Lattice QCD study of four-quark components of the iso-singlet scalar mesons — significance of disconnected diagrams —

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(Dated: December 15, 2014)

Abstract

We study the possible significance of four-quark states in the iso-singlet scalar mesons (\(J^{PC} = 0^{++}, I = 0\)) by performing two-flavor full lattice QCD simulations on an \(8^3 \times 16\) lattice using the improved gauge action and the clover-improved Wilson quark action. In particular, we evaluate the propagators of molecular and tetra-quark states together with singly disconnected diagrams. For the computation of the singly disconnected diagrams we employ the \(Z_2\)-noise method with the truncated eigenmode approach. We show that the quark loops given by the disconnected diagrams play an essential role in making the four-quark states exist. We find that the light iso-singlet scalar meson \(\sigma\) may be the molecular state. The main component of the propagator of the tetra-quark state originates from the singly disconnected diagrams.

Usage

PACS numbers

Structure
I. INTRODUCTION

The approximate chiral symmetry and its spontaneous breaking in QCD are indispensable basic ingredients for understanding the low-energy phenomena of hadrons. The pions should be the remnants of the Nambu-Goldstone (NG) bosons associated with the spontaneous breaking of chiral $SU(2) \otimes SU(2)$ symmetry with $\langle \bar{u}u + \bar{d}d \rangle / \sqrt{2}$ being the order parameter; their small masses come from the tiny current quark masses of $u$ and $d$ quarks. The other would-be NG boson is the $\eta$, which is massive even in the chiral limit where the quarks are massless due to the axial anomaly in QCD. In the linear representation of $SU(2) \otimes SU(2)$, the four scalar bosons appear, one of which is traditionally called the $\sigma$ meson. The scalar bosons are the amplitude fluctuations of the chiral order parameter, while the NG bosons the phase fluctuations. In view of the success of the nonlinear realization of the chiral symmetry in describing the low-energy hadron phenomena, the curvature of the effective potential might be large, and accordingly the $\sigma$ might appear only as a high-lying state coupled with other states. Nevertheless, the picture given by the linear representation where the $\sigma$ exists as a basic ingredient should become relevant around the (pseudo-) critical region of the chiral transition, which is found to be a crossover with a transitional region in the lattice QCD.

Interestingly enough, recent experiments and precise and systematic analyses of the $\pi-\pi$ scattering respecting the crossing symmetry as well as the chiral symmetry have revealed the existence of the low-mass scalar meson with a mass from 400 to 700 MeV. Then the physical content and the mechanism for realizing such a low-lying state in the $J^{PC} = 0^{++}$ state have prompted much debate. One of the most popular ideas is that all the low-lying scalar states can be realized as tetra-quark states, i.e., diquark-antidiquark states, as first advocated by Jaffe. On the other hand, the appearance of the $\sigma$ in the $\pi-\pi$ scattering may simply suggest that the meson is a $\pi-\pi$ resonance state with the pion maintaining its identity; if the pions were heavy, the resonance state may turn into a molecular state of the heavy pion. Note that such four-quark states, irrespective whether they are molecular states or tetra-quark states, are more likely to exist in the heavy-quark sectors: such exotic states include $X(3872)$, $Y(4260)$, $Z(4430)$, $Z_b(10610)$, and $Z_b(10650)^{+,-}$. It would be interesting to see how the four-quark states or the components of a hadron change as the quark masses are changed.

In the present work, we explore the possible significance of the four-quark components in
the iso-singlet scalar mesons by performing two-flavor full lattice QCD simulations. Many quenched lattice simulations have been carried out for the iso-singlet scalar mesons. The first full QCD calculation of the $\sigma$ meson was performed by the SCALAR Collaboration, where the $(\bar{q}q)$ interpolation field was used and a disconnected diagram, i.e., a quark-loop diagram in the normal language of the quantum field theory, was evaluated using the $Z_2$-noise method with the truncated eigenmode approach. It was found that the inclusion of the disconnected diagram is indispensable for obtaining a clear signal showing the existence of the low-lying scalar meson. They also showed a significant quark mass dependence of the clearness and the resultant mass of the $\sigma$. There have been many subsequent studies of the scalar mesons including the $\kappa$ based on lattice simulations of full QCD. The possible four-quark nature of the iso-nonsinglet scalar mesons has also been examined on a lattice. More recently, Prelovsek et al. explored the possibility that the $\sigma$ meson is well described as a four-quark state, i.e., a molecular or tetra-quark state, without taking into account the disconnected diagrams, which may unfortunately make the physical significance of their result obscure in view of the essential significance of the disconnected diagram observed in Ref. 13. We show that the quark loops given by the disconnected diagrams play an essential role in making the four-quark states exist. We perform simulations both with and without disconnected diagrams and compare them. Although the quark masses used in the present work are admittedly not small, and hence it may not be straightforward to extract direct implications regarding the nature of the $\sigma$, our work may be an important milestone to understand the role of the four-quark states possibly changing from light to heavy quark sectors.

In the present work, we prepare two types of interpolation operators for the creation of four-quark states: a molecular operator $(\bar{q}q)(\bar{q}q)$ with $(\bar{q}q)$ and a tetra-quark operator $(\bar{q}qqq)$ composed of a diquark $(qq)$ and an antidiquark $(\bar{q}\bar{q})$ being color-singlet. There are many other operators with the same quantum number as the $\sigma$, which include $(\bar{q}q)$, $(\bar{q}q)(\bar{q}q)$, $(\bar{q}qqq)$, the glueballs $(gg)$, the hybrids $(\bar{q}qq)$, and their excited modes. It would certainly be desirable to include all the operators for a precise calculation. In the present work, however, we do not include these operators as interpolation operators. Note that our calculation is a full QCD calculation and hence all the states that couple to the $\sigma$ should, in principle, be created in the intermediate states, provided that the prepared interpolation operators well coupled with these states. Moreover, it has been reported that the scalar glueball is
heavy with a mass of approximately 1500 MeV and will be decoupled from the low-lying \(\sigma\). Therefore, the neglect of the glueball state as well as hybrids including glueball states should be valid for the description of the \(\sigma\). It is needless to say that the numerical cost will become huge for full QCD calculations incorporating all the above interpolation operators. This numerical cost is especially huge, when we include the disconnected diagrams.

The present article is organized as follows. We begin in Section II by showing the formulation of the four-quark propagators. In Section III we give the numerical results of our simulations and discuss the significance of the disconnected diagrams in the four-quark propagators, effective masses, and the iso-singlet scalar mesons. We end in Section IV with our conclusions.

II. FOUR-QUARK STATES IN THE ISO-SINGLET SCALAR MESONS

We investigate the possible significance of the four-quark states in the iso-singlet scalar mesons by performing the two-flavor full lattice QCD simulations. In particular, we focus on the ingredients in the four-quark states that might consist of the molecular state \((\bar{q}q)(\bar{q}q)\) and/or the tetra-quark state \((\bar{q}qqq)\).

The molecular interpolation operators are defined as

\[
O_{\text{molec}}(t) = \frac{1}{\sqrt{3}} \left[ O_{\pi}^{\pi^+}(t)O_{\pi}^{\pi^-}(t) - O_{\pi}^{\pi^0}(t)O_{\pi}^{\pi^0}(t) + O_{\pi}^{\pi^-}(t)O_{\pi}^{\pi^+}(t) \right],
\]

where \(O_{\pi}^{\pi^+}(t)\), \(O_{\pi}^{\pi^-}(t)\), and \(O_{\pi}^{\pi^0}(t)\) are the \(\pi\) meson operators made up of two quarks. They are given by

\[
O_{\pi}^{\pi^+}(t) = -\sum_{x,a} \bar{d}^a(t,x)\gamma_5 u^a(t,x),
\]

\[
O_{\pi}^{\pi^-}(t) = \sum_{x,a} \bar{u}^a(t,x)\gamma_5 d^a(t,x),
\]

\[
O_{\pi}^{\pi^0}(t) = \frac{1}{\sqrt{2}} \sum_{x,a} \left[ \bar{u}^a(t,x)\gamma_5 u^a(t,x) - \bar{d}^a(t,x)\gamma_5 d^a(t,x) \right],
\]

where \(a\) is the index of the color. We assume that the molecular state is composed of two pions to take into account the possibility that the \(\sigma\) meson exists as a bound state of two heavy pions instead of as a \(\pi-\pi\) resonance state.
The tetra-quark interpolation operators are given by

\[ O_{\text{tetra}}(t) = \sum_a [ud]^a(t)[\bar{ud}]^a(t) , \]  

(3)

where \([ud]^a(t)\) and \([\bar{ud}]^a(t)\) are diquark and antidiquark operators, respectively, written as

\[ [ud]^a(t) = \frac{1}{2} \sum_{x,b,c} \epsilon^{abc} \left[ u^T b(t, x) C_5 d^c(t, x) - d^T b(t, x) C_5 u^c(t, x) \right] , \]

\[ [\bar{ud}]^a(t) = \frac{1}{2} \sum_{x,b,c} \epsilon^{abc} \left[ \bar{u}^b(t, x) C_5 \bar{d}^c(t, x) - \bar{d}^b(t, x) C_5 \bar{u}^c(t, x) \right] , \]  

(4)

with the charge conjugation matrix \(C\).

For the components of the molecular and tetra-quark states there are other possible candidates. For example, in Ref.\(^{22}\), vector- and axial-vector-type operators as well as pseudo-scalar-type operators were used for the molecular states. For the tetra-quark state, in addition to the (anti)pseudo-scalar diquark operators, the (anti)scalar diquark operators are also employed. Because there is no conclusive understanding of appropriate operators for describing the iso-singlet scalar mesons, we have chosen the simplest operators.

The propagator \(G^i(t)\) for the four-quark states is written as

\[ G^i(t) = \langle \mathcal{O}^i(t)\mathcal{O}^{i\dagger}(0) \rangle , \quad i = \text{molec or tetra}, \]  

(5)

where \(\mathcal{O}^i\) is the molecular or tetra-quark interpolation operator.

We show the diagrams for the elements of the propagator \(G^i(t)\): the molecular state \(G^{\text{molec}}(t)\) and the tetra-quark state \(G^{\text{tetra}}(t)\). Through the functional integral of Eq. (5) with the quark fields, the propagator of the molecular state \(G^{\text{molec}}(t)\) is written as

\[ G^{\text{molec}}(t) = 2 \left[ D(t) + \frac{1}{2} C(t) - 3A(t) + \frac{3}{2} V(t) \right] , \]  

(6)

where \(D(t)\), \(C(t)\), \(A(t)\), and \(V(t)\) correspond to direct, crossed, single annihilation (singly disconnected), and vacuum (doubly disconnected) diagrams, respectively (Fig. [1]). The detailed expression for each diagram is given in Appendix A. The tetra-quark propagator is given by

\[ G^{\text{tetra}}(t) = 2 \left[ 2(D_1(t) + D_2(t)) - 2(A_1'(t) + A_2'(t) + A_3'(t) + A_4'(t)) + (V_1'(t) + V_2'(t) + V_3'(t) + V_4'(t)) \right] , \]  

(7)
where $D'(t)$, $A'(t)$, and $V'(t)$ are shown in Fig. 2 and their detailed formulas are given in Appendix A. The number index of $D'(t)$, $A'(t)$, and $V'(t)$ represents the difference of the combination of the color index, which is described in detail in Appendix A. The difference between Figs. 1 and 2 is in the directions of the arrows on the quark lines.

Both propagators $G^{\text{molec}}(t)$ and $G^{\text{tetra}}(t)$ contain doubly disconnected diagrams $V(t)$ and $V'(t)$, which are neglected in our calculations. Assuming that the $N_c$ counting scheme also works for $N_c = 3$, we apply it to the contraction in the diagrams. We estimate the orders of the diagrams in Figs. 1 and 2: $D(t)$ and $D'(t) \sim \mathcal{O}(N_c^2)$, $C(t) \sim \mathcal{O}(N_c)$, $A(t)$ and $A'(t) \sim \mathcal{O}(N_c)$ and $V(t)$ and $V'(t) \sim \mathcal{O}(1)$. Under the above assumption, we may neglect the doubly disconnected diagrams $V(t)$ and $V'(t)$ compared with other diagrams. Moreover, the large-$N_c$ counting suggests that the singly disconnected diagrams $A(t)$ and $A'(t)$ become the same order as the crossed diagram $C(t)$. The singly disconnected diagrams may play an essential role in the understanding of four-quark states and should not be neglected.

However, the calculation of the singly disconnected diagrams has a huge computational cost because the evaluation of the quark loop on all lattice sites is necessary. To reduce the computational time, we use the $Z_2$-noise method with the truncated eigenmode approach to estimate the quark loop and to evaluate the vacuum expectation value. Another key issue in the calculation of the singly disconnected diagrams is the subtraction of the contribution of the vacuum expectation value, which does not vanish for the iso-singlet scalar mesons. Therefore, taking account of the vacuum expectation value $v(t)$, we replace the
quark propagators \( (W^{-1})_{t,x;x',y}^{ab \alpha \beta} \) with \( (W^{-1})_{t,x;x',y}^{ab \alpha \beta} - v(t) \delta^{ab} \delta^{\alpha \beta} \delta_{tt'} \delta_{xy} \), where \( \alpha \) and \( \beta \) are the indexes of the Dirac spinor, \( (t, x) \) and \( (t', y) \) are sink and source sites on the lattice, \( v(t) = 1/(12N_L^3) \langle \text{Tr}[(W^{-1})_{t,x;x,x}] \rangle \), and \( N_L \) is the number of a spatial lattice site. Although we keep the possible time dependence of \( v(t) \) in our computation, we end up with verifying that it does not depend on \( t \) with high statistics.

### III. CALCULATED RESULTS

We generate two-flavor full QCD configurations using the same simulation parameters (clover coefficient \( C_{SW} = 1.68 \) and coupling \( \beta = 1.7 \)) as those in Ref.\(^\text{25} \), except for the lattice size. The lattice size in our calculation is set to \( 8^3 \times 16 \), which is smaller than that in Ref.\(^\text{25} \). First we produce the two-flavor full QCD configurations using the hybrid Monte Carlo (HMC) method with the clover-improved Wilson quark action. The first 2000 trajectories are updated in the quenched QCD, then we switch to simulations with the dynamical fermion. The next 100 HMC trajectories are discarded for thermalization, then we start to store the configurations every 10 trajectories. The numbers of configurations at the dynamical hopping parameter values of \( \kappa = 0.146, 0.147, \) and 0.148 are 16496, 14344, and 11720, respectively. Our estimated critical hopping parameter \( \kappa_c \) and the lattice size are \( \kappa_c = 0.152(6) \) and \( a = 0.269(9) \) fm, respectively. The lattice spacing is determined so that the \( \rho \) meson mass at the inverse of the critical hopping parameter reproduces the physical mass \( m_V = m_\rho = 770 \) MeV, which is extracted linearly from the calculated \( \rho \) meson masses at \( \kappa = 0.146, 0.147, \) and 0.148 on the lattice. We list the values of the \( \pi \) and \( \rho \) meson masses together with the number of configurations at \( \kappa = 0.146, 0.147, \) and 0.148 in Table I.

We calculate the quark propagators using a point source and sink with the clover-improved Wilson quark action. For the disconnected diagrams we employ the \( Z_2 \)-noise method with the truncated eigenmode approach. We carry out the dilution in the temporal direction\(^\text{26} \), in which the numbers of noise vectors and eigenvalues are 120 and 12, respectively.

#### Importance of the Singly Disconnected Diagrams

We focus on the importance of the disconnected diagrams in four-quark states. Here we neglect the contribution of the doubly disconnected diagrams in the four-quark states under
TABLE I: Masses of $\pi$ and $\rho$ and number of configurations.

| $\kappa$ | $m_\pi a$ | $m_\pi$ MeV | $m_\rho a$ | $m_\rho$ MeV | configurations $^a$ |
|----------|------------|-------------|------------|-------------|------------------|
| 0.146    | 1.018(2)   | 747(27)     | 1.431(4)   | 1050(39)    | 16496            |
| 0.147    | 0.930(2)   | 682(25)     | 1.358(6)   | 996(38)     | 14344            |
| 0.148    | 0.827(4)   | 607(23)     | 1.304(10)  | 956(39)     | 11720            |

$^a$Number of configurations separated by 10 trajectories to each other.

the assumption that their order is smaller than that of other diagrams in the case of large-$N_c$ counting. We shall analyze the propagators of the molecular state $G_{\text{molec}}$ and tetra-quark state $G_{\text{tetra}}$.

First we show the propagators of the molecular state at $\kappa = 0.146, 0.147, \text{ and } 0.148$ in Fig. 3 together with the propagators of diagrams $D(t)$, $C(t)$, and $A(t)$ in Fig. 1. They are weighted with the coefficients in Eq. (6) to make it clear which propagator is important in the molecular state. In the propagator of the molecular state $G_{\text{molec}}$ the connected diagram $D(t)$ and the singly disconnected diagram $A(t)$ are dominant compared with the connected diagram $C(t)$. We emphasize that the contribution from the singly disconnected diagram $A(t)$ is the same order of magnitude as that from the connected diagram $D(t)$, which suggests that the singly disconnected diagram should not be neglected in the propagator of the molecular state.

Next the propagators of the tetra-quark state at $\kappa = 0.146, 0.147, \text{ and } 0.148$ are shown in Fig. 4. We also plot the elements of the tetra-quark diagrams $D'(t)$ and $A'(t)$, in Fig. 2 where $D'(t)$ and $A'(t)$ are given by $D'(t) = D'_1(t) + D'_2(t)$ and $A'(t) = A'_1(t) + A'_2(t) + A'_3(t) + A'_4(t)$. The propagators of the singly disconnected diagrams $A'(t)$ at $\kappa = 0.147$ and 0.148 have some error around $5 \leq t \leq 10$ in spite of the high-statistics calculation. We can see that the main component of the propagator of the tetra-quark state originates from the singly disconnected diagrams $A'(t)$. The absolute values of the propagator of the connected diagrams $D'(t)$ are much smaller than those of the singly disconnected diagrams $A'(t)$. We thus cannot neglect the singly disconnected diagram in the investigation of the tetra-quark state. From the comparison between Figs. 3 and 4, the propagators of the molecular state have smaller errors than those of the tetra-quark state. The propagators of the molecular state have only small errors because the interpolation operators of it are composed of two pseudo-scalar...
FIG. 3: (color online). The propagators of the molecular state and its components at \( \kappa = 0.146, 0.147, \) and 0.148. The solid diamonds represent the propagators of the molecular state. The open circles, squares, and triangles represent the components of the molecular states \( 2D(t), C(t), \) and \( -6A(t) \) in Eq. (6), respectively. The \( D(t) \) and \( A(t) \) diagrams are dominant in the molecular states. The plots of \( 2D(t) \) and \( -6A(t) \) are shifted to \( t/a \pm 0.2 \) for visibility.

From Figs. 3 and 4 we see that the singly disconnected diagrams play the key role in understanding the molecular and tetra-quark states. In particular, the singly disconnected diagrams are dominant in the four-quark states, which is also found in the two-quark state.\(^{13}\)

We show the effective masses obtained from the propagators \( G^{\text{molec}} \) and \( G^{\text{tetra}} \) in Figs. 5 and 6.
FIG. 4: (color online). The propagators of the tetra-quark state and its components at \( \kappa = 0.146 \), 0.147, and 0.148. The solid squares represent the propagators of tetra-quark state. The open circles and triangles represent \( 4D'(t) \) and \( -4A'(t) \), respectively, which are plotted at \( t/a \pm 0.2 \) for visibility. The singly disconnected diagrams \( A'(t) \) are dominant in the tetra-quark states.

and (6) The effective masses are defined by

\[
m^{i}_{\text{eff}}(t) = - \ln \left[ \frac{G^{i}(t+1)}{G^{i}(t)} \right], \quad i = \text{molec or tetra}. \tag{8}
\]

Figure 5 shows the effective masses without the singly disconnected diagrams as a function of time. The molecular state has a clear plateau in the behavior of the effective masses in the range \( 1 \leq t \leq 5 \), which suggests that a stable one-particle state whose mass is approximately
FIG. 5: (color online). The effective masses of the molecular (open triangles) and tetra-quark states (open squares) without the singly disconnected diagrams at $\kappa = 0.146$, 0.147, and 0.148. The data are plotted at $t/a \pm 0.2$ for visibility.

$2m_\pi$ exists. However, reliable plateaus in the effective masses of the molecular state are not found in computations with lighter quark masses\textsuperscript{22}. The fact that the stable one-particle state was successfully extracted for the larger quark masses implies that the behavior of the molecular state strongly depends on the quark mass. On the other hand, the values of effective masses of the tetra-quark state are larger than those of the molecular state at small $t$ and decrease significantly with time as reported in Ref.\textsuperscript{22}. We do not observe a clear plateau in the effective masses of the tetra-quark state. Without the singly disconnected diagrams, the ground state of the iso-singlet scalar meson may be dominated by the molecular state and its mass is approximately $2m_\pi$. However, the plateau in the effective masses of the molecular state disappears at $t = 6$ and the effective masses start to drop again, which may indicate that the effect of $\pi-\pi$ scattering states, i.e., two-particle states such as $|\pi\pi\rangle$, appears
FIG. 6: (color online). The effective masses of the molecular (solid triangles) and tetra-quark (solid squares) states with the singly disconnected diagrams at $\kappa = 0.146$, 0.147, and 0.148. The data are plotted at $t/a \pm 0.2$ for visibility.

in the channel. A similar drop in the effective masses of the molecular and tetra-quark states at large $t$ was reported in Ref.22. To take into account this effect, we need to include the $\pi-\pi$ scattering states properly in the lattice calculation22.

In Fig. 6 we show the effective masses as a function of time for the molecular and tetra-quark states with the singly disconnected diagrams. The behavior of the effective masses of the molecular state with the singly disconnected diagram is almost the same as that without the singly disconnected diagram. There is a clear plateau in effective masses at small time and the effective mass decreases at large time. In the molecular state there is a stable one-particle state whose mass is approximately $2m_\pi$. On the other hand, we find a dramatic change in the behavior of the effective masses of tetra-quark states because of the existence of the singly disconnected diagrams. A plateau-like structure appears in the range
FIG. 7: (color online). The quark mass dependence of the square of the $\pi$ meson mass (solid circles), double the $\pi$ meson mass (open triangles), the $\rho$ meson mass (open circles), the mass of the molecular state (diamonds), and the mass of the tetra-quark state (open squares). We plot the masses of the molecular state both with (solid diamonds) and without (open diamonds) the singly disconnected diagram. The chiral limit is given by $\kappa_c = 0.152(6)$.

$1 \leq t \leq 4$, which might imply the existence of a one-particle state.

In Fig. 7 we display $(m_\pi)^2$, $2m_\pi$, $m_\rho$, $m_{\text{molec}}$, $m_{\text{molec}}$, and $m_{\text{tetra}}$ in the lattice unit as a function of the inverse hopping parameter. The masses of the molecular states are obtained from plateaus of the effective masses in the range $2 \leq t \leq 5$. The difference between the masses of the molecular state with the singly disconnected diagram and that without the singly disconnected diagram is small at $\kappa = 0.146, 0.147$, and 0.148. The masses of the molecular states with and without the singly disconnected diagram decrease as the chiral limit is approached. In the chiral limit the mass of the molecular state is smaller than the $\rho$ meson mass, which indicates that the light iso-singlet scalar meson $\sigma$ may be the four-quark state as the molecular state.

On the other hand, from the behavior of the effective masses of the tetra-quark state, it is difficult to give a clear interpretation. If we assume that the plateau-like structure of the effective masses of the tetra-quark state with the singly disconnected diagrams in $1 \leq t \leq 4$ implies the existence of a pole, we can evaluate the mass of the tetra-quark state. We plot the quark mass dependence of the tetra-quark state in Fig. 7. The mass of the tetra-quark state shows little dependence of the quark mass compared with that of the molecular state,
and in the chiral limit it becomes much larger than the $\rho$ meson mass.

To obtain conclusive results, we need to perform the variational method with not only four-quark interpolation operators but also two-quark ones. Moreover, the computation with a lighter quark mass is indispensable to more precisely evaluate the precious values of masses in the chiral limit.

**IV. CONCLUSION AND OUTLOOK**

We investigated the possible significance of the four-quark states, i.e. the molecular and tetra-quark states in the iso-singlet scalar mesons, whose quantum numbers are $J^{PC} = 0^{++}$, $I = 0$, with the two-flavor dynamical quarks on the lattice. We reported the results of the propagators and the effective masses of the molecular and tetra-quark states, including the estimate of the singly disconnected diagrams, for the first time. We showed that the quark loops given by the disconnected diagrams play an essential role in making the four-quark states exist. We found that the light iso-singlet scalar meson $\sigma$ may be the four-quark state as the molecular state. Furthermore, the main component of the tetra-quark propagator originates from the singly disconnected diagrams.

We evaluated the effective masses of the molecular state with and without the singly disconnected diagram. The difference between the mass of the molecular state with the singly disconnected diagram and that without the singly disconnected diagram is small at $\kappa = 0.146, 0.147,$ and $0.148$. The masses extracted from plateaus in the effective masses of the molecular state with or without the singly disconnected diagram are approximately $2m_\pi$. In the chiral limit, the mass of the molecular state is smaller than the $\rho$ meson mass, which indicates that the light iso-singlet scalar meson $\sigma$ may be the four-quark state as the molecular state. In the molecular state, the amplitude of the propagator of the singly disconnected diagram is as large as that of the connected diagram. The singly disconnected diagram includes the process $(\bar{q}qqq) \leftrightarrow (\bar{q}q)$. This might suggest the importance of two-quark mixing in the molecular state. The $\sigma$ may be the molecular state but it may also contain the two-quark state.

On the other hand, for the tetra-quark states we found that the singly disconnected diagrams markedly affect the effective masses. By virtue of the singly disconnected diagrams, the plateau-like structure appears in the effective masses, which might imply the existence
of a one-particle state. If we assume that the plateau-like structure suggests the existence of a pole, we can evaluate the mass of the tetra-quark state. The mass of the tetra-quark state shows little dependence of the quark mass compared with that of the molecular state, and in the chiral limit it becomes much larger than the $\rho$ meson mass. In the tetra-quark state, the amplitude of the singly disconnected diagrams is much larger than that of the connected diagrams. In particular, the propagator is dominated by the singly disconnected diagrams in the entire time region, which suggests that the mixing between the tetra-quark state and the two-quark state might be large.

From the feature of the $(\bar{q}qqq) \leftrightarrow (\bar{q}q)$ mixing in the molecular and tetra-quark states, we can get the following conjecture in accordance with the analysis using a generalized linear sigma model in Ref.27. Both the molecular and tetra-quark states contain the four-quark states as well as the two-quark state through the singly disconnected diagrams. However, the proportion of the two-quark state in the tetra-quark state is larger than that of the molecular state because the singly disconnected diagrams in the tetra-quark state are more crucial than those in the molecular state.

To extract conclusive results regarding the possible significance of four-quark states in the iso-singlet scalar mesons, further improvement of the computation is indispensable such as calculation on a larger lattice, estimation of the doubly disconnected diagrams in the molecular and tetra-quark states, inclusion of other possible interpolation operators for the four-quark states, and the use of the variational method with possible interpolation operators. In particular, to investigate the existence of a pole, the calculation of all diagrams in the four-quark states is indispensable. The evaluation of the doubly disconnected diagrams is important because they make the scattering amplitudes unitary28.

In addition to the four-quark states, there are many possible states with the same quantum number as that of the iso-singlet scalar mesons: two-quark states $(\bar{q}q)$, glueballs $(gg)$, hybrid states $(\bar{q}qg)$, and so on. For the comprehensive understanding of the iso-singlet scalar mesons, these interpolation operators should be taken into account. We carried out the calculation with heavy quark masses of $m_\pi = 607, 682,$ and 747 MeV, which are far from the physical $\pi$ mass. Computation with light quark masses close to the physical point would change the masses of the molecular and tetra-quark states.
Acknowledgments

This work was supported in part by the Nagoya University Program for Leading Graduate Schools ”Leadership Development Program for Space Exploration and Research”, Grant-in-Aid for Scientific Research (S) (22224003), the Kurata Memorial Hitachi Science and Technology Foundation, and the Daiko Foundation. This work was partially supported by Grants-in-Aid for Research Activity of Matsumoto University (No.14111048). This work was supported by Grants-in-Aid for Scientific Research (Kakenhi) Numbers 24340054 and 26610072. The simulation was performed on an NEC SX-9 supercomputer at RCNP, Osaka University, and was conducted using the Fujitsu PRIMEHPC FX10 System (Oakleaf-FX, Oakbridge-FX) in the Information Technology Center, The University of Tokyo.

Appendix A: Propagators of the four-quark states

The detailed descriptions of diagrams $D(t)$, $C(t)$, $A(t)$, and $V(t)$ in Eq. (6) are given by

\[ D(t) = \left\langle \sum_{x,y,a,b,c,d} \text{Tr} \left[ \gamma_5 (W^{-1})_{t,0}^{ac} \gamma_5 (W^{-1})_{0,x,t}^{ca} \right] \text{Tr} \left[ \gamma_5 (W^{-1})_{t,y;0,w}^{bd} \gamma_5 (W^{-1})_{0,w;0}^{db} \right] \right\rangle, \tag{A1} \]

\[ C(t) = \left\langle \sum_{x,y,a,b,c,d} \text{Tr} \left[ \gamma_5 (W^{-1})_{t,0}^{ac} \gamma_5 (W^{-1})_{0,z,t,y}^{cb} \gamma_5 (W^{-1})_{t,y;0,w}^{bd} \gamma_5 (W^{-1})_{0,w;0}^{da} \right] \right\rangle, \tag{A2} \]

\[ A(t) = \left\langle \sum_{x,y,a,b,c,d} \text{Tr} \left[ \gamma_5 (W^{-1})_{t,x;0,z}^{ab} \gamma_5 (W^{-1})_{0,z,t,y}^{bc} \gamma_5 (W^{-1})_{t,y;0,w}^{cd} \gamma_5 (W^{-1})_{0,w;0}^{da} \right] \right\rangle, \tag{A3} \]

\[ V(t) = \left\langle \sum_{x,y,a,b,c,d} \text{Tr} \left[ \gamma_5 (W^{-1})_{t,x;0,z}^{ab} \gamma_5 (W^{-1})_{t,y;0,w}^{ba} \gamma_5 (W^{-1})_{0,z;0,w}^{cd} \gamma_5 (W^{-1})_{0,w;0,z}^{dc} \right] \right\rangle. \tag{A4} \]

where the brackets represent the functional integral over gauge configurations and Tr operates on the Dirac spinor. Because the mass difference between the up and down quarks is neglected, the propagators of each of them are expressed by $W^{-1}$. In Eqs. (A1) ~ (A4), the superscripts $a$, $b$, $c$, and $d$ of $W^{-1}$ are the indexes of the color. We put the source points at $w$ and $z$ in the calculation of the propagators and sum over sink points $x$ and $y$. 

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The explicit descriptions of $D'(t)$, $A'(t)$, and $V'(t)$ in Eq. (7) are written by

$$D_1'(t) = \sum_{x,y,b,c,d,e} \text{Tr} \left[ (C_{\gamma_5})^T (W^{-1})^{bd}_{t,x;0,z} C_{\gamma_5} (W^{-1T})^{ce}_{0,z,t,x} \right]$$

$$D_2'(t) = \sum_{x,y,b,c,d,e} \text{Tr} \left[ (C_{\gamma_5})^T (W^{-1})^{db}_{0,w;y} C_{\gamma_5} (W^{-1T})^{ce}_{t,y;0,w} \right], \quad (A5)$$

$$A_1'(t) = \sum_{x,y,b,c,d,e} \text{Tr} \left[ (C_{\gamma_5})^T (W^{-1})^{bb}_{t,x;y} C_{\gamma_5} (W^{-1T})^{dc}_{t,y;0,w} \right]$$

$$A_2'(t) = \sum_{x,y,b,c,d,e} \text{Tr} \left[ (C_{\gamma_5})^T (W^{-1})^{db}_{t,x;y} C_{\gamma_5} (W^{-1T})^{de}_{0,w;0,z} \right], \quad (A6)$$

$$A_3'(t) = \sum_{x,y,b,c,d,e} \text{Tr} \left[ (C_{\gamma_5})^T (W^{-1})^{bc}_{t,x;y} C_{\gamma_5} (W^{-1T})^{bd}_{t,y;0,w} \right]$$

$$A_4'(t) = \sum_{x,y,b,c,d,e} \text{Tr} \left[ (C_{\gamma_5})^T (W^{-1})^{be}_{t,x;y} C_{\gamma_5} (W^{-1T})^{de}_{0,w;0,z} \right], \quad (A7)$$

$$V_1'(t) = \sum_{x,y,b,c,d,e} \text{Tr} \left[ (C_{\gamma_5})^T (W^{-1})^{bb}_{t,x;y} C_{\gamma_5} (W^{-1T})^{cc}_{t,y;0,w} \right]$$

$$V_2'(t) = \sum_{x,y,b,c,d,e} \text{Tr} \left[ (C_{\gamma_5})^T (W^{-1})^{bb}_{t,x;y} C_{\gamma_5} (W^{-1T})^{cc}_{t,y;0,w} \right], \quad (A8)$$

$$V_3'(t) = \sum_{x,y,b,c,d,e} \text{Tr} \left[ (C_{\gamma_5})^T (W^{-1})^{bc}_{t,x;y} C_{\gamma_5} (W^{-1T})^{bc}_{t,y;0,w} \right]$$

$$V_4'(t) = \sum_{x,y,b,c,d,e} \text{Tr} \left[ (C_{\gamma_5})^T (W^{-1})^{bc}_{t,x;y} C_{\gamma_5} (W^{-1T})^{bc}_{t,y;0,w} \right], \quad (A9)$$

$$V_5'(t) = \sum_{x,y,b,c,d,e} \text{Tr} \left[ (C_{\gamma_5})^T (W^{-1})^{dd}_{0,w;0,z} C_{\gamma_5} (W^{-1T})^{de}_{0,z;0,w} \right], \quad (A10)$$

$$V_6'(t) = \sum_{x,y,b,c,d,e} \text{Tr} \left[ (C_{\gamma_5})^T (W^{-1})^{dd}_{0,w;0,z} C_{\gamma_5} (W^{-1T})^{de}_{0,z;0,w} \right], \quad (A11)$$

$$V_7'(t) = \sum_{x,y,b,c,d,e} \text{Tr} \left[ (C_{\gamma_5})^T (W^{-1})^{dd}_{0,w;0,z} C_{\gamma_5} (W^{-1T})^{de}_{0,z;0,w} \right], \quad (A12)$$

$$V_8'(t) = \sum_{x,y,b,c,d,e} \text{Tr} \left[ (C_{\gamma_5})^T (W^{-1})^{dd}_{0,w;0,z} C_{\gamma_5} (W^{-1T})^{de}_{0,z;0,w} \right], \quad (A13)$$

$$V_9'(t) = \sum_{x,y,b,c,d,e} \text{Tr} \left[ (C_{\gamma_5})^T (W^{-1})^{dd}_{0,w;0,z} C_{\gamma_5} (W^{-1T})^{de}_{0,z;0,w} \right], \quad (A14)$$
where $C$ is the charge conjugation matrix.

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