

# Scale Setting in Nf=2+1 QCD with Wilson fermions

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RQCD Collaboration: arXiv:2211.03744



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# Overview

Determine the gradient flow scale at the physical point  $t_{0,ph}$  using  $m_{\Xi}$ .

- ★ Introductory remarks on setting the scale in lattice simulations.
- ★ Gradient flow scale.
- ★ CLS ensembles.
- ★ Continuum, quark mass and finite volume fits to the baryon octet masses (also consider decuplet baryons). Fit forms for quark mass dependence. Estimation of systematics.
- ★ Extraction of the baryon sigma terms  $\sigma_{\pi B}$  and  $\sigma_{sB}$  using the Feynman-Hellmann theorem.
- ★ Determination of  $m_\ell$ ,  $m_s$ ,  $m_u - m_d$ .
- ★ Summary and outlook

# Setting the scale

**Input** to lattice simulations:  $g$ ,  $m_q$ .

**Output:** dimensionless quantities  $X^{latt} = (a^n X^{phys})$  for  $X$  with dimension  $n$ .

**Need to fix  $m_q$  and  $a$  using input from Nature.**

Predictions for some quantities are reaching sub-percent precision:

$m_s$  (0.6%),  $m_c$  (0.4%),  $m_b$  (0.3%),  
 $f_\pi$  (0.6%),  $f_K$  (0.2%),  $f_D$  (0.3%),  $f_{D_s}$  (0.2%)

**Precision determinations of the scale are needed.**

Dimensionless combinations less sensitive to scale setting: ratios ( $m_c/m_s$ ,  $f_\pi/f_K$ ), form factors ( $f_+^{K\pi}(0)$ ) ...

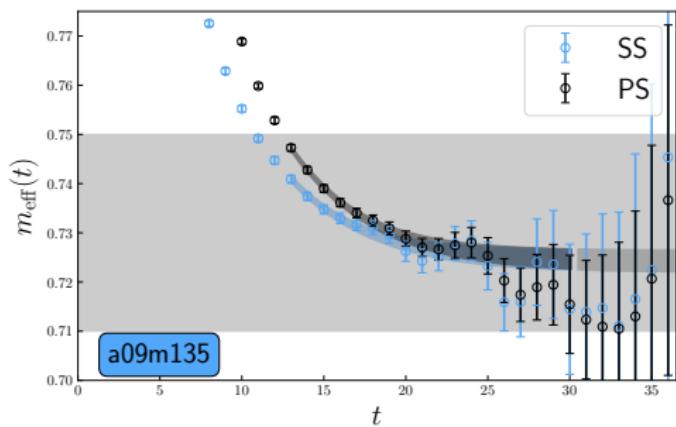
However,  $a_\mu^{\text{HVP}}$  to better than 1% requires scale to a few per mille accuracy (through  $am_\mu$ ) [Aoyama et al., 2006.04822].

# Setting the scale

Choice for expt. input should be well defined and precisely determined in expt. and also on the lattice.

For  $m_{u,d,s}$ :  $M_\pi$  and  $M_K$ , sensitive to quark mass:  $M_{PS}^2 \sim B_0(m_{q1} + m_{q2})$ .

**Not so many choices for setting the scale**  $a = (X^{phys}/X^{latt})^{-n}$  (at the physical point): need a stable particle (under strong decay).



**Baryon masses,  $m_N$ ,  $m_\Xi$ ,  $m_\Omega$**

Signal to noise problem

e.g. [CalLat,2011.12166],  $m_\Omega$

Gray band, prior for the ground state.

## Setting the scale

**Leptonic decay constants:**  $f_\pi$ , and  $f_K$ .

Experimental decay rates give  $|V_{ud}|f_\pi$  and  $|V_{us}|f_K$  plus QED.

**Heavy-light or quarkonium spectrum below decay thresholds:** problem of discretisation effects.

**If the simulations reproduce nature then it does not matter which quantity is used to set the scale.**

For some quantities lattice precision is such that deviations from Nature may be seen for ( $m_u = m_d$ , electrically neutral) iso-QCD simulations.

$m_u \neq m_d$  and QED effects are  $O(1\%)$ .

Some QCD+QED simulations with are being performed. Different approaches,  $\text{QED}_L$  [[Hayakawa and Uno,0804.2044](#)],  $\text{QED}_M$  [[Endres et al.,1507.08916](#)],  $\text{QED}_{C^*}$  [[Lucini et al.,1509.01636](#)], . . .

Dynamical  $N_f = 1 + 1 + 1 + 1$  QCD+QED<sub>L</sub> [[BMWc,1406.4088](#)]. Most simulations include QED in the electro-quenched approximation. Alternatively, compute isospin breaking effects perturbatively, e.g. [[RM123,1303.4896](#)].

Subtracting isospin-breaking effects is ambiguous. Choose a prescription.

## Setting the scale

**Intermediate scales:** cannot be directly related to expt..

Aim: dependence on  $m_q$  is mild and very precisely computed. Defined in terms of the gauge fields.

Sommer scale  $r_0$  defined through the static quark force [Sommer,hep-lat/9310022]

$$r_0^2 F(r) = c = 1.65$$

A related scale:  $r_1$  with  $c = 1.0$  [Bernard et al.,hep-lat/0002028].

Also in use: **gradient flow scales  $t_0$  and  $w_0$ .**

**Consider combinations with other observables,**

e.g.  $(\sqrt{t_0} M_\Xi)^{latt} = (\sqrt{t_0} M_\Xi)^{phys}$ .

# Gradient flow scale $t_0$

**Gradient flow equation** [Lüscher,1006.4518]:

$$a^2 \frac{d}{dt} V_t(x, \mu) = -g_0^2 \cdot \partial_{x,\mu} S_G(V_t) \cdot V_t(x, \mu) \quad V_t(x, \mu)|_{t=0} = U(x, \mu)$$

where  $S_G$  is a lattice gauge action.

**Flow time  $t$  has dimensions  $a^2$ .**

Useful properties: local gauge-invariant combinations of the smoothed fields do not require renormalization at  $t > 0$  and their correlation functions have no short-distance singularities.

**Define the gradient flow time  $t_0$  in terms of the**

**average action density  $E(t)$**

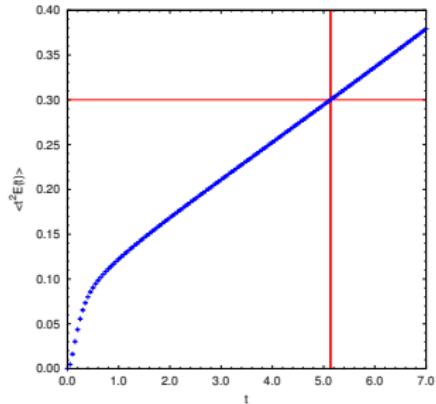
$$t^2 E(t)|_{t=t_0} = c = 0.3, \quad E(t) = \frac{1}{V_4} \int_{V_4} d^4x \frac{1}{4} G_{\mu\nu}^a(x, t) G_{\mu\nu}^a(x, t)$$

where  $G_{\mu\nu}^a(x, t)$  is the field strength tensor evaluated using  $V_t$ .

# Gradient flow scale $t_0$

Value of  $c = 0.3$  chosen so that errors are small and there is a linear dependence on  $t$ .

Discretisation effects:  $S_G$ ,  $E(t)$ , ensemble action, . . .

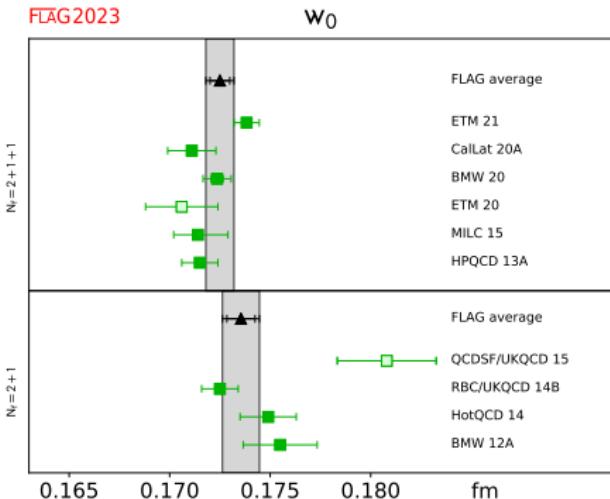
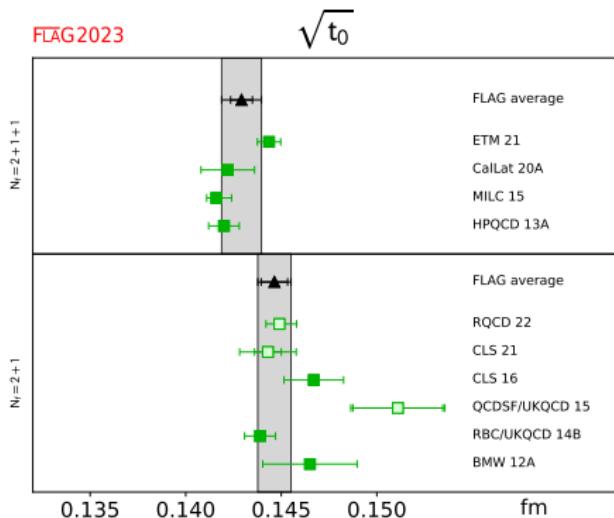


Different choices: e.g. Zeuthen flow, [Ramos and Sint, 1508.05552], Symanzik flow [Fodor et al., 1203.4469], [MILC, 1311.1474]. Also [Cheng et al., 1404.0984],

This work: Wilson flow and clover leaf definition of  $E(t)$ .

Alternative scale  $w_0$ , where  $w_0^2 \partial_t (t^2 \langle E(t) \rangle)_{t=w_0^2} = 0.3$  [BMWc, 1203.4469]

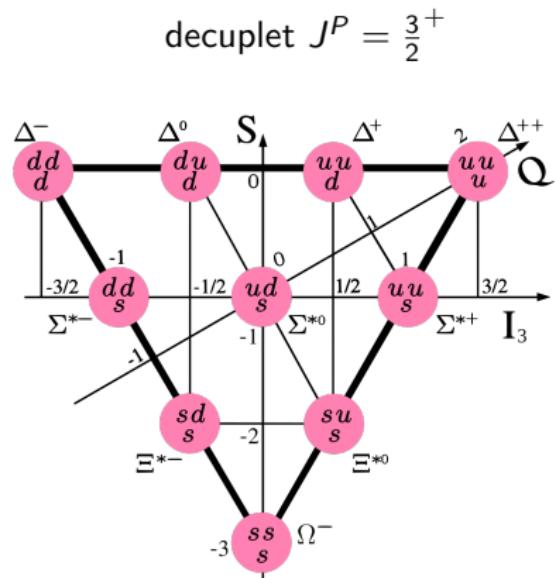
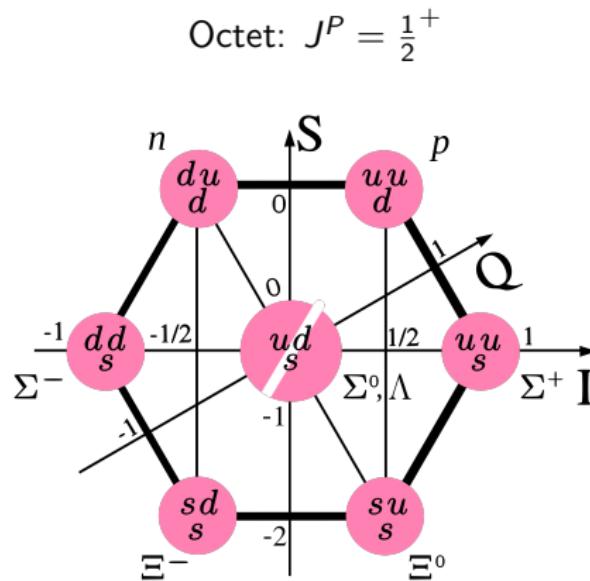
# $t_0$ and $w_0$



FLAG average  $N_f = 2 + 1$ :  $\sqrt{t_0} = 0.14464(87)$  fm,  $w_0 = 0.17355(92)$  fm.

ETM 21 ( $f_\pi$ ), CalLat 20 ( $m_\Omega$ ), MILC 15 ( $f_\pi, f_K$ ), HPQCD 13 ( $f_\pi$ ), CLS 16, CLS 21 ( $f_\pi, f_K$ ), QCDSF/UKQCD 15 ( $m_O, m_V$ ), RBC/UKQCD 14 ( $m_\Omega$ ), BMWc 12 ( $m_\Omega$ ).

# Baryon spectrum



Simulating QCD (isospin-symmetric, electrically neutral):  $N$ ,  $\Sigma$ ,  $\Lambda$ ,  $\Xi$  and  $\Delta$ ,  $\Sigma^*$ ,  $\Xi^*$ ,  $\Omega$ .

**Unstable under strong decay:**  $\Delta \rightarrow N\pi$ ,  $\Sigma^* \rightarrow \Lambda\pi$ ,  $\Sigma\pi$  and  $\Xi^* \rightarrow \Xi\pi$ .

# Correcting expt. masses for electrical and quark mass isospin breaking effects

QCD values for  $M_\pi$  and  $M_K$  from [FLAG 16,1607.00299].

mass	value/MeV	Expt./MeV	mass	value/MeV	Expt./MeV
$M_\pi$	<b>134.8(3)</b>	134.98 ( $\pi^0$ )			
$M_K$	<b>494.2(3)</b>	497.61 ( $K^0$ )			
$m_N$	937.53(6)	938.27 ( $p$ )	$m_\Delta$	1231(60)	1231(56) ( $\Delta^0$ )
$m_\Lambda$	1115.68(1)	1115.68	$m_{\Sigma^*}$	1383(20)	1383(18) ( $\Sigma^{*+}$ )
$m_\Sigma$	1190.67(12)	1192.64 ( $\Sigma^0$ )	$m_{\Xi^*}$	1532(5)	1532(5) ( $\Xi^{*0}$ )
$m_\Xi$	<b>1316.9(3)</b>	1314.86 ( $\Xi^0$ )	$m_\Omega$	1669.5(3.0)	1672.45(29)

$$\overline{M}_\pi = \hat{M}_{\pi^+}, \quad \overline{M}_K = \sqrt{\frac{1}{2}(\hat{M}_{K^+}^2 + \hat{M}_{K^0}^2)}.$$

cf. [FLAG 21,2111.09849],  $\overline{M}_\pi = M_{\pi^0}$ ,  $\overline{M}_K = M_{K^0}$ .

For the unstable decuplet baryons, the Breit-Wigner mass is given with an error of  $\Gamma/2$  (with rounding).

# Correcting expt. masses for electrical and quark mass isospin breaking effects

**Assume**  $\Delta m_B = \Delta Q^2 \delta m^{\text{QED}} - \Delta I_3 \delta m^{\text{QCD}}$

Consistent with convention that neutral particles do not receive QED corrections.

Also with  $\Delta m_N - \Delta m_\Sigma - \Delta m_{\Xi} = 0$ , Coleman-Glashow theorem (verified to within 0.13 MeV by [\[BMWc,1406.4088\]](#)), while expt gives 0.06(23) MeV.

**Wrong**, e.g. single  $\delta m^{\text{QCD}}$  means (CVC relation) all  $g_{S,B}$  are equal.

$$\Delta m_N = m_p - m_n \approx -\delta m^{\text{QCD}} + \delta m^{\text{QED}}, \quad \Delta m_\Sigma = m_{\Sigma^+} - m_{\Sigma^-} \approx -2\delta m^{\text{QCD}},$$

$$\Delta m_{\Xi} = m_{\Xi^0} - m_{\Xi^-} \approx -\delta m^{\text{QCD}} - \delta m^{\text{QED}}, \quad m_{\Xi} = \frac{1}{2} (m_{\Xi^0} + m_{\Xi^-} - \delta m^{\text{QED}})$$

$\delta m^{\text{QCD}} \approx 4$  MeV and  $\delta m^{\text{QED}} \approx 2.7$  MeV. Assume same  $\delta m^{\text{QED}}$  for  $m_\Omega$ .

**Note:** 1 MeV is a 0.75 % effect on  $m_{\Xi}$ .

## CLS ensembles

Coordinated Lattice Simulations (CLS): Berlin, CERN, Mainz, UA Madrid, Milano Bicocca, Münster, Odense, Regensburg, Rome I and II, Wuppertal, DESY-Zeuthen.

$N_f = 2 + 1$  flavours of non-perturbatively  $O(a)$  improved Wilson fermions on tree level Symanzik improved glue. Leading  $O(a^2)$  errors in hadron masses.

★ **High statistics:** typically 6000-8000 MDUs, 1000-2000 configurations.

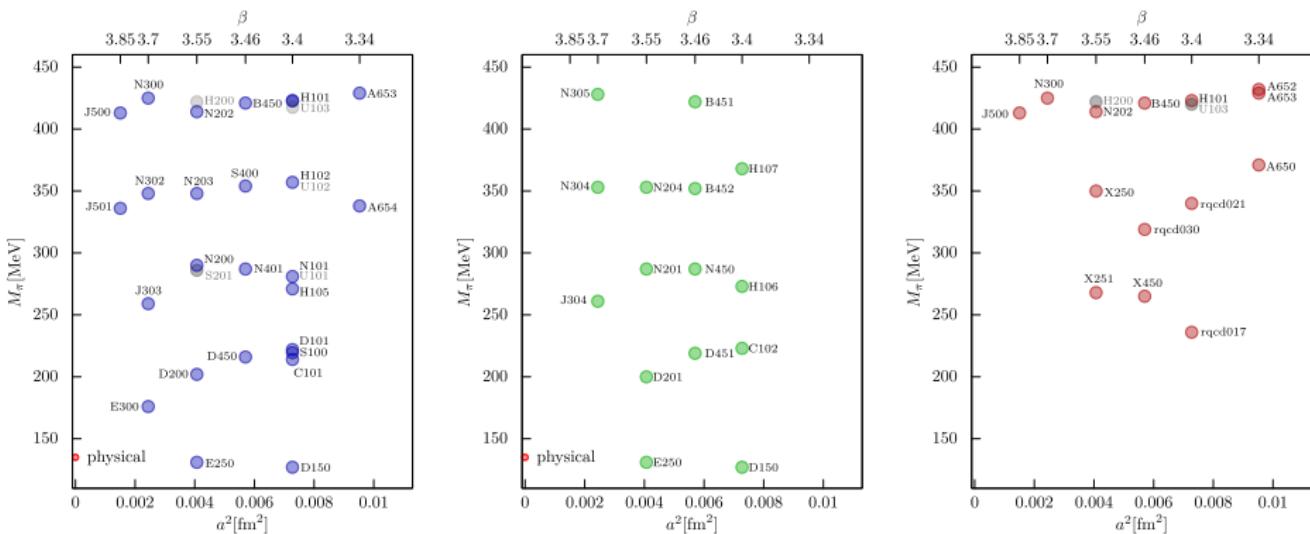
**Aim to control all main sources of systematics** ( $a$ ,  $m_q$  and  $V$ ).

★ **Discretisation:** Six lattice spacings:  $a = 0.1 - 0.04$  fm.

★ **Finite volume:**  $Lm_\pi \gtrsim 4$  with additional smaller volumes.

★ **Quark mass:**  $m_\pi = 410$  MeV down to  $m_\pi^{phys}$ .

# CLS ensembles: $m_\pi$ vs $a^2$



$$2m_\ell + m_s = \text{const.}$$

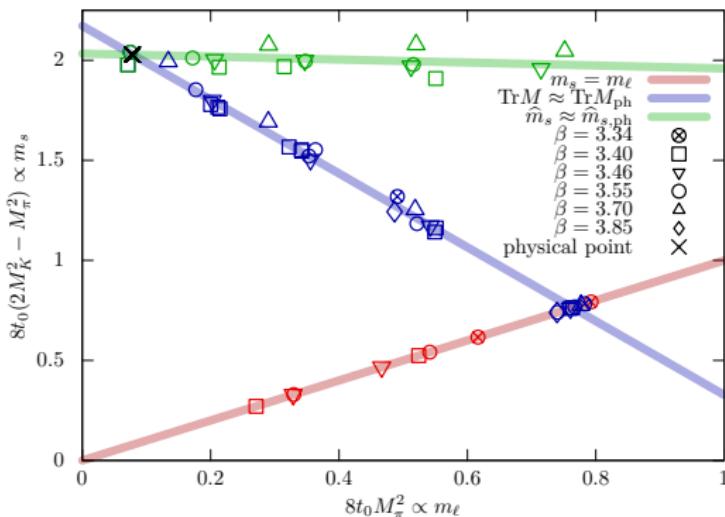
$$m_s = \text{const.}$$

$$m_\ell = m_s$$

$a < 0.06$  fm open-boundary conditions in time.

$a > 0.06$  fm mixture of ensembles with periodic and open-boundary conditions.

# CLS ensembles: $m_\ell$ - $m_s$ plane



**Three trajectories:** good control over the quark mass dependence. Can correct for mis-tuning of the trajectories. Observables sensitive to  $m_s$  are tightly constrained.

$2m_\ell + m_s = \text{const.}$ : investigate SU(3) flavour breaking (flavour average quantities roughly constant), approach to physical point involves  $m_\pi \downarrow$  and  $m_K \uparrow$ .

$m_\ell = m_s$ : important for determination of SU(3) ChPT low energy constants (and renormalisation factors).

$t_{0,ph}$ ,  $t_0^*$  and  $t_{0,ch}$

Determine  $t_0$  at three points in the quark mass plane.

- ▶ Physical point:  $t_{0,ph}$  using  $(\sqrt{t_0} m_\Xi)^{latt} = \sqrt{t_{0,ph}} m_\Xi^{ph}$ .
- ▶ Chiral limit:  $t_{0,ch}$  at  $m_\ell = m_s = 0$ , needed for the extraction of LECs.
- ▶ Reference point:  $t_0^*$  [Bruno et al., 1608.08900] Defined at the point along the symmetric line  $m_s = m_\ell$  where

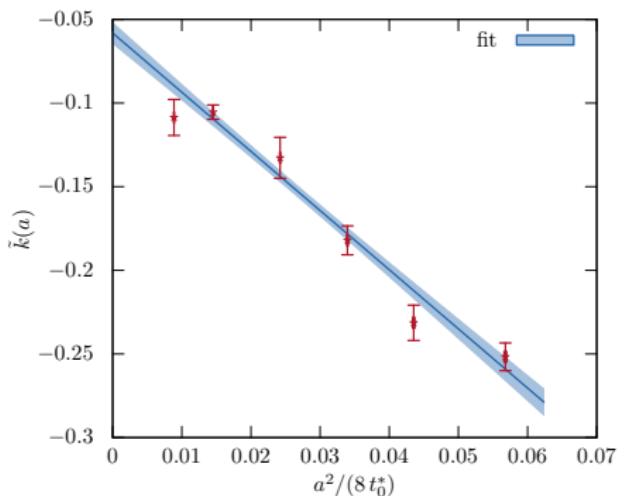
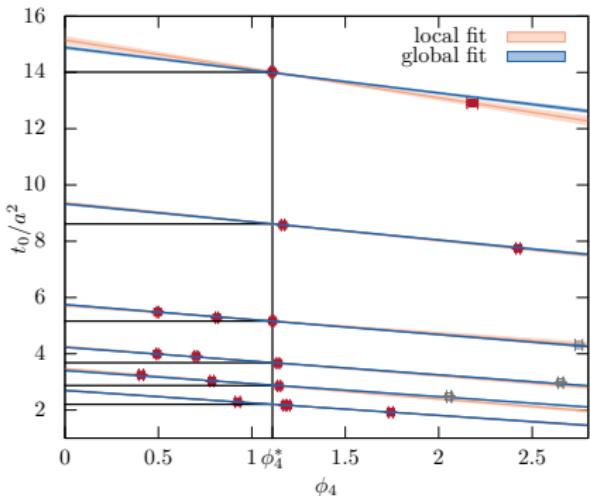
$$\phi_4^* = 8t_0^* \left( M_K^2 + \frac{M_\pi^2}{2} \right) = 12t_0^* M_\pi^2 = 1.110.$$

**Only requires an interpolation.** Useful for representing relative change in the lattice spacing.

$t_0$  depends (mildly) on the quark mass. Known to NNLO SU(3) ChPT  
 [Bär and Golterman, 1312.4999].

Only able to resolve NLO behaviour.

$$t_0(\bar{M}, \delta M) = t_{0,\text{ch}} \left( 1 + k_1 \frac{3\bar{M}^2}{(4\pi F_0)^2} \right) \approx t_{0,\text{ch}} \left( 1 + \tilde{k}_1 8 t_0 \bar{M}^2 \right),$$



From a global fit to  $t_0$ : in the continuum,

$$\tilde{k}_1 = -0.0466(62), \quad t_0^* = 0.9655(46) t_{0,\text{ch}}, \quad t_0^* = 0.99947(7) t_{0,\text{ph}}.$$

# Extracting meson and baryon masses

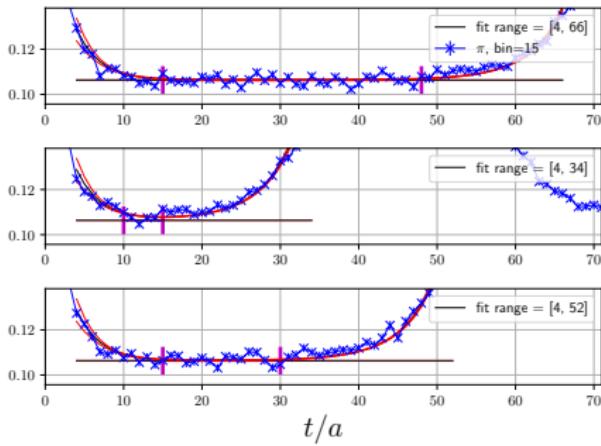
Multiple measurements of the two-point functions on every configuration.

Smeared sources optimized to reduce excited state contamination.

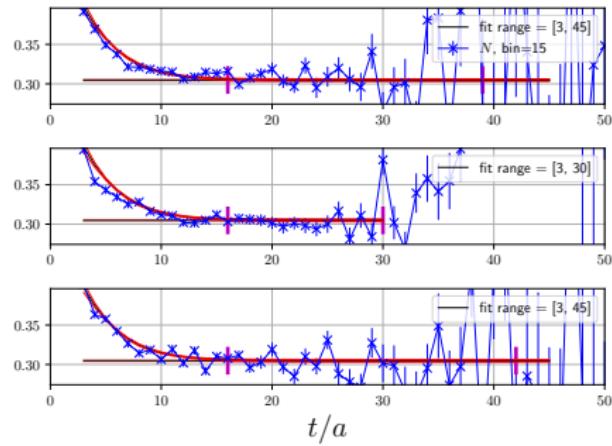
For ensembles with open boundary conditions in time, hadron masses can only be extracted in the bulk.

N300  $m_s = m_\ell$ ,  $a = 0.05$  fm,  $M_\pi = 425$  MeV

Pion



Nucleon



Autocorrelations taken into account: errors estimated via a binsize analysis.

# Extrapolation of baryon multiplets

Determine  $t_{0,ph}$  using  $m_{\Xi}$

Perform a continuum, quark mass and finite volume extrapolation of the baryon octet (and decuplet) masses.

$$\overline{M}^2 = \frac{1}{3}(2M_K^2 + M_\pi^2) \propto \overline{m} = \frac{1}{3}(2m_\ell + m_s), \quad \delta M^2 = 2(M_K^2 - M_\pi^2) \propto \delta m = m_s - m_\ell$$

Rescale all masses by  $\sqrt{8t_0}$ :  $B \in \{N, \Lambda, \Sigma, \Xi, \Delta, \Sigma^*, \Xi^*, \Omega\}$

$$m_B = \sqrt{8t_0} m_B, \quad \overline{M} = \sqrt{8t_0} \overline{M}, \quad \delta \overline{M} = \sqrt{8t_0} \delta M, \quad a = \frac{a}{\sqrt{8t_0^*}},$$

# Extrapolation of baryon multiplets

## Extrapolation performed using the fit form

$$m_B(M_\pi, M_K, L, a) = [m_B(M_\pi, M_K, \infty, 0) + \delta m_B^{FV}(M_\pi, M_K, L)] \\ \times [1 + a^2 (c + \bar{c} \bar{M}^2 + \delta c_B \delta M^2)].$$

Simultaneous fit to baryon multiplets with **all correlations taken into account.**

**Discretisation coefficients:** 6 parameters for the octet and decuplets baryons separately.

[Husung et al., 1912.08498]  $a^2 \sum_i [\bar{g}(1/a)]^{\hat{r}_i} c_i$ .

[Husung et al., 2111.02347]: dominant contribution expected to be  $g^{1.52} a^2$ ,  
This work:  $g^2$  varies by a factor of 1.15, while  $a$  changes by a factor of 2.5.

Natural choice for  $m_B(M_\pi, M_K, \infty, 0)$  is to use SU(3) baryon ChPT  
(and in a finite volume for  $\delta m_B^{FV}$ ).

# NNLO BChPT

BChPT:  $O(p^3)$  baryon ChPT with EOMS regularisation [Ellis et al.,nucl-th/9904017]

$$m_O(M_\pi, M_K, \infty, 0) = m_0 + \bar{b} \overline{M}^2 + \delta b_O \delta M^2 + \frac{m_0^3}{(4\pi F_0)^2} \left[ g_{O,\pi} f_O \left( \frac{M_\pi}{m_0} \right) + g_{O,K} f_O \left( \frac{M_K}{m_0} \right) + g_{O,\eta_8} f_O \left( \frac{M_{\eta_8}}{m_0} \right) \right],$$

where

$$f_O(x) = -2x^3 \left[ \sqrt{1 - \frac{x^2}{4}} \arccos \left( \frac{x}{2} \right) + \frac{x}{2} \ln(x) \right].$$

and  $M_{\eta_8}^2 = (4M_K^2 - M_\pi^2)/3$ .

**Depends on 6 low energy constants (LECs):  $m_0$ ,**

$\bar{b}$  and  $\delta b_O$  (depending only on  $b_0$ ,  $b_F$  and  $b_D$  due to SU(3) constraints),

$g_{O,\pi,K,\eta_8}$  (depending only on  $F$  and  $D$ , also appearing in ChPT expressions for  $g_A^O$ ), appear in combination with  $F_0$ .

## NNLO BChPT

**Heavy limit (HBChPT)** [Jenkins and Manohar, Phys. Lett. B 255 (1991) 558.]:  
 $f(x) = -x^3 + \mathcal{O}(x^4)$ .

Analogous expression for the decuplet baryons ([Martin Camalich et al., 1003.1929]) involves 4 LECs.

**BChPT in a finite volume (FV)** gives the finite volume dependence of  $m_B$  (see e.g. [Ren et al., 1209.3641]). **No additional LECs!**

## Joint baryon octet and decuplet fits: small scale expansion

If  $M_\pi$  not much smaller than the gap  $m_D - m_O$  then at NNLO in BChPT need to consider both baryon loops in addition to meson loops.

**Small scale expansion (SSE)**, see e.g. [Martin Camalich et al., 1003.1929]

$$m_B \mapsto m_B + \mathcal{C}^2 \frac{\delta^3}{(4\pi F_0)^2} \left[ \xi_{B,\pi} h_B \left( \frac{M_\pi}{\delta} \right) + \xi_{B,K} h_B \left( \frac{M_K}{\delta} \right) + \xi_{B,\eta_8} h_B \left( \frac{M_{\eta_8}}{\delta} \right) \right],$$

for  $B \in \{N, \Lambda, \Sigma, \Xi, \Delta, \Sigma^*, \Xi^*, \Omega\}$  and

$$h_O(x) = - \left( 2 - 3x^2 \right) \ln \left( \frac{x}{2} \right) - \frac{1}{2} x^2 - 2w(x),$$

$$h_D(x) = \left( 2 - 3x^2 \right) \ln \left( \frac{x}{2} \right) + \frac{1}{2} x^2 - 2w(-x),$$

$$w(x) = \begin{cases} \left( x^2 - 1 \right)^{3/2} \arccos \left( x^{-1} \right) & , \quad |x| \geq 1 \\ \left( 1 - x^2 \right)^{3/2} \ln \left( \left| x^{-1} + \sqrt{x^{-2} - 1} \right| \right) & , \quad |x| < 1 \end{cases}.$$

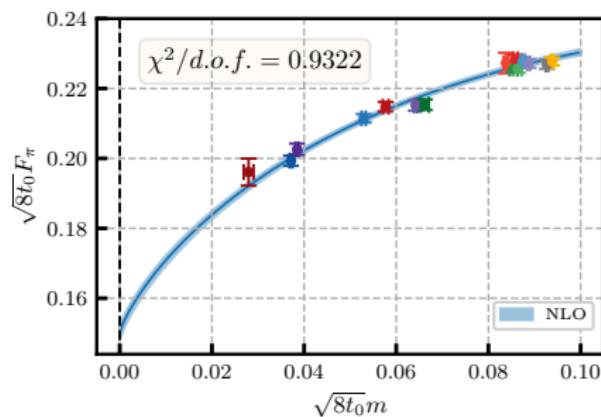
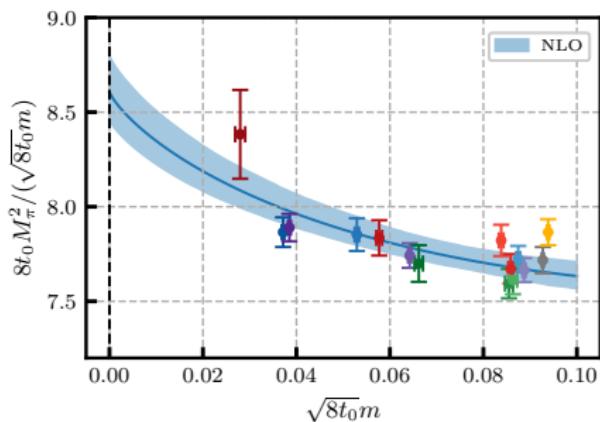
$\xi_{B,\pi,K,\eta_8}$  are known group theoretical factors.

**Two new LECs:**  $\mathcal{C}$  and  $\delta = m_{D0} - m_0$ .

# Future: simultaneous fit to several observables

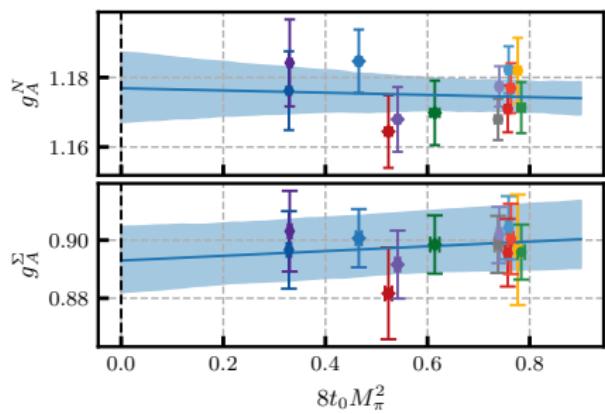
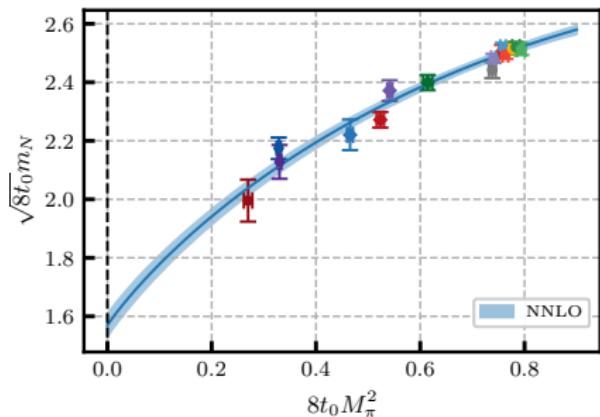
[RQCD,2201.05591]: CLS  $N_f = 3$  ( $m_s = m_\ell$ ) ensembles,  $a = 0.04 - 0.1$  fm,  $M_\pi = 430 - 240$  MeV.

Fit  $M_\pi^2$  and  $F_\pi$  as a function of the renormalised quark mass  $m = m_\ell$  to extract the ChPT low energy constants  $B_0$  and  $F_0$ .



## Future: simultaneous fit to several observables

Fit  $m_N$  and  $g_A^{N,\Sigma}$  as a function of  $M_\pi^2$  to extract the ChPT low energy constants  $m_0$ ,  $F$  and  $D$ .



## Taylor expansion a la Gell-Mann-Okubo (GMO)

Not clear how well SU(3) NNLO BChPT or HBChPT expressions describe the baryon masses for our range of  $M_\pi$  and  $M_K$  (also at the physical point!).

Also consider a **Taylor expansion** about **the symmetric point** ( $m_s = m_\ell$ )  
[QCDSF,1102.5300].

$$m_O(M_\pi, M_K, \infty, 0) = m_0 + \bar{b}, \overline{M}^2 + \delta b_O \delta M^2 + \overline{d} \overline{M}^4 + \delta d_O \delta M^2 \overline{M}^2 + \delta e_O \delta M^4$$

Equivalent to form obtained expanding about  $\overline{M}^{*,2}$  at the symmetric point, with different coefficients.

At NLO the expression (and LECs) is the same as in BChPT (1+3 parameters).

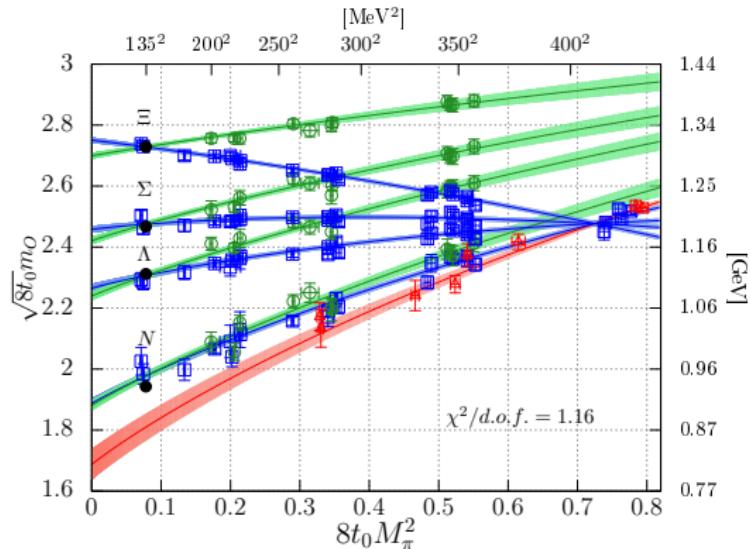
SU(3) constraints on  $\delta d_O$  mean NNLO terms introduce  $1(\bar{d}) + 2(\delta d_O) + 4(\delta e_O)$  parameters.

**Less constrained than BChPT fit** (11 compared to 6 parameters).

Expression for the decuplet baryons involves 8 coefficients.

# NNLO BChPT fit to the baryon octet: $m_q$ dependence

FV terms included in the fit. 12 parameters to fit the 4 octet baryon masses.

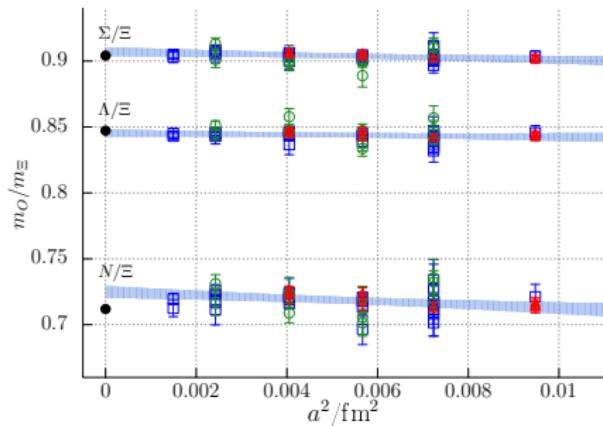
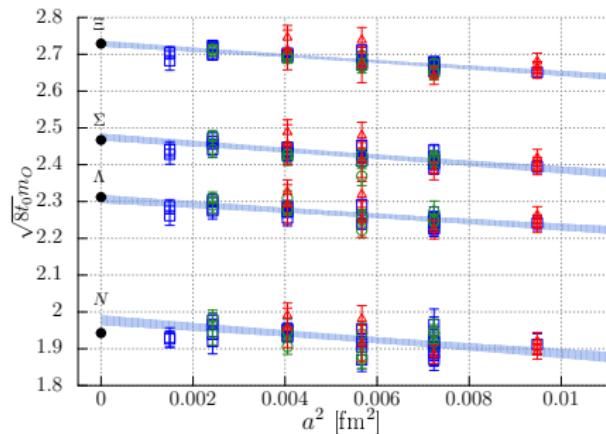


The data points are shifted to correct for finite  $a$ , finite  $V$  and mis-tuning of the trajectory.

$t_{0,ph}$  determined via an iterative procedure with corrected expt. values for  $M_{\pi,ph}$ ,  $M_{K,ph}$  and  $m_{\Xi,ph}$ .  $\sqrt{8t_{0,ph}} \sim 0.409$  fm.

# NNLO BChPT fit to the baryon octet: discretisation effects

The data points are shifted to the physical point ( $M_{\pi,ph}$ ,  $M_{K,ph}$ ).

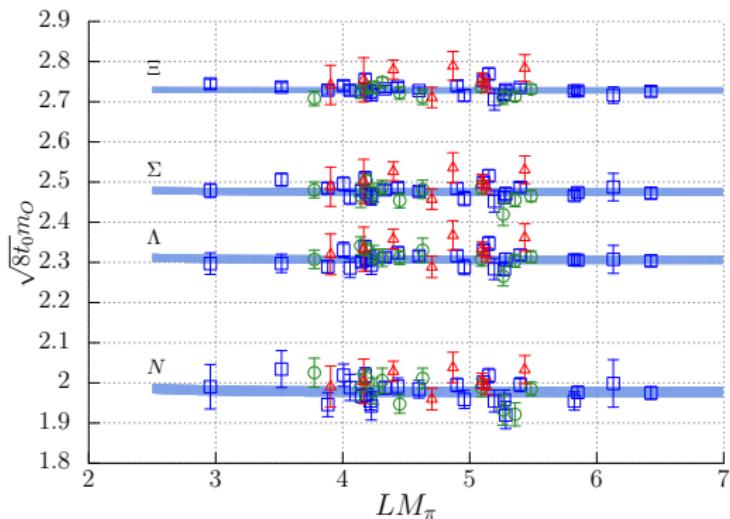


Discretisation effects are mild:  $1 + a^2 (c + \bar{c} \bar{\mathbb{M}}^2 + \delta c_O \delta \mathbb{M}^2)$ . Around 3% from  $a = 0.1$  fm to  $a = 0$ .

$a^2 \delta c_O \delta \mathbb{M}^2$  terms are small. Higher order terms not significant.

# NNLO BChPT fit to the baryon octet: finite volume effects

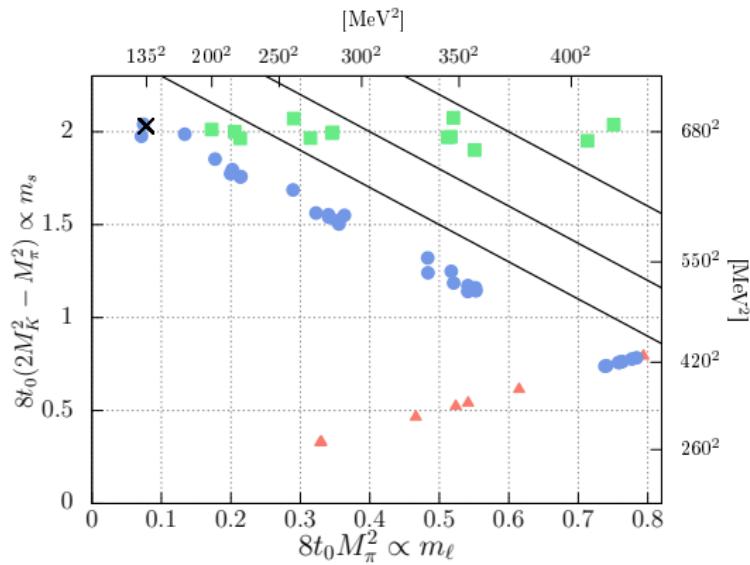
The data points are shifted to the physical point in the continuum limit.



Finite volume effects are small, however, including FV terms in the fit (which involves no extra coefficients) improves the fit quality.

## Assess the systematics of the fits: cuts on the data

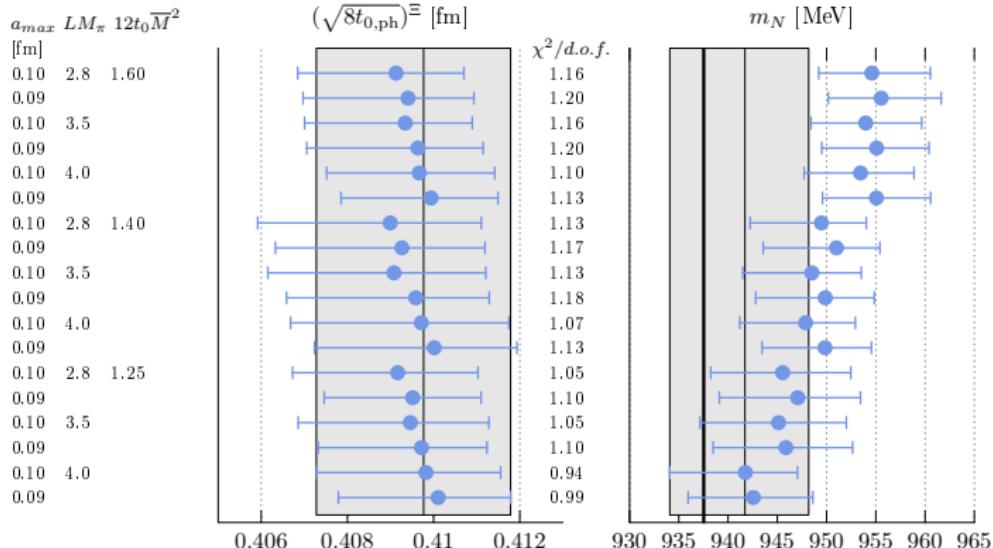
$m_q$  dependence: (SU(3) BChPT) include  $\overline{M}^2 < (498)^2$  [MeV $^2$ ] and impose further cuts  $\overline{M}^2 < (466)^2$  [MeV $^2$ ],  $\overline{M}^2 < (440)^2$  [MeV $^2$ ].



Finite  $V$ : start with  $L > 2.3$  fm and impose cuts  $LM_\pi > 3.5$  and  $LM_\pi > 4.0$ .

Finite  $a$ : only consider cut  $a < 0.09$  fm.

# Variation with cuts on the data



$\chi^2/d.o.f$  improves with cuts on  $\bar{M}^2$ .

Values of  $\sqrt{8t_{0,ph}}$  obtained are consistent. Agreement of  $m_N$  with corrected expt. value improves with cuts on  $\bar{M}^2$ .

Grey bands indicate the weighted average of the results.

## Weighted average of the results

Use a modified Akaike Information Criterion (AIC) [[Akaike,\(1998\)](#)] (following [[BMWc,2002.12347](#)])

Perform a weighted average of fit the results by weighting each fit  $j$  with

$$O_{\text{weighted}} = \sum_j^{N_M} w_j O_j$$
$$w_j = A \exp \left[ -\frac{1}{2} (\chi_j^2 - N_{\text{DF},j} + p_j) \right], \quad \sum_i^{N_M} w_i = 1$$

**Standard AIC**: fixed data, exponent  $\chi_j^2 + 2p_j$ , favours fits with low  $\chi^2$  and a small number of parameters.

**Modification** (subtract  $n_{\text{data},j} = N_{\text{DF},j} + p_j$ ): fix the parametrization and vary the data, favours larger  $N_{\text{DF},j}$ .

Alternatives: [[Jay and Neil,2008.01069](#)], equivalent to subtracting  $2N_{\text{DF},j}$ .

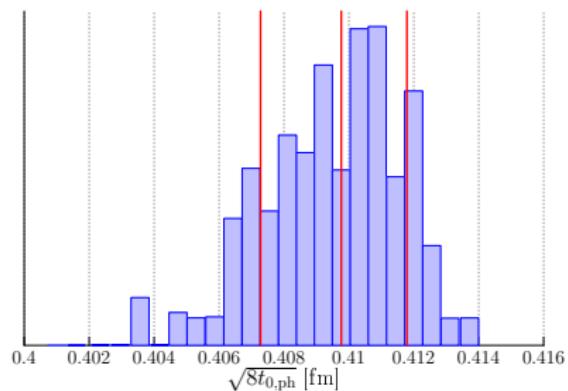
## Weighted average of the results

Final result:  $\sqrt{8t_{0,ph}} = 0.4098^{(20)}_{(25)} \text{ fm}$

Fits to 18 different cuts on the data.

$18 \times 100$  bootstraps weighted with  $w_j$ .

(0.5% total uncertainty)

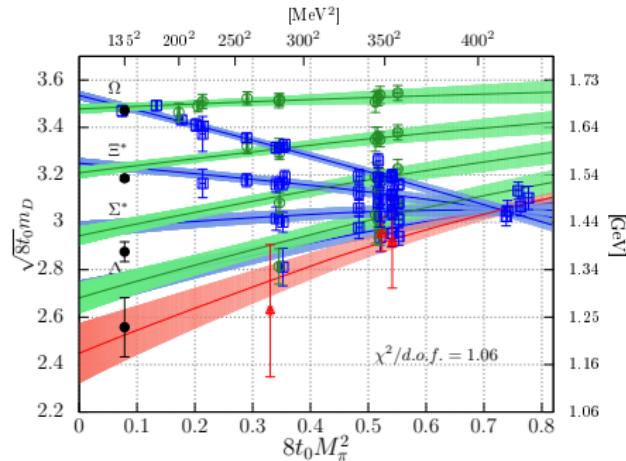
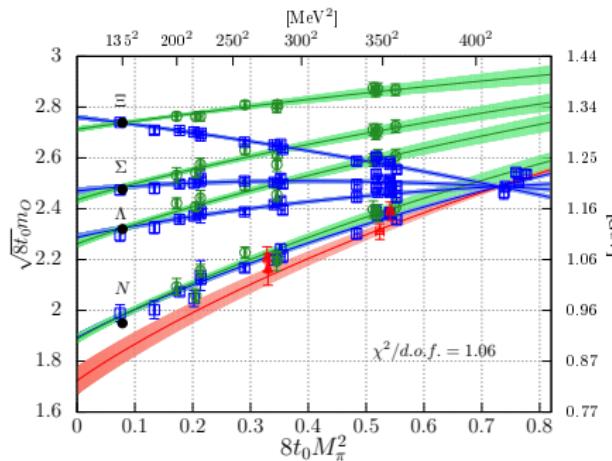


Dominated by fits with  $\chi^2/d.o.f.$  of 0.94 ( $N_{\text{DF}} = 80$ ) and 0.99 ( $N_{\text{DF}} = 73$ ).

# Variation with the continuum fit form

Fit the octet and decuplet masses simultaneously using NNLO BChPT + SSE + FV terms (23 parameters).

$\Delta$ ,  $\Sigma^*$ ,  $\Xi^*$  baryons are unstable: cut out data where  $D \rightarrow O\pi$  in the infinite volume limit.



$\sqrt{8t_{0,ph}}$  set using  $m_\Xi$ . Best fit shown (fit form gives reasonable description of data).  $m_\Omega$  consistent with corrected expt. value.

Unstable baryons: expt. masses not reproduced.

# Variation with the continuum fit form

Fit the octet masses using GMO fit form (17 parameters).

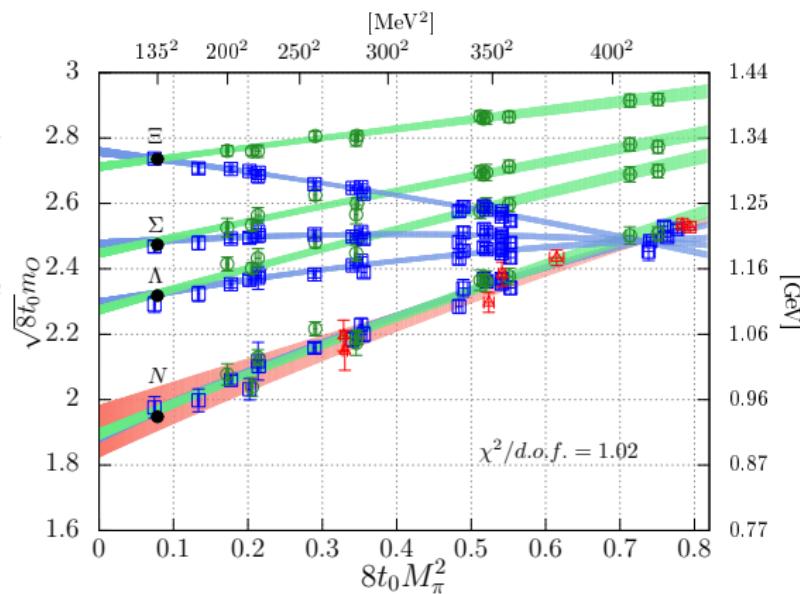
Fit is less constrained compared to BChPT (11 parameters compared to 6).  
Best fit shown (fit form gives reasonable description of data).

Convergence determined by  
 $\delta M^2 / \overline{M}^2$ .

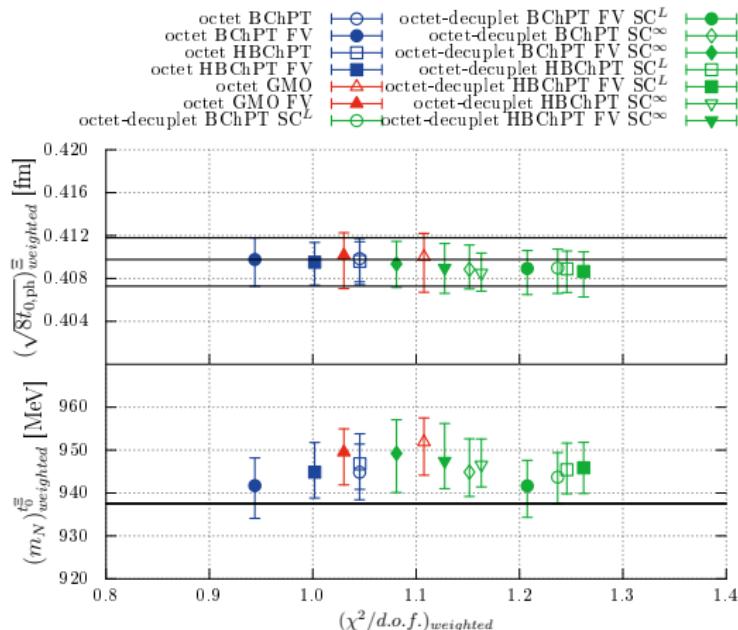
Want to include data from ensembles at or close to the physical point

→ no  $m_q$  cut imposed.

$\sqrt{8t_{0,ph}}$  set using  $m_{\Xi}$ .



# Variation with the continuum fit form



Results for  $\sqrt{8t_{0,ph}}$  are very stable ( $m_{\Xi}$  tightly constrained).

Including FV terms in the fit improves the fit quality.

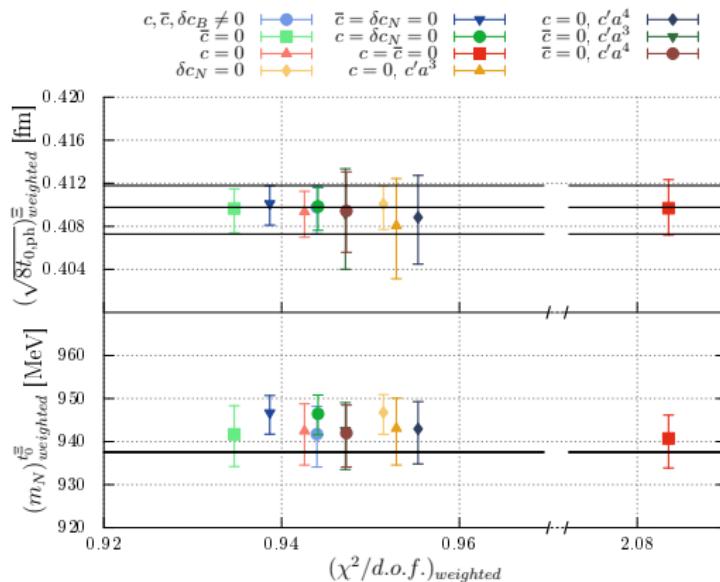
Poorer fit quality: HBChPT and GMO fit forms compared to EOMS BChPT, also when including the decuplet masses.

# Variation with the fit form: discretisation effects

Discretisation effects are mild, however, only varying  $a$ -effects by cutting out the coarsest lattice spacing (only 4 ensembles).

Investigate importance of  $O(a^2)$  terms:  $1 + a^2 (c + \bar{c} \overline{M}^2 + \delta c_O \delta M^2)$  and higher order terms using NNLO BChPT continuum fit form + FV terms:

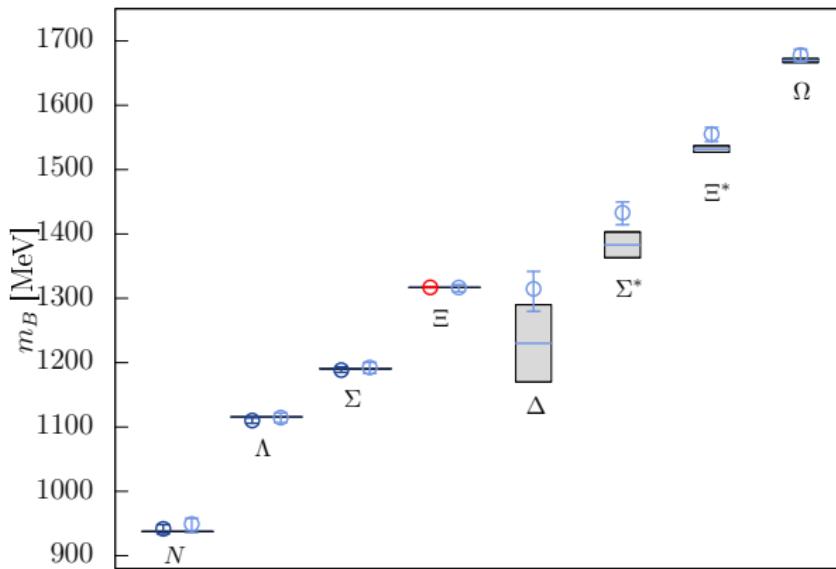
Results are very stable, even though the fit quality varies.  $m_N$  sensitive to  $\delta c_N$ .



## Low lying baryon spectrum

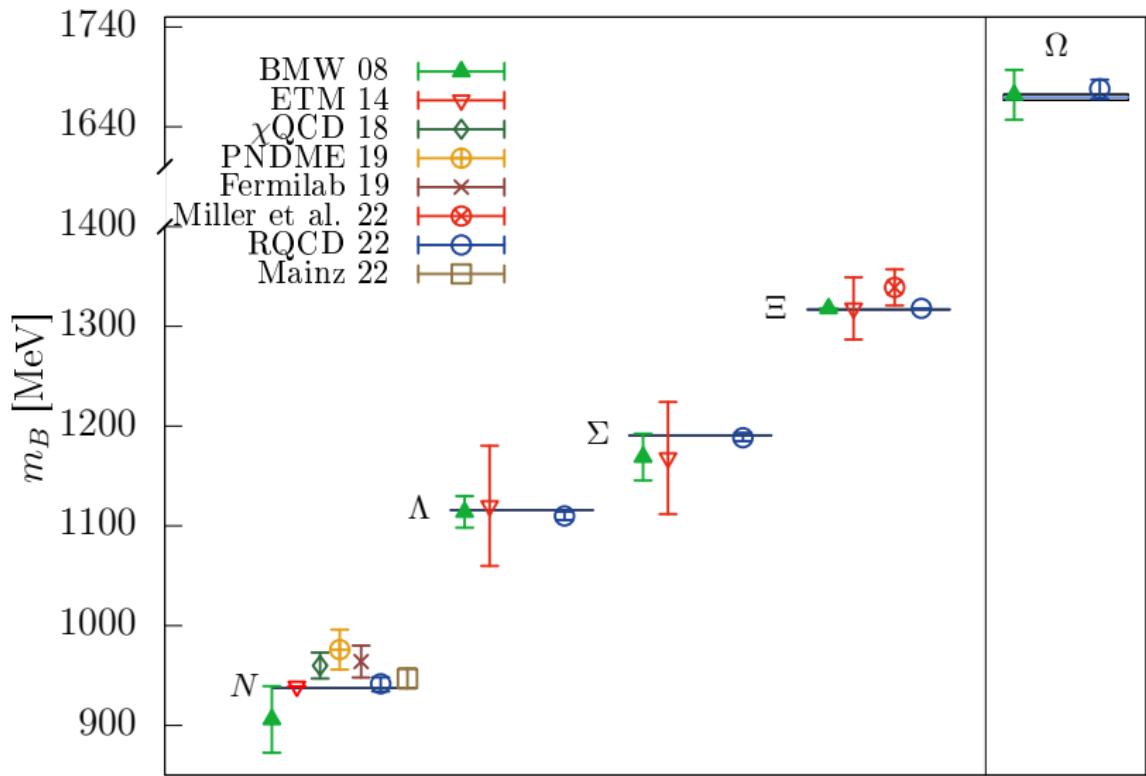
Octet baryon spectrum from BChPT fits + FV terms (determine  $\sqrt{8t_{0,ph}}$ )  
Agreement with corrected expt. masses within 1% overall uncertainty.

Octet and decuplet masses from BChPT + SSE + FV terms.



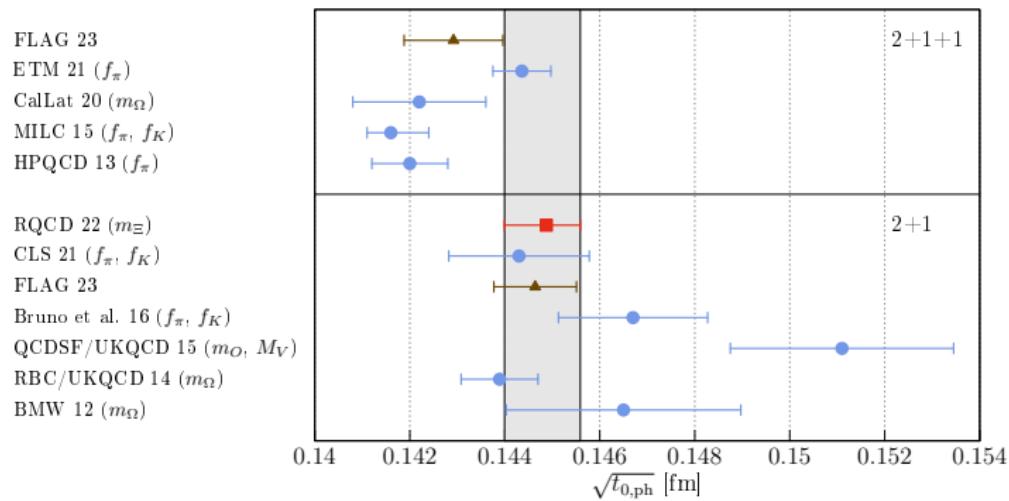
Proper treatment of the unstable decuplet baryons via the Lüscher formalism required.

## Low lying baryon spectrum



# Comparison with other determinations of $\sqrt{t_{0,ph}}$

Final result:  $\sqrt{t_{0,ph}} = 0.1449^{(7)}_{(9)} \text{ fm}$



CLS ensembles: [\[Bruno et al., 1608.08900\]](#) and [\[CLS 21, 2112.06696\]](#) (proceedings).

Also: Saez-Gonzalvo et al. (Lattice 2023, preliminary) 15 ensembles, twisted mass and improved Wilson valence quarks:

$$\sqrt{t_{0,ph}} = 0.1446(5)(3) \text{ fm from } f_\pi \text{ and } f_K.$$

## Baryon sigma terms: $\sigma_{\pi B}$ and $\sigma_{sB}$

The sigma terms, can be obtained via the Feynman-Hellmann theorem.

$$\sigma_{q,B} = m_q \left[ \frac{\langle B | \bar{q} \mathbb{1} q | B \rangle}{\langle B | B \rangle} - \langle \Omega | \bar{q} \mathbb{1} q | \Omega \rangle \right] = m_q \frac{\partial m_B}{\partial m_q},$$

where  $|\Omega\rangle$  denotes the vacuum. Consider  $\sigma_{\pi B} = \sigma_{uB} + \sigma_{dB}$  and  $\sigma_{sB}$ .

Using the Gell-Mann-Oakes-Renner (GMOR) relation:  $M_{PS}^2 \approx B_0(m_{q1} + m_{q2})$

$$\sigma_{\pi B} \approx \tilde{\sigma}_{\pi B} = M_\pi^2 \frac{\partial m_B}{\partial M_\pi^2} \quad \sigma_{sB} \approx \tilde{\sigma}_{sB} = M_{s\bar{s}}^2 \frac{\partial m_B}{\partial M_{s\bar{s}}^2}$$

where  $M_{s\bar{s}}^2 = 2M_K^2 - M_\pi^2$ .

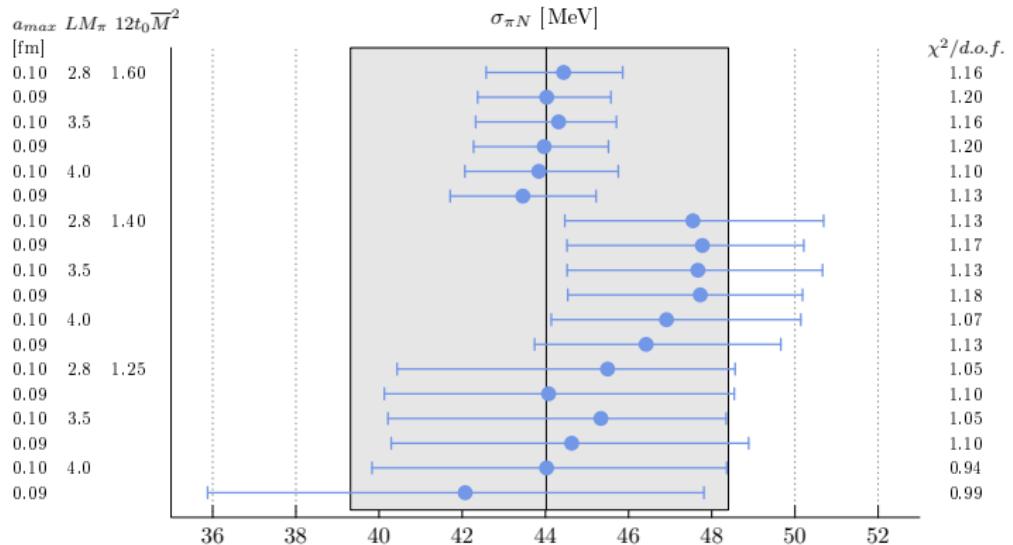
Nucleon sigma terms are relevant for computing WIMP-nucleon spin-independent cross-sections for direct dark matter detection experiments.  $q \in \{c, b, t\}$  are also interesting.

Difficult to determine  $\sigma_{s,N}$  via indirect (FH) approach (in particular if  $m_s$  is kept roughly constant).

Direct determinations of  $\sigma_{qB}$  ( $q \in \{u, d, s, c\}$ ) have been performed.

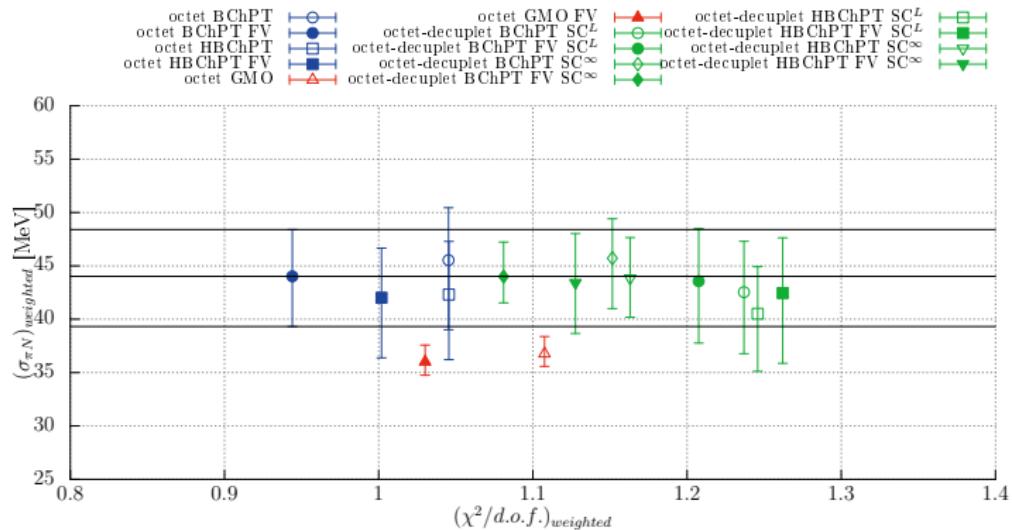
# Variation of $\tilde{\sigma}_{\pi N}$ with cuts on the data

Using NNLO BChPT for  $m_O(\mathbb{M}_\pi, \mathbb{M}_K, \infty, 0)$ .



Weighted average of the fits:  $\tilde{\sigma}_{\pi N} = 44.0^{(4.4)}_{(4.7)}$  MeV.

# Variation of $\tilde{\sigma}_{\pi N}$ with continuum fit form for $m_O$



## Additional considerations

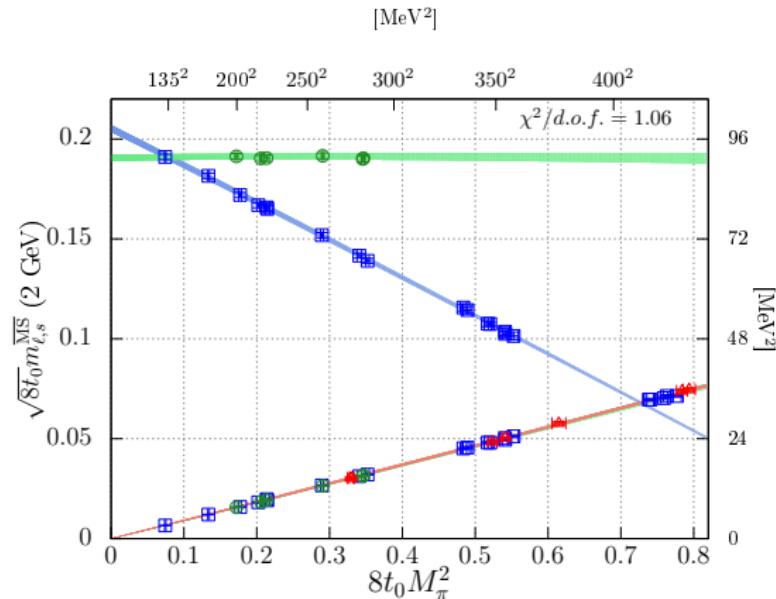
Fit to  $\sqrt{8t_0}m_B$ , however,  $t_0$  depends on  $M^2$ :  $\tilde{\sigma}_{\pi B}$  and  $\tilde{\sigma}_{sB}$  shown are corrected for this.

Want  $\sigma_{\pi B}$  not  $\tilde{\sigma}_{\pi B}$  etc.  $\rightarrow$  Need  $\partial M_\pi / \partial m_\ell$ ,  $\partial M_K / \partial m_\ell$ ,  $\partial M_K / \partial m_s$ .

Consistent to use GMOR relation with NNLO BChPT.

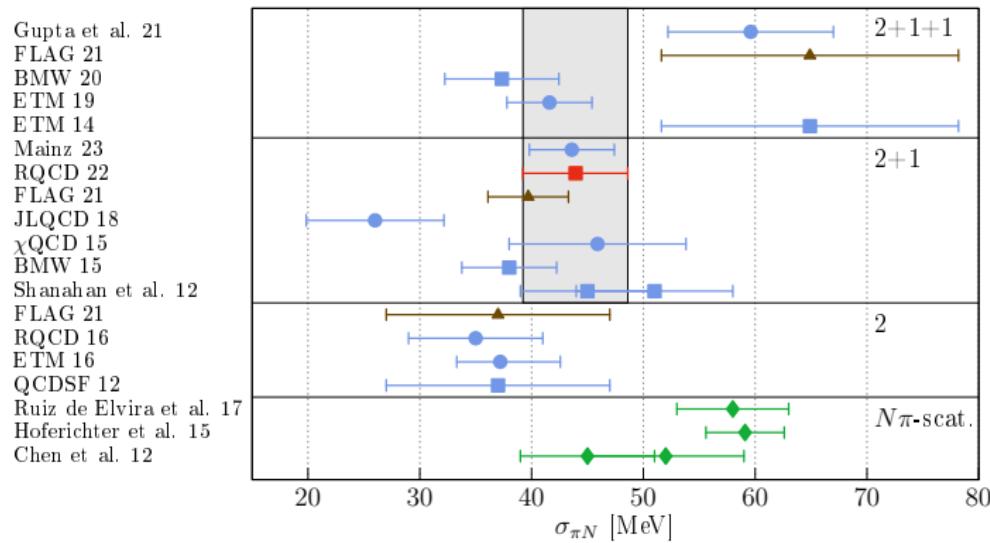
Note: all  $m_\ell$  trajectories go to zero as  $M_\pi^2 \rightarrow 0$ .

To  $O(p^4)$  in SU(3) ChPT [Gasser and Leutwyler, Nucl. Phys. B250 (1985)]. PCAC quark masses renormalised to  $\overline{MS}$  at 2 GeV using  $Z_A/Z_P$  from [RQCD, 2012.06284] determined using RI-SMOM (used  $O(a)$  improvement coefficients from [ALPHA, 1906.03445]).



# Comparison with other determinations of $\sigma_{\pi N}$

$$\tilde{\sigma}_{\pi N} = 44.4^{(4.4)}_{(4.7)} \text{ MeV} \rightarrow \sigma_{\pi N} = 43.9^{(4.7)}_{(4.7)} \text{ MeV},$$

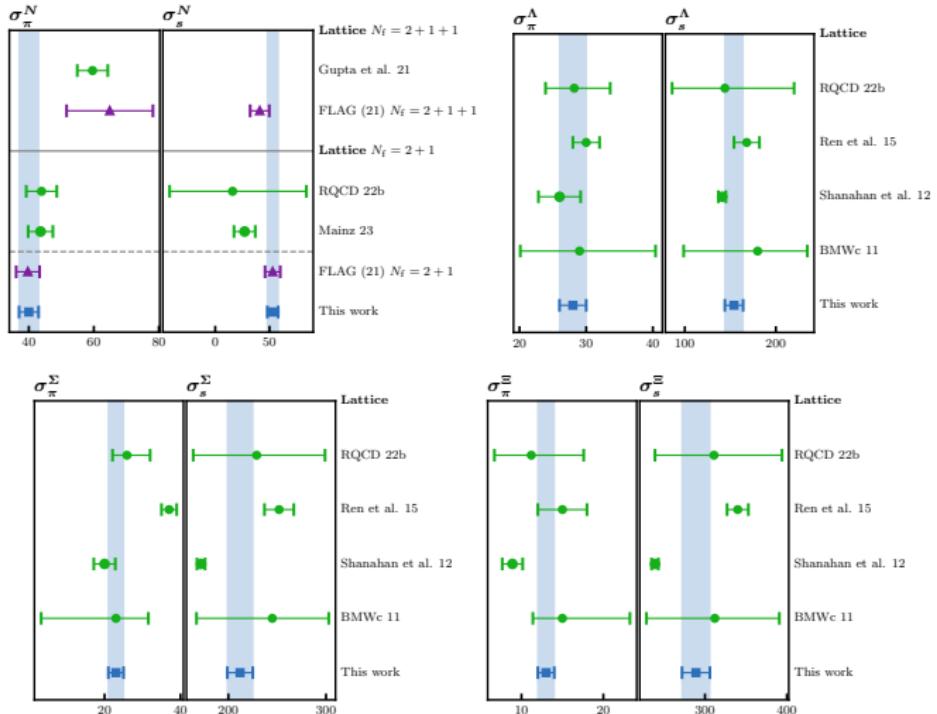


Some tension with the phenomenological results of [\[Hoferichter et al.,1506.04142\]](#) obtained using  $N\pi$  scattering data.

[\[Hoferichter et al.,2305.07045\]](#) ( $m_{\pi^\pm}$  vs  $m_{\pi^0}$ )  $\sigma_{\pi N} = 55.9 \pm 3.5$  MeV.

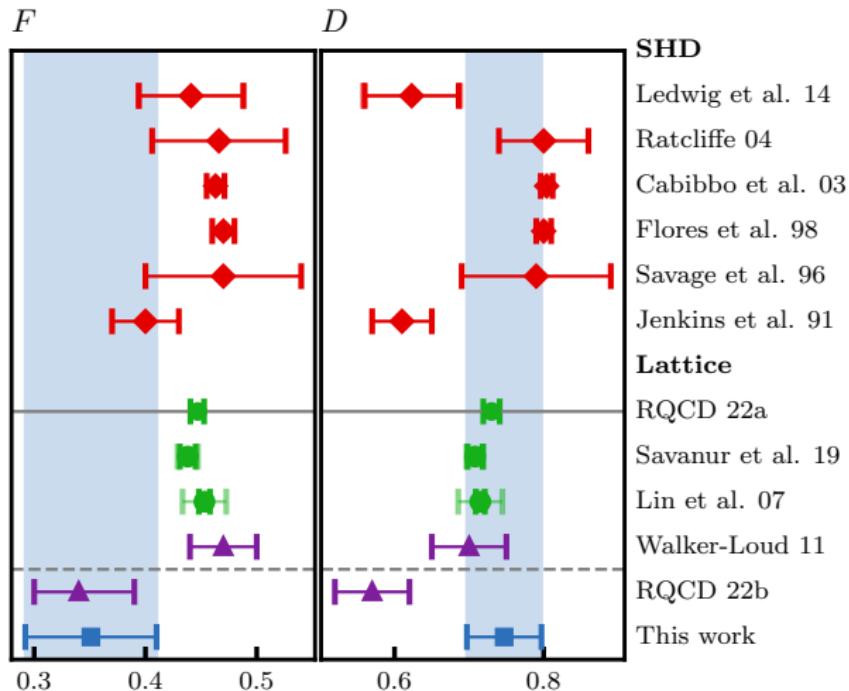
Direct determination by [\[Gupta et al.,2105.12095\]](#) is also larger.

# Sigma terms of the octet baryons



"This work": RQCD, Pia Petrak and J. Heitger, direct determination of the sigma terms on a sub-set of the CLS ensembles ( $M_\pi \gtrsim 200$  MeV). **Not all systematics are estimated.**

# Low energy constants $F$ and $D$

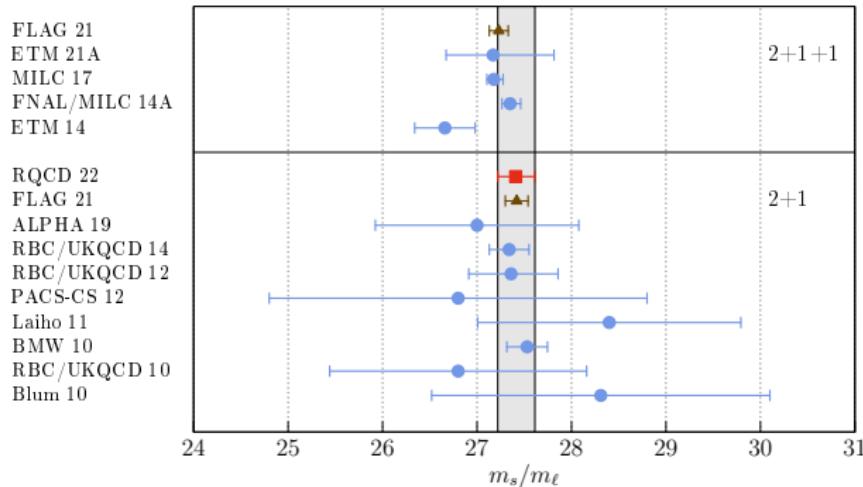


SHD: phenomenological analyses of semi-leptonic hyperon decays.

Lattice: Axial charges at the physical point (Savanur et al., Lin et al.), baryon masses (Walker-Loud)

# Light and strange quark masses

$$N_f = 3, m_\ell^{\overline{MS}}(2 \text{ GeV}) = 3.37^{(+4)}_{(-5)} \text{ MeV}, m_s^{\overline{MS}}(2 \text{ GeV}) = 92.2^{(+8)}_{(-10)} \text{ MeV}$$



[RQCD,2305.04717]: CVC relation  $\delta_m = m_u - m_d = \frac{g_V^\Sigma}{g_S^\Sigma} \Delta m_\Sigma^{QCD}$ .

Estimate  $\Delta m_\Sigma^{QCD} \approx (m_{\Sigma^+} - m_{\Sigma^-})/2 = -4.04(4) \text{ MeV}$  (PDG) and using  $g_S^\Sigma = 3.98^{(22)}_{(24)}$  gives

$$\delta_m = m_u - m_d = -2.03(12) \text{ MeV}.$$

Leads to, with  $m_\ell = (m_u + m_d)/2$ ,  
compared to FLAG ( $N_f = 2 + 1$ )

$$m_u/m_d = 0.54(2), \\ m_u/m_d = 0.485(19) \quad [\text{BMWc,1604.07112}].$$

## Summary and outlook

Precision determinations of the lattice scale are important as lattice predictions for key quantities relevant for expt. and phenomenology become more precise.

Determination of Wilson flow scale at the physical point with 0.5% uncertainty via  $m_{\Xi}$ :

$$\sqrt{8t_{0,ph}} = 0.4098^{(20)}_{(25)} \text{ [fm]}$$

- ★ Performed continuum, finite volume, quark mass simultaneous fits to the baryon octet with all correlations taken into account. Systematics on the fits were evaluated via cuts to the data and utilising the modified AIC criterion.
- ★ Utilising data along three trajectories in the quark mass plane means mistuning of the trajectories can easily be corrected. Provided tight constraints on  $m_{\Xi}$  at the physical point.
- ★ Discretisation and finite volume effects are mild for our ensembles.
- ★ Covariant BChPT provided a reasonable description of the data for our range of  $M_\pi$  and  $M_K$  ( $\overline{M}^2 < 440^2 \text{ [MeV}^2]$ ). (Large  $N_{DF}$  for the fits).
- ★ Corrected expt. octet baryon spectrum reproduced to within 1% uncertainties.
- ★ As a by product extract the sigma terms  $\sigma_{\pi B}$  and  $\sigma_{sB}$ .
- ★ Also extracted the LECs which are not well known for SU(3) BChPT.

- ★ HBChPT and GMO expansions gave consistent results for  $t_{0,ph}$  and the baryon spectrum. Including SSE terms enabled a reasonable fit of both the octet and decuplet baryons.

In the future:

Improve the  $t_{0,ph}$  determination:

- ★ Already have additional measurements on many ensembles, which are not included in the current analysis.
- ★ Perform a simultaneous fit of  $m_B$  and direct determinations of  $\sigma_{\pi B}$  and  $\sigma_{sB}$ .

In addition:

- ★ Test ChPT further through determination of LECs via simultaneous fits to related observables, e.g.  $M_{\pi,K}$ ,  $m_{\ell,s}$  and  $F_{\pi,K}$  and  $m_B$  and  $g_A^B$ .
- ★ ...

Back-up slides

## Global interpolation of $t_0/a^2$

$$\begin{aligned}\frac{t_0}{a^2} &= \frac{t_0^*}{a^2}(g^2) [1 + \tilde{k}_1 A - 2b_a(a\bar{m} - am^*)] + \bar{c}A + \delta c 8t_0 \delta M^2 \\ &= [f(g^2) + c_{t_0} + d_{t_0} f^{-1/2}(g^2)] (1 + \tilde{k}_1 A - 2b_a a \bar{m}) + \bar{c}A + \delta c 8t_0 \delta M^2,\end{aligned}$$

where

$$A = 8t_0 (\bar{M}^2 - M^{*2}).$$

and

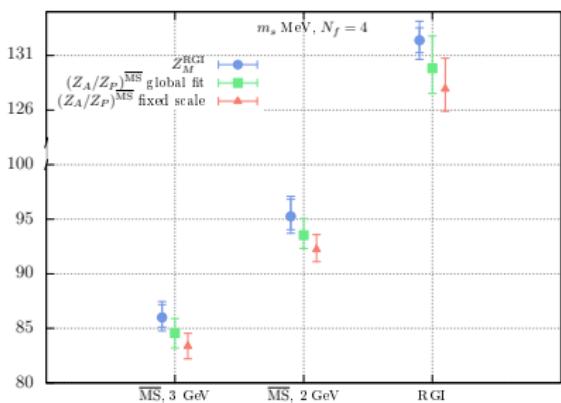
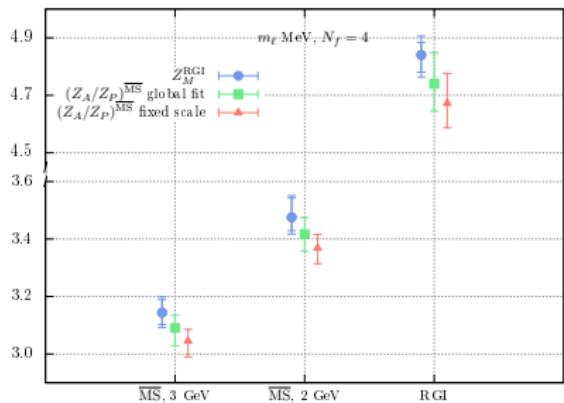
$$\begin{aligned}\frac{t_0^*}{a^2(g^2)} &= \frac{t_0^*}{a_0^2(g^2)} [1 - 2b_a(g^2)am^*] = [f(g^2) + c_{t_0} + d_{t_0} f^{-1/2}(g^2)] \times \\ &\quad [1 - 2b_a(g^2)am^*],\end{aligned}$$

where

$$f(g^2) = \frac{t_0^* \Lambda_L^2}{h^2(g^2)} = 0.00528(36) \exp \left( \frac{16\pi^2}{\beta_0 g^2} + \frac{\beta_1}{\beta_0^2} \ln \frac{\beta_0 g^2}{16\pi^2} - b_{t_0} g^2 + \dots \right).$$

# Quark masses $m_\ell$ and $m_s$

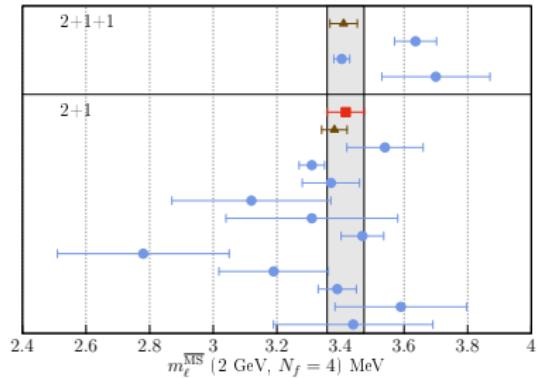
Renormalisation: RGI [ALPHA,1906.03445], RI'-SMOM [RQCD,2012.06284]



# Quark masses $m_\ell$ and $m_s$

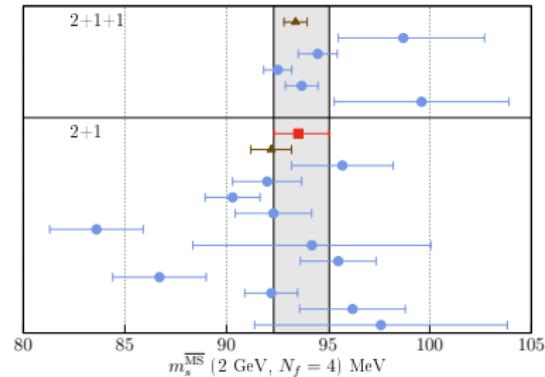
FLAG 21  
 ETM 21  
 FNAL/MILC/TUMQCD 18  
 ETM 14

RQCD 22  
 FLAG 21  
 ALPHA 19  
 RBC/UKQCD 14  
 RBC/UKQCD 12  
 PACS-CS 12  
 Laiho 11  
 BMW 10  
 PACS-CS 10  
 MILC 10  
 HP QCD 10  
 RBC/UKQCD 10  
 Blum 10

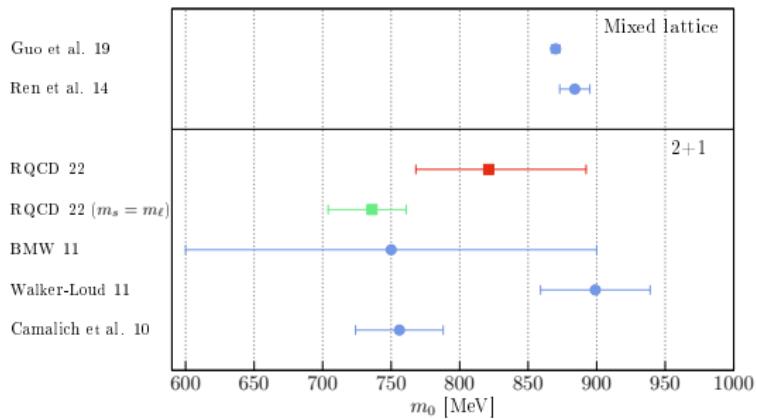


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 ETM 21  
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 HP QCD 14  
 ETM 14

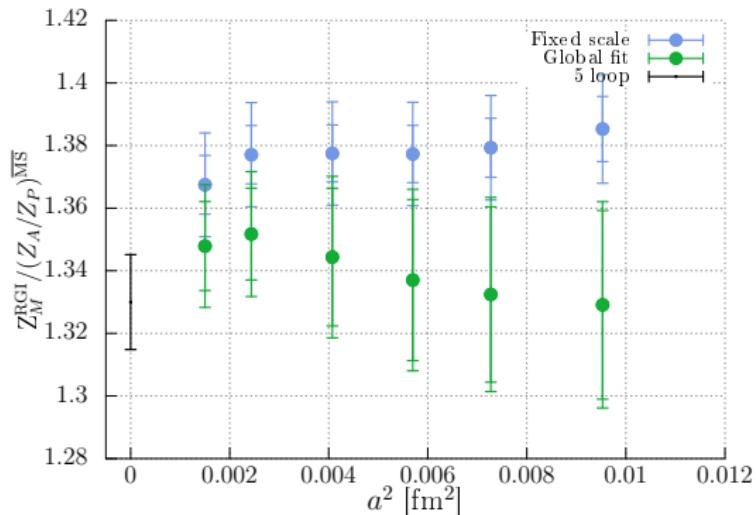
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 FLAG 21  
 ALPHA 19  
 Mazewawa 16  
 RBC/UKQCD 14  
 RBC/UKQCD 12  
 PACS-CS 12  
 Laiho 11  
 BMW 10  
 PACS-CS 10  
 HP QCD 10  
 RBC/UKQCD 10  
 Blum 10



# Octet baryon mass in the chiral limit



# Quark masses $m_\ell$ and $m_s$



# Estimates of QED and QCD isospin breaking effects

[RQCD,2305.04717]: CVC relation  $\Delta m_B^{\text{QCD}} = g_{S,B}(m_u - m_d)$

For the baryon octet

$$\begin{aligned}\Delta m_N^{\text{QED}} &= \Delta m_N - g_S^N(m_u - m_d) \\ &= \Delta m_N - \frac{2g_S^N}{g_S^\Sigma} \Delta m_\Sigma^{\text{QCD}}, \\ \Delta m_\Xi^{\text{QED}} &= \Delta m_\Xi - \frac{2g_S^\Xi}{g_S^\Sigma} \Delta m_\Sigma^{\text{QCD}}.\end{aligned}$$

This gives

$$\begin{array}{ll}\Delta m_N^{\text{QED}} = 0.97^{(31)}_{(36)} \text{ MeV}, & \Delta m_N^{\text{QCD}} = -2.26^{(31)}_{(36)} \text{ MeV}, \\ \Delta m_\Sigma^{\text{QED}} = 0.77(05) \text{ MeV}, & \Delta m_\Sigma^{\text{QCD}} = -4.04(04) \text{ MeV, (Expt)} \\ \Delta m_\Xi^{\text{QED}} = -1.65^{(37)}_{(39)} \text{ MeV}, & \Delta m_\Xi^{\text{QCD}} = -5.20^{(42)}_{(44)} \text{ MeV.}\end{array}$$