# $\eta,~\eta^\prime$ mixing from the lattice

Konstantin Ottnad

Institut für Kernphysik, Johannes Gutenberg-Universität Mainz

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Introducti	on				

Quarks cannot be observed directly but are bound in hadrons (at low energies):

- The lightest hadrons  $\pi^{\pm}$ ,  $\pi^{0}$ ,  $K^{\pm}$ ,  $K^{0}$ ,  $\bar{K}^{0}$ ,  $\eta$  ("octet mesons") have masses from 135 MeV to 548 MeV.
- In addition there is a "flavor-singlet", the  $\eta'$ .
- For exact flavor symmetry  $(m_u = m_d = m_s)$  all 9 mesons should have the same mass.

However:  $M_{n'} \approx 958 \,\mathrm{MeV} \gg M_{octet}$ 

Theoretical solution to this puzzle in QCD:

• Large mass of the  $\eta'$  is caused by the QCD vacuum structure and the  $U(1)_A$  anomaly. Weinberg (1975), Belavin et al. (1975), t'Hooft (1976), Witten (1979), Veneziano (1979)

 The U(1) axial current is anomalously broken, i.e. even for m<sub>q</sub> = 0: Adler (1969), Jackiw and Bell (1969)

$$\partial_{\mu}A^{0}_{\mu} = \frac{N_{f}g^{2}}{32\pi^{2}}G^{a}_{\mu\nu}\tilde{G}^{a,\mu\nu} \neq 0$$

- Instantons with non-trivial topology provide non-perturbative explanation. Belavin et al. (1975), t'Hooft (1976)
- The flavor-singlet η' remains massive as m<sub>l</sub>, m<sub>s</sub> → 0.

# Does lattice QCD reproduce the large $\eta'$ mass from first principles?

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For exact SU(3) flavor symmetry one expects

- Flavor octet state  $|\eta_8\rangle = \frac{1}{\sqrt{6}}(|\bar{u}u\rangle + |\bar{d}d\rangle 2|\bar{s}s\rangle)$  (Pseudo-Goldstone boson)
- Flavor singlet state  $|\eta_0\rangle = \frac{1}{\sqrt{3}}(|\bar{u}u\rangle + |\bar{d}d\rangle + |\bar{s}s\rangle)$  (related to  $U(1)_A$  anomaly)

However, SU(3) flavor symmetry is broken by large  $m_s \gg m_u \approx m_d \equiv m_l$ :

• Physical  $\eta$ ,  $\eta'$  states are not flavor eigenstates but **mixtures**, e.g.

$$\begin{pmatrix} |\eta\rangle \\ |\eta'\rangle \end{pmatrix} = \begin{pmatrix} \cos\phi_l & -\sin\phi_s \\ \sin\phi_l & \cos\phi_s \end{pmatrix} \begin{pmatrix} |\eta_l\rangle \\ |\eta_s\rangle \end{pmatrix}$$

in the quark flavor basis  $|\eta_l\rangle = \frac{1}{\sqrt{2}}(|\bar{u}u\rangle + |\bar{d}d\rangle), \quad |\eta_s\rangle = |\bar{s}s\rangle.$ 

- In nature further mixing possible, e.g. with  $\pi^0$  ( $m_u \neq m_d$ ),  $\eta_c$  (including c quark)
- How did nature arrange the mixing pattern?

# Use lattice QCD to determine the mixing parameters.

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Outline					

- **1**  $\eta, \eta'$  in Lattice QCD
- 2 Lattice setup
- **③** Physical extrapolations for  $M_{\eta,\eta'}$  and mixing parameters
- Model averages and (preliminary!) results

#### Contributions by many collaborators over the years:

Krzysztof Cichy Elena Garcia-Ramos Karl Jansen Bastian Knippschild Liuming Liu Marcus Petschlies \* Siebren Reker Urs Wenger \* Falk Zimmermann Petros Dimopoulos Christopher Helmes Christian Jost Bartosz Kostrzewa\* Chris Michael Ferenc Pittler \* Carsten Urbach \* Markus Werner ut ended Twister

people involved in the current analysis (this work)

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Information on masses and mixing is encoded in (expectation values of) meson two-point correlation functions:

$$\mathcal{C}_{ij}\left(t
ight)\sim\sum_{ec{ extsf{x}}}\left\langle 0
ight| \left. \textit{O}_{i}\left( extsf{x}
ight) \textit{O}_{j}^{\,\dagger}\left(0
ight) \left|0
ight
angle$$

• For  $\eta$ ,  $\eta'$  use local, pseudoscalar interpolating operators  $O_{i,j}$ :

$$\eta_l = rac{1}{\sqrt{2}} (ar{u} i \gamma_5 u + ar{d} i \gamma_5 d), \qquad \eta_s = ar{s} i \gamma_5 s, \qquad \eta_c = ar{c} i \gamma_5 c$$

• For e.g. 
$$i = j$$
:  $C_{ii}(t) = \sum_{n} \frac{\left|\langle 0|O_i|n\rangle \right|^2}{2M_n} \exp\left(-M_n t\right) \stackrel{t \gg 0}{\longrightarrow} \frac{\left|\langle 0|O_i|n\rangle \right|^2}{2M_\eta} \exp\left(-M_\eta t\right)$ 

 $\rightarrow$  Ground state mass  $M_\eta$  can be extracted directly at sufficiently large t.

 $\rightarrow$  Decay constants / mixing parameters related to physical amplitudes  $A_i^n = \langle 0 | O_i | n \rangle$ .

• Information on higher states ( $\eta'$ ) from solving GEVP:  $C(t)v^{(n)}(t,t_0) = \lambda^{(n)}(t,t_0)C(t_0)v^{(n)}(t,t_0)$ 

 $\rightarrow$  Eigenvalues  $\lambda^{(n)}(t, t_0)$  give mass of *n*-th state at  $t \gg 0$ .

 $\rightarrow$  Eigenvectors  $v^{(n)}(t, t_0)$  carry information on physical amplitudes  $A^{\eta, \eta', \dots}_{l,s,c,\dots}$ 

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# Quark disconnected diagrams

• Consider 
$$O_i = O_j = \eta_l$$

$$\begin{aligned} \mathcal{C}_{II}(t) &\sim \sum_{\vec{x}} \langle 0 | \, \bar{u}(x) i \gamma_5 u(x) \bar{u}(0) i \gamma_5 u(0) | 0 \rangle \\ &\sim \mathrm{tr} \left[ D_{0t}^{-1} \gamma_5 D_{t0}^{-1} \gamma_5 \right] + \mathrm{tr} \left[ D_{tt}^{-1} \gamma_5 \right] \mathrm{tr} \left[ D_{00}^{-1} \gamma_5 \right] \end{aligned}$$

Quark connected and disconnected pieces:

Lattice Dirac operator D<sub>xy</sub> is a very large (3 · 4 · L<sup>3</sup> · T) × (3 · 4 · L<sup>3</sup> · T) – matrix



Quark-connected and disconnected correlators;  $M_{\pi}=139\,{
m MeV},~a=0.080\,{
m fm}$ 

• Disconnected diagrams need all-to-all propagator  $D_{xx}^{-1} \Rightarrow$  prohibitively expensive

Use stochastic method + one-end trick instead

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# Quark disconnected diagrams

• Consider 
$$O_i = O_j = \eta_I$$

$$\begin{split} \mathcal{C}_{II}(t) &\sim \sum_{\vec{x}} \langle 0 | \, \bar{u}(x) i \gamma_5 u(x) \bar{u}(0) i \gamma_5 u(0) | 0 \rangle \\ &\sim \mathrm{tr} \left[ D_{0t}^{-1} \gamma_5 D_{t0}^{-1} \gamma_5 \right] + \mathrm{tr} \left[ D_{tt}^{-1} \gamma_5 \right] \mathrm{tr} \left[ D_{00}^{-1} \gamma_5 \right] \end{split}$$

Quark connected and disconnected pieces:



Lattice Dirac operator D<sub>xy</sub> is a very large (3 · 4 · L<sup>3</sup> · T) × (3 · 4 · L<sup>3</sup> · T) – matrix



Quark-connected vs. full correlators;  $M_{\pi} = 139 \,\mathrm{MeV}, a = 0.080 \,\mathrm{fm}$ 

 $\rightarrow$  Severe signal-to-noise problem; signal typically lost at  $t \gtrsim 1 \, \text{fm} \dots$ 

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# How to tackle the signal-to-noise problem?

Assumption:

Disconnected diagrams couple only to  $\eta$ ,  $\eta'$ .

- No signal-to-noise problem in quark-connected contribution.
- Replace connected contributions by respective ground state contributions.
   PRD 64 (2001), 114509. EPJ C58 (2008), 261-269
   PRL 111 (2013) 18, 181602
- Charm quark contributions are neglected (they are very small)
- If this assumption is correct we should see a plateau at very small values of  $t/a \dots$



Connected contribution with and w/o excited states  $M_\pi = 270\,{\rm MeV},\; a = 0.78\,{\rm fm}$ 

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... We observe plateaux in both states starting at very small values of t.

- M<sub>η</sub> agrees very well with asymptotic behavior of M<sub>η</sub>(t) from standard method.
- Significant improvement in the statistical error for M<sub>η</sub>.
- Can check validity of assumption from Monte-Carlo data.



In finite volume and for fixed top. charge  $Q_t$  one finds

$$\langle \omega(x)\omega(0) \rangle_{Q_t=\mathrm{fixed}} 
ightarrow rac{1}{V} \left( \chi_t - rac{Q_t^2}{V} + rac{c_4}{2V\chi_t} 
ight) + \dots,$$

for correlators of winding number densities  $\omega(x)$  at large |x|.

S. Aoki et al., Phys.Rev. D76, 054508 (2007)

 $\Rightarrow$  Expect constant offset in  $\eta'(\eta)$  correlator at large *t*:

$$<\lambda^{\eta'}(t)>_{Q_t= ext{fixed}}\rightarrow\sim rac{a^5}{T}\left(\chi_t-rac{Q_t^2}{V}+rac{c_4}{2V\chi_t}
ight).$$





 $\eta, \eta'$  principal correlators  $M_{\pi} = 137 \,\mathrm{MeV}, \ a = 0.068 \,\mathrm{fm}, \ L \approx 5.4 \,\mathrm{fm}$ 

- Always present for finite volume + finite statistics.
- Often masked by statistical point errors!
- (Correlated) Noise in 
   <sup>'</sup>
   <sup>'</sup>
   signal largely due to fluctuation + autocorrelation of this constant.



Topological finite volume effect (II)



#### Simple but efficient way to correct for this effect:

Remove constant using discrete derivative correlator:

$$C(t) \rightarrow \tilde{C}(t) = C(t) - C(t + \Delta t)$$

- Resulting data are much less correlated.
- Further analysis (GEVP, physical extrapolation) can be carried out in the standard way.

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How to ol	otain physical	results?				

- Fix bare parameters (a, m<sub>1</sub>, m<sub>s</sub>,...):
  - Use known hadronic quantities (e.g.  $M_{\pi}^{\text{phys}}$ ,  $M_{K}^{\text{phys}}$ , ...)  $\rightarrow$  Further observables are predictions.

#### Control discretization effects:

- Simulate at different (small) values of a.
- Perform continuum extrapolation.
- With modern LQCD calculations lattice artifacts are typically  $\propto a^2$ .
- Correct for unphysical quark masses:
  - Simulate at several light and strange quark masses, or tune  $m_s = m_s^{\rm phys}$
  - Perform chiral extrapolation.
  - State-of-the-art lattice simulations include physical quark masses.

#### • Control finite volume effects:

- Simulate several physical volumes.
- Perform infinite volume extrapolation OR correct for finite volume effects (if possible)

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Lattice set	tup					

ID	β	a/fm	T/a	L/a	$M_{\pi}/\mathrm{MeV}$	$M_{\pi}L$	$N_{\rm conf}$	$\Delta N_{ m conf}$
cA211.12.48	1.726	0.0922	96	48	172	3.85	287	4
cA211.15.48			96	48	191	4.27	1853	2
cA211.30.32			64	32	268	4.01	1261	4
cA211.40.24			48	24	311	3.48	1320	2
cA211.53.24			48	24	357	4.00	624	8
cB211.072.64	1.778	0.0800	128	64	139	3.62	779	4
cB211.14.64			128	64	193	5.01	456	4
cB211.25.48			96	48	257	5.01	574	2
cB211.25.32			64	32	260	3.37	989	1
cB211.25.24			48	24	271	2.64	654	4
cC211.06.80	1.836	0.0684	160	80	137	3.80	738	4
cC211.20.48			96	48	248	4.12	611	4
cD211.054.96	1.900	0.0573	192	96	139	3.89	492	2

- Gauge configurations generated by the Extended Twisted Mass Collaboration (ETMC).
- $N_f = 2 + 1 + 1$  flavors of Wilson Clover twisted-mass sea quarks. PRD 98 (2018) 054518 PRD 104 (2021) 074520
- Automatic O(a) improvement at maximal twist. JHEP 08 (2004) 007 JHEP 10 (2004) 070
- Degenerate light quark doublet, i.e.  $m_u^{\text{sea}} = m_d^{\text{sea}}$ .
- Non-degenerate heavy quark doublet with  $m_s^{\text{sea}} = \text{phys}$ ,  $m_c^{\text{sea}} = \text{phys}$ .

New action and (much) more chiral + finer ensembles compared to "old" analysis (2012–2018) JHEP 11 (2012) 048, PRL 111 (2013) 18, 181602, JHEP 09 (2015) 020, PRD 97 (2018) 5, 054508

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a/fm	T/a	L/a	$M_{\pi}/\mathrm{MeV}$	$M_{\pi}L$	$N_{ m conf}$	$\Delta N_{ m conf}$
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	a/fm 0.0922 0.0800 0.0684 0.0573	a/fm T/a 0.0922 96 96 64 48 0.0800 128 96 64 48 0.0684 160 96 0.0573 192	a/fm         T/a         L/a           0.0922         96         48           96         48         64           64         32         48           48         24         48           0.0800         128         64           128         64         32           48         24         48         24           0.0800         128         64         32           48         24         48         24           0.0800         128         64         32           48         24         32         48         24           0.0684         160         80         96         48           0.0573         192         96         96	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$ \begin{array}{c c c c c c c c c c c c c c c c c c c $

#### • Ensembles cover four values of the lattice spacing a

- $\rightarrow$  continuum extrapolation
- Various physical volumes with  $L \approx 2...5.5 \,\text{fm}$ ,  $2.6 \le M_{\pi}L \le 5.0$ .
  - $\rightarrow$  extrapolation to infinite volume / check for finite size effects.
- Pion masses from  $\sim 140 \,\mathrm{MeV}$  to  $\sim 360 \,\mathrm{MeV}$ ; six boxes with  $M_{\pi} < 200 \,\mathrm{MeV}$ .
  - $\rightarrow$  chiral extrapolation and checking its convergence
- Three boxes at physical quark masses.

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- Many different physical volumes with L ≈ 2...5.5 fm, 2.6 ≤ M<sub>π</sub>L ≤ 5.0.
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In this study we use a mixed action setup

$$\mathcal{S} = \mathcal{S}_{\mathcal{G}}[U] + \mathcal{S}_{\mathcal{F}}^{\text{sea}}[\psi_{l}, \psi_{h}, U] + \mathcal{S}_{\mathcal{F}}^{\text{val}}[\{q_{f}, q_{f}'\}, U] + \text{ghosts},$$

where

- S<sub>G</sub>[U] is the Iwasaki gauge action. Nucl. Phys. B 258 (1985) 141
- $S_F^{\text{sea}}[\psi_l, \psi_h, U]$  is the Wilson clover twisted-mass action with  $\psi_l = (u_{\text{sea}}, d_{\text{sea}})^T$  and  $\psi_h = (c_{\text{sea}}, s_{\text{sea}})^T$ .
- $S_F^{\text{val}}[\{q_f, q_f'\}, U]$  is the Osterwalder-Seiler action for quark flavors  $f = u, d, s, \dots$  Annals Phys. 110 (1978) 440

This setup has several advantages over a unitary setup:

- Avoids strange-charm mixing through cutoff effects.
- One-end trick variance reduction can be used for heavy quarks (i.e. for the strange).
- Preserves automatic O(a)-improvement.

Physical results require fixing  $\mu_s$  by matching with an observable and taking the continuum limit:

- Compute all the desired observables for a set of μ<sub>s</sub> values at each β.
- Perform linear interpolation of observables to target µ<sub>s</sub> value.

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μ <sub>s</sub> –matchi	ng				



We employ four choices for the  $\mu_s$  matching conditions

"Ω-matching": m<sub>Ω</sub>(M<sup>phys</sup><sub>π</sub>, β) = m<sup>phys</sup><sub>Ω</sub> → μ<sub>s</sub>(β).
 "kaon-matching": M<sub>K</sub>(M<sub>π</sub>, β) = M<sup>phys</sup><sub>K</sub> → μ<sub>s</sub>(M<sub>π</sub>, β).
 "η<sub>s</sub>-matching": M<sub>ηs</sub>(M<sub>π</sub>, β) = M<sup>phys</sup><sub>ηs</sub> → μ<sub>s</sub>(M<sub>π</sub>, β) using M<sup>phys</sup><sub>ηs</sub> = 689.89 MeV. Nature 593 (2021) 7857, 51-55
 Using LO χPT proxy for μ<sub>s</sub>, i.e. M<sup>2</sup><sub>K</sub> - <sup>1</sup>/<sub>2</sub>M<sup>2</sup><sub>π</sub> = phys → μ<sub>s</sub>(M<sub>π</sub>, β).
 Different choices lead to different slopes ~ a<sup>2</sup> for continuum extrapolation (+ higher order effects).

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Mixing observables							

Decay constants  $f_{\rm P}^i$  are defined from axial-vector matrix elements (amplitudes)

$$\langle 0 | A^{i}_{\mu} | P(p) \rangle = i f^{i}_{P} p_{\mu} , \qquad P = \eta, \eta' ,$$

On the lattice: quark flavor basis (i=l,s) is a more "natural" choice

$$A'_{\mu} = rac{1}{\sqrt{2}} (ar{u} \gamma_{\mu} \gamma_5 u + ar{d} \gamma_{\mu} \gamma_5 d), \qquad A^s_{\mu} = ar{s} \gamma_{\mu} \gamma_5 s.$$

 $\eta$  and  $\eta'$  are not flavor eigenstates; most general parametrization:

$$\begin{pmatrix} f_{\eta}^{l} & f_{\eta}^{s} \\ f_{\eta'}^{l} & f_{\eta'}^{s} \end{pmatrix} = \begin{pmatrix} f_{l}\cos\phi_{l} & -f_{s}\sin\phi_{s} \\ f_{l}\sin\phi_{l} & f_{s}\cos\phi_{s} \end{pmatrix}$$

From  $\chi$ PT one expects  $|\phi_l - \phi_s|$  to be small, i.e.  $\frac{|\phi_l - \phi_s|}{|\phi_l + \phi_s|} \ll 1$ 

- $|\phi_l \phi_s| \sim \frac{1}{N_c}$  is OZI-suppressed, unlike e.g.  $|\phi_0 \phi_8|$  which receives  $SU(3)_F$ -breaking contributions.
- Small difference in one basis does NOT imply small difference in another basis!

$$\Rightarrow \text{Approximate, single angle } \phi \approx \phi_l \approx \phi_s \text{ (FKS) scheme: } \tan^2(\phi) = -\frac{f_l^{\eta'} f_s^{\eta}}{f_l^{\eta} f_s^{\eta'}}.$$

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Mixing of	servables				

Axial vector matrix elements are very noisy  $\Rightarrow$  Difficult to directly determine  $\phi_{l,s}$  and  $f_{l,s}$ .

Consider pseudoscalar matrix elements

$$h^i_{\mathrm{P}} = 2m_i < 0 | \boldsymbol{P}^i | \mathrm{P} >, \quad \mathrm{P} = \eta, \eta' \,,$$

which can be related to axial vector ones via the anomaly equation using  $\chi PT$ :

$$\begin{pmatrix} h_{\eta}^{l} & h_{\eta}^{s} \\ h_{\eta'}^{l} & h_{\eta'}^{s} \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \operatorname{diag} \left( f_{l} M_{\pi}^{2}, f_{s} \left( 2M_{K}^{2} - M_{\pi}^{2} \right) \right) \,.$$

Th. Feldmann et al., PRD 58 (1998), 114006 Th. Feldmann et al., Phys.Lett. B449 (1999) 339-346

- This expression holds to LO χPT.
- Scale dependence due to Z<sup>0</sup><sub>A</sub> is neglected; expect deviations at high(er) energies. → cf. recent study by the Regensburg group (RQCD) on CLS ensembles JHEP 08 (2021) 137
- $\phi$  does not depend on renormalization at all,  $f_{l,s}$  depend only on  $Z_P/Z_S$ .
- Can check whether  $|\phi_l \phi_s|$  is small!

Introduction	$\eta,\eta'$ in LQCD	Setup	Physical extrapolations	Results	Summary & Outlook
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# Chiral, continuum and finite size (CCF) fit models

We use the following, basic ansätze for physical extrapolations:

$$M_{\eta}^{2} = A_{0}(m_{l} + 2m_{s}) + B_{0}a^{2}, \qquad (1)$$

$$M_{\eta'}^2 = \dot{M}_0^{SU(3)} + A_1(2m_l + m_s) + B_1 a^2, \qquad (2)$$

$$\phi = \operatorname{atan}(\sqrt{2}) + A_2(m_l - m_s) + B_2 a^2, \qquad (3)$$

$$f_{\{l,s\}} = \mathring{f}_{\{l,s\}}^{SU(2)} + A_{\{3,4\}} m_l + B_{\{3,4\}} a^2, \qquad (4)$$

$$f_{\{l,s\}}/f_{\{\pi,K\}} \equiv R_{l,s} = \mathring{R}_{l,s}^{SU(2)} + A_{\{5,6\}} m_l + B_{\{5,6\}} a^2,$$
(5)

• where 
$$m_l \cong M_\pi^2$$
 and  $m_s \cong (2M_K^2 - M_\pi^2)$ ,

• and  $\mathring{M}_{0}^{SU(3)}$ ,  $\mathring{f}_{l,s}^{SU(2)}$ ,  $\mathring{R}_{l,s}^{SU(2)}$ ,  $A_i$ ,  $B_i$  are free parameters of the fits.

Additional fit models are obtained by any combination of the following changes:

- including a term  $C_i \frac{M_{\pi}^2}{\sqrt{M_{\pi}L}} e^{-M_{\pi}L}$  (not for  $M_{\eta}^2$ ;  $M_{\pi,K,\eta}$  are explicitly FS-corrected Nucl.Phys.B 721 (2005) 136-174)
- including a term D<sub>i</sub> M<sup>4</sup><sub>π</sub>,
- with and w/o explicit m<sub>s</sub> dependence (where applicable),
- applying a data cut  $\in \{ \text{no cut}, M_{\pi} < 270 \, \text{MeV}, a < 0.08 \, \text{fm}, M_{\pi}L > 3.5 \}.$

All statistical errors are computed using the non-parametric (binned) bootstrap  $N_B = 10000$ .

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Introduction	$\eta, \eta'$ in LQCD	Setup	Physical extrapolations	Results	Summary & Outlook





- Light chiral extrapolation very mild.
- Steep continuum extrapolation for M<sub>η</sub>, i.e. up to ~ 30% corrections.
- $M_{\eta'}$  tends to be overfitted.
- Physical results in good agreement with experiment.
- Statistically precise results, i.e.  $\Delta M_{\eta}/M_{\eta} \sim 1\%..2\%, \ \Delta M_{\eta'}/M_{\eta'} \sim 2\%..3\%$



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Data cuts	$-M_n, M_{n'}$				



- Cuts in  $M_{\pi}$ , a typically reduce  $\chi^2/N_{
  m dof}$  for  $M_{\eta}$
- Here: M<sub>π</sub>L cut has virtually no effect.
   → similar for adding an explicit FS term
- Physical results remain very stable.
- Statistical errors may increase (as expected).





### Physical extrapolation for $\phi$ – comparison of $\mu_s$ -matchings



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Physical extrapolations for  $\phi$ ,  $\phi_I$ ,  $\phi_s$ 



- Data for  $\phi_l$ ,  $\phi_s$  even more precise than for  $\phi$ .
- Results for  $\phi_l$  and  $\phi_s$  almost identical.
- $\phi$  and  $\phi_{I,s}$  differ by  $1\sigma 2\sigma$ .
- Some tension fitting full set of data with basic fit ansatz
- $\chi^2/N_{\rm dof}$  improved by e.g. applying cut in  $M_{\pi}$ .



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- Data for f<sub>s</sub> tends to be more statistically precise; less fluctuations.
- Fits generally work much better for  $f_s$ .  $\rightarrow$  already seen in "old" analysis PRD 96 (2018) 5, 054508 However: data more chiral, i.e.  $M_{\pi} \in \{140...360 \,\mathrm{MeV}\}$  vs  $M_{\pi} \in \{230...500 \,\mathrm{MeV}\}$ )
- Ratios  $f_l/f_{\pi}$  and  $f_s/f_K$  may cancel some quark mass and FS effects.

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- Data for f<sub>s</sub> tends to be more statistically precise; less fluctuations.
- Fits generally work much better for  $f_5$ .  $\rightarrow$  already seen in "old" analysis PRD 96 (2018) 5. 054508 However: data more chiral, i.e.  $M_{\pi} \in \{140...360 \,\mathrm{MeV}\}$  vs  $M_{\pi} \in \{230...500 \,\mathrm{MeV}\}$ )
- Ratios  $f_l/f_{\pi}$  and  $f_s/f_K$  may cancel some quark mass and FS effects.
- Applying cuts, e.g.  $M_{\pi}L > 3.5$  and including finite size term  $\sim e^{-M_{\pi}L}$  improves fits.

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Model aver	aging				

We assign a weight to each fit

Phys. Rev. D 103,114502 (2021)

$$w_i \sim e^{-\frac{1}{2} \left( \chi^2 + 2(N_{\rm para} - N_{\rm prio}) - 2N_{\rm data} \right)}, \quad N_{\rm prio} = 0.$$

Central value and total err for an observable y are given by median and the 16% and 84% percentiles of the CDF

$$CDF(y,\lambda) = \int_{-\infty}^{y} d\tilde{y} \sum_{i} w_{i} N(\tilde{y}, m_{i}, \sigma_{i} \sqrt{\lambda}).$$

Statistical ( $\sigma_{\rm stat}$ ) and systematic ( $\sigma_{\rm sys}$ ) errors are separated by solving

$$\lambda \sigma_{\rm stat}^2 + \sigma_{\rm sys}^2 = \left(\frac{y_{\rm hi} - y_{\rm lo}}{2}\right)^2 \quad {\rm where} \quad {\it CDF}(y_{\rm hi}, \lambda) = 0.84\,, \quad {\rm and} \quad {\it CDF}(y_{\rm lo}, \lambda) = 0.16\,,$$

where  $\lambda$  is used to rescale the statistical errors  $_{\it Nature \ 593\ (2021)\ 7857,\ 51-55}$ 

The set of models for each observable is given by

$$\{\mu_s\text{-matchings}\}\bigotimes\{\text{CCF models}\}\bigotimes\{\text{data cuts}\}$$
(6)

Typically, this yields  $\mathcal{O}(100)$  models per observable:

$$\# \left\{ \mu_s \text{-matchings} \right\} = 4 \,, \qquad 4 \leq \# \left\{ \text{CCF models} \right\} \leq 8 \,, \qquad \# \left\{ \text{data cuts} \right\} = 4 \,.$$

Introduction $\eta, \eta'$ in LQCD	Setup	Physical extrapolations	Results	Summary & Outlook
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### Masses



- Agreement with experiment  $(M_{\eta}^{exp} = 547.862(17) \,\mathrm{MeV}, M_{\eta'}^{exp} = 957.78(6) \,\mathrm{MeV}).$
- Error on M'<sub>n</sub> improved by factor ~ 3 compared to our previous results

$$M_{\eta} = 557(11)_{\text{stat}}(03)_{\chi PT} \text{ MeV}, \quad M'_{\eta} = 911(64)_{\text{stat}}(03)_{\chi PT} \text{ MeV}$$

PRD 97 (2018) 5, 054508 PRL 111 (2013) 18, 181602

- Improved control over systematic effects (chiral + continuum + FS).
- Scale is set using  $\sqrt{t_0^{
  m phys}}=0.14436(61)\,{
  m fm}.$  PRD 104 (2021) 7, 074520

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Introduction	$\eta,\eta'$ in LQCD	Setup	Physical extrapolations	Results	Summary & Outlook



- $\Delta \phi$  improved by factor ~ 1.5 compared to old result  $\phi = 38.8(2.2)_{\text{stat}}(2.4)^{\circ}_{\chi PT}$ . PRD 97 (2018) 5, 054508
- Value for \u03c6 mostly in agreement with pheno determinations, e.g.

	$\phi_l$	$\phi_s$	
R. Escribano et al. (2016)	39.6(2.3)°	$40.8(1.8)^{\circ}$	PRD 94 (2016), 054033
R. Escribano et al. (2015)	39.3(1.2)°	39.2(1.2)°	EPJC 75, 414 (2015)
Th. Feldmann (2000)	39.3(1.0)°	39.3(1.0)°	Int. J. Mod. Phys. A 15 (2000)

• Slight tension with RQCD results  $\phi_l(\mu = 1 \text{ GeV}) = 38.3(1.8)^\circ$  and  $\phi_s(\mu = 1 \text{ GeV}) = 36.8(1.6)^\circ$ , possibly due to (neglecting) scale dependence. JHEP OS (2021) 137



### Decay constant parameters



f<sub>l</sub> increased, f<sub>s</sub> decreased compared to 2018 analysis, i.e.

 $f_l = 125(5)_{\text{stat}}(6)_{\chi PT} \text{ MeV}, \quad f_s = 178(4)_{\text{stat}}(1)_{\chi PT} \text{ MeV}$ 

Improved control over systematic effects of physical extrapolations; particularly for f<sub>1</sub>.

• Physical extrapolation of ratios:  $f_l/f_{\pi} = 1.057(28)_{\text{stat}}(27)_{\text{sys}}$  and  $f_s/f_K = 1.105(20)_{\text{stat}}(13)_{\text{sys}}$ 

 $\Rightarrow \quad f_l = 137.6(3.6)_{\rm stat}(3.5)_{\rm sys}\,{\rm MeV}, \quad f_s = 172.0(3.1)_{\rm stat}(2.3)_{\rm sys}\,{\rm MeV}$ 



# Decay constant parameters



• Errors on  $f_s$  quite competitive; new analysis in better agreement with pheno results for  $f_l$ 

	$f_l$	$f_s$	
R. Escribano et al. (2016)	134.2(5.2) MeV	177.2(5.2) MeV	PRD 94 (2016), 054033
R. Escribano et al. (2015)	139.6(12.7) MeV	181.0(18.3) MeV	EPJC 75, 414 (2015)
Th. Feldmann (2000)	$139.3(2.5){ m MeV}$	$174.5(7.8)\mathrm{MeV}$	Int. J. Mod. Phys. A 15 (2000)
G. Bali et al., RQCD (2021)	129.7(4.7) MeV	$179.1(6.1){ m MeV}$	JHEP 08 (2021) 137

RQCD results at μ = 1 GeV compatible within 1σ to 2σ.

Introduction	η,η′ in LQCD	Setup	Physical extrapolations	Results	Summary & Outlook
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Summary	and outlook				

Lattice study of  $\eta$ ,  $\eta'$  with  $N_f = 2 + 1 + 1$  dynamical quark flavors:

- Physical extrapolations for all observables with controlled systematics.
- Three boxes at physical quark mass; generally much more chiral ensembles.
- Reduced statistical and systematic (!) errors compared to older analysis (2012–2018).
- Mass of  $\eta'$  reproduced from first principles with 2% error;  $M_{\eta,\eta'}$  in agreement with experiment.
- Precise results for (FKS scheme) mixing parameters  $\phi$ ,  $f_l$  and  $f_s$  in good agreement with phenomenology.

#### **Possible future plans:**

- Study scale dependence of mixing parameters.
  - $\rightarrow$  Requires computation of  $Z^0_A(\mu)$
  - $\rightarrow$  Need different strategy to extract axialvector matrix elements.
- Add ensembles with different m<sub>s</sub><sup>sea</sup>
- Further increase statistics for physical quark mass ensembles (?)
  - $\rightarrow$  Direct continuum extrapolations.
  - $\rightarrow$  Remove need of chiral extrapolation entirely.