# CHARMONIUM SPECTRUM FROM $N_\mathrm{f} = 3 + 1$ LATTICE QCD*

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We produced a set of gauge configurations generated with a new $N_\mathrm{f} = 3+1$ massive renormalization scheme for three degenerate light quarks with a mass that equals the average light-quark mass in nature and a physical charm-quark mass, and a non-perturbatively determined clover coefficient for dynamical Wilson quarks on the lattice. We present the details of the algorithmic setup and tuning procedure of ensembles with three different volumes. We discuss finite volume effects and lattice artifacts, and present physical results for the charmonium spectrum and dimensionless quantities in a first continuum limit study.

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## 1. Introduction

Heavy quarks have only little effect on low-energy physics which in practice can be neglected for the bottom and the top quark. The omission of a dynamical charm quark from QCD simulations has been shown to have only minor influence on low-energy observables [1], but can affect quantities with valence charm quarks at a few-percent level [2]. Moreover, when the strong coupling is determined on the lattice in $N_\mathrm{f} = 3$ QCD, the perturbation theory at the scale of the charm quark is necessary to relate it to the phenomenologically relevant $N_\mathrm{f} = 5$ result. This can introduce an error of up to 1.5% on the $\Lambda$ parameter [3].

In [4], a new action with a novel $\mathrm{O}(a)$ improvement scheme, specially tailored towards simulations including a charm quark, has been proposed. We report on first large volume simulations using this action, concentrating on the scale setting, which provides a relation between the bare coupling $g_0$ and the lattice spacing $a$ in fm. This relation is, up to lattice artifacts, independent of the quark masses. The standard procedure is to determine an experimentally accessible dimensionful quantity at the physical mass point

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in lattice units, and obtain the lattice spacing by using the experimental input. This usually requires simulations of the whole chiral trajectories at each lattice spacing. We propose a method for scale setting that is orders of magnitude cheaper and requires only simulations at the flavor SU(3) symmetric point, where the three light-quark masses are equal and

$$\phi_4 \equiv 8t_0\left(m_K^2 + \frac{m_\pi^2}{2}\right) = 12t_0 m_{\pi,K}^2 = 1.11\,, \tag{1}$$

$$\phi_5 \equiv \sqrt{8t_0}\,(m_{D_s} + 2m_D) = \sqrt{72t_0}\, m_{D,D_s} = 11.94\,. \tag{2}$$

At this mass point, $\sqrt{8t_0^\star} = 0.413(5)(2)$ fm has been determined in [5, 6]. Due to decoupling, it has the same value in the $3+1$ flavor theory up to a couple per mille, as long as the fourth quark's mass is at least as heavy as a charm quark, but this is what is enforced by the second condition of Eq. (2). Once the relation between $g_0$ and $a$ is mapped out at this particular mass point, one can proceed constructing chiral trajectories, *e.g.*, along lines where $\phi_4$ and $\phi_5$ are constant. However, already the SU(3) symmetric ensembles are highly useful. They can be the starting point for the determination of fundamental parameters of QCD, but also can be used directly for charm physics, where the unphysical light-quark masses play only a small role. The dynamical charm quark will allow to determine disconnected contributions to charmonium states.

## 2. Simulations

For our simulations, we choose a mass-dependent renormalization scheme, proposed in [4], using a mass-dependent clover coefficient $c_{\mathrm{SW}}$ in the clover action term $S_{\mathrm{SW}} = a^5 c_{\mathrm{SW}}(g_0^2, M_q)\sum_x \bar\psi(x)\frac{i}{4}\sigma_{\mu\nu}\hat F_{\mu\nu}(x)\psi(x)$, which has been determined non-perturbatively. We apply this action for the first time to large volume simulations with a physical charm-quark mass. For a first estimate of the bare coupling and quark masses, we use the tuning results in [4], determined on a line of constant physics (LCP). For our first simulation, we choose a bare coupling $\beta = 3.24$, light-quark masses given by $\kappa_{u,d,s} = 0.134484$ and a charm-quark mass by $\kappa_c = 0.12$. For the algorithmic parameters, we started with the setup of CLS's H400 simulation, *cf.* [7], to which we added the charm quark. The new contribution to the action was not further factorized and the corresponding forces were integrated on the second level of our three-level integrator. For our simulations, we use openQCD version 1.6 [8] with open boundary conditions in time direction and twisted-mass reweighting, 2$^{\mathrm{nd}}$ and 4$^{\mathrm{th}}$ order OMF integrators [9], SAP preconditioning and low-mode-deflation based on local coherence [10, 11]. For a full specification of the action with open boundary conditions, we also need

$c_0 = 5/3$ for the Lüscher–Weisz action, boundary improvement coefficients $c_F = c_G = 1.0$ and the clover coefficient from the fit formula [4]

$$c_{\rm SW}(g_0^2 = 6/3.24) \;=\; \tfrac{1+Ag_0^2+Bg_0^4}{1+(A-0.196)g_0^2} = 2.18859\,,\;\; A = -0.257\,,\;\; B = -0.050\,.$$

The $u/d$ quark doublet is simulated with a weight proportional to

$$\det\left[D^\dagger D\right] \to \det\left[(D_{\rm oo})^2\right] \det\frac{\hat{D}^\dagger\hat{D} + \mu_0^2}{\hat{D}^\dagger\hat{D} + 2\mu_0^2} \det\left[\hat{D}^\dagger\hat{D} + \mu_0^2\right] \tag{3}$$

in terms of the even–odd preconditioned Dirac operator $\hat{D} = D_{\rm ee} - D_{\rm eo}\,(D_{\rm oo})^{-1}D_{\rm oe}$, with $D = D_W + m_0$, where we introduced an infrared cutoff by the twisted mass $\mu_0$. The strange and charm quarks are simulated with RHMC, and the two rational functions have degrees 12 and 10, respectively, with ranges optimized during the tuning process. Both the doublet and the rational parts need reweighting and are further factorized according to [12]

$$\det\!\left[\hat{D}^\dagger\hat{D}+\mu_0^2\right] = \det\!\left[\hat{D}^\dagger\hat{D}+\mu_N^2\right] \times \frac{\det\!\left[\hat{D}^\dagger\hat{D}+\mu_0^2\right]}{\det\!\left[\hat{D}^\dagger\hat{D}+\mu_1^2\right]} \times \ldots \times \frac{\det\!\left[\hat{D}^\dagger\hat{D}+\mu_{N-1}^2\right]}{\det\!\left[\hat{D}^\dagger\hat{D}+\mu_N^2\right]}\,,$$

with $a\mu_i$ given by $\{0.0005, 0.005, 0.05, 0.5\}$ for all our ensembles, such that we have 13 pseudo-fermion fields and 14 actions in total.

After thermalization on spatially smaller lattices and subsequent doubling of the spatial dimensions, flow observables and meson masses were computed on a more-or-less thermalized subset of configurations. It turned out that the desired tuning point was missed by quite a bit. What makes the tuning process non-trivial is the fact that in $\phi_4$ and $\phi_5$, the mass dependence of $t_0$ and the meson masses go in opposite directions. The final tuning point turns out to be

$$\kappa_{u,d,s} \;=\; 0.13440733\,, \qquad \kappa_c = 0.12784\,.$$

With these final parameters, we produced two high statistics ensembles A1 and A2 with two different lattice sizes given in Table I and a short ensemble A0 on a smaller lattice to study finite size effects. A computation of $t_0^\star/a^2$ on these ensembles, together with the known value of $\sqrt{8t_0^\star} = 0.413(5)(2)$ fm [5, 6], yields values for the lattice spacings in fm. A setup with open boundaries in the temporal direction and periodic boundaries in spatial directions allows us to reach fine lattice spacings [13], which is crucial for simulations with a dynamical charm quark in the sea. The measurements of the mesonic two-point functions were carried out with the open-source (GPL v2) program "mesons" [14] — the degenerate pion/kaon and $D$-/$D_s$-meson masses in lattice units as well as our final tuning parameters are shown in Table II.

Assuming decoupling, *i.e.*, $t_0^\star|_{N_\mathrm{f}=3+1} = t_0^\star|_{N_\mathrm{f}=3} + O(1/m_\mathrm{charm}^2)$, our value of $t_0/a^2 \approx 7.4$ corresponds to a lattice spacing $a \approx 0.054$ fm. The physical size of our $L/a = 32$ lattice is $L \approx 1.73$ fm with $m_\pi L = 3.5$, which is a bit small, but finite size effects seem to be under control, as the comparison with $L/a = 48$ shows, see also [15]. In a next step, we tuned an ensemble B at a finer lattice spacing on a $144 \times 48^3$ lattice with a bare coupling $\beta = 3.43$ using the same procedure as described above, yielding final parameters $\kappa_{u,d,s} = 0.13599$ and $\kappa_c = 0.13088$, and a lattice spacing $a \approx 0.043$ fm. This gives a physical lattice extent $L \approx 2.06$ fm and $m_\pi L = 4.3$.

TABLE I

Simulation parameters, lattice sizes and statistics of the new ensembles.

| Ens. | $\frac{T}{a} \times \frac{L^3}{a^3}$ | $6/g_0^2$ | $am_{u,d,s}$ | $am_c$ | $a$ [fm] | $Lm_\pi^\star$ | $N_\mathrm{traj}$ (MDU) |
|---|---|---|---|---|---|---|---|
| A0 | $96 \times 16^3$ | 3.24 | −0.27996 | −0.08886 | 0.054 | 1.75 | 1000 (2000) |
| A1 | $96 \times 32^3$ | 3.24 | −0.27996 | −0.08886 | 0.054 | 3.5 | 3908 (7816) |
| A2 | $128 \times 48^3$ | 3.24 | −0.27996 | −0.08886 | 0.054 | 5.3 | 3868 (7736) |
| B | $144 \times 48^3$ | 3.43 | −0.32326 | −0.17971 | 0.041 | 4.4 | 4000 (8000) |

TABLE II

Tuning results of the new ensembles.

| Ens. | $N_\mathrm{ms}$ | $t_0/a^2$ | $am_{\pi,K}$ | $am_{D,D_s}$ | $\phi_4$ | $\phi_5$ |
|---|---|---|---|---|---|---|
| A0 | 500 | 8.83(23) | 0.310(6) | 0.614(17) | 10.22(90) | 15.48(43) |
| A1 | 1954 | 7.42(4) | 0.1141(8) | 0.5232(7) | 1.161(22) | 12.098(36) |
| A2 | 1934 | 7.37(2) | 0.1111(3) | 0.5234(4) | 1.092(6) | 12.058(17) |
| B | 2000 | 11.60(6) | 0.0896(5) | 0.4135(7) | 1.116(12) | 11.950(30) |

## 3. Charmonium spectrum

Our ensembles with fine lattice spacings are very well suited for a study of charmonia — already at the coarsest lattice, the charmonium masses that we measure, neglecting disconnected contributions at the moment, are very close to their values in nature. In Fig. 1, we show the meson spectrum of our ensemble B. We get a very clear signal up to the $J/\Psi$ state and can extract reasonable plateau values for higher charmonium states summarized in Table III. We find good agreement for charmonia with PDG data because they contain only charm valence quarks which in our simulations have their physical mass value. Further, the sum of the degenerate light-quark masses is at its physical value, and since there are no light quarks in the valence sector, the derivatives of the charmonium masses with respect to light quark masses are equal, *i.e.* $\mathrm{d}m_x/\mathrm{d}m_{\mathrm{up}} = \mathrm{d}m_x/\mathrm{d}m_{\mathrm{down}} = \mathrm{d}m_x/\mathrm{d}m_{\mathrm{strange}}$. If we want to correct the degenerate light-quark masses to their physical values via $m_x^{\mathrm{phys}} = m_x + (\Delta_{\mathrm{up}} + \Delta_{\mathrm{down}} + \Delta_{\mathrm{strange}})\frac{\mathrm{d}m_x}{\mathrm{d}m_u} + \mathrm{O}(\Delta^2)$, it is clear that the linear term vanishes, because $\phi_4$ is chosen such that $\Delta_{\mathrm{up}} = \Delta_{\mathrm{down}} = -0.5\Delta_{\mathrm{strange}}$ $(m_{u,d,s} = \sum_{i=u,d,s} m_i^{\mathrm{phys}}/3)$, and we only have $\mathrm{O}(\Delta^2)$ corrections.

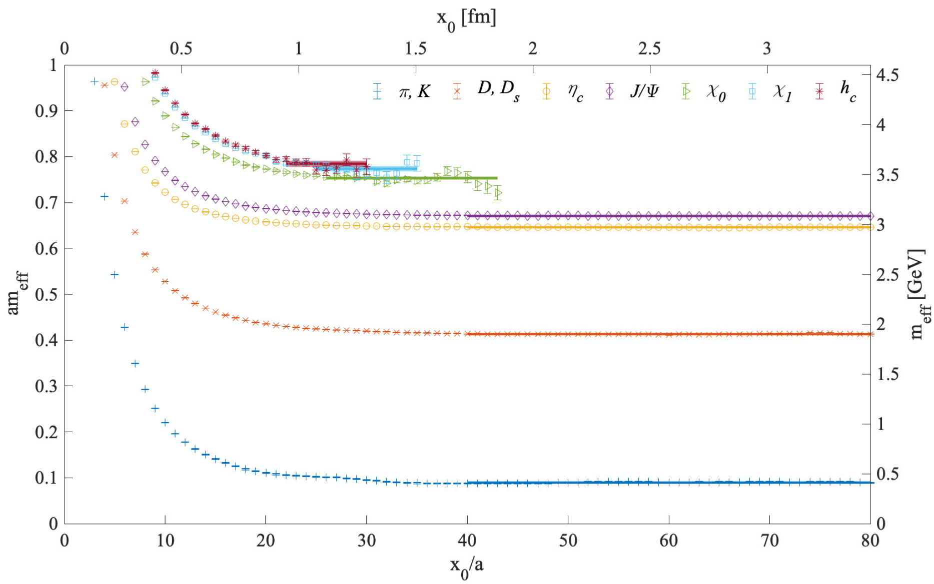


Fig. 1. Effective masses of the pion/kaon, $D$- and $D_s$-meson, charmonium states $\eta_c$, $J/\Psi$, $\chi_0$, $\chi_1$ and $h_c$ (from bottom to top) on ensemble B.

TABLE III

Effective masses of charmonium states together with their PDG values.

| [GeV] | $\eta_c$ | $J/\psi$ | $\chi_{c_0}$ | $\chi_{c_1}$ | $h_c$ |
|---|---|---|---|---|---|
| $m_{\mathrm{eff}}$ | 2.973(52) | 3.086(55) | 3.456(79) | 3.54(10) | 3.62(11) |
| PDG | 2.9834(5) | 3.096900(6) | 3.4148(3) | 3.51066(7) | 3.52538(11) |

## 4. Conclusions and outlook

We produced a new set of gauge configurations generated with $N_{\mathrm{f}} = 3+1$ Wilson quarks with a non-perturbatively determined clover coefficient in a massive $\mathrm{O}(a)$ improvement scheme with lattice spacings $a = 0.054$ fm and $a = 0.043$ fm. The three light quarks are degenerate, with the sum of their masses being equal to its value in nature and the charm quark having its physical mass. As a first physics result, we measure the masses of the charmonium states $\eta_c$, $J/\psi$, $\chi_{c_0}$, $\chi_{c_1}$ and $h_c$, which we find in good agreement with their PDG values. The highlight of our analysis is the charmonium hyperfine splitting, $(m_{J/\Psi} - m_\eta)/m_\eta = 0.0380(3)$ on ensemble B, within per mille level precision of the experimentally known value 0.038. On ensemble A2, we measure a value of 0.0382(3), hence we observe almost no lattice artifacts. We further plan to study decoupling of the charm quark with light quarks on our ensembles, measure the charmonium sigma terms and disconnected quark loop contributions. For a good continuum limit study, we plan an even larger and finer ensembles. For more details, see also [15].

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