. Results for $L/a = 8$

Preliminary results for $L/a = 8$ are listed in Tab. 1. The bare parameters were tuned such that the Φ_i satisfy the LCP conditions (4.8) with allowed deviations of up to 5% for Φ_1, Φ_3 and 10% for Φ_2. The results for $L^\star \Delta M^{ud}$ as a function of c_{sw} are interpolated to the point where the improvement condition (4.11) is fulfilled, as shown in the left panel of Fig. 1. A subsequent interpolation of g_0^2 to the previously obtained c_{sw} gives the corresponding g_0^2, see the right panel of Fig. 1. The results of this procedure are

$$c_{sw} = 2.26(4), \qquad g_0^2 = 1.87(1). \tag{5.1}$$

6. Summary and outlook

We have developed a strategy to determine c_{sw} in $N_f = 3+1$ with a massive charm quark. In the framework of a massive renormalization and improvement scheme, a line of constant physics is set up which aims at keeping in particular the charm quark mass fixed to an approximately

physical value in order to avoid large mass-dependent cutoff effects. The first point for c_{sw} as a function of g_0^2 on the coarsest lattice with $L/a = 8$, $a \approx 0.1$fm, has been computed. Simulations on finer lattices, which correspond to smaller g_0^2 and will enable contact with perturbation theory, are on the way. So far, the main effort was in tuning to the proper line of constant physics, but this step will become easier due to the gained knowledge. The invested effort is also valuable as the approximate knowledge of $\kappa_c(g_0^2)$ will help to plan subsequent simulations in the improved theory with a massive charm.

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