Scale setting for CLS 2+1 simulations

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Scale setting: Precision lattice QCD for particle and nuclear physics



Overview

This talk is based on

Original 2017 publication

[M. Bruno, T. K. and S. Schaefer, "Setting the scale for the CLS 2 + 1 flavor ensembles",

Phys. Rev. D 95 (2017) no.7, 074504]

2021 update

[B. Straßberger, M. Cè, S. Collins, A. Gérardin, G. von Hippel, P. Korcyl, T. K., D. Mohler, A. Risch, S. Schaefer, W. Söldner and R. Sommer, "Scale setting for CLS 2+1 simulations",

PoS LATTICE2021 (2022), 135]

Ben's PhD thesis

[B. Straßberger,

"Towards Higher Precision Lattice QCD Results: Improved Scale Setting and Domain Decomposition Solvers",

doi:10.18452/26517]

Recent r₀ determination (→ Tom Asmussen's talk)

[T. M. B. Asmussen, R. Höllwieser, F. Knechtli and T. K., "The determination of potential scales in 2+1 flavor QCD",

arXiv:2412.10215 [hep-lat]]

Goal

A precise scale is necessary for all dimensionful predictions of QCD The goals of this work are

- Determine precise values in [fm] for widely used reference scales like
 - $\sqrt{t_0}$, the original gradient flow scale

[M. Lüscher, JHEP 08 (2010) 071]

- w₀, a modified gradient flow scale
 [S. Borsányi, JHEP 09 (2012)]
- ► *r*₀, the "Sommer Scale" from the static potential

[R. Sommer, Nucl. Phys. B 411 (1994)]

r₁, a shorter distance cousin of r₀
 [W. Bernard et al., Phys. Rev. D 62 (2000)]

(In continuum iso-QCD at well-defined mass points)

• Map out the relation between simulation parameter $\beta \equiv \frac{6}{g_0^2}$ and the lattice spacing *a* for the lattice action used by CLS

The original precision goal was modest, 1% - 2%, based on our aspiration to compute Λ_{QCD} to $\approx 3\%$

- CLS = Coordinated Lattice Simulations consortium of several European lattice-QCD groups
- Since 2013: generation of $N_{\rm f} = 2 + 1$ ensembles
- Action
 - [M. Bruno et al. JHEP 02 (2015) 043]
 - ► Tree-level Symanzik O(a²) improved gauge action ☐, ☐ [M. Lüscher, P. Weisz (1985)]
 - ► Non-perturbatively O(a) improved Wilson fermions

[B. Sheikholeslami, R. Wohlert, Nucl.Phys.B 259 (1985)][J. Bulava, S. Schaefer, Nucl.Phys.B 874 (2013)]

- Open boundaries in time (mostly)
- Chiral trajectory with tr[M_q] = const

[W. Bietenholz et al., Phys.Lett. B690 (2010)] Reason: with Wilson fermions same $\tilde{g}_0^2 = g_0^2 \left(1 + \frac{b_g}{a} \operatorname{tr}[M_q]/3\right) \Leftrightarrow$ same lattice spacing *a* up to $O(a^2)$

Ensembles and Statistics



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Ensembles and Statistics

- Area \propto MDUs
- Gray = original (2017)
- Blue = update (2021)



T.Korzec (BUW)



- Inputs
- Iteration
- Results

To fix three bare parameters $a m_{u,d}$, $a m_s$, β we use three experimental inputs

- Pion mass *m*_π
- Kaon mass *m_K*
- Pseudo-scalar decay constant $f_{\pi K} \equiv \frac{2}{3} \left(f_K + \frac{1}{2} f_\pi \right)$

We assume that these are already "corrected" for

- QED effects (standard model \neq QCD)
- $N_f = 2 + 1$ is not $N_f = 1 + 1 + 1 + 1 + 1 + 1$ effects
- \rightarrow Yesterday's talk by Alberto Ramos

We want to use leptonic decay constants f_{π} , f_K to set the scale

Lowest order:
$$\Gamma^0(P \to l\nu) = \frac{G_F^2}{8\pi} f_P^2 m_l^2 m_P \left(1 - \frac{m_l^2}{m_P^2}\right)^2 |V_{q_1q_2}|^2$$

And $ip_\mu f_P = \langle 0|\bar{q}_1\gamma_\mu\gamma_5 q_2|P(p)\rangle$ is computable in QCD

- Advantages
 - Low energy quantity
 - Pseudo-scalar correlators are extremely precise (signal/noise=constant)
 - χ_{PT} to known to high orders
 - Finite volume effects are well understood
- Disadvantages
 - ► Indirect connection to experiment via V_{ud}, V_{us}
 - Conceptually difficult beyond QCD
 - \blacktriangleright Not a spectral quantity \rightarrow needs renormalization and improvement

Iteration

We would like to

• Compute for each β : $af_{\pi K}|_{\text{phys. mass}}$

• Divide by $f_{\pi K}^{\text{iso-QCD}}$ to obtain *a* in fm

In practice: The physical mass point is only known after scale setting.

Iterate

- Take best value of $\sqrt{t_0}$ [fm]
- Express masses in t₀ units

$$\phi_2 = 8t_0 m_\pi^2$$

$$\phi_4 = 8t_0 \left(m_K^2 + \frac{1}{2} m_\pi^2 \right) , \qquad p$$

proxy for light quark mass proxy for tr[M^R]

- Perform simulations on chiral trajectories that go through $\phi_{2}^{\text{iso-QCD}}, \phi_{4}^{\text{iso-QCD}}$
- On this set of ensembles, compute $\sqrt{t_0} f_{\pi K}$
- Continuum / chiral extrapolate to $\phi_2^{\text{iso-QCD}}$, $\phi_4^{\text{iso-QCD}}$
- Divide by $f_{\pi K}^{\text{iso-QCD}}$ to obtain $\sqrt{t_0}$ [fm]

Quark Mass Derivatives

Instead of re-doing all simulations several times, we correct existing ones

• For every relevant observable \mathcal{O} , compute derivatives with respect to the bare quark masses

 $\frac{d\langle \mathcal{O} \rangle}{d \, am_u}, \ \frac{d\langle \mathcal{O} \rangle}{d \, am_d}, \ \frac{d\langle \mathcal{O} \rangle}{d \, am_s}$

• Use these to shift to slightly different chiral trajectories $\langle \mathcal{O} \rangle \rightarrow \langle \mathcal{O} \rangle + \sum A^{d \langle \mathcal{O} \rangle}$

 $\langle \mathcal{O} \rangle \rightarrow \langle \mathcal{O} \rangle + \sum_{f} \Delta_{f} \frac{d \langle \mathcal{O} \rangle}{d \, am_{f}}$

• We neglect $O(\Delta^2) \rightarrow$ shifts must be small



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Results

$$\begin{array}{rcl} \sqrt{t_0} &=& 0.1443(7)(13) \ {\rm fm} \,, \\ \sqrt{t_0^\star} &=& 0.1439(7)(13) \ {\rm fm} \,, \\ r_0 &=& 0.4729(74) \ {\rm fm} \,, \\ r_1 &=& 0.3128(40) \ {\rm fm} \end{array}$$

physical mass

$$m_u = m_d = m_s, \phi_4 = 1.11$$

 $\leftarrow \text{Tom Asmussen}$

Lattice spacings with CLS action

β	<i>a</i> [fm]		
3.40	0.0849(5)(8)		
3.46	0.0749(4)(7)		
3.55	0.0633(4)(6)		
3.70	0.0491(3)(4)		
3.85	0.0385(2)(3)		

Details and Sources of Errors

- Systematic Errors
- Statistical Errors

Errors from Inputs

Experimentally one finds

- $m_\pi^\pm =$ 139.5704 MeV, $m_\pi^0 =$ 134.9768 MeV o 3.3%
- $m_{K}^{\pm} =$ 493.68 MeV, $m_{K}^{0} =$ 497.61 MeV ightarrow 0.8%
- $(f_{\pi^+} f_{\pi^0})/f_{\pi^+} \approx 0.3\%$

Spread too big \rightarrow needs correction \rightarrow we use as inputs

"Corrected" iso-QCD values

- $m_{\pi}^{\text{isoQCD}} = 134.9768(5) \text{ MeV}$
- $m_K^{isoQCD} = 497.611(13) \text{ MeV}$ [PDG]

•
$$f_{\pi}^{\text{isoQCD}} = 130.56(02)(13)(02) \text{ MeV}$$

• $f_{K}^{\text{isoQCD}} = 157(2)(2)(4) \text{ MeV}$
[FLAG 2021]

This is precise enough for us. More care maybe needed in the future \rightarrow Alberto Ramos, Andreas Risch

Decoupling

Can these values be used also for $N_{\rm f} = 2 + 1$ QCD? How much are dimensionless ratios like $\sqrt{t_0} f_{\pi}$ affected?



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Scale Setting

Other Parameters

Our calculation also relies on various renormalization and improvement factors

- $c_{sw} = \frac{1-0.1921g_0^2 0.1378g_0^4 + 0.0717g_0^6}{1-0.3881g_0^2}$ (non-perturbative) O(a) improvement of the (bulk) Wilson action [J. Bulava, S. Schaefer, Nucl.Phys.B 874 (2013)] • Z_A (non-perturbative) known to $\approx 0.04\%$ accuracy Axial current renormalization factors [M. Dalla Brida, T.K., S. Sint, P. Vilaseca, Eur.Phys.J.C 79 (2019)] • $c_A = -0.006033 g_0^2 \times \left[1 + \exp\left(9.2056 - \frac{13.9847}{g_0^2}\right)\right]$ (non-perturbative) Axial current improvement coefficient [J. Bulava, M. Della Morte, J. Heitger, C. Wittemeier, Nucl.Phys.B 896 (2015) 555-568]
- *b_A*,*b_P*,... (perturbative) Improvement coefficients that come with mass factors *am_q* Error=Difference between last known orders

[Y. Taniguchi, A. Ukawa, Phys.Rev. D58 (1998)]

Systematic Monte-Carlo Errors - Distribution

Often it is not possible to sample exactly from a desired PDF $\propto e^{-S_A}$. Instead a similar PDF $\propto e^{-S_B}$ is used.

We correct for such deviations by reweighting

$$\langle \mathcal{O} \rangle_A = \frac{\langle \mathcal{O} | W \rangle_B}{\langle W \rangle_B}$$

 $W = e^{S_B - S_A}$

- Protect simulations from exceptionally small eigenvalues of \hat{D} $det[\hat{D}^{\dagger}\hat{D}] \rightarrow det[\hat{D}^{\dagger}\hat{D} + \mu^{2}]^{2}/det[\hat{D}^{\dagger}\hat{D} + 2\mu^{2}]$ (twisted mass reweighting 2. kind) [M. Lüscher, F. Palombi, PoS (LATTICE2008) 049]
- $\det[\hat{D}] = \pm \det[\sqrt{\hat{D}^{\dagger}\hat{D}}] \rightarrow \pm \det[R(\hat{D}^{\dagger}\hat{D})]$
 - One reweighting factor for rational $R(x) \neq \sqrt{x}$
 - One reweighting factor for \pm

[D. Mohler, S. Schaefer, Phys.Rev.D 102 (2020)]

 \rightarrow No systematic error for us

Typical Reweighting Factor

Overall reweighting factor on H100



Systematic Monte-Carlo Errors - Topology

Even at our smallest lattice spacings, the topology moves



J501: $a \approx 0.038$ fm, *Q* from GF fields at $t \approx t_0$ in the bulk

- Topology sampling is not more problematic than other quantities
- Ordinary critical slowing down $\propto a^{-2}$ is bad enough
- What would happen if we were stuck in a "sector" with |Q| < 1?

All sectors: $t_0/a^2 = 14.01(7)$ $w_0/a = 4.46(2)$ Stuck: $t_0/a^2 = 14.06$ $w_0/a = 4.46$

 \rightarrow Effect not very clear, needs a dedicated study

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Systematic Monte-Carlo Errors - Plateaus

- Hadron correlators usually suffer from a signal/noise problem
- But not Pions nor Kaons!
 - ightarrow We observe long and precise plateaus even without quark smearing
- Fixed source time-slice (at $x_0 = a$) + correlations
 - ightarrow "waves" in effective masses

$$\begin{split} f_{P}^{r,s}(x_{0},y_{0}) &= -\frac{a^{6}}{L^{3}} \sum_{\mathbf{x},\mathbf{y}} \langle P^{r,s}(x) P^{s,r}(y) \rangle \\ f_{A}^{r,s}(x_{0},y_{0}) &= -\frac{a^{6}}{L^{3}} \sum_{\mathbf{x},\mathbf{y}} \langle A_{0}^{r,s}(x) P^{s,r}(y) \rangle \\ m_{\text{PS}} &= \log \left[f_{P}(a,y_{0}) / f_{P}(a,y_{0}+a) \right] \end{split}$$

with local

- Pseudo-scalar density P
- Axial current A_µ



typical case (here J303)

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with local

Pseudo-scalar density P

Axial current A_µ



difficult case (here D200)

Systematic Monte-Carlo Errors - Plateaus

Matrix elements are isolated from ratios

$$R(x_0, y_0) = \sqrt{\frac{f_A^{\text{imp}}(x_0, y_0) f_A^{\text{imp}}(x_0, T - y_0)}{f_P(T - y_0, y_0)}}$$

 $f_{PS} = Z_A [1 + \overline{b}_A \ a \ {
m tr} M_q + \widetilde{b}_A \ a m_{
m PCAC}] \sqrt{2/m_{PS}} \ R^{
m aver}$



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We deal with reweighted "primary" observables

$$oldsymbol{o} = \langle \mathcal{O}
angle_{oldsymbol{Q} \mathcal{C} \mathcal{D}} = rac{\langle \mathcal{O} \ oldsymbol{W}
angle}{\langle oldsymbol{W}
angle} \,.$$

As well as with "derived" observables

$$f(\langle \mathcal{O}_1 \rangle_{QCD}, \ldots, \langle \mathcal{O}_n \rangle_{QCD}, m)$$

The bare quark mass derivative of the latter is given by

$$\frac{df}{dm} = \frac{\partial f}{\partial o_i} \left\langle \frac{\partial \mathcal{O}_i}{\partial m} \right\rangle_{QCD} - \frac{\partial f}{\partial o_i} \left(\left\langle \mathcal{O}_i \frac{\partial S}{\partial m} \right\rangle_{QCD} - o_i \left\langle \frac{\partial S}{\partial m} \right\rangle_{QCD} \right) + \frac{\partial f}{\partial m} \\
= \frac{\partial f}{\partial o_i} \frac{\left\langle \frac{\partial \mathcal{O}_i}{\partial m} W \right\rangle}{\langle W \rangle} - \frac{\partial f}{\partial o_i} \left(\frac{\left\langle \mathcal{O}_i \frac{\partial S}{\partial m} W \right\rangle}{\langle W \rangle} - \frac{\left\langle \mathcal{O}_i W \right\rangle \left\langle \frac{\partial S}{\partial m} W \right\rangle}{\langle W \rangle^2} \right) + \frac{\partial f}{\partial m}.$$

- All observables will need: sea quark mass dependence $\frac{\partial S}{\partial m} \rightarrow tr[D^{-1}] \rightarrow stochastic estimation, 1 solve per noise$
- Fermionic observables also: valence quark mass dependence E.g. pion correlator $(\bar{u}\gamma_5 d)$: $\mathcal{O} = -\sum \operatorname{tr}[\gamma_5 D^{-1}(x, y)\gamma_5 D^{-1}(y, x)]$ estimated stochastically $\mathcal{O} = -\sum_{\mathbf{y}} \langle \xi^{\dagger}(\mathbf{y}) \xi(\mathbf{y}) \rangle_{\text{noise}}$ with $\xi = D^{-1}\eta$ and $\eta =$ vector with noise on x_0 . (1 solve per noise) Each mass derivative needs an additional inversion $rac{\partial \mathcal{O}}{\partial m_u} = -\sum_{m{y}} \langle \xi^\dagger(m{y}) rac{\partial \xi(m{y})}{\partial m_u}
 angle_{ ext{noise}}$ $\frac{\partial \xi}{\partial m} = -D^{-2}\eta$

Two $m_{u,d} = m_s$ ensembles with 7% difference in ϕ_4



Largest shift: 5%, majority $\approx 2\% \rightarrow$ We assume that $O(\Delta^2)$ is negligible

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04.03.2025

Since we are already changing the chiral trajectories: one more change:

- Instead of trajectories with $tr[M_q] = const.$
- Create trajectories with $\phi_4 = \text{const.} \sim \text{tr}[M^R]$



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Scale Setting

Our volumes are finite, but large

- Smallest $m_{\pi}L \approx 3.8$ on D452 (only case below 4)
- Largest $m_{\pi}L \approx 6.4$ on N202
- Smallest $L \approx 2.35$ fm

Finite volume effects in $f_{\pi,K}$ and $m_{\pi,K}$ have been worked out in χ_{PT}

[G. Colangelo, S. Dürr, Nucl. Phys. B 721 (2005)] We apply these corrections

- Average correction: 0.1%
- Biggest correction: 0.6%

Uncanceled finite size effects are assumed to be negligible

Statistical Monte-Carlo Errors

To calculate the statistical errors of a MC estimate

$$\sigma_f = \sqrt{\frac{\operatorname{var}(f)}{N/(2\tau_{\operatorname{int},f})}}$$

We use the Γ -method, i.e. explicitly compute $\tau_{int,f}$ from the data [U. Wolff, Comput.Phys.Commun. 156 (2004)]

- We use rough estimates of τ_{exp} to attach exponential tails to Γ [S. Schaefer, R. Sommer, F. Virotta, Nucl.Phys.B 845 (2011)]
- Projected Observables

[A. Ramos, Comput.Phys.Commun. 238 (2019)] For "derived" observables $f(\langle a_1 \rangle, \dots, \langle a_n \rangle)$, store a projected time series

$$f^{i}_{\text{proj}} = f(\langle a_{1} \rangle, \dots, \langle a_{n} \rangle) + \sum_{\alpha} \frac{\partial f}{\partial \langle a_{\alpha} \rangle} (a^{i}_{\alpha} - \langle a_{\alpha} \rangle), \qquad i = 1, \dots, N$$

Analyzed like a "primary" observable, this yields the correct error

Example: action density at flow time $t \approx t_0$ on N = 4032 measurements on H101



Example: action density at flow time $t \approx t_0$ on N = 3804 measurements of N202



How Much Statistics is Necessary?

Experiment: let us use different fractions of H101 statistics

Ν	<i>N</i> /14	$ au_{int}$
4032	287	14 ± 6
1400	100	$\textbf{22}\pm\textbf{8}$
700	50	9 ± 6
350	25	6 ± 2

ightarrow statistics of at least $N/ au_{exp} >$ 50 is necessary

Using full statistics and attaching a tail with $\tau_{exp} = 13.3$, we obtain

$$\tau_{\rm int} = 24 \pm 6$$

Chiral / Continuum Extrapolations

Lattice results $\sqrt{t_0} f_{\pi K}$ vs ϕ_2 at $\phi_4 = \text{const.}$ is fitted globally:

- Continuum part of the fit
 - I. Order Taylor in φ₂ − φ₂^{sym}
 2. Order Taylor in φ₂ − φ₂^{sym}

 - SU(3) χ_{PT}
 - $SU(2) \chi_{PT}$ for f_{π} only in [B.Straßberger PhD thesis]
- Lattice artifacts
 - Factor $(1 + c_1 \frac{a^2}{t_{a}^{sym}})$
 - As above $+c_2 a^2 m_{\pi}^2$
- Cuts
 - neglect coarse ensembles
 - neglect heavy ensembles
 - both

Variation = leading source of (systematic) error!

type	cut	$\chi^2/{ m dof.}$	$\sqrt{t_0}f_{\pi}$	$\sqrt{t_0} f_{\pi K}$
Taylor	-	2.05		0.1083(3)
Taylor	$\beta > 3.4$	2.07		0.1088(4)
Taylor	$\beta > 3.5$	2.68		0.1084(5)
Taylor	$\phi_2 < 0.6$	1.77		0.1086(3)
Taylor	$\phi_2 < 0.4$	2.16		0.1086(4)
Taylor	$\beta>3.4, \phi_2<0.6$	2.03		0.1090(5)
Taylor(4)	-	1.98		0.1081(3)
Taylor(4)	$\beta > 3.4$	1.69		0.1083(4)
Taylor(4)	$\beta > 3.5$	2.26		0.1078(5)
Taylor(4)	$\phi_2 < 0.6$	1.64		0.1084(4)
Taylor(4)	$\phi_2 < 0.4$	2.03		0.1083(4)
Taylor(4)	$\beta>3.4, \phi_2<0.6$	1.43		0.1086(5)
$SU(3) \chi PT$	-	1.84		0.1081(3)
$SU(3) \chi PT$	$\beta > 3.4$	1.63		0.1085(4)
$SU(3) \chi PT$	$\beta > 3.5$	2.09		0.1081(5)
$SU(3) \chi PT$	$\phi_2 < 0.6$	1.50		0.1084(3)
$SU(3) \chi PT$	$\phi_2 < 0.4$	1.86		0.1084(4)
$SU(3) \chi PT$	$\beta>3.4, \phi_2<0.6$	1.48		0.1088(5)
$SU(3) \chi PT + a^2 m_\pi^2$	-	1.82		0.1085(4)
$SU(3) \chi PT + a^2 m_{\pi}^2$	$\beta > 3.4$	1.77		0.1084(6)
$SU(3) \chi PT + a^2 m_{\pi}^2$	$\beta > 3.5$	2.39		0.1080(8)
SU(3) $\chi PT + a^2 m_{\pi}^2$	$\phi_2 < 0.6$	1.63		0.1085(5)
$SU(3) \chi PT + a^2 m_{\pi}^2$	$\phi_2 < 0.4$	2.16		0.1086(7)
SU(3) $\chi PT + a^2 m_\pi^2$	$\beta>3.4, \phi_2<0.6$	1.18		0.1078(7)
$SU(2) \chi PT$	-	1.82	0.0933(4)	0.1074(3)
$SU(2) \chi PT$	$\beta > 3.4$	1.58	0.0937(4)	0.1079(4)
$SU(2) \chi PT$	$\beta > 3.5$	1.94	0.0933(6)	0.1075(5)
$SU(2) \chi PT$	$\phi_2 < 0.6$	1.26	0.0941(4)	0.1078(3)
$SU(2) \chi PT$	$\phi_2 < 0.4$	1.30	0.0945(5)	0.1079(4)
$SU(2) \chi PT$	$\beta > 3.4, \phi_2 < 0.6$	0.96	0.0947(6)	0.1085(5)

[B.Straßberger PhD thesis]

Lattice Artifacts Beyond $O(a^2)$

- Our fits assume that we see only leading corrections to scaling, i.e. pure O(a²)
- Other cutoff effects that could be expected
 - $O(a^3)$, next order of the Symanzik action
 - O(a² log(a)^Γ), taking the leading order more seriously. There are O(10) such terms with largely known Γ
 [N. Husung, P. Marguard, R. Sommer, Phys.Lett.B 829 (2022)]
 - ► O(a) from uncanceled am_q
- With "only" 5 lattice spacings it is difficult to fit more than 1-2 lattice-artifact terms.

Practical approach: use only pure $O(a^2)$, but study cuts and χ^2 values.

Extrapolations are a major source of uncertainty

Conclusions

Conclusions

- We obtained $\sqrt{t_0}$ to $\approx 1\%$ accuracy
- At this level of precision the errors are dominated by
 - Statistical error
 - Systematic error due to extrapolations
- Negligible sources of errors
 - External parameters
 - Charm quark effects
 - Mass shifts beyond linear approximation
 - Finite Volume

Wish-list / Possible Improvements

- Longer MC chains
- *m_s* = const. trajectory
- Improved flow