Properties of the η and η' mesons
Part I: Masses and decay constants

arxiv:2106.05398

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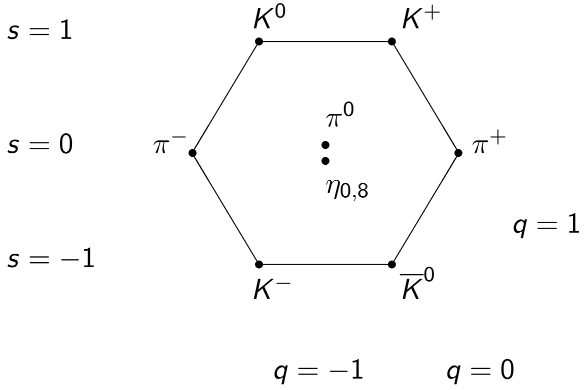
talk held at Lattice 2021, MIT

July 26, 2021

Quark model: "periodic table of pseudoscalar mesons"



$$SU(3)_L \times SU(3)_R \to SU(3)_V$$

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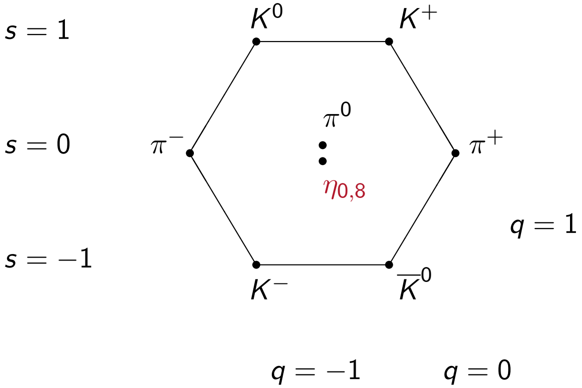

$$SU(3)_L \times SU(3)_R \to SU(3)_V$$

The QCD vacuum: Axial symmetry breaking

- η_0 becomes heavy compared to the octet mesons due to anomalous breaking of $U_A(1)$ axial symmetry:

$$\partial_\mu \widehat{A}^{a\mu} = \left(\overline{\psi}\gamma_5 \widehat{\{M, t^a\}}\psi\right) + \sqrt{2N_f}\delta^{a0}\widehat{q}_t, \quad a = 0, \ldots, 8$$

- $SU(3)$ flavour symmetry for $m_s = m_\ell$:

$$\eta = \eta_8 = \frac{u\bar{u} + d\bar{d} - 2s\bar{s}}{\sqrt{6}}, \qquad \eta' = \eta_0 = \frac{u\bar{u} + d\bar{d} + s\bar{s}}{\sqrt{3}}$$

- Away from flavour symmetric limit, η and η' states are not flavour eigenstates and

$$\eta \neq \eta_8, \qquad \eta' \neq \eta_0$$

Motivation

- Masses well-known from experiment, but important benchmark quantity
- Decay constants have never before been obtained from first principles and without model assumptions, see, e.g., *ETMC (arxiv:1710.07986)* for a lattice determination relating them to the pseudoscalar matrix elements
- Decay constants required for many phenomenological applications, e.g. transition form factors $F_{\gamma\gamma^*\to\eta^{(\prime)}}$ at large Q^2.
- Check of NLO large-N_c $U(3)$ ChPT using two mass trajectories and including the physical point
- Renormalization scale dependence of the singlet decay constants have frequently been ignored in the literature

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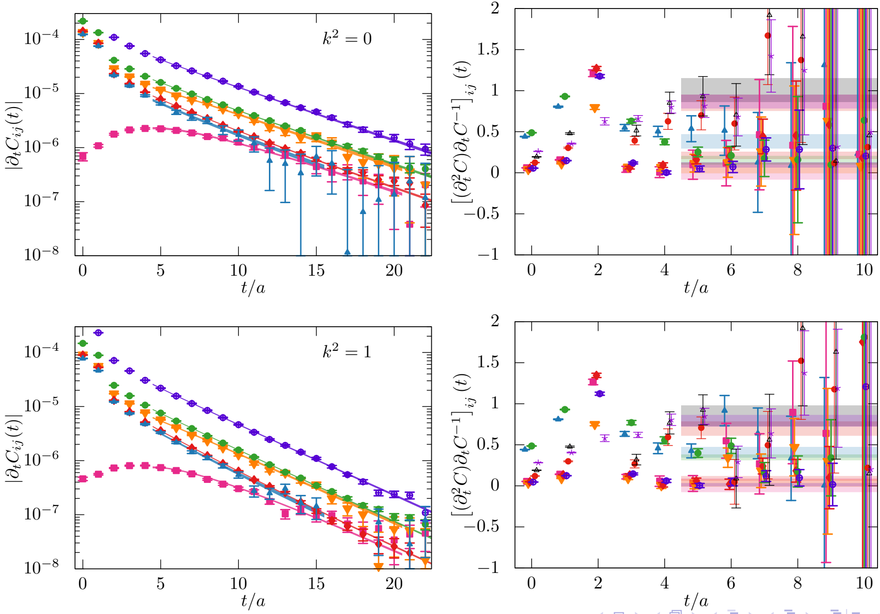
but: technically challenging

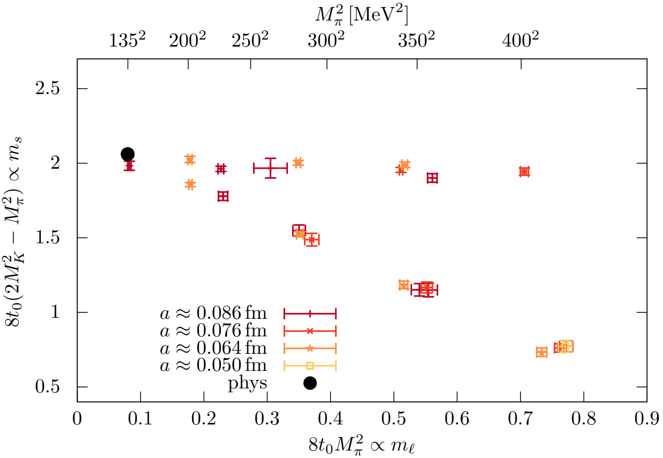
Extracting masses and matrix elements

- 300k to 800k stochastic probes per ensemble, employing time dilution and hopping parameter expansion
- Two smearing levels (to enhance our operator basis) + local (to enable the extraction of matrix elements)
- Instead of GEVP: direct fits to matrices and matrix generalization of effective masses
- Improve signal by fitting to derivative and including finite-momentum data

Fitting (example: H105, $M_\pi \approx 280\,\mathrm{MeV}$)

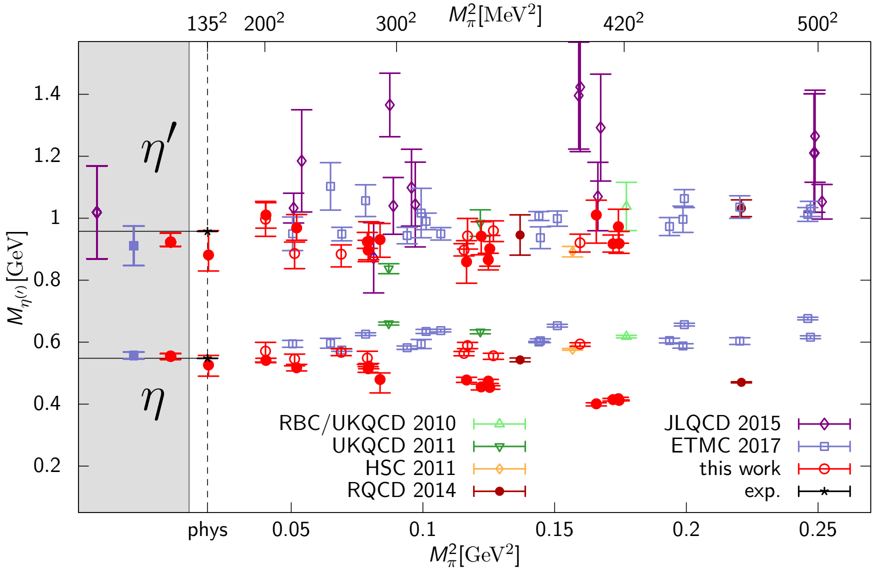


Lattice setup



- 21 large volume CLS ensembles
- Four lattice spacings $0.050\,\mathrm{fm} \lesssim a \lesssim 0.086\,\mathrm{fm}$
- Two quark mass trajectories leading to and including the physical point

Masses: Results and comparison



Decay constants: Definitions and renormalization

$$\langle\Omega|A^a_\mu|\mathcal{M}(p)\rangle = ip_\mu F^a_{\mathcal{M}}, \quad \text{where} \quad a \in \{0,8\}, \quad \mathcal{M} \in \{\eta, \eta'\}$$

- Flavour basis representation is connected by an orthogonal transformation
- Singlet and octet decay constants renormalize differently
- Non-singlet Z_A known non-perturbatively *Bulava et al. (arxiv:1604.05827)*
- Singlet: difference to non-singlet known perturbatively to two loops *Constantinou et al. (arxiv:1610.06744)*
- Non-vanishing anomalous dimension $\rightarrow$ singlet decay constants depend on renormalization scale
- However, 1-loop coefficient $\gamma^s_{A0} = 0 \rightarrow$ finite renormalization at $\mu = \infty$.
- Perform fits at $\mu = \infty$ and run down results in the end

NLO Large-N_c ChPT

$$R(\theta)\begin{pmatrix}\mu_8^2 & \mu_{80}^2\\ \mu_{80}^2 & \mu_0^2\end{pmatrix}R^{\mathsf{T}}(\theta)=\begin{pmatrix}M_\eta^2 & 0\\ 0 & M_{\eta'}^2\end{pmatrix},$$

where $\mu_i=\mu_i(\overline{M}^2,\delta M^2|F,L_5,L_8,M_0^2,\Lambda_1,\Lambda_2)$

- Expand simultaneously around $m=0$ and $1/N_c=0$ (no anomaly in $N_c=\infty$) Leutwyler, Gasser
- Parametrizations of masses and decay constants by six low energy constants
- 3 of which depend on the QCD scale: $M_0^2(\mu)=6\tau_0(\mu)/F^2$, $\Lambda_1(\mu)$, $\Lambda_2(\mu)$
- Chiral logarithms are NNLO
- NNLO exists, but involves many more parameters *Guo et al. (arxiv:1503.02248)*,*Bickert et al. (arxiv:1612.05473)*

$\mathcal{O}(a)$ improvement of flavour diagonal matrix elements

Bhattacharya et al. (arxiv:hep-lat/0511014):

non-singlet:

$$\widehat{\text{tr}\,\lambda\mathcal{O}} = Z_O \left[(1 + a\tilde{b}_O \,\text{tr}\, M)\,\text{tr}(\lambda\mathcal{O})^I + \frac{a}{2} b_O \,\text{tr}\,(\{\lambda, M\}\mathcal{O}) + a f_O \,\text{tr}(\lambda M)\,\text{tr}\,\mathcal{O} \right]$$

singlet: $$\widehat{\text{tr}\mathcal{O}} = Z_O^s \left[(1 + a\tilde{d}_O \text{tr} M)\text{tr}\mathcal{O}^I + a d_O \text{tr} M\mathcal{O} \right],$$

where, e.g., $\mathcal{O} = \overline{\psi}\gamma_\mu\gamma_5\psi$ and $\lambda = t^8$ Gell-Mann matrix

- Octet acquires singlet contribution at finite lattice spacing
- $\tilde{b}_A, b_A, c_A$ known from *Bali et al. (arxiv:1607.07090)* and *Bulava et al. (arxiv:1502.04999)*
- unknown improvement coefficients $d_A, \tilde{d}_A, f_A, c_A^s$ are parameterized for the fits:

$$f_A(g^2) = f_A^l g^6, \qquad d_A(g^2) = b_A(g^2) + d_A^l g^4,$$
$$\tilde{d}_A(g^2) = \tilde{d}_A^l g^4, \qquad c_A^s(g^2) = c_A + \delta c_A^l g^4,$$

$\rightarrow$ 4 fit parameters for full $\mathcal{O}(a)$ improvement of all decay constants

Physical point extrapolation

$$f_O(a, \overline{M}^2, \delta M^2) =$$

$$f_O^{\mathrm{cont}}(\overline{M}^2, \delta M^2 | F, L_5, L_8, M_0^2, \Lambda_1, \Lambda_2) \qquad \text{continuum}$$

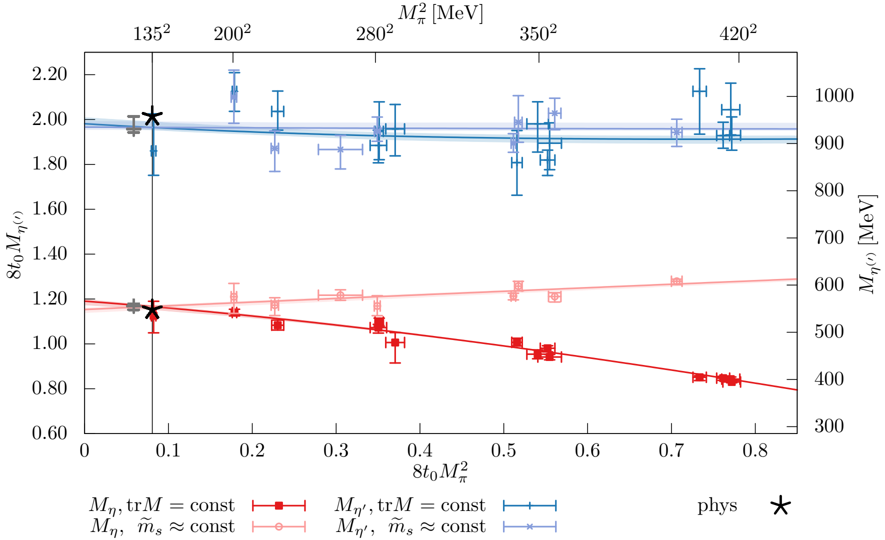
$$\times\, h_O^{(1)}(a, am_\ell, am_s | f_A^l, d_A^l, \tilde{d}_A^l, \delta c_A^l) \qquad \mathcal{O}(a) \text{ improvement}$$

$$\times\, h_O^{(2)}(a^2/t_0^*, a^2\overline{M}^2, a^2\delta M^2 | l_O, m_O, n_O) \qquad \mathcal{O}(a^2) \text{ terms}$$

where $O \in \{M_\eta, M_{\eta'}, F_\eta^8, F_\eta^0, F_{\eta'}^8, F_{\eta'}^0\}$ and $h_{M_\eta}^{(1)} = h_{M_{\eta'}}^{(1)} = 1$

- Fix numerically irrelevant lattice spacing terms to zero
- $\mathcal{O}(a)$ improvement for decay constants: d_A (singlet) and f_A (octet) seem to be particularly important
- Combined, fully correlated fit gives $\chi^2/N_{\mathrm{df}} \approx 179/122 \approx 1.47$

Physical point results: masses



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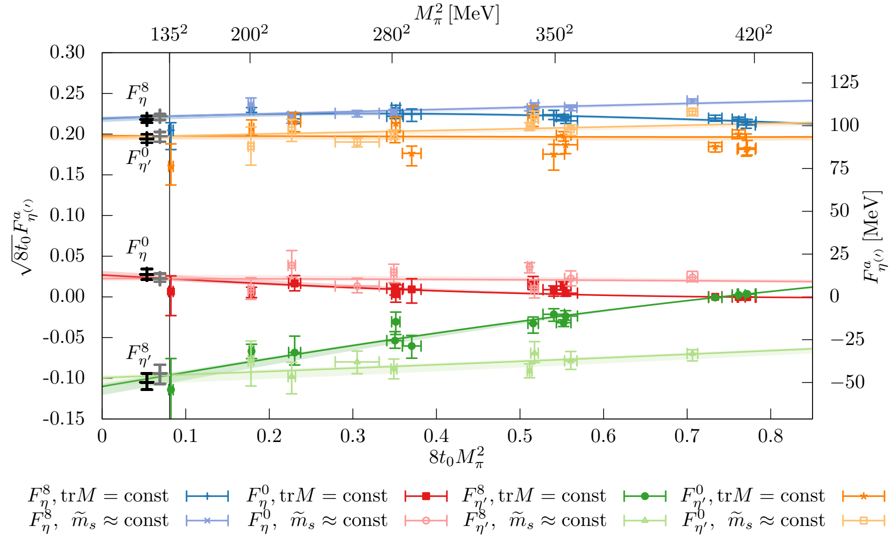

Systematics

- Volume: only large volumes: $L_s^3 > (2.2\,\mathrm{fm})^3 \gg R_\eta^3 \approx R_\pi^3$ *Bernstein (arxiv:1511.03242)* and typically $L_s M_\pi > 4$
- Lattice spacing: vary parametrization of discretization effects
- NLO large-N_c ChPT: impose cutoffs on the average (non-singlet) pseudoscalar mass: $\overline{M}^2 \leq \overline{M}^2_{\mathrm{max}}$, $12 t_0 \overline{M}^2_{\mathrm{max}} \in \{1.2, 1.4, 1.6\}$
- Renormalization: matching to PT done at $\mu \in \{a^{-1}/2, a^{-1}, 2a^{-1}\}$

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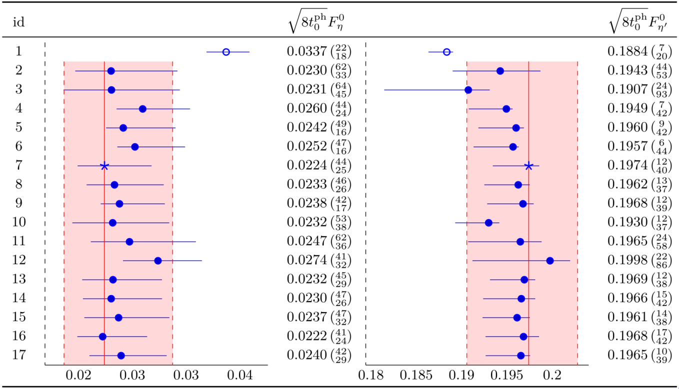

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- Renormalization: matching to PT done at $\mu \in \{a^{-1}/2, a^{-1}, 2a^{-1}\}$
- Take spread of the central values around our central fit and assign them to the respective systematic error
- Errors added in quadrature

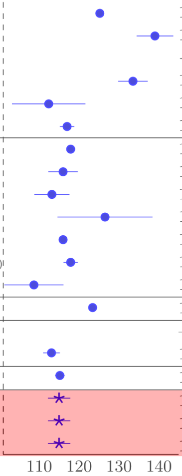
Physical point results

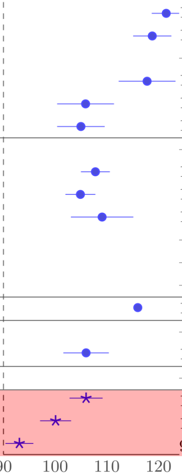
- Scale setting using $(8t_0^{\mathrm{ph}})^{-1/2} = 475(6)\,\mathrm{MeV}$
  Bruno et al. (arxiv:1608.08900)
- Masses agree with experiment ($M_\eta^{\mathrm{phys}} = 547.9\,\mathrm{MeV}$ and $M_{\eta'}^{\mathrm{phys}} = 957.8\,\mathrm{MeV}$, PDG)

$$M_\eta = 554.7\,\binom{4.0}{6.6}_{\mathrm{stat}}\binom{2.4}{2.7}_{\mathrm{syst}}(7.0)_{t_0},\ \mathrm{MeV}$$
$$M_{\eta'} = 929.9\,\binom{12.9}{6.0}_{\mathrm{stat}}\binom{22.9}{3.3}_{\mathrm{syst}}(11.7)_{t_0}\ \mathrm{MeV},$$

Physical point results

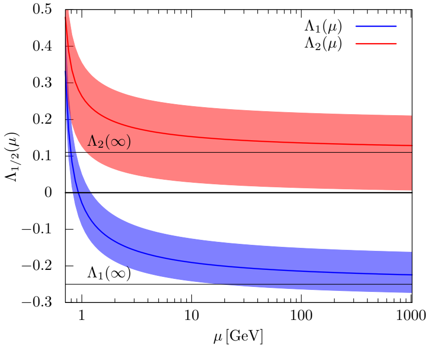
ref	F^8/MeV	F^0/MeV
Benayoun et al. [101]	125.2(9)	121.5(2.8)
Escribano and Frere [102]	139.0(4.6)	118.8(3.7)
Escribano et al. [103]	– – –	—
Chen et al. [104]	133.5(3.7)	117.8(5.5)
Escribano et al. [105]	112.4(9.2)	105.9(5.5)
Escribano et al. [98]	117.0(1.8)	105.0(4.6)
Leutwyler [6]	118	—
Feldmann [97]	116.0(3.7)	107.8(2.8)
Guo et al. [81] NLO-A	113.2(4.4)	104.9(2.9)
Guo et al. [81] NNLO-B	126(12)	109.1(6.0)
Bickert et al. [42] NLO-I	116.0(9)	—
[42] NNLO w/o Ci ($\mu_{\text{EFT}} = 1\text{GeV}$)	117.9(1.8)	—
[42] NNLO w/ Ci ($\mu_{\text{EFT}} = 1\text{GeV}$)	109(7)	—
Ding et al. [106]	123.4	116.0
ETMC [19]	—	—
Gu et al. [107] NNLO-A9p(F_π)	113.1(2.1)	106.0(4.4)
eq. (7.16)	115.2(1.2)	—
this work ($\mu = 1\text{GeV}$)	115.0(2.8)	106.0(3.2)
this work ($\mu = 2\,\text{GeV}$)	115.0(2.8)	100.1(3.0)
this work ($\mu = \infty$)	115.0(2.8)	93.1(2.7)





$$F^8 = \sqrt{(F^8_\eta)^2 + (F^8_{\eta'})^2} \qquad F^0 = \sqrt{(F^0_\eta)^2 + (F^0_{\eta'})^2}$$

QCD scale dependence of LECs

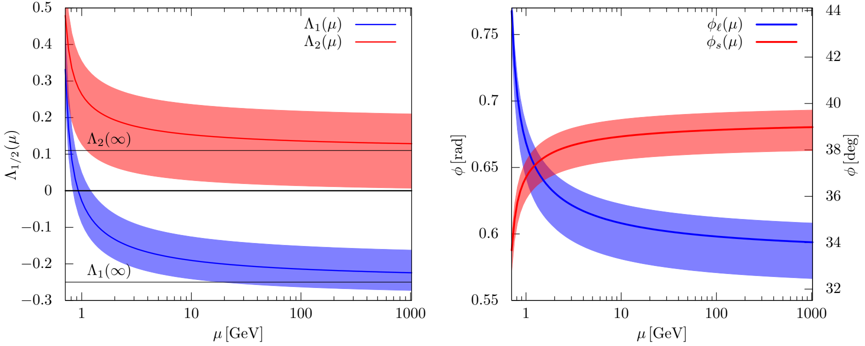


Scale dependence of singlet current translates to scale dependence of LECs, e.g.,

$$\mu \frac{\mathrm{d}}{\mathrm{d}\mu} \frac{F_0(\mu)}{\sqrt{1+\Lambda_1(\mu)}} = 0.$$

→ assuming $\Lambda_1 = 0$ renders F_0 scale independent

QCD scale dependence of LECs



"Feldmann-Kroll-Stech" scheme:

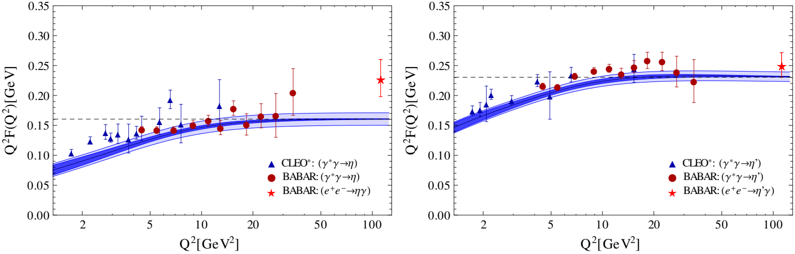
4 decay constants reduce to three parameters in the flavour basis (two decay constants + 1 angle)*FKS (arxiv:hep-ph/9802409)*:

$$\frac{\sqrt{2}}{3} F_\pi^2 \Lambda_1 = F^\ell F^s \sin(\phi_\ell - \phi_s)$$

→ Very good agreement at low scales

extent of validity of approximation previously unknown

Transition form factors $Q^2 F_{\gamma\gamma^* \to \eta^{(\prime)}}$



- Use decay constants at a well defined scale as input for the QCD light cone sum rule calculation *Agaev et al. (arxiv:1409.4311)*
- Asymptotic values obtained from

$$\lim_{Q^2\to\infty} Q^2 F_{\gamma\gamma^*\to\eta^{(\prime)}} = \frac{2}{\sqrt{3}}\left(F^8_{\eta^{(\prime)}} + 2\sqrt{2}F^0_{\eta^{(\prime)}}(\mu=\infty, N_f=4)\right).$$

- Results confirm phenomenological inputs, tensions to experiment at high Q^2 persist

$$\lim_{Q^2\to\infty} Q^2 F_{\gamma\gamma^*\to\eta}(Q^2) = 161(10)\,\mathrm{MeV}, \lim_{Q^2\to\infty} Q^2 F_{\gamma\gamma^*\to\eta'}(Q^2) = 231(10)\,\mathrm{MeV}$$

Summary

- Physical point extrapolation employing 21 CLS ensembles along two mass trajectories and four lattice spacings
- Precise determination of η and η' masses
- First ab-initio determination of all four η and η' decay constants
- NLO large N_c ChPT provides good description of all data with just six parameters
- Scale dependence explicitly taken into account
  $\rightarrow$ Agreement with FKS scheme based determinations due to smallness of Λ_1 at scales $0.8\,\mathrm{GeV} \leq \mu \leq 2\,\mathrm{GeV}$

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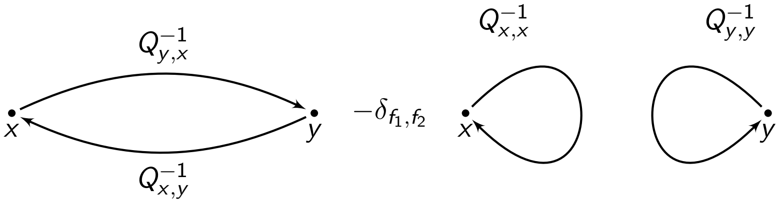
more details: *arxiv:2106.05398*

Backup

Stochastic estimation of disconnected loops

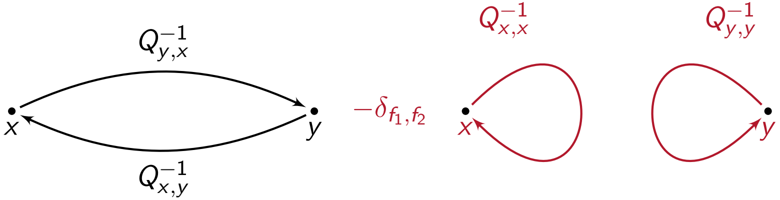


Wick contractions of mesons:

$$\langle q_{f_1}(y)\gamma_5\bar{q}_{f_2}(y)\bar{q}_{f_1}(x)\gamma_5 q_{f_2}(x)\rangle = q_{f_1}(y)\gamma_5\bar{q}_{f_2}(y)\bar{q}_{f_1}(x)\gamma_5 q_{f_2}(x)$$

$$= Q^{-1}_{f_1,f_1}(y,x)Q^{-1}_{f_2,f_2}(x,y) - \delta_{f_1,f_2}Q^{-1}_{f_1,f_2}(y,y)Q^{-1}_{f_1,f_2}(x,x)$$

Stochastic estimation of disconnected loops



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$$= Q^{-1}_{f_1,f_1}(y,x)Q^{-1}_{f_2,f_2}(x,y) - \delta_{f_1,f_2}Q^{-1}_{f_1,f_2}(y,y)Q^{-1}_{f_1,f_2}(x,x)$$

$\rightarrow$ disconnected loops arise

Stochastic Estimation of Disconnected loops

Stochastic estimation is required for the inversion of Q: The N_{stoch} linear systems $Q \mid s_i\rangle = \mid \eta_i\rangle$ are solved on random sources $\eta_{ix\alpha a} \in (\mathbb{Z}_2 + i\mathbb{Z}_2)/\sqrt{2}$

$$Q^{-1} = \frac{1}{N_{stoch}} \sum_{i}^{N_{stoch}} \mid s_i\rangle\langle\eta_i \mid + \mathcal{O}(\frac{1}{\sqrt{N_{stoch}}})$$

→ extra stochastic noise in addition to the gauge noise.

Time dilution Bernardson et al.,1993; Viehoff et al.,1998; O'Cais et al.,2005

- put random sources at every 4th time slice
- set source at (open) boundaries to zero

Hopping parameter expansion Thron et al.,1998; Michael et al., 2000; Bali et al.2005

- use locality of the Wilson Dirac operator and expand in small κ
- using two and four applications for the pseudoscalar and axialvector loops, respectively

Matrix correlators

- Construct N bases from n biquark fields:

$$b_i(t,\vec{p}) = \sum_{j=0}^{n-1} B_{ij} \sum_{\vec{x}} e^{-i\vec{p}\vec{x}} \left(\bar{q}_j \gamma_5 q_j\right)(x),$$

  where $B \in \mathbb{R}^{N\times n}$ matrix that defines a basis and subscripts are superindices defining flavour and smearing.

- matrix correlator

$$C(t) = \frac{1}{N_t} \sum_{t'=0}^{N_t-1} \begin{pmatrix} \langle b_1(t'+t) \mid b_1(t') \rangle & \cdots & \langle b_1(t'+t) \mid b_N(t') \rangle \\ \vdots & \ddots & \vdots \\ \langle b_N(t'+t) \mid b_1(t') \rangle & \cdots & \langle b_N(t'+t) \mid b_N(t') \rangle \end{pmatrix}.$$

- Note: C is a real, positive semidefinite and symmetric matrix.

Fitting to matrices

- Usually: solve GEVP to diagonalize C
- Instead: decompose correlator in terms of orthogonal (mass) eigenstates:

$$C(t)_{ij} = \sum_n \frac{1}{2E_n} \langle b_i \mid n \rangle \langle n \mid b_j \rangle \exp(-E_n t)$$
$$= \left[Z D(t) Z^T \right]_{ij},$$

where

$$Z_{in} = \frac{1}{\sqrt{2E_n}} \langle b_i \mid n \rangle, \qquad \text{and} \qquad D(t) = \mathrm{diag}_{n=0}(\exp(-E_n t))$$

- Note that Z does *not* depend on t.
- Need to truncate the sum: $Z : N \times \infty \to Z : N \times N_{\mathrm{st}}$
- There is no need for Z to be quadratic, may fit more or fewer states N_{st} than available bases N.

Improving the signal

Derivative trick

Replacing correlators with their derivatives removes any constant shifts in the correlator and decreases autocorrelations (similar to *Takashi (arxiv:hep-lat/0701005)*, *Feng et al. (arxiv:0909.3255)*):

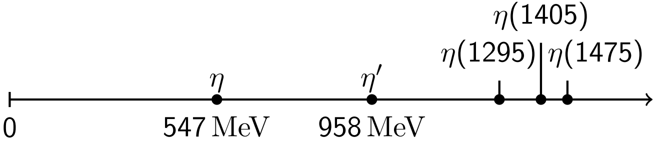
$$\partial_t C(t) = -ZED(t)Z^T$$

Combine data with dispersion relation

Signals typically better at $p^2 > 0$: Combine several correlators in a joint fit, using the dispersion relation:

$$E(p) = \sqrt{m^2 + p^2}, \qquad p_i = \frac{2\pi k_i}{L}$$

Excited states



- η' signal deteriorates at short Euclidean times
- plethora of states nearby
- coverage of excited states depends on the (octet or singlet) nature of these states and the overlap with the chosen basis
- need to include these states in the fit $\rightarrow$ need at least a 3x3 matrix
- typical fit windows $t \in [0.35, 1]\,\mathrm{fm}$
- fit functions contain multi-exponentials:

$$C_{ij}(t) = \sum_{n=0}^{N-1} Z_{in} D_{nn} Z_{jn} = \sum_{n=0}^{N-1} Z_{in} Z_{jn} \exp(-E_n t)$$

Generalized effective masses

- Excited states become visible when looking at

$$(\partial_t C(t))C^{-1} = -ZEZ^{-1} + \mathcal{O}(\exp(-(E_{N_{st}} - E_{N_{st}-1})t))$$

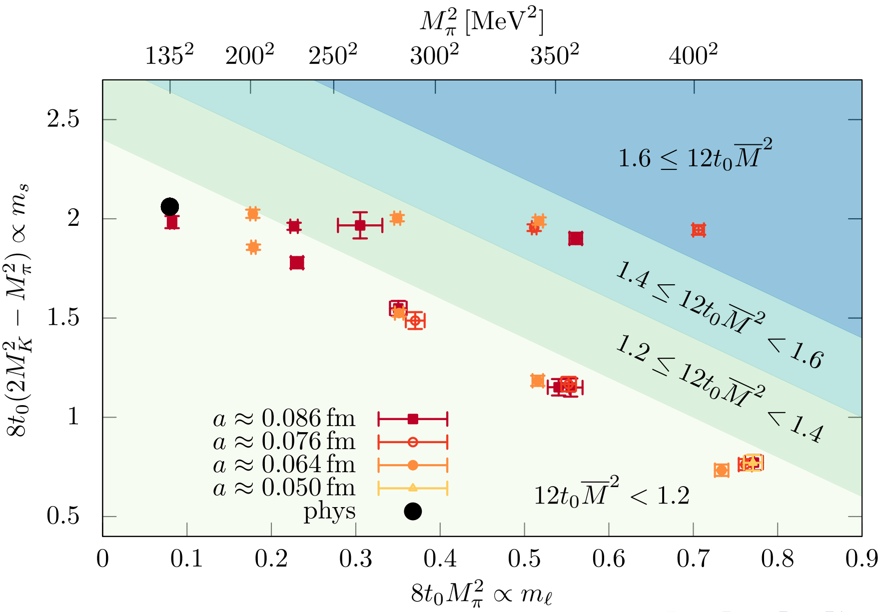
- leading term ZEZ^{-1} does not depend on time
- generalization of simple effective masses (for single correlators):

$$(\partial_t C(t))C^{-1} = \partial_t \log(C(t))$$

- can be included in a (joint) fit and helps constraining amplitudes (Z)
- leading term unchanged when using higher derivatives

$$(\partial_t^2 C(t))(\partial_t C)^{-1} = -ZEZ^{-1} + \mathcal{O}(\exp(-(E_{N_{st}} - E_{N_{st}-1})t))$$

ChPT cuts



M_π^2 [MeV^2]
135^2 200^2 250^2 300^2 350^2 400^2
$1.6 \leq 12t_0\overline{M}^2$
$1.4 \leq 12t_0\overline{M}^2 < 1.6$
$1.2 \leq 12t_0\overline{M}^2 < 1.4$
$12t_0\overline{M}^2 < 1.2$
$a \approx 0.086$ fm
$a \approx 0.076$ fm
$a \approx 0.064$ fm
$a \approx 0.050$ fm
phys
$8t_0(2M_K^2 - M_\pi^2) \propto m_s$
0.5 1 1.5 2 2.5
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9
$8t_0M_\pi^2 \propto m_\ell$