The π^0, η and η' mesons from lattice QCD+QED

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Broken flavour symmetry

Our starting point for understanding the flavour wavefunctions of the pseudoscalar (PS) mesons is the limit of SU(3)-flavour symmetry

- In this limit the π^0 and η belong to the familiar meson octet, and the η' is a singlet

$$\mathcal{O}_{\pi_3} = (\bar{u}\gamma^5 u - \bar{d}\gamma^5 d)/\sqrt{2}, \quad \mathcal{O}_{\eta_8} = (\bar{u}\gamma^5 u + \bar{d}\gamma^5 d - 2\bar{s}\gamma^5 s)/\sqrt{6},$$

$$\mathcal{O}_{\eta_1} = (\bar{u}\gamma^5 u + \bar{d}\gamma^5 d + \bar{s}\gamma^5 s)/\sqrt{3}$$

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- In reality SU(3)-flavour symmetry is broken due to non-degenerate up/down/strange quarks, and the flavour wavefunctions of the mass eigenstates are (orthogonal) linear combinations of these states
- This ‘mixing’ hasn’t been studied before on the lattice with isospin breaking or QED

Broken flavour symmetry

One particular point of interest here is the U(1)-axial anomaly associated with the PS singlet, which is distributed amongst the π^0, η, η' mesons as they acquire singlet admixture.

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Primary concern is to find the linear combinations of PS operators, $\mathcal{O}_f = \bar{q}_f \gamma^5 q_f$, that couple diagonally to the π^0, η, η':

$$\langle \Omega | \sum_f c_{mf} \mathcal{O}_f | n \rangle \propto \delta_{nm} , \quad c_{mf} \in \mathbb{R}$$

Lattice approach

We employ interpolating operators for each light quark flavour

$$\mathcal{O}_f = (\bar{q}_f \gamma^5 q_f), \quad f = u, d, s,$$

and additionally apply two different levels of gauge-covariant Gaussian smearing, denoted by superscript.

From this basis of operators we construct the correlation functions

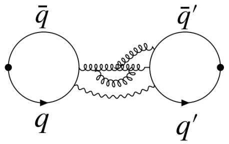
$$C_{ij}(t) = \sum_{\vec{x},\vec{y}} \langle \mathcal{O}_j(\vec{y}, t)\, \mathcal{O}_i^\dagger(\vec{x}, t_0) \rangle, \quad \mathcal{O}_{i,j} = \mathcal{O}_u^1, \mathcal{O}_d^1, \mathcal{O}_s^1, \mathcal{O}_u^2, \mathcal{O}_d^2, \mathcal{O}_s^2,$$

which can also be interpreted as a matrix

Lattice approach

The Wick contractions for our correlation functions lead to two distinct combinations of propagator traces:

$$C(t)_{disc} = \sum_{\vec{x},\vec{y}} \mathrm{Tr}\left[S_{q'}(\vec{y},t;\vec{y},t)\gamma^5\right] \mathrm{Tr}\left[S_q(\vec{x},t_0;\vec{x},t_0)\gamma^5\right],$$



are disconnected contributions and

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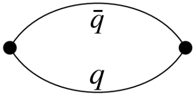

are typical connected 2-point functions which could be calculated using point-to-all propagators.

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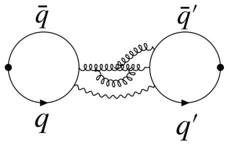

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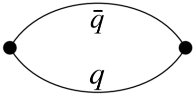


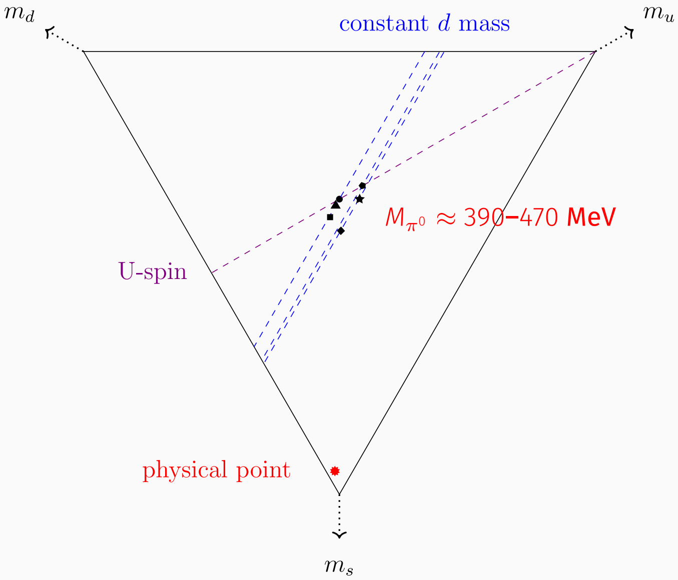
are typical connected 2-point functions which could be calculated using point-to-all propagators.

The disconnected contributions however require computation of the 'self-to-self' propagator, which is in practice as expensive as the all-to-all propagator.

Simulation details

- All gauge configurations are $24^3 \times 48$, $n_f = 1 + 1 + 1$ dynamical QCD+QED with $\mathcal{O}(a)$ improved Clover fermions
- In this work we approximate the all-to-all propagators using $\mathbb{Z}_2$-noise wall sources with spin, colour and time dilution
- We use 3 independent noise sources on each configuration and 1000 configurations on each ensemble
- Our ensembles are chosen so that the average quark mass is held constant between them: $\bar{m} = (m_u + m_d + m_s)/3 = \mathrm{constant}$
- We have 6 ensembles in total that can be visualized on the plane defined by $\bar{m}$:

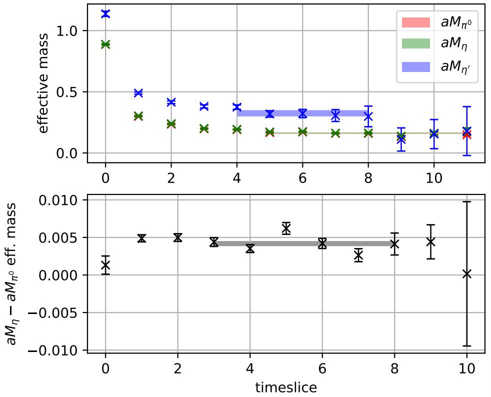
Simulation details



GEVP Diagonalization

Having calculated each element of the 6×6 matrix of correlation functions, we diagonalize using the generalized eigenvalue problem (GEVP) method at large times:

$$C(t)^{-1}\, C(t+\delta t)\, \vec{v}_n = e^{-M_n \delta t}\, \vec{v}_n$$



GEVP Diagonalization

Using the GEVP eigenvectors we also calculate the overlaps as

$$e^{M_n t} \sum_{j=1}^{6} C_{ij}(t) v_{j,n} = \langle n | \mathcal{O}_i^\dagger | 0 \rangle,$$

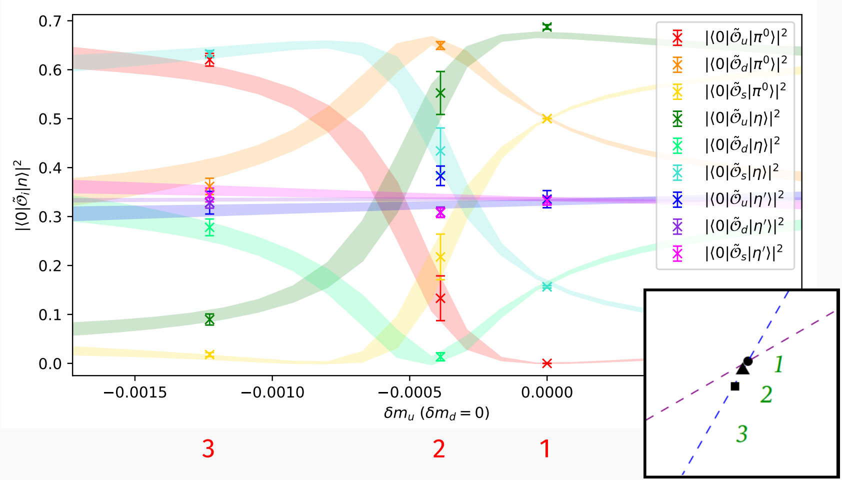
which can be used to diagonalize our operators since

$$\delta_{nm} \propto \langle n | m \rangle \propto \sum_{f=u,d,s} \langle n | \mathcal{O}_f^\dagger | 0 \rangle \langle 0 | \mathcal{O}_f | m \rangle = \langle 0 | \sum_{f=u,d,s} \left(\langle n | \mathcal{O}_f^\dagger | 0 \rangle \mathcal{O}_f \right) | m \rangle,$$

i.e. they are the Clebsch-Gordan coefficients relating the eigenstates to the states created by our flavour operators

State composition extrapolation

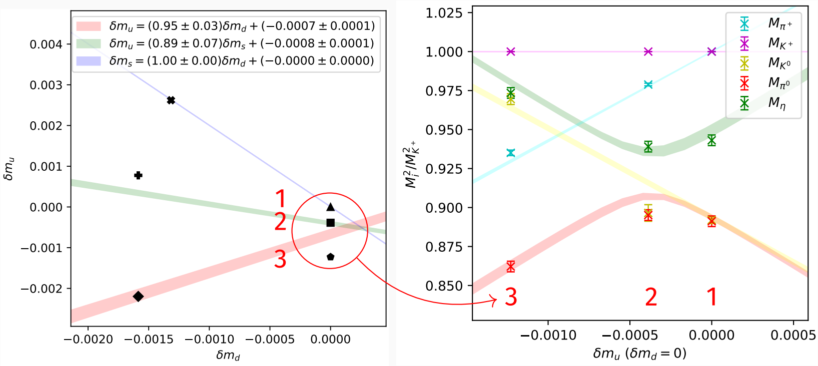
Global fit to flavour compositions (ensembles 1–3 pictured):



$(\bar{u}\gamma^5 u - \bar{d}\gamma^5 d)/\sqrt{2}$, $(\bar{u}\gamma^5 u - \bar{s}\gamma^5 s)/\sqrt{2}$, $(\bar{d}\gamma^5 d - \bar{s}\gamma^5 s)/\sqrt{2}$

Symmetry lines and masses

We can also use our global fit to determine where one of the flavour neutral mesons is a pure iso-, U- or V-spin ”pion” :



The avoided level crossing observed between the π^0 and η masses corresponds to proximity to the extrapolated SU(3) “symmetric” point

Conclusion

Summary:

- We have determined, for the first time including QED and quark mass isospin-breaking, the π^0, η and η' masses and mixing parameters ‘near’ an SU(3) symmetric point
- We have observed that the flavour compositions of these states can be sensibly parametrized and help us to understand the relevant masses

Outlook:

- Proper treatment of systematic uncertainties in this analysis and resolved physical mixing
- Use our diagonalized operators to isolate the corresponding states in studies of the decay constants, $\pi^0 \to \gamma\gamma$ etc.

Bonus: noise source methods

In this work we approximate the all-to-all propagators using $\mathbb{Z}_2$-noise wall sources with spin, colour and time dilution:

$$\eta_r(\vec{x},t;t_0)^{ab}_{\mu\nu} = \xi_r(\vec{x})\,\delta_{tt_0}\,\delta_{ab}\,\delta_{\mu\nu}, \qquad \lim_{N_r\to\infty}\frac{1}{N_r}\sum_{r=1}^{N_r}\xi_r(\vec{x})\,\xi_r(\vec{y}) = \delta_{\vec{x}\vec{y}},$$

and calculating solution vectors for each source spin, colour and time as

$$\psi_r(\vec{y},t;t_0)^{ab}_{\mu\nu} = \sum_{\vec{z}} M^{-1}(\vec{y},t;\vec{z},t_0)^{ab}_{\mu\nu}\,\xi_r(\vec{z}),$$

leads to an approximation of the all-to-all propagator for a finite number (N_r) of independent noise sources:

$$S(\vec{y},t;\vec{x},t_0)^{ab}_{\mu\nu} \approx \frac{1}{N_r}\sum_{r=1}^{N_r}\psi_r(\vec{y},t;t_0)^{ab}_{\mu\nu}\,\xi_r(\vec{x})$$

Bonus: smearing couplings comparison

We find that the overlaps of each flavour operator with an eigenstate agree between the two smearings used, eg.

$$\frac{\langle 0|\mathcal{O}_u^{(1)}|\eta\rangle}{\langle 0|\mathcal{O}_d^{(1)}|\eta\rangle} = -2.097(23), \quad \frac{\langle 0|\mathcal{O}_u^{(2)}|\eta\rangle}{\langle 0|\mathcal{O}_d^{(2)}|\eta\rangle} = -2.080(25),$$

and so we normalize both sets as

$$\langle 0|\tilde{\mathcal{O}}_f|n\rangle \equiv \frac{1}{\sqrt{\sum_{f=u,d,s} |\langle 0|\mathcal{O}_f^{(l)}|n\rangle|^2}}\langle 0|\mathcal{O}_f^{(l)}|n\rangle, \quad f = u, d, s,$$

and refer to the quantities $\langle 0|\tilde{\mathcal{O}}_f|n\rangle$ as the flavour contents of the eigenstate $|n\rangle$

Bonus: physical point mixings

Assessing our global fit at the physical quark masses we find

$$|\pi^0\rangle = 0.96(9)|\pi_3\rangle \,-\, 0.06(17)|\eta_8\rangle \,+\, 0.09(16)|\eta_1\rangle$$

$$|\eta\rangle = -0.04(8)|\pi_3\rangle \,+\, 0.90(12)|\eta_8\rangle \,+\, 0.37(18)|\eta_1\rangle$$

$$|\eta'\rangle = -0.004(7)|\pi_3\rangle \,-\, 0.30(9)|\eta_8\rangle \,+\, 0.95(3)|\eta_1\rangle$$

We cannot resolve any mixing between the π^0 and η/η', but we see mixing between the η and η' consistent with a mixing angle of

$$|\theta_{\eta\eta'}| = \sin^{-1}(-0.30 \pm 0.09) = (-17.3^{+5.3}_{-5.5})^{\circ}$$