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Towards the determination of the charm quark mass on $N_\mathrm{f} = 2+1$ CLS ensembles

ALPHA Collaboration

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We present the current status of our lattice QCD determination of the charm quark mass using $N_\mathrm{f} = 2+1$ dynamical, non-perturbatively $\mathrm{O}(a)$ improved Wilson fermions. A subset of CLS ensembles with five different lattice spacings along the $\mathrm{Tr}[M_\mathrm{q}] = \mathrm{const.}$ trajectory is used. For the computation of the correlation functions involving valence charm quark propagators, we employ distance preconditioning to gain the necessary precision. To stabilize the extrapolations to the physical point, we consider different definitions of the bare charm quark mass and corresponding renormalization procedures.

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1. Introduction

As fundamental parameters of the Standard Model, the masses of the quarks are of great phenomenological interest. Particularly the precise knowledge of the charm and bottom quark mass values is crucial for the search for new physics, because decay rates and branching ratios of the Higgs boson depend critically on the masses of these heavy quarks (see, e.g., [1]) and at future lepton colliders it will be possible to measure their Yukawa couplings to very high accuracy.

As a consequence of confinement, any determination of quark masses must relate them to the observable, low-energy hadronic world and thus requires a reliable quantitative control over this genuinely non-perturbative regime of QCD. Therefore, lattice QCD has emerged as an ideal calculational tool to provide precise quark mass results. Nevertheless, some difficulties have to be overcome. Apart from properly dealing with the inherent renormalization scheme and scale dependence of quark masses, mass dependent cut-off effects can become sizable towards the charm sector, when Wilson fermions are considered, such that full $\mathrm{O}(a)$ improvement and the use of small lattice spacings are needed.

Here we report the status of our ongoing computation to determine the mass of the charm quark in $N_f = 2+1$ lattice QCD with Wilson fermions, which applies recent non-perturbative results for the (scale dependent) quark mass renormalization factor [2], as well as for some of the improvement coefficients (multiplying the quark mass dependent terms involved) [3]. A calculation of the light and strange quark masses for the same lattice discretization is also under way [4].

2. Setup

We work on CLS ensembles with $N_f = 2+1$ flavors of $\mathrm{O}(a)$ improved Wilson fermions and Lüscher-Weisz gluons [5, 6]. In this work we constrain ourselves to the mass trajectory with $\mathrm{Tr}[M_q] = 2m_l + m_s = \mathrm{const.}$ All considered ensembles feature open boundary conditions in time to allow for a proper sampling of the topological charge. Measurements for five different lattice spacings a down to $\approx 0.04\,\mathrm{fm}$ and pion masses m_π down to $\approx 200\,\mathrm{MeV}$ are included. An overview of the considered ensembles is given in Fig. 1. In the near future, we will increase the statistics on the finest ensembles and add ensembles with smaller pion masses for some couplings.

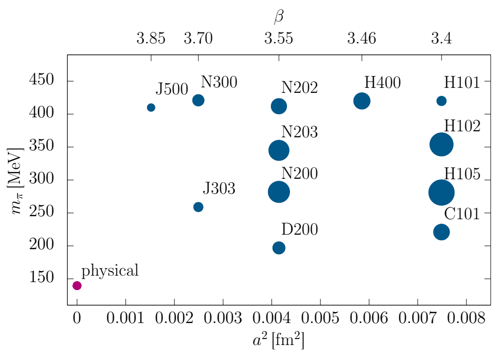

Figure 1: Status of the measurements. The area of the circles is proportional to the number of measurements. Ensemble ids are given in [5, 6].

We work in a partially quenched setup, where the charm quark only enters in the valence sector. To determine effective meson masses and the quark masses, we calculate the two-point correlation functions

$$f_O^{rs}(x_0, y_0) = -\frac{a^6}{L^3} \sum_{\vec{x},\vec{y}} \langle O^{rs}(x_0,\vec{x}) P^{rs}(y_0,\vec{y}) \rangle \,, \quad O^{rs} = \bar{\psi}^r(x)\,\Gamma\,\psi^s(x)\,, \tag{2.1}$$

where P is the pseudoscalar density, for all possible flavor combinations rs and various Dirac structures Γ. The sources are placed at the boundaries, i.e., at $y_0 = a$ and $y_0 = T - a$. To decrease the statistical error, we use 16 $U(1)$ noise sources per time slice.

Bare quark masses can be calculated from the $\mathrm{O}(a)$ improved PCAC relation via

$$am_{rs}(x_0) = \frac{\tilde{\partial}_0 f_{\mathrm{A}_0}^{rs}(x_0) + ac_\mathrm{A}\partial_0^*\partial_0 f_\mathrm{P}^{rs}(x_0)}{2f_\mathrm{P}^{rs}(x_0)}, \tag{2.2}$$

where A_0 is the temporal component of the axial current and $\tilde{\partial}_0$, ∂_0^* and ∂_0 are lattice representations of the central, backward and forward derivative. The improvement coefficient c_A is known non-perturbatively from ref. [7].

We consider two heavy valence quarks with masses above and below the physical charm quark mass. For both choices we determine the effective masses of the pseudoscalar mesons corresponding to D and D_s and of the vector mesons corresponding to D^* and D_s^*. The hopping parameter κ_c for a physical charm quark is determined on each ensemble by an interpolation of the meson masses to their physical values. In principle, each of the aforementioned mesons could be chosen to fix κ_c and the resulting values from different choices are expected to differ only by cut-off effects.

Since $\mathrm{Tr}[M_\mathrm{q}]$ is kept constant for all our ensembles, we can choose the flavor-averaged meson mass $M = \frac{1}{3}(2m_\mathrm{D} + m_{\mathrm{D_s}})$ for the calibration and expect the dependence on the light quark masses to be rather mild. In addition, we can use insights from heavy quark effective theory [8, 9] concerning the heavy meson masses, to remove short-distance effects from spin-interactions of the heavy quark. Therefore, the appropriate spin average on top of the flavor average, leading to the average mass

$$M = \frac{1}{12}(6m_{\mathrm{D}^*} + 2m_\mathrm{D} + 3m_{\mathrm{D}_\mathrm{s}^*} + m_{\mathrm{D_s}}), \tag{2.3}$$

is expected to decrease cut-off effects in the tuning procedure. At the same time, however, the statistical error on the vector meson masses is significantly larger than the error on the pseudoscalar meson masses. This could propagate into the final result. We thus consider both possibilities and judge the quality of the chiral-continuum extrapolations afterwards.

On top of the expected cut-off effects, heavy quarks can also introduce numerical difficulties. When the iterative solution of the Dirac equation is based on a global residuum

$$\left|\sum_z \mathbb{D}_{x,z} S_\mathrm{h}(z) - \eta(x)\right| < r_\mathrm{gl} \quad \text{with} \quad \mathbb{D} = D[U] + m_\mathrm{h}, \tag{2.4}$$

and the mass m_h is heavy, time slices far away from the source are exponentially suppressed, leading to incorrect solutions at late times [10]. Distance preconditioning [11] can be used to achieve numerically accurate results at all time slices. Instead of the original Dirac equation, the preconditioned system [12], in matrix notation

$$(P\mathbb{D}P^{-1})(PS) = (P\eta), \quad P = \mathrm{diag}(p_i), \quad p_i = \exp\left(\alpha\,|y_0 - x_0^{(i)}|\right), \tag{2.5}$$

is solved and the desired solution is obtained by the multiplication of the preconditioned solution with the inverse of the preconditioning matrix P. With an appropriate choice for the parameter α, the exponential decay of the propagator is counteracted such that, effectively the heavy quark acts as a light quark. To keep the additional cost under control, α has to be tuned carefully. Figure 2 shows the local residuum

$$r_\mathrm{loc}(x_0,y_0) \equiv \frac{|(\mathbb{D}S_\mathrm{h})(x_0,y_0) - \eta(x_0,y_0)|}{|S_\mathrm{h}(x_0,y_0)|}, \quad \text{with} \quad y_0 = a,\ x_0 = \frac{7}{8}T, \tag{2.6}$$

against α together with the number of iterations to reach $r_{gl} = 10^{-8}$. When α is increased above some threshold, r_{loc} starts to decrease exponentially, while the cost increases exponentially.

The effect of the preconditioned solver can be seen on the right hand side of Fig. 2, where we show the effective mass of the pseudoscalar heavy-light meson on the H400 ensemble for the preconditioned and the standard solver. Without preconditioning, the identification of a plateau is ambiguous since the effect of the numerical instabilities already dominates at comparably small times, leading to possibly large systematic uncertainties. We use the implementation of the distance preconditioned SAP-GCR solver [12] in the open source package `mesons` [13].

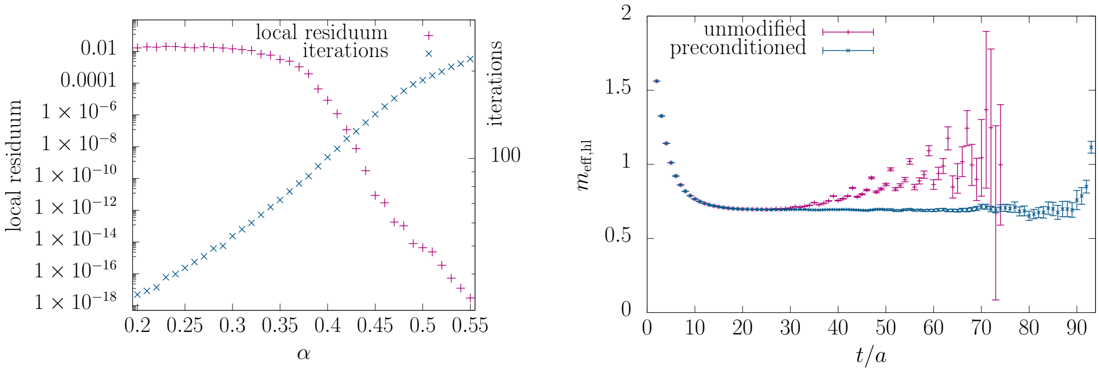

Figure 2: *Left:* The local residuum at $x_0 = \frac{7}{8}T$ and the number of iterations to reach the global residuum depending on the preconditioning parameter α on one configuration of the H400 ensemble. *Right:* Effective mass of the D meson determined on all configurations with and without distance preconditioning. The rise in $m_{\mathrm{eff,hl}}$ at late time slices for the preconditioned mass is due to the boundary at $T/a = 95$.

3. Renormalized quark masses

With κ_c at hand, we can interpolate the PCAC masses involving a heavy propagator to obtain the bare charm quark mass. To determine physical and O(a) improved masses, we need to renormalize and improve the bare quark masses. Taking the relevant formulae from refs. [2, 3], we arrive at

$$M_{rs}^{\mathrm{RGI}} = \frac{M}{\overline{m}(\mu_{\mathrm{had}})} m_{rs,\mathrm{R}} \equiv \frac{M}{\overline{m}(\mu_{\mathrm{had}})} \frac{Z_{\mathrm{A}}}{Z_{\mathrm{P}}(\mu_{\mathrm{had}})} m_{rs} \left[1 + \frac{(b_{\mathrm{A}} - b_{\mathrm{P}})}{Z} a m_{rs} - b_M a \mathrm{Tr}[M_{\mathrm{q}}] \right] \tag{3.1}$$

as general formula for a non-degenerate renormalized renormalization group invariant (RGI) quark mass. The running factor $M/\overline{m}$ to evolve the mass from the hadronic scale μ_{had} to the RGI value, as well as the non-perturbatively determined renormalization constant for the pseudoscalar density Z_{P}, are available from [2]. The renormalization constant for the axial current Z_{A} was determined in [14, 15]. We work with the value from ref. [15] because of its smaller statistical uncertainties. The combination of the improvement coefficients $(b_{\mathrm{A}} - b_{\mathrm{P}})$ and the normalization constant $Z = Z_{\mathrm{m}} Z_{\mathrm{P}}/Z_{\mathrm{A}}$ have recently been determined non-perturbatively [3]. They allow for correcting for the valence quark dependent piece of the O(a) effects, which are expected to be dominating for valence quark in the charm region. Whereas non-perturbative results for r_{m} are available in [16], the full factor multiplying the sum of the sea quark masses, defined as

$$b_M \equiv (r_{\mathrm{m}} - 1) \frac{(b_{\mathrm{A}} - b_{\mathrm{P}})}{N_{\mathrm{f}}} + (\overline{b}_{\mathrm{A}} - \overline{b}_{\mathrm{P}}) \,, \tag{3.2}$$

is not known non-perturbatively so far. Therefore we neglect this subleading piece of the improvement and investigate the possibility of residual $\mathrm{O}(a)$ effects in the continuum extrapolation.

By choosing different combinations of flavors rs, we can arrive at various definitions of the renormalized charm quark mass. Imposing two mass degenerate flavors c and c′ at the mass of the physical charm quark allows us to employ the clean signal of the PCAC mass from the heavy-heavy propagator to calculate the RGI mass via

$$M_\mathrm{c}^\mathrm{RGI} = \frac{M}{\overline{m}(\mu_\mathrm{had})} m_{\mathrm{cc'},\mathrm{R}} \,. \tag{3.3}$$

Since we expect the mass dependent cut-off effects to be rather large for this choice, we also consider the definition based on the light-heavy correlation functions,

$$2m_{\mathrm{lc},\mathrm{R}} - m_{\mathrm{ll'},\mathrm{R}} \equiv 2\,\frac{m_{\mathrm{c},\mathrm{R}} + m_{\mathrm{l},\mathrm{R}}}{2} - \frac{m_{\mathrm{l},\mathrm{R}} + m_{\mathrm{l},\mathrm{R}}}{2} = m_{\mathrm{c},\mathrm{R}} \,, \tag{3.4}$$

and the analogous expression from the strange-heavy correlation functions, where the non-degenerate quark masses have been defined in eq. (2.2). Combining both to a flavor averaged mass, to reduce the slope in the chiral extrapolation, we arrive at

$$M_\mathrm{c}^\mathrm{RGI} = \frac{M}{\overline{m}(\mu_\mathrm{had})} \frac{1}{3} \left[2(2m_{\mathrm{lc},\mathrm{R}} - m_{\mathrm{ll'},\mathrm{R}}) + (2m_{\mathrm{sc},\mathrm{R}} - m_{\mathrm{ss'},\mathrm{R}})\right] \tag{3.5}$$

as second definition for a renormalized charm quark. Both definitions can be used to determine a chiral-continuum extrapolated quark mass. This leads to a reduction of systematic effects.

4. Preliminary results

In Figure 3 we present the preliminary results of our analysis. On the left hand side the RGI charm quark mass determined from the definition in eq. (3.5) against the pion mass m_π is shown for the five values of the bare inverse coupling β. From the ensembles at $\beta = 3.40$ and $\beta = 3.55$ it can be seen, that there is no significant dependence of $M_\mathrm{c}^\mathrm{RGI}$ on the light quark masses. At the same time, the cut-off effects are rather large.

On the right hand side of Fig. 3 the preliminary chiral-continuum fits for both definitions (3.3) and (3.5) are shown. As expected, the masses based on the heavy-heavy current seem to suffer from larger cut-off effects. At this stage of the analysis we perform a fit to the polynomial form

$$M_\mathrm{c}^\mathrm{RGI}\left(t_0\delta_M^2, \frac{a^2}{t_0}\right) = c_0\left(1 + c_1 t_0 \delta_M^2\right)\left(1 + c_2\frac{a^2}{t_0}\right) \quad \text{with} \quad t_0\delta_M^2 = t_0(m_K^2 - m_\pi^2)\,, \tag{4.1}$$

with the fit parameters c_i which parameterize the leading chiral and cut-off effects. The chiral point is defined at the physical value of $t_0\delta_M^2$. The gluonic quantity t_0 is defined from the gradient flow and its physical value has been computed in ref. [17]. No linear dependence on a can be resolved. For the two coarsest lattice spacings, we observe higher-order effects in $M_\mathrm{c}^\mathrm{RGI}$ from definition (3.3) (blue points). Therefore we decide to exclude these points from our fit with the ansatz (4.1). For the definition (3.5) (red points), all ensembles are taken into account.

As it can be seen from Fig. 3, both definitions nicely coincide in the continuum limit. Although the different PCAC masses are partly correlated, we see this as evidence that possible systematic errors in the fit are under good control.

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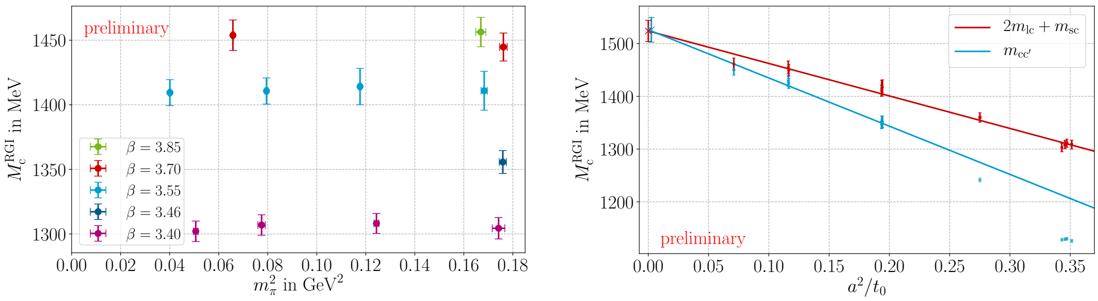

Figure 3: *Left:* Overview of the RGI charm quark masses evaluated on the considered ensembles depending on the pion mass. Different bare couplings and thus lattice spacings are indicated with different colors. *Right:* Chiral-continuum fits for both definitions of the charm quark mass. The higher-dimensional fits and the data points are projected onto the plane of the chiral trajectory.

5. Outlook

We have presented preliminary results of our determination of the RGI charm quark mass on the $N_f = 2+1$ CLS ensembles. To arrive at stable plateaus for the heavy-light mesons, we used a distance preconditioned solver. Our continuum extrapolations are monitored by extrapolating several definitions of the renormalized charm quark mass. Barely any effect of the sea quarks on the charm quark mass can be seen in our parameter region down to $m_\pi = 200\,\text{MeV}$. Although we refrain from quoting a number for $M_c^{\rm RGI}$ at this preliminary stage, we note that our extrapolated value is close to the FLAG average quoted in [18]. With the current status, we can foresee that the final precision will almost reach the $\approx 1\%$ limit dictated by the uncertainty on the running factor.

To arrive at final results, further steps will be done: As it can be concluded from Fig. 1, we have to increase the statistics on the most demanding ensembles. Additional ensembles on the $\text{Tr}[M_q] = \text{const.}$ trajectory are available for three lattice spacings and will be considered. This effort is ongoing. Especially the ensembles at the finest lattice spacing will help to stabilize the fit to the continuum. Other definitions of the renormalized quark mass, e.g., from the bare current quark mass and the ratio-difference method [19] can be explored to investigate possible systematic effects. The impact of a combined fit of several definitions will be studied. Although we do not expect any finite-volume effects on our charm observables, we will explicitly check this for one representative point in the parameter space.

As it is described in ref. [17], our ensembles deviate slightly from the chiral trajectory chosen for the $\text{Tr}[M_q] = \text{const.}$ trajectory. This can be corrected by a slight shift in the sea quark masses. In order to incorporate the effect on our observables, we calculated the derivatives of the correlation functions with respect to a shift in the sea quark masses.

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