Tuning of QCD+QED simulations with C⋆ boundary conditions

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Introduction

We give an update on the ongoing effort of the RC⋆ collaboration to generate fully dynamical QCD+QED ensembles with C⋆ boundary conditions and with O(a) improved Wilson fermions using the openQ⋆D code.

ensemble	lattice	a [fm]	α_R	Quark Content
A400a00b324	64×32^3	0.05393(24)	0	$m_u = m_d = m_s \neq m_c$
B400a00b324	80×48^3	0.05400(14)	0	$m_u = m_d = m_s \neq m_c$
A450a07b324	64×32^3	0.05469(32)	0.007076(24)	$m_u \neq m_d = m_s \neq m_c$
A380a07b324	64×32^3	0.05323(28)	0.007081(19)	$m_u \neq m_d = m_s \neq m_c$
A500a50b324	64×32^3	0.05257(14)	0.040772(85)	$m_u \neq m_d = m_s \neq m_c$
A360a50b324	64×32^3	0.05054(27)	0.040633(80)	$m_u \neq m_d = m_s \neq m_c$
C380a50b324	96×48^3	0.050625(79)	0.04073(11)	$m_u \neq m_d = m_s \neq m_c$

Table 1: List of our ensembles.

Lines of Constant Physics

For our QCD+QED ensembles we defined the following *surfaces of constant physics*:

$$\phi_0 = 8t_0\left(M_{K^\pm}^2 - M_{\pi^\pm}^2\right) = 0,$$
$$\phi_1 = 8t_0\left(M_{\pi^\pm}^2 + M_{K^\pm}^2 + M_{K^0}^2\right) = 2.13,$$
$$\phi_2 = 8t_0\left(M_{K^0}^2 - M_{K^\pm}^2\right)\alpha_R^{-1} = 2.37,$$
$$\phi_3 = \sqrt{8t_0}\left(M_{D_s} - M_{D^0} + M_{D^\pm}\right) = 12.1.$$

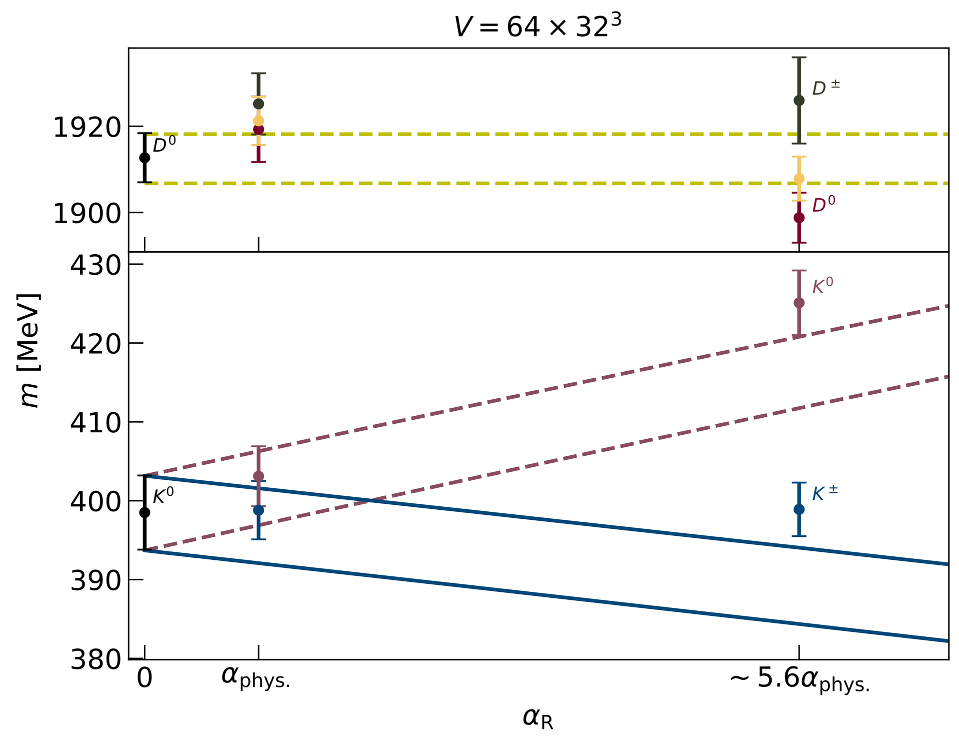
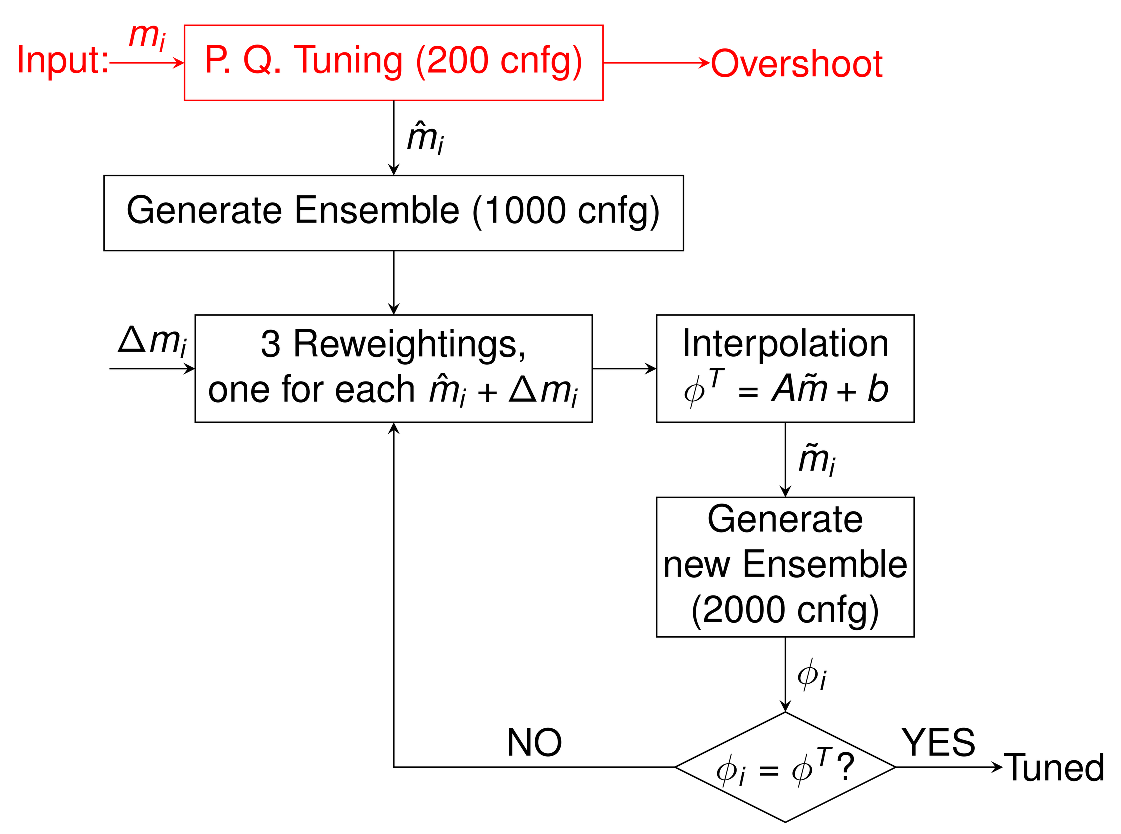


Fig. 1: Lines of constant physics.

Tuning Strategy

For fixed values of α and β, the bare quark masses need to be tuned to obtain the desired values of the ϕ variables. Since we have chosen to work with $m_d = m_s \equiv m_{ds}$, this is a three-parameter tuning problem. In practice, we have followed the steps in the flowchart.



Sign of the Pfaffian

The fermionic Pfaffian is a consequence of C⋆ boundary conditions and its sign flip is a lattice artefact. It can be written:

$$\mathrm{pf}(CKD) = \sqrt{\det(Q)} = \prod_{n=1}^{12V} \lambda_n$$

the sign of the Pfaffian is estimated following the λ_ns (eigenvalues of $Q = \gamma_5 D$) flow from the target mass m to larger mass M.

λ_n crossing zero even → positive sign

λ_n crossing zero odd → negative sign

The code first reduces the interval $I \in [m, M]$ in which the flip can occur by looking if the smallest λ increase from m to M (Fig. 2). Only if $I \neq \{0\}$ we track the eigenvalues and eigenvectors flow.

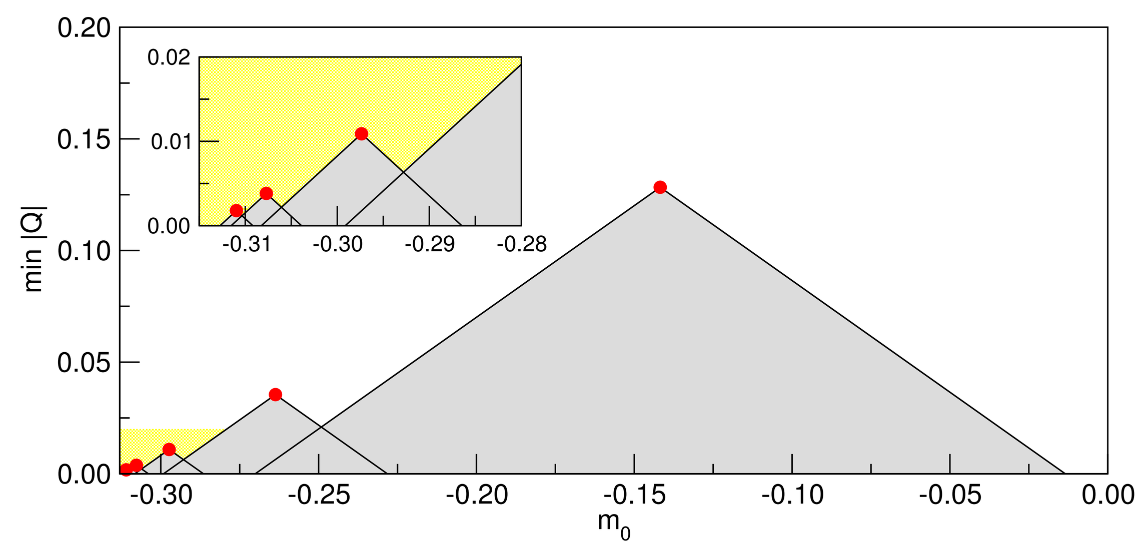


Fig. 2: Smallest eigenvalue of up Q as a function of the valence mass, calculated on the 96×48^3 volume. The eigenvalue can not flow in the grey region.

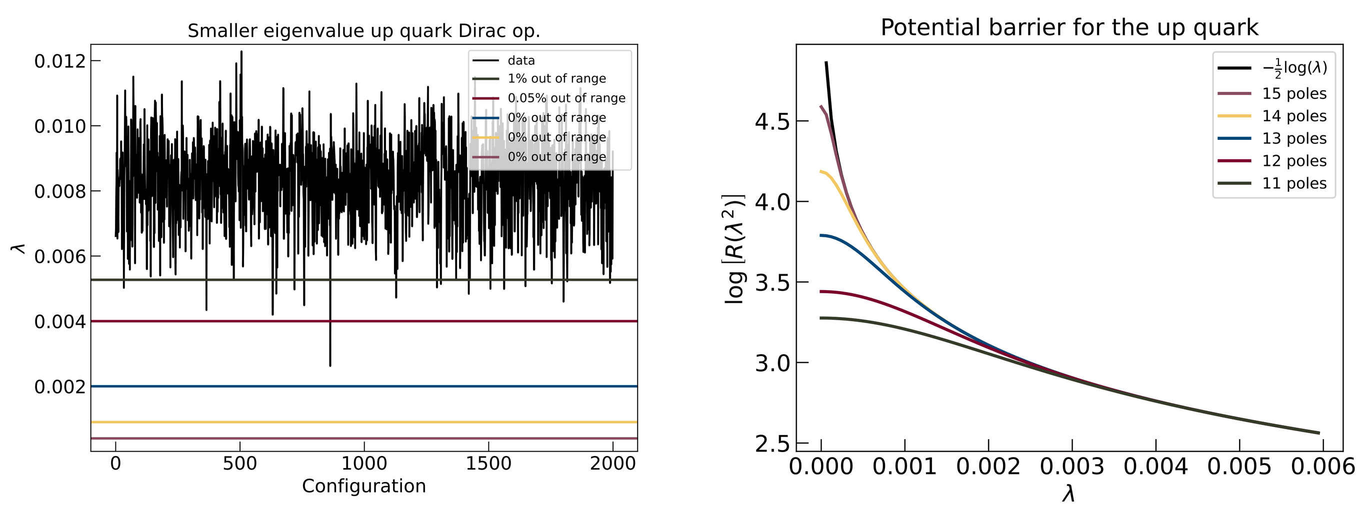


Fig. 3: We systematically increased the value of the lower bound of the rational approximation (left) to decrease the tunnelling barrier for the up quark (right).

We investigated the source of the absence of sign flip by lowering the tunnelling barrier for the smallest eigenvalue as proposed in [1] (Fig. 3). The result was no sign flip which could be due to:

- ergodicity problem,
- lattice spacing enough small to remove the artifact,
- the up quark too massive.

Finite Volume Effects

QCD finite volume corrections can be estimated by LO χ-PT:

$$M_P(L) = M + \frac{\xi}{3}\sum_{\vec{n}\in\mathbb{Z}^3\setminus\{0\}} \frac{2}{nL} K_1(nL)\,,$$
$$M_C(L) = M - \frac{\xi}{3}\sum_{\vec{n}\in\mathbb{Z}^3\setminus\{0\}} \frac{1-3(-1)^{\sum_i n_i}}{nL} K_1(nL)\,,$$

where $\xi = M^2/(4\pi F)^2$, K_1 is a modified Bessel function of the second kind, for periodic and C⋆ boundary conditions. On the larger volume, the QCD finite volume effects on pion mass are smaller than 1%.

In the case of QED with C⋆ boundary conditions the power-law finite-volume effects have been derived in [3]:

$$M_C(L) = M - \alpha\left\{\frac{q^2\zeta(1)}{2L} + \frac{q^2\zeta(2)}{\pi M L^2} + o\left(\frac{1}{L^4}\right)\right\},$$

the higher order terms in $1/L$ depend on the derivative of the Compton tensor. The first two terms of the $1/L$ expansion are structure-independent.

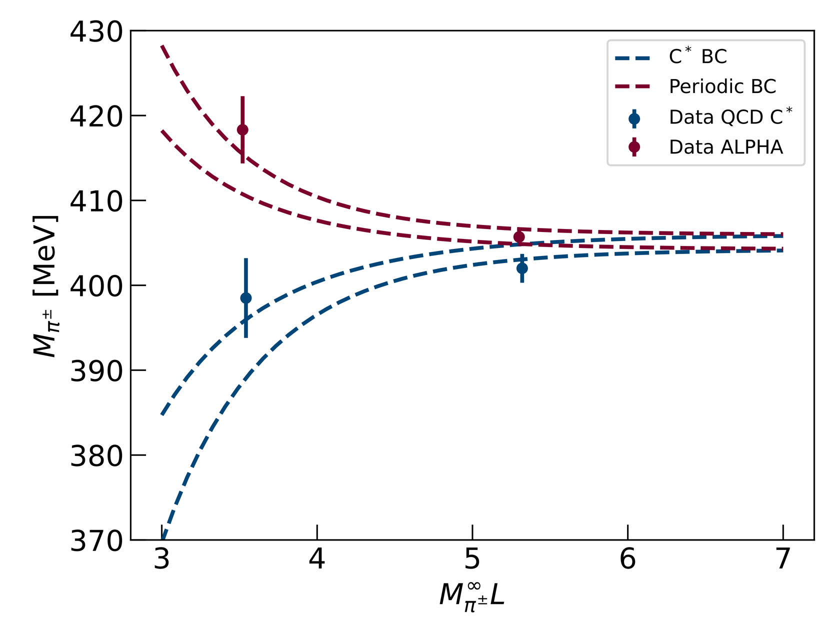


Fig. 4: Pion masses for our QCD ensembles, and ALPHA ensembles from [2].

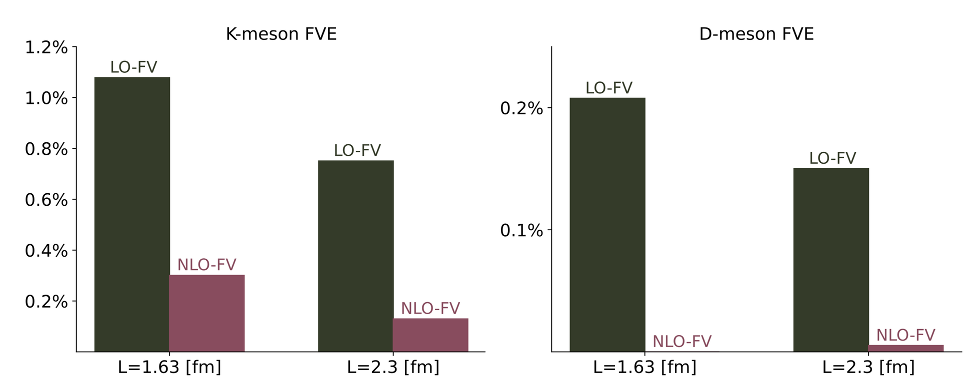


Fig. 5: QED finite volume effects on the mesons masses for $\alpha_R \approx 0.04$.

Conclusion and outlook

- The three-parameter tuning can not rely on a strategy like the Partially Quenching due to the significant Sea-Quarks contribution, which forbids us to tune the masses one per time.
- The errors on our $64x32^3$ volume are probably dominated by FVE. An accurate tuning thus requires much larger statistics.
- From the hierarchy of the FVE as seen in Fig. 5 we suppose that the contributions of the non-universal terms in the 1/L expansion are in the sub-0.1% range.

References

[1] Daniel Mohler, Stefan Schaefer, *Remarks on strange-quark simulations with Wilson fermions*, (2020).

[2] Roman Höllwieser, Francesco Knechtli, Tomasz Korzec, *Scale setting for $N_f = 3+1$ QCD*, (2020).

[3] Lucini, B., Patella, A., Ramos, A. et al., *Charged hadrons in local finite-volume QED+QCD with C⋆ boundary conditions. J. High Energ. Phys.*, **76** (2016).

Other contributions of the collaboration

- Tue. 8:00 pm, P. Tavella, *Strange and charm contribution to the HVP from C⋆ boundary conditions.*
- Thur. 9:00 am, R. Gruber, *A first look at the HVP from QCD and QCD+QED with C⋆ boundary conditions.*
- Thur. 9:20 am, A. Altherr, *A first look at the HVP from QCD and QCD+QED with C⋆ boundary conditions II.*
- Thur. 9:40 am, S. Martins, *Finite-Size Effects of the HVP Contribution to the Muon $(g-2)$ with C⋆ Boundary Conditions.*
- Fri. 4:40 pm, J. Lücke, *An update on QCD+QED simulations with C⋆ boundary conditions.*