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 $\chi$PT 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 $\chi$PT 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 $N_{\text{cfg}}$ 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 $M_\pi$ and decay constant $F_\pi$
  - Also with strange quark ($\rightarrow M_K, F_K$)

- Ensembles produced by CLS and analysed by ALPHA
  - 10 to 20 stochastic sources/config. for correlators
  - Typical mass/decay constant known to percent accuracy:

  \[
  \begin{array}{ll}
  m_\pi & = 192 \text{ MeV} \\
  a & = 0.065 \text{ fm} \\
  \frac{L_T}{a} & = 128
  \end{array}
  \]

- 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 $m_\pi$ is 192 MeV
- All systems have $L_T = 2L$ and periodic b.c.

The graph shows:

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

(more chiral = more expensive!)
(finier 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_{\text{exp}} \Rightarrow \sim \rho

  (previously measured) \Rightarrow \text{final error}

- A large contribution to the error from $Z_A$ renorm. factor, e.g. for $F_\pi$:

- 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 (→ infinitely many low-energy constants)
- Written in terms of pion field
- Lowest-order Lagrangian (schematically):

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

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

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

- Starting from one-loop diagrams one get “chiral logs”, e.g. $M^2 \log(M^2)$
SU(2) $\chi$PT for pion quantities

Consider (as functions of quark mass and lattice spacing)

$$M_\pi, \quad F_\pi$$

and build

$$y = \frac{M^2_\pi}{8\pi^2 F^2_\pi} \quad \text{i.e.} \quad y_{\text{chir}} = 0, \quad y_{\text{phys.}} = y_\pi \simeq 0.013$$

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

$$M^2_\pi = M^2 \left\{ 1 + y + y \log y + y^2 + y^2 \log y + y^2(\log y)^2 \ldots \right\}$$

$$F_\pi = \underbrace{F}_{\text{LO}} \left\{ 1 + y + y \log y + y^2 + y^2 \log y + y^2(\log y)^2 \ldots \right\} \underbrace{1}_{\text{NLO}} \underbrace{1}_{\text{NNLO}}$$

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

- 15 Ensembles \( \times \{ F_\pi, M_\pi \} \rightarrow 30 \) datapoints to fit (simultaneous fits to all of them)

- Which fit function?
  - Truncate to NLO
  - NLO + linear (“junction”) \( \Rightarrow \)
  - Full-fledged NNLO fit

- These choices + fit-range cuts \([m_\pi \leq 650, 500, 390, 345 \text{ MeV}]\)

\( \Rightarrow \) systematic uncertainties on the outcome

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Chiral point in \( N_f = 2 \) simulations

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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 $\Sigma$!
    (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 $\ell_3, \ell_4$: (note $\ell_i = \log(\Lambda^2_i/M_{\pi,\text{phys}}^2)$)
  There are several estimates, uncertainty about 20% [FLAG 2013]

- NNLO LECs $\ell_{12}, c_M, c_F$:
  Nowadays still virtually undetectable
  E.g. [BWM Collaboration ’13] quote (w/ grain of salt) errors of 30-70%
All data coming from lattice are *adimensional* ("lattice units"): e.g. $M = a m$ and not $m$ itself.

"Setting the scale" means: finding $a$ in fermi.

To do this, choose an observable (e.g. kaon decay constant) and:

\[ \text{measure } F_K \Rightarrow \text{set } F_K = a \cdot f_K \equiv 155 \text{ MeV} \Rightarrow a = \cdots \text{ fm} \]

Once this is done, all other quantities can be *made physical*.
Here, $F_K$ is used to set the scale

As for $F_\pi$, measurements at various quark masses and chiral fits!

Can compare two ways to get to physical point:
(each requiring its own version of $\chi$PT)

- 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)
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)

Can $\chi$PT be trusted there? How much?

Effect of this all:

For $F_\pi$ (phys. point) and $\Sigma$, “no big deal”

For $y \to 0$ extrapolations and (N)NLO low-energy constants: large systematic uncertainty!
Fit curves 1: $F_{\pi}$

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

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Chiral point in $N_f = 2$ simulations
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Fit curves 1: $F_\pi$ (zoom for $\beta = 5.3$)

All fits have 7 total free parameters except NNLO (10).
Fit curves 2: $M_{\pi}^2$

- NLO, 500 MeV
- NLO, 345 MeV
- Junction 0.02, 500 MeV
- NNLO, 500 MeV

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Fit-range dependence corroborates NNLO result.

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Chiral point in $N_f = 2$ simulations

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

Final answer: $f_\pi = 129.7 \pm 1.1$ MeV [i.e. $\sqrt{2}(91.71 \pm 0.78)$].
Practically trouble-free. In the continuum and chiral limits:

\[ \sqrt[3]{\Sigma} = 269 \pm 3_{\text{stat}} \pm 4_{\text{syst}} \text{ MeV} \quad \overline{\text{MS}}(2 \text{ GeV}) \]
Condensate, $N_f = 2$ determinations [FLAG 2013 prelim. report]

This analysis

Σ₀^{1/3} [MeV]
Trust in NNLO here, $\ell_4 = 3.3 \pm 0.9_{\text{stat.}} \pm 2_{\text{syst.}}$

NLO looks more convincing – cf. latest world-average of $4.59 \pm 0.26$

Can’t say much for $\ell_3 \sim 2.26 \pm \infty$!

(believed to be in fact around 3.5)

NNLO: just mentioning $\ell_{12} \sim 1.6$, $c_F \sim -19$, $c_M \sim -10$
Closing remarks

- Chiral condensate and pion decay constant: well determined – stable and with percent accuracy
- But, as opposed to analogous $F_K$ analysis,
  - NLO $\chi$PT 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 $N_F = 2 + 1$
  (guess: the same precocious breakdown of NLO will be seen there)
The End.
Slow modes in autocorrelation analysis

(Integrated autocorrelation time “converts naïve error into actual one”:

\[
\sigma^2 = \frac{2\tau_{\text{int}}^0}{N} \Gamma(0) ; \quad \tau_{\text{int}}^0 = \frac{1}{2} + \sum_{t=1}^{\infty} \rho(t) \quad \text{with} \quad \rho(t) = \frac{\Gamma(t)}{\Gamma(0)}
\]

In practice, signal on \( \rho \) soon lost: danger!

(\text{despite trying to balance uncertainty in } \rho \text{ and remainder of the tail})

Observable can couple, undetected, to a slow mode

\( \Rightarrow \) underestimation of error!

\textbf{Solution}: where the measured \( \rho \) 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: \( \tau_{\text{int}} = \tau_{\text{int}}^0 + \tau_{\exp} \rho(W) \)
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- All systems have $L_T = 2L$ and periodic b.c.

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Chiral point in $N_f = 2$ simulations

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From 2-point functions to PCAC masses

Define

\[ P^{rs} = \overline{\psi}_r \gamma_5 \psi_s ; \quad A_0^{rs} = \overline{\psi}_r \gamma_0 \gamma_5 \psi_s \]

with the 2-point functions

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

one finds

\[ \frac{1}{2} \left( \partial_0 + \partial_0^* \right) f_{AP}(x_0) + c_A a \partial_0^* \partial_0 f_{PP}(x_0) \]

\[ \frac{1}{2f_{PP}(x_0)} \rightarrow m_{rs} , \quad x_0 \rightarrow \infty , \]

renormalised then as:

\[ m_{R}^{rs} = \frac{Z_A}{Z_P} \frac{(1 + \overline{b}_A a m_{\text{sea}} + \tilde{b}_A a m_{rs}) m_{rs}}{(1 + \overline{b}_P a m_{\text{sea}} + \tilde{b}_P a m_{rs})} m_{rs} . \]
From 2-point functions to $m_{PS}$ and $f_{PS}$

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

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

![Graph showing measured points and one-state fit.](image)
Generate $U(1)$ random noise source on timeslice $t$: $\eta_t(x)$

Solve $\zeta'_t = a^{-1}(D + m_{0,r})^{-1}\gamma_5\eta_t$

Estimator for the two-point functions:

\[
a^3 f^{rs}_{PP}(x_0) = \sum_x \left\langle \zeta'^r_t(x_0 + t, x) \dagger \zeta^s_t(x_0 + t, x) \right\rangle ;
\]

\[
a^3 f^{rs}_{AP}(x_0) = \sum_x \left\langle \zeta'^r_t(x_0 + t, x) \dagger \gamma_5 \zeta^s_t(x_0 + t, x) \right\rangle ,
\]

(averages are over sources and configurations).
ChiPT formulae (LECs: $M$, $F$, $\ell_3$, $\ell_4$, $\ell_{12}$, $c_M$, $c_F$)

\[
M^2_\pi(\beta, y) = M^2_\beta \times \left\{ 1 - \frac{1}{2} \left[ \ell_3 + 2y_\pi \ell_4 + \log y_\pi \right] \cdot y + \frac{1}{2} \cdot y \log y \\
+ \left[ c_M + \ell_4 + \frac{1}{4} (\ell_3 + \log y_\pi)^2 + \frac{q_M^2}{90} \right] \cdot y^2 \\
- \frac{1}{2} \left[ (\ell_3 + \log y_\pi) + \frac{q_M}{6} \right] \cdot y^2 \log y + \frac{7}{8} \cdot y^2 (\log y)^2 \right\};
\]

\[
F(\beta, y) = F_\beta \times \left\{ 1 + \left[ \ell_4 + \log y_\pi + 2y_\pi \ell_4 \right] \cdot y - 1 \cdot y \log y \\
+ \left[ -c_F - 2\ell_4 + (\ell_4 + \log y_\pi)^2 + \frac{q_F^2}{36} \right] \cdot y^2 \\
- \left[ 2(\ell_4 + \log y_\pi) + \frac{q_F}{6} \right] \cdot y^2 \log y + \frac{5}{4} \cdot y^2 (\log y)^2 \right\};
\]

\[
q_M = 60\ell_{12} - 33\ell_3 - 12\ell_4 + 52 + 15 \log y_\pi
\]

\[
q_F = 18\ell_4 - 15\ell_{12} + 3 \log y_\pi - \frac{29}{2}.
\]
Ratio $f_\pi/f$

![Graph showing the ratio $f_\pi/f$ as a function of $y_{cut}^2$ with different lines representing NLO, Junction 0.03, Junction 0.02, and NNLO.]
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