Lattice simulations with \( N_f = 2 + 1 \) improved Wilson fermions at a fixed strange quark mass

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The explicit breaking of chiral symmetry of the Wilson fermion action results in additive quark mass renormalization. Moreover, flavour singlet and non-singlet scalar currents acquire different renormalization constants with respect to continuum regularization schemes. This complicates keeping the renormalized strange quark mass fixed when varying the light quark mass in simulations with \( N_f = 2 + 1 \) sea quark flavours. Here we present and validate our strategy within the CLS (Coordinated Lattice Simulations) effort to achieve this in simulations with non-perturbatively order-\( a \) improved Wilson fermions. We also determine various combinations of renormalization constants and improvement coefficients.

I. INTRODUCTION

With the gradual removal and reduction of systematic sources of error, including finite volume, unphysical quark mass and lattice spacing effects, Lattice QCD simulations have gained prominence in predicting non-perturbative matrix elements that are of phenomenological importance. Present-day large scale simulations employ a multitude of quark actions, namely, overlap and domain wall actions, staggered actions, twisted mass Wilson actions at maximal twist and Wilson actions.

On the one hand overlap and domain wall actions (with a large extent in the fifth direction) have the theoretically most desirable properties, including automatic order-\( a \) improvement and an exact chiral symmetry at non-vanishing values of the lattice spacing \( a \). On the other hand Wilson fermions are cheaper to simulate in comparison and no approximations such as the uncontrollable rooting of fermionic determinants are required. Furthermore, unlike in the staggered or twisted mass formulations, no taste or unphysical isospin symmetry breaking takes place: Simulating QCD with \( N_f = 2 + 1 \) flavours, where we assume the light quarks to be mass-degenerate, there is only one pion mass \( M_\pi \) and one kaon mass \( M_K \).

While in the other fermion formulations mentioned above lattice effects are of order \( a^2 \) for most matrix elements, the naive Wilson action has artefacts of order \( a \) that need to be removed non-perturbatively, in order to improve the action and operators. Another draw-back is additive quark mass renormalization. While in the continuum only for the axialvector current a distinction between flavour singlet and non-singlet dimension three quark bilinears needs to be made, in the Wilson formalism these quark mass combinations (or, equivalently, scalar currents) renormalize differently. In simulations with dynamical sea quarks this complicates parameter tuning within the quark mass plane.

Traditionally, simulations with \( N_f = 2 + 1 \) (or \( N_f = 2 + 1 + 1 \)) fermions have been performed, keeping the strange quark mass approximately fixed while reducing the light quark mass towards its physical point value. For an overview of simulation points of many lattice collaborations that were available a few years ago, see Fig. 1 taken from Ref. \(^1\). For details, see also Refs. \(^2\)\(^3\).

![FIG. 1. Positions of some lattice simulations in the quark mass plane, taken from Ref. \(^1\) (\( M_m \sim \sqrt{m_\pi} \), \( 2M_K^2 - M_\pi^2 \)). For details, see also Refs. \(^2\)\(^3\).](image_url)

\( ETMC '10 \)\(^{(2+1+1)}\)
\( MILC '10 \)
\( QCDSF-UKQCD '10 \)
\( BMWc'10 \)
\( PACS-CS '09 \)
\( RBC-UKQCD '10 \)
\( HSC '08 \)

\( M_\pi \) \([\text{MeV}]\)
\( M_K \) \([\text{MeV}]\)

For \( (M_\pi \sim \sqrt{m_\pi} , (2M_K^2 - M_\pi^2)^{1/2} \sim \sqrt{m_\pi}) \). For details, see also Refs. \(^2\)\(^3\).
It was realized by the QCDSF collaboration [4] that extrapolating along a line where the sum of lattice quark masses \( m_u + m_d + m_s = 2m_{\ell} + m_s \) is kept constant (the green outliers in Fig. [1]) can be very advantageous, since gluonic observables or the centres of mass of meson and baryon multiplets dominantly depend on the trace of the quark mass matrix but are only mildly affected by the difference \( m_s - m_{\ell} \). This allows for a better controlled approach of the physical point along this mass plane trajectory, with only a small variation of the lattice scale, minimizing the risk of missing the physical point. Therefore, only a very moderate subsequent reweighting of quark masses — if at all — may become necessary. Within the \( N_f = 2 + 1 \) CLS effort [7] we follow this strategy.

At moderately fine lattice spacings, \( a \gtrsim (3 \text{GeV})^{-1} \), physical point simulations with a spatial extent of the lattice \( L > 4/M_{\pi} \) are possible. However, for complicated observables or at finer lattice spacings, obtaining meaningful physical point results is still prohibitively expensive. In this situation it is desirable to have a second line in the quark mass plane at hand to validate any extrapolation strategy. This has motivated us within the CLS effort to generate ensembles not only at fixed valence quark mass (close) to its physical value while lowering the light quark mass. This additional trajectory allows us to benefit from SU(2) chiral perturbation theory (ChPT) and to determine the corresponding low energy constants. SU(2) ChPT should be more reliable than SU(3) ChPT as the \( K \) and the (hypothetical) octet \( \eta_8 \) mesons are not particularly light in nature or in the simulations envisaged here. The additional line in the quark mass plane also provides an alternative to Gell-Mann–Okubo style expansions in the SU(3) flavour symmetry breaking parameter [5] [6] [17].

Due to the different renormalization patterns of singlet and non-singlet quark mass combinations, it is not straightforward to keep the renormalized strange quark mass fixed in simulations with Wilson fermions. This is evident from Fig. [1] where no single group managed to keep the renormalized strange quark mass constant, illustrating that even when employing other fermion actions the correct tuning may not be entirely trivial. Here we describe how we achieved an almost constant renormalized strange quark mass, starting from a few existing simulation points with \( 2m_{\ell} + m_s = 3m_{\text{symm}} = \text{const.} \) and additional points along the \( m_s = m_{\ell} \) line that usually will exist, either from searches for the starting point of the \( 2m_{\ell} + m_s = 3m_{\text{symm}} \) trajectory or from non-perturbative renormalization efforts.

This article is organized as follows. In Sec. [II] we introduce our notations and describe the basic method to achieve a fixed strange quark mass in our simulations, including order-\( a \) improvement. In Sec. [III] we give a brief overview of the action used and ensembles generated. We then parameterize our quark mass data and also fit previously undetermined improvement coefficients. In Sec. [IV] we describe our determination of the physical quark mass point. More details on the numerical results and fits are presented in Sec. [V] where we also discuss combinations of improvement coefficients, before we conclude in the final section.

## II. THE METHOD

We define our notation and derive useful relations, which enable us to relate the strange quark and light quark hopping parameters, defining a line of an (almost) constant renormalized strange quark mass. We then order-\( a \) improve this result and discuss how to keep constant renormalized masses of additional valence quark flavours.

### A. Definitions and useful relations

We closely follow the notation of Ref. [18], however, substituting \( \text{Tr} M = 2\pi M_{\pi} \), see below. We assume two mass-degenerate flavours of light sea quarks with masses \( m_1 = m_2 = m_{\ell} \) and one strange sea quark \( m_3 = m_s \). We define \( \kappa_{\text{crit}} \) as the hopping parameter value at which the quark mass from the axial Ward-Takahashi identity (AWI mass) in the flavour-symmetric case \( m_1 = m_2 = m_3 \) vanishes. Lattice quark masses are then defined as:

\[
m_j = \frac{1}{2a} \left( \frac{1}{\kappa_j} - \frac{1}{\kappa_{\text{crit}}} \right).
\]

We introduce the following conventions for averages:

\[
m_{jk} \equiv \frac{1}{2} (m_j + m_k), \quad (2)
\]

\[
\bar{m} \equiv \frac{1}{3} (m_s + 2m_{\ell}), \quad (3)
\]

\[
\bar{m}^2 \equiv \frac{1}{3} (m_{s}^2 + 2m_{\ell}^2). \quad (4)
\]

We consider flavour non-singlet \( (j \neq k) \) pseudoscalar \( P_{jk} = \bar{q}^j \gamma_5 q^k \) and axialvector \( A_{jk}^{A,0} = \bar{q}^j \gamma_\mu \gamma_5 q^k \) currents. The pseudoscalar current is automatically order-\( a \) improved while the improved axial current reads \( A_{jk}^{A} = A_{jk}^{A,0} + \kappa C A \partial_\mu P_{jk}, \) where \( \partial_\mu \) is the symmetrized discrete next neighbour derivative and the improvement coefficient \( C A \) was determined non-perturbatively in Ref. [19].

We define renormalized, order-\( a \) improved currents:

\[
\tilde{A}_{jk}^{A} = Z_A A_{jk}^{A} \left [ 1 + a (3b_{\ell} \bar{m} + b_A m_{jk}) \right ], \quad (5)
\]

\[
\tilde{P}_{jk} = Z_P P_{jk} \left [ 1 + a (3b_{\ell} \bar{m} + b_P m_{jk}) \right ]. \quad (6)
\]

Note that, away from the \( m_s = m_{\ell} \) line, \( m_{\ell} \) defined in this way can be negative for positive AWI masses. The average mass \( \bar{m} \) remains positive.
Note that $Z_P$ will depend on the target renormalization scheme and scale. The factors of 3 are due to the conventions used for $N_f = 3$ in Ref. [18]. For the action we use, $Z_A$ was calculated in Ref. [20]. Renormalized quark masses can be obtained from the axial Ward identity (AWI)

$$\tilde{m}_j + \tilde{m}_k = 2 \tilde{m}_{jk} = \frac{\partial J(0|\tilde{A}^{jk}||\pi^{jk})}{\partial (0|\tilde{P}^{jk}||\pi^{jk})},$$

(7)

where $\pi^{jk}$ is a pseudoscalar state with quark $q^j$ and antiquark $q^k$.

Finally, we define unrenormalized (but improved) non-singlet AWI masses:

$$\tilde{m}_{jk} = \frac{\partial J(0|A^{jk}||\pi^{jk})}{\partial (0|P^{jk}||\pi^{jk})}.$$ 

(8)

These can easily be related to the renormalized quark masses via Eqs. [5]–[7]. The main CLS ensembles are generated along trajectories of constant average lattice quark masses $\overline{m}$ (and therefore $\overline{m}$ is constant up to $\mathcal{O}(a)$ corrections). For non-perturbative renormalization purposes we generated additional ensembles along the SU(3) flavour symmetric trajectory, i.e. $m_s = m_\ell$. We now wish to keep $\overline{m}_s$ fixed, varying $m_\ell$ and adjusting $\kappa_s$ as required.

The renormalized quark masses can be related to the lattice quark masses:

$$\tilde{m}_j = Z_m \left\{ m_j + (m_\ell - 1)\overline{m} + a \left[ b_m m_j^2 + 3 b_m m_j m_\ell \right] + 3 (r_m \overline{d}_m - \overline{b}_m) \overline{m}_s^2 + (r_m d_m - b_m) m_\ell \overline{m}_s^2 \right\}. \quad (9)$$

At an average quark mass $\overline{m} > 0$ the coupling $g^2 = 6/\beta$ that corresponds to a given lattice spacing $a$ will undergo renormalization too, $g_{\text{lat}}^2 \rightarrow g_{\text{lat}}^2 = g^2(1 + b_g a \overline{m})$, where $b_g = 0.012000(2)N_f g_0^2 + \mathcal{O}(g^4)$ [21]. This means that $Z_J = Z_J[g_j^2, a(g_j^2)\mu]$, where we consider $J \in \{m, P, A\}$ and $r_m = r_m[g_j^2, a(g_j^2)\mu]$. The dependence on the renormalization scale $\mu$ is absent in the case of $Z_A$, as the non-singlet axial current does not carry an anomalous dimension. Also the order-$a$ improvement coefficients are functions of $g_j^2$, however, in these cases we can neglect the effect of the difference between $g_j^2$ and $\tilde{g}_j^2$, which is of a higher order in $a$.

Expanding $Z_J$ around $g_j^2$ gives

$$Z_J \left[ g_j^2, a(g_j^2)\mu \right] = Z_J \left[ g_j^2, a(g_j^2)\mu \right] \left\{ 1 + \left[ \frac{\partial \ln Z_J(g_j^2, a\mu)}{\partial g_j^2} + \frac{d \ln Z_J(g_j^2, a\mu)}{d a} \frac{\partial \ln a(g_j^2)}{\partial g_j^2} \right] g_j^2 b_j a \overline{m} + \ldots \right\}$$

and similarly for $r_m$. Note that in this case $d \ln r_m / d \ln a = 0$. The same holds for the scale dependence of $Z_A$ while $Z_m$ carries an anomalous dimension.

Above, we have introduced the $\beta$-function

$$\beta(g_j^2) = -\frac{1}{4\pi} \frac{d g_j^2}{d \ln a} = -\frac{g_j^2}{2\pi} \left( \beta_0 \frac{g_j^2}{16\pi^2} + \ldots \right),$$

(11)

where our normalization convention corresponds to $\beta_0 = 11 - \frac{2}{3}N_f$, and the anomalous dimension of the current (or quark mass) $J$, which reads

$$\gamma_J(g_j^2) = \frac{d \ln Z_J}{d \ln a}.$$ 

(12)

We can eliminate $b_j$ by redefining

$$\tilde{b}_J(g_j^2) \equiv b_j(g_j^2)$$

and

$$\tilde{b}_J(g_j^2) \equiv \frac{\partial \ln Z_J(g_j^2, a\mu)}{\partial g_j^2} + \frac{\gamma_J(g_j^2)}{4\pi \beta(g_j^2)} g_j^2.$$ 

(13)

Analogously, the $\tilde{d}_m$ improvement coefficient can be replaced by $\tilde{d}_m$ to absorb the effect of $b_j$ on $r_m$. Note that the anomalous dimension cancels from the above combination. Both $b_J$ and $b_J$ are of $\mathcal{O}(g^4)$ in perturbation

theory and at present unknown. With these substitutions Eq. (9) becomes

$$\tilde{m}_j = Z_m \left\{ m_j + (m_\ell - 1)\overline{m} + a \left[ b_m m_j^2 + 3 b_m m_j m_\ell \right] + 3 (r_m \overline{d}_m - \overline{b}_m) \overline{m}_s^2 + (r_m d_m - b_m) m_\ell \overline{m}_s^2 \right\},$$ 

(14)

where $Z_m$ now is a function of $g_j^2$, rather than of $\tilde{g}_j^2$. The only other difference between the two equations is the replacement of the bar-coefficients by tilde-coefficients.

Equation (14) implies that we can re-express the (unrenormalized) AWI masses in terms of the lattice masses, see Eqs. (48)–(53) of Ref. [18]:

$$\tilde{m}_{jk} = \frac{Z_P Z_m}{Z_A} \left[ m_{jk} + (m_\ell - 1)\overline{m} + a \left( A m_{jk}^2 + 3 B m_{jk} \overline{m} + 9 C \overline{m}^2 + 3 D \overline{m}_s^2 \right) \right].$$ 

(15)
where
\[ A = b_P - b_A - 2b_m, \]  
\[ B = \bar{b}_P - \bar{b}_A + b_m + 2b_m + \frac{1}{3}(r_m - 1)(b_P - b_A), \]  
\[ C = \frac{1}{3} \left[ (r_m - 1)(\bar{b}_P - \bar{b}_A) + r_m d_m - b_m \right] - \frac{b_m}{2}, \]  
\[ D = \frac{1}{3} \left[ r_m d_m + \frac{b_m}{2} \right]. \]

Note that we independently verified these results of Ref. [13]. However, we replaced \( b_j \mapsto \bar{b}_j \) and \( d_m \mapsto d_m \), absorbing the effect of \( b_2 \) into these new coefficients. The difference between these two sets of improvement coefficients is of \( O(g^4) \) and is given in Eq. (13). The relation between \( N_f = 3 \) quark masses \( m_j^2 + m_\ell^2 = -4m_\ell^2 + 12m_\ell \bar{m} - 9\bar{m}^2 + 3\bar{m}^2 \) was used to derive Eq. (20).

For mass-degenerate up and down quarks it will turn out more convenient to rewrite the order-\( a \) corrections in terms of their functional dependence on \( (m_s - m_\ell)^2 \), \( (m_s - m_d)\bar{m} \) and \( \bar{m}^2 \).

Some of the above improvement coefficients as well as \( Z_m, Z_P \) and \( Z_A \) have been computed to one-loop order in perturbation theory [22] for the tree-level Symanzik improved gauge action that we use in our simulations.

\[ Z \equiv \frac{Z_mZ_P}{Z_A} = 1 + (0.09546 - 0.11058 + 0.06786)C_F g^2, \] \[ b_m = d_m = -\frac{1}{2} - 0.05727(5)C_F g^2, \] \[ b_A = 1 + 0.0881(1)C_F g^2, \] \[ b_P = 1 + 0.0890(1)C_F g^2, \]

where \( C_F = 4/3 \) and terms of \( O(g^4) \) are ignored. This means the difference \( b_A - b_P \) practically vanishes to \( O(g^2) \) while \( b_A - \bar{b}_P \), being a sea quark effect, exactly vanishes to this order. Therefore, keeping the renormalized strange quark mass \( \tilde{m}_s \) constant amounts to keeping the AWI mass \( \tilde{m}_s \equiv 2\tilde{m}_{13} - \tilde{m}_{12} \)

\[ = \tilde{m}_s \frac{Z_P}{Z_A} \left\{ 1 + a \left[ 3(\bar{b}_P - \bar{b}_A)\bar{m} + (b_P - b_A)m_s \right] \right\} \]

fixed, up to \( O(g^4a^m) \) and \( O(g^4am_s) \) corrections with small coefficients. It has been confirmed non-perturbatively [24] that the \( am_s \) term is not unnaturally large. In the absence of other information from non-perturbative approaches, in particular on \( b_A - b_P \), we will keep \( \tilde{m}_s \) fixed instead of \( \tilde{m}_s \).

We remark that for the gauge and fermion action that we use \( r_m \) has been computed perturbatively [25], with the result

\[ r_m = 1 + 0.001158(1)C_F N_f g^4. \]

From our study we will see that the non-perturbative values are much larger.

Differences of AWI quark masses are related by the non-singlet renormalization constant \( Z \) of Eq. (20) to differences of the above lattice quark masses while the average AWI quark mass \( \bar{m} \) is related by \( Z r_m \) to the average lattice quark mass [18, 26–28]. Below we will make use of the relations

\[ 2 \left( m_{13}^2 - m_{12}^2 \right) = \frac{1}{2} \left( m_s + m_\ell \right)^2 - 2m_\ell^2 \]

\[ = -\frac{1}{6} \left( m_s - m_\ell \right)^2 + 2\left( m_s - m_\ell \right)\bar{m}, \] \[ \bar{m} = m^2 + \frac{2}{9} \left( m_s - m_\ell \right)^2. \]

Differences and sums of AWI masses read:

\[ \tilde{m}_s - \tilde{m}_\ell = 2 \tilde{m}_{13} - \tilde{m}_{12} \]

\[ = \tilde{m}_s \frac{Z_P}{Z_A} \left\{ 1 + a \left[ \left( \frac{3}{2} (b_P - b_A) + (b_P - b_A)m_s \right) \right] \right\} \]

\[ = Z \left\{ (m_s - m_\ell) + a \left[ \frac{A}{6} (m_s - m_\ell)^2 + (2A + 3B)(m_s - m_\ell)\bar{m} \right] \right\}, \]

\[ \bar{m} = \frac{1}{3} (\tilde{m}_{12} + \tilde{m}_{23} + \tilde{m}_{31}) = \frac{1}{3} (\tilde{m}_s + 2\tilde{m}_\ell) \]

\[ = Z \left\{ \frac{r_m\bar{m}}{a} + \frac{1}{18} \left( A + 12D \right) (m_s - m_\ell)^2 \right\} \]

\[ + \left( A + 3B + 9C + 3D \right) \bar{m}^2 \] \[ \left\{ \right\}, \]

where \( \tilde{m}_\ell \equiv \tilde{m}_{12}, \) assuming \( \kappa_1 = \kappa_2 \). Having rewritten everything in terms of differences of quark masses and average quark masses, we can re-express the improvement terms through AWI masses, which will allow us to eliminate \( \kappa \) from most equations:

\[ \tilde{m}_s - \tilde{m}_\ell = Z(m_s - m_\ell) \]

\[ = -\frac{a}{Z} \left[ \frac{A}{6} \left( \tilde{m}_s - \tilde{m}_\ell \right)^2 + \frac{B_0}{r_m} \bar{m} (\tilde{m}_s - \tilde{m}_\ell) \right], \]

\[ \bar{m} = Z r_m \bar{m} - \frac{a}{Z} \left[ \frac{C_0 r_m}{9} (\tilde{m}_s - \tilde{m}_\ell)^2 + \frac{D_0}{2r_m} \bar{m}^2 \right], \]

where we substituted the combinations \( B_0, \ldots, B_0, \ldots \), that are normalized such that \( A = B_0 = C_0 = D_0 = 1 \) at

2 For the \( Z_f \) we quote the more precise values given in Ref. [24], using \( c_{SW} = 1 \), which is consistent to this order. The ordering of the numerical values in the first line corresponds to \( Z_m = Z_g^{-1} \), \( Z_P \) and \( Z_A \), where \( Z_m \), and \( Z_P \) are the conversions to the \( \overline{\text{MS}} \) scheme at the scale \( \mu = a^{-1} \). The scale and scheme dependence cancels from the combination \( Z \).
We also made the masses significantly larger than one. Note that
\begin{equation}
\tilde{\kappa} \equiv \kappa_{\text{crit}} \text{,}
\end{equation}

\begin{align}
\kappa_{\text{crit}} &= \lambda \left( 1 + \frac{1}{2} \frac{\kappa_{\ell}}{\kappa_s} \right) \\
\kappa_{\text{crit}}^2 &= \lambda \left( 1 + \frac{1}{2} \frac{\kappa_{\ell}}{\kappa_s} \right) \left( 1 + \frac{1}{2} \frac{\kappa_{\ell}}{\kappa_s} \right)
\end{align}

for 1/2 + O(\kappa^2) and 1 + O(\kappa^2) [see Eqs. (20)–(23)] while all improvement coefficients \( \lambda \) and \( \lambda_1 \) only receive contributions at O(\kappa^4).

Although not needed here, for completeness we also express lattice quark mass combinations through AWI masses:

\begin{align}
m_s - m_\ell &= \frac{1}{2a} \left( \frac{1}{\kappa_s} - 1 \right) \\
\tilde{m}_s &= \left( \frac{1}{\kappa_s} - 1 \right) a Z \text{,}
\end{align}

where we have the left hand side constant. Solving \( \tilde{m}_s = \tilde{m}_{s,\text{ph}} \) for 1/\( \kappa_s \) gives

\begin{align}
\frac{1}{\kappa_s} &= \frac{2}{2 + r_m} \left( 3 \frac{\kappa_{\ell}}{Z} \tilde{m}_{s,\text{ph}} + (1 - r_m) \frac{1}{\kappa_\ell} + \frac{3r_m}{2} \frac{1}{\kappa_{\text{crit}}} \right).
\end{align}

\( \kappa_{\text{crit}} \) and \( \tilde{m}_{s,\text{ph}} \) can be eliminated by subtracting the result at the physical point from both sides of this equation:

\begin{align}
\frac{1}{\kappa_s} &= \frac{1}{\kappa_{s,\text{ph}}} + \frac{2(1 - r_m)}{2 + r_m} \left( \frac{1}{\kappa_\ell} - \frac{1}{\kappa_{\text{crit}}} \right),
\end{align}

i.e. for predicting the target \( \kappa_s \) as a function of \( \kappa_\ell \), up to O(\kappa) corrections, we only need to know the value of the parameter \( r_m \), in addition to determining the physical point. Note that \( r_m > 1 \), which means that as we decrease \( \kappa_\ell \) away from the physical point, we have to increase \( \kappa_s \).

The equality \( 3\tilde{m}_\ell = (\tilde{m}_\ell - \tilde{m}_s) + 3\tilde{m} \) results in the relation

\begin{align}
3\tilde{m}_\ell &= Z \left( \frac{r_m - 1}{\kappa_s} + \frac{2r_m + 1}{\kappa_\ell} - \frac{3r_m}{\kappa_{\text{crit}}} \right),
\end{align}

in analogy to Eq. (37). We can again eliminate \( \kappa_{\text{crit}} \), by subtracting the result at the physical point. Furthermore, we substitute the difference \( \kappa_s^{-1} - \kappa_{s,\text{ph}}^{-1} \) of Eq. (39), giving

\begin{align}
a(\tilde{m}_\ell - \tilde{m}_{s,\text{ph}}) &= Z \left( \frac{r_m - 1}{\kappa_s} + \frac{2r_m + 1}{\kappa_\ell} - \frac{3r_m}{\kappa_{\text{crit}}} \right).
\end{align}

If we are now targeting a value \( \tilde{m}_s \neq \tilde{m}_{s,\text{ph}} \), we can extract the corresponding shift in \( \kappa_s^{-1} \) relative to the physical point from the above equation.

**C. Order-\( a \) improvement**

Here we show how to order-\( a \) improve Eq. (39). However, we refrain from working out the equivalent expression for the light quark mass shift Eq. (41) as for our purposes an approximate determination of the target \( \kappa_\ell \) value is sufficient. Above we have not only related AWI masses to lattice masses, introducing \( Z \) and \( r_m \), but also improvement terms with coefficients \( A \), \( B_0 \), \( C_0 \) and \( D_0 \) have been worked out.

Multiplying Eq. (30) by two and Eq. (31) by three, it is easy to derive an order-\( a \) improved version of Eq. (37):

\begin{align}
3\tilde{m}_s &= Z \left( \frac{2 + r_m}{2a \kappa_s} + \frac{r_m - 1}{\kappa_s} - \frac{3r_m}{2 \kappa_{\text{crit}}} \right) \\
&- \frac{a}{2Z} \left( 4 + C_0 r_m \right) \left( \tilde{m}_s - \tilde{m}_\ell \right)^2 \\
&+ \frac{6B_0}{r_m} \left( \tilde{m}_s - \tilde{m}_\ell \right) \frac{m}{\tilde{m}} + \frac{9D_0 m}{2Z r_m} \frac{m}{\tilde{m}}.
\end{align}

Next we keep \( \tilde{m}_s \equiv \tilde{m}_s(\kappa_s, \kappa_\ell) = \tilde{m}_{s,\text{ph}} \) fixed and compute differences between simulated and physical mass values:
\[
(m_s - \bar{m})^2 - (m_s - \bar{m}_{\text{ph}})^2 = \frac{Z}{2a} \left( \frac{1}{\kappa_s} - \frac{1}{\kappa_{s,\text{ph}}} \right) (\bar{m} + \bar{m}_{\text{ph}} - 2\bar{m}_s),
\]

\[
(m_s - \bar{m}) m - (m_s - \bar{m}_{\text{ph}}) \bar{m}_{\text{ph}} = \frac{Z}{6a} \left( \frac{1}{\kappa_s} - \frac{1}{\kappa_{s,\text{ph}}} \right) [\bar{m}_s - 2(\bar{m} + \bar{m}_{\text{ph}})],
\]

\[
\bar{m}^2 - \bar{m}_{\text{ph}}^2 = \frac{2Z}{9a} \left( \frac{1}{\kappa_s} - \frac{1}{\kappa_{s,\text{ph}}} \right) (\bar{m}_s + \bar{m} + \bar{m}_{\text{ph}}).
\]

Above we have re-expressed the non-singlet combination \( \bar{m} - \bar{m}_{\text{ph}} \) through differences of inverse hopping parameters. We now isolate \( 1/\kappa_s \) in Eq. 42 and subtract the physical point values from both sides of the resulting equation:

\[
\frac{1}{\kappa_s} - \frac{1}{\kappa_{s,\text{ph}}} = \frac{2}{2 + r_m} \left( \frac{1}{\kappa_s} - \frac{1}{\kappa_{s,\text{ph}}} \right) \left\{ 1 - r_m + \frac{a}{6Z} (A + C_0 r_m) (-2\bar{m}_{s,\text{ph}} + \bar{m}_{\text{ph}} + \bar{m}_\ell) + \frac{2B_0}{r_m} (\bar{m}_{s,\text{ph}} - 2(\bar{m}_{\text{ph}} + \bar{m}_\ell)) + \frac{2D_0}{r_m} (\bar{m}_{s,\text{ph}} + \bar{m}_{\text{ph}} + \bar{m}_\ell) \right\}.
\]

Using Eq. (41), we can re-express \( \bar{m}_\ell \) above in terms of \( \kappa_s, \kappa_{s,\text{ph}}, \) and \( \bar{m}_{\text{ph}} \). This gives

\[
\frac{1}{\kappa_s} = \frac{1}{\kappa_{s,\text{ph}}} + \frac{2}{3} \left\{ 1 - r_m + \frac{1}{3} \left[ \frac{B_0 + D_0}{r_m} - (A + C_0 r_m) \right] \frac{\bar{m}_{s,\text{ph}}}{Z} + \frac{1}{3} \left( A + C_0 r_m + \frac{2D_0}{r_m} - 4B_0 \right) \left( \frac{\bar{m}_{\text{ph}}}{Z} + \frac{r_m}{4} \right) \right\},
\]

where

\[
x = \frac{3}{2 + r_m} \left( \frac{1}{\kappa_s} - \frac{1}{\kappa_{s,\text{ph}}} \right).
\]

We employ Eq. (47) to determine the order-\( a \) improved value of \( \kappa_s \). The last term of this equation is numerically subleading since \( \bar{m}_{s,\text{ph}} \approx 0 \) and terms quadratic in \( x \) can be neglected too as long as \( \bar{m}_\ell \ll \bar{m}_s \). Therefore, the dominant order-\( a \) correction amounts to a constant shift of \( \kappa_s^{-1} \), relative to Eq. (29). Note that at tree-level \( r_m = A = B_0 = C_0 = D_0 = 1 \) and therefore, \( \kappa_s = \text{const.} \), as it should be in the non-interacting case.

**D. Comment on additional valence quark flavours**

We now consider the partially quenched situation, introducing additional “charm” valence quarks of the lattice mass

\[
m_c = m_4 = m_5 = \frac{1}{2a} \left( \frac{1}{\kappa_c} - \frac{1}{\kappa_{\text{crit}}} \right),
\]

where \( \kappa_{\text{crit}} \) is still the hopping parameter for the \( N_f = 3 \) case at vanishing quark masses. Again, one can obtain the AWI charm quark mass from Eq. (7). As the charm quark is quenched, rather than using the currents \( A^i_\mu \) and \( \tilde{A}^i_\mu \) with \( j \in \{1, 2, 3\} \), we can also just compute \( \tilde{A}^4_\mu \) and \( \tilde{A}^5_\mu \), pretending we have two distinct (but mass-degenerate) charm quark flavours. In this partially quenched situation, rather than working with the flavour symmetry group SU(3), we have to work with the graded group SU(5|2), replacing mass traces in Eq. (14) by supertraces. The changes can be worked out easily and reduce to the preceding formulæ when replacing the flavour combination 45 by 12 and \( m_c \) by \( m_\ell \). In particular we have

\[
\tilde{m}_c = \frac{Z_\mu}{Z} \tilde{m}_c \left\{ 1 + a \left[ (b_P - b_A) m_c + 3(b_P - b_A) m \right] \right\},
\]

where

\[
\tilde{m}_c = \partial_\mu \langle \sigma_4^A [\pi_4^{45}] \rangle / \langle \pi_4^{45} [\pi_4^{45}] \rangle.
\]

Note that \( m \) above still denotes the mass average over the three sea quark flavours only.

Expressing the renormalized charm quark mass through lattice quark masses, we obtain the following relation between the AWI charm mass and partially
are at the same time on the trajectory ensemble $\sqrt{s_0}/a$, estimates of pion and kaon masses from assigning $\sqrt{s_0}/a = 0.4144(70)$ fm \cite{22} (also the lattice spacings $a$ are estimated in this way), the AWI quark masses in lattice units and the number of molecular dynamics units $N_{MD}$. In most cases the trajectory length is two and measurements are taken every four units. We complement the $\sqrt{s_0}/a$ values determined in Ref. \cite{17} by preliminary estimates obtained on the newly generated ensembles. Note that the ensembles H101, H200 and N202 are at the same time on the $\overline{m} = m_{\text{symm}}$ and $m_s = m_c$ lines. All D100 results are very preliminary due to insufficient statistics. We exclude D100, H200 and rqcd019 from further analysis. Preliminary results are typset in Italic.

| trajectory | ensemble | $\kappa_c$ | $\kappa_s$ | $L\overline{m}_c$ | $N_1 \times N_2^2$ | $\sqrt{s_0}/a$ | $aM_{\text{symm}}$ | $N_{\text{MD}}$ |
|------------|----------|-----------|-----------|-----------------|-----------------|-----------------|-----------------|-------------|
| $\overline{m} = m_{\text{symm}}$ | H101 | 0.13675962 | 0.13675962 | 5.8 | 96 x 32 x 3 | 4.772(5) | 422 | 422 | 0.009201(39) | 0.009201(39) | 800 |
| | H102 | 0.136857 | 0.13649339 | 4.9 | 96 x 32 x 3 | 4.800(6) | 356 | 442 | 0.006502(46) | 0.013836(43) | 7988 |
| | H105 | 0.13697 | 0.13634979 | 3.9 | 96 x 32 x 3 | 4.819(6) | 282 | 467 | 0.003951(52) | 0.018672(52) | 11332 |
| | C101 | 0.13703 | 0.13622041 | 4.6 | 96 x 48 x 3 | 4.824(4) | 223 | 476 | 0.002466(32) | 0.021242(34) | 6208 |
| | D100 | 0.13709 | 0.136103607 | 3.2 | 128 x 64 x 3 | 4.860(4) | 129 | 482 | 0.006801(30) | 0.025552(43) | 492 |
| $m_s = m_c$ | rqcd019 | 0.1366 | 1.366 | 8.4 | 32 x 32 x 3 | 4.545(5) | 607 | 607 | 0.018694(77) | 0.018694(77) | 1686 |
| | rqcd021 | 0.136813 | 0.136813 | 4.7 | 32 x 32 x 3 | 4.925(12) | 340 | 340 | 0.005983(63) | 0.005983(63) | 1541 |
| | rqcd017 | 0.136865 | 0.136865 | 3.3 | 32 x 32 x 3 | 5.100(7) | 238 | 238 | 0.002799(92) | 0.002799(92) | 1849 |
| $\overline{m}_s = \overline{m}_{s,\text{ph}}$ | H107 | 0.136045565908 | 0.136201185143 | 3.1 | 96 x 32 x 3 | 4.665(6) | 368 | 549 | 0.006662(50) | 0.029981(60) | 6236 |
| | H106 | 0.13701570024 | 0.1364870478 | 3.8 | 96 x 32 x 3 | 4.751(6) | 272 | 519 | 0.003775(70) | 0.024029(68) | 6212 |
| | C102 | 0.1370508458 | 0.13619026556 | 4.6 | 96 x 48 x 3 | 4.790(4) | 223 | 504 | 0.002467(34) | 0.029356(54) | 6000 |

In the situation $\overline{m} = m_{\text{symm}}$, unsurprisingly, at least up to order-$a$ effects, $m_c$ (and therefore $\kappa_c$) should be kept constant. One may wonder if, owing to the heavy charm quark mass, discretization effects may be substantial. Examining Eq. (52) we notice that as long as $\overline{m}$ is kept constant only the parametrically small second last term ($m_s - m_c \ll m_{s,\text{ph}}$) changes. Therefore, along the $\overline{m} = m_{\text{symm}}$ trajectory, also keeping track of the dominant order-$a$ effects, $m_c$, i.e. $\kappa_c$, should remain constant. In Secs. $\text{II B}$ and $\text{II C}$ we worked out how $\kappa_c$ has to be varied to keep $\overline{m}_s = \overline{m}_{s,\text{ph}}$ constant. What happens along this line? In this case

$$
\overline{m}_{c,\text{ph}} - \overline{m}_{s,\text{ph}} = Z(m_c - m_s) \left[ 1 + O(a) \right]
$$

should remain constant. This means that in this situation the difference between $1/\kappa_c$ and $1/\kappa_s$ should be kept approximately fixed, too:

$$
\frac{1}{\kappa_c} = \frac{1}{\kappa_s} + \frac{1}{\kappa_{c,\text{ph}}} - \frac{1}{\kappa_{s,\text{ph}}}. \tag{55}
$$

The order-$a$ contributions are again captured by Eq. (52) and the compensation term can be worked out if needed, in analogy to the discussion of Sec. ITIC above.

In fact of the spike that the charm quark is quenched, $r_m$ still appears in the above equation since we defined the lattice quark mass relative to the inverse sea quark critical hopping parameter. It is now clear how to keep the AWI (or the renormalized) charm quark mass approximately constant:

$$
\overline{m}_c - \overline{m} = Z(m_c - \overline{m}) \left[ 1 + O(a) \right]. \tag{53}
$$

Note that when setting $\overline{m}_c = \overline{m}$ and $m_c = m_c$, substituting $m^2 = \overline{m} - \frac{1}{2}(m(m_c - m_c) + \frac{1}{2}(m_c - m)^2) + m m_c$ and $m m_c = \overline{m}^2 - \frac{1}{2}(m(m_c - m_c))$, Eq. (52) reduces to the unquenched case discussed previously, as it should.
We were unable to reliably fit seven (or six) parameters to data from seven ensembles, covering just the \( m = m_{symm} \) and \( m_s = m_{\ell} \) lines. Moreover, \( D_0 \) is insensitive to the \( m = m_{symm} \) points, \( A \) does not depend on the \( m_s = m_{\ell} \) points and a determination of \( B_0 \) requires points at additional positions in the quark mass plane. Therefore, we initially made use of the one-loop estimates

\[
A = 1 + 0.1153(2)C_F g^2, \tag{58}
\]

\[
B_0 = D_0 = 1 + 0.1126(3)C_F g^2, \tag{59}
\]

\[
C_0 = 1 + 0.1140(1)C_F g^2, \tag{60}
\]

see Eqs. \((16), (21) - (25)\) and \((22) - (24)\). After investigating various fits with different combinations of \( A, C_0 \) and \( D_0 \) as free parameters, we found that fixing \( A, B_0 \) and \( D_0 \) to the above one-loop estimates but allowing \( C_0 \) to float gave a good and stable description of the data. Note that the non-perturbatively determined values of \( A \) \cite{24} were not available at the beginning of this study. This then enabled us to predict the \( \kappa_s \) values that corresponded to our target AWI strange quark mass (see Sec. \( \text{IV} \) below), using Eq. \((47)\). Table \( \text{II} \) demonstrates that indeed we managed to keep the AWI strange quark mass \( \hat{m}_s \) constant in simulations with Wilson fermions within statistical errors of 0.3\% and 0.1\% at \( \beta = 3.4 \) and \( \beta = 3.55 \), respectively, see also Fig. \( \text{F} \) below.

After simulating three additional points along the \( \tilde{m}_s = \tilde{m}_{s,ph} = \text{const.} \) trajectory for each lattice spacing, we used the non-perturbative values \( A = 2.91(33) \) and \( A = 2.27(14) \) for \( \beta = 3.4 \) and \( \beta = 3.55 \), respectively, that were obtained employing coordinate space methods \cite{24}, to determine the remaining six parameters from a combined correlated fit to all data. Varying \( A \) within its uncertainty \cite{24} had only a very insignificant impact on the remaining six fit parameters. After excluding the rather heavy (in lattice units) \( \beta = 3.4 \) rqcd019 point from the fit, we have nine and ten ensembles with 15 and 16 different quark mass values at our disposal at \( \beta = 3.4 \) and \( \beta = 3.55 \), respectively.

The resulting fit parameters are shown in Table \( \text{II} \). The data only mildly constrain the parameter \( D_0 \), which comes out to be compatible with zero within large errors. \( r_m, B_0 \), and \( C_0 \) deviate substantially from the perturbative expectations and \( B_0 \) even comes out negative. However, as one would expect, \( r_m \) as well as the improvement parameters are closer to unity at the larger \( \beta \) value. The fits are discussed in more detail in Secs. \( \text{V A} \) and \( \text{V B} \) below. Repeating the \( \beta = 3.4 \) fit, excluding the lightest \( m_s = m_{\ell} \) data point (rqcd017) as this was obtained on a small volume \( L M_x = 3.2 \times 4 \), did not significantly impact on any of the fit parameters but resulted in increased errors in some cases: \( r_m = 2.50(20) \), \( \kappa_{crit} = 0.1369159(66) \) and \( D_0 = -0.7 \pm 17.0 \). Note that the central value of \( D_0 \) moved down by one standard deviation while the errors on \( r_m \) and \( \kappa_{crit} \) approximately doubled. Including the heavy rqcd019 point hardly affected any of the fit parameters, with the exception of \( D_0 = 16.5 \pm 4.4 \), indicating a large positive value of this parameter. However, in view

### III. SIMULATION PARAMETERS AND FIT PROCEDURE

In this article we present results obtained at two \( \beta \) values: \( \beta = 3.4 \), corresponding to \( a \approx 0.085 \) fm, and \( \beta = 3.55 \) (\( a \approx 0.064 \) fm). Investigations at further lattice spacings are in progress. At each lattice spacing the simulations cover four mass points ranging from a pion mass \( M_{\pi} \approx 200 \) MeV up to \( M_{\pi} \approx 420 \) MeV along the \( m = m_{symm} = \text{const.} \) line with \( M_{\pi} L > 4 \) (3.9 in one case). At \( \beta = 3.4 \) one additional point exists along this line at \( M_{\pi} \approx 129 \) MeV \((D100)\). However, as in this case we have only limited statistics and \( M_{\pi} L < 4 \), we will discard this ensemble from any fit. For an overview of the analysed ensembles, see Table \( \text{I} \). The lattice spacing and meson mass estimates are based on the continuum limit value of the scale \( \sqrt{s_0} = 0.4144(59)(37) \) fm that was obtained by the BMW Collaboration \cite{29}. We utilize open boundary conditions in time \((31)\), with the exception of the rqcd017, rqcd019, rqcd021, B250, X250 and X251 ensembles, which are periodic in time for gauge fields and antiperiodic for fermions. Note that the ensembles under investigation correspond to lattice spacings at which topological freezing is not yet a major problem \cite{7}, enabling us to use (anti)periodic boundary conditions.

We remark that at \( \beta = 3.55 \) and \( \kappa_s = \kappa_s = 0.137 \) there exist two ensembles, H200 and N202, both with \( L M_x > 4 \). However, in the first case \( L \approx 2 \) fm is rather small in physical units. While this does not appear to affect the AWI mass, the measured pion mass on the larger volume comes out somewhat lighter. Therefore, we discard H200 from further analysis.

In addition to the already existing \( m = m_{symm} \) point at \( m_s = m_{\ell} \), we first generated three other points along the flavour symmetric line for both lattice spacings, one at a bigger and two at smaller values of the quark mass. The data along these two lines in the quark mass plane enabled us to estimate \( Z_r' r_m' \) and \( \kappa_{crit} \) from fits of the form \([\text{see Eqs.} (30) \text{ and } (31)]\):

\[
\hat{m}_s - \hat{m}_u = \frac{Z_r}{2} \left( \frac{1}{\kappa_s} - \frac{1}{\kappa_{crit}} \right) \times \left[ 1 - \frac{A}{12} \left( \frac{1}{\kappa_s} - \frac{1}{\kappa_{crit}} \right) - B_0 a m \right], \tag{56}
\]

\[
\overline{m} = Z_r m \left[ a m - \frac{C_0}{36} \left( \frac{1}{\kappa_s} - \frac{1}{\kappa_{crit}} \right)^2 - \frac{D_0}{2} (a m)^2 \right]. \tag{57}
\]

The combination \( a m = (2\kappa_1^{-1} + \kappa_3^{-1} - 3\kappa_{crit}^{-1})/6 \) above depends on \( \kappa_{crit} \). To this order in \( a \) this parameter can in principle be substituted by the measured value of \( a m / (Z_r m) \) if desired. This is possible because we will neither need the value of \( \kappa_{crit} \) for our determination of the physical point nor for predicting the \( \kappa_s \) trajectory (as a function of \( \kappa_s \)) along which \( \hat{m}_s \approx (Z_r / Z_{\lambda}) \hat{m}_s \) is kept fixed, see Eqs. \((59)\) and \((47)\).

The resulting fit parameters are shown in Table \( \text{II} \). The data only mildly constrain the parameter \( D_0 \), which comes out to be compatible with zero within large errors. \( r_m, B_0 \) and \( C_0 \) deviate substantially from the perturbative expectations and \( B_0 \) even comes out negative. However, as one would expect, \( r_m \) as well as the improvement parameters are closer to unity at the larger \( \beta \) value. The fits are discussed in more detail in Secs. \( \text{V A} \) and \( \text{V B} \) below.
TABLE II. Results of global fits to our AWI quark mass data according to Eqs. \([51]\) and \([77]\). The \(A\) values were determined in Ref. \([23]\). In the cases where varying \(A\) within its uncertainty had an effect, a second error is given to reflect the associated systematics.

| \(\beta\) | \(\chi^2/N_{\text{DF}}\) | \(Z\) | \(r_m\) | \(\kappa_{\text{symm}}\) | \(A\) (no fit) | \(B_0\) | \(C_0\) | \(D_0\) |
|----------|-----------------|-----|-----|-----------------|-------------|-------|-------|-------|
| 3.4      | 32.1/9          | 0.8710(30)(10) | 2.6335(94)(5) | 0.13691(15)(27)(1) | 2.91(33) | -1.55(76)(1) | 3.43(30) | 10.9(91)(0.3) |
| 3.55     | 26.2/10         | 0.9841(25)(3) | 1.530(14)(1) | 0.1371718(10) | 2.27(14) | -0.81(45)(1) | 1.89(25)(1) | 1.2(1.2) |

of the rather large improvement coefficients at \(\beta = 3.4\), the rqcd019 results may very well be polluted by significant \(O(a^2)\) effects, which is why we chose to discard this point from further analysis.

IV. DETERMINATION OF THE PHYSICAL QUARK MASS VALUES

At each lattice spacing the average lattice quark mass \(m_{\text{symm}}\) for the \(\overline{m} = m_{\text{symm}}\) trajectory is fixed by imposing a target value for the combination \([7]\)

\[
\phi_4 \equiv 8t_0 \left( m_{\pi}^2 + \frac{1}{2} M_{\pi}^2 \right) \propto \overline{m} \tag{61}
\]

\[
\propto \overline{m} + a \left[ \frac{2}{9} m_{\pi} (m_s - m_{\ell})^2 + (d_m + 3d_\pi) m_{\pi} \right] + O(a^2)
\]

at \(\kappa_{\ell} = \kappa_{\text{symm}}\), where \(t_0\) is the gluonic scale defined in Ref. \([30]\) and we have made use of the Gell-Mann–Oakes–Renner relation as well as of Eqs. \([14]\) and \([27]\). At the physical point the numerical value

\[
\phi_{4,\text{ph}} = 1.17(38) \tag{62}
\]

can be obtained from the pion and kaon masses in the electrically neutral isospin symmetric limit, \(M_s = 134.8(3)\) MeV and \(M_{\pi} = 494.2(4)\) MeV \([22]\), and the result \(\sqrt{M_0} = 0.4144(59)(37)\) fm of the BMW Collaboration \([29]\) for the continuum limit \(N_f = 2 + 1\) theory. In the future we will independently determine a lattice scale and at that stage the value Eq. \([62]\) may change.

The combination \(\phi_4\) will not vary strongly along the \(\overline{m} = m_{\text{symm}}\) trajectory: At fixed renormalized quark masses \(m_4\) (and \(\phi_2\) defined below) can only be subject to \(O(a^2)\) lattice artefacts. This also holds when \(\overline{m}\) is varied as the effect of the renormalization of the charge through \(b_g\) cancels from this combination. However, the proportionality of \(\phi_4\) to the average lattice quark mass \(\overline{m}\) is subject to order-\(a\) corrections, see Eqs. \([14]\) and \([61]\). The latter of the correction terms in Eq. \([61]\) does not change along the \(\overline{m} = m_{\text{symm}}\) line. The remaining \(O(a)\) correction term is proportional to \((m_s - m_{\ell})^2\). On the continuum side, generalizing the Ademollo–Gatto theorem \([53]\) and also as a consequence of the Gell-Mann–Okubo expansion \([5, 16, 17]\), \(\phi_4\) cannot depend linearly on the symmetry breaking parameter \(m_s - m_{\ell}\), i.e. it can only depend on \((M_{\pi}^2 - M_{\ell}^2)^2\) and higher powers. Indeed, to next-to-leading order SU(3) ChPT \([33, 35]\) \(\phi_4\) is constant as long as \(\overline{m}\) is constant and it will only receive corrections at next-to-next-to-leading order \([57]\). Therefore, the \(\overline{m} = m_{\text{symm}}\) line with \(\phi_{4,\text{symm}} = \phi_{4,\text{ph}}\), where \(\phi_{4,\text{symm}}\) refers to the \(\phi_4\) value at the point \(m_s = m_{\ell}\), should go through the physical point, up to continuum and lattice effects that are both quartic in the pseudoscalar meson masses in units of the chiral symmetry breaking scale \(4\pi F_0 \sim 1\) GeV. In view of these corrections that depend on \((M_{\pi}^2 - M_{\ell}^2)^2\) and \(\phi_4\) itself, we targeted a slightly larger value \(\phi_{4,\text{symm}} \approx 1.15 > \phi_{4,\text{ph}}\), see Ref. \([7]\).

In the overview plot Fig. \([2]\) the positions of our analysed ensembles in the \(\phi_4\) vs. \(\phi_2\) plane are shown, where at the physical point:

\[
\phi_{2,\text{ph}} = 0.0801(28), \tag{64}
\]

using again the physical values for \(t_0\) and \(M_{\pi}\) from above.

Averbach and ordinate are approximately proportional to the light and average lattice quark masses, respectively. The physical target ranges \(\phi_{4,\text{ph}}\) and \(\phi_{2,\text{ph}}\) are shown as horizontal and vertical error bands. The line for \(m_s = m_{\ell}\) corresponds to \(\phi_4 = 3\phi_2/2\), for \(m_s = \hat{m}_{s,\text{ph}}\) we show a linear fit to the data while for \(\overline{m} = m_{\text{symm}}\) we plot a constant plus quadratic function of \(\phi_{2,\text{symm}} - \phi_2 \propto t_0(M_{\pi}^2 - M_{\ell}^2)\). Indeed, the \(\phi_4\) combination only mildly varies between the \(\overline{m} = m_{\text{symm}}\) simulation points but changes significantly along the other two mass plane trajectories. The orange point at \(\beta = 3.4\) corresponds to the ensemble D100 (see Table I) that does not enter any of our fits.

Along the \(\overline{m} = m_{\text{symm}}\) trajectory order-\(a\) lattice artefacts as well as the leading continuum chiral correction both are proportional to \((m_s - m_{\ell})^2\). Because of this variation the target value at the SU(3) symmetric point was deliberately chosen larger than its physical point estimate Eq. \([62]\). At both couplings we have somewhat underestimated this target value \(\phi_{4,\text{symm}} = 1.15\): For our \(\beta = 3.4\) and \(\beta = 3.55\) data we obtain \(\phi_{4,\text{symm}} = 1.139(6)\) and \(\phi_{4,\text{symm}} = 1.111(4)\), respectively. This then results in smaller than physical central \(\phi_{4,\text{ph}}\) values. From the fit
to the $\bar{m} = m_{\text{symm}}$ points we find

$$\frac{\phi_{4,\text{ph}}}{\phi_{4,\text{symm}}} = 0.945(9), \quad \phi_{4,\text{ph}} = 1.076(8),$$

(65)

$$\frac{\phi_{4,\text{ph}}}{\phi_{4,\text{symm}}} = 0.985(6), \quad \phi_{4,\text{ph}} = 1.094(5),$$

(66)

at $\beta = 3.4$ and $\beta = 3.55$, respectively. In both cases the slope of $\phi_4$ as a function of $(\phi_{2,\text{symm}} - \phi_2)^2$ is small but significant. It decreases towards the smaller lattice spacing, indicating that the main effect may be due to lattice artefacts. In hindsight, if we would have chosen $\phi_{4,\text{symm}} \approx 1.18$ and $\phi_{4,\text{symm}} \approx 1.13$ at $\beta = 3.4$ and $\beta = 3.55$, respectively, we would have hit the central physical target value for $\phi_4$ at $\phi_2 = \phi_{2,\text{ph}}$ along our $\bar{m} = m_{\text{symm}}$ line. Nevertheless, both extrapolated $\phi_{4,\text{ph}}$ values agree with the physical value $\phi_{4,\text{ph}} = 1.117(38)$ within errors. We remark that also this value is not final but depends on a future independent determination of the scale parameter $\tilde{\tau}_0$.

In Fig. 3 we plot the ratio $\sqrt{t_0/t_{0,\text{ph}}}$ as a function of the light AWI quark mass ratio $\tilde{m}_\ell/\tilde{m}_{\ell,\text{ph}}$ where we normalize with respect to the corresponding physical mean values (see below). At both lattice spacings $\sqrt{t_0}$ along the $\bar{m} = m_{\text{symm}}$ line depends only mildly on $m_\ell$ but — as expected — it changes considerably along the other lines, and in particular along $m_s = m_\ell$. The dependence on the quark masses can be parameterized in terms of lattice spacing and continuum effects [35]. The latter are to leading

FIG. 2. Our simulation points in the $\phi_4 \sim \bar{m}$ [see Eq. (51)] vs. $\phi_2 \sim m_\ell$ [see Eq. (63)] plane. The bands correspond to the uncertainties of the physical point values Eqs. (62) and (64). $\phi_4 = (3/2) \phi_2$ along the $m_s = m_\ell$ line and the other curves represent fits to the data, including (tiny) error bands. Orange point: ensemble D100. The data points corresponding to ensembles rqcd019 and B250 are outside of the plotted range. Left: $\beta = 3.4$. Right: $\beta = 3.55$.

FIG. 3. $\sqrt{t_0}$ as a function of the AWI quark mass $\tilde{m}_\ell$, normalized with respect to the extrapolated physical point values $\sqrt{t_{0,\text{ph}}}$ and $\tilde{m}_{\ell,\text{ph}}$, for our three quark mass plane trajectories. The lines are fits to the data. Orange point: ensemble D100. The data points corresponding to ensembles rqcd019 and B250 are outside of the plotted range. Left: $\beta = 3.4$. Right: $\beta = 3.55$. 

$\beta = 3.4$ and $\beta = 3.55$, respectively. In both cases the slope of $\phi_4$ as a function of $(\phi_{2,\text{symm}} - \phi_2)^2$ is small but significant. It decreases towards the smaller lattice spacing, indicating that the main effect may be due to lattice artefacts. In hindsight, if we would have chosen $\phi_{4,\text{symm}} \approx 1.18$ and $\phi_{4,\text{symm}} \approx 1.13$ at $\beta = 3.4$ and $\beta = 3.55$, respectively, we would have hit the central physical target value for $\phi_4$ at $\phi_2 = \phi_{2,\text{ph}}$ along our $\bar{m} = m_{\text{symm}}$ line. Nevertheless, both extrapolated $\phi_{4,\text{ph}}$ values agree with the physical value $\phi_{4,\text{ph}} = 1.117(38)$ within errors. We remark that also this value is not final but depends on a future independent determination of the scale parameter $\tilde{\tau}_0$.

In Fig. 3, we plot the ratio $\sqrt{t_0/t_{0,\text{ph}}}$ as a function of the light AWI quark mass ratio $\tilde{m}_\ell/\tilde{m}_{\ell,\text{ph}}$ where we normalize with respect to the corresponding physical mean values (see below). At both lattice spacings $\sqrt{t_0}$ along the $\bar{m} = m_{\text{symm}}$ line depends only mildly on $m_\ell$ but — as expected — it changes considerably along the other lines, and in particular along $m_s = m_\ell$. The dependence on the quark masses can be parameterized in terms of lattice spacing and continuum effects [35]. The latter are to leading
order linear functions of $\bar{m} \propto m$ and $(\bar{m}_s - \bar{m}_t)^2 \propto (\bar{m}_s - \bar{m}_t)^2$, where the proportionality holds up to tiny residual $O(a)$ effects (see above). Extrapolating the $\bar{m} = m_{\text{symm}}$ data quadratically in $\bar{m}_s - \bar{m}_t \propto \bar{m} - \bar{m}_t$, we obtain the physical point values
\begin{align}
\frac{\sqrt{t_0,\text{ph}}}{\sqrt{t_0,\text{symm}}} &= 1.0167(18), \quad \frac{\sqrt{6t_0,\text{ph}}}{a} = 4.852(7), \quad (67) \\
\frac{\sqrt{t_0,\text{ph}}}{\sqrt{t_0,\text{symm}}} &= 1.0009(13), \quad \frac{\sqrt{6t_0,\text{ph}}}{a} = 6.433(6), \quad (68)
\end{align}
for $\beta = 3.4$ and $\beta = 3.55$, respectively. Note that some of the $t_0$ values shown in the figure are preliminary, see Table[1] and may have underestimated errors, due to very large autocorrelations times for this observable, that we may not yet have taken fully into account. Therefore, the $\sqrt{6t_0,\text{ph}}/a$ values quoted above should also be considered as preliminary. The curves shown in the figure are linear fits to the $\bar{m}_s = \bar{m}_t, \text{ph}$ and $m_s = m_t, \text{data}$ and the constant plus quadratic fit in $\bar{m} - \bar{m}_t$ to the $\bar{m} = m_{\text{symm}}$ data described above.

Note that linear lattice artefacts along the $m = m_s = m_t = m_{\text{line}}$ line are due to the change of the coupling $g^2 = (1 + b_\text{m} am) g^2$. This means that in this case the dependence on the lattice spacing $a$ of the linear slope of $\sqrt{t_0(m)}$ as a function of $m$ could serve to isolate the effect of $b_g$, when compared to the continuum limit mass dependence $t_0,c(\bar{m})$ along this line: From
\begin{equation}
\begin{aligned}
a(g^2) &= \Lambda^{-1} \exp \left(-\frac{8\pi^2}{\beta_0 g^2} + \cdots \right) \\
&= a(g^2) (1 + b_a am + \cdots) \quad (69)
\end{aligned}
\end{equation}
it follows that $b_a = 8\pi^2 b_g/\beta_0 = 8\pi^2 b_g/9$ for $N_f = 3$. This coefficient is related to the change of the slope
\begin{equation}
\begin{aligned}
\sqrt{t_0(\bar{m})} &= \frac{a(g^2)}{a(0)} \sqrt{t_{0,c}(\bar{m})} \left(1 - b_a am \sqrt{t_{0,c}(\bar{m})} \right). \quad (70)
\end{aligned}
\end{equation}
Note that $d_m + 3d_m$ and $Z_m r_m$ are required to relate $\sqrt{t_0(m)}$ to $\sqrt{t_0(\bar{m})}$. As the slope becomes more negative for the coarser lattice spacing, $b_g$ must be positive, in agreement with the one-loop perturbative expectation (21). A larger average quark mass results in a coarser effective lattice spacing.

As AWI masses can be determined more precisely than pseudoscalar masses and are less susceptible to finite volume effects, we will use these to set the physical quark masses, by imposing the FLAG value (72).
\begin{equation}
\frac{\hat{m}_{\ell,\text{ph}}}{\bar{m}_{\text{ph}}} \approx \frac{\hat{m}_{\ell,\text{ph}}}{\bar{m}_{\text{ph}}} = 0.1018(15), \quad (71)
\end{equation}
to define the physical quark mass point. Also this target value may undergo a slight change in the future, once we have independently extrapolated the combination
\begin{equation}
\frac{3M_K^2}{2M_K^2 + M_\pi^2} = 0.1076(5) \quad (72)
\end{equation}
to the continuum limit.

We remark that there are slight differences between ratios of renormalized and AWI quark masses $\bar{m}$ and $\hat{m}$, see Eq. (2). Since we keep $\bar{m}$ fixed along our main mass plane trajectory, the dependence on $b_\text{p} - b_\text{g}$ cancels from the ratio Eq. (71). However, a correction term
\begin{equation}
\frac{b_\text{p} - b_\text{A}}{3}(m_{\ell,\text{ph}} - m_{s,\text{ph}}) = \frac{b_\text{p} - b_\text{A}}{3Z}(\hat{m}_{\ell,\text{ph}} - \hat{m}_{s,\text{ph}})
\end{equation}
survives, see Eq. (23). Non-perturbatively, one finds (23)
\begin{equation}
b_\text{p} - b_\text{A} = 0.90(32) \quad (73)
\end{equation}
and $b_\text{p} - b_\text{A} = 0.59(14)$, respectively, at $\beta = 3.4$ and $\beta = 3.55$. At $\beta = 3.4$, where the above order-$a$ correction is largest, using $Z^{-1} \approx 1.15$ and $a(\hat{m}_{s,\text{ph}} - \hat{m}_{t,\text{ph}}) \approx 0.023$ (see Table[1] and Eq. (73)), we obtain a change of about 0.8% from substituting the ratio of renormalized quark masses Eq. (71) by the ratio of AWI masses. This effect, that reduces to 0.4% at $\beta = 3.55$, is well below the 1.5% relative error of the FLAG average (22), that we use.

The global fit of Eqs. (55) and (57) to our mass data provides a parametrization of the AWI masses as functions of $\kappa_t$ and $\kappa_s$. The fit parameters can be found in Table[11] and the fit is discussed in detail in Secs. [1A and [1B below. At each lattice spacing we then determine the physical hopping parameter values $\kappa_t,\text{ph}$ and $\kappa_s,\text{ph}$ as well as the corresponding AWI masses $\hat{m}_{\ell,\text{ph}}$ and $\hat{m}_{s,\text{ph}}$ that satisfy Eq. (71) along the chiral trajectory $\bar{m} = m_{\text{symm}}$. Note that since we have a parametrization of light and strange AWI masses as functions of the hopping parameters, we can also determine the physical point along any other chiral trajectory that incorporates it (5). Our procedure of finding the physical point is illustrated in Fig [4], where we plot this ratio as a function of $\kappa_t^{-1}$. In addition to the $\bar{m} = m_{\text{symm}}$ points (blue) that follow lines with little curvature, as expected from Eqs. (56) and (57), we also show the results of our subsequent measurements along the $\bar{m}_s = \bar{m}_{s,\text{ph}}$ trajectory (green), which nicely coincide with the parametrization, thereby validating our strategy. Note that the $m_t = m_{\text{line}}$ points (with the exception of the symmetric point on the $\bar{m} = m_{\text{symm}}$ line) are not shown as the ratio displayed is trivial in this case. The error band of the target value is dominated by the uncertainty of Eq. (71).

The physical point values, postdicted including more statistics and the newly generated fixed AWI strange quark mass ensembles, read:
\begin{equation}
\kappa_{t,\text{ph}} = 0.1370906(13), \quad \kappa_{s,\text{ph}} = 0.1361024(25), \quad (74)
\end{equation}
\begin{equation}
\hat{m}_{\ell,\text{ph}} = 0.000866(48), \quad \hat{m}_{s,\text{ph}} = 0.023780(65), \quad (75)
\end{equation}

4 In the absence of an independent determination of the scale parameter $t_0$, for the moment being we fix $\frac{1}{2} \sum_i \kappa_i^{-1} = 0.13675962$ and $\sum_i \kappa_i^{-1} = 0.137$ at $\beta = 3.4$ and $\beta = 3.55$, respectively, i.e. we assume that our $\bar{m} = m_{\text{symm}}$ curves go exactly through the physical point. As can be seen in Fig[2] this assumption is justified. Along this line the physical point is then defined by Eq. (71).
where we neglected the uncertainty of $m$, are dominated by the uncertainty of the target value Eq. (71), as a function of $m$.

The strange quark AWI masses along the $\tilde{m}_s = \tilde{m}_{s,ph}$ curves correspond to Eqs. (56) and (57) with the parameter values of Table II. Orange point: ensemble D100. Left: $\beta = 3.4$. Right: $\beta = 3.55$.

In Fig. 5 we plot our measured AWI strange quark masses determined on the newly generated ensembles along the predicted $\tilde{m}_s = \tilde{m}_{s,ph}$ trajectory, normalized with respect to the postdicted values from the global fit shown in Eqs. (75) and (77) above as a function of the light quark AWI mass. Indeed, the two sets of AWI strange quark masses are constant within errors. The $\beta = 3.55$ data perfectly coincide with the expectation (see also the N204, N201 and D201 entries of Table I). The $\beta = 3.4$ data agree reasonably well with the original target value (see ensembles H107, H106 and C102 of Table I) but they are off by almost 3 standard deviations, corresponding to 1%, from the postdiction Eq. (75), that was obtained using an altered value of $c_A$.

Neglecting any uncertainty on $2m_\ell + m_s = 3m_{symm}$, the 1.5% error of the target range Eq. (71) translates into a small error on $\tilde{m}_{s,ph}$ and a larger relative error on $\tilde{m}_s$. These uncertainties contribute to the horizontal and vertical error bands shown in the figure. Note that these would be wider if we could include a realistic error estimate for $m_{symm}$. The figure demonstrates that it is possible to tune the AWI strange quark mass to the desired value within a few per mille and even in the case where, due to the incomplete information on $c_A$, we mistuned to an incorrect target value the difference is extremely small.

V. DISCUSSION OF THE FITS AND THE RESULTING PARAMETERS

We will first investigate in more detail lattice spacing effects for the $m = m_{symm}$ and $m_s = m_\ell$ data, before presenting an overview of all AWI mass data, and discussing combinations of improvement coefficients.
A. $\overline{m} = m_{\text{symm}}$ and $m_s = m_\ell$ data and improvement coefficients

Here we compare different projections of our quark mass data to the global fits Eqs. (56) and (57) with the parameter values shown in Table II.

In Fig. 6 we show the ratio of the AWI over the lattice quark mass along the $m_s = m_\ell$ trajectory, as a function of $\overline{m} = m_s = m_\ell$, normalized to the mass $m_{\text{symm}}$ = $\overline{m}_{\text{ph}}$. The value of $\overline{m}/\overline{m}$ at $\overline{m} = 0$ corresponds to the combination of renormalization constants $Z_{\text{symm}}$. Orange point: ensemble rqc019 (excluded from the global fit). The curves correspond to Eq. (78), with the parameter values of Table II.

From Eq. (57) we can see that

$$x_{\text{symm}} - C = 1$$

Moreover, the average deviation of this parameter from the tree-level expectation $D_0 = 1$ is hard to extract. This also means that our results are quite insensitive regarding the value of $D_0$.

In Fig. 7 we show a combination that isolates the effect of $C_0$: $\overline{m}$ over $\overline{m}_{\text{symm}}$ as a function of $(m_s - m_\ell)^2$, normalized to the corresponding physical point value, for the constant average lattice quark mass data $\overline{m} = m_{\text{symm}}$.

FIG. 6. The ratio of the AWI over the lattice quark mass along the $m_s = m_\ell$ trajectory, as a function of $\overline{m} = m_s = m_\ell$, normalized to the mass $m_{\text{symm}}$ = $\overline{m}_{\text{ph}}$. The value of $\overline{m}/\overline{m}$ at $\overline{m} = 0$ corresponds to the combination of renormalization constants $Z_{\text{symm}}$. Orange point: ensemble rqc019 (excluded from the global fit). The curves correspond to Eq. (78), with the parameter values of Table II.

FIG. 7. The dependence of the average AWI quark mass on the difference of the lattice quark masses squared, along the $\overline{m} = m_{\text{symm}}$ trajectory. Orange point: ensemble D100. Both mass combinations are normalized with respect to their $m_s = m_\ell$ value $m_{\text{symm}}$ and their physical point value, respectively. The curves correspond to Eq. (79) with the parameter values of Table II.

As the light quark mass decreases the ratio shown deviates from one. The parametrization can be read off from Eq. (79):

$$\frac{\overline{m}}{m_{\text{symm}}} = 1 - \frac{C_0}{g m_{\text{symm}}} \left( \frac{m_s - m_\ell}{m_s - m_\ell, \text{ph}} \right)^2.$$
This means the negative slope is proportional to \( C_0 \), which decreases considerably, increasing \( \beta \) from 3.4 to 3.55, see also Table I. For \( \beta = 3.4 \) we show the preliminary D100 physical point result (orange) that did not enter our global fit. The left-most point at \( \beta = 3.4 \) (corresponding to the H102 ensemble of Table I) exhibits the largest deviation of our data from the two global fits to data from 9 and 10 ensembles (15 and 16 quark mass values), respectively. Since \( a\overline{m} \) is constant for all the \( \beta = 3.4 \) data shown in the figure and \( a(m_s - m_\ell) \) is larger for the other points, we would not expect the average AWI quark mass on ensemble H102 to be particularly sensitive to higher order discretization effects. Therefore, we assume the deviation seen is a statistical fluctuation.

Finally, in Fig. 8 we show the ratio of AWI and lattice quark mass differences as a function of \( m_s - m_\ell \) for the \( \overline{m} = m_{\text{symm}} \) data. We normalize the ordinate with respect to its physical point value, to enable comparison between different lattice spacings. We also display the global fits. Note that the right-most orange \( \beta = 3.4 \) point (D100) did not enter the fit as we regard its error as unreliable, due to limited statistics. From Eq. (56) we see that

\[
\frac{\tilde{m}_s - \tilde{m}_\ell}{m_s - m_\ell} = Z \left\{ 1 - a \left[ \frac{A}{6} (m_s - m_\ell) + B_0 \overline{m} \right] \right\}.
\]

Therefore, at \( m_s = m_\ell \) we can read off the combination \( Z(1 - B_0 a m_{\text{symm}}) \). This is somewhat larger than the \( Z \) parameters that are listed in Table I because \( B_0 \) is negative in both cases. The slope corresponds to \(- Z A a (m_{s,ph} - m_{\ell,ph})/6 \). Note that the value of the parameter \( A \) that was obtained independently is consistent with our data.

We have demonstrated that \( A, C_0 \) and \( D_0 \) can be constrained from data along the \( \overline{m} = m_{\text{symm}} \) and \( m_s = m_\ell \) lines. While the sensitivity to \( D_0 \) is small, \( B_0 \) cannot be constrained at all from data points along these two lines.

Obviously, \( \overline{m} \) needs to be varied for \( m_s \neq m_\ell \) for the results to become sensitive to \( B_0 \). Unfortunately, to enable a precise determination of \( Z \) [and of \( r_m = (Z\tau_m)/Z \)] some knowledge of \( B_0 \) is required but we were only able to constrain \( B_0 \), once data points from other regions of the quark mass plane were added, in our case along the \( \tilde{m}_s = \tilde{m}_{s,ph} \) line. Another possibility of achieving this would have been to follow a partially quenched strategy, computing valence quark AWI masses along the sea quark symmetric line \( m_s = m_\ell \). Nevertheless, in order to determine the \( \tilde{m}_s = \tilde{m}_{s,ph} \) line from the two chiral trajectories \( \overline{m} = m_{\text{symm}} \) and \( m_s = m_\ell \), there is no need for a very accurate value of \( B_0 \) since the \( B_0 a m_{\text{symm}} \) contribution to \( Z \) only amounts to a 0.6\% correction, even on the coarser \( \beta = 3.4 \) ensemble.

**B. AWI and pseudoscalar mass data**

In Fig. 9 we plot the average AWI mass in lattice units as a function of \( \kappa^{-1}_\ell \) for our three quark mass plane trajectories: \( \overline{m} = m_{\text{symm}}, \tilde{m}_s = \tilde{m}_{s,ph} \) and \( m_s = m_\ell \). The curves correspond to our fit according to Eq. (57) with parameters as shown in Table I. The \( \overline{m} = m_{\text{symm}} \) curve is almost constant as along this line \( \overline{m} \) only changes due to an \( \mathcal{O}(a) \) term that is parameterized by \( C_0 \), see Fig. 8. The curvature is not visible on the scale of Fig. 9.

In Fig. 10 a comparison is shown between strange and light AWI mass differences \( \tilde{m}_s - \tilde{m}_s \) and the fit Eq. (56). In this representation the \( m_s = m_\ell \) points obviously coincide with zero and are therefore not shown. Overall, we have good coverage of the quark mass plane and the data are described reasonably well by the fit. Like in Fig. 9 at both lattice spacings that we investigated, the \( \overline{m} = m_{\text{symm}} \) and \( \tilde{m}_s - \tilde{m}_{s,ph} \) curves intersect very close to (and in statistical agreement with) the preferred position of the physical point.
Finally, in Fig. 11 we display the ratio $3M^2/(2M^2_K + M^2_\pi)$ as a function of $8t_0,phM^2_\pi$ for the $\overline{m} = m_{\text{symm}}$ and $\overline{m}_s = \overline{m}_{s,\text{ph}}$ mass plane trajectories. The vertical and horizontal bands correspond to the physical point. The parametrization of the fit curves is given in Eqs. (81) and (82). Orange point: ensemble D100. Left: $\beta = 3.4$. Right: $\beta = 3.55$.

The fitted parameter values read

$$\alpha = 0.235(19), \quad \gamma = 2.054(12),$$

$$\alpha = -0.025(15), \quad \gamma = 2.062(6)$$
for $\beta = 3.4$ and $\beta = 3.55$, respectively. Both $\gamma$ values agree well with the physical point expectation $2(\phi_{2,\text{ph}} - \phi_{2,\text{ph}}) = 2.075(70)$. The curvature of the $m = m_{\text{symm}}$ line is of a higher order in ChPT and also subject to an $O(\alpha)$ lattice effect. The change of the parameter $\alpha$ with $\beta$ indicates that the latter dominates.

At the physical point we obtain the following values for the ratio Eq. (72) from the fits Eqs. (81)–(82): $0.1087(6)(37)$ and $0.1086(6)(35)$ for the $m = m_{\text{symm}}$ and $\tilde{m}_s = \tilde{m}_{s,\text{ph}}$, data, respectively, at $\beta = 3.4$ and $0.1074(4)(37)$ and $0.1082(3)(35)$ at $\beta = 3.55$. The first errors are statistical only while the second errors given include the propagation of the uncertainty of $\phi_{2,\text{ph}}$ errors are statistical only while the second errors given include the propagation of the uncertainty of $\phi_{2,\text{ph}}$. The change of the parameter $\alpha$ with $\beta$ indicates that the latter dominates.

We outlined a strategy to keep the strange quark mass, determined through the axial Ward identity, constant in simulations with $N_f = 2 + 1$ flavours of Wilson fermions, implementing full order-$\alpha$ improvement, see Eqs. (39), (41) and (47). This was successfully tested to very high precision at two lattice spacings, $a \approx 0.805$ fm and $a \approx 0.604$ fm, see Fig. 5. We estimated this procedure to differ, due to as yet only partially known flavour singlet $O(\alpha)$ effects, from keeping the renormalized strange quark mass constant by less than one percent, even at the coarser lattice spacing. Furthermore, we worked out how valence quark hopping parameters need to be adjusted, see Sec. 11. This will be used in future studies of charm physics.

| coefficient | perturbation theory | $\beta = 3.4$ | $\beta = 3.55$ |
|-------------|---------------------|--------------|--------------|
| $b_m$       | $-1/2 - 0.0703g^2$  | $-1.04(31)$  | $-0.85(14)$  |
| $d_m$       | $-1/2 - 0.0703g^2$  | $-1.80(16)$  | $-1.04(13)$  |
| $b_P - b_A$ | $0.0012g^2$         | $0.90(32)$   | $0.59(14)$   |
| $\tilde{b}_m + b_P - b_A$ | $O(g^4)$         | $0.12(51)$   | $0.34(21)$   |
| $d_m - b_m$ | $O(g^4)$            | $-1.5(1.5)$  | $-0.39(27)$  |

### VI. SUMMARY AND OUTLOOK

We outlined a strategy to keep the strange quark mass, determined through the axial Ward identity, constant in simulations with $N_f = 2 + 1$ flavours of Wilson fermions, implementing full order-$\alpha$ improvement, see Eqs. (39), (41) and (47). This was successfully tested to very high precision at two lattice spacings, $a \approx 0.805$ fm and $a \approx 0.604$ fm, see Fig. 5. We estimated this procedure to differ, due to as yet only partially known flavour singlet $O(\alpha)$ effects, from keeping the renormalized strange quark mass constant by less than one percent, even at the coarser lattice spacing. Furthermore, we worked out how valence quark hopping parameters need to be adjusted, see Sec. 11. This will be used in future studies of charm physics.

We computed several combinations of renormalization constants and order-$\alpha$ improvement coefficients, see Tables I and II. We observed that the parameters that are either related to flavour singlet quark mass combinations ($b_m$, $b_P$, $b_A$), flavour singlet currents ($r_m$, $d_m$) or both ($\tilde{d}_m$) come out very different from the corresponding perturbative expectations. However, these seem to converge rapidly in the direction of the tree-level results when increasing $\beta = 6/g^2$ from 3.4 to 3.55. Non-perturbative order-$\alpha$ improvement of all currents of interest is ongoing, see, e.g., Refs. 19, 24.

In order to set the physical strange quark mass we also determined the physical point in the $\kappa^{-1}_s$ vs. $\kappa^{-1}_f$ plane. Its position may still undergo changes in the future, once the continuum limit has been taken independently, which then might necessitate a slight reweighting of the strange quark mass. Having ensembles along three lines in the quark mass plane ($2m_c + m_s = 3m_{\text{symm}}$, $m_s = m_{s,\text{ph}}$ and $m_s = m_t$) enables tests of the convergence of SU(2) and SU(3) ChPT and of expansions in the SU(3) symmetry breaking parameter $\xi$ as well as highly constrained physical point extrapolations. It also allows us to pursue a non-perturbative renormalization and order-$\alpha$ improvement programme.

Results on baryon distribution amplitudes along the $2m_c + m_s = \text{const.}$ trajectory at one lattice spacing have already been published 10. Further results on distribution amplitudes, also utilizing the constant strange quark
mass points, are in preparation and an article on light hadron spectroscopy is forthcoming.

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