Approaching the chiral point in two-flavour lattice simulations

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Introduction

- How to study the low-energy regime of QCD?
  No analytical first-principle tools there!
  - Effective theories on one hand ...
  - ... and lattice numerical simulations on the other.

- General idea:
  - measure masses and decay constants on the lattice
  - fit to χPT functional forms $\Rightarrow$ fix its low-energy constants

  ALPHA dealt mainly with kaons so far - this is focused on pions.
  [Fritzsch et al. 2012], but see [SL 2013]

- Caveats/questions:
  - Data from discretised lattice reliable (continuum limit) ?
  - Are we in the χPT regime ?

Data collection 1: lattice

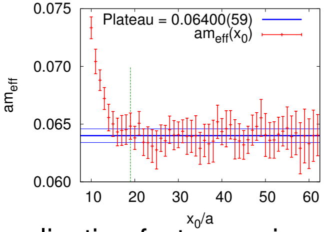
- Discretised spacetime (spacing $a \geq 0.05$ fm).
- Discretised version of (Euclidean) QCD action and observables.
- Hit 'Run' on the computer, wait some (very long) time, get results.

Real-world issues:

- Choice of action: "Wilson action"
  (not the best for going chiral, but reliable and relatively fast)
- Discretisation effects? (our goal is: $a \to 0$)
  With "$O(a)$-improvement", disturbances are at most $O(a^2)$
- In the computer the volume is finite:
  don't worry as long as $m_\pi L \geq 4$ (thumb rule)
- At each set of coupling, measure over N_{cfg} configurations:
  statistics, autocorrelations issues, etc...
- Two-flavour (i.e. u, d-quarks only) ?
  The s might count: can be added as *valence* (i.e. no loops)

Data collection 2: measurements

- What to measure in practice?
  - Two-point functions in time: $\langle P(0)P(t)\rangle$, $\langle P(0)A_0(t)\rangle$
  - Extract from those (lattice units: $M_\star = am_\star$, $F_\star = af_\star$):
    quark mass M_q, pion mass M_π and decay constant F_π
  - Also with strange quark ($\rightarrow M_{\mathrm{K}}, F_{\mathrm{K}}$)
- Ensembles produced by CLS and analysed by ALPHA
  - 10 to 20 stochastic sources/config. for correlators
  - Typical mass/decay constant known to percent accuracy:

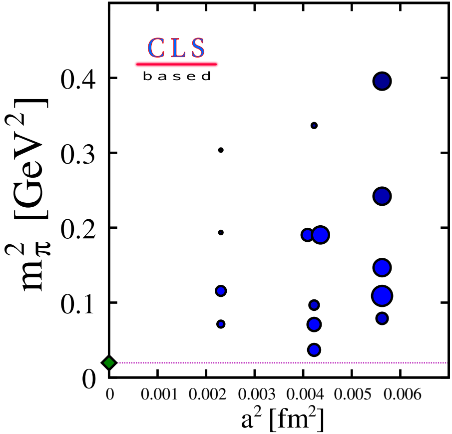


$$m_\pi = 192 \text{ MeV}$$
$$a = 0.065 \text{ fm}$$
$$\frac{L_T}{a} = 128$$

- Renormalisation factors as in [ALPHA 2012]:
  - b-factors from one-loop PT [Sint, Weisz 1997]
  - Z_A, Z_P determined nonperturbatively.

Data collection 3: ensembles at hand

- $m_\pi L$ range is: 4.0 – 7.7 (i.e. enough not to worry much)
- Lowest m_π is 192 MeV
- All systems have $L_T = 2L$ and periodic b.c.



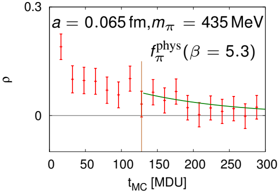
- Downward: chiral limit
- To the left: continuum limit

(more chiral = more expensive!)
(finer lattice = more expensive!)

Data collection 4: error analysis

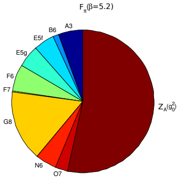
- Correlations are propagated to the final quantities
- Sophisticated error analysis includes slow-mode contributions [Schäfer, Sommer, Virotta, 2010]:

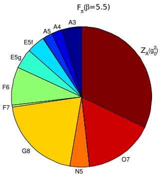
slow modes $\sim \tau_{\exp}$ (previously measured) $\Rightarrow$



$\Rightarrow$ final error

- A large contribution to the error from Z_A renorm. factor, e.g. for F_π:





- Systematic errors still lurking out there ...

Chiral perturbation theory [Weinberg '79; Gasser, Leutwyler '80s]

"χPT"

- An effective field theory for low-energy QCD
- Order-by-order renormalisable ($\rightarrow$ infinitely many *low-energy constants*)
- Written in terms of pion field
- Lowest-order Lagrangian (schematically):

$$\mathcal{L}^{(\mathrm{LO})} = \frac{1}{4} F^2 \left[(D_\mu U)(D^\mu U^\dagger) + M^2 (U + U^\dagger) \right]$$

($U \leftrightarrow$ pion field, $M^2 \sim m_q \sim$ pion mass)

- Higher orders: derivatives of U, powers of M, e.g.:
  $\sim M^2 U^2,\ U^2 (DU)^2, \ldots$
  $\Rightarrow$ Proliferation of terms ($\leftrightarrow$ parameters) in $\mathcal{L}$

- Starting from one-loop diagrams one get "chiral logs", e.g. $M^2 \log(M^2)$

$SU(2)$ χPT for pion quantities

Consider (as functions of quark mass and lattice spacing)

$$M_\pi \;,\; F_\pi$$

and build

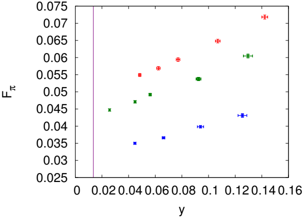
$$y = \frac{M_\pi^2}{8\pi^2 F_\pi^2} \quad \text{i.e.} \quad y_{\rm chir} = 0 \;,\; y_{\rm phys.} = y_\pi \simeq 0.013$$

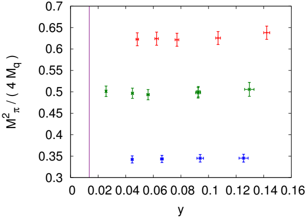
$SU(2)$ χPT (i.e. only up and down) predicts then (asymptotic series!)

$$\begin{aligned} M_\pi^2 &= M^2\left\{1 + y + y\log y + y^2 + y^2\log y + y^2(\log y)^2 \ldots\right\} \\ F_\pi &= \underbrace{F}_{LO}\left\{1 + \underbrace{y + y\log y}_{NLO} + \underbrace{y^2 + y^2\log y + y^2(\log y)^2}_{NNLO} \ldots\right\} \end{aligned}$$

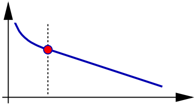
Low-energy constants: 2 $\rightarrow$ 4 $\rightarrow$ 7, for LO $\rightarrow$ NLO $\rightarrow$ NNLO !

Extracting LECs by fitting





- 15 Ensembles $\times\{F_\pi, M_\pi\} \to$ 30 datapoints to fit
  (simultaneous fits to all of them)
- Which fit function?
  - Truncate to NLO
  - NLO + linear ("junction") $\Longrightarrow$
  - Full-fledged NNLO fit



- These choices + fit-range cuts $[m_\pi \leq 650, 500, 390, 345\ \text{MeV}]$
  $\Rightarrow$ systematic uncertainties on the outcome

LECs, closer inspection

- LO low-energy constants:
  - F is $\sim$ pion decay constant
  - $M^2 \sim 4M_q(\Sigma/F^2)$: used to get the chiral condensate Σ!
    (after clever rewriting of fit function)

  Lots of accurate determinations (percent-level).
  Also used to set the scale.
  (here: the scale a is set through F_{K})
- NLO LECs $\bar{\ell}_3, \bar{\ell}_4$: (note $\bar{\ell}_i = \log(\Lambda_i^2/M^2_{\pi,\mathrm{phys}})$)
  There are several estimates, uncertainty about 20% [FLAG 2013]
- NNLO LECs $\bar{\ell}_{12}, c_M, c_F$:
  Nowadays still virtually undetectable
  E.g. [BWM Collaboration '13] quote (w/ grain of salt) errors of 30-70%

Intermezzo: F_{K} scale-setting I

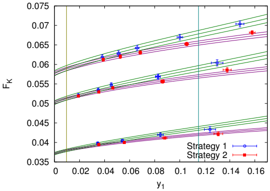
- All data coming from lattice are *adimensional* (“lattice units”):
  e.g. $M = am$ and not m itself.
- “Setting the scale” means: finding a in fermi.
- To do this, choose an observable (e.g. kaon decay constant) and:

$$\text{measure } F_{\mathrm{K}} \;\Rightarrow\; \text{set } F_{\mathrm{K}} = a \cdot f_{\mathrm{K}} \equiv 155\text{ MeV} \;\Rightarrow\; a = \cdots \text{ fm}$$

- Once this is done, all other quantities can be *made physical*

F_{K} scale-setting II

- Here, F_{K} is used to set the scale
- As for F_{π}, measurements at various quark masses and chiral fits!
- Can compare two ways to get to physical point:
  (each requiring its own version of χPT)
  - Kaon mass fixed
  - Strange mass fixed



- There, NLO behaviour is very well seen and that's it !
- (as a result, lattice spacing known with percent accuracy or better)

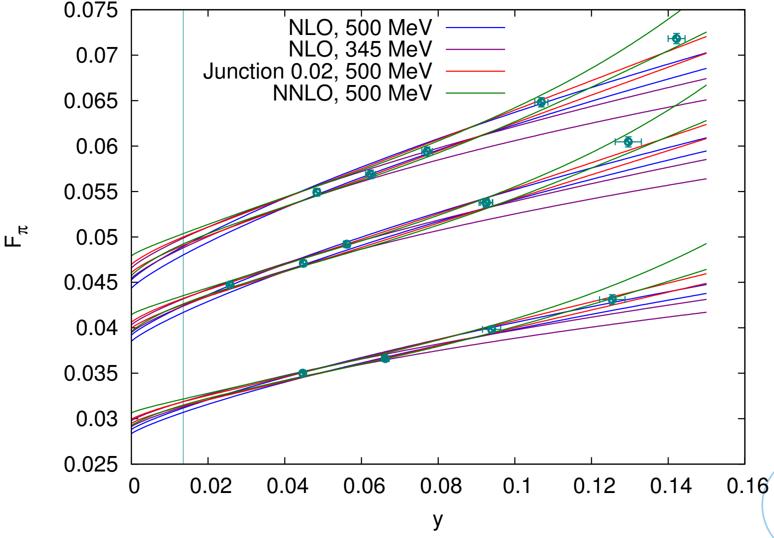
Back to F_π

- For pion-related observables, much more problematic
  (as observed by various groups as well)
- Quite some fit-range-cut dependence
- y^2-terms effectively cancel "$y \log y$" over a wide interval
  (which led to "junction fits" at some point)
- $\star$ Can χPT be trusted there? How much?

Effect of this all:

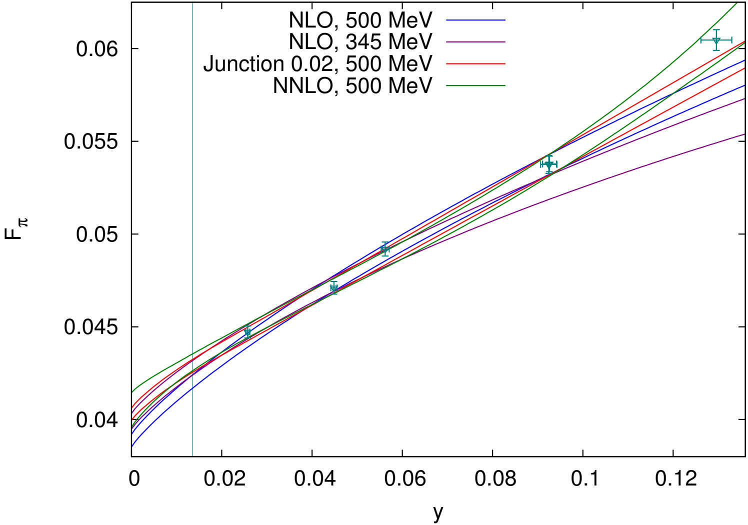
- For F_π(phys. point) and Σ, "no big deal"
- For $y \to 0$ extrapolations and (N)NLO low-energy constants:
  large systematic uncertainty!

Fit curves 1: F_π



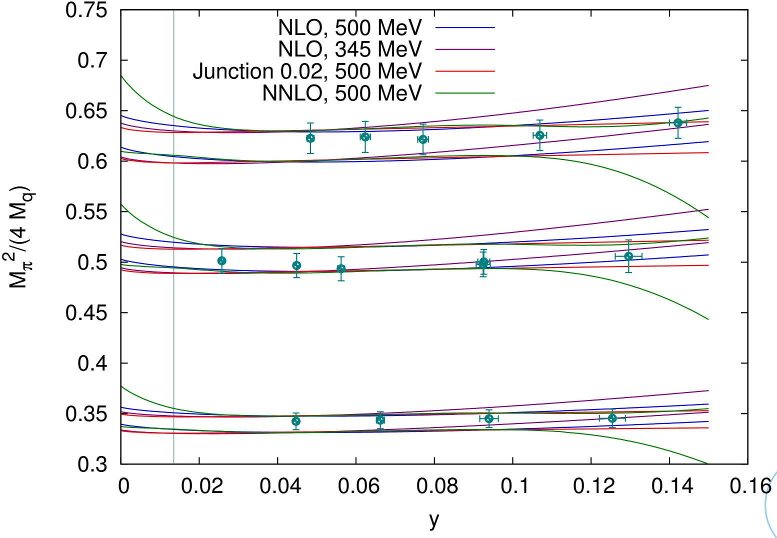
All fits have 7 total free parameters except NNLO (10).

Fit curves 1: F_π (zoom for $\beta = 5.3$)

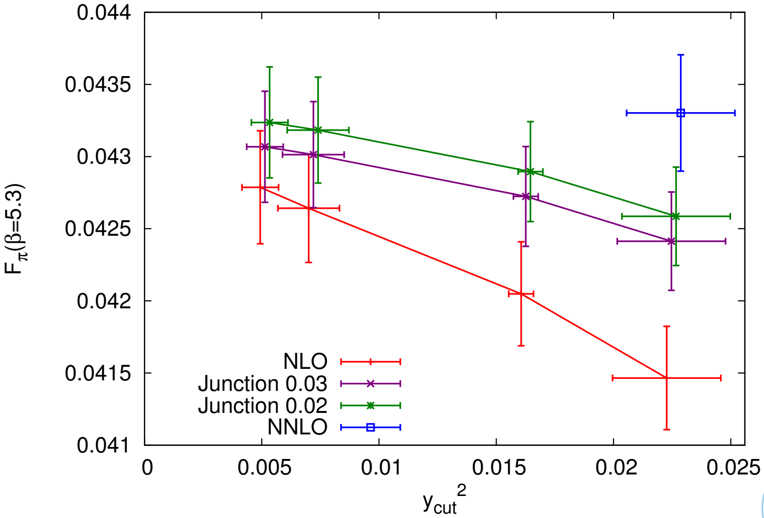


All fits have 7 total free parameters except NNLO (10).

Fit curves 2: M_π^2

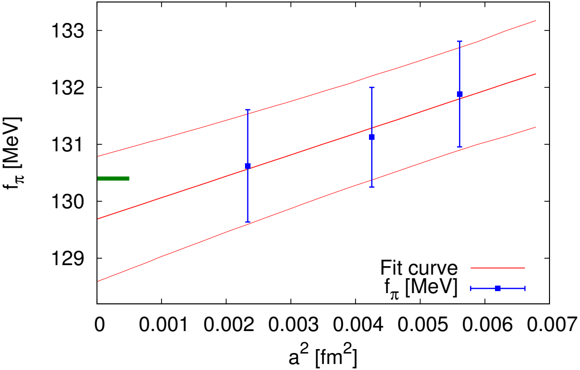


F_π, outcome



Fit-range dependence corroborates NNLO result.

Plugging in the scale from F_K, take the continuum limit:

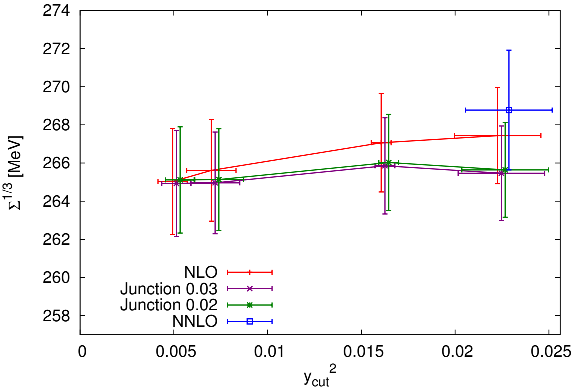


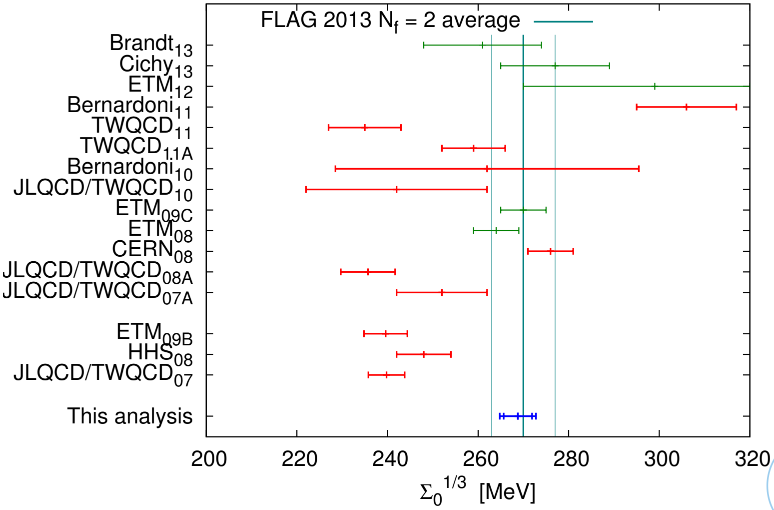
Final answer: $f_\pi = 129.7 \pm 1.1$ MeV [i.e. $\sqrt{2}(91.71 \pm 0.78)$].

Chiral condensate Σ

Practically trouble-free. In the continuum and chiral limits:

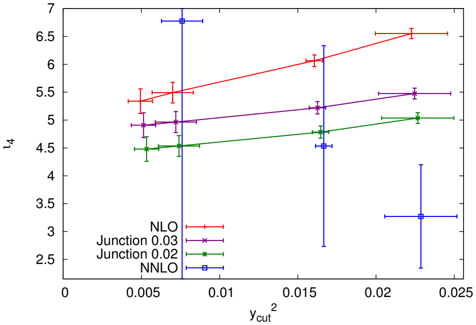
$$\sqrt[3]{\Sigma} = 269 \pm 3_{\rm stat} \pm 4_{\rm syst} \ \text{MeV} \qquad \overline{\text{MS}}(2\ \text{GeV})$$





FLAG 2013 N_f = 2 average
$Brandt_{13}$
$Cichy_{13}$
ETM_{12}
$Bernardoni_{11}$
$TWQCD_{11}$
$TWQCD_{11A}$
$Bernardoni_{10}$
$JLQCD/TWQCD_{10}$
ETM_{09C}
ETM_{08}
$CERN_{08}$
$JLQCD/TWQCD_{08A}$
$JLQCD/TWQCD_{07A}$
ETM_{09B}
HHS_{08}
$JLQCD/TWQCD_{07}$
This analysis
200
220
240
260
280
300
320
$\Sigma_0^{1/3}$ [MeV]

(N)NLO LECs



- Trusting NNLO here, $\bar{\ell}_4 = 3.3 \pm 0.9_{\text{stat.}} \pm 2_{\text{sist!}}$

  NLO looks more convincing – cf. latest world-average of 4.59 ± 0.26
- Can't say much for $\bar{\ell}_3 \sim 2.26 \pm \infty$!

  (believed to be in fact around 3.5)
- NNLO: just mentioning $\bar{\ell}_{12} \sim 1.6$, $c_F \sim -19$, $c_M \sim -10$

Closing remarks

- Chiral condensate and pion decay constant:
  well determined – stable and with percent accuracy
- But, as opposed to analogous F_{K} analysis,
  - NLO χPT fades out at $m_\pi \simeq 300$ MeV already
    Same issue recently seen by BMW in 2+1 flavours
    (partial explanation: higher amplitude in chiral logs)
- Data not enough for proper NNLO fitting
  (which affects NLO LECs as well as $f(m \to 0)$ extrapolations)
- More datapoints would be desired . . .
  but CLS now has switched to $N_{\mathrm{F}} = 2 + 1$
  (guess: the same precocious breakdown of NLO will be seen there)

The End.

Slow modes in autocorrelation analysis

(cf. [Schäfer, Sommer, Virotta 2010] for details)

Integrated autocorrelation time "converts naïve error into actual one":

$$\sigma^2 = \frac{2\tau^0_{\rm int}}{N}\Gamma(0) \quad ; \quad \tau^0_{\rm int} = \frac{1}{2} + \sum_{t=1}\rho(t) \quad \text{with} \quad \rho(t) = \Gamma(t)/\Gamma(0)$$

In practice, signal on ρ soon lost: danger!

(despite trying to balance uncertainty in ρ and remainder of the tail)

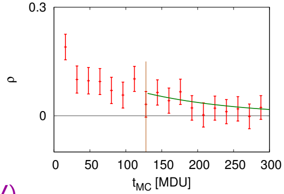
Observable can couple, undetected, to a slow mode

$\Rightarrow$ underestimation of error!

Solution: where the measured ρ vanishes ($t \equiv W$), attach an exponential tail

- It represents the observable's coupling to slow modes
- Its decay rate is measured (or estimated) previously

Use rather: $\tau_{\rm int} = \tau^0_{\rm int} + \tau_{\rm exp}\rho(W)$



Ensemble table

Tag	β, a [fm]	m_π [MeV]	$m_\pi L$	$N_{\rm cnfg.}$	$\frac{N_{\rm cnfg.}}{\tau_{\rm int}}$	$\frac{N_{\rm cnfg.}}{\tau_{\rm exp}}$	$N_{\rm src}$	trj.	Alg.	r_0?
A2	5.2	629	7.7	1000	817	120.6	10	8	DD	X
A3	(0.075)	492	6.0	1004	633	121.1	10	8	DD	X
A4		383	4.7	1012	861	122.0	10	8	DD	X
A5		330	4.0	1001	1100	163.5	10	4	MP	X
B6		281	5.2	636	639	51.9	20	2	MP	X
E4	5.3	580	6.2	156	97	9.3	10	16	DD	-
E5f	(0.065)	436	4.6	1000	354	59.9	10	16	DD	-
E5g		436	4.7	1000	571	119.8	10	16	DD	X
F6		311	5.0	600	410	35.9	10	8	DD	X
F7		266	4.3	1177	569	70.5	10	8	DD	X
G8		192	4.1	878	720	35.6	20	2	MP	X
N4	5.5	551	6.5	469	30	4.2	10	8	DD	X
N5	(0.048)	440	5.2	476	82	4.2	10	8	DD	X
N6		340	4.0	2010	386	40.2	10	4	MP	X
O7		267	4.2	980	211	19.6	20	4	MP	X

- All systems have $L_T = 2L$ and periodic b.c.

From 2-point functions to PCAC masses

Define

$$P^{rs} = \overline{\psi}_r \gamma_5 \psi_s \quad ; \qquad A_0^{rs} = \overline{\psi}_r \gamma_0 \gamma_5 \psi_s \quad :$$

with the 2-point functions

$$f_{PP}^{rs} = \int \langle P^{rs}(x) P^{sr}(0) \rangle \quad ; \qquad f_{AP}^{rs} = \int \langle A_0^{rs}(x) P^{sr}(0) \rangle \ .$$

one finds

$$\frac{\frac{1}{2}(\partial_0 + \partial_0^*) f_{AP}(x_0) + c_A a \partial_0^* \partial_0 f_{PP}(x_0)}{2 f_{PP}(x_0)} \to m_{rs} \ , \quad x_0 \to \infty \ ,$$

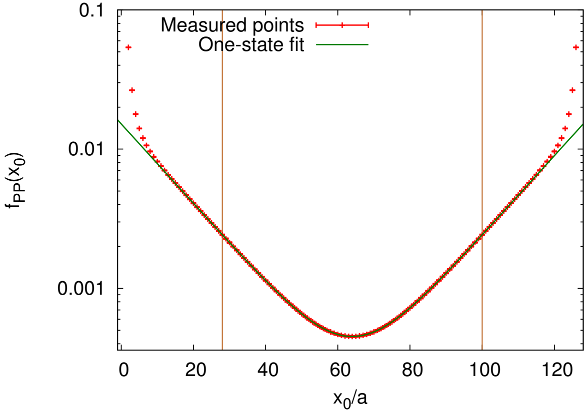
renormalised then as:

$$m_R^{rs} = \frac{Z_A}{Z_P} \frac{(1 + \overline{b}_A a m_{\mathrm{sea}} + \widetilde{b}_A a m_{rs})}{(1 + \overline{b}_P a m_{\mathrm{sea}} + \widetilde{b}_P a m_{rs})} m_{rs} \ .$$

From 2-point functions to m_{PS} and f_{PS}

$$f_{PP}(x_0) = c_1 \left[e^{-m_{PS} x_0} + (echo) \right] + higher\ states$$

$$f_{PS}^{\text{bare}} = 2\sqrt{2c_1}\, m_{rs} m_{PS}^{-3/2} \quad , \quad f_{PS} = Z_A (1 + \overline{b}_A a m_{\text{sea}} + \widetilde{b}_A a m_{rs}) f_{PS}^{\text{bare}} \quad .$$



2-point functions: stochastic evaluation

- Generate $U(1)$ random noise source on timeslice t: $\eta_t(x)$
- Solve $\zeta_t^r = a^{-1}\left(D + m_{0,r}\right)^{-1}\gamma_5\eta_t$
- Estimator for the two-point functions:

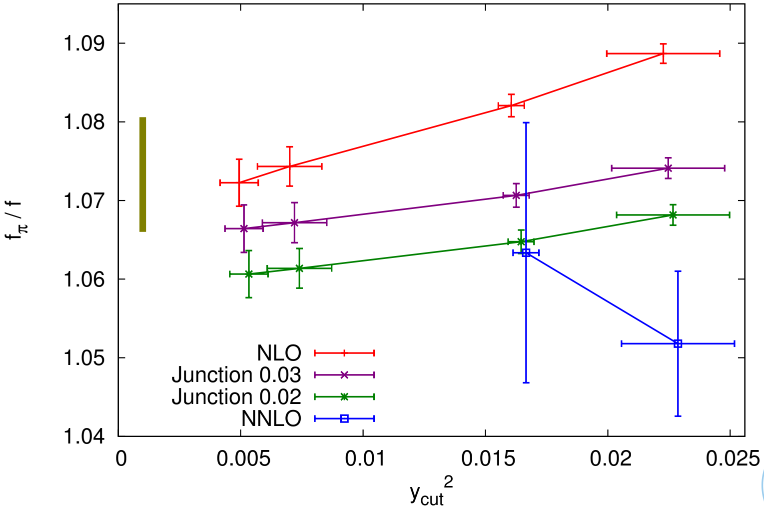
$$
\begin{aligned}
a^3 f_{PP}^{rs}(x_0) &= \sum_{\mathbf{x}} \left\langle\!\!\left\langle \zeta_t^r(x_0+t,\mathbf{x})^\dagger \quad \zeta_t^s(x_0+t,\mathbf{x}) \right\rangle\!\!\right\rangle \quad ; \\
a^3 f_{AP}^{rs}(x_0) &= \sum_{\mathbf{x}} \left\langle\!\!\left\langle \zeta_t^r(x_0+t,\mathbf{x})^\dagger \gamma_5 \zeta_t^s(x_0+t,\mathbf{x}) \right\rangle\!\!\right\rangle \quad ,
\end{aligned}
$$

(averages are over sources and configurations).

ChiPT formulae (LECs: $M, F, \bar\ell_3, \bar\ell_4, \bar\ell_{12}, c_M, c_F$)

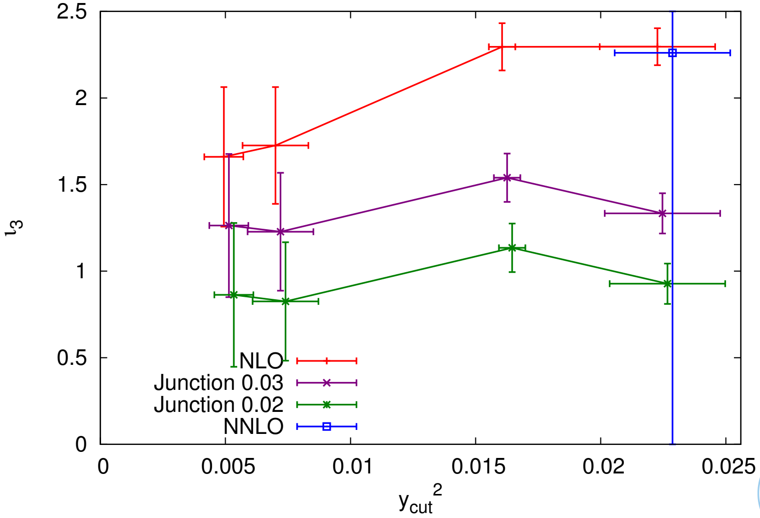
$$
\begin{aligned}
M_\pi^2(\beta,y) &= M_\beta^2 \times \Big\{ 1 - \frac{1}{2}\Big[\bar\ell_3 + 2y_\pi\bar\ell_4 + \log y_\pi\Big]\cdot y + \frac{1}{2}\cdot y\log y \\
&\quad + \Big[c_M + \bar\ell_4 + \frac{1}{4}(\bar\ell_3 + \log y_\pi)^2 + \frac{q_M^2}{90}\Big]\cdot y^2 \\
&\quad - \frac{1}{2}\Big[(\bar\ell_3 + \log y_\pi) + \frac{q_M}{6}\Big]\cdot y^2\log y + \frac{7}{8}\cdot y^2(\log y)^2 \Big\} \quad ; \\
F(\beta,y) &= F_\beta \times \Big\{ 1 + \Big[\bar\ell_4 + \log y_\pi + 2y_\pi\bar\ell_4\Big]\cdot y - 1\cdot y\log y \\
&\quad + \Big[-c_F - 2\bar\ell_4 + (\bar\ell_4 + \log y_\pi)^2 + \frac{q_F^2}{36}\Big]\cdot y^2 \\
&\quad - \Big[2(\bar\ell_4 + \log y_\pi) + \frac{q_F}{6}\Big]\cdot y^2\log y + \frac{5}{4}\cdot y^2(\log y)^2 \Big\} \quad ; \\
q_M &= 60\bar\ell_{12} - 33\bar\ell_3 - 12\bar\ell_4 + 52 + 15\log y_\pi \\
q_F &= 18\bar\ell_4 - 15\bar\ell_{12} + 3\log y_\pi - \frac{29}{2} \quad .
\end{aligned}
$$

Ratio f_π / f



1.09
1.08
1.07
1.06
1.05
1.04
f_π / f
0
0.005
0.01
0.015
0.02
0.025
y_cut^2
NLO
Junction 0.03
Junction 0.02
NNLO

$\bar{\ell}_3$



2.5
2
1.5
1
0.5
0
l3
0
0.005
0.01
0.015
0.02
0.025
ycut 2
NLO
Junction 0.03
Junction 0.02
NNLO
DESY