

# An estimate of the $\eta$ and $\eta'$ meson masses in $N_f = 2 + 1$ lattice QCD

CP-PACS and JLQCD Collaborations:

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Masses of the  $\eta$  and  $\eta'$  mesons are estimated in  $N_f = 2 + 1$  lattice QCD with the non-perturbatively  $O(a)$  improved Wilson quark action and the Iwasaki RG-improved gluon action, using CP-PACS/JLQCD configurations on a  $16^3 \times 32$  lattice at  $\beta = 1.83$  (lattice spacing is 0.122 fm). We apply a stochastic noise estimator technique combined with smearing method to evaluate correlators among flavor  $SU(2)$  singlet pseudoscalar operators and strange pseudoscalar operators for 10 combinations of up/down and strange quark masses. The correlator matrix is then diagonalized to identify signals for mass eigenstates. Masses of the ground state and the first excited state extrapolated to the physical point are  $m_\eta = 0.545(16)$  GeV and  $m_{\eta'} = 0.871(46)$  GeV, being close to the experimental values of the  $\eta$  and  $\eta'$  masses.

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## 1. Introduction

The U(1) problem [1] is an outstanding issue in hadron spectroscopy. The large mass of the  $\eta'$  relative to the  $\pi$  is believed to be related to QCD vacuum structure and anomaly of the axial current. In order to reproduce the  $\eta'$  mass from first principles calculations, a number of lattice QCD simulations have been carried out. Early attempts [2, 3] were made in quenched QCD. Recent studies [4, 5, 6] shifted to full QCD with two degenerate up and down ( $u/d$ ) quarks.

In the real world the role of strange ( $s$ ) quark is important since the mass difference between the  $s$  quark and  $u/d$  quarks is the cause of mixing between the singlet and octet pseudoscalars, that leads to the physical  $\eta$  and  $\eta'$  mesons. In this article, we report on an attempt to estimate masses of the  $\eta$  and  $\eta'$  in  $N_f = 2 + 1$  QCD, in which degenerate  $u/d$  quarks and an  $s$  quark are treated dynamically. The mixing effect is taken into account by diagonalizing a correlator matrix for operators coupled to both  $\eta$  and  $\eta'$ . We use Wilson quark formulation. An attempt to calculate the  $\eta'$  mass with staggered fermions is made in Ref. [7].

The calculation is carried out on a set of gauge configurations generated previously for a study of the flavor non-singlet hadron spectrum and light quark masses in  $N_f = 2 + 1$  QCD [8]. This report presents results for the  $\eta$  and  $\eta'$  masses calculated for the coarsest of the three lattice spacings.

A technical difficulty in the study of the  $\eta$  and  $\eta'$  masses lies in the evaluation of the two-loop quark diagram contribution to the singlet part of propagators. Due to configuration fluctuations in the two-loop diagram, errors of the  $\eta$  and  $\eta'$  propagators increase rapidly as time slice. On the other hand, we have to suppress contamination from higher excited states. Calculations have to be setup in a way that signals of the  $\eta$  and  $\eta'$  appear at small time slices. For this purpose, we combine a smearing method with a stochastic noise estimator technique (SET), as carried out in Ref. [6].

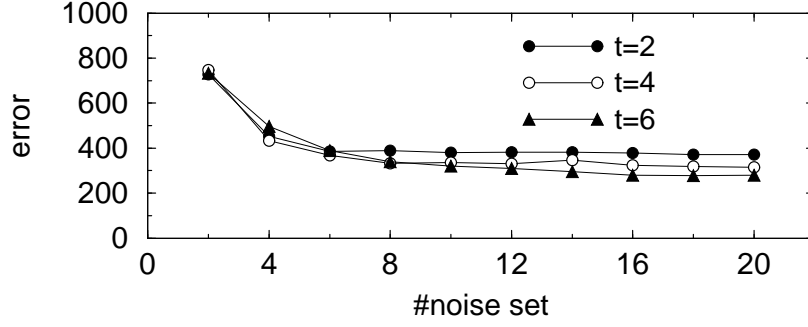
The organization of this article is as follows. Numerical calculations including our procedure to calculate the two-loop diagram are described in Sec. 2. In Sec. 3 we give an account of analysis procedure and the  $\eta$  and  $\eta'$  masses at the physical point. Conclusions are given in sec. 4. Data presented here should be regarded as preliminary since detailed analysis is still ongoing.

## 2. Numerical Calculations

### 2.1 Configuration

We use a set of  $N_f = 2 + 1$  full QCD configurations [8] generated with the Iwasaki RG-improved gauge action and the non-perturbatively  $O(a)$  improved Wilson fermion action at  $\beta = 1.83$  on a  $16^3 \times 32$  lattice. Polynomial hybrid Monte Carlo simulations have been carried out for 10 quark mass combinations; we choose five hopping parameters  $K_{ud} = 0.13655, 0.13710, 0.13760, 0.13800$  and  $0.13825$  for the  $u/d$  quarks, and two  $K_s = 0.13710$  and  $0.13760$  for the  $s$  quark. The pseudoscalar to vector mass ratio ranges from 0.78 to 0.61. The lattice spacing is  $a = 0.122$  fm which is determined from experimental values of the  $\pi$ ,  $\rho$  and  $K$  meson masses.

The trajectory length is 7000 – 8600 for each mass combination. Measurements are carried out at every 10 trajectories. Errors are estimated by the jack-knife method with a bin size of 10 configurations (100 trajectories).



**Figure 1:** Error of the two-loop diagram versus number of noise sets for ( $K_s = 0.13710, K_{ud} = 0.13825$ ). The vertical scale is arbitrary.

## 2.2 Two-loop quark diagram

When one determines the  $\eta$  and  $\eta'$  masses from propagators around a time slice, contamination from higher excited states has to be small at that time slice. For this condition to be satisfied, it is desirable that contamination is small also for octet pseudoscalars. In Ref. [8], we adopted an exponential-like smearing function

$$K(\vec{n} - \vec{m}) = A \exp(-B|\vec{n} - \vec{m}|) \quad \text{for } \vec{n} \neq \vec{m}, \quad K(\vec{0}) = 1, \quad (2.1)$$

with  $A = 1.2$  and  $B = 0.1$ , and find that effective masses of octets obtained with doubly smeared source and unsmeared (point) sink operators reach an approximate plateau at a small time slice; the mass estimated at  $t \approx 4$  is only a few percent different from accurate value of the ground state mass. With this observation in mind, we construct the two-loop diagram using a doubly smeared loop diagram at the source with the kernel (2.1) and an unsmeared loop diagram at the sink, and combine it with the corresponding one-loop diagram.

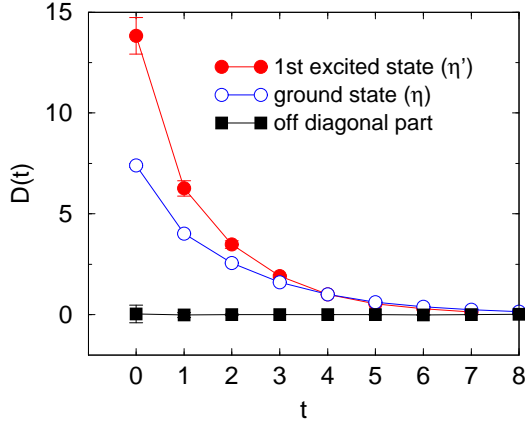
The two-loop diagram is estimated by a combined method of SET and smearing applied to configurations fixed to Coulomb gauge. We prepare a  $U(1)$  random number  $\exp(i\theta(\vec{n}, t))$  for each site  $(\vec{n}, t)$  of the whole lattice and solve a quark propagator  $q(\vec{n}, t)$  for the random source. The propagator is then smeared twice at a source time slice  $t_{\text{src}}$ , multiplied by the inverse of the random number and summed over sites on the time slice,

$$\xi(t_{\text{src}}) = \sum_{\vec{l}, \vec{m}, \vec{n}} \exp(-i\theta(\vec{l}, t_{\text{src}})) K(\vec{l} - \vec{m}) K(\vec{m} - \vec{n}) q(\vec{n}, t_{\text{src}}). \quad (2.2)$$

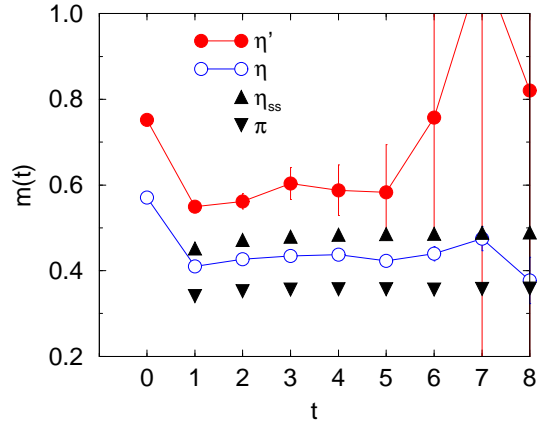
The loop diagram  $\zeta(t_{\text{snk}})$  at a sink time slice  $t_{\text{snk}}$  is calculated similarly without smearing. The two-loop diagram is estimated by averaging the product of the two loops over 20 stochastic noise sets generated for each color and spin at a time,

$$G_{2\text{-loop}}(t) = \frac{1}{L^3 T} \sum_{t=t_{\text{snk}}-t_{\text{src}}} \langle \text{Tr}(\gamma_5 \zeta(t_{\text{snk}})) \text{Tr}(\gamma_5 \xi(t_{\text{src}})) \rangle_{\text{noise}}. \quad (2.3)$$

In any stochastic noise methods, error consists of stochastic noise and configuration fluctuations. In our case, the error of the two-loop diagram decreases rapidly with a number of noise sets and reaches a plateau for a range of time slices we use for later analysis. See Fig. 1. This means that our final error obtained with full 20 noise sets is dominated by configuration fluctuations.



**Figure 2:** Diagonalized propagator for ( $K_s = 0.13710, K_{ud} = 0.13825$ ). For off-diagonal part,  $D_{12}(t)$  in eq. (3.4) are plotted.



**Figure 3:** Effective masses of the  $\eta$  and  $\eta'$  for ( $K_s = 0.13710, K_{ud} = 0.13825$ ). Those for  $\pi$  and  $\eta_{ss}$  are overlaid.

### 3. Analysis and Results

#### 3.1 $\eta$ and $\eta'$ masses at simulation points

In order to derive masses of the  $\eta$  and  $\eta'$ , we consider flavor  $SU(2)$  singlet and strange pseudoscalar operators

$$\eta_n = (\bar{u}\gamma_5 u + \bar{d}\gamma_5 d)/\sqrt{2}, \quad \eta_s = (\bar{s}\gamma_5 s), \quad (3.1)$$

and calculate the  $2 \times 2$  correlators

$$G(t) = \begin{pmatrix} \eta_n^P(t)\eta_n^S(0) & \eta_n^P(t)\eta_s^S(0) \\ \eta_s^P(t)\eta_n^S(0) & \eta_s^P(t)\eta_s^S(0) \end{pmatrix}, \quad (3.2)$$

where superscripts  $S$  and  $P$  denote smeared and point operators. If the correlator matrix is dominated by the contribution of the ground state ( $\eta$ ) and the first excited state ( $\eta'$ ) at a time slice  $t$ , we obtain a relation

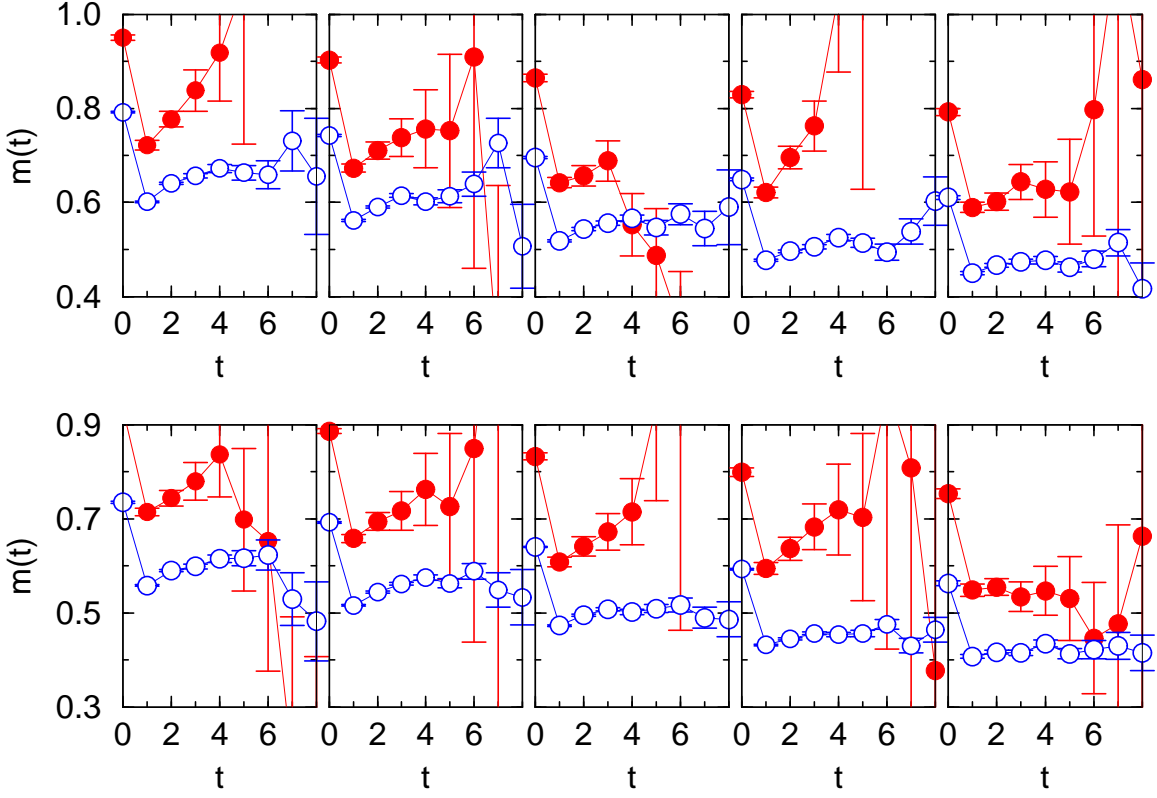
$$(CG(t)G^{-1}(t_0)C^{-1})_{ij} \approx \delta_{ij} \exp(-m_i(t-t_0)) \quad i, j = \eta, \eta', \quad (3.3)$$

where the matrix  $C$  diagonalizes the basis operators  $\eta_k^P$  ( $k = n, s$ ) to give the physical ones  $O_i$  ( $i = \eta, \eta'$ ),  $O_i = \sum_{k=n,s} C_{ik} \eta_k^P$ , and  $t_0$  is a reference time slice. The matrix  $C$  is independent of time slice. Selecting a representative time slice  $t_D$ , we estimate the matrix  $C$  by diagonalizing the matrix  $G(t_D)G^{-1}(t_0)$ . We then calculate the “diagonalized” propagator

$$D_{ij}(t) = (CG(t)G^{-1}(t_0)C^{-1})_{ij}. \quad (3.4)$$

Note that  $D_{ij}(t_0) = \delta_{ij}$  and  $D_{ij}(t_D) = 0$  ( $i \neq j$ ) by definitions.

Figure 2 shows the diagonalized propagator obtained with  $t_0 = 4$  and  $t_D = 3$  for the mass combination of the heaviest  $s$ -quark and the lightest  $u/d$ -quarks. Diagonal parts (signals for  $\eta$  and  $\eta'$ ) decay exponentially as indicated by effective masses plotted in Fig. 3, while off-diagonal parts



**Figure 4:** Effective masses of the  $\eta$  (open symbols) and  $\eta'$  (filled symbols) for  $K_s = 0.13710$  (top panels) and  $0.13760$  (bottom panels).  $u/d$ -quark mass decreases from left panels to right panels.

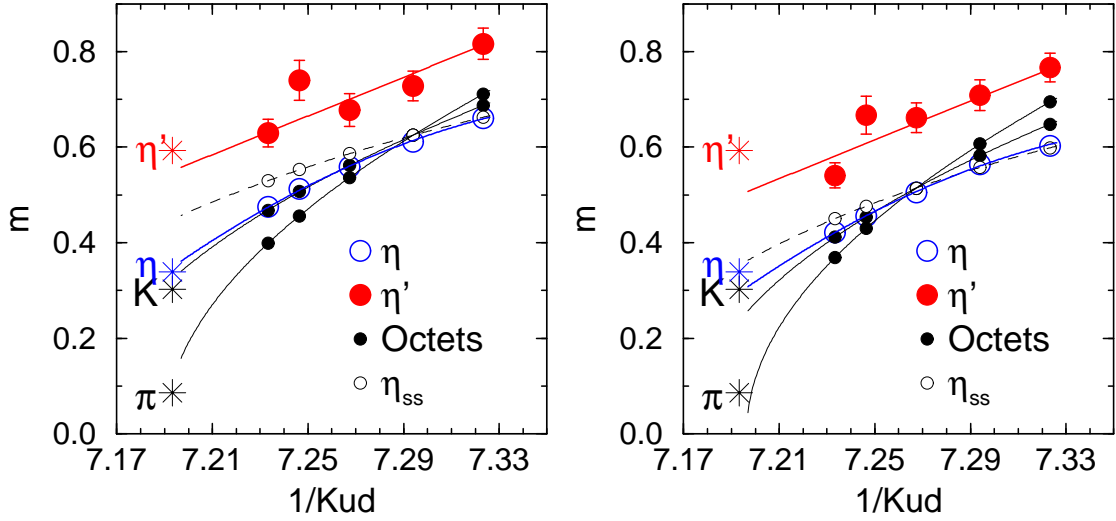
are negligible for all  $t$ . In other words, the relation (3.3) is realized. This result suggests that the  $\eta$  and  $\eta'$  contribution dominates our correlator matrix at small time slice, e.g., already at  $t \approx 2$ .

In Fig. 3, we overlay effective masses of an octet pseudoscalar  $\bar{u}\gamma_5 d$  ( $\pi$ ) and those of  $\bar{s}\gamma_5 s$  determined by ignoring the two-loop diagram contribution (“ $\eta_{ss}$ ”). The mass of the  $\eta'$  is much larger than masses of the  $\pi$  and  $\eta_{ss}$ , which demonstrates the importance of the two-loop diagram contribution for the large mass of the  $\eta'$

Figure 4 shows effective masses of the  $\eta$  and  $\eta'$  for all quark mass combinations. Because effective masses of the  $\eta$  show approximate plateaus around  $t \approx 4$ ,  $m_\eta$  are determined from fits in the range  $t = 3 - 5$ . For  $\eta'$ , plateaus are clear for the lightest  $u/d$ -quarks, while they are not so apparent for heavier  $u/d$ -quarks. Nonetheless off-diagonal parts of the diagonalized propagator are consistent with zero already at  $t = 2$  for all cases, which suggests that contribution from higher excited states is small. Therefore, we estimate  $m_{\eta'}$  from fits in the range  $t = 2 - 4$ . Table 1 summarizes masses of the  $\eta$  and  $\eta'$ .

For degenerate  $u/d$  and  $s$  quarks, the  $\eta$  is a pure octet state, and therefore  $m_\eta$  should agree with  $m_{\eta_{ss}}$ . Values of  $m_\eta$  in Table 1 are determined by the procedure explained above even for these cases. On the other hand, one-mass fits to  $\eta_{ss}$  propagators in the range  $t = 8 - 16$  give  $m_{\eta_{ss}} = 0.6251(13)$  and  $0.5136(09)$  for  $K_{ud} = K_s = 0.13710$  and  $0.13760$  respectively. They are larger than

$K_{ud}$	$K_s = 0.13710$		$K_s = 0.13760$	
	$m_\eta$	$m_{\eta'}$	$m_\eta$	$m_{\eta'}$
0.13655	0.6605(35)	0.816(33)	0.6022(39)	0.767(30)
0.13710	0.6116(31)	0.728(31)	0.5645(23)	0.709(32)
0.13760	0.5588(34)	0.678(34)	0.5055(22)	0.662(31)
0.13800	0.5122(32)	0.740(42)	0.4555(23)	0.667(39)
0.13825	0.4751(45)	0.629(29)	0.4220(37)	0.541(26)

**Table 1:** Masses of the  $\eta$  and  $\eta'$  mesons.**Figure 5:** Pseudoscalar meson masses versus  $1/K_{ud}$  for  $K_s=0.13710$  (left figure) and  $0.13760$  (right figure). Stars marked at the physical  $u/d$  quark mass point indicate experimental values.

$m_\eta$  by about 2 percent. We regard the 2 percent as an estimate of systematic error in  $m_\eta$  arising from excited state contaminations.

### 3.2 Chiral extrapolations

Chiral fits to  $m_\eta$  and  $m_{\eta'}$  are made using low order polynomial functions of quark masses defined by  $m_{ud} = (1/K_{ud} - 1/K_c)/2$  and  $m_s = (1/K_s - 1/K_c)/2$  ( $K_c$  is the critical hopping parameter). Masses of pseudoscalar mesons are plotted in Fig. 5 as a function of  $1/K_{ud}$ . The figure suggests that  $m_{\eta'}$  shows a linear dependence in  $m_{ud}$  within our errors, so we assume a simple linear function

$$m_{\eta'} = A + B_{ud}m_{ud} + B_s m_s. \quad (3.5)$$

We obtain  $\chi^2/\text{dof} = 1.4$ , which is acceptable. We include a quadratic term of  $m_{ud}$  for  $m_\eta$ ,

$$m_\eta = C + D_{ud}m_{ud} + D_s m_s + E m_{ud}^2, \quad (3.6)$$

because a linear function does not fit to data due to curvatures shown in Fig. 5. The quadratic term reduces  $\chi^2$  of the fit greatly to  $\chi^2/\text{dof} = 1.0$ . We note that linear fits to  $m_{\eta, \eta'}$  give masses at the physical point consistent with those from the fits above within  $3\sigma$  for the  $\eta$  and  $1\sigma$  for the  $\eta'$ .

Masses of the  $\eta$  and  $\eta'$  extrapolated to the physical point, as determined from experimental  $m_\pi$ ,  $m_\rho$  and  $m_K$ , read

$$m_\eta = 0.545(16) \text{ GeV}, \quad (3.7)$$

$$m_{\eta'} = 0.871(46) \text{ GeV}. \quad (3.8)$$

#### 4. Conclusions and Future Plan

We have estimated the masses of the  $\eta$  and  $\eta'$  in  $N_f = 2 + 1$  lattice QCD, albeit at one lattice spacing. Our result  $m_\eta=0.545(16)$  GeV is consistent with the experimental value of 0.550 GeV. The  $\eta'$  meson mass  $m_{\eta'}=0.871(46)$  GeV is also close to experiment, 0.960 GeV. This is encouraging since the small difference of 100 MeV between our value for  $m_{\eta'}$  and experiment may well be accounted for by systematic errors.

Finite lattice spacing is one of possible origins of systematic errors. Another shortcoming of this work is a relatively large value of  $u/d$  quark masses. We expect to improve our program for the U(1) problem using CP-PACS/JLQCD configurations already generated for finer lattices and configurations which will be generated by the PACS-CS collaboration [9] soon for lighter quarks.

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