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Tuning QCD+QED ensembles via reweighting

Introduction

From *First results on QCD+QED with C⋆ boundary conditions*, JHEP 03 (2023) 012

$N_f = 1+2+1$ **QCD+QED ensembles with C⋆ boundary conditions**

ensemble	lattice	β	α	κ_u	$\kappa_d = \kappa_s$	κ_c
A400a00b324	64×32^3	3.24	0	0.13440733	0.13440733	0.12784
B400a00b324	80×48^3	3.24	0	0.13440733	0.13440733	0.12784
A450a07b324	64×32^3	3.24	0.007299	0.13454999	0.13441323	0.12798662
A380a07b324	64×32^3	3.24	0.007299	0.13459164	0.13444333	0.12806355
A500a50b324	64×32^3	3.24	0.05	0.135479	0.134524	0.12965
A360a50b324	64×32^3	3.24	0.05	0.135560	0.134617	0.129583
C380a50b324	96×48^3	3.24	0.05	0.1355368	0.134596	0.12959326

Tuned according to the following scheme

$$\phi_0^{\mathrm{phys}} = 8t_0\left(M_{K_\pm}^2 - M_{\pi_\pm}^2\right) = 0.992$$
$$\phi_1^{\mathrm{phys}} = 8t_0\left(M_{\pi_\pm}^2 + M_{K_\pm}^2 + M_{K_0}^2\right) = 2.26$$
$$\phi_2^{\mathrm{phys}} = 8t_0\left(M_{K_0}^2 - M_{K_\pm}^2\right)\alpha_{\mathrm{R}}^{-1} = 2.36$$
$$\phi_3^{\mathrm{phys}} = \sqrt{8t_0}\left(M_{D_s^\pm} + M_{D_0} + M_{D_\pm}\right) = 12.0$$

$$\phi_0 = 0 \quad \rightarrow \quad m_d = m_s$$
$$\phi_1 = 2.11$$
$$\phi_2 = 2.36$$
$$\phi_3 = 12.1$$

Goal

- Use **reweighting factors to tune** ϕ_0 close to the physical value while keeping fixed $\phi_{1,2,3}$

- Reweighting factors allow to recycle **simulated** configurations to calculate the path integral wrt a different **target** probability distribution

$$\langle \mathcal{O} \rangle_{\text{target}} = \frac{\langle \mathcal{O} W \rangle_{\text{sim}}}{\langle W \rangle_{\text{sim}}} \qquad W \sim \frac{\rho_{\text{target}}(U)}{\rho_{\text{sim}}(U)}$$

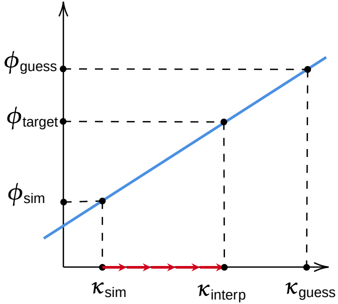
price: **noise**

Outline of the strategy

- Choose a new set of bare masses $\vec{\kappa}_{\text{guess}} \neq \vec{\kappa}_{\text{sim}}$

$$\kappa = \frac{1}{2(m+4)}$$

- Consider $\vec{\kappa}_{\text{sim}}$ + 4 new sets by shifting one flavour at a time
- Use **linear interpolation** to get $\vec{\kappa}_{\text{interp}}$ for ϕ_0^{target}
- Compute the reweighting factors for $\vec{\kappa}_{\text{interp}}$



Imagine this in 5 dimensions!

flavour f	κ_{sim}	κ_{guess}	m_{sim}	m_{guess}	δm
u	0.13459164	0.13464294	-0.28505901	-0.286474434	-0.001415424
d	0.13444333	0.13454895	-0.28096090	-0.283880328	-0.002919428
s	0.13444333	0.13428372	-0.28096090	-0.276540447	0.004420453
c	0.12806355	0.12801713	-0.09568842	-0.094273001	0.001415419

RHMC

The probability distribution generated in a HMC simulation reads

$$\rho_{\rm sim}(U) \sim \mathrm{d}U e^{-S_g[U]} |\det(\hat{D})|^{2\alpha} \qquad\qquad \hat{D} = D_{ee} - D_{eo} D_{oo}^{-1} D_{oe}$$

- $\alpha = 1$ for 2 degenerate flavours with Periodic Boundary Conditions
- $\alpha = \frac{1}{2}$ for 1 non-degenerate flavour with PBC or 2 degenerate flavours with C* BC
- $\alpha = \frac{1}{4}$ for 1 non-degenerate flavour with C* BC

Better work with the γ_5-hermitian operator $\hat{Q} = \gamma_5 \hat{D}$

$$|\det(\hat{D})|^{2\alpha} = \det(\hat{Q}^2)^\alpha \qquad\qquad \hat{Q}^2 = \hat{D}^\dagger \hat{D}$$

RHMC

In Rational HMC $(\hat{Q}^2)^\alpha$ is replaced by a **rational approximation** $R_\alpha(x) \sim x^{-\alpha}$

$$|\det(\hat{D})|^{2\alpha} = \det(\hat{Q}^2)^\alpha = \det\left[(\hat{Q}^2)^\alpha R_\alpha(\hat{Q}^2)\right] \det\left[R_\alpha(\hat{Q}^2)^{-1}\right]$$

and the distribution actually simulated is

$$\rho_{\rm sim}^{\rm RHMC}(U) \sim \mathrm{d}U e^{-S_g[U]} \det\left[R_\alpha(\hat{Q}^2)^{-1}\right]$$

$W_{\rm rat} \equiv \det\left[(\hat{Q}^2)^\alpha R_\alpha(\hat{Q}^2)\right]$ is a correction to the rational approximation $\rightarrow$ **reweighting factor**

In $N_f = 1 + 2 + 1$ ensemble

$$\rho_{\rm sim}^{\rm RHMC}(U) \sim e^{-S_g[U]} \det\left[R_{\frac{1}{4}}(\hat{Q}_u^2)^{-1}\right] \cdot \det\left[R_{\frac{1}{2}}(\hat{Q}_{ds}^2)^{-1}\right] \cdot \det\left[R_{\frac{1}{4}}(\hat{Q}_c^2)^{-1}\right]$$

Mass reweighting factors: shift one non-degenerate flavour ($f = u, c \qquad \alpha = \frac{1}{4}$)

$$\rho_{\mathrm{sim}}(U) \sim e^{-S_g[U]} \det\left[R_{\frac{1}{4}}(\hat{Q}_f^2)^{-1}\right] \qquad \rho_{\mathrm{target}}(U) \sim e^{-S_g[U]} \det\left[(\hat{Q}_{f'}^2)^{\frac{1}{4}}\right]$$

Assuming the same rational approximation for the new mass

$$W_{\mathrm{MSRW}}^{f \to f'} = \frac{\rho_{\mathrm{target}}}{\rho_{\mathrm{sim}}} = \frac{\det\left[(\hat{Q}_{f'}^2)^{\frac{1}{4}}\right]}{\det\left[R_{\frac{1}{4}}(\hat{Q}_f^2)^{-1}\right]} \cdot \frac{\det\left[R_{\frac{1}{4}}(\hat{Q}_{f'}^2)\right]}{\det\left[R_{\frac{1}{4}}(\hat{Q}_{f'}^2)\right]} = \underbrace{\det\left[(\hat{Q}_{f'}^2)^{\frac{1}{4}} R_{\frac{1}{4}}(\hat{Q}_{f'}^2)\right]}_{W_{\mathrm{rat}}^{f'}} \cdot \underbrace{\frac{\det\left[R_{\frac{1}{4}}(\hat{Q}_f^2)\right]}{\det\left[R_{\frac{1}{4}}(\hat{Q}_{f'}^2)\right]}}_{W_{Q_f \to Q_{f'}}}$$

Shift two degenerate flavours ($ds \to d's'$)

$$\rho_{\mathrm{sim}}(U) \sim e^{-S_g[U]} \det\left[R_{\frac{1}{2}}(\hat{Q}^2_{ds})^{-1}\right] \qquad \rho_{\mathrm{target}}(U) \sim e^{-S_g[U]} \det\left[(\hat{Q}^2_{d'})^{\frac{1}{4}}\right] \det\left[(\hat{Q}^2_{s'})^{\frac{1}{4}}\right]$$

In this case we need an extra factor to compensate for the mismatch in the power of the rational approximations

$$W = \frac{\rho_{\mathrm{target}}}{\rho_{\mathrm{sim}}} = W^{ds \to d'}_{\mathrm{MSRW}} \cdot W^{ds \to s'}_{\mathrm{MSRW}} \cdot \underbrace{\frac{\det\left[R_{\frac{1}{2}}(\hat{Q}^2_{ds})^{-1}\right]}{\det\left[R_{\frac{1}{4}}(\hat{Q}^2_{ds})^{\mathbf{2}}\right]}}_{W_{\mathrm{SPLIT}}}$$

Shift one of the two degenerate flavours ($ds \to d's$ or $ds \to ds'$)

$$\rho_{\text{sim}}(U) \sim e^{-S_g[U]} \det\left[R_{\frac{1}{2}}(\hat{Q}_{ds}^2)^{-1}\right] \qquad \rho_{\text{target}}(U) \sim e^{-S_g[U]} \det\left[(\hat{Q}_{d'}^2)^{\frac{1}{4}}\right] \det\left[(\hat{Q}_{ds}^2)^{\frac{1}{4}}\right]$$

We need an extra correction to the rational approximation of power $\frac{1}{4}$

$$W = \frac{\rho_{\text{target}}}{\rho_{\text{sim}}} = W_{\text{MSRW}}^{ds \to d'} \cdot W_{\text{SPLIT}} \cdot \underbrace{\det\left[(\hat{Q}_{ds}^2)^{\frac{1}{4}} R_{\frac{1}{4}}(\hat{Q}_{ds}^2)\right]}_{W_{\text{rat}}^{ds}}$$

Codes

- **Reweighting factors** openQxD-devel/18-msrw/extras/msrw rw2.c
- **Correction to rational approximations** main/ms1.c or rw2.c
- **Rational approximations** minmax/minmax.c
- **Meson correlators** main/ms6.c

Analysis

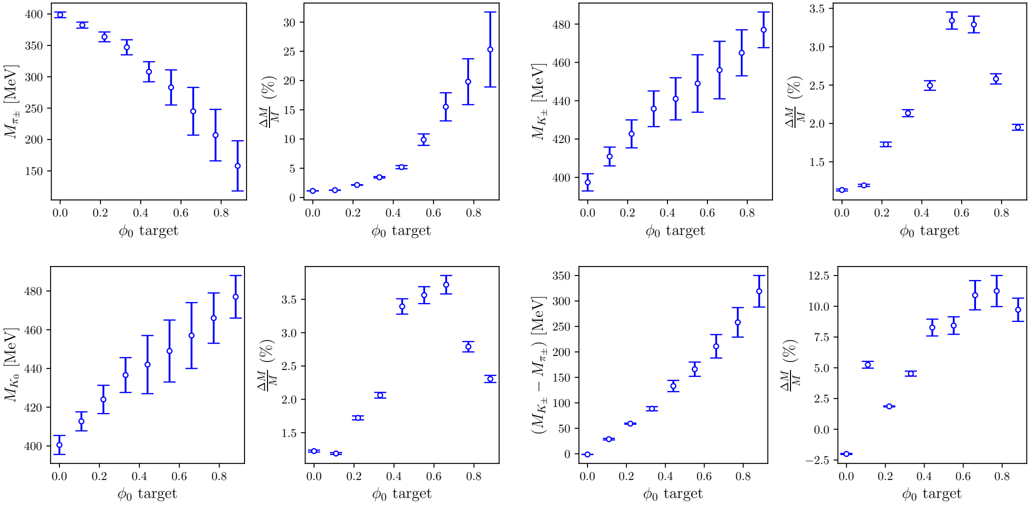
- Due to exceptional configurations only computation up to $\phi_0^{\mathrm{target}} \simeq 0.9$ successful
- The analysis is done with the **JQxDAnalysis** (Gitlab) routines implementing the gamma method for the error propagation
- All the reweighting factors are calculated and included
- Universal approximation of Finite Volume Corrections subtracted to charged mesons

Results: ϕ's (from meson masses)

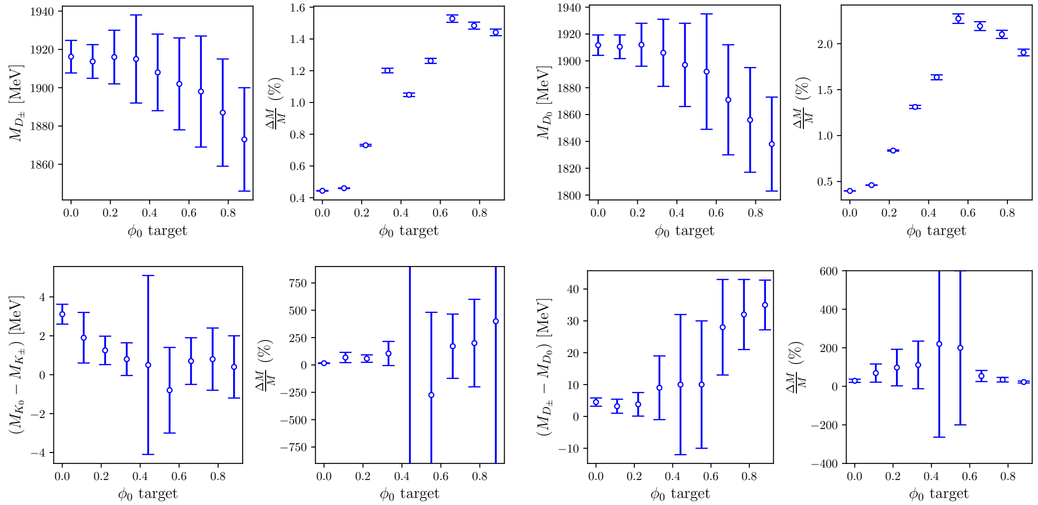
ϕ_0 target	α_R	ϕ_0	ϕ_1	ϕ_2	ϕ_3
0.000	0.007091(28)	-0.004738(96)	2.111(49)	1.55(23)	12.079(51)
0.110	0.007101(31)	0.1003(54)	2.146(52)	0.95(69)	12.089(54)
0.220	0.007135(45)	0.2056(42)	2.170(79)	0.66(38)	12.120(86)
0.331	0.007147(44)	0.306(11)	2.22(11)	0.43(45)	12.12(13)
0.441	0.00724(10)	0.442(31)	2.15(13)	0.3(2.5)	12.09(12)
0.551	0.007088(58)	0.539(18)	2.14(19)	-0.4(1.2)	12.07(16)
0.661	0.007084(66)	0.654(23)	2.11(21)	0.42(71)	12.00(15)
0.772	0.007066(59)	0.766(29)	2.11(18)	0.45(92)	11.95(15)
0.882	0.007041(42)	0.896(18)	2.13(14)	0.24(99)	11.89(13)

- ϕ_0 close to target value
- ϕ_1 and ϕ_3 roughly constant
- $\phi_2 = 8t_0\left(M_{K_0}^2 - M_{K_\pm}^2\right)\alpha_{\mathrm{R}}^{-1}$ unstable and far from 2.36
- Strong sensitivity to the effective mass

Results: light mesons masses



Results: heavy mesons masses



Discussion and outlooks

- Is the level of precision satisfactory?
- How can we do better?
- What's next?

Backup slides

Computational cost

Simulation cost for 4096 cores on HLRN. In each row the reweighting factors include four mass reweighting factors and one splitting factor. Second and third columns refer to the average number of seconds per configuration.

ϕ_0 target	Rew. factors	Mesons	config.
0.000	362	59.6	2000
0.110	366	68.0	2000
0.220	355	55.2	2000
0.331	344	70.3	2000
0.441	369	64.1	2000
0.551	377	68.5	2000
0.661	361	72.4	2000
0.772	368	72.8	2000
0.882	400	69.3	1934
Core-hours	$\sim$ 7.5M	$\sim$ 1.36M	

```
#!/bin/bash
#SBATCH -t 12:00:00
#SBATCH -n 4096 -N 43
#SBATCH -p standard96
#SBATCH -A bep00102
```

Results: pseudoscalar mesons masses

ϕ_0 target	$M_{\pi_\pm}$ [MeV]	$M_{K_\pm}$ [MeV]	M_{K_0} [MeV]	$M_{D_\pm}$ [MeV]	M_{D_0} [MeV]
0.000	398.7(4.5)	397.4(4.5)	400.5(4.9)	1916.2(8.5)	1911.7(7.6)
0.110	382.3(4.8)	410.9(4.9)	412.7(4.9)	1913.7(8.8)	1910.5(8.8)
0.220	363.6(7.8)	422.7(7.3)	424.0(7.3)	1916(14)	1912(16)
0.331	347(12)	435.8(9.3)	436.6(9.0)	1915(23)	1906(25)
0.441	308(16)	441(11)	442(15)	1908(20)	1897(31)
0.551	283(28)	449(15)	449(16)	1902(24)	1892(43)
0.661	245(38)	456(15)	457(17)	1898(29)	1871(41)
0.772	207(41)	465(12)	466(13)	1887(28)	1856(39)
0.882	158(40)	477.0(9.3)	477(11)	1873(27)	1838(35)

Results: difference in pseudoscalar meson masses

ϕ_0 target	$M_{K_\pm} - M_{\pi_\pm}$ [MeV]	$M_{K_0} - M_{K_\pm}$ [MeV]	$M_{D_\pm} - M_{D_0}$ [MeV]
0.000	-1.346(27)	3.11(51)	4.5(1.3)
0.110	28.6(1.5)	1.9(1.3)	3.2(2.2)
0.220	59.1(1.1)	1.25(73)	3.8(3.7)
0.331	88.4(4.0)	0.80(84)	9(10)
0.441	133(11)	0.5(4.6)	10(22)
0.551	166(14)	-0.8(2.2)	10(20)
0.661	211(23)	0.7(1.2)	28(15)
0.772	258(29)	0.8(1.6)	32(11)
0.882	319(31)	0.4(1.6)	35.0(7.8)

Interpolated hopping parameters

ϕ_0 target	κ_u^{interp}	κ_d^{interp}	κ_s^{interp}	κ_c^{interp}	config.
0.000	0.134578	0.134436	0.134438	0.128090	2000
0.110	0.134592	0.134452	0.134399	0.128126	2000
0.220	0.134606	0.134469	0.134359	0.128162	2000
0.331	0.134618	0.134485	0.134320	0.128199	2000
0.441	0.134633	0.134502	0.134281	0.128238	2000
0.551	0.134647	0.134517	0.134242	0.128271	2000
0.661	0.134662	0.134535	0.134202	0.128304	2000
0.772	0.134677	0.134550	0.134163	0.128337	2000
0.882	0.134691	0.134568	0.134123	0.128370	1934
0.992	0.134706	0.134582	0.134085	0.128403	0