Project ID **bep00102** — Initial Application

Towards QCD+QED Simulations with C* Boundary Conditions at physical QED coupling

Application for CPU-time on Lise

collaboration

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Contents

Abstract

This project is a natural continuation of the previous project **bep00085** (allocation period: January 2020 – December 2020), and it is part of a long-term research programme aiming at calculating isospin-breaking and QED radiative corrections in hadronic quantities from first principles in QCD+QED. We propose the generation of three QCD+QED gauge ensembles with lattice spacing $a \simeq 0.05$ fm, with three values of the fine-structure constant $\alpha_R \simeq 1/137, 0.02, 0.04$, at the U-symmetric point i.e. $m_d = m_s$. The quark masses need to be tuned to a suitably-chosen line of constant physics. Two different lattice volumes are considered: 64×32^3 and 96×48^3 with C* boundary conditions in the spatial directions and periodic boundary conditions in the temporal direction. These ensembles will allow to study finite-volume effects of various observables on the one hand, and the linearity of observables in α_R on the other hand. We apply to a total of **4.73M NPL** on Lise.

1 Overview of the application

Isospin-breaking and QED radiative corrections to hadronic observables are generally rather small but they become phenomenologically relevant when the target precision is at the percent level. For example, leptonic and semileptonic decay rates of π and K mesons are presently known from lattice simulations at the sub–percent level of accuracy [1]. At the same time, QED radiative corrections to these quantities are estimated to be of the order of a few percent, by means of chiral perturbation theory [2], and must be included at this level of precision.

This project is a natural continuation of the previous project **bep00085** (allocation period: January 2020 – December 2020), and it is part of a long-term research programme aiming at calculating isospin-breaking and QED radiative corrections in hadronic quantities from first principles in QCD+QED. The signature of the proposed project is the use of C* boundary conditions [3, 4, 5, 6] which allow for a local and gauge-invariant formulation of QED in finite volume and in the charged sector of the theory [7, 8, 9]. In particular, full QCD+QED configurations will be generated at various values of the fine-structure constant α_R (including $\alpha_R = 0$) in such a way that physical observables can be interpolated at the physical value of $\alpha_R \simeq 1/137$. The generated configurations will be used to explore a variety of observables: from baryon correlators and masses to decay rates of mesons in QCD+QED.

The open-source `openQ*D-1.1` code [10] will be used to generate gauge configurations. This code has been developed by the RC* collaboration (several investigators of this application are among its developers). It is an extension of the `openQCD-1.6` code [11] for QCD.

We plan to extend our previous work in two directions, organized in two distinct and independent subprojects.

1. We will generate two ensembles of $N_f = 1+2+1$ QCD+QED configurations (`Q*D-32-4-GEN` and `Q*D-32-6-GEN`) with lattice spacing $a \simeq 0.054$ fm, and two values of the fine-structure constant $\alpha_R \simeq 1/137, 0.02$. Unphysically large values of the fine-structure constant produce an amplification of isospin-breaking effects. This strategy will allow a first investigation of the linearity of observables in this range of α_R, of the deterioration of the signal-to-noise ratio for isospin-breaking effects at smaller values of α_R, and the possibility to use a linear interpolation with several values of α_R in order to reduce the error. Tuning the bare masses to the chosen line of constant physics (described in section 3) is particularly complicated in the presence of electromagnetic interactions, because of the large number of parameters. Building on the experience accumulated with the project **bep00085**, we will follow a partially quenched stategy for tuning the bare masses while α is gradually increased, and the pion mass is gradually decreased. Dedicated runs (`Q*D-32-3-TUN`, `Q*D-32-3-GEN`, `Q*D-32-4-TUN`, `Q*D-32-4-GEN`) are designed for this purpose. The tuning strategy is described in detail in section 4. Finally, the goal of the `Q*D-32-4-OBS` and `Q*D-32-6-OBS` runs is to calculate all mesonic masses including reweighting factors on the full set of configurations.

2. Understanding finite-volume effects is one of the biggest challenges in QCD+QED simulations, since the photon introduces corrections that are proportional to inverse powers of the volume. Specific runs have been designed to investigate this source of systematic errors in a quantitative way. We will generate one ensemble of $N_f = 1+2+1$ QCD+QED configurations (`Q*D-48-1-GEN`) at $\alpha_R = 0.04$, with the parameters obtained with our project **bep00085**, and we will measure all mesonic masses including reweighting factors (`Q*D-48-1-OBS`) on this set of configurations.

A summary of the cost analysis for the proposed application is presented in table 1, and motivated in section 6. We therefore apply for computer time on Lise for a total amount of

$$\textbf{32.42M core}\times\textbf{hours on Lise} = \textbf{0.34M (Lise node)}\times\textbf{hours} = \textbf{4.73M NPL}$$

equally distributed over the four quarters

$$\textbf{4.73M NPL} = \textbf{1.19M NPL} + \textbf{1.18M NPL} + \textbf{1.18M NPL} + \textbf{1.18M NPL}\ .$$

run	volume	n. cnfgs	cnfgs from run	nodes	time per cnfg	total time	total cost
`Q*D-32-3-TUN`	64×32^3	500	`QCD-32-1`	43	490 s	3 d	0.28 Mch
`Q*D-32-3-GEN`	64×32^3	1000	—	43	1300 s	15 d	1.49 Mch
`Q*D-32-4-TUN`	64×32^3	500	`Q*D-32-3-GEN`	43	490 s	3 d	0.28 Mch
`Q*D-32-4-GEN`	64×32^3	2500	—	43	1300 s	38 d	3.73 Mch
`Q*D-32-4-OBS`	64×32^3	2000	`Q*D-32-4-GEN`	43	600 s	14 d	1.38 Mch
`Q*D-32-5-TUN`	64×32^3	500	`Q*D-32-4-GEN`	43	490 s	3 d	0.28 Mch
`Q*D-32-5-GEN`	64×32^3	1000	—	43	1300 s	15 d	1.49 Mch
`Q*D-32-6-TUN`	64×32^3	500	`Q*D-32-5-GEN`	43	490 s	3 d	0.28 Mch
`Q*D-32-6-GEN`	64×32^3	2500	—	43	1300 s	38 d	3.73 Mch
`Q*D-32-6-OBS`	64×32^3	2000	`Q*D-32-6-GEN`	43	600 s	14 d	1.38 Mch
`Q*D-48-1-GEN`	96×48^3	1500	—	32	10600 s	184 d	13.6 Mch
`Q*D-48-1-OBS`	96×48^3	1000	`Q*D-48-1-GEN`	32	4100 s	48 d	3.50 Mch
							31.42 Mch

Table 1: Estimate of time and cost for each run. The reported volume corresponds to the physical volume. In the `openQ*D` code, C* boundary conditions are implemented by means of an orientifold construction which effectively doubles the simulated volume. For instance the 64×32^3 physical volume is simulated with a $64^2 \times 32^2$ volume. All runs with a 64×32^3 physical volume can be parallelized with a local lattice of $8 \times 8 \times 4 \times 4$. All runs with a 96×48^3 physical volume can be parallelized with a local lattice of $8 \times 12 \times 12 \times 6$. For a justification of the estimated cost, see section 6. The column “cnfgs from run” is relevant only for measurement runs; runs generating configurations report here “—”. In the last column, Mch = Mcore-hours.

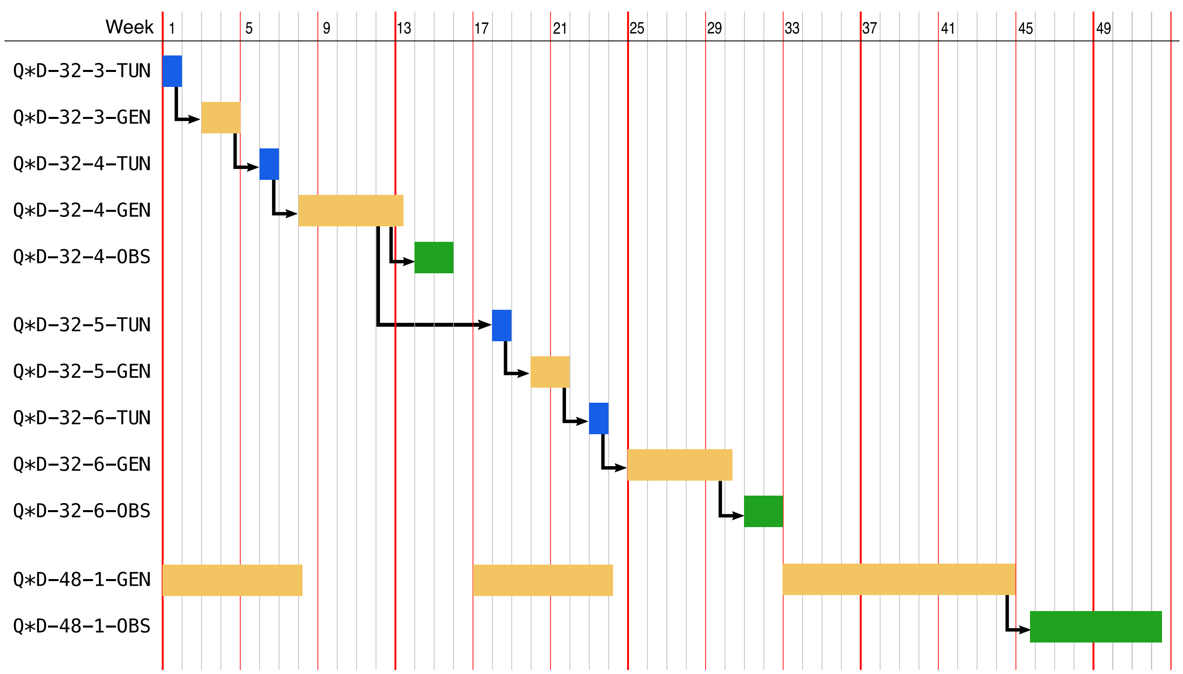

Figure 1: Gantt diagram of the planned workflow with dependencies. The first 10 runs are sequential, since the parameters for each `*-GEN` run are determined by the previous `*-TUN` run, and each `*-TUN` or `*-OBS` run needs the configurations generated by the previous `*-GEN` run. The first run `Q*D-32-3-TUN` will make use of configurations generated with our previous project **bep00085**. The last two runs are independent from the others. In particular run `Q*D-48-1-GEN` can be split and spread over a long period of time, allowing for efficient use of the quarterly allocated computing quotas.

2 Preliminary work

In our previous project **bep00085** we have generated two QCD ensembles and two QCD+QED ensembles. In all cases the lattice spacing was $a \simeq 0.05$ fm. In the QCD case, we have simulated the SU(3) symmetric point, i.e. $m_u = m_d = m_s \simeq (m_u + m_d + m_s)^{\mathrm{phys}}/3$. In the QCD+QED case, we have simulated an unphysically large value of the fine-structure constant $\alpha_R \simeq 5.5\alpha_R^{\mathrm{phys}}$ in order to amplify the isospin-breaking effects. Moreover we have chosen to work at the U-symmetric point, i.e. $m_d = m_s$, and we have chosen m_u in such a way that the strong isospin-breaking effects are rescaled with the same factor as the QED isospin-breaking effects. More details on our simulation strategy, and the definition of our line of constant physics are given in section 3. The most important parameters and observables for those 4 ensembles have been summarized in tables 2, 3, 4, 5. In these tables we include also the run `Q*D-32-2+RW` which is obtained by reweighting the `Q*D-32-2` ensemble in the bare quark masses (chosen in such a way to hit the target tuning point). Preliminary results have been presented at the APLAT 2020 conference, and we are presenting an update at this year's Lattice conference. We are finalizing the analysis of these ensemble, and a publication with these results is in preparation.

We have also invested a significant amount of human time in the `openQ*D` code, in particular:

- We have released the 1.1 version, which includes now the fully-tested calculation of the dressing factors needed for correlators of charged hadrons.
- We have developed a code to calculate the sign of the Pfaffian of the Dirac operator, needed because of the C* boundary conditions. Our code is based on the well established strategy to follow the eigenvalue flow with the bare mass (see e.g. [12]), but we include also some innovative idea which makes the calculation faster. At this stage, this code is still private, but we plan to include it in the public repository in the near future. We have found that only 1 out of 1500 thermalized configurations of the `Q*D-32-2` run have a negative sign for the Pfaffian, showing that the sign problem is practically inexistent at the cosidered values of the parameters.
- We have developed a code to reweight configurations in the bare quark masses. This is useful to correct for small mistunings, and we are already using it successfully in our `Q*D-32-2+RW` run.
- We are developing a code for the calculation of (smeared) baryon two-point functions. This code is at the moment in testing phase, and it will be ready in the next few months.

3 Choice of parameters

The QCD+QED action with four flavours of $O(a)$-improved Wilson fermions depends on 10 parameters: the SU(3) bare coupling constant β, the bare fine-structure constant α, the bare masses m_f with $f = u, d, s, c$, and the improvement coefficients $c^q_{\mathrm{sw,SU(3)}}$ and $c^q_{\mathrm{sw,U(1)}}$ for $q = 2/3, -1/3$.

For the proposed simulations, we choose the Lüscher-Weisz gauge action for the SU(3) field with

$$\beta = 3.24 \ . \tag{1}$$

In QCD at the symmetric point, this corresponds to a lattice spacing $a \simeq 0.054$ fm. This has been determined in [13] using periodic boundary conditions in space. C* boundary conditions do not affect this value (see `QCD-32-1` run in table 2). In QCD+QED at $\alpha_R = 0.04$ we obtain a marginally lower value $a \simeq 0.050$ fm. In all cases the lattice spacing is determined from the auxiliary observable t_0, by using the central value of the CLS determination $(8t_0)^{1/2} = 0.415$ fm. This has been taken only as an indicative value, keeping in mind that it contains an $O(\alpha)$ ambiguity which can be resolved only when the scale is set with a physical observable, e.g. the mass of the Ω baryon.

Isospin-breaking corrections are expected to be of the order of percent, and hence particularly hard to resolve. As done in [14, 15, 16, 17], we simulate at several values of the fine-structure constant α

ensemble	n. cnfgs	a	α_R	L	$m_{\pi^\pm}L$
`QCD-32-1`	2000	0.0539(3) fm	0	1.736(8) fm	3.52(4)
`QCD-48-1`	1082	0.0539(3) fm	0	1.736(8) fm	3.52(4)
`Q*D-32-1`	1993	0.0526(2) fm	0.04077(6)	1.682(5) fm	4.18(2)
`Q*D-32-2`	1500	0.0505(4) fm	0.04053(7)	1.617(11) fm	2.83(4)
`Q*D-32-2+RW`	200	0.050(5) fm	0.0408(3)	1.60(2) fm	3.11(8)

Table 2: Column by column: *(1)* Ensemble name. *(2)* Number of thermalized configurations for the first four ensembles, or number of reweighted configurations for `Q*D-32-2+RW` (extension to the full set of configuration is in progress). *(3)* Lattice spacing a, calculated by assuming $\sqrt{8t_0} = 0.415$ fm with no error; the error in a comes from the propagation of the statistical error on t_0/a^2. *(4)* Renormalized fine-structure constant α_R. *(5), (6)* Linear size L of the spatial box in fermi and in units of the inverse pion mass.

ensemble	volume	β	α	κ_u	$\kappa_d = \kappa_s$	κ_c	$c_{\mathrm{sw,SU(3)}}$	$c_{\mathrm{sw,U(1)}}$
`QCD-32-1`	64×32^3	3.24	0	0.13440733	0.13440733	0.12784	2.18859	0
`QCD-48-1`	80×48^3	3.24	0	0.13440733	0.13440733	0.12784	2.18859	0
`Q*D-32-1`	64×32^3	3.24	0.05	0.135479	0.134524	0.12965	2.18859	1
`Q*D-32-2`	64×32^3	3.24	0.05	0.135560	0.134617	0.129583	2.18859	1
`Q*D-32-2+RW`	64×32^3	3.24	0.05	0.1355368	0.134596	0.12959326	2.18859	1

Table 3: Simulation parameters for the five analyzed runs. All ensembles have C* boundary conditions in space and periodic boundary conditions in time. For the first four ensembles, the values of $\kappa_{u,d,s}$ are the ones actually used to generate the configurations. For `Q*D-32-2+RW`, the values of $\kappa_{u,d,s}$ are the ones used in the reweighting procedure.

ensemble	$m_{\pi^\pm} = m_{K^\pm}$	$m_{K^0} - m_{K^\pm}$	$m_{D^0} = m_{D_s}$	$m_{D^\pm} - m_{D^0}$	$\pi\sqrt{3}L^{-1}$
`QCD-32-1`	402(3) MeV	0 MeV	1914(11) MeV	0 MeV	—
`QCD-48-1`	402(2) MeV	0 MeV	1910(10) MeV	0 MeV	—
`Q*D-32-1`	496(2) MeV	23.2(5) MeV	1870(5) MeV	32(1) MeV	638(2) MeV
`Q*D-32-2`	351(3) MeV	30.5(8) MeV	1902(8) MeV	26(1) MeV	664(5) MeV
`Q*D-32-2+RW`	390(12) MeV	22(5) MeV	1910(14) MeV	19(1) MeV	671(8) MeV

Table 4: Summary of masses. The masses for charged hadrons have been corrected for the universal $O(\alpha)$ finite-volume corrections. The quantity $\pi\sqrt{3}L^{-1}$ is the smallest energy of a free photon in the considered finite box with C* boundary conditions in all directions. The larger errors in the reweighted run `Q*D-32-2+RW` is due partly to the reduced statistics and partly to the reweighting procedure.

ensemble	ϕ_1	ϕ_2	ϕ_3
`QCD-32-1`	2.13(5)	—	12.1(8)
`QCD-48-1`	2.14(3)	—	12.0(6)
`Q*D-32-1`	3.37(3)	2.56(5)	11.92(3)
`Q*D-32-2`	1.73(3)	2.44(7)	12.11(6)
`Q*D-32-2+RW`	2.1(1)	2.3(2)	12.1(2)

Table 5: Summary of tuning observables. All ensembles are at the U-symmetric point, i.e. $m_d = m_s$ or $\phi_0 = 0$. The $\phi_{0,1,2,3}$ are described in the main text. Our main goal in project **bep00085** was to tune the QCD+QED parameters in such a way that $\phi_{1,3}$ are equal to the QCD runs, while $\phi_2 = \phi_2^{\mathrm{phys}} \simeq 2.37$.

(including $\alpha = 0$) in order to interpolate to the physical value. We have already generated a gauge ensemble at $\alpha = 0$ and $\alpha = 0.05$ on a 64×32^3 volume, and we propose here the generation of three gauge ensembles with

$$\alpha = 1/137 \ , \qquad \text{on a } 64 \times 32^3 \text{ volume} \ , \tag{2}$$

$$\alpha = 0.02 \ , \qquad \text{on a } 64 \times 32^3 \text{ volume} \ , \tag{3}$$

$$\alpha = 0.05 \ , \qquad \text{on a } 96 \times 48^3 \text{ volume} \ . \tag{4}$$

Notice that the bare α does not coincide with the renormalized α_R, which we define as

$$\alpha_R = \frac{8\pi}{3} t_0^2 \langle F_{\mu\nu} F_{\mu\nu}(0, t_0) \rangle \ , \tag{5}$$

where $F_{\mu\nu}(x,t)$ is some discretization of the U(1) field tensor calculated in terms of the gauge field at positive flow time t.

We employ C* boundary conditions in space and periodic boundary conditions in time for all our ensembles. We have already verified at $\alpha = 0$ and $\alpha = 0.5$, that we are free from the problem of topological freezing at the chosen lattice spacing, which justifies the use of periodic boundary conditions in time.

The *lines of constant physics* are determined by keeping the following quantities

$$\phi_0 = 8t_0(M_{K^\pm}^2 - M_{\pi^\pm}^2) \ , \tag{6}$$

$$\phi_1 = 8t_0(M_{\pi^\pm}^2 + M_{K^\pm}^2 + M_{K^0}^2) \ , \tag{7}$$

$$\phi_2 = 8t_0(M_{K^0}^2 - M_{K^\pm}^2)\alpha_R^{-1} \ , \tag{8}$$

$$\phi_3 = \sqrt{8t_0}(M_{D_s} + M_{D^0} + M_{D^\pm}) \ , \tag{9}$$

constant as α is varied. Eventually we will want to vary β as well in order to study the continuum limit, but this is outside of the scope of the proposed project. While these quantities can be determined quite accurately from lattice simulations, their real-world value is unknown, since t_0 cannot be measured experimentally. In practice one needs to simulate different lines of constant physics, and then one needs to interpolate/extrapolate to the real-world one by setting the scale with a physical observable.

- Notice that $\phi_0 = 0$ if and only if $m_d = m_s$, where the theory is invariant under an SU(2) flavour symmetry which rotates down and strange (which is often called *U-spin symmetry*). We will refer to the $\phi_0 = 0$ as the *U-symmetric point.* At the physical point

$$\phi_0^{\text{phys}} \simeq 0.992 \ . \tag{10}$$

- The quantity ϕ_1 has been already used in other contexts [18, 19]. At the physical point

$$\phi_1^{\text{phys}} \simeq 2.26 \ . \tag{11}$$

- In χPT, the quantity

$$8t_0(M_{K^0}^2 - M_{K^\pm}^2) = E(m_{d,R} - m_{u,R}) + F\alpha_R + \text{NLO} + O(\alpha_R^2) \tag{12}$$

receives two contributions: a term proportional to $m_{d,R} - m_{u,R}$ from strong-isospin effects and a term from QED corrections proportional to α_R. At the physical point, the two effects have the same order of magnitude. We choose to keep this feature along our lines of constant physics by scaling the above quantity (and therefore $m_{d,R} - m_{u,R}$) proportionally to α_R. This corresponds to the choice of keeping ϕ_2 fixed and equal to its value at the physical point

$$\phi_2^{\text{phys}} \simeq 2.37 \ . \tag{13}$$

Notice that with this choice, at $\alpha = 0$ one has $M_{K^0} = M_{K^\pm}$ which corresponds to the isospin symmetric limit $m_u = m_d$.

- The quantity ϕ_3 is used essentially to fix the charm quark mass [13]. We will take it equal to its value at the physical point

$$\phi_3^{\text{phys}} \simeq 12.0 \; . \tag{14}$$

The aim of this project is to simulate on the U-symmetric line of constant physics defined by

$$\phi_0 = 0 \; , \quad \phi_1 \simeq \phi_1^{\text{phys}} \; , \quad \phi_2 \simeq \phi_2^{\text{phys}} \; , \quad \phi_3 \simeq \phi_3^{\text{phys}} \; . \tag{15}$$

For $\alpha = 0$ this corresponds to the widely studied QCD SU(3)-symmetric point $m_u = m_d = m_s$. In this setup the $\pi^{\pm}$ is heavier than the real-world one, making simulations easier. As routinely done in QCD (and more so in the past), one wants to start from heavier pions and then to approach the physical pion mass in steps.

We finally comment on the SW improvement coefficients: $c_{\text{sw,SU(3)}}$ is associated to the operator $\bar{\psi}\sigma_{\mu\nu}G_{\mu\nu}\psi$, and $c_{\text{sw,U(1)}}$ is associated to the operator $\bar{\psi}\sigma_{\mu\nu}F_{\mu\nu}\psi$. Each of these coefficients depends on the electric charge of the quark, for a total of four improvement coefficients in a QCD+QED simulation. We take the two SU(3) coefficients equal to the non-perturbatively determined ones in pure-QCD [20] at $\beta = 3.24$, i.e.

$$c_{\text{sw,SU(3)}}^{q=2/3} = c_{\text{sw,SU(3)}}^{q=-1/3} = 2.18859 \tag{16}$$

and the two U(1) coefficients equal to the tree-level ones

$$c_{\text{sw,U(1)}}^{q=2/3} = c_{\text{sw,U(1)}}^{q=-1/3} = 1 \; . \tag{17}$$

In practice this means that $O(a)$ corrections are not entirely eliminated, however they are suppressed with one power of α.

4 Tuning strategy

For $\alpha = 1/137$ and $\alpha = 0.02$, the bare quark masses need to be tuned in order to obtain the desired values of the $\phi_{1,2,3}$ variables. This tuning represents an important fraction of the requested computer time. We design a tuning strategy building on our experience accumulated with project **bep00085**. We describe here the main steps, diagrammatically represented in figure 1.

1. We use QCD configurations from the run `QCD-32-1` (previous project) to calculate meson masses in the electroquenched setup at $\alpha = 1/137$. This means that we will need to combine these configurations with pure U(1) configurations that will be generated elsewhere (this can be done on a small cluster). We tune the value of the valence quark masses to obtain

$$\phi_1 \simeq 1.5\phi_1^{\text{phys}} \; , \quad \phi_2 \simeq \phi_2^{\text{phys}} \; , \quad \phi_3 \simeq \phi_3^{\text{phys}} \; . \tag{18}$$

   Notice that $\phi_0 = 0$ is ensured by requiring $m_d = m_s$. The three masses m_u, $m_{d,s}$, m_c can be tuned independently. One first calculates the K^0 mass which depends only on $m_{d,s}$, and tunes it to the desired value. This can be achieved with a simple scan in $m_{d,s}$ (five values are estimated to be sufficient). Once $m_{d,s}$ is fixed, one calculates the mass of $K^{\pm}$ as a funcion of m_u (five values are estimated to be sufficient), and tunes it to the desired value. Finally one calculates ϕ_3 as a function of m_c (five values are estimated to be sufficient), and tunes it to the target value. These scans have been grouped under the collective name `Q*D-32-3-TUN`.

   Notice that in this first step we choose to tune ϕ_1 to a larger value ($1.5\phi_1^{\text{phys}}$) than the one we are ultimately interested in. This is done because we have observed a large number of exceptional configurations in the electroquenched setup at $\alpha = 0.05$ and $M_{K^{\pm}} \simeq 390$ MeV. Choosing heavier mesons reduces this problem drastically. Notice also that exceptional configurations are produced by the non-unitary setup, and they are therefore expected to occur less often at smaller α. Nevertheless we have decided to opt for a safe strategy.

2. We produce 1000 QCD+QED configurations (`Q*D-32-3-GEN`) with the parameters determined in step 1. We plan to start the Markov chain from thermalized (independent) QCD and pure U(1) configurations. We expect a thermalization no longer than 500 configurations.

3. We repeat the tuning dicussed in point 1, on the thermalized configurations generated in point 2. This time we aim for the target values

$$\phi_1 \simeq \phi_1^{\rm phys} \ , \quad \phi_2 \simeq \phi_2^{\rm phys} \ , \quad \phi_3 \simeq \phi_3^{\rm phys} \ . \tag{19}$$

   The needed scans have been grouped under the collective name `Q*D-32-4-TUN`.

4. We produce 2500 QCD+QED configurations (`Q*D-32-4-GEN`) with the parameters determined in step 3. We plan to start the Markov chain from a thermalized configurations produced in step 2. We expect a thermalization no longer than 500 configurations. In our experience with the project **bep00085**, the residual small mistuning obtained by this procedure can be easily corrected with a reweighting in the bare masses.

5. We measure all mesons and reweighting factors (`Q*D-32-4-OBS`), on the thermalized configurations generated in point 4.

This procedure is repeated for $\alpha = 0.2$, except that the first tuning is performed on the configurations of the `Q*D-32-4-GEN` ensemble. The corresonding runs in figure 1 are `Q*D-32-5-TUN`, `Q*D-32-5-GEN`, `Q*D-32-6-TUN`, `Q*D-32-6-GEN`, `Q*D-32-6-OBS`.

Finally notice that the large-volume runs `Q*D-48-1-GEN` and `Q*D-48-1-OBS` do not require any additional tuning: the quark masses used for this run are the same as the `Q*D-32-2+RW` run in table 3.

5 Code, algorithm, performance

The production of gauge field ensembles and measurement of physical observables is based on the `openQ*D-1.1` code base, publicly available under the GNU General Public License []. It is an extension of the `openQCD` code [11] which has been extensively used to generate QCD configurations e.g. by the ALPHA collaboration, c.f. [21] and by the CLS network, c.f. [19].

The programs are highly optimized for machines with current x86-64 processors, but will run correctly on any system that complies with the ISO C89 and the MPI 1.2 standards. The code is structured to ensure a very good data locality. Nevertheless, the performance of the programs is mainly limited by data movement, i.e., the memory-to-processor bandwidth and network latency.

The simulation program implements the RHMC algorithm which evolves the physical fields in phase space. Each trajectory starts with momentum fields randomly chosen from a normal distribution. Then the fields are evolved according to the molecular dynamics (MD) of the Hamiltonian equations. The equations are integrated for a fixed molecular dynamics time (trajectory length), using nested hierarchical symplectic integrators such as the 4th-order Omelyan–Mryglod–Folk integrator. At the end of each trajectory, the fields are submitted to an accept-reject step that corrects for the integration errors.

The code has a highly-optimized lattice Dirac operator (e.g. even-odd preconditioning) and implements frequency-splitting for the quark determinant. The use of the rational approximation and twisted masses requires standard reweighting techniques which are supported by calculating the corresponding factors a posteriori. During the MD evolution, the Dirac operator has to be inverted multiple times which is accelerated using modern techniques like deflation, multi-shift and chronological solvers. The choice of solvers (CGNE, MSCG, SAP+GCR, DFL+SAP+GCR) is separately configurable for each force component and pseudo-fermion action. Additional features are an implementation of the Fast Fourier Transform as well as Fourier acceleration for the electromagnetic gauge fields.

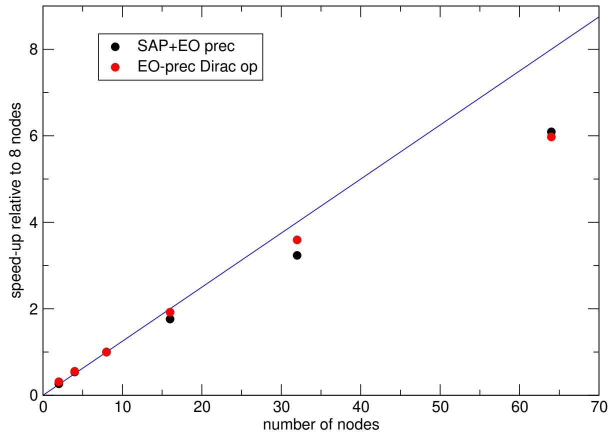

Figure 2: Strong-scaling and performance analysis of the SAP preconditioner (black circles) and of the EO-preconditioned Dirac operator (red circles). For this study we have chosen a QCD+QED setup, a $96 \times 64 \times 64 \times 32$ lattice with C* boundary conditions in space and periodic in time, and we have varied the number of nodes. The speed-up is plotted as a function of the number of nodes n. The speed-up is defined as the ratio of the running time on 8 nodes divided by the running time on n nodes. In the right pane, we plot the relative performance as a function of the number of nodes n.

The inversion of the Dirac operator constitutes the bulk of the calculation in the proposed runs. In particular the Dirac operator for light quarks is inverted with a deflated SAP-preconditioned GCR solver. In order to illustrate the scalability of the code, we have studied the strong scaling of the SAP preconditioner and of the Dirac operator itself on Lise, see fig. 2. The code shows almost perfect scaling up to 16 nodes, and a degradation for 32 and 64 nodes. In order to be able to conclude this project within a year, we choose to run our jobs either with 32 or 43 nodes (compare with table 1 and figure 1).

6 Justification of resources

We expect the generation of the configurations for runs `Q*D-32-3-GEN`, `Q*D-32-4-GEN`, `Q*D-32-5-GEN`, `Q*D-32-6-GEN` to be as expensive as the `Q*D-32-2` run, which we have executed and timed on Lise under project **bep00085**. In fact the cost of simulations is determined by the number of terms in the rational approximation used for the RHMC, and by the cost of the inversion of the Dirac operator. In turn, these are determined by the pion masses, the gap of the Dirac operator, and the physical volume, which are roughly the same in all these runs. In table 1 we use the measured value of 1300s per configuration, corresponding to a trajectory length $\tau = 2$ and to an acceptance rate of about 96%. We choose 2500 configurations for the `Q*D-32-4-GEN` and `Q*D-32-6-GEN` runs, which lie on the chosen line of constant physics. We expect a total of 2000 thermalized configurations, which will allow us to have a statistics similar to the `Q*D-32-2` run from our previous project. The `Q*D-32-3-GEN` and `Q*D-32-5-GEN` runs are used only for tuning, and a smaller number of configurations is sufficient. Notice that these runs can be continued later on (e.g. to use them for interpolations or extrapolations).

The `Q*D-32-3-TUN`, `Q*D-32-4-TUN`, `Q*D-32-5-TUN`, `Q*D-32-6-TUN` runs involve the measurement of meson correlators in a partially quenched setup. We will need a scan of five values of $m_d = m_s$ to tune the K^0 mass to the desired value, then a scan of five values of m_u to tune the $K^\pm$ mass, and finally a scan of five values of m_c to tune the value of D^0. The time needed for this tuning can be take from the similar tuning that we have already performed for the `Q*D-32-2` run on Lise in our previous project. In table 1 we use the measured value of 490s per configuration for the full scan.

The `Q*D-32-4-OBS` and `Q*D-32-6-OBS` runs involve the measurement of meson correlators, the measurement of the reweighting factor which corrects the rational approximation of the RHMC, the measurement of the sign of the Pfaffian of the Dirac operator (which appears instead of the usual determinant because of the C* boundary conditions). Again, the time needed for all these elements have been measured on Lise on the `Q*D-32-2` run, and has been used for an estimate of the required computer time in 1.

In contrast the time needed for the `Q*D-48-1-GEN` run has not been measured, and it has been estimated by rescaling the time needed for the `Q*D-32-2` run from our previous project. In particular the time has been rescaled proportionally to the volume and with the inverse of the number of cores, times an extra factor 1.2 which accounts for increased number of poles of the rational approximation and the smaller integration step, both needed when the volume increases. The time needed for the `Q*D-48-1-OBS` run has been estimated by means of a similar rescaling, without the extra factor 1.2.

We need to store all gauge configurations generated by the runs `Q*D-32-3-GEN`, `Q*D-32-4-GEN`, `Q*D-32-5-GEN`, `Q*D-32-6-GEN`, `Q*D-48-1-GEN`. We plan to use these configurations for the measurement of other interesting observables (e.g. baryon masses) in the future. A disk space of 136 Tb is needed on the WORK filesystem. These configurations will be moved to available storage space at DESY Zeuthen, via ssh, at the end of the project.

A Previously funded projects

- HLRN, **bep00085** project, *QCD+QED Simulations with C* Boundary Conditions*, 2M NPL allocated computer time from Jan 2020 until Dec 2020.

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