Properties of Pseudoscalar Flavor-Singlet Mesons from 2+1+1 Twisted Mass Lattice QCD

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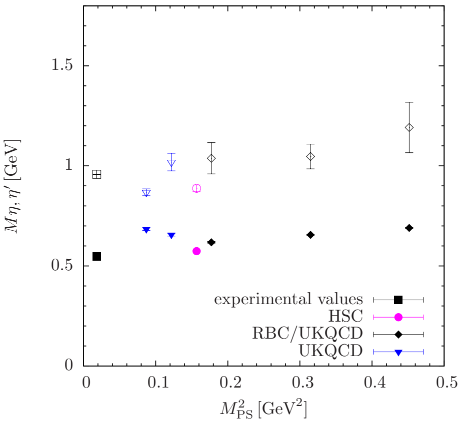
Outline

- Want to calculate properties of η, η'-mesons using 2+1+1 dynamic quark flavours
- This allows to determine masses of η, η' (in principle also for η_c)
- Study quark mass dependence
- Perform scaling test to estimate systematic errors
- Extract flavour contents of the states
- Check for possible c-quark contribution to η, η'
- Determine mixing angle

2+1 flavour results available so far:



J. J. Dudek et al., Phys. Rev. D83, 111502 (2011)

N. Christ et al., Phys. Rev. Lett. 105, 241601 (2010)

E. B. Gregory et al., arXiv:1112.4384

Wilson tmLQCD for light quarks (1)

Consider the QCD action

$$\mathcal{S}_{QCD} = \int d^4x \left(-\frac{1}{4} G^a_{\mu\nu} G^{a,\mu\nu} + \sum_f \bar{\psi}_f \left(i\not{D} - \mathcal{M}_f \right) \psi_f \right) = \mathcal{S}_G[G] + \mathcal{S}_F\left[G, \psi, \bar{\psi}\right]$$

with four quark flavours, i.e. one light $\psi_l = (u, d)$ and one heavy doublet $\psi_h(c, s)$.

The Wilson twisted mass lattice action for the light doublet reads

$$\mathcal{S}_{F,l}[U, \chi_l, \bar{\chi}_l] = a^4 \sum_x \bar{\chi}_l \left(D_W + m_0 + i\mu_l \gamma_5 \tau^3 \right) \chi_l$$

Frezzotti et. al., JHEP 0108:058 (2001)

D_W: Wilson operator, m_0: bare untwisted quark mass, μ_l: bare twisted quark mass

$\mathcal{S}_F$ is related to the physical basis (in the continuum only!) via

$$\psi = \exp\left(i\omega\gamma_5\tau^3/2\right)\chi \quad \text{and} \quad \bar{\psi} = \bar{\chi}\exp\left(i\omega\gamma_5\tau^3/2\right) \; .$$

Wilson tmLQCD for light quarks (2)

- Wilson and tmWilson basis are different lattice regularizations
- "twist-rotation" is NOT a symmetry on the lattice → different lattice artefacts compared to Wilson formulation

→ Can be used to cancel $\mathcal{O}(a)$-effects

- It can be shown that at maximum twist $\omega = \frac{\pi}{2}$, one has:

$$\left\langle O^{cont}\left[\psi,\bar{\psi}\right]\right\rangle = \left\langle O^{tm}\left[\chi,\bar{\chi}\right]\right\rangle + \mathcal{O}\left(a^2\right)$$

i.e. we have automatic $\mathcal{O}(a)$ improvement

R. Frezzotti and G. C. Rossi, Nucl. Phys. B 129&130, 880-882 (2004)

- No tuning of further, operator-specific improvement coefficients
- Flavor symmetry and parity are broken at finite a (but $\mathcal{O}\left(a^2\right)$-effect)
- Light sector is flavour-diagonal

Heavy quark sector

The action for the heavy doublet reads

$$\mathcal{S}_{F,h}[U,\chi_h,\bar{\chi}_h] = a^4 \sum_x \bar{\chi}_h \left(D_W + m_0 + i\mu_\sigma \gamma_5 \tau^1 + \mu_\delta \tau^3 \right) \chi_h \ .$$

R. Frezzotti and G.C. Rossi, Nucl. Phys. Proc. Suppl.128 193-202 (2004)

m_0: bare untwisted quark mass, μ_σ: bare twisted mass, μ_δ: c,s-mass splitting

- strange and charm quark masses are given by

$$m_{c,s} = \mu_\sigma \pm \frac{Z_P}{Z_S} \mu_\delta$$

- Again automatic $\mathcal{O}(a)$ improvement is achieved
- Heavy sector is NOT flavour-diagonal → two additional progagators G^{xy}_{cs} G^{xy}_{sc}

⇒ Heavy sector requires a much larger number of contractions for correlation functions

Interpolating operators for η, η'

In the physical basis 2 γ-combinations ($i\gamma_5$, $i\gamma_0\gamma_5$) available; consider only $i\gamma_5$:

$$\eta_l^{phys} = \frac{1}{\sqrt{2}}\bar{\psi}_l i\gamma_5 \psi_l \quad \eta_{c,s}^{phys} = \bar{\psi}_h \left(\frac{1\pm\tau^3}{2} i\gamma_5\right) \psi_h = \begin{cases} \bar{c} i\gamma_5 c \\ \bar{s} i\gamma_5 s \end{cases} .$$

At maximal twist this reads in the twisted basis:

$$\eta_l^{tm} = \frac{1}{\sqrt{2}}\bar{\chi}_l \left(-\tau^3\right) \chi_l \quad \eta_{c,s}^{tm} = \frac{1}{2}\bar{\chi}_h \left(-\tau^1 \pm i\gamma_5\tau^3\right) \chi_h \quad .$$

$\Rightarrow$ heavy operators are a sum of scalars and pseudoscalars!

Considering renormalization we have

$$\begin{aligned} \eta_{c,renormalized}^{tm} &= Z_P\left(\bar{\chi}_c i\gamma_5 \chi_c - \bar{\chi}_s i\gamma_5 \chi_s\right) - Z_S\left(\bar{\chi}_s \chi_c + \bar{\chi}_c \chi_s\right) \\ \eta_{s,renormalized}^{tm} &= Z_P\left(\bar{\chi}_s i\gamma_5 \chi_s - \bar{\chi}_c i\gamma_5 \chi_c\right) - Z_S\left(\bar{\chi}_s \chi_c + \bar{\chi}_c \chi_s\right) . \end{aligned}$$

$\rightarrow$ Need $\frac{Z_P}{Z_S}$; how can we avoid this when calculating masses?

Correlation function matrix for η, η'

Choose different set of „heavy“ operators

$$\eta_{S,P} = \eta_c^{tm} \pm \eta_s^{tm} = \begin{cases} \frac{1}{\sqrt{2}}(\bar{\chi}_c\chi_s + \bar{\chi}_s\chi_c) \\ \frac{1}{\sqrt{2}}(\bar{\chi}_c i\gamma_5\chi_c - \bar{\chi}_s i\gamma_5\chi_s) \end{cases} .$$

$\Rightarrow$ This corresponds to an additional rotation of the basis.

In the twisted basis we have to calculate this correlation matrix:

$$\mathcal{C}^\eta(t) = \begin{pmatrix} \eta_l(t)\eta_l(0) & \eta_l(t)\eta_S(0) & \eta_l(t)\eta_P(0) \\ \eta_S(t)\eta_l(0) & \eta_S(t)\eta_S(0) & \eta_S(t)\eta_P(0) \\ \eta_P(t)\eta_l(0) & \eta_P(t)\eta_S(0) & \eta_P(t)\eta_P(0) \end{pmatrix} .$$

- Eigenvectors of $\mathcal{C}^\eta(t)$ give access to flavour contents
- Eigenvalues allow to extract masses for η and η'

Setup

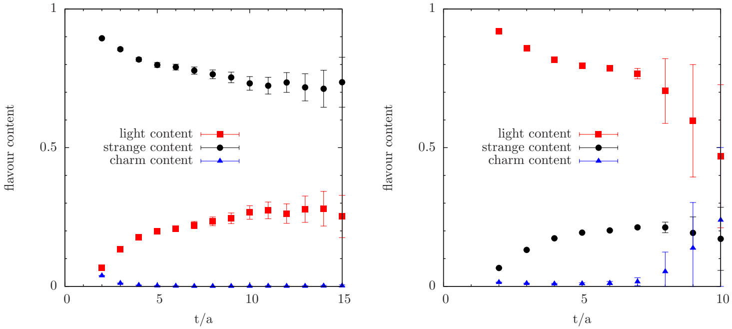
We used the following setup:

- Gauge configurations were provided by ETM Collaboration; we use 15 ensembles

R. Baron et. al., JHEP 06 111 (2010)

- Computations are done on the JUGENE and JUDGE systems at Jülich and our GPU-Cluster
- Three lattice spacings $a_A = 0.086\,\text{fm}$, $a_B = 0.078\,\text{fm}$ and $a_D = 0.061\,\text{fm}$
- Physical lattice size $L \geq 3\,\text{fm}$ for many ensembles
- We use ≈ 600 up to ≈ 2500 gauge configuration per ensemble
- Charged pion masses range from $\approx 230\,\text{MeV}$ to $\approx 500\,\text{MeV}$
- μ_σ, μ_δ fixed for each β

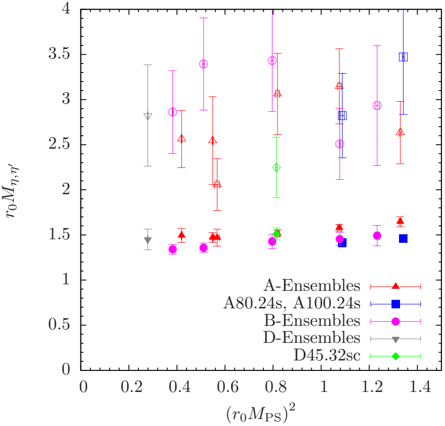
Identifying the states



Flavor contents for η (left) and η' (right) from B25.32 ensemble, 3x3-matrix, local-correlators only

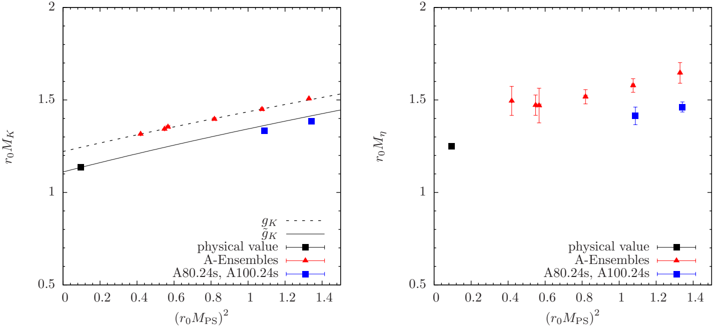
- Groundstate (η) has large strange contribution $\rightarrow$ expected from quark model
- Second state (η') is dominated by light quark contributions
- No charm contribution to any of the two states
- Third state (not shown) contains almost only charm

Masses for η, η'



- M_η has rather small statistical error, mostly $\lesssim 5\%$
- M_η shows moderate m_l-dependence
- M_η not at physical point yet
  $\rightarrow$ m_S-dependence
- η' even with 2500 gauges still hard to extract; shows large autocorrelation
- Need to study systematic errors especially for $M_{\eta'}$

m_S-dependence of M_K, M_η



M_K (left) and M_η (right) for A-Ensembles as function of M_{PS}^2

- In both cases the untuned points miss the physical value
- Blue points have different strange mass
- Dependence on m_s sizeable for K and η
- Bare m_s is fixed for each lattice spacing (but $m_{s,A} \neq m_{s,B} \neq m_{s,D}$)
- Perform linear fit $g_K[(r_0 M_{\mathrm{PS}})^2]$ and shift to hit physical point ($\tilde{g}_K$)

$\Longrightarrow$ Shift M_K for all ensembles by $\delta_{\mathrm{K}}[(r_0 M_{\mathrm{PS}})^2] = (r_0 M_{\mathrm{K}})^2[(r_0 M_{\mathrm{PS}})^2] - \tilde{g}_{\mathrm{K}}[(r_0 M_{\mathrm{PS}})^2]$

Correction for m_s

- Two different kaon masses M_K^A, $M_{K,s}^A$ for the A-Ensembles at $\mu_l = 0.008$ and $\mu_l = 0.010$
- Use them to estimate $D_\eta = \frac{d(aM_\eta)^2}{d(aM_K)^2}$
- Neglect possible M_{PS}, β-dependence
- Extrapolate all ensembles via

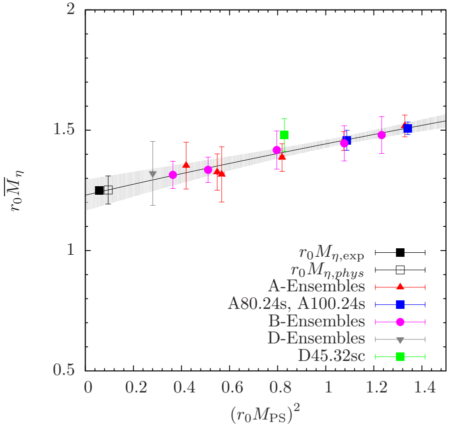
$$(r_0\overline{M}_\eta)^2[(r_0 M_{\mathrm{PS}})^2] = (r_0 M_\eta)^2 + D_\eta \cdot \delta_{\mathrm{K}}[(r_0 M_{\mathrm{PS}})^2]$$

Fitting $(r_0\overline{M}_\eta)^2[(r_0 M_{\mathrm{PS}})^2]$ we find

$$M_\eta(M_\pi) = 549(33)_{\mathrm{stat}}(44)_{\mathrm{sys}}\mathrm{MeV}$$

with $r_{0,\mathrm{phys}} = 0.45(2)\,\mathrm{fm}$

R. Baron et. al. PoS LATT2010, 123



Scaling behavior

- Use 3 points at different a and shift to fixed $r_0 \bar{M}_K \approx 1.34$ via

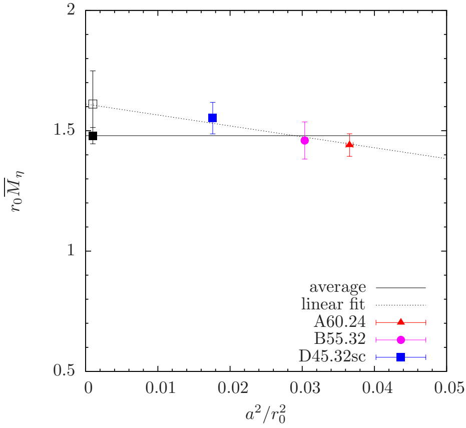
$$(r_0 \overline{M}_\eta)^2 = (r_0 M_\eta)^2 + D_\eta \cdot \Delta_\mathrm{K}$$

- Points have almost similar $r_0 M_{PS} \approx 0.9$
- Residual M_{PS}-dependence neglected
- $\Delta M = M_\mathrm{lin} - M_\mathrm{const} = 0.13(13)_\mathrm{stat}$

→ data compatible with constant fit!

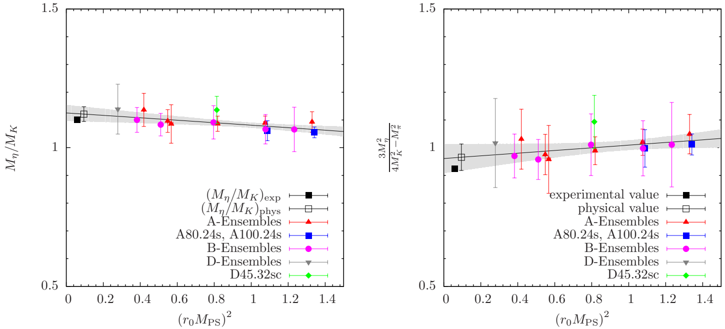
→ rather small lattice artefacts

However, we assume $\Delta M / M_\mathrm{const} \approx 8\%$ for our systematic error.



Scaling behavior using A60.24, B55.32 and D45.32

Mass ratios



$M_\eta/M_K[(r_0 M_{PS})^2]$ (left) and quadratic GMO (right)

For additional cross-check of our result for M_η, we study mass ratios:

- $M_\eta/M_K = 1.121(26)$ (exp value ≈ 1.100) gives $M_\eta = 558(13)_{stat}(45)_{sys}\mathrm{MeV}$
- $\frac{3M_\eta^2}{4M_K^2-M_\pi^2} = 0.966(48)$ (exp value ≈ 0.925) gives $M_\eta = 559(14)_{stat}(45)_{sys}\mathrm{MeV}$

$\Rightarrow$ Results from all three methods agree, combined fit gives
$M_\eta = 557(15)_{stat}(45)_{sys}\mathrm{MeV}$

Mixing

In the quark basis (neglecting charm)

$$|\eta_l\rangle = \frac{1}{2}(|u\bar{u}\rangle + |d\bar{d}\rangle) \ , \quad |\eta_s\rangle = |s\bar{s}\rangle$$

the η and η' are not pure states:

$$\begin{pmatrix} |\eta\rangle \\ |\eta'\rangle \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \cdot \begin{pmatrix} |\eta_\ell\rangle \\ |\eta_s\rangle \end{pmatrix} \ .$$

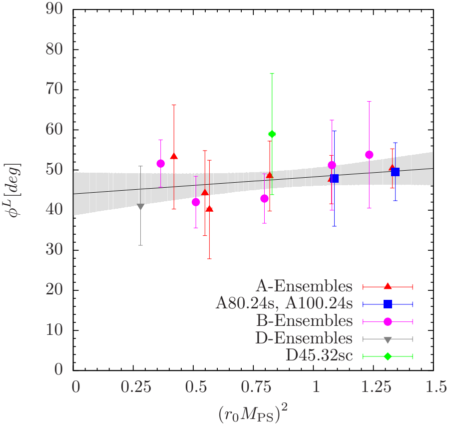
(single angle mixing scheme)

Expressed in amplitudes from matrix fit:

$$\tan^2(\phi) = -\frac{A_{\ell\eta'} A_{s\eta}}{A_{\ell\eta} A_{s\eta'}}$$

From linear fit we obtain:

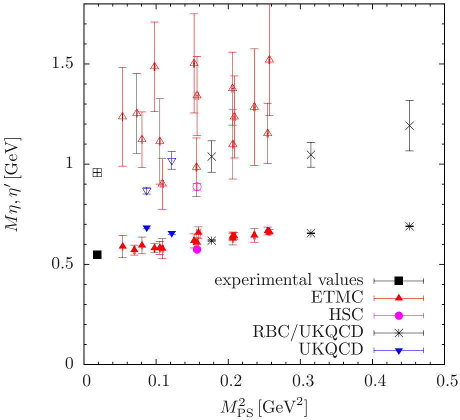
$\phi = 44^\circ(5)_{\mathrm{stat}}$



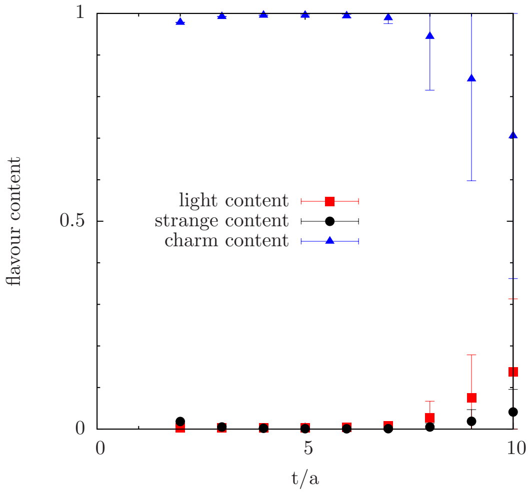
Mixing angle from 4×4 matrix using local amplitudes $A_{q,n}$

Summary and Outlook

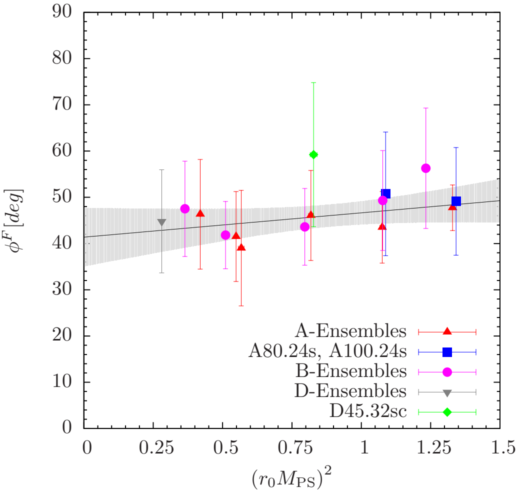
- First calculation with 2+1+1 dynamical quark flavours
- Small lattice artefacts for η
- No charm contribution to η and η'
- $M_\eta = 557(15)_{\text{stat}}(45)_{\text{sys}}\text{MeV}$ in good agreement with $M_\eta^{\text{exp}} \approx 548\text{MeV}$
- $M_{\eta'}$ strongly affected by noise and autocorrelation
- Mixing angle $\phi = 44°(5)_{\text{stat}}$
- Need better variance reduction for heavy disc loops
- Study flavour singlet decay constants from $\langle 0|A_\mu|\eta\rangle$, $\langle 0|A_\mu|\eta'\rangle$ (?)
- Additional scaling tests; vary m_s for more ensembles



Flavor contents for third state



Mixing angles from 6×6-matrix using fuzzed amplitudes



Factorizing fit model

$$\mathcal{C}_{qq'}(t) = \sum_n \frac{A_{q,n}A_{q',n}}{2m^{(n)}}\left[\exp(-m^{(n)}t) + \exp(-m^{(n)}(T-t))\right]$$

Generalized eigenvalue problem

Use of n operators allows to extract n excited states:

$$C^{\eta}_{ij}(t) \simeq \sum_{k=1}^{n} \phi_i^{(k)} \exp\left(-E_k t\right) \left(\phi_j^{(k)}\right)^*, \qquad \phi_i^{(k)} = \langle 0|\eta_i|k\rangle \ .$$

For $\eta_i = \eta_i^{\dagger}$, $C^{\eta}_{ij} = \left(C^{\eta}_{ij}\right)^{\dagger}$ one has to solve a generalized eigenvalue problem:

$$\mathcal{C}^{\eta}(t)\,\phi^{(k)}(t,t_0) = \lambda^{(k)}(t,t_0)\,C^{\eta}(t_0)\,\phi^{(k)}(t,t_0) \ ,$$

where $\phi^{(k)}$ is the eigenvector corresponding to k-th state.

- Masses are obtained from

$$\frac{\lambda_k(t,t_0)}{\lambda_k(t+1,t_0)} = \frac{\exp\left(-m^{(k)}t'\right) - \exp\left(-m^{(k)}(T-t')\right)}{\exp\left(-m^{(k)}(t'+1)\right) - \exp\left(-m^{(k)}(T-(t'+1))\right)} \ .$$

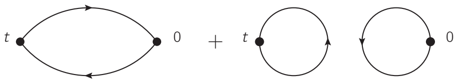
- Flavor contents of the states are given by

$$c_l^{(k)} = \frac{1}{N}\left(\phi_1^{(k)}\right)^2 , \quad c_s^{(k)} = \frac{1}{N}\left(\phi_2^{(k)}\right)^2 , \quad c_c^{(k)} = \frac{1}{N}\left(\phi_3^{(k)}\right)^2 \ ,$$

with N s.t. $c_l^{(k)} + c_s^{(k)} + c_c^{(k)} = 1$.

Variance reduction

Typical matrix element C_η^{ij} consists of connected and disconnected pieces:



Disconnected diagrams have large intrinsic noise → use stochastic sources ξ:

$$\phi = M^{-1}\xi \ , \qquad M_u = 2\kappa \mathrm{tr}\left[aD_{tmW}\left(1+\tau^3\right)/2\right]$$

In WtmLQCD there is a very efficient way to evaluate loops with light quarks:

Use $(M_d - M_u) = 4i\kappa a\mu_l\gamma_5$ and $M_u^\dagger = \gamma_5 M_d \gamma_5$ to obtain

$$\sum_{s,c,x} X\left(M_u^{-1} - M_d^{-1}\right) = 4i\kappa a\mu_l \sum_{s,c,x} X\left(M_u^{-1}\right)^\dagger M_u^{-1}\gamma_5$$

$$= 4i\kappa a\mu_l \sum_{s,c,x} \{\phi^*\gamma_5 X\phi\}_{n\ samples} + \mathrm{noise}$$

- Signal / noise ratio of $\sim V/\sqrt{V^2} = 1$ compared to $\sim 1/\sqrt{V}$
- Restricted to certain loops
- Cannot be applied in the heavy sector due to the additional mass splitting

K. Jansen et. al., Eur. Phys. J C58 261-269 (2008)