η and η′ mixing from Lattice QCD

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We present a lattice QCD computation of η and η′ masses and mixing angles, for the first time controlling continuum and quark mass extrapolations. The results for $M_\eta = 551(8)_{\text{stat}}(6)_{\text{sys}}$ MeV and $M_\eta' = 1006(54)_{\text{stat}}(38)_{\text{sys}}(+61)_{\text{sys}}$ MeV are in excellent agreement with experiment. Our data show that the mixing in the quark flavour basis can be described by a single mixing angle of $\phi = 46(1)_{\text{stat}}(3)_{\text{sys}}$ indicating that the η′ is mainly a flavour singlet state.

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Introduction.—Quantum Chromodynamics (QCD) is established as the theory of hadrons. Many of the properties of hadrons can be understood qualitatively from quark models, in which the gluons contribute only indirectly, being responsible for the force between quarks. A more direct consequence of the gluonic degrees of freedom in QCD is that quark loop contributions (also known as disconnected diagrams or OZI-rule violating contributions) are present – see Figure 1 – and they are important as disconnected diagrams or OZI-rule violating contributions in QCD are that quark loop contributions (also known as disconnected diagrams or OZI-rule violating contributions) are present – see Figure 1 – and they are important in a description of the ninth pseudoscalar meson, the η′ with mass 958 MeV. In fact, if the disconnected contributions were not present, the η would have the mass of the (neutral) pion. And the η′ would have a mass of about $\sqrt{2M_K^2 - M_\pi^2}$, which is much lighter than the physical η mass.

The large mass of the η′ meson is in contrast to the masses of the other eight light pseudoscalar mesons. Their small masses are qualitatively explained by the spontaneous breaking of chiral symmetry in QCD and the small quark mass values of up (u), down (d) and strange (s) quarks. The mass of the η′, the ninth pseudoscalar meson, is thought to be caused by the anomalous breaking of the $U(1)_A$ symmetry. This anomaly arises from the gluonic degrees of freedom in QCD and can be linked to the presence of topological excitations (of a pseudoscalar nature) in the QCD vacuum.[1–3].

This scenario – based on arguments from effective field theory and perturbation theory – should be checked by a non-perturbative evaluation directly from QCD itself. The non-perturbative method which allows most control over systematic errors is lattice QCD. Extrapolation to the continuum limit requires computing hadronic properties for several values of the lattice spacing (a). Formalisms which have modifications at finite lattice spacing of size $a^2$ allow this extrapolation to be made more reliably. Here we use the twisted mass lattice formalism which has this desirable property. It also has the attractive feature of allowing very efficient evaluation of disconnected contributions. To study the η and η′, it is essential to include u, d and s quarks. Here we go further and make use of a twisted mass formalism with the charm quark (c) also included. Loop contributions from even heavier quarks (b and t) can safely be neglected.

Because of the essential contribution of disconnected diagrams, which are noisy when evaluated in lattice QCD, previous results for η and η′ using u, d and s quarks are quite limited[4–8]. Previously, we have presented lattice results including also the c quark in Ref. [9] where we were able to determine the mass of the η meson. Here we extend this study, using powerful methods to separate ground and excited states, which will enable us to determine η and η′ mass and the corresponding mixing angle, for the first time extrapolated to the continuum limit and to physical values of up/down and strange quark masses. This result is fundamental for our understanding of QCD and confirms the role of the ABJ anomaly in generating the observed large mass of the η′ meson.

Lattice computation.—The results presented in this paper are based on gauge configurations generated by the European Twisted Mass collaboration (ETMC) with Iwasaki gauge action[10] and Wilson twisted mass fermions at maximal twist[11,12] with up, down, strange and charm dynamical quark flavours. Up and down quarks are mass degenerate and, therefore, mostly de-
noted with $\ell$ in the following. One important advantage of this fermion action is that physical quantities are $O(a)$ improved \([12]\) (c.f. Refs. \([11,13]\)). The main drawback of this action is that flavour and parity symmetries are broken at finite values of the lattice spacing, but restored in the continuum limit.

The details of the three sets of ETMC ensembles (called $A$, $B$ and $D$) were presented in Ref. \([15]\) and we adopt the notation therein for labeling the ensembles. A study of light meson masses and couplings (e.g. $f_\pi$), using chiral perturbation theory gave lattice spacings of $a_A = 0.0863(4)$ fm, $a_B = 0.0779(4)$ fm and $a_D = 0.0607(2)$ fm, respectively \([16]\). This can be summarised conveniently by specifying the Sommer scale (which we measure accurately on our lattices) as $\Lambda_0 = 0.45(2)$ fm, see Refs. \([9,10]\) for details. These ensembles cover a factor of two in $a^2$ so allow a reliable determination of the continuum limit ($a = 0$). The physical volumes are, with only a few exceptions, larger than 3 fm and $M_{\pi}L \geq 3.5$.

For each lattice spacing, the values of bare strange and charm quark masses are kept fixed, while the bare average up/down quark mass value is varied giving a lightest pseudoscalar meson (here called $M_\pi$) in the range $230–510$ MeV which allows reliable extrapolation to the physical value. The value of the strange quark mass is $230(510)$ MeV which allows reliable extrapolation to the physical value. The physical volumes are, with only a few exceptions, larger than 3 fm and $M_{\pi}L \geq 3.5$.

For fixing average up/down and strange quark masses to their physical values we use $M_{\pi\eta} = 135$ MeV and $M_{K_0} = 498$ MeV. All statistical errors are determined using a blocked bootstrap procedure with 1000 samples to account for autocorrelations.

We compute the Euclidean correlation functions

$$C(t)_{q'q} = \langle O_{q'}(t')O_q(t)\rangle, \quad q,q' \in \ell,s,c,$$  \hspace{1cm} (1)

with operators $O_{\ell} = (ui\gamma_5 u + di\gamma_5 d)/\sqrt{2}$, $O_s = \bar{s}i\gamma_5 s$ and $O_c = \bar{c}i\gamma_5 c$. We enlarge our correlator matrix $C$ by including also fuzzed operators. Note that in twisted mass lattice QCD there are several steps required to reach these correlation functions, as explained in detail in Ref. \([9]\). We estimate the disconnected contributions to the correlation functions Eq. \([1]\) using Gaussian volume sources and the one-end trick for the connected contribution \([14]\). For the light disconnected contributions a powerful noise reduction technique is available \([8,18]\). For the strange and charm disconnected loops, we use the hopping parameter noise reduction technique.

We solve the generalised eigenvalue problem (GEVP) \([15,21]\)

$$C(t)\eta^{(n)}(t,t_0) = \lambda^{(n)}(t,t_0)C(t_0)\eta^{(n)}(t,t_0) \hspace{1cm} (2)$$

for eigenvalues $\lambda^{(n)}(t,t_0)$ and eigenvectors $\eta^{(n)}$. $n$ labels the states $\eta, \eta', \ldots$ contributing. Masses of these states can be determined from the exponential fall-off of $\lambda^{(n)}(t,t_0)$ at large $t$. The pseudoscalar matrix elements $A_{q,n} \equiv \langle n|O_q|0\rangle$ with $q \in \ell,s,c$ and $n \in \eta, \eta', \ldots$ can be extracted from the eigenvectors \([21]\). It turns out that the charm quark contributions to $\eta, \eta'$ are negligible and, thus, we drop the $c$ quark in what follows.

As an example for the masses determined from the GEVP we show in Figure \([a]\) the effective masses $aM^{(*)} = -\log\{\lambda^{(*)}(t,t_0)/\lambda^{(*)}(t+1,t_0)\}$ as a function of $t/a$ for ensemble A100. One observes a clear plateau for the lowest state from $t/a = 6$ on. For the first excited state, the $\eta'$, a plateau is barely visible.

To improve the $\eta'$ (and $\eta$) mass determinations, we use a method first proposed in Ref. \([22]\) and successfully applied for the $\eta_2$ (the $\eta'$ in $N_f = 2$ flavour QCD) in Ref. \([18]\). The method is based on the following assumption: disconnected contributions are only big for the $\eta$ and $\eta'$ states, but negligible for higher excited states. The assumption would be justified if topological charge fluctuations in the vacuum, which give a large contribution to the $\eta'$ mass, mainly coupled to the $\eta, \eta'$ states, and not to other heavier states. Of course, the validity of this assumption needs to be checked in the Monte-Carlo data.

The connected contractions, shown in Figure \([a]\) have a constant signal to noise ratio in time, so we can reliably determine the ground states in these two connected correlators and subtract the excited state contributions. We then use these to build a correlation matrix $C^{emb}$ from subtracted connected and original disconnected contractions. If disconnected contributions were relevant only for $\eta$ and $\eta'$, one should find – after diagonalising $C^{emb}$ – a plateau for both $\eta$ and $\eta'$ from small values of $t/a$ on.

The effect of this procedure can be seen in Figure \([b]\).
FIG. 3: $\eta$ (filled) and $\eta'$ (open) masses versus $(r_0 M_\pi)^2$ and chiral extrapolations with errorbands.

A plateau appears at much earlier $t/a$ values as compared to Figure 2(a), while the plateau values agree very well within errors. Therefore, we use this procedure – which allows to determine in particular the $\eta'$ mass value with much better accuracy – for the results presented here.

The $\eta$ and $\eta'$ mesons will be flavour mixtures in general. For the determination of the corresponding mixing angle, it is convenient on the lattice to work in the quark flavour basis. Our mixing determination builds on the angle, it is convenient on the lattice to work in the quark flavour basis. Our mixing determination builds on the pseudoscalar matrix elements $A_{q,n}$ which enter the fit to the correlators and which can be expressed with two mixing angles $\phi_\ell, \phi_s$ and two constants $c_\ell, c_s$

\[
\begin{pmatrix} A_{\ell,\eta} & A_{s,\eta} \\ A_{\ell,\eta'} & A_{s,\eta'} \end{pmatrix} \approx \begin{pmatrix} c_\ell \cos \phi_\ell & -c_s \sin \phi_\ell \\ c_\ell \sin \phi_\ell & c_s \cos \phi_\ell \end{pmatrix} .
\]

(3)

Given data for $A_{q,n}$, the mixing angles can be extracted:

\[
\tan \phi_\ell = \frac{A_{\ell,\eta'}}{A_{\ell,\eta}}, \quad \tan \phi_s = -\frac{A_{s,\eta}}{A_{s,\eta'}} .
\]

(4)

Note that $c_\ell, c_s$ and renormalisation constants drop out in Eqs. 4. In chiral perturbation theory combined with large $N_c$ arguments one can show that in the quark flavour basis $|\phi_s - \phi_\ell| \ll 1$ should hold (see Refs. 23–27 and references therein). If this is the case, a single mixing angle $\phi \approx \phi_s \approx \phi_\ell$ can be determined from

\[
\tan^2(\phi) = -\frac{A_{\ell,\eta'} A_{s,\eta}}{A_{\ell,\eta} A_{s,\eta'}} .
\]

(5)

Results.—To compare different lattice spacings, we plot values for $r_0 M_\eta$ (corrected for any mismatch of the strange quark mass [9]) as filled symbols in Figure 3 with an error band dominated by the error of the strange quark mass mismatch correction. The data from all three values of the lattice spacing fall onto a single line, indicating small lattice artifacts and successful mismatch correction. The line represents a linear fit of $(r_0 M_\eta)^2$ in the squared pion mass to our data, resulting in $M_\eta = 551(11)_{\text{stat}}$ MeV. Alternatively, we extrapolate $(M_\eta/M_K)^2$ or the GMO ratio $3M_\eta^2/(4M_K^2 - M_\pi^2)$ linearly in the squared pion mass, leading to $M_\eta = 547(8)_{\text{stat}}$ MeV and $M_\eta = 554(8)_{\text{stat}}$ MeV, respectively. We estimate the systematic uncertainties from fitting the different lattice spacings separately and quote as a final result the weighted average (accounting for correlations) over the three methods

\[
M_\eta = 551(8)_{\text{stat}}(6)_{\text{sys}} \text{ MeV} .
\]

The data for $M_\eta'$ are plotted as open symbols in Figure 3 showing, within the statistical errors, no visible lattice spacing or strange quark mass dependence. Therefore, we extrapolate the data of $(r_0 M_\eta)^2$ for all values of the lattice spacing, again linearly in the squared pion mass, to the physical point and obtain

\[
M_\eta' = 1006(54)_{\text{stat}}(38)_{\text{sys}}(+61)_{\text{ex}} \text{ MeV} ,
\]

where again the systematic error comes from separate fits to the data at the different lattice spacing values. In order to estimate the potential systematic error stemming from the excited state removal procedure, we use the difference of the extrapolations of data with and without excited state removal.

It is worth noting that our estimates for $M_\eta$ and $M_\eta'$ are in excellent agreement with the experimental values of 547.85(2) MeV and 957.78(6) MeV [28], respectively.

Using Eqs. 4 we can evaluate $\phi_\ell$ and $\phi_s$ for all ensembles. We first study the difference $\phi_\ell - \phi_s$ shown in Figure 3: the difference is indeed rather small and mostly compatible with zero with no significant dependence of the strange quark mass. A linear extrapolation
in \((r_0 M_\pi)^2\) of all the data yields \(3(1)_{\text{stat}}(3)_{\text{sys}}\,^\circ\), where the systematic error is estimated from the maximal difference compared to extrapolating the data sets for the three different lattice spacings separately.

In Figure 5 we show estimates for the single angle \(\phi\) computed from Eq. 5. Due to correlations of the data used in the ratio, the statistical errors are smaller than for \(\phi_\ell\) and \(\phi_\pi\) separately. The data appear to confirm the smallness of \(|\phi_\ell - \phi_\pi|\), as the overall picture is rather consistent. Within the statistical accuracy, we cannot resolve (but also not exclude) a residual lattice spacing and strange quark mass dependence. Therefore, we perform a linear fit in the squared pion mass to our data for \(\phi\) and obtain

\[
\phi = 46(1)_{\text{stat}}(3)_{\text{sys}}\,^\circ.
\]

This value of \(\phi\) indicates that the \(\eta\) meson is dominated by the flavour octet and the \(\eta'\) mainly by the flavour singlet state. It is in good agreement with other lattice determinations [4, 6–8] and slightly higher than the average phenomenological estimate [20]. We recall that we defined the angles for the pseudoscalar densities. Due to the anomaly they are, therefore, not directly related to the mixing angles defined via the axial vector current.

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FIG. 5: \(\phi\) as a function of \((r_0 M_\pi)^2\). Note that the data are consistent with the SU(3) flavour symmetry requirement \(\phi_{SU(3)} = \text{arctan} \sqrt{2} \approx 54.7^\circ\) for \(m_\ell = m_\pi\).