Scale setting from precise Omega baryons

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Motivation – what physics are we interested in?

Main interests (among the authors)

- Hadron-hadron interactions in Lattice QCD and Effective field theory
- Quark-mass dependence of hadron masses, with a particular focus on strangeness physics and charmed hadrons
- Interface to FAIR experiments (including CBM, PANDA)
- Exotic hadrons and their structure

Approaches

- Lattice QCD and Effective field theory

What we encountered

- Scale setting uncertainty relevant in many (unexpected) places
- In some cases, determined point (finite a, fixed quark masses) uncertainties of QCD resonances seem better determined than the scale
- Scale-setting uncertainty very relevant for tuning of RHQ actions (charm and bottom)

What none of use care about:

- Flow scales

What did we do in a nutshell?

R.J.Hudpsith, Matthias Lutz, DM, arXiv:2404.02769

- Precise determination of $I(J^P) = 0(3/2)^+$ and $= 0(3/2)^-$ Ω-baryon ground states on $\mathrm{Tr}(M) = const.$ CLS ensembles.
- Description with N^{3}LO $\mathrm{SU}(3)_f$ chiral perturbation theory.
(This was surprisingly successful and had unexpected implications.)
- These fits allow for a determination of the lattice spacings.
- As an afterthought, we also determine $\sqrt{t_0}$.

Outline

Why the Ω-baryon?

- On the surface: Known very precisely from experiment.
  (some people think one should and can do better)
- M_Ω is relatively straight-forward to determine with high precision (using a combination of standard lattice spectroscopy methods).
  In our case: At small time separation more precise than the pion.
- The strange-quark propagators are relatively cheap;
  no large noise to signal ratio.
- No complicated improved currents and renormalization.
- QCD stable state; strong isospin-breaking effects expected to be negligible; QED effects expected to be small;

Outline

1. Features of our calculation
   - Correlator methods
   - Omega baryon masses
   - Flavor $SU(3)$ chiral fits
2. Results
3. Challenges
4. Conclusions

Correlator basis and methods

- We use simple local Ω operators

$$\Omega_i^{\kappa}(x) = \epsilon_{abc}(s_a^T C\gamma_i s_b)s_c^{\kappa}(x).$$

- A parity projection is performed in the usual manner

$$C_{\Omega}^{\pm}(t-t') = \frac{1}{2}(1 \pm \gamma_t)^{\kappa\kappa'}\frac{1}{3}\sum_{i=x,y,z}\sum_{x}^{L^3}\Omega_i^{\kappa}(x,t)(\Omega_i^{\kappa'}(0,t'))^{\dagger}\,.$$

- Average over appropriate forward- and backward propagating states
- Truncated solver method

  G.S. Bali, S. Collins, A. Schäfer, CPC **181**, 1570 (2010)

  Our setup: sloppy solves on every timeslice (periodic bc) or in the bulk (open bc) and a single high-precision solve.

Quark sources

We use Coulomb-gauge-fixed wall sources

A. Billoire, E. Marinari, G. Parisi, Phys. Lett. B **162**, 160 (1985)
R. Gupta, G. Guralnik, G.W. Kilcup, S.R. Sharpe, PRD **43**, 2003 (1991)

- Gauge fixing through a Fourier-accelerated non-linear conjugate gradient algorithm

  R.J. Hudspith, CPC **187**, 115 (2015)

- Negligible calculational overhead
- Superior volume-scaling of the signal compared to other choices
  $\rightarrow$ Leverages large (lattice) volume of CLS ensembles with close-to-physical quark masses.
- Effective masses tend to approach their asymptotic values from below.

Generalized Pencil of Functions

C. Aubin, K. Orginos, AIP Conf. Proc. **1374,** 621 (2011)
J.R. Green *et al.* PRD **90,** 074507 (2014)
M. Fischer *et al.* EPJ A **56,** 206 (2020)

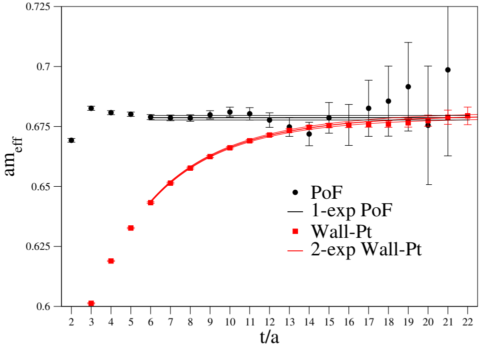
- The best way to deal with this is to form a generalized Pencil of Functions (PoF) matrix built from the Wall-point correlator $C^{\pm}_{\Omega}(t)$
- We use s simple 2x2 matrix

$$M^{\pm}_{\Omega}(t) = \begin{pmatrix} C^{\pm}_{\Omega}(t) & C^{\pm}_{\Omega}(t+1) \\ C^{\pm}_{\Omega}(t+1) & C^{\pm}_{\Omega}(t+2) \end{pmatrix} . \quad (1)$$

- This is solved as a symmetric GEVP at fixed metric time τ_0 and with approximate diagonalization at a later reference time τ.
- τ_0 and τ are varied as appropriate;
  chosen dimension and $\Delta\tau$ of the PoF were investigated.
- This part is similar to BMW scale setting for $(g-2)_{\mu}$.

Wall-point sources versus PoF – consistency check

- Principal correlator from the PoF approaches asymptotic behavior fast; benefit at the expense of noisier data
- Empirically, the PoF leads to reduced correlations in time
- Methods lead to consistent results
  $\rightarrow$ Final results from PoF (less afflicted by systematics)



Representative result from the C101 ensemble.

Wall-point sources versus PoF – consistency check

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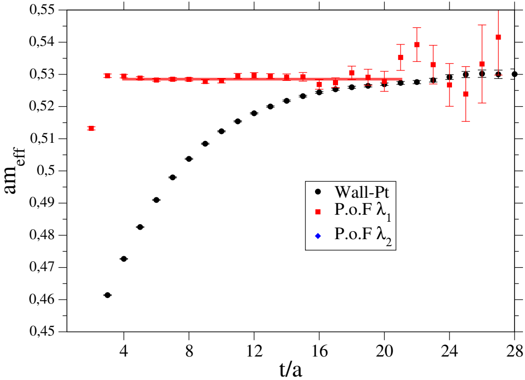
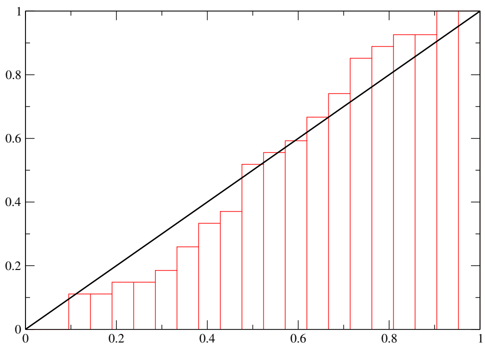


Result for the E250 ensemble requested by referee.

Consistency check: p-value histogram

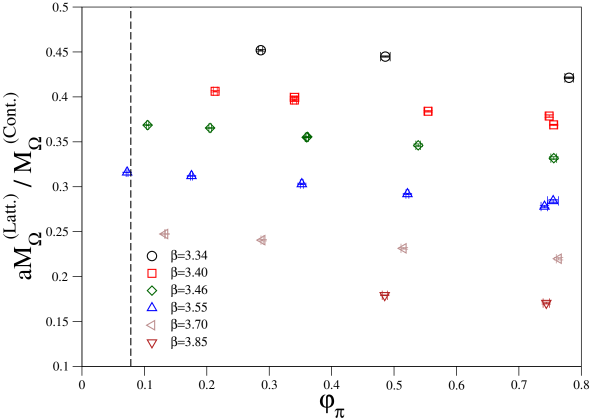
- We use correlated fits based on separated/binned measurements $\rightarrow$ meaningful χ^2/d.o.f and p-values
- We can test if resulting p-values are distributed as expected.
- We see no need to attach a systematic uncertainty to our mass determination.

Cumulative histogram of our fit p-values



Ensembles and overview of the data

- We use 2+1 flavor CLS ensembles on the $Tr(M) = \text{const.}$ trajectory
- 27 ensembles at 6 lattice spacing (one non-CLS)
- This will turn out to be an unfortunate choice



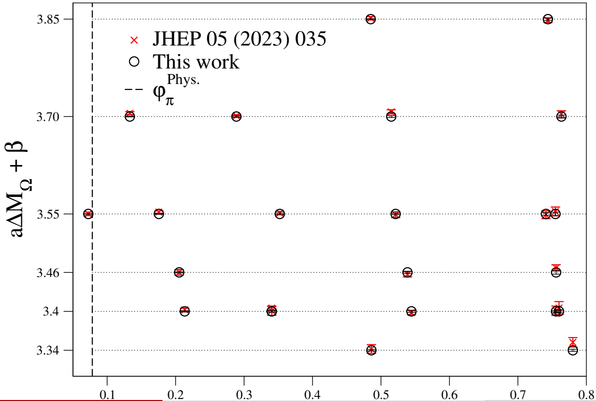
Some first observations

- As can be seen, our data shows significant slope in $\varphi_\pi = 8t_0 m_\pi^2$.
- Several pairs of ensembles used differ only by volume
  - $(U103, H101)$ and $(H200, N202)$ are such pairs at the $SU(3)_f$ symmetric point
  - $(H105, N101)$ and $(X451, N451)$ are at intermediate pion masses
  - We see the largest finite-volume effects for ensembles with $m_\pi = m_K = m_\eta$.
  - At intermediate pion masses, we have large $m_\pi L$ differences but observe tiny differences in the Ω baryon mass.

$\rightarrow$ Non-trivial finite-volume effects

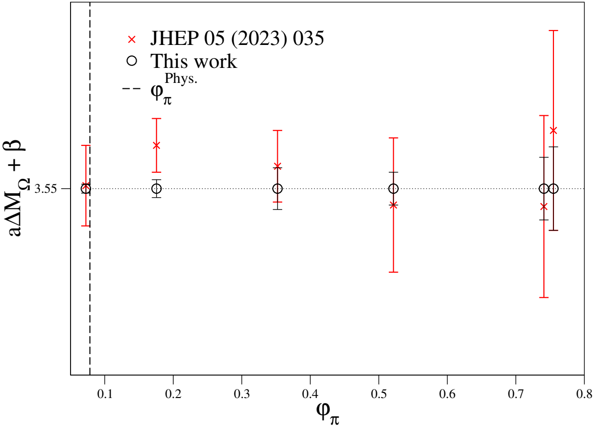
Comparing our masses to the RQCD results I

- Most of the results consistent within 1 standard deviation
- Largest tension on E300 with 2.3 σ
  (we would expect some deviations $> 1\sigma$)
- Data most precise in large volumes
  (low pion masses, finer lattice spacing)



Comparing our masses to the RQCD results II

- For small-volume lattices our data is only slightly more precise.
- For large volumes the wall sources are more efficient.
- On E250: Method significantly cheaper yet much more precise.



SU(3) chiral fits

- Simplified approach compared to

M.F.M. Lutz, Y. Heo, X.-Y. Guo, EPJ C **83**, 440 (2023);
M.F.M. Lutz, Y. Heo, R.J. Hudspith, PRD **110**, 094046 (2024)
+ many references therein

- There, $SU(3)\chi$PT fits are done for the whole octet and decuplet.
- Particular emphasis on on-shell masses in the one-loop contributions.
- Lead to improved convergence properties in earlier studies.
- Well-known Lüscher-type finite-box effects are included.
- Baryon masses obtained through solving coupled non-linear equations.

- Simplified approach uses lattice values in the loop expressions, focuses on the Ω baryon, and employs some other simplifications to the full setup.

SU(3) chiral fits

Rewrite in terms of dimensionless quantities ($\varphi_Q = \tilde{m}_Q^2 = 8t_0 m_Q^2$, etc.)

$$\frac{aM_\Omega^{\text{Latt.}}}{M_\Omega^{\text{Phys.}}} = a\Big\{1 - 4\,(\tilde{d}_0 + \tilde{d}_D/3)\Delta(\tilde{m}_K^2 + \tilde{m}_\pi^2/2) - \frac{8}{3}\,\tilde{d}_D\,\Delta[\tilde{m}_K^2 - \tilde{m}_\pi^2]$$
$$+ \frac{1}{\tilde{f}^2}\,\tilde{c}_\Omega^2\,\Delta[\tilde{J}_{K\Xi}(\tilde{M}_\Omega)/Z_\Omega] + \frac{1}{3\,\tilde{f}^2}\,\tilde{h}_\Omega^2\,\Delta[\tilde{J}_{\eta\Omega}(\tilde{M}_\Omega)/Z_\Omega] + \frac{1}{3\,\tilde{f}^2}\,\tilde{h}_\Omega^2\,\Delta[\tilde{J}_{K\Xi^*}(\tilde{M}_\Omega)/Z_\Omega]$$
$$- \frac{1}{\tilde{f}^2}\sum_{Q=\pi,K,\eta}\Big(\tilde{g}_{\Omega Q}^{(S)}\,\Delta[\tilde{m}_Q^2\,\tilde{I}_Q^{(0)}] + \tilde{g}_{\Omega Q}^{(V)}\,\Delta[\tilde{I}_Q^{(2)}]\Big)$$
$$+ \tilde{e}_\Omega^{(\pi)}\,\Delta[\tilde{m}_\pi^4] + \tilde{e}_\Omega^{(K)}\,\Delta[\tilde{m}_K^4] + \tilde{e}_\Omega^{(\eta)}\,\Delta[(\tilde{m}_K^2 - \tilde{m}_\pi^2)\,(4\,\tilde{m}_K^2 - \tilde{m}_\pi^2)/3]\Big\},$$

The terms are organized by order in the chiral expansion

- terms with d_0 and d_D contribute at next-to-leading-order (NLO)
- “bubble" terms C_A and H_A contribute at N^{2}LO
- “tadpole" terms $g_{\Omega(\pi/K/\eta)}^{(S/V)}$, $e_\Omega^{(\pi/K/\eta)}$ contribute at N^{3}LO

SU(3) chiral fits

- $\Delta[\cdots]$ indicates subtraction by corresponding physical-point expression (i.e. at physical quark masses, infinite volume, and in the continuum)
- Note that we are using the values for t_0 on each ensemble to make most quantities dimensionless.
  $\rightarrow$ To the order we work at, the small mass-dependence of t_0 can be absorbed into a redefinition of the LECs.
- Promoting the physical t_0 in the subtractions to a fit parameter provides our t_0 determination.
- There are 13 combinations of LECs and our current dataset for m_Ω is not sufficient to determine all.

More on the chiral fits

- We need N^3LO for a good fit.

LO	NLO	N^2LO	N^3LO $\left(\text{no } \tilde{g}_{\Omega\eta}^{(S/V)}\right)$	N^3LO $\left(\text{no } \tilde{g}_{\Omega(\pi/\eta)}^{(S/V)}\right)$
323	4.1	3.1	0.54	0.69

- Observed volume effects are dominated by $m_{K/\eta}L$.
- The chosen approach ($SU(3)\chi$PT) and the need for N^3LO terms limits our possibility for (sensible) fit variations.
- Note that the η contributions are estimated using the GMOR relation with $m_\eta^2 = (4m_K^2 - m_\pi^2)/3$.
- Along our trajectory, we cannot distinguish the finite-volume tadpole terms $\tilde{I}_\eta^{(n)}$ and $\tilde{I}_K^{(n)}$ and drop all tadpole and bubble terms with the η.

Outline

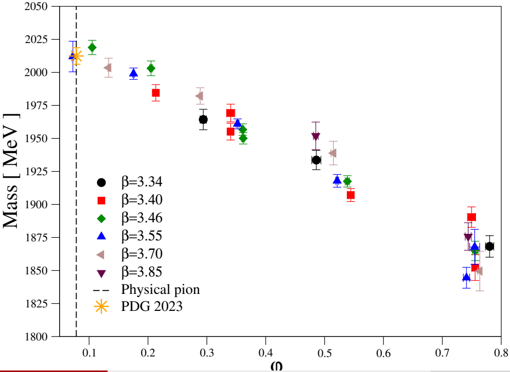
Chiral parameter and resulting lattice scales

- Some (largely unimportant) chiral parameters are fixed form the literature.
- Results for the lattice scales as well as (most-important) LECs are shown.
- The remaining LECs are set to zero.
- Resulting lattice spacings with relative uncertainties of $0.17\% \ldots 0.32\%$.

f [MeV]	92.4	μ [MeV]	770
M [MeV]	804.3	$M + \Delta$ [MeV]	1115.2
$a(\beta = 3.34)$	$0.09329(27)(5)$ fm	$a(\beta = 3.40)$	$0.08262(18)(4)$ fm
$a(\beta = 3.46)$	$0.07380(14)(4)$ fm	$a(\beta = 3.55)$	$0.06268(10)(3)$ fm
$a(\beta = 3.70)$	$0.04884(13)(3)$ fm	$a(\beta = 3.85)$	$0.03806(12)(2)$ fm
d_0	$-0.39(13)$ GeV^{-1}	d_D	$-0.51(15)$ GeV^{-1}
C_A	$1.7(4)$	H_A	$0.6(2)$
$g^{(S)}_{\Omega K}$	$-13(4)$ GeV^{-1}	$g^{(V)}_{\Omega K}$	$48(12)$ GeV^{-1}
$e^{(\eta)}_{\Omega}$	$-0.13(4)$ GeV^{-3}	$\sqrt{t_0}$	to be shown

Negative parity Ω ground state

- Comparison to the PDG 3-star $\Omega(2012)$ discovered by Belle; for the experimental state the width is plotted as the error bar.
- At intermediate pion masses we see a state well below $\Theta^* K$
- At light pion mass our results approach the $\Theta^* K$ threshold; Θ^* is a resonance decaying into $\Theta\pi$
- Small discretization and noticeable (pion-based) finite-volume effects.



Resulting determination of the flow-scale

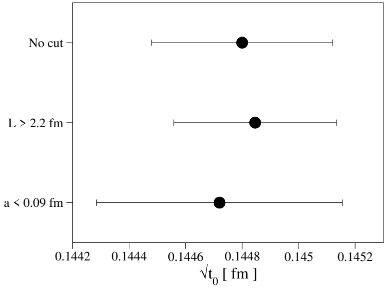
- Initially we fixed t_0 to the Regensburg value. As a final step, we allowed it to float

$$\sqrt{t_0} = 0.14480(32)_{\text{Stat.}}(6)_{\text{QED}}(7)_{\text{Cuts}}\ \text{fm}\,.$$

- QED effects (input M_Ω)
  - The Ω carries electric charge
  - This is expected to result in a mass-correction at or below the 0.2% level

    R. Horsley *et al.* J. Phys. G **46**, 115004 (2019).
  - We use the prediction $M_\Omega^{(3/2)^+} = 1.6695$ GeV (from the Regensburg paper) close to this bound for another fit.
  - The difference between the two results yields our QED uncertainty.
- Data cuts
  - Due to the need for an N^{3}LO description and the (exclusive) use of the $Tr(M)$ =const. trajectory, our options for sensible data cuts are limited.
- We are only aware of one well-motivated EFT-based approach describing low-energy QCD along our mass trajectory: $SU(3)\chi$PT.

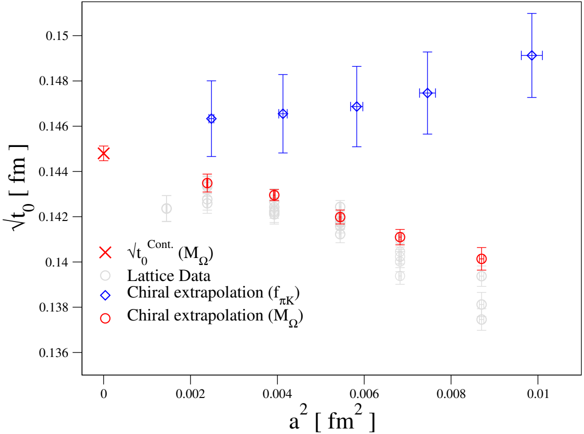
Additional data cuts performed



- Cutting more lattice spacings is not sensible with our data

Consistency-check: Cutoff dependence in $\sqrt{t_0}$

- We can perform a naive chiral-extrapolation of $\sqrt{t_0}$ on each ensemble (grey)
- Using our lattice spacings the following plot results (no continuum extrapolation performed)



Outline

Used LECs and priors

- Unfortunately, we currently must add priors for the LECs for some of the flattest directions

$$\tilde{d}_D = -0.07 \pm 0.03 \,,$$
$$\tilde{c}_\Omega = 0.9 \pm 0.9 \,,$$
$$\tilde{h}_\Omega = 0.4 \pm 0.2 \,.$$

- We also set to zero $\tilde{e}_\Omega^{(\pi)}$ and $\tilde{e}_\Omega^{(K)}$.
- Our final result also omits $\tilde{g}_{\Omega\pi}^{(S)}$ and $\tilde{g}_{\Omega\pi}^{(V)}$; this has negligible influence on the lattice spacings.
- Our final fit has 27 data points, 14 fit parameters and 3 priors.

Mass-dependent discretization effects: A non-trivial story

- Mass-independent discretization effects are absorbed into scales a.
- Exclusively using data along the CLS $Tr(M)$ =constant trajectory limits our control over the $SU(3)$ chiral LECs and over the leading mass-dependent discretization effects.
- This can be seen by the poor precision of the NLO LECs

$$\tilde{d}_0 = -0.054(18) \qquad \tilde{d}_D = -0.071(20)$$

- The following lattice-scale dependence has previously been considered

$$d_0 \to d_0 + a^2 \gamma_{d_0}$$
$$d_D \to d_D + a^2 \gamma_{d_D}$$

M.F.M. Lutz, Y. Heo, X.-Y. Guo, EPJ C **83**, 440 (2023);
M.F.M. Lutz, Y. Heo, R.J. Hudspith, PRD **110**, 094046 (2024).

- Contributions are much smaller than our uncertainties on these LECs.

Mass-dependent discretization effects: A non-trivial story

- Our conclusion: Effects on d_0 and d_D are small compared to uncertainties on these LECs;
  Resolving them needs data on other CLS trajectories.
- Additional fit to test that mass-independent discretization effects get absorbed as intended:
  - Fit with an explicit $O(a^2)$-correction term (replacing the 1 with $1 + C_a a^2$)
  - Prior of 0 ± 0.1 to stabilize the fit
  - Fit yielded a coefficient compatible with zero:

$$C_a = 0.00058(150)$$

  - This resulted in $\sqrt{t_0} = 0.14477(38)$ fm
- Additional fit with a mass-dependent discretization correction term to the NLO parameter $\tilde{d}_D$:
  - This resulted in the mild change $\sqrt{t_0} = 0.14482(18)$ fm

What other challenges exist?

- Pole masses and t_0 values in Eq. 17 are mostly taken from CLS papers.

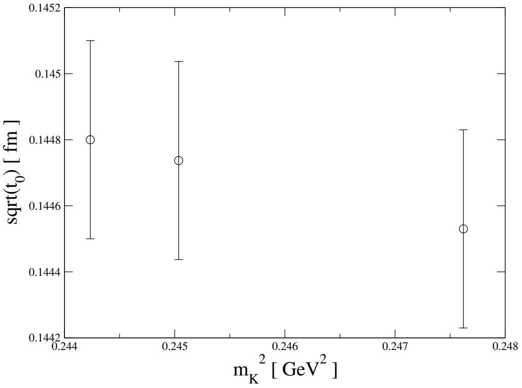
  G.S. Bali *et al.*, JHEP **05**, 035 (2023);
  M. Cè *et al.*, PRD **106**, 114502 (2022).

- We do not have the bootstrap samples for these.
- We draw a pseudo-resampling from random Gaussian noise distributions with widths corresponding to the total uncertainty. We treated them either as uncorrelated or fully correlated with a negligible effect on our t_0 uncertainty.
- To investigate this procedure, we calculate the actual correlations between aM_Ω, φ_π and φ_K on a newly generated ensemble.

	aM_Ω	φ_π	φ_K
aM_Ω	1.0000	0.0503	0.1583
φ_π		1.0000	0.6122
φ_K			1.0000

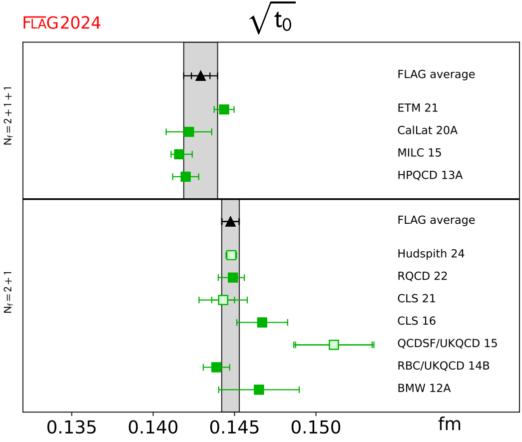
Scheme for iso-symmetric QCD

- In our preprint we use $m_\pi = 134.8(3)$ MeV and $m_K = 494.2(3)$ MeV.
- (Preliminary) plot shows our result for the definitions from FLAG2018 (left), FLAG(2021)(right) and the consensus from Monday (middle)



Comparison provided by FLAG

- In our view: All current calculations have clear limitations
- No tension among the recent 2+1 flavor results, but we are surely not at a satisfactory level yet



Outline

Conclusions

- Chiral behavior of the Omega baryon masses can be surprisingly-well described by the used $SU(3)$ formalism
- Finite-volume effects are often modeled too naively.
- Reliable determinations of $SU(3)$ LECs will require more ensembles and more observables. Interesting steps in

  M.F.M. Lutz, Y. Heo, X.-Y. Guo, EPJ C **83**, 440 (2023);
  M.F.M. Lutz, Y. Heo, R.J. Hudspith, PRD **110**, 094046 (2024).
- People should stop using point-sources when better alternatives exist (and they are not needed).
- The (experimentally not-known) quantum numbers of the $\Omega(2012)$ are likely $I(J^P) = 0(\frac{3}{2}^-)$.

In an ideal world: better data

- Use all three CLS trajectories
- Calculate all pseudoscalar mesons and all baryons occurring in χPT description
- Use full data covariance (bootstrap or pseudo-resampling)
- Prolong several HMC chains

- We currently pursue other (scientific) hobbies.

Backup slides

Fit ranges and p values

Ensemble	$(t_{\min}, t_{\max})/a$	p	Ensemble	$(t_{\min}, t_{\max})/a$	p
A653	$(3, 17)$	0.32	H200	$(4, 11)$	0.50
A654	$(3, 12)$	0.52	N202	$(5, 16)$	0.61
GSI_B650	$(4, 23)$	0.14	N203	$(8, 22)$	0.13
U103	$(4, 13)$	0.71	N200	$(10, 21)$	0.76
H101	$(4, 15)$	0.91	D200	$(3, 23)$	0.71
H102	$(3, 23)$	0.62	E250	$(4, 21)$	0.22
H105	$(3, 17)$	0.73	N300	$(4, 12)$	0.40
N101	$(5, 20)$	0.48	N302	$(12, 25)$	0.76
C101	$(6, 21)$	0.78	J303	$(15, 32)$	0.66
B450	$(4, 19)$	0.52	E300	$(15, 31)$	0.38
S400	$(4, 17)$	0.81	J500	$(24, 36)$	0.38
X451	$(3, 16)$	0.46	J501	$(18, 39)$	0.42
N451	$(5, 17)$	0.91			
D450	$(7, 25)$	0.13			
D452	$(5, 25)$	0.56			

Comparison to other CLS results