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An Update on QCD+QED simulations with C* boundary conditions

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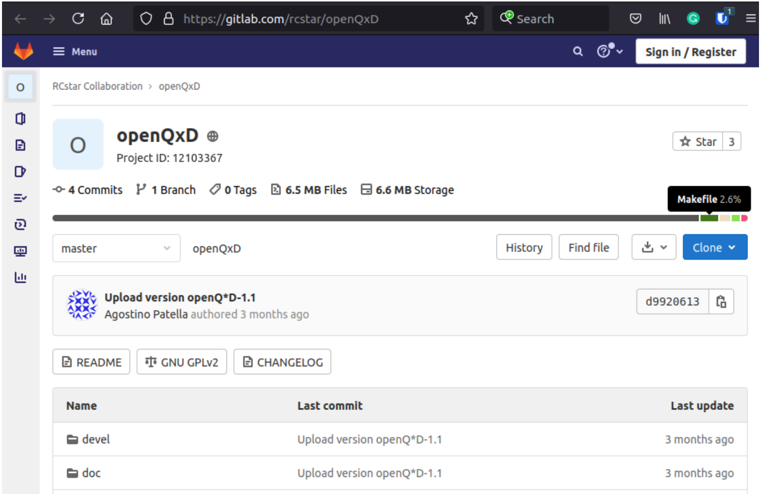
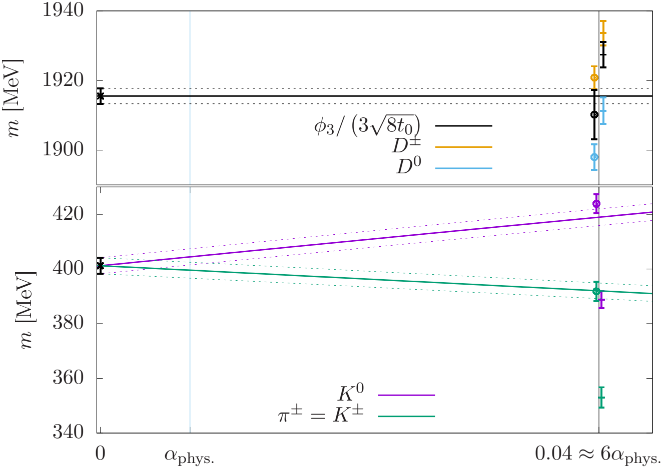
- Ensembles generated with the openQ*D code[a]



Available at `https://gitlab.com/rcstar/openQxD`

[a] Isabel Campos et al., 'openQ*D code: a versatile tool for QCD+QED simulations'.

Line of Constant Physics



Setup:

- Wilson fermions
- $N_f = 1+2+1$
- PBCs in time
- C* BCs in space
- $a \approx 0.05$ fm
- $Lm_{\pi^{\pm}} \approx 3$

Plot:

\+ without RW

o with RW

$$\phi_0 = 8t_0\left(m^2_{K^{\pm}} - m^2_{\pi^{\pm}}\right) = 0 \qquad \phi_1 = 8t_0\left(m^2_{K^0} + m^2_{K^{\pm}} + m^2_{\pi^{\pm}}\right) \simeq \phi_1^{\text{phys.}}$$

$$\phi_2 = \frac{8t_0}{\alpha_{\text{R}}}\left(m^2_{K^0} - m^2_{K^{\pm}}\right) \simeq \phi_2^{\text{phys.}} \qquad \phi_3 = \sqrt{8t_0}\left(m_{D_s^{\pm}} + m_{D^{\pm}} + m_{D^0}\right) \simeq \phi_3^{\text{phys.}}$$

Reweighting - Sign of the Pfaffian

- Weight for a single quark flavor with C* boundary conditions

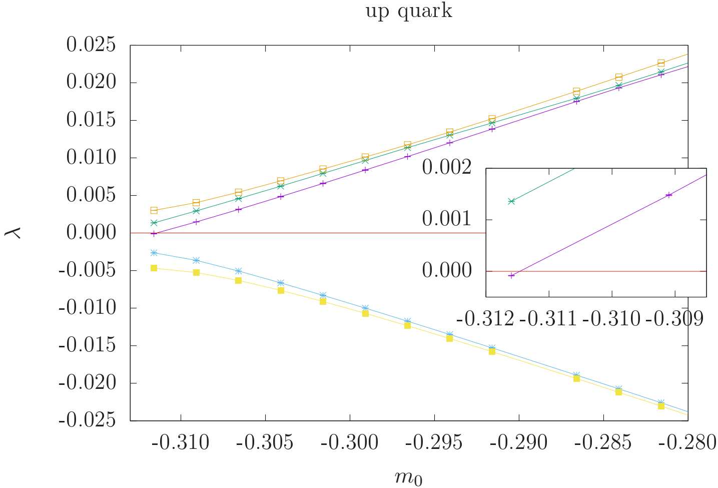
$$\int_{C^*\mathrm{bcs}} \left[\mathrm{d}\bar{\psi}\right] \left[\mathrm{d}\psi\right] \, e^{-\bar{\psi} D \psi} = \mathrm{Pf}\,(CTD) = W_{\mathrm{sgn}} \left|\det\left(D^{\dagger} D\right)\right|^{1/4}$$

- C is charge conjugation matrix: $\psi^{\mathcal{C}} = C^{-1} \bar{\psi}^{T}$
- T translates the fermion by one spatial length: $T\psi(x) = \psi(x + \hat{L}_1)$
- At small lattice spacing mild sign problem
- Pfaffian can be written in terms of the eigenvalues λ_j of operator $Q = \gamma_5 D$

$$\mathrm{Pf}\,(CTD) = \prod_{j=1}^{12V} \lambda_j, \quad \lambda_j \in \mathbb{R}$$

Reweighting - Mass Flow

- Sign of the Pfaffian W_{sgn} is estimated via spectral flow[b,c]
- For large mass $Q \approx \gamma_5 m$ has equal number of positive and negative EVs



[b] I. Campos et al., ‘Monte Carlo simulation of SU(2) Yang-Mills theory with light gluinos’.

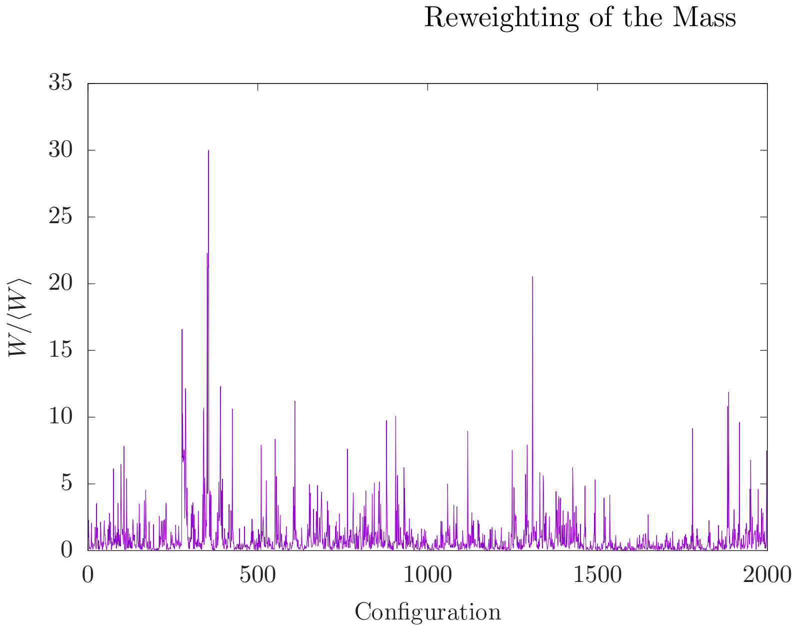
[c] Mohler and Schaefer, ‘Remarks on strange-quark simulations with Wilson fermions’.

Reweighting of the Mass

- Idea: Go from $\langle O \rangle_m$ to $\langle O \rangle_{m'}$ without generating a new ensemble
- Focus on the mass reweighting:

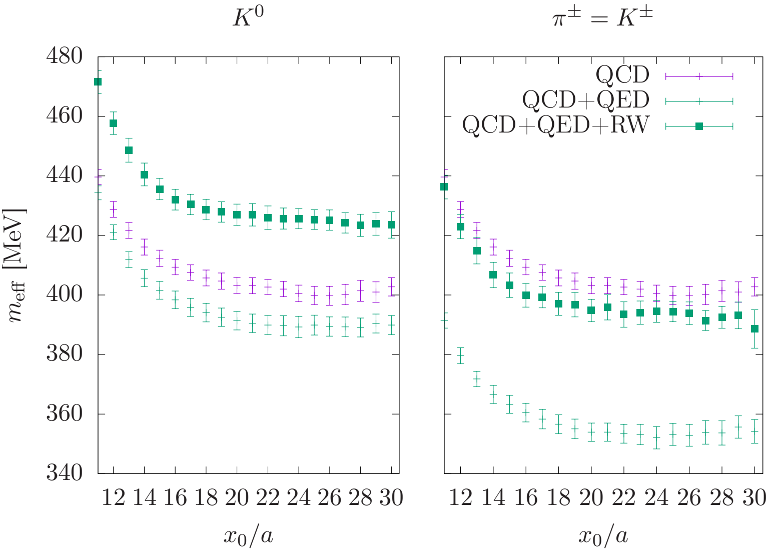
$$W_{\mathrm{mass}} = \det \left[R\left(\hat{Q}_m^2\right) R^{-1}\left(\hat{Q}_{m'}^2\right)\right]$$

- $\hat{Q} = \gamma_5 \hat{D}$ is the even-odd-preconditioned hermitian Dirac operator
- $R\left(\hat{Q}^2\right)$ is a rational approximation for $\left(\hat{Q}^2\right)^{-1/4}$


Reweighting of the Mass
$W/\langle W\rangle$
Configuration
0
5
10
15
20
25
30
35
0
500
1000
1500
2000

Reweighting of the Mass

Charged masses are extracted from gauge invariant interpolating operators[d]



[d] Hansen et al., 'Gauge invariant determination of charged hadron masses'.

Summary and Outlook

✓ Production of $N_f = 1 + 2 + 1$ fully dynamical QCD+QED configurations
- Using openQ*D with C* boundary conditions
- $\alpha_{\mathrm{R}} \approx 0.04$

✓ Computation of the sign of the Pfaffian
- Hence a simulation of the **full** path integral
- No negative sign in the thermalized configurations

✓ Reweighting of the mass in the context of the RHMC
- No significant increase in the errors

➤ Generate more ensembles along the LCP at different values of α_{R} and V
- Goal 1: Finite volume effects? (Currently generating $L = 24, 32, 48$)
- Goal 2: How far can we reweight?
- Goal 3: Can we resolve isospin-breaking effects at $\alpha_{\mathrm{phys.}}$?

Thank you!

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References I

Sz. Borsanyi et al. ‘Ab initio calculation of the neutron-proton mass difference’. In: *Science* 347 (2015), pp. 1452–1455. DOI: 10.1126/science.1257050. arXiv: 1406.4088 [hep-lat].

Mattia Bruno, Tomasz Korzec and Stefan Schaefer. ‘Setting the scale for the CLS 2+1 flavor ensembles’. In: *Physical Review D* 95.7 (2017). ISSN: 24700029. DOI: 10.1103/PhysRevD.95.074504. arXiv: 1608.08900.

I. Campos et al. ‘Monte Carlo simulation of SU(2) Yang-Mills theory with light gluinos’. In: *Eur. Phys. J. C* 11 (1999), pp. 507–527. DOI: 10.1007/s100520050651. arXiv: hep-lat/9903014.

Isabel Campos et al. ‘openQ*D code: a versatile tool for QCD+QED simulations’. In: (Aug. 2019). arXiv: 1908.11673. URL: http://arxiv.org/abs/1908.11673.

Patrick Fritzsch et al. ‘Symanzik improvement with dynamical charm: a 3+1 scheme for Wilson quarks’. In: *JHEP* 06 (2018). [Erratum: JHEP 10, 165 (2020)], p. 025. DOI: 10.1007/JHEP06(2018)025. arXiv: 1805.01661 [hep-lat].

Martin Hansen et al. ‘Gauge invariant determination of charged hadron masses’. In: *JHEP* 05 (2018), p. 146. DOI: 10.1007/JHEP05(2018)146. arXiv: 1802.05474 [hep-lat].

References II

Roman Höllwieser, Francesco Knechtli and Tomasz Korzec. 'Scale setting for $N_f = 3 + 1$ QCD'. In: (2020). arXiv: 2002.02866.

Biagio Lucini et al. 'Charged hadrons in local finite-volume QED+QCD with C* boundary conditions'. In: 2016 (2015). DOI: 10.1007/JHEP02(2016)076. arXiv: 1509.01636.

Daniel Mohler and Stefan Schaefer. 'Remarks on strange-quark simulations with Wilson fermions'. In: *Phys. Rev. D* 102.7 (2020), p. 074506. DOI: 10.1103/PhysRevD.102.074506. arXiv: 2003.13359 [hep-lat].

Backup - Setup

- Lüscher-Weisz $SU(3)$ gauge action
- Compact $U(1)$ with Fourier acceleration
- Non-perturbatively $\mathcal{O}(a)$ improved Wilson fermions for the QCD ensembles[e]
- For QCD+QED ensemble same value of c_{SW} as for the QCD ones
- Periodic boundary conditions in time
- C* boundary conditions in all spatial directions[f]
- RHMC with rational approximation for all quarks
- Deflation solvers for up and down/strange quarks

[e] Fritzsch et al., 'Symanzik improvement with dynamical charm: a 3+1 scheme for Wilson quarks'.

[f] Lucini et al., 'Charged hadrons in local finite-volume QED+QCD with C* boundary conditions'.

Backup - Setup

- All ensembles at $\beta = 3.24$[g]
- Lattice spacing is determined using $N_f = 2+1$ value of $\sqrt{8t_0} = 0.415(4)(2)$ fm[h]

Ens.	QCD	QCD+QED	QCD+QED+RW
N_{cfg}	2000	2001	2001
Volume	64×32^3	64×32^3	64×32^3
α	0.0	0.05	0.05
α_R	0.0	0.04063(6)	0.0407(11)
a [fm]	0.0539(3)	0.0505(3)	0.0510(2)
$m_{\pi^\pm}$ [MeV]	399(3)	359(3)	398(3)
$Lm_{\pi^\pm}$	3.49(3)	2.90(3)	3.24(3)

[g] Höllwieser, Knechtli and Korzec, 'Scale setting for $N_f = 3+1$ QCD'.
[h] Bruno, Korzec and Schaefer, 'Setting the scale for the CLS 2+1 flavor ensembles'.

Backup - Reweighting

For the computation the determinant for the mass reweighting is split into factors:

$$W_{\mathrm{mass}} = \det\left[R\left(\hat{Q}_m^2\right) R^{-1}\left(\hat{Q}_{m'}^2\right)\right] = \det\left[\prod_{j=1}^{n} \frac{\hat{Q}_m^2 + \nu_j^2}{\hat{Q}_m^2 + \mu_j^2} \frac{\hat{Q}_{m'}^2 + \mu_j^2}{\hat{Q}_{m'}^2 + \nu_j^2}\right]$$
$$= \prod_{j=1}^{n} \det\left[B_j^\dagger B_j\right]$$

with

$$B_j = 1 + \delta\hat{D}S_j$$
$$S_j = \left(\hat{D}_{m'} + i\gamma_5\nu_j\right)^{-1} - \left(\hat{D}_m + i\gamma_5\mu_j\right)^{-1} -$$
$$- \left(\hat{D}_m + i\gamma_5\mu_j\right)^{-1} \delta\hat{D} \left(\hat{D}_{m'} + i\gamma_5\nu_j\right)^{-1}$$

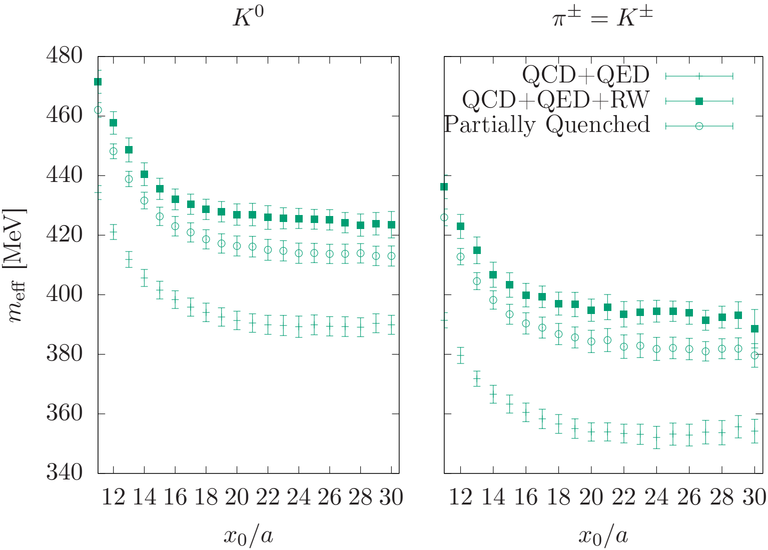
and hence

$$W_{\mathrm{mass}} = \prod_{j=1}^{n} \det\left[1 + R_j\right]$$

with

$$R_j = \left(\delta\hat{D}S_j\right)^\dagger + \left(\delta\hat{D}S_j\right) + \left(\delta\hat{D}S_j\right)^\dagger \left(\delta\hat{D}S_j\right)$$

Backup - Effect of the Reweighting



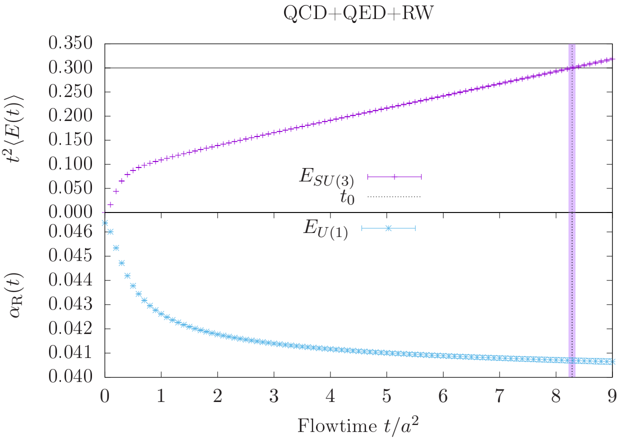
Backup - Setting the Scale - Wilson Flow

- t_0 is obtained by solving the equation

$$t^2 \left\langle E_{SU(3)}(t) \right\rangle \Big|_{t_0} = 0.3$$

- α_R is extracted via[i]

$$\alpha_R = \left. \frac{t^2 \left\langle E_{U(1)}(t) \right\rangle}{4\pi \mathcal{N}} \right|_{t_0}$$



[i] Borsanyi et al., 'Ab initio calculation of the neutron-proton mass difference'.

Backup - Results - Algorithm

Ens.	N_{cfg}	Acceptance	$\left\langle e^{-\Delta H} \right\rangle$	$\tau_{\langle E(t_0) \rangle}$
QCD	2000	95%	0.998(5)	57(29)
QCD+QED	2001	95%	0.8(1)	61(38)