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QCD+QED simulations with C* boundary conditions

RC*QR collaboration

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Motivations and introduction

- Isospin transformations (i.e. unitary transformations of the up/down doublet) are are approximated symmetries of Nature.
- Isospin symmetry is broken by $m_u \neq m_d$ and $q_u \neq q_d$.
- Isospin-breaking effects are typically of order 1% on hadronic observables.
- In order to calculate hadronic observables at the percent or subpercent precision level, one needs to consider QCD+QED.
- The RC* collaboration is exploring (not only!) the possibility to generate QCD+QED configurations with C-periodic boundary conditions. A brief account in this talk, for more: A. Altherr *et al.* [RC*], "First results on QCD+QED with C* boundary conditions," JHEP 03 (2023), 012, 1452-1455.

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Theoretical intro

Three ways for QCD+QED on the lattice

1. RM123 method

G. M. de Divitiis *et al.* [RM123], "Leading isospin breaking effects...," Phys.Rev.D 87 (2013) 11, 114505.

Expand action and observables in powers of e, $\delta\beta = O(e^2)$, $\delta m_f = O(e^2)$, e.g.

$$
\begin{aligned}
S_{\mathrm{QCD+QED}} = & S_{\mathrm{QCD}} + S_\gamma + \frac{\delta\beta}{\beta} S_{gluon} + \sum_{xf} \delta m_f \, \bar{\psi}_f \psi_f(x) \\
& + e \sum_{x\mu} A_\mu(x) \mathcal{J}_\mu(x) + e^2 \sum_{x\mu} A_\mu(x)^2 \mathcal{T}_\mu(x) + O(e^3)
\end{aligned}
$$

Pros:

- Calculate directly isospin-breaking and radiative correction to QCD (10% precision is enough).
- Reuse QCD configurations (careful with the finite-volume effects).
- Tuning is trivial: QED counterterms are calculated by solving linear equations.

Cons:

- Complicated observables, quark-disconnected pieces, expensive variance-reduction techniques.
- Correction-to-QCD noise ratio diverges with $V^{1/2}$ and some power of a^{-1}. Bad scaling with V can be killed with coordinate-space techniques, bad scaling with a is irreducible.

Three ways for QCD+QED on the lattice

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Expand action and observables in powers of e, $\delta\beta = O(e^2)$, $\delta m_f = O(e^2)$. Used in:

S. Borsanyi *et al.* [BMW], "Leading hadronic contribution to the muon magnetic moment from lattice QCD," Nature 593 (2021) 7857, 51-55.

Any other work uses the *electroquenched approximation*, i.e. sea quarks are considered electrically neutral (unjustified big simplification).

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Gluon and photon fields are treated on equal footing. Fully interacting $SU(3) \times U(1)$ configurations are generated. Used in:

S. Borsanyi *et al.* [BMW], "Ab initio calculation of the neutron-proton mass difference," Science 347 (2015), 1452-1455.

R. Horsley *et al.* [QCD-SF], "QED effects in the pseudoscalar meson sector," JHEP 04 (2016), 093. R. Horsley *et al.* [QCD-SF], "Isospin splittings of meson and baryon masses from three-flavor lattice QCD + QED," J.Phys.G 43 (2016) 10, 10LT02.

A. Altherr *et al.* [RC*], "First results on QCD+QED with C* boundary conditions," JHEP 03 (2023), 012, 1452-1455.

Pros:

- Standard algorithms can be used.
- Simpler observables.
- The scaling of the noise in QCD+QED with V and a is like in QCD.

Cons:

- Expensive simulations.
- Observables need to be calculated at the permille precision level.
- Up and down quark masses need to be tuned independently.

Three ways for QCD+QED on the lattice

3. Reweighting on QCD

Reweight observables with $e^{-S_{\text{QCD+QED}}+S_{\text{QCD}}}$.

S. Aoki *et al.* [PACS-CS] "1+1+1 flavor QCD + QED simulation at the physical point," Phys.Rev.D 86 (2012), 034507.

T. Ishikawa *et al.* '''Full QED+QCD low-energy constants through reweighting," Phys.Rev.Lett. 109 (2012), 072002.

Notice: RM123 is nothing but an expansion of the reweighting factor.

Pros:

- Reuse QCD configurations (careful with the finite-volume effects).
- Use correlations to calculate isospin-breaking and radiative correction to QCD.
- Relatively simple to implement.

Cons:

- Tuning is more complicated than RM123, but simpler than full simulations.
- Correction-to-QCD noise ratio diverges with $V^{1/2}$ and some power of a^{-1}.

Charged states

The Gauss's law forbids charged states with periodic boundary conditions:

$$Q = \int_0^L d^3x \, \rho(\boldsymbol{x}) = \int_0^L d^3x \, \nabla \cdot \boldsymbol{E}(\boldsymbol{x}) = 0 \; .$$

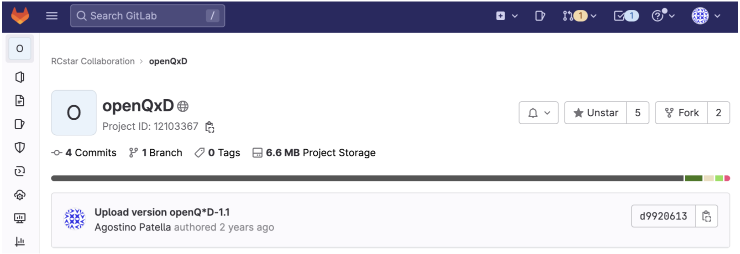
Some popular solutions:

- $\mathrm{QED_L}$: non-local constraint $\int d^3x \, A_\mu(t, \boldsymbol{x}) = 0$.
- $\mathrm{QED_m}$: massive photon.
- $\mathrm{QED_\infty}$: (only with RM123) reconstruct infinite-volume QCD n-point functions and integrate them with infinite-volume photon propagators.
- $\mathrm{QED_C}$: C-periodic boundary conditions in space $\phi(t, \boldsymbol{x} + L\boldsymbol{e}_k) = \phi^C(t, \boldsymbol{x})$.

Some properties of $\mathrm{QED_C}$:

- Continuum limit described by Symanzik effective theory (like $\mathrm{QED_m}$).
- Leading finite-volume effects dominated by low-energy states (like $\mathrm{QED_m}$).
- Power-like finite-volume effects to single-particle masses and matrix elements (like $\mathrm{QED_L}$).
- Incompatible with θ-periodic boundary conditions.
- Partially-broken flavour symmetry.

Numerical simulations

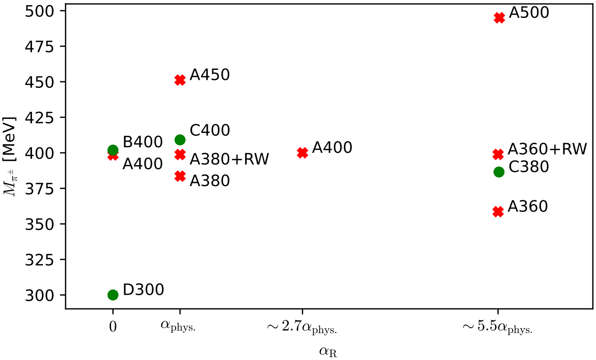


Campos, Fritzsch, Hansen, Marinkovic, Patella, Ramos, Tantalo + Lücke
`https://gitlab.com/rcstar/openQxD`

- Extension of openQCD-1.6
- Simulation of QCD and QCD+QED
- C* boundary conditions in space
- Compact photon action
- Wilson flow for photon field
- Fourier acceleration for photon field
- Multiple deflation subspaces
- U(1)-invariant quark propagators
- Sign of determinant/Pfaffian (soon)
- Mass reweighting (soon)

I. Campos *et al.*, "openQ*D code: a versatile tool for QCD+QED simulations," Eur.Phys.J.C 80 (2020) 3, 195.

Ensembles



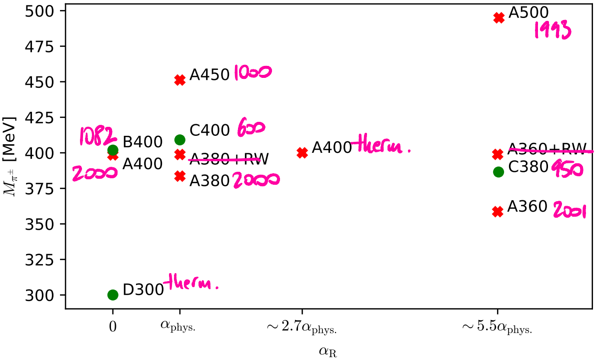
$a \simeq 0.05$ fm
u+d+s+c quarks

A $= 64 \times 32^3$
B $= 80 \times 48^3$
C $= 96 \times 48^3$
D $= 128 \times 64^3$

✖ $m_\pi L \lesssim 4$
● $m_\pi L \gtrsim 5$

Ensembles

configurations



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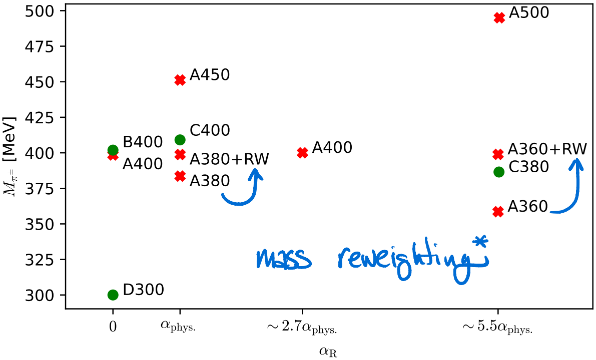

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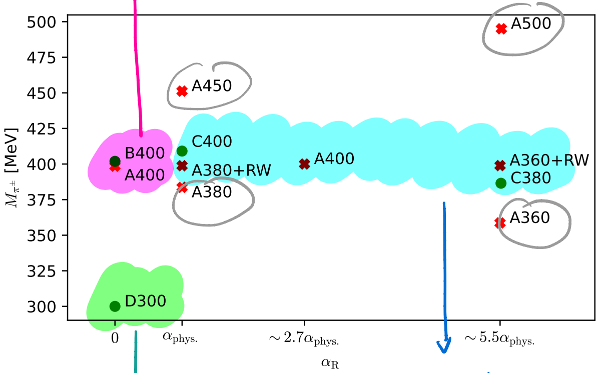
* of $\det(D^\dagger D)^\alpha$ with $\alpha = 1/4, 1/2$ [Lücke, AP, to appear soon]

Ensembles

SU(3) symmetric point $m_u = m_d = m_s$

$M_{\pi^\pm} = M_{K^\pm} = M_{K_0}$

used for tuning



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$M_{\pi^\pm} < M_{K^\pm} < M_{K^0}$

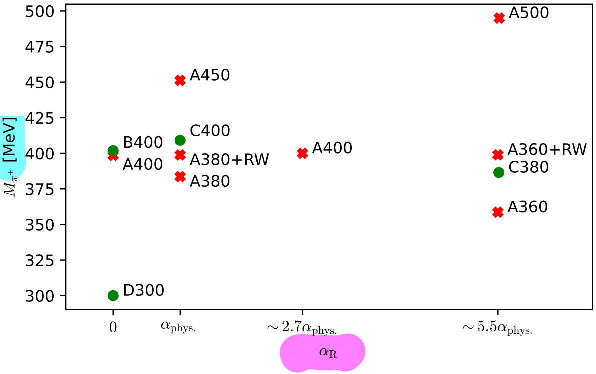
U-symmetric line $m_d = m_s$

$M_{\pi^\pm} = M_{K^\pm} < M_{K^0}$

Ensembles

Ideally : $M_{\Omega^-} = 1672.45(29)$ MeV

Here : $\sqrt{8t_0} = 0.415$ fm



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u+d+s+c quarks

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$m_\pi L \lesssim 4$

$m_\pi L \gtrsim 5$

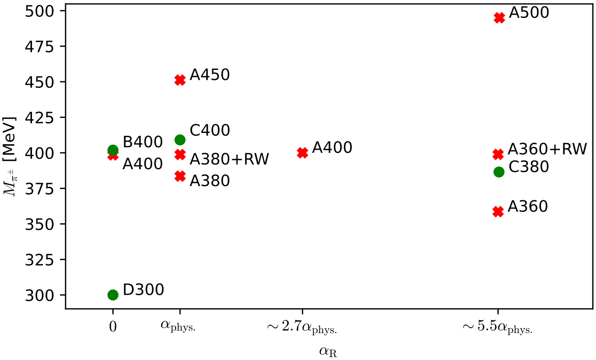
Ideally $\alpha_{phys} = \lim_{t\to\infty} \frac{32\pi^2}{3} t^2 \langle F^2_{\mu\nu}(t) \rangle$

Here $\alpha_R = N(a)\, t_0^2 \langle F^2_{\mu\nu}(t_0) \rangle$

Notice $\alpha_{phys} = \alpha_R + O(\alpha_R^2)$

Quark masses are tuned by choosing

$\sqrt{8t_0}\, M_{\pi^\pm}$, $\sqrt{8t_0}\, M_{K^\pm}$, $\sqrt{8t_0}\, M_{K_0}$, $\sqrt{8t_0}\, M_{D_{ave}} = \sqrt{8t_0}\, \frac{M_{D^\pm} + M_{D_s^\pm} + M_{D_0}}{3}$



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u+d+s+c quarks

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C = 96×48^3

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✖ $m_\pi L \lesssim 4$

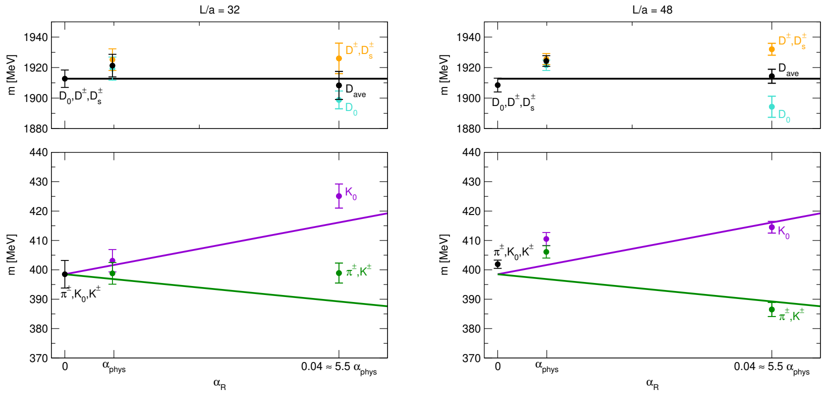
● $m_\pi L \gtrsim 5$

"Trajectories" defined by keeping $\phi_{0,1,2,3}$ constant as α_R is varied.

$\phi_0 = 8t_0 \left(M_{K^\pm}^2 - M_{\pi^\pm}^2 \right)$ $\qquad \phi_2 = \frac{8t_0}{\alpha_R} \left(M_{K_0}^2 - M_{K^\pm}^2 \right)$

$\phi_1 = 8t_0 \left(M_{K^\pm}^2 + M_{K_0}^2 + M_{\pi^\pm}^2 \right)$ $\qquad \phi_3 = \sqrt{8t_0} \left(M_{D^\pm} + M_{D_s^\pm} + M_{D_0} \right)$

Meson masses



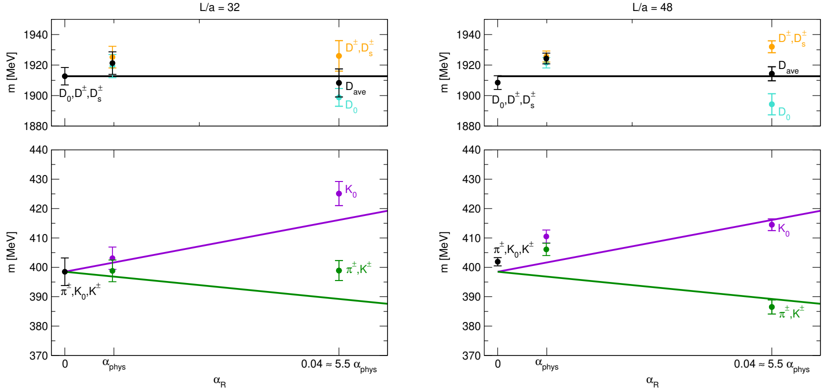
$$\phi_0 = 8t_0(M^2_{K^\pm} - M^2_{\pi^\pm}) = 0$$

$$\phi_1 = 8t_0(M^2_{\pi^\pm} + M^2_{K^\pm} + M^2_{K_0}) \simeq \phi_1^{\text{phys}}$$

$$\phi_2 = 8t_0\alpha_R^{-1}(M^2_{K_0} - M^2_{K^\pm}) \simeq \phi_2^{\text{phys}}$$

$$\phi_3 = \sqrt{8t_0}(M_{D_0} + M_{D^\pm} + M_{D_s^\pm}) \simeq \phi_3^{\text{phys}}$$

Meson masses

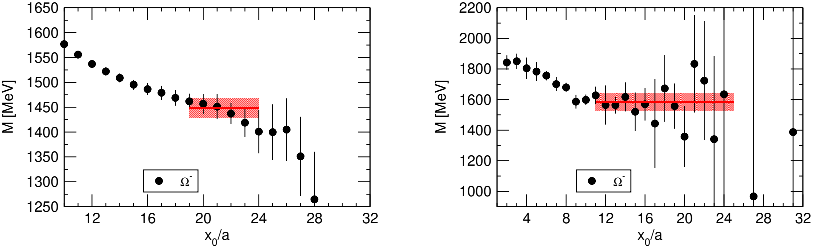


$$M(L) = M(\infty) - \frac{\alpha_R q^2 c_1}{2L} - \frac{\alpha_R q^2 c_2}{2ML^2} + O\left(\frac{1}{L^4}\right)$$

Universal FV correction for $K^{\pm}$ at $\alpha_R \simeq 5.6\alpha_{\text{phys}}$

$L/a = 32$: $1.09(1)\% + 0.308(8)\%$
$L/a = 48$: $0.751(4)\% + 0.145(2)\%$

Omega mass



Summary and possible points for discussion

- Simulations run as well/bad as QCD ones. More expensive because of $C^\star$ boundary conditions and RHMC for all quarks.
- We calculate the sign of the quark Pfaffian on all configurations. We have a faster algorithm that can be useful for QCD as well.
- Tuning of quark masses is difficult but not hopeless. Which precision do we need?
- Meson effective masses are obtained with a statistical precision similar to QCD. Finite-volume effects need to be quantified better.
- Correlations are essential in order to calculate isospin-breaking effects (e.g. mass splittings).
- We calculated p, n, Ξ^-, Λ_0, Ω^- masses. Too noisy for now. We are neglecting extra Wick contractions due to $C^\star$ boundary conditions.
- We are calculating HVP contribution to muon $g-2$ on QCD+QED configurations.