HUMBOLDT-UNIVERSITÄT ZU BERLIN

RTG 2575: Rethinking Quantum Field Theory

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

Jens Lücke

RC*

A. Altherr, L. Bushnaq, I. Campos, M. Catillo, A. Cotellucci, M. Dale, P. Fritzsch, R. Gruber, M. K. Marinkovic, A. Patella, J. C. Pinto Barros, N. Tantalo, P. Tavella

12 August 2022

CINECA

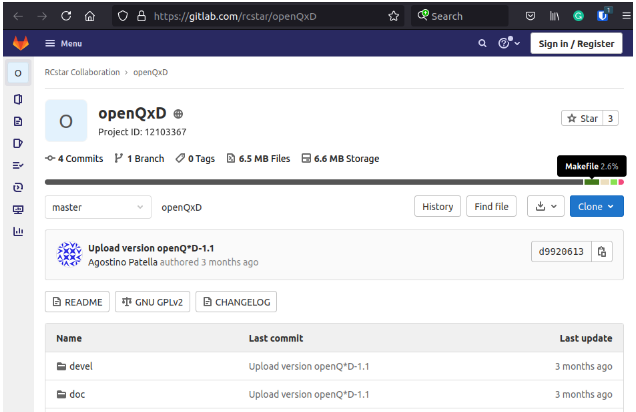
HLRN NORDDEUTSCHER VERBUND FÜR HOCH- UND HÖCHSTLEISTUNGSRECHNEN

PSNC

CSCS Centro Svizzero di Calcolo Scientifico Swiss National Supercomputing Centre

Code

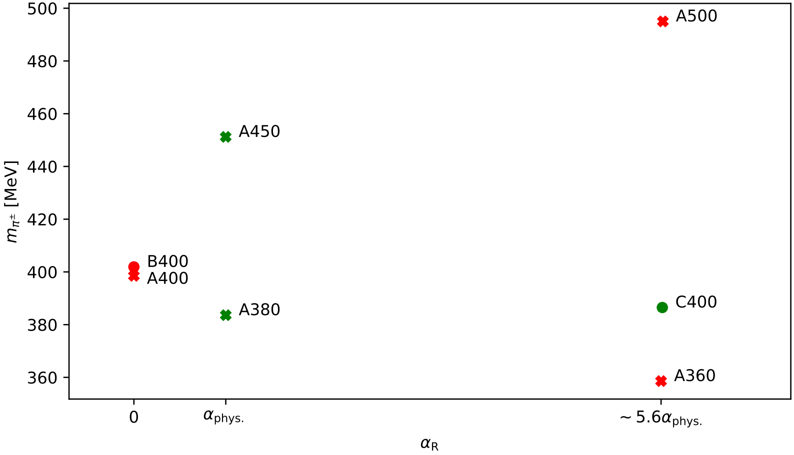
Ensembles generated with the openQ*D code[a]



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

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

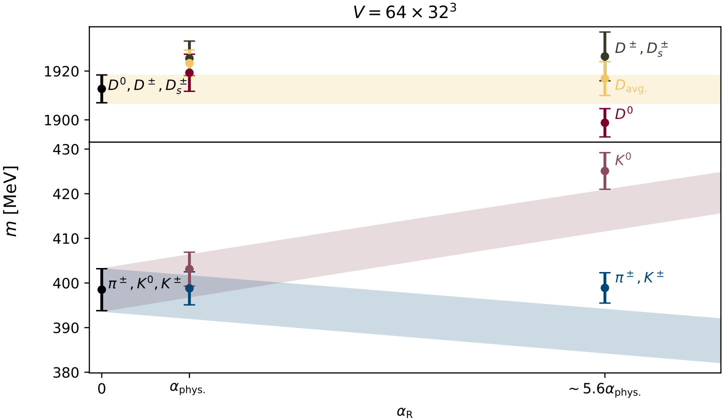
Overview - Ensembles



Setup:

- Wilson fermions
- $N_f = 1 + 2 + 1$
- RHMC for all quarks
- PBCs in time
- C* BCs in space
- $a \approx 0.05$ fm
- $Lm_{\pi^\pm} \approx 3$ and $Lm_{\pi^\pm} \approx 5$

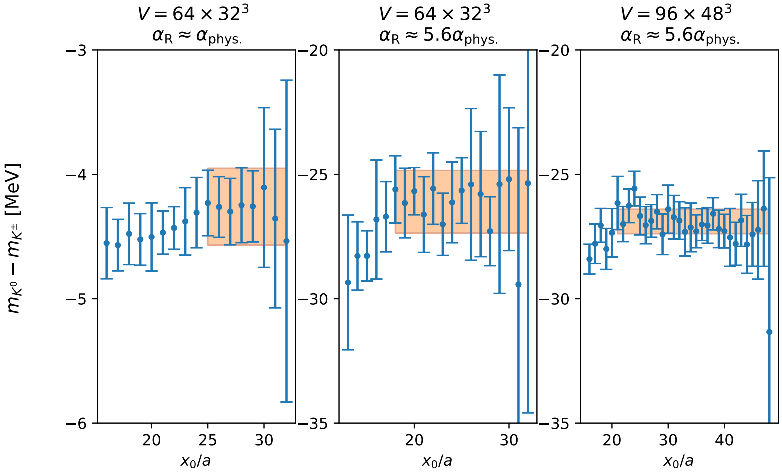
Line of Constant Physics



- QCD+QED has 6 free parameters
- We use the scheme:

1) $t_0 = 0.415$ fm
2) $\alpha_R \in \{0, 1/137, 0.04\}$
3) $\phi_0 = 8t_0\left(m_{K^\pm}^2 - m_{\pi^\pm}^2\right) = 0$
4) $\phi_1 = 8t_0\left(m_{K^0}^2 + m_{K^\pm}^2 + m_{\pi^\pm}^2\right) \simeq \phi_1^{\text{phys.}}$
5) $\phi_2 = 8t_0\left(m_{K^0}^2 - m_{K^\pm}^2\right)\alpha_R^{-1} \simeq \phi_2^{\text{phys.}}$
6) $\phi_3 = \sqrt{8t_0}\left(m_{D_s^\pm} + m_{D^\pm} + m_{D^0}\right) \simeq \phi_3^{\text{phys.}}$

Observables - Mesons



Charged masses are extracted using gauge invariant interpolating operators[b]

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

Baryons - Theory

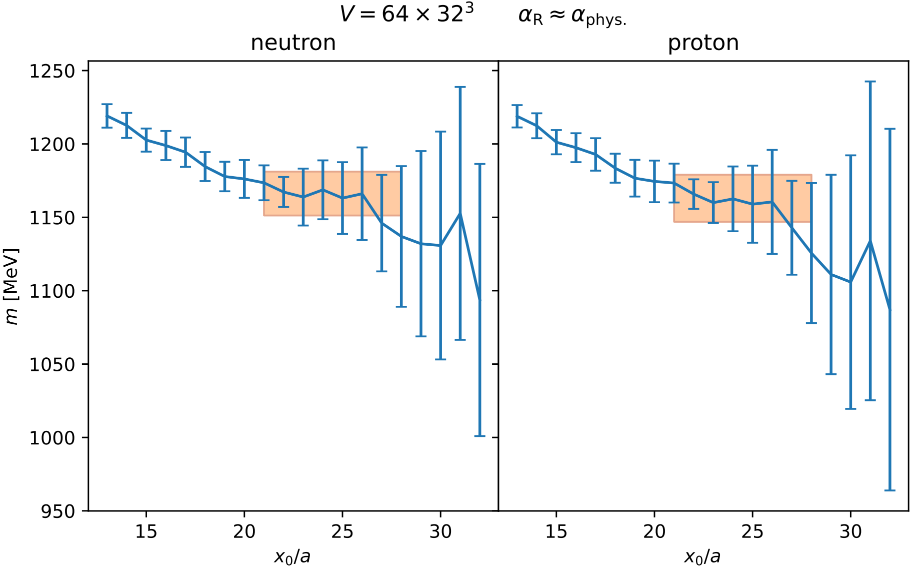
- Baryon operators are constructed from smeared, gauge invariant fermion fields and smeared gauge links
- Gaußian smearing for gauge invariant quark operator Ψ:

$$\Psi_{(\mathrm{s})} = (1 + \omega H[U_s])^n \Psi$$

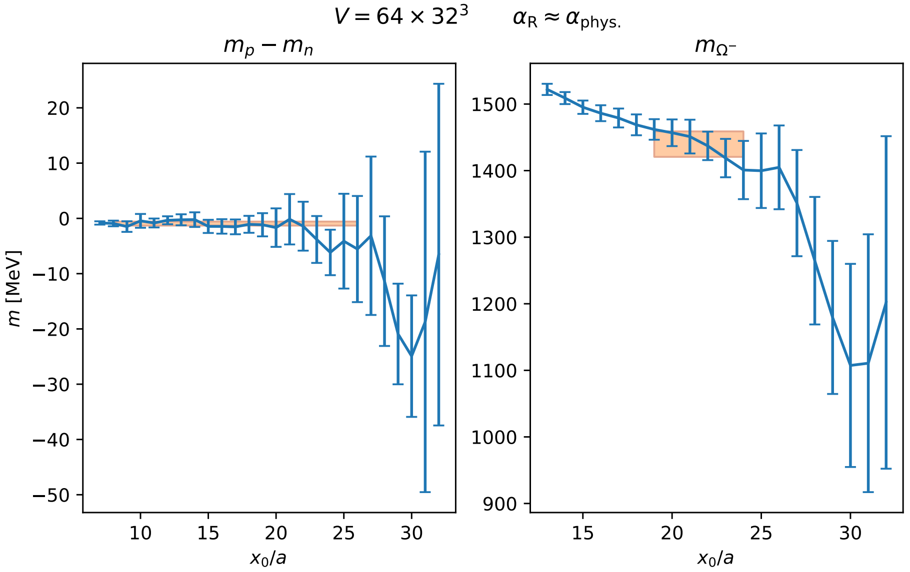
- $H[U_s]$ is spatial hopping operator depending on smeared gauge field U_s
- Gauge smearing with modified gradient flow:

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

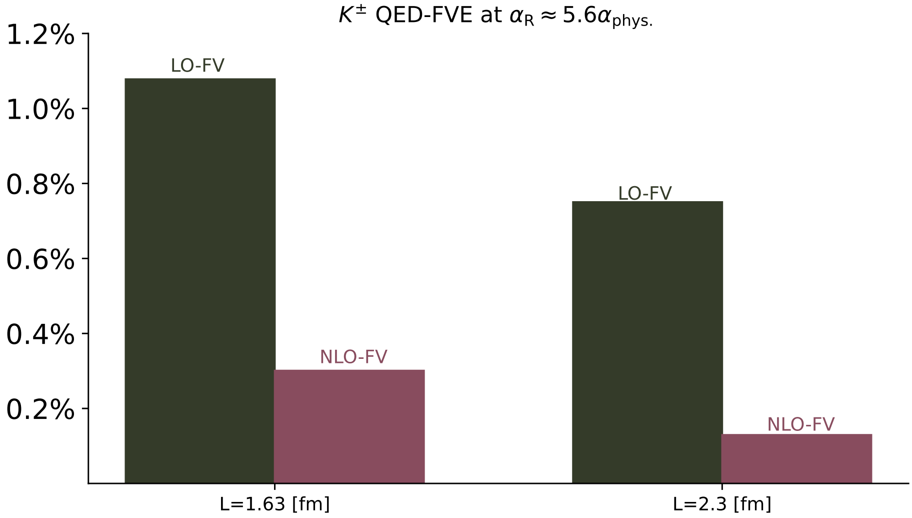
- Flowtime s and parameters n and ω are optimized using the GEVP
- Currently still neglecting quark-quark Wick contractions! $\Rightarrow$ expected to be $\mathcal{O}\left(e^{-L}\right)$



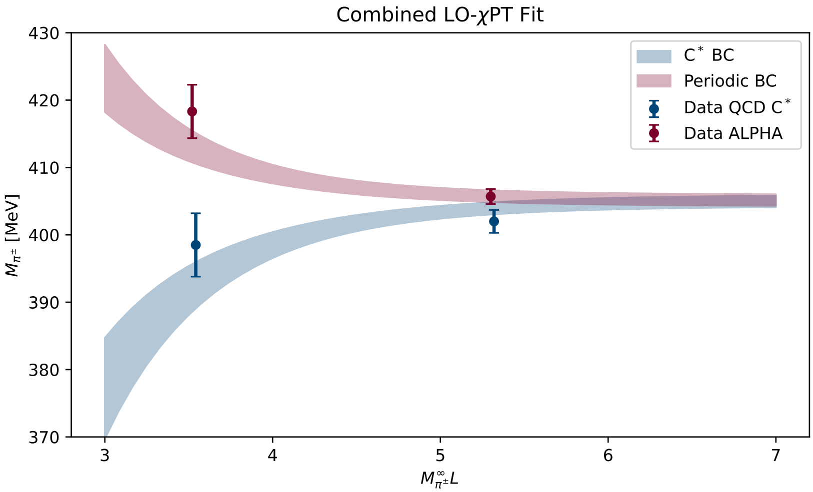
$V = 64 \times 32^3$
$\alpha_R \approx \alpha_{phys.}$
neutron
proton
1250
1200
1150
1100
1050
1000
950
m [MeV]
15
20
25
30
x_0/a


$V = 64 \times 32^3$ $\alpha_R \approx \alpha_{phys.}$
$m_p - m_n$
m_{Ω^-}
m [MeV]
x_0/a
20
10
0
−10
−20
−30
−40
−50
10
15
20
25
30
1500
1400
1300
1200
1100
1000
900

Finite volume corrections - QED



Finite volume corrections - QCD



[c] Höllwieser, Knechtli and Korzec, 'Scale setting for $N_f = 3+1$ QCD'.

Cost analysis

ensemble	global volume	$\frac{\text{core} \times \text{hours}}{\text{MDU}}$	$\frac{\text{core} \times \text{secs}}{\text{MDU} \times \text{point}}$
`A1`[d]	96×32^3	303	0.35
`A400a00b324`	64×32^3	242	0.42
`B400a00b324`	80×48^3	1516	0.62
`A450a07b324`	64×32^3	622	1.07
`A380a07b324`	64×32^3	599	1.03
`A500a50b324`	64×32^3	512	0.88
`A360a50b324`	64×32^3	616	1.05
`C380a50b324`	96×48^3	4115	1.40

[d] Höllwieser, Knechtli and Korzec, 'Scale setting for $N_f = 3 + 1$ QCD'.

Summary and Outlook

✓ Production of $N_f = 1 + 2 + 1$ fully dynamical QCD+QED configurations
  - Using openQ*D with C* boundary conditions
  - $\alpha_R \in \{0, \alpha_{phys.}, 5.6\alpha_{phys.}\}$
  - $V = 64 \times 32^3$, 80×48^3 , 96×48^3

✓ Refined tuning strategy using reweighting of the mass in the context of the RHMC

- Computation of hadron masses
  - Goal: Lower the errors on the baryons

➤ Generate more ensembles along the LCP at different values of α_R and V
  - Goal: Finite volume effects? Generate larger volumes!

➤ Split down and strange quark to approach physical point

➤ Generate more QCD ensembles to explore RM123-method with C* boundary conditions

Thank you!

Other contributions from the collaboration:

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

[1] 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].

[2] 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.

[3] 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.

[4] 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].

[5] 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].

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

[7] Roman Höllwieser, Francesco Knechtli and Tomasz Korzec. 'Scale setting for $N_f = 3 + 1$ QCD'. In: *Eur. Phys. J. C* 80.4 (2020), p. 349. DOI: 10.1140/epjc/s10052-020-7889-7. arXiv: 2002.02866 [hep-lat].

[8] 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.

Acknowledgments

The work was supported by the North-German Supercomputing Alliance (HLRN) with the projects bep00085 and bep00102. The work was supported by CINECA that granted computing resources on the Marconi supercomputer to the LQCD123 INFN theoretical initiative under the CINECA-INFN agreement. The authors acknowledge access to Piz Daint at the Swiss National Supercomputing Centre, Switzerland under the ETHZ's share with the project IDs go22, go24 and eth8. The work was supported by the Poznan Supercomputing and Networking Center (PSNC) through grant numbers 450 and 466.

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'.

- All ensembles at $\beta = 3.24$[g]
- Improvement coefficients are $c_{\mathrm{sw}}^{\mathrm{SU(3)}} = 2.18859$ and $c_{\mathrm{sw}}^{\mathrm{U(1)}} = 1$
- Lattice spacing is determined using $N_f = 2 + 1$ value of $\sqrt{8t_0} = 0.415(4)(2)$ fm[h]

ensemble	lattice	α	α_{R}	a [fm]	$m_{\pi^\pm}$ [MeV]
`A400a00b324`	64×32^3	0	0	0.05393(24)	398.5(4.7)
`B400a00b324`	80×48^3	0	0	0.05400(14)	401.9(1.4)
`A450a07b324`	64×32^3	0.007299	0.007076(24)	0.05469(32)	451.2(4.3)
`A380a07b324`	64×32^3	0.007299	0.007081(19)	0.05323(28)	383.6(4.4)
`A500a50b324`	64×32^3	0.05	0.040772(85)	0.05257(14)	495.0(2.8)
`A360a50b324`	64×32^3	0.05	0.040633(80)	0.05054(27)	358.6(3.7)
`C380a50b324`	96×48^3	0.05	0.04073(11)	0.050625(79)	386.5(2.4)

[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 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:

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

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

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

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

with the definition

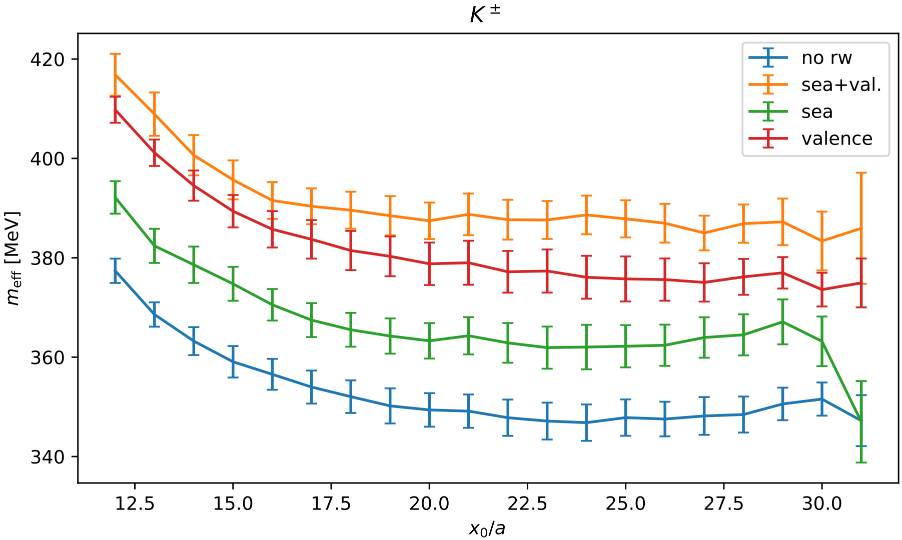
$$B_j = \frac{\hat{Q}_m + i\mu_j}{\hat{Q}_m + i\nu_j} \frac{\hat{Q}_{m'} + i\nu_j}{\hat{Q}_{m'} + i\mu_j} = 1 - iC_j \ . \tag{1}$$

$$C_j = (\nu_k - \mu_k) \frac{1}{\hat{Q}_m + i\nu_k} (\hat{Q}_{m'} - \hat{Q}_m) \frac{1}{\hat{Q}_{m'} + i\mu_k} \tag{2}$$

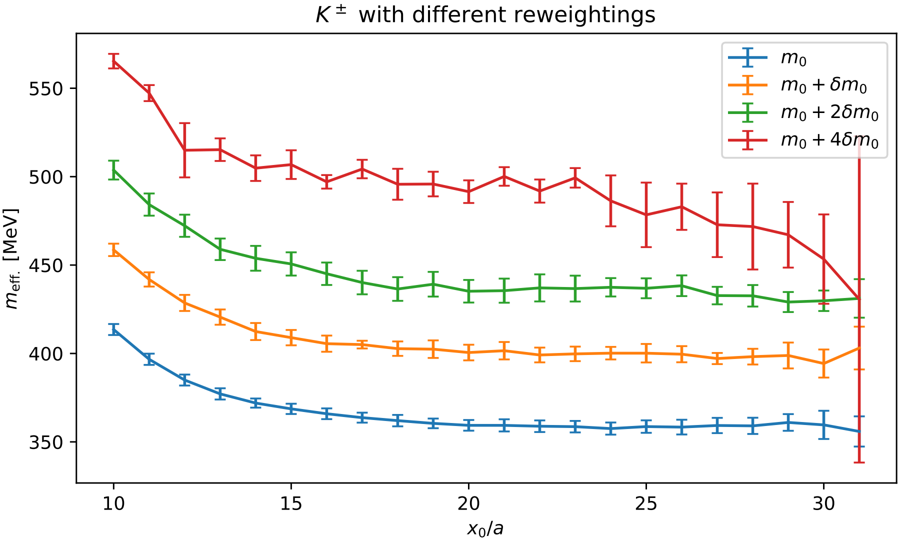
and hence

$$W_{\text{mass}} = \prod_{j=1}^{n} \left\langle e^{-\phi_j^\dagger (B_j^\dagger B_j - 1)\phi_j} \right\rangle_\phi = \prod_{j=1}^{n} \left\langle e^{-2\text{Im}\phi_j^\dagger C_j \phi_j - (C_j\phi_j)^\dagger (C_j\phi_j)} \right\rangle_\phi$$

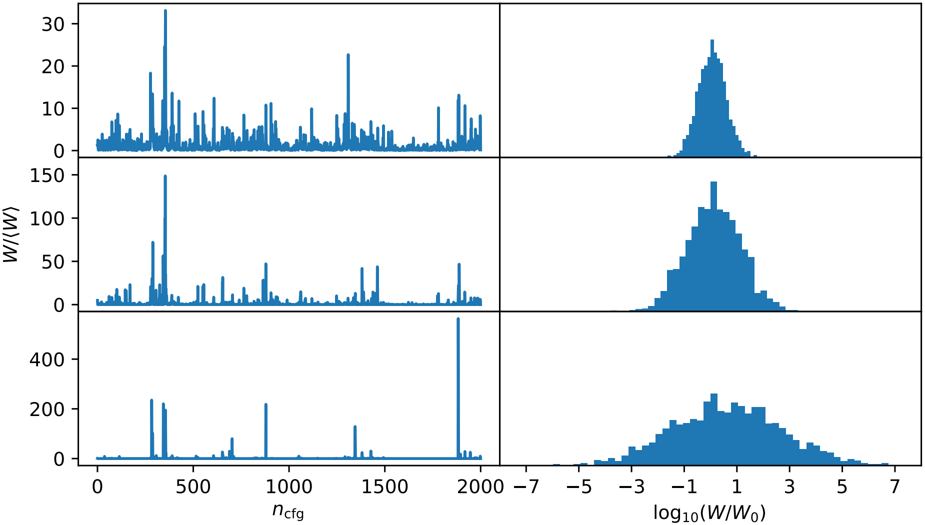
Backup - Effect of the Reweighting



Backup - Reweighting of the Mass



Backup - Reweighting of the Mass



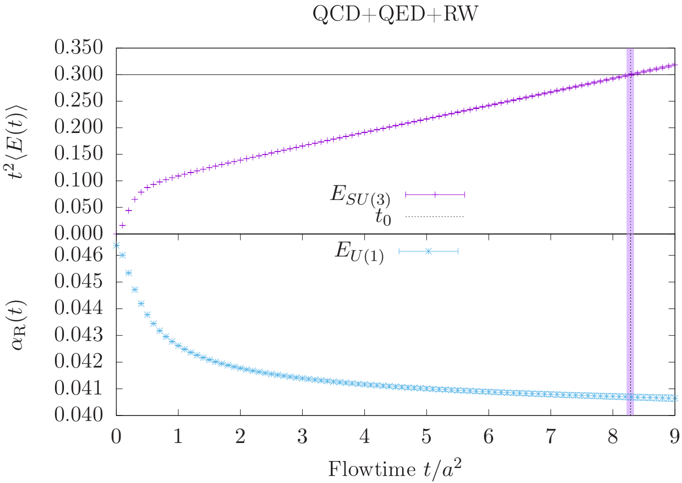
Backup - Setting the Scale - Wilson Flow

- 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'.

ensemble	n. cnfg	acc. rate	$\langle e^{-\Delta H} \rangle$	$\tau_{\rm int}(t_0)$	$\tau_{\rm int}(Q^2)$	$\tau_{\rm int}(\alpha_R)$
A400a00b324	2000	95%	0.9979(55)	51(18)	6.4(2.3)	—
B400a00b324	1082	98%	0.9950(25)	31(10)	8.0(2.8)	—
A450a07b324	1000	94%	0.9978(46)	44(19)	6.5(3.0)	2.3(1.6)
A380a07b324	2000	92%	1.0017(46)	46(15)	10.3(3.5)	2.7(1.5)
A500a50b324	1993	97%	0.9961(21)	21.4(5.5)	11.6(2.6)	1.40(55)
A360a50b324	2001	95%	0.9956(45)	47(16)	8.5(2.6)	1.1(1.0)
C380a50b324	600	98%	1.004(12)	12.5(3.9)	10.6(4.1)	3.0(1.2)