Scalar Mesons in Lattice QCD

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We explore whether “f0(600) or σ” exists as a pole in QCD, by a full lattice QCD simulation on the \(8^3 \times 16\) lattice using the plaquette action and Wilson fermions. It is shown that a low-mass \(σ\) pole exists owing to the disconnected diagram of the meson propagator. A discussion is given on the physical content of the \(σ\).

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Recently there has been renewed and growing interest in scalar mesons.1 2 One of the most noteworthy developments in this field is the re-identification of the \(σ(600)\) after some twenty years. The results of re-analyses of the \(ππ\) scattering phase shift of the scattering \((S)\) matrix strongly suggest the existence of the pole of the \(σ\) meson with \(I = 0\) and \(J^{PC} = 0^{++}\) in the \(s\) channel as well as the \(ρ\) pole in the \(t\) channel. In confirming the \(σ\) pole, it was essential to respect chiral symmetry, analyticity, unitarity and crossing symmetry in constructing the \(S\) matrix.3 4 5 6. The significant contributions of the \(σ\) pole were also identified in the decay processes of heavy particles such as \(D^0 \rightarrow ππ\) and \(Υ(3S) \rightarrow ππ\).7 8 9. The meson called “\(f_0(600)\) or \(σ\)” appeared in the 2002 edition of PDG.8. It should be noted that a recent analysis clearly shows phase motion consistent with resonance behavior.

As stressed above, the significance of the \(σ\) pole is intimately related to chiral symmetry in QCD; the \(σ\) may be identified as the chiral partner of the \(π\) in the linear representation of chiral \(SU(2)\otimes SU(2)\) symmetry.11 Here, it is noteworthy that the \(κ\) meson with \(I = 1/2\) is reported to exist with a mass \(m_κ\) of about 800 MeV8 12 13; the \(κ\) is supposed to constitute the nonet scalar states of chiral \(SU(3)\otimes SU(3)\) symmetry together with the \(σ\). See ‘Meson Particle Listings \(f_0(600)\)’ in Ref.4 (pp.010001-450 ~ 453), and references therein.

Even with the confirmed existence of the low lying scalar mesons, there are long standing controversies on their nature.2 Are they usual \(q\bar{q}\) mesons, four quark states like \(qqqq\), or \(πκ (KK)\) molecules, rather than pre-existing resonances? How large is the mixing among them or with glueballs?15 Although not mentioned in2, the \(σ\) may be a collective \(q\bar{q}\) state described as a superposition of many atomic \(q\bar{q}\) states.16 17 In fact, the dynamical models of chiral symmetry breaking, such as the Nambu-Jona-Lasinio model17 and the Schwinger-Dyson approaches18, describe the \(σ\) as well as the \(π\) as collective states.

Confronting these problems with the \(σ\), it would be intriguing to explore whether QCD accommodates the \(σ\) and other possible low-lying scalar mesons, as well as to examine their nature by a first-principles calculation of QCD.

DeTar and Kogut19 were the first who measured the screening mass of the \(σ\) meson in lattice QCD, although in the quenched approximation. In the same approximation, Alford and Jaffe explored possible light scalar mesons described as \(q^2\bar{q}^2\) states20, while the masses of the \(q\bar{q}\) states and their mixing with glueball states in the scalar channel were investigated by Lee and Weinberg21. It was pointed out22 that the so-called disconnected diagram, which is not properly treated in the quenched approximation, gives almost the same amount of contribution to the propagator as the connected diagram does; this indicates that using the dynamical quarks is essential to study the \(σ\) on a lattice.

A simulation with dynamical quarks was carried out by McNeile and Michael25, who computed the masses of the iso-singlet scalar states given by a superposition of \(q\bar{q}\) and glueball states. In their simulation, the \(σ\) meson was found to be lighter than the \(π\); hence the relevance of the simulation in reality is obscure.

Since the existence and the nature of the \(σ\) may be related to chiral symmetry and its dynamical breaking, it is desirable to examine the behavior of the chiral limit of the calculated quantities for a proper description of the \(σ\) meson. Of course, it is preferable to adopt lattice fermions which have better chiral properties. Using the domain wall fermions, RBC (Riken-Brookhaven-Columbia) collaboration examined the \(σ\) propagator on the lattice, unfortunately, however, in the quenched approximation and with an approximate estimate of the disconnected diagram based on the chiral perturbation theory24.

In this letter, we present a lattice calculation of the scalar particles using full QCD with the inclusion of the disconnected diagrams. We employ the most standard
lattice QCD numerical techniques, and show that there exists a σ pole, whose mass is similar to that of the ρ meson for the quark masses used for the simulation but tends to become as low as 2mπ in the chiral limit. We shall show that the incorporation of the disconnected diagram is responsible for realizing such a low mass of the σ meson. We shall briefly discuss the physical content of the σ meson. We shall also mention that our simulation suggests the existence of the η meson, another member of the nonet of the scalar mesons.

We adopt the following interpolation operator for creating the σ meson with I = 0 and JPC = 0++,

$$\hat{\sigma}(x) \equiv \frac{3}{4} \sum_{c=a=1}^{4} \frac{\bar{u}_{a}^{c}(x)u_{a}^{c}(x) + \bar{c}_{a}^{c}(x)c_{a}^{c}(x)}{\sqrt{2}},$$

where u (d) denotes the up-quark (down-quark) operator with c and α being the color and Dirac-spinor indices, respectively. Then the σ meson propagator reads

$$G(y, x) = \langle T \hat{\sigma}(y)\hat{\sigma}(x) \rangle = \frac{1}{Z} \int DU D\bar{u} Du D\bar{d} Dd \times \hat{\sigma}(y)\hat{\sigma}(x) e^{-S_G - \bar{u}Wu - \bar{d}WDd}.$$  \hspace{1cm} (2)

Here W−1’s are the u- and d-quark propagators, U’s the link variables of the gluon, and $S_G$ the gauge action. By integration over the quark fields, the σ meson propagator is reduced to

$$G(y, x) = -\langle T W^{-1}(x, y) W^{-1}(y, x) \rangle + 2\langle \sigma(y) - \langle \sigma(y) \rangle \sigma(x) - \langle \sigma(x) \rangle \rangle, \hspace{1cm} (3)$$

where

$$\sigma(x) \equiv \text{Tr}W^{-1}(x, x),$$

with “Tr” being the trace operation over the color and Dirac indices. Here we set the u and d quark propagators to be the same. Equation 3 shows that the σ propagator consists of two terms: one corresponds to a connected diagram and the other to a disconnected diagram. Since the vacuum expectation value $\langle \sigma(x) \rangle$ does not vanish, it should be subtracted from the σ operator. We employ Wilson fermions and the plaquette gauge action. We perform a full QCD simulation in which the disconnected diagrams are included.

As for the simulation parameters, we first note that CP-PACS performed a full-QCD calculation of the light meson spectroscopy with great success [22]. Therefore, we use the same values of the simulation parameters as those used by CP-PACS, i.e., $\beta = 4.8$ and the hopping parameter, $\kappa = 0.1846, 0.1874$ and 0.1891, except for the lattice size; our lattice size is $8^3 \times 16$. We shall use the point source and sink, which together with the smaller lattice size, leads to larger masses due to a mixture of higher mass states. In other words, the masses to be obtained in our simulation should be considered as upper limits. We show in Table 1 the value of $m_\pi/m_\rho$ together with that of CP-PACS. They are consistent within the error bars. We generate the gauge configurations in full QCD using the hybrid Monte Carlo (HMC) algorithm. The first 1500 trajectories are updated in quenched QCD, then we switch to a simulation with the dynamical fermion. The next 2000 trajectories of HMC are discarded for thermalization and the σ, π and ρ propagators are calculated every ten trajectories.

It is not an easy task to evaluate the disconnected part of the propagator, since one must calculate TrW−1(x, x) for all lattice sites x. We used the $Z_2$ noise method to calculate the disconnected diagrams, σ(x), and the subtraction terms of the vacuum ⟨σ⟩. Each of these terms is the order of ten, and ⟨(σ − ⟨σ⟩)(σ − ⟨σ⟩)⟩ becomes less than 10−4, as shown in Fig 11. Therefore, in order to obtain the signals correctly as the difference between these terms, numerical simulations with a high precision and careful analyses are necessary. One thousand random $Z_2$ numbers are generated for each configuration: We refer to our previous report [22] for the relationship between the amount of $Z_2$ noise and the achieved accuracy. Gauge configurations are created by HMC in a vector supercomputer, while most of the disconnected propagator is calculated in a parallel machine.

The propagators of the π, ρ and σ for $\kappa = 0.1874$ are shown in Fig 12. From our results, we estimate the critical value of the hopping parameter and the lattice space as $\kappa_c = 0.195(3)$ and $a = 0.207(9)$ fm, respectively, which are to be compared with the CP-PACS values, $\kappa_c = 0.19286(14)$ and $a = 0.197(2)$ fm. The mass ratios of $m_\pi/m_\rho$ and $m_\sigma/m_\rho$ together with $m_{\text{connect}}/m_\rho$ are summarized in Table 1, where $m_{\text{connect}}$ is the mass evaluated only from the connected diagram. We have extracted the π and ρ masses using two-pole formula from their propagators. The small errors of the π and ρ propagators indicate the high precision of our simulation. Our result for the mass ratios $m_\pi/m_\rho$ in Table 1 is in a good agreement with that of CP-PACS, with unavoidable small differences owing to the different lattice sizes. To extract the σ meson mass, we have used the one-pole ansatz, since its propagator has large error bars.

<table>
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<th>Table 1: Summary of the results.</th>
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<td>κ</td>
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<td>$m_\pi/m_\rho$</td>
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<td>$m_\sigma/m_\rho$</td>
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<td>$m_{\text{connect}}/m_\rho$</td>
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1) Number of configurations separated by 10 trajectories to each other. 2) CP-PACS. 3) Our result. $m_{\text{connect}}$ is the σ mass estimated only from the connected part.
at large $t \sim 6$ in spite of our high statistics; it implies that the obtained value gives an upper limit of the scalar meson mass. Figure 1 and Table 1 show that the mass of the $\sigma$ is of the same order as the mass of the $\rho$; we remark that the $2\pi$ threshold is higher than the $\sigma$ in our simulation. We have checked that the effective mass method gives essentially the same result as that given above.

![Figure 1](image1.png)

**FIG. 1:** Propagators of the connected and disconnected diagrams of the $\sigma$ for $\kappa = 0.1874$.

Figure 2 shows the individual contributions of the connected and disconnected parts of the $\sigma$ propagator, which reaches a plateau at $t \geq 5$, since the precision of our calculation is limited to $O(G(t)) \sim 10^{-4}$. The connected part shows clear signals of a rapid damping with small error bars. We note that the connected part of the $\sigma$ propagator can be regarded as the one of the $a_0$ meson provided that the difference between the $u$-quark and the $d$-quark is neglected. Therefore, the rapid damping of the connected part of the $\sigma$ propagator is in accordance with the fact that the $a_0$ is heavier than the $\rho$. Figure 2 shows that the disconnected part dominates the $\sigma$ propagator. By comparing Fig. 1 with Fig. 2 we see that the $\sigma$ as a light meson results from the disconnected part of the $\sigma$ propagator with the background vacuum condensate subtracted, which are odd with the constituent quark model. In the naive sense, the connected quark diagram corresponds to the constituent quarks in the SU(3) non-relativistic quark model where the OZI rule is satisfied. This may give a clue to clarify the physical content of the $\sigma$ meson, as will be discussed later. The mass of the connected $\sigma$ (the $a_0$) shown in Table 1 is almost 2.5 times of the $\rho$ mass and exhibits only a weak dependence on the hopping parameter, suggesting an irrelevance of chiral symmetry to the $a_0$ meson.

![Figure 2](image2.png)

**FIG. 2:** Propagators of the $\pi$, $\rho$ and $\sigma$ for $\kappa = 0.1874$.

In Fig. 3 we display $m_\pi^2$, $m_\rho$, $m_\sigma$ and $2m_\sigma$ in lattice units as a function of the inverse hopping parameter. As the chiral limit is approached, the $\sigma$ meson mass obtained from the full $\sigma$ propagator decreases and eventually becomes smaller than the $\rho$ meson mass in the chiral limit.

![Figure 3](image3.png)

**FIG. 3:** $m_\pi^2$, $m_\rho$, $m_\sigma$ and $2m_\sigma$ in the lattice unit as a function of the inverse hopping parameter. The chiral limit is given by $\kappa_c = 0.195(3)$.

We have also calculated the $\kappa$ meson using the same configurations. We take the same hopping parameter values for $u$ and $d$ quarks and use the following three values for the $s$ quark hopping parameter, $\kappa_s = 0.1835$, 0.1840 and 0.1845. The ratios $m_\kappa/m_K$ and $m_K/m_K^*$ at the chiral limit are listed in Table 2. One may notice that all the three values of $\kappa_s$ fairly reproduce the physical mass ratio, $m_K/m_K^*$ in the chiral limit of the $u$- and $d$-quarks. A more notable point is that the resultant $\kappa$ mass hardly changes with the variation of $\kappa_s$ and it is almost twice as heavy as the $K^*$; i.e., the $\kappa$ is not degenerated with the $\sigma$, although they should belong to the same nonet. The origin to lift the octet-singlet degeneracy may be attributed the following facts; because of the strangeness content,
the $\kappa$ propagator is solely composed of a connected diagram and contains no disconnected part, the latter of which was the origin of the light mass of the $\sigma$. In fact, the $\kappa$ mass listed in Table 2 is almost the same as the $a_0$ mass estimated using the connected part of the $\sigma$ with the corresponding hopping parameters. Thus we can understand why the $\sigma$ is light while the $\kappa$ is heavy, consistently.

<table>
<thead>
<tr>
<th>$s$ quark hopping parameter</th>
<th>0.1835</th>
<th>0.1840</th>
<th>0.1845</th>
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<tr>
<td>$m_\kappa/m_K^*$</td>
<td>0.639(6)</td>
<td>0.631(6)</td>
<td>0.623(6)</td>
</tr>
<tr>
<td>$m_\sigma/m_K^*$</td>
<td>2.039(43)</td>
<td>2.037(43)</td>
<td>2.044(44)</td>
</tr>
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</table>

Table 2: The mass ratios $m_\kappa/m_K^*$ versus $m_\sigma/m_K^*$ at $\kappa = 0.1945(29)$. The $s$ quark hopping parameters were taken to be 0.1835, 0.1840 and 0.1845.

The dominance of the disconnected diagram in the $\sigma$ meson propagator in contrast to the octet scalar mesons suggests possible physical contents of the light $\sigma$: The disconnected diagram includes the process $q\bar{q} \leftrightarrow G$ where $G$ denotes a glueball states. This might suggest an importance of the glueball mixing in the light $\sigma$ if the glueball states were not heavy. Instead, we notice that such a fluctuation process of the $q\bar{q}$ states with the heavy $G$ giving an effective vertex for $q\bar{q} \rightarrow q\bar{q}$ may form a collective state mentioned before. One may also notice that the disconnected diagram contains four quark states of dipiiclqurk and anti-diquark states, i.e., $qq$-$\bar{q}\bar{q}$. Clearly more works are needed to elucidate the physical content of the scalar mesons.

We have reported the first study of the scalar mesons based on the full QCD lattice simulation with dynamical fermions, including analysis of the disconnected diagram effects. We have used the most standard lattice QCD techniques, which have worked well for the established mesons and baryons, and clarified the accuracy and statistics required to obtain signals in the scalar channel.

Our results indicate the existence of a light isoscalar $J^{PC} = 0^{++}$ scalar meson, i.e., the $\sigma$ meson with a mass of almost the same order as that of the $\rho$ meson (see Table 1). We have also shown that the $\kappa$ meson belonging to the flavor octet is almost twice as heavy as the $K^*$. Of course, the results reported here are in far from final quantitative stage because our quark masses are much heavier than those in the real world and our scalar mesons cannot decay on our lattice. Nevertheless, it is now clear that the $\sigma$ meson as well as other scalar mesons can be studied in the lattice QCD. We hope that the present work prompts other lattice studies which will give a deeper and more quantitative understanding of the scalar mesons, especially the $\sigma$.

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