PROCEEDINGS OF SCIENCE

$N_f = 1 + 2 + 1$ QCD+QED simulations with C* boundary conditions

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We give an update on the ongoing effort of the RC* collaboration to generate fully dynamical QCD+QED configurations with C* boundary conditions using the openQ*D code. The simulations are tuned to the U-symmetric point ($m_d = m_s$) with pions at $m_{\pi^\pm} \approx 400$ MeV. The splitting of the light mesons is used as one of three tuning observables and fixed to $m_{K^0} - m_{K^\pm} \approx 5$ MeV and $m_{K^0} - m_{K^\pm} \approx 25$ MeV on ensembles with renormalized electromagnetic coupling $\alpha_\mathrm{R} \approx \alpha_\mathrm{phys.}$ and $\alpha_\mathrm{R} \approx 5.5\alpha_\mathrm{phys.}$ respectively. We will discuss some details concerning our tuning strategy and present the calculation of the meson and baryon masses. Finally, we will also present a cost analysis for our simulations. More technical details on finite-volume effects and the tuning can be found in A. Cotellucci's proceedings [1].

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1. Introduction

We present an update on a long-term research program aiming at calculating isospin-breaking and QED radiative corrections in hadronic quantities, with C* boundary conditions [2–5] and fully-dynamical QCD+QED simulations. C* boundary conditions allow for a local and gauge-invariant formulation of QED in finite volume and in the charged sector of the theory [6–8]. In particular, three new ensembles were generated at the values of the fine-structure constant $\alpha_R \approx 0.04$ and $\alpha_R \approx 1/137$. The larger value of α_R was chosen to amplify QED corrections.

The open-source `openQ*D-1.1` code [9, 10] was used to generate all gauge configurations presented in this work. This code has been developed by the RC* collaboration. It is an extension of the `openQCD-1.6` code [11] for QCD.

In this proceedings, we will give a very broad overview of the ensembles we have generated and some observables that were computed on them. Starting from our renormalization scheme (section 2) we will show some baryon masses computed at physical electromagnetic coupling (section 3). This is followed by a short overview of the cost of the fully dynamical QCD+QED simulations we have done so far (section 4). The section on the finite volume effects, mentioned in the talk can be found in Alessandro Cotellucci's proceedings [12].

2. Ensembles and Setup

We have generated two $N_f = 3+1$ QCD ensembles and five $N_f = 1+2+1$ QCD+QED ensembles. For the SU(3) field the Lüscher-Weisz action with $\beta = 3.24$ was used, while for the U(1) field the Wilson action with $\alpha_0 = 0.05$ and $\alpha_0 = 1/137$ (for the QCD+QED ensembles), and $O(a)$-improved Wilson fermions. We employ C* boundary conditions in all three spatial and periodic boundary conditions in the time direction for all our ensembles. We have verified that we are free from the problem of topological freezing in all our ensembles, which justifies the use of periodic boundary conditions in time. More information on the setup and choice of parameters can be found in [13, 14].

Compared to [14], the major updates are three new ensembles. There are two new ones at $\alpha_0 = 1/137$ on a 64×32^3 lattice and one at $\alpha_0 = 0.05$ on a 96×48^3 lattice. An overview of all ensembles can be found in figure 1. QCD+QED with four fermion flavors is parameterized by six inputs. The parameters of our ensembles are fixed via the (unphysical) scheme

$$\sqrt{8t_0} = 0.415\,\text{fm} \qquad \alpha_\mathrm{R} \in \{0, 1/137, 0.05\} \tag{1a}$$

$$\phi_0 = 8t_0\left(M_{\pi^\pm}^2 - M_{K^\pm}^2\right) \stackrel{!}{=} 0 \qquad \phi_1 = 8t_0\left(M_{K^0}^2 + M_{\pi^\pm}^2 + M_{K^\pm}^2\right) \stackrel{!}{=} \phi_1^{\text{phys.}} \tag{1b}$$

$$\phi_2 = 8t_0\left(M_{K^0}^2 - M_{K^\pm}^2\right)/\alpha_\mathrm{R} \stackrel{!}{=} \phi_2^{\text{phys.}} \qquad \phi_3 = \sqrt{8t_0}\left(M_{D^0} + M_{D^\pm} + M_{D_s^\pm}\right) \stackrel{!}{=} \phi_3^{\text{phys.}}\,. \tag{1c}$$

Taking the meson masses from the PDG [15], the value of $\sqrt{8t_0}$ from [16] and the Thompson limit of the electromagnetic coupling $\alpha_\mathrm{R} = 1/137$ one gets

$$\phi_0^{\text{phys.}} = 0.992\,, \qquad \phi_1^{\text{phys.}} = 2.26\,, \qquad \phi_2^{\text{phys.}} = 2.36\,, \qquad \phi_3^{\text{phys.}} = 12.0\,. \tag{2}$$

The scheme defined in eq. (1) is unphysical in multiple ways. First of all, the overall scale t_0 cannot be measured directly in an experiment. Furthermore, choosing $\phi_0 = 0$ implies that the down and

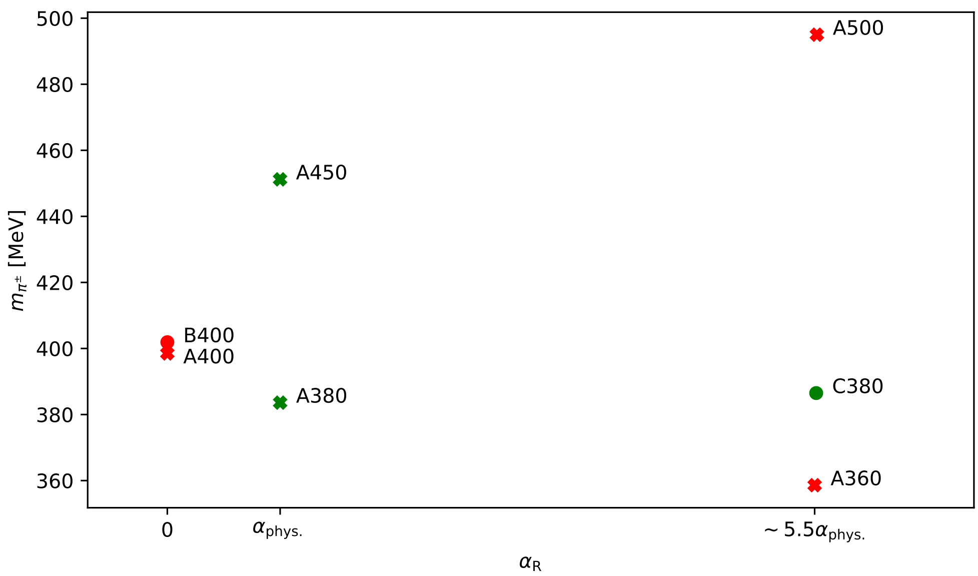


Figure 1: Overview of all ensembles generated so far. The first letter in the naming convention denotes the geometry of the ensemble. For example, A corresponds to a 64×32^3 lattice, while C stands for a 96×48^3 lattice. The number after the first letter stands for the mass of the lightest excitation in the system, i.e. the pion. Dots denote large volumes, while crosses denote the smaller 64×32^3 lattices. In green are the new ensembles, while the red ones were already discussed in [13].

strange quark need to be degenerate. At some point in the future, the goal is to replace the scale t_0 by the mass of the omega baryon M_{Ω^-} and split the down and strange quark to be able to do simulations closer to the physical point. A plot of the chosen lines of constant physics can be found in figure 2.

3. Hadron masses

Both the meson and baryon masses are extracted in a gauge-invariant way by dressing the bare quark fields with Dirac factors [8]. For the mesons, this is sufficient to build interpolating operators that have a good overlap with the meson states on our ensembles. For the baryons, the procedure is slightly more involved. Baryon operators are constructed from smeared, U(1)-gauge-invariant fermion fields and smeared gauge links. Gaußian smearing is used for gauge invariant, dressed quark operator Ψ

$$\Psi_{(s)} = (1 + \omega H[U_s])^n \Psi \, . \tag{3}$$

Here $H[U_s]$ is the spatial hopping operator depending on smeared gauge field U_s. The gauge smearing is done with a modified gradient flow defined by the flow equation

$$\partial_s U_s(x,k) = \partial_{x,k} \sum_{i \neq j} \mathrm{tr} P_{s,ij}(x) \qquad \text{with} \qquad U_0 = U \, . \tag{4}$$

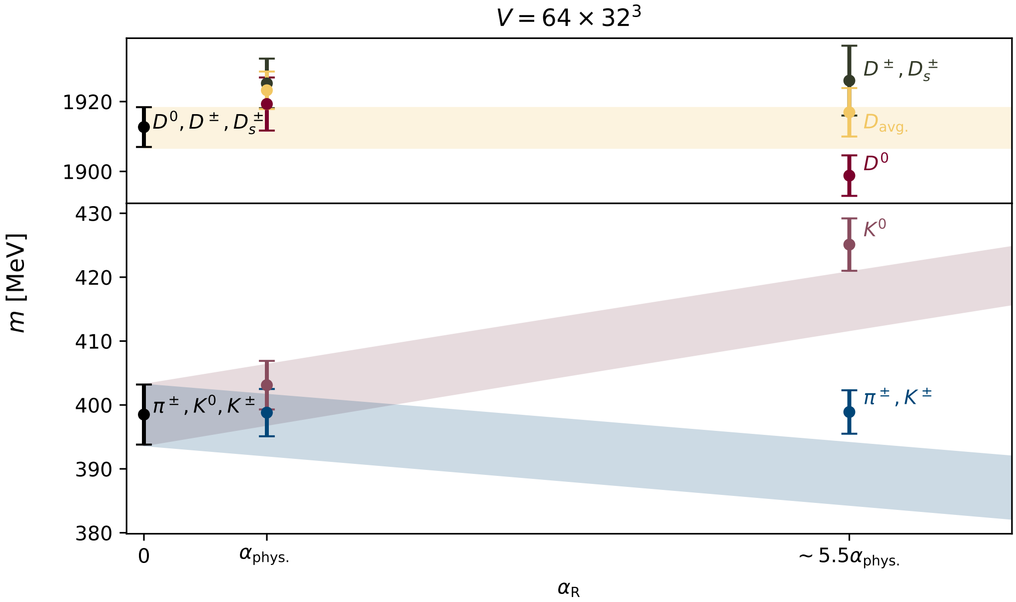


Figure 2: Illustration of the tuning procedure. On the left in black one can see the light meson masses in pure QCD at $\alpha_{\mathrm{R}} = 0$, at the SU(3)-symmetric point (thus the degeneracy of the low-lying mesons). The yellow, red, and blue bands depict the lines of constant physics for the light (lower section) and heavy (upper section) mesons. On the QCD+QED ensemble at $\alpha_{\mathrm{R}} \approx 1/137$ one can see, that the light mesons are straight on the line of constant physics, while the heavy ones are slightly too heavy. The opposite situation is the case for the ensemble at the artificially large value of $\alpha_{\mathrm{R}} \approx 0.04$.

The spatial plaquettes in the point x, built from U(1)-gauge-links at positive flow-time s are denoted by $P_{s,ij}(x)$. The flowtime s and parameters n and ω are optimized using the GEVP. The modified version of the flow is used since it preserves locality in time. The interpolating operator for a spin-1/2 baryon is then given by

$$B(x_0) = \sum_{\vec{x}} \sum_{\substack{abc\\fgh}} \epsilon_{abc} F_{fgh} \left\{ \Psi_{(\mathrm{s})fa} \Psi^t_{(\mathrm{s})gb} C\gamma_5 \Psi_{(\mathrm{s})hc}(x_0,\vec{x}) - C\bar{\Psi}^t_{(\mathrm{s})fa} \bar{\Psi}_{(\mathrm{s})gb} C\gamma_5 \bar{\Psi}^t_{(\mathrm{s})hc}(x_0,\vec{x}) \right\} . \tag{5}$$

Here, a, b, c are color indices and f, g, h are flavor indices (spin indices are implicit or contracted). The matrix C is the charge conjugation operator acting on the spin indices. Different baryons are obtained by choosing particular tensors F_{fgh}, according to the table 1. Projecting the two-point function onto the positive parity component, the $1/2^+$ correlation functions at zero momentum are

$$C(x_0) = \langle B^t(0) C \frac{1+\gamma_0}{2} B(x_0) \rangle . \tag{6}$$

Working out the quark contractions, it turns out, that the correlation function decomposes into a single-quark-line-connected $C_1(x_0)$ and a three-quark-line-connected part $C_3(x_0)$. The contribution from C_1 is exponentially suppressed with the volume: With C⋆ boundary conditions, one has quark-quark and antiquark-antiquark contractions, because the quark and antiquark are related via the

$(1/2)^+$ Baryon	Non-zero components of F_{fgh}
p	$F_{uud} = 1$
n	$F_{ddu} = 1$
Λ_0	$F_{sud} = 2$, $F_{dus} = 1$, $F_{uds} = -1$
Σ^+	$F_{uus} = 1$
Σ^-	$F_{dds} = 1$
Ξ_0	$F_{ssu} = 1$
Ξ^-	$F_{ssd} = 1$

Table 1: Flavor tensor F_{fgh} defining the interpolating operators for spin-1/2 baryons via eq. (5). The flavor indices can take values u, d, s, and c.

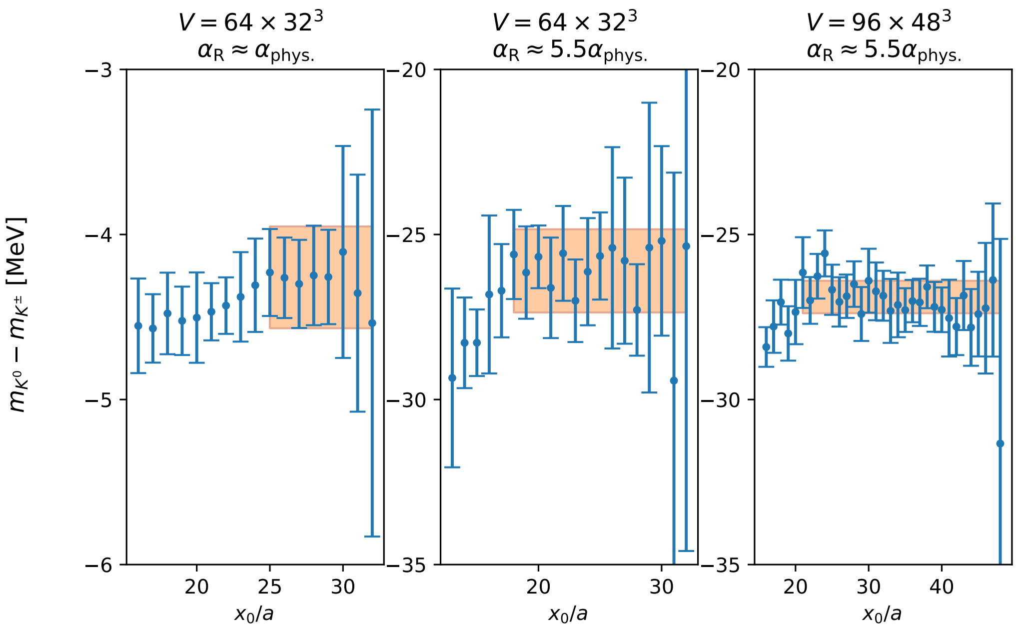
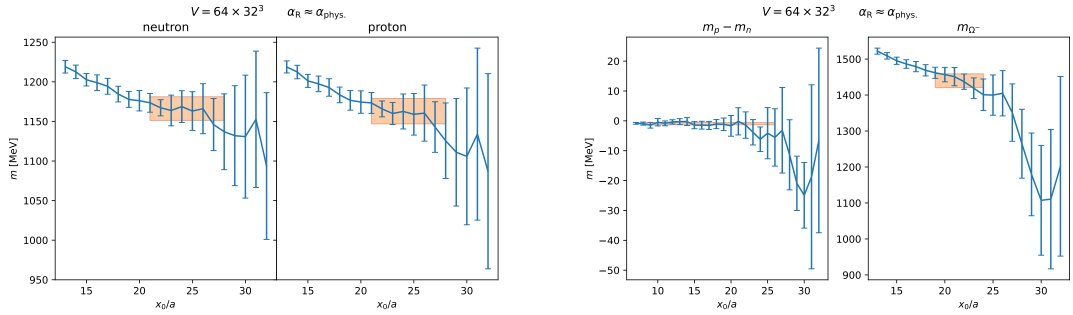


Figure 3: Splitting of the light mesons. In the left plot, one can see the splitting of the kaons on the ensemble A380. In the middle, the absolute value of the splitting is much larger as it was extracted from the ensemble A360. Keeping ϕ_2 constant it follows that the splitting is proportional to α_R. Finally, on the right-hand side, the splitting is extracted on C380. The error bar is significantly smaller, compared to the smaller volume. In all plots, the orange error band denotes the effective mass and indicates the fit range that was used.

boundary conditions. Such flavor-violating artefacts are pure finite volume effects and are proven to vanish in the $L \to \infty$ limit [6]. So, in this work, only the C_3 parts of the baryon correlation functions are computed. The masses that have been extracted from our smeared baryon interpolating operators are displayed in figure 4.



(a) Proton and neutron effective masses.

(b) Proton and neutron splitting and omega effective mass.

Figure 4: Baryon observables. Compared to the mesons in figure 3, the baryon observables need to be extracted from intermediate times, since the large times are clearly dominated by noise. The small volume at physical electromagnetic coupling is currently not suitable to extract a signal for the nucleon splitting.

4. Cost analysis

At past conferences, the question about the cost of simulations with $C^\star$ boundary conditions was asked a couple of times. While we can not yet make an estimate of how the cost will scale to the physical point, we can compare a simulation of QCD with periodic boundary conditions with one with $C^\star$ boundaries. On top of that, we can give a number on the overhead of including dynamical QED in the simulations for the ensembles we have generated so far. In order to be able to compare the production cost, we have measured the time needed to generate a thermalized configuration on Lise[1] at HLRN for all gauge ensembles. The results are shown in table 2; in particular, we report the specific cost, i.e. the cost in core$\times$seconds per molecular dynamics unit divided by the number of lattice points.[2] Comparing `A1` with `A400a00b324` one would naively expect that the latter was a factor of 2 more expensive since it uses $C^\star$- instead of periodic boundary conditions. Looking at the specific cost shows that the factor is in fact much smaller. This can be explained by a change in the algorithmic parameters. While both simulations used a three-level integrator and a similar number of fermionic forces, our ensemble `A400a00b324` integrates six instead of eight forces on the mid-level. This results in a factor of $6/8$ and reduces the cost gap. This gap is even further reduced by the fact that in the generation of `A1` smaller residues were used for the solvers. Comparing the number of times the Dirac operator is applied by the various solvers, we estimate the difference in residues to account for another factor of 0.84. Thus, in total we estimate the specific cost of the QCD simulation with $C^\star$ boundary conditions to be $2 \times 6/8 \times 0.84 = 1.26$ times larger than the one with periodic boundary conditions. Comparing that with the actual factor of $0.42/0.35 = 1.2$

[1]Lise has 1236 standard nodes with 384 GB memory, each of them with 2 CPUs. The CPUs are Intel Cascade Lake Platinum 9242 (CLX-AP) with 48 cores each. The nodes are connected with an Omni-Path network with a fat tree topology, 14 TB/s bisection bandwidth, and 1.65 μs maximum latency. Source: `https://www.hlrn.de/supercomputer-e/hlrn-iv-system/?lang=en`.

[2]The reader familiar with `openQ*D` knows that $C^\star$ boundary conditions are implemented by means of an orbifold procedure which effectively doubles the lattice size. In the code, one distinguishes between physical and extended (i.e. doubled) lattice. Throughout this paper, we always refer to the physical lattice. When we talk about lattice volume, we always refer to the volume of the physical lattice. In particular, in order to reconstruct the total cost from table 2, one needs to multiply the specific cost times the number of points of the physical lattice.

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ensemble	global volume	n. cores	specific cost $\left[\frac{\text{cores}\times\text{secs}}{\text{MDUs}\times\text{points}}\right]$
`A1` [17]	96×32^3	6144	0.35
`A400a00b324`	64×32^3	4096	0.42
`B400a00b324`	80×48^3	2560	0.62
`A450a07b324`	64×32^3	4096	1.07
`A380a07b324`	64×32^3	4096	1.03
`A500a50b324`	64×32^3	4096	0.88
`A360a50b324`	64×32^3	4096	1.05
`C380a50b324`	96×48^3	3072	1.40

Table 2: Cost comparison of all production runs presented in this work with a $N_f = 3+1$ QCD ensemble `A1` produced by the ALPHA collaboration [17]. For comparability, all times were measured on Lise at HLRN.

we can conclude that we have a good understanding of where the overhead comes from. Similar estimations for the other ensembles can be found in [14].

5. Summary and outlook

Up to the time of publication, we have generated five tuned QCD+QED ensembles at two different volumes. Comparing the cost of the generation of our current ensembles with QCD simulations at the SU(3)-symmetric point and periodic boundary conditions, we conclude that we understand the origin of the overhead of our simulations. We are currently generating another ensemble at $\alpha = 0.02$. Unfortunately, we have also shown that the small-volume ensembles that we have generated suffer from considerable QED and QCD finite-volume effects. Hence in order to achieve an actual precise tuning, future simulations need to be done at much larger volumes. This is especially true once one wants to attempt to reach the physical point. In that case, the quarks, and thus the mesons used for tuning, will become much lighter and suffer from larger finite-volume effects. Switching to a physical scheme makes it also necessary to have a much more precise estimation of the omega mass. Hence, we want to improve the computation of the baryon masses by applying noise reduction techniques.

Since the tuning and the generation of fully dynamical QCD+QED ensembles is rather expensive our collaboration is also investigating the RM123 method [18] in conjunction with C* boundary conditions. Here, QED effects are included perturbatively in iso-symmetric QCD ensembles. This has the advantage, that the tuning is much simpler due to the smaller number of parameters. The disadvantage is that every new order in α poses a new challenge in the sense that the operator insertions in the correlations functions become more and more complicated. Investigating, how the fully dynamical approach and the RM123 method compare and what the limitations of each approach are is important not only from a conceptual but also from an economical point of view.

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