Search for the possible S=+1 Pentaquark states in Quenched Lattice QCD

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We study spin $\frac{1}{2}$ hadronic states in quenched lattice QCD to search for a possible $S = +1$ pentaquark resonance. Simulations are carried out on $8^3 \times 24, 10^3 \times 24, 12^3 \times 24$ and $16^3 \times 24$ lattices at $\beta=5.7$ at the quenched level with the standard plaquette gauge action and the Wilson quark action. We adopt two independent operators with the quantum numbers $(I, J) = (0, \frac{1}{2})$ to construct $2 \times 2$ correlation matrices. After the diagonalization of the correlation matrices, we successfully obtain the energies of the lowest-state and the 2nd-lowest-state in this channel. The analysis of the volume dependence of the energies and spectral weight factors indicates that a resonance state is likely to exist slightly above the NK threshold in $(I, J^P) = (0, \frac{1}{2}^-)$ channel.

I. INTRODUCTION

After the discovery [1] of $\Theta^+(1540)$ followed by the other experiments [2, 3, 4, 5, 6, 7, 8, 9], identifying the properties of the particle is one of the central problems in hadron physics. While the isospin of $\Theta^+$ is likely to be zero [10], the spin and the parity and the origin of its tiny width still remain open questions [10]. In spite of many theoretical studies on $\Theta^+$ [11, 12, 13], the nature of this exotic particle, including the question about the existence of the particle, is still controversial. Among the theoretical approaches, the lattice QCD calculation is considered as one of the most reliable ab initio methods for studying the properties of hadronic states, which has been very successful in reproducing the non-exotic hadron mass spectra [14]. Up to now, several lattice QCD studies have been reported, which aim to look for pentaquarks in various different ways. However, the conclusions are unfortunately contradictory with each other. On one hand, in Refs. [12, 16, 17], the authors conclude that the parity of $\Theta^+$ is likely to be negative, while in Ref. [13] the state with the similar mass to $\Theta^+$ in the positive parity channel is reported. In Refs. [11, 20], the absence of $\Theta^+$ is suggested.

One of the difficulties in the spectroscopy calculation with lattice QCD arises from the fact that the hadron masses suffer from systematic errors due to the discretization, the chiral extrapolation, the quenching effect, the finite volume effect and the contaminations from higher excited states. Another difficulty specific to the present problem is that the signal of $\Theta^+$ is embedded in the discrete spectrum of NK scattering states in finite volume. In order to verify the existence of a resonance state, one needs to isolate the first few low energy states including the lowest NK scattering state, identify a resonance state and study its volume dependence which can distinguish itself from other scattering states. Therefore, ideally one should extract multistates from a high statistics unquenched calculation for several different lattice volumes with thousands of gauge configurations so that the careful separation of states and the studies of volume dependence are possible. Although, giving well controlled continuum and chiral extrapolations may be important, we simply assume that the spectra would not be drastically changed based on the experience from the past lattice QCD studies. Even with such a compromise we hope we can learn much about the existence and the qualitative properties of $\Theta^+$.

In this paper, we study $(I, J) = (0, \frac{1}{2})$ channel in quenched lattice QCD to search for the possible resonance state. We adopt two independent operators with $I = 0$ and $J = \frac{1}{2}$ and diagonalize the $2 \times 2$ correlation matrices by the variational method for all the combinations of lattice sizes and quark masses to extract the first excited state slightly above the NK threshold in this channel. After the careful separation of the states, we investigate the volume dependence of the energy as well as the spectral weight [14] of each state so that we can distinguish the resonance state from simple scattering states.

The paper is organized as follows. We present the formalism used in the analysis in Sec. III and show the simulation conditions in Sec. IV. The process of the analysis is shown in Sec. V. Secs. VI-VIII are devoted to the interpretation...
of the obtained results in $(I, J) = (0, \frac{1}{2})$ channel and the verification of the existence of the resonance state, as well as some checks on the consistency and the reliability of the obtained data. In Sec. IX we discuss the operator dependence of the results and compare our results with the previous works. We finally summarize the paper in Sec. X.

II. FORMALISM

As $\Theta^+$ lies above the NK threshold, any hadron correlators, which have the $\Theta^+$ signal, also contain the discrete-level NK scattering states in a finite volume lattice. In order to isolate the resonance state from the scattering states, one needs to extract at least two states before anything else.

Since a double exponential fit of a single correlator is numerically extremely difficult, we adopt the variational method using correlation matrices constructed from independent operators $\{O^I_{\text{snk}}\}$ for $\{O^J_{\text{src}}\}$ is needed to construct correlation matrices $C^{IJK}(T) \equiv \langle O^I_{\text{snk}}(T)O^J_{\text{src}}(0) \rangle$, which can be decomposed into the sum over the energy eigenstates $|i\rangle$ as

$$C^{IJK}(T) = \langle O^I_{\text{snk}}(T)O^J_{\text{src}}(0) \rangle = \sum_i \sum_j C^{I}_{\text{snk}Ii} \Lambda(T)_{ij} C_{\text{src}jJ}, = (C^{I}_{\text{snk}} \Lambda(T)C_{\text{src}})_{JJ},$$

(1)

with the general matrices which depend on the operators as

$$C^{I}_{\text{snk}Ii} \equiv \langle 0|O^I_{\text{snk}}|i\rangle, C_{\text{src}jJ} \equiv \langle j|O^J_{\text{src}}|0\rangle,$$

(2)

and the diagonal matrix

$$\Lambda(T)_{ij} \equiv \delta_{ij} e^{-E_i T}.$$  

(3)

From the product

$$C^{-1}(T + 1)C(T) = C_{\text{src}}^{-1} \Lambda(-1)C_{\text{src}},$$

(4)

we can extract the energies $\{E_i\}$ as the logarithm of eigenvalues $\{e^{E_i}\}$ of the matrix $C^{-1}(T + 1)C(T)$. While there are $N$ independent operators for the correlation matrix, the number of the intermediate states $|i\rangle$ which effectively contributes to this matrix may differ from $N$ in general. Let us call this number as $N_{\text{eff}}$. If $N_{\text{eff}}$ is larger than $N$, the higher excited states are non negligible and their contaminations give rise to a $T$-dependence of eigenvalues as $\{e^{E_i(T)}\}$. If on the other hand $N_{\text{eff}}$ is smaller than $N$, $\mathcal{C}$ becomes non-invertible so that the extracted energies become numerically fairly unstable. In order to have a reliable extraction of states, we therefore need to find an appropriate window of $T$ ($T_{\text{min}} \leq T \leq T_{\text{max}}$) so that $N_{\text{eff}} = N$. The stability of $\{e^{E_i(T)}\}$ against $T$ is expected in this $T$ range and we can obtain $N$ eigenenergies $\{E_i\}$ ($0 \leq i \leq N - 1$) by fitting the eigenvalues $e^{-E_i(T)}$ as $E_i = E_i(T) \equiv \ln(e^{E_i(T)})$ in $T_{\text{min}} \leq T \leq T_{\text{max}}$. Since finding the stability of the energies against $T$ in noisy data could be quite subjective, the result may suffer from uncontrollable biases. In order to avoid such biases, one should impose a certain concrete criteria to judge the stability as will be explained in later sections and select only those data which satisfies this criteria. After the separation of the states, we need to distinguish a possible resonance state from NK scattering states by the criteria to judge the stability as will be explained in later sections and select only those data which satisfies this criteria.

III. LATTICE SET UP

We carry out simulations on four different sizes of lattices, $8^3 \times 24$, $10^3 \times 24$, $12^3 \times 24$ and $16^3 \times 24$ with 2900, 2900, 1950 and 950 gauge configurations using the standard plaquette (Wilson) gauge action at $\beta = 5.7$ and the Wilson quark action. The hopping parameters for the quarks are $(\kappa_{u,d}, \kappa_s) = (0.1600, 0.1650)$, $(0.1625, 0.1650)$, $(0.1650, 0.1650)$, $(0.1600, 0.1600)$ and $(0.1650, 0.1600)$, which correspond to the current quark masses $(m_{u,d}, m_s) \sim (240, 100)$, $(170, 100)$, $(100, 100)$, $(240, 240)$ and $(100, 240)$, respectively in the unit of MeV $22$. The lattice spacing $a$ from
the ρ meson mass is is set to be 0.17 fm, which implies the physical lattice sizes are $1.4^3 \times 4.0$ fm$^4$, $1.7^3 \times 4.0$ fm$^4$, $2.0^3 \times 4.0$ fm$^4$ and $2.7^3 \times 4.0$ fm$^4$.

We adopt the following two operators used in Ref. [15] for the interpolating operators at the sink \{O$_{\text{sink}}^I$\}:

$$\Theta^I(x) \equiv \varepsilon^{abc}[u_a^T(x)C\gamma_5 d_b(x)]u_c(x)[\overline{\sigma}(x)\gamma_5 d_c(x)] - (u \leftrightarrow d), \quad (5)$$

which is expected to have a larger overlap with \(\Theta^+\) state, and

$$\Theta^2(x) \equiv \varepsilon^{abc}[u_a^T(x)C\gamma_5 d_b(x)]u_c(x)[\overline{\sigma}(x)\gamma_5 d_c(x)] - (u \leftrightarrow d), \quad (6)$$

which we expect to have larger overlaps with NK scattering states. Here, Dirac fields $u(x), d(x)$ and $s(x)$ are up, down and strange quark fields respectively and the Roman alphabets \{a,b,c\} denote color indices. For measuring the energy spectrum, the two operators at the source \{O$_{\text{src}}^I$\} are chosen to be \(\Theta^I_{\text{wall}}(t)\) and \(\Theta^2_{\text{wall}}(t)\) defined using spatially spread quark fields $\sum_x q(x)$ under the Coulomb gauge:

$$\Theta^I_{\text{wall}}(t) \equiv \left(\sqrt{\frac{1}{V}}\right)^5 \sum_{x_1 \sim x_5} \varepsilon^{abc}[u_a^T(x_1)C\gamma_5 d_b(x_2)]u_c(x_3)[\overline{\sigma}(x_4)\gamma_5 d_c(x_5)] - (u \leftrightarrow d), \quad (7)$$

and

$$\Theta^2_{\text{wall}}(t) \equiv \left(\sqrt{\frac{1}{V}}\right)^5 \sum_{x_1 \sim x_5} \varepsilon^{abc}[u_a^T(x_1)C\gamma_5 d_b(x_2)]u_c(x_3)[\overline{\sigma}(x_4)\gamma_5 d_c(x_5)] - (u \leftrightarrow d). \quad (8)$$

The above operators give a $2 \times 2$ correlation matrix in the channel with the quantum number of $(I,J) = (0, \frac{1}{2})$. We note here that the baryonic correlators have the spinor indices, which we omit in the paper, and they contain the propagations of both the positive and negative parity particles. For the projection of the parity, we multiply $\frac{1}{2}(1 \pm \gamma_5)$.

We fix the source operator $\Theta^I_{\text{wall}}(t)$ on $t = t_{\text{src}} \equiv 6$ plane to reduce the effect of the Dirichlet boundary on the spatial extent. We adopt the operators $\sum_x \Theta^I(x,t)$ as sink operators, which is summed over all space to project out the zero-momentum states. We finally calculate

$$C^{1I}(T) = \sum_x \langle \Theta^I(x,T + t_{\text{src}})\overline{\Theta}^I_{\text{wall}}(t_{\text{src}}) \rangle. \quad (9)$$

Using two independent operators, we can extract the first two states, namely the lowest and the next-lowest states. The lowest state is considered to be the “lowest” NK scattering state. In order to extract a possible resonance state with controlled systematic errors, we need to choose the physical volume of the lattice in an appropriate range. If we choose $L$ too large, the resonance state becomes heavier than the 2nd-lowest NK state whose energy is naively expected to scale as $\sqrt{M_N^2 + (\frac{2\pi}{L})^2} + \sqrt{M_K^2 + (\frac{2\pi}{L})^2}$ according to the spatial lattice extent $L$. In this case we need to extract the 3rd state using a $3 \times 3$ correlation matrix, which requires more computational time. The energy difference between the lowest and the next-lowest NK scattering states $\sqrt{M_N^2 + (\frac{2\pi}{L})^2} + \sqrt{M_K^2 + (\frac{2\pi}{L})^2} - (M_N + M_K)$, for example, ranges from 180 MeV to 880 MeV in $1.4\text{fm} \leq L \leq 3.5\text{fm}$. Taking into account that \(\Theta^\uparrow\) lies about 100 MeV above the NK threshold, we take 3.5 fm as the upper limit of $L$. On the other hand, if we choose $L$ too small, unwanted finite-volume artifacts from the finite sizes of particles become non-negligible. It is however difficult to estimate the lower limit of $L$, because the finite-volume effect is rather uncontrollable. We shall take the spatial extents $L = 8, 10, 12, 16$ at $\beta = 5.7$ as a trial.

We take periodic boundary conditions in all directions for the gauge field, whereas we impose periodic boundary conditions on the spatial directions and the Dirichlet boundary condition on the temporal direction for the quark field. The reason for choosing the Dirichlet boundary condition for the quark field is to avoid possible contaminations from those propagating beyond the boundary at $t = 0$ in periodic boundary conditions. This is in contrast to the case of ordinary 3-quark baryons, where we can cancel out these unwanted contributions using the combination of the periodic and antiperiodic boundary conditions on the temporal direction. However, the situation is different for the cases of pentaquark. If the temporal length $N_t$ is not long enough, we indeed encounter contaminations from the particles which go beyond the temporal boundary. For example, with the periodic boundary condition, the correlation $\langle \Theta(T + t_{\text{src}})\overline{\Theta}(t_{\text{src}}) \rangle$ contains the unwanted contributions such as

$$\langle K|\Theta(T + t_{\text{src}})|N\rangle\langle N|\overline{\Theta}(t_{\text{src}})|K\rangle \sim e^{-E_NT + E_K(T - N_t)} \approx e^{-E_NT + E_KT}. \quad (10)$$
In this case, the effective mass plot approaches $E_N - E_K$ below the NK threshold as $T$ is increased. We find that it would be safest to impose the Dirichlet boundary condition on the temporal direction, since no quark can go over the boundary on $t=0$ in the temporal direction. Although the boundary is transparent for the particles composed only by gluons; i.e. glueballs, due to the periodicity of the gauge action, taking into account that these particles are rather heavy, it would be however safe to neglect these gluonic particles going beyond the boundary. Then, the correlation 

$$\langle \Theta(T + t_{src})\overline{\Theta}(t_{src}) \rangle$$

mainly contains such terms as $\langle \text{vac}|\Theta(T + t_{src})|NK \rangle \langle NK|\overline{\Theta}(t_{src})|\text{vac} \rangle$ and we can use exactly the same prescription mentioned in the last section. Some of the previous lattice QCD studies on $\Theta^+$ adopted a parity projection method using the combination with periodic and antiperiodic boundary conditions [15, 19]. We stress that one should in principle be careful whether the result is free from the contamination from higher excited states.

After obtaining the energy spectrum, we carry out a study of the spectral weight for $(\kappa_u, \kappa_s) = (0.1600, 0.1600)$. Introducing two smeared operators $\overline{\Theta}_{\text{smea}}$, $\Theta_{\text{smea}}$ we compute the following correlators

$$C^{IJ}_{\text{smea}}(T) = \sum_{x} \langle \overline{\Theta}^I(x, T + t_{src}) \Theta^J_{\text{smea}}(t_{src}) \rangle,$$

from which we extract the spectral weights using a constrained double exponential fit. The details will be explained in Sec. VII

IV. LATTICE QCD DATA

Before obtaining the energies of the lowest-state and the 2nd lowest-state, there are only a few simple steps. First, we calculate the $2 \times 2$ correlation matrix $C(T)$ defined in Eq. (14) and obtain the “energies” $\{E_i(T)\}$ as the logarithm of eigenvalues $\{e^{E_i(T)}\}$ of the matrix product $C^{-1}(T + 1)C(T)$. After finding the $T$ range $(T_{\text{min}} \leq T \leq T_{\text{max}})$, where $\{E_i(T)\}$ are stable against $T$, we can extract the energies $E_i$ by the least $\chi$-squared fit of the data as $E_i = E_i(T)$ in $T_{\text{min}} \leq T \leq T_{\text{max}}$.

Since the volume dependence of the energy is crucial to judge whether the state is a resonance or not, a great care must be paid in extracting the energy. Therefore, systematic error by the contamination from higher excited
FIG. 2: The “effective mass” plot $E_i(T)$ as the function of $T$, the separation between source operators and sink operators, in $(I, J^F) = (0, 1/2^-)$ channel with the hopping parameters $(\kappa_{u,d}, \kappa_s) = (0.1600, 0.1650)$ on $8^3 \times 24, 10^3 \times 24, 12^3 \times 24, 16^3 \times 24$ lattice at $\beta = 5.7$.

FIG. 3: The “effective mass” plot $E_i(T)$ as the function of $T$, the separation between source operators and sink operators, in $(I, J^F) = (0, 1/2^-)$ channel with the hopping parameters $(\kappa_{u,d}, \kappa_s) = (0.1650, 0.1600)$ on $8^3 \times 24, 10^3 \times 24, 12^3 \times 24, 16^3 \times 24$ lattice at $\beta = 5.7$. 
FIG. 4: The “effective mass” plot $E_i(T)$ as the function of $T$, the separation between source operators and sink operators, in $(I, J^F) = (0, 1/2^-)$ channel with the hopping parameters $(\kappa_{u,d}, \kappa_s) = (0.1625, 0.1650)$ on $8^3 \times 24, 10^3 \times 24, 12^3 \times 24, 16^3 \times 24$ lattice at $\beta = 5.7$.

FIG. 5: The “effective mass” plot $E_i(T)$ as the function of $T$, the separation between source operators and sink operators, in $(I, J^F) = (0, 1/2^-)$ channel with the hopping parameters $(\kappa_{u,d}, \kappa_s) = (0.1650, 0.1650)$ on $8^3 \times 24, 10^3 \times 24, 12^3 \times 24, 16^3 \times 24$ lattice at $\beta = 5.7$. 
states should be avoided by a careful choice of fitting ranges. For this reason, we impose the following criteria for the reliable extraction of the energies. Although the criteria is nothing more than just one possible choice, we believe it is important to impose some concrete criteria for the fit so that we can reduce the human bias for the fit, though not completely.

1. The effective mass plot should have “plateau” for both the lowest and the 2nd-lowest states simultaneously in a fit range \([T_{\text{min}}, T_{\text{max}}]\), where the length \(N_{\text{fit}} \equiv T_{\text{max}} - T_{\text{min}} + 1\) should be larger than or equal to 3 (\(N_{\text{fit}} \geq 3\)).

2. In the plateau region, the signal for the ground and the 1st excited states should be distinguishable, so that the gap between the central values of the lowest and the 2nd-lowest energies should be larger than their errors.

3. The fitted energies should be stable against the choice of the fit range; i.e. the results of the fit with \(N_{\text{fit}}\) time slices and with \(N_{\text{fit}} - 1\) time slices should be consistent within statistical errors for both the ground and the 1st excited states.

4. The ground state energy obtained by the diagonalization method using the \(2 \times 2\) correlation matrix should be consistent with the value from a single exponential fit for a sufficiently large \(t\).

If the fit does not satisfy the above conditions, we discard the result since the data in the fit range may be either contaminated by higher excited-states or the 2nd-lowest state signal is too noisy for a reliable fit.

Figs. 4 show the “effective mass” plot \(E_i(T)\) for the heaviest combination of quarks \((\kappa_{u,d,\kappa_s} = 0.1600,0.1600)\). As is mentioned in Sec. II, we need to find the \(T\) region \((T_{\text{min}} \leq T \leq T_{\text{max}})\) where each \(E_i(T)\) shows a plateau. In the case of \(12^3 \times 24\) lattice in Fig. 4, for example, We choose the fit range of \(T_{\text{min}} = 6\) and \(T_{\text{max}} = 9\) (\(N_{\text{fit}} = 4\)). The plateau in this region satisfies the above criteria so that we consider the fit \(E_0\) and \(E_1\) for the range \(6 \leq T \leq 9\) as being reliable. The situation is similar for the cases of \(10^3 \times 24\) and \(16^3 \times 24\) lattices. On the other hand, in the case of \(8^3 \times 24\) lattice we do not find a plateau region satisfying the above criteria.

Figs. 2, 3, 4, 5 shows the “effective mass” plots for the combinations with smaller quark masses. We find that the signal is noisier for the lighter quarks and the fit with the smaller volumes \(8^3 \times 24\) and \(10^3 \times 24\) lattices do not satisfy the criteria.

V. LOWEST-STATE ENERGY IN \((I, J^P) = (0, \frac{1}{2}^-)\) CHANNEL

A. The volume dependence of the lowest-state energy

Now we show the lattice QCD results of the lowest-state in \(I = 0\) and \(J^P = \frac{1}{2}^-\) channel. The filled circles in Fig. 6 show the lowest-state energies \(E_0\) in \(I = 0\) and \(J^P = \frac{1}{2}^-\) channel on four different volumes. Here the horizontal axis denotes the lattice extent \(L\) in the lattice unit and the vertical axis is the energy of the state. The lower line denotes the simple sum \(M_N + M_K\) of the nucleon mass \(M_N\) and Kaon mass \(M_K\) obtained with the largest lattice. Though \(M_N\) and \(M_K\) are slightly affected by finite volume effects, the deviation of \(M_N + M_K\) \((L = 8)\) from \(M_N + M_K\) \((L = 16)\) is about a few \% (Table II). We therefore simply use \(M_N + M_K\) \((L = 16)\) as a guideline.

At a glance, we find that the energy of this state takes almost constant value against the volume variation and coincides with the simple sum \(M_N + M_K\). We can therefore conclude that the lowest-state in \(I = 0\) and \(J^P = \frac{1}{2}^-\) channel is the NK scattering state with the relative momentum \(|p| = 0\). The good agreement with the sum \(M_N + M_K\) implies the weakness of the interaction between N and K. In fact, the scattering length in the \(I = 0\) channel is known to be tiny \((a_0^{KN}(I = 0) = -0.0075\text{ fm})\) from compilations of hadron scattering experiments \(^{24, 22}\), whereas the current algebra prediction from PCAC with SU(3) symmetry predicts that the scattering length \(a_0^{KN}(I = 0) = 0\).

B. Comparison with the previous lattice work

The lowest-state in \(I = 0\) and \(J^P = \frac{1}{2}^-\) channel coincide with the simple sum of the nucleon mass and the Kaon mass and is very likely to be the NK scattering state with the relative momentum \(|p| = 0\). Furthermore, the data indicate that the interaction between N and K is very weak. We here compare our data with the previous lattice QCD studies, which were performed with almost the same conditions as ours, in order to confirm the reliability of our data.

The well-known hadron masses \(m_N, m_K\) and \(m_N\) listed in Table I can be compared with the values in Ref. 22. Our data are consistent with those in Ref. 22. The lowest NK scattering state in \((I, J^P) = (0, \frac{1}{2}^-)\) channel is carefully investigated in Ref. 26 with almost the same parameters as our present study. It is worth comparing
VI. 2ND LOWEST-STATE ENERGY IN $(I, J^P) = (0,\frac{1}{2}^-)$ CHANNEL

The $(I, J^P) = (0,\frac{1}{2}^-)$ state is one of the candidates for $\Theta^+(1540)$. Since $\Theta^+$ is located above the NK threshold, it would appear as an excited-state in this channel. We show the lattice data of the 2nd lowest-state in this channel.

In order to distinguish a possible resonance state from NK scattering states, we investigate the volume dependence of both the energy and the spectral weight of each state. It is expected that the energies of resonance states have small volume dependence, while the energies of NK scattering states are expected to scale as $\sqrt{M_N^2 + |\frac{2\pi}{T} n\vec{u}|^2} + \sqrt{M_K^2 + |\frac{2\pi}{T}\kappa\vec{u}|^2}$ varying according to the relative momentum $\frac{2\pi}{T}\vec{u}$ between N and K on a finite periodic lattice, provided that the NK interaction is weak and negligible. We can take advantage of the above difference for the discrimination.

A. Possible corrections to the volume dependence of NK scattering states

A possible candidate for the volume dependence of the energies of NK scattering states is the simple formula as $E_{NK}^R(L) \equiv \sqrt{M_N^2 + |\frac{2\pi}{T} n\vec{u}|^2} + \sqrt{M_K^2 + |\frac{2\pi}{T}\kappa\vec{u}|^2}$ with the relative momentum $\frac{2\pi}{T}\vec{u}$ between N and K in finite periodic lattices, which is justified on the assumption that nucleon and Kaon are point particles and that the interaction between them is negligible. In practice, there may be some corrections to the volume dependence of $E_{NK}^R(L)$. We therefore estimate here two possible corrections; the existence of the NK interaction and the application of the momenta on a finite discretized lattice.

There can be small hadronic interactions between nucleon and Kaon, which may lead to correction to naively expected energy spectrum $E_{NK}^R(L)$ of the NK scattering states. Using L"uscher formula, one can relate the scattering phase shift to the energy shift from $E_{NK}^R(L)$ on finite lattices. For example, in the case when a system belongs to the representation $A_1^+$ of cubic groups, which are relevant in the present case, the relation between the phase shift and the possible momentum spectra is

$$e^{2i\delta_0(k)} = \frac{Z(1; q^2) + i\pi\frac{q^2}{2}}{Z(1; q^2) - i\pi\frac{q^2}{2}}.$$  \hspace{1cm} (12)

Here $Z(s; q^2)$ is the Zeta function defined as

$$Z(s; q^2) \equiv \frac{1}{\sqrt{4\pi}} \sum_{n \in \mathbb{Z}^3} \frac{1}{(n^2 - q^2)^s}.$$  \hspace{1cm} (13)

with the eigenenergy $q$ on a finite lattice. We have simply omitted the corrections from the partial waves with angular momentum higher than the next smallest one ($l = 4$). Although our current quark masses are heavier than those of the real quarks, we use the empirical values of the phase shift in NK scattering in Ref. 28, by simply neglecting the quark mass dependence. The correction using the empirical values results in at most a few % larger energy than the simple formula $E_{NK}^R(L)$ within the volume range under consideration; the energies are slightly increased by the weak repulsive force between nucleon and Kaon.

The reader may claim that one has to adopt momenta on a finite discretized lattice: $|\vec{p}|^2 = 4\sin^2\left(\frac{\pi t}{L}\right) \cdot |\vec{u}|^2$ for Kaon and $|\vec{p}|^2 = \sin^2\left(\frac{2\pi}{T}\right) \cdot |\vec{u}|^2$ for nucleon respectively. This correction turns out to be within only a few % lower.
energy than $E_{\text{NK}}^\Omega(L)$, although it is not certain whether this correction is meaningful or not for composite particles like nucleon or Kaon.

We find that these corrections lead to at most a few % deviations from $E_{\text{NK}}^\Omega(L)$. We then neglect these corrections for simplicity in the following discussion and use the simple form $E_{\text{NK}}^\Omega(L)$. Note here that there are other possible finite volume effects due to the finite size of N, K and possible pentaquark states, than the volume dependence arising from $\frac{2\pi}{L^3}$. We then need to take account of this fact in the following analysis.

B. The volume dependence of the 2nd lowest-state energy

The filled squares in Fig. 6 show the 2nd lowest-state energies in this channel. The black and gray symbols are calculated with the fit with $N_{\text{fit}} - 1$ and $N_{\text{fit}}$ time slices, respectively (see the criteria.3 in the Sec. IV). The upper line shows the energies of the 2nd lowest NK scattering state $E_{\text{NK}}^{|\vec{n}|=1} \equiv \sqrt{M_N^2 + (2\pi/L)^2} + \sqrt{M_K^2 + (2\pi/L)^2}$ with the next smallest relative momentum between N and K on the $L = 16$ lattices. In addition to the naive expectation of the volume dependence of the 2nd lowest NK scattering state, we also calculate the sum $E_{\text{NK}}^{|\vec{n}|=1} + E_{\text{NK}}^{|\vec{n}|=1}$ of energies of nucleon $E_{\text{NK}}^{|\vec{n}|=1}$ and Kaon $E_{\text{NK}}^{|\vec{n}|=1}$ with the smallest lattice momentum $|\vec{p}| = \frac{2\pi}{L} |\vec{n}| = 2\pi/L$. We extract $E_{\text{NK}}^{|\vec{n}|=1}$ and $E_{\text{NK}}^{|\vec{n}|=1}$ from the correlators $\sum_\vec{x} e^{i\vec{n} \cdot \vec{x}} \langle N(\vec{x}, t + t_{\text{src}})|N(0, t_{\text{src}})\rangle$ and $\sum_\vec{x} e^{i\vec{n} \cdot \vec{x}} \langle K(\vec{x}, t + t_{\text{src}})|K(0, t_{\text{src}})\rangle$. These results are denoted by the open squares in Fig. 6 as the sum $E_{\text{NK}}^{|\vec{n}|=1} + E_{\text{NK}}^{|\vec{n}|=1}$. The deviations of $E_{\text{NK}}^{|\vec{n}|=1} + E_{\text{NK}}^{|\vec{n}|=1}$ from $E_{\text{NK}}^{|\vec{n}|=1}$ are very small. If we assume the weak interaction between nucleon and Kaon, the naive expectation for the 2nd lowest NK scattering states denoted by the upper line in Fig. 6 would be realized even on the $L = 8$ lattices in our setup.

Next we compare the 2nd lowest state energy with the expected energy of the 2nd lowest NK scattering states. Although these values almost coincide with each other on the $L = 16$ lattices, the energies do not change even in the smaller lattices as compared with the expected volume dependence for the 2nd lowest NK scattering state. At the smallest lattices with $L = 8$, some results coincide with each other again. However we consider that the volume with $L \sim 1.4$ fm is too small for the pentaquarks; it is difficult to tell which is the origin of the changes, uncontrollable finite volume effects or expected volume dependence for the 2nd lowest NK scattering state. Especially, when the quarks are heavy, composite particles will be rather compact and we expect smaller finite size effects other than those from the lattice momenta $\frac{2\pi}{L}$. Thus, the significant deviations in $1.5 \lesssim L \lesssim 3$ fm with the combination of the heavy quarks, such as $(\kappa_{u,d}, \kappa_s) = (0.1600, 0.1600)$, is reliable and the obtained state is difficult to explain as the NK scattering state. Moreover the statistical error is also well controlled for the heavy quarks.

Therefore one can understand this behavior with the view that this state is a resonance state rather than a scattering state. In fact, while the data with the lighter quarks has rather strong volume dependence which can be considered to arise due to the finite size of a resonance state, the lattice data exhibit almost no volume dependence with the combination of the heavy quarks especially in $1.5 \lesssim L \lesssim 3$ fm, which can be regarded as the characteristic of resonance states.

VII. THE VOLUME DEPENDENCE OF THE SPECTRAL WEIGHT

For further confirmation, we investigate the volume dependence of the spectral weight. As mentioned in Sec III, the correlation function $\langle O(T)O(0) \rangle$ can be expanded as $\langle O(T)O(0) \rangle = \sum W_i e^{-E_i T}$. The spectral weight of the $i$-th state is defined as the coefficient $W_i$ corresponding to the overlap of the operator $O(t)$ with the $i$-th excited-state. The normalization conditions of the field $\psi$ and the states $|i\rangle$ give rise to the volume dependence of the weight factors $W_i$ in accordance with the types of the operators $O(t)$.

For example, in the case when a correlation function is constructed from a point-source and a zero-momentum point-sink, as $\sum_\vec{x} \langle \Theta(\vec{x}, T + t_{\text{src}})|\bar{O}(0, t_{\text{src}})\rangle$, the weight factor $W_i$ takes an almost constant value if $|i\rangle$ is the resonance state where the wave function is localized. If the state $|i\rangle$ is two-particle state, the situation is more complicated. Nevertheless if there is almost no interaction between the two particles, the weight factor is expected to be proportional to $\frac{1}{V}$. In the case when a source is a wall operator $\bar{O}_{\text{wall}}(t_{\text{src}})$ as taken in this work, a definite volume dependence of $W_i$ is not known. Therefore, we re-examine the lowest-state and the 2nd lowest-state in $(I, J^P) = (0, \frac{1}{2}^-)$ channel using the locally-smeared source $\bar{O}_{\text{smear}}(t_{\text{src}}) \equiv \sum_{\vec{x}\in\Gamma} \bar{O}(\vec{x}, t_{\text{src}})$ with $\Gamma \equiv \{0, 3\}, \{0, 3\}, \{0, 3\}$, which we introduce to partially enhance the ground-state overlap. Since smeared operators whose typical sizes are much smaller than the total volume can be regarded as local operators, we can discriminate the states using the locally-smeared operators as in the case of point operators. We adopt the hopping parameter $(\kappa_{u,d}, \kappa_s) = (0.1600, 0.1600)$ and additionally employ $14^3 \times 24$ lattice for this aim.
FIG. 6: The filled squares denote the lattice QCD data of the 2nd lowest-state in \((I, J^P) = (0, \frac{1}{2}^-)\) channel plotted against the lattice extent \(L\). The filled circles represent the lattice QCD data \(E_0\) of the lowest-state in \((I, J^P) = (0, \frac{1}{2}^-)\) channel. The open symbols are the sum \(E^{|\vec{n}|=1}_N + E^{|\vec{n}|=1}_K\) of energies of nucleon \(E^{|\vec{n}|=1}_N\) and Kaon \(E^{|\vec{n}|=1}_K\) with the smallest lattice momentum \(|\vec{p}| = \frac{2\pi}{L}\). The upper line represents \(\sqrt{M_N^2 + |\vec{p}|^2} + \sqrt{M_K^2 + |\vec{p}|^2}\) with \(|\vec{p}| = 2\pi/L\) the smallest relative momentum on the lattice. The lower line represent the simple sum \(M_N + M_K\) of the masses of nucleon \(M_N\) and Kaon \(M_K\). We adopt the central values of \(M_N\) and \(M_K\) obtained on the largest lattice to draw the two lines.
We extract $W_0$ and $W_1$ using the two-exponential fit as 
\[ \sum_{\mathbf{x}} \Theta^2(\mathbf{x}, T + t_{\text{src}}) \Theta_{\text{smear}}^2(\mathbf{0}, t_{\text{src}}) = W_0 e^{-E_0^+ T} + W_1 e^{-E_1^+ T}. \]

The weight factors $W_0$ and $W_1$ are then obtained through the two-parameter fit as
\[ \sum_{\mathbf{x}} \theta^2(\mathbf{x}, T + t_{\text{src}}) \Theta_{\text{smear}}^2(\mathbf{0}, t_{\text{src}}) = W_0 e^{-E_0^+ T} + W_1 e^{-E_1^+ T} \]
in as large $t$ range ($T_{\text{min}} \leq T + t_{\text{src}} \leq T_{\text{max}}$) as possible in order to avoid the contaminations of the higher excited-states than the 2nd excited-state (3rd lowest-state), which will bring about the instability of the fitted parameters. The fluctuations of $E_0^+$ and $E_1^+$ are taken into account through the Jackknife error estimation. Fig. 7 includes all the results with the various fit range as $(T_{\text{min}}, T_{\text{max}}) = (16.18, 17.19, 18.20)$ to see the fit-range dependence. Though the results have some fit-range dependences, the global behaviors are almost the same among the three.

The left panel in Fig. 7 shows the weight factor $W_0$ of the lowest-state in $(I, J^P) = (0, \frac{1}{2}^-)$ channel against the lattice volume $V$. We find that $W_0$ decreases as $V$ increases and that the dependence on $V$ is consistent with $\frac{1}{V}$, which is expected in the case of two-particle states. It is again confirmed that the lowest-state in this channel is the NK scattering state with the relative momentum $|p| = 0$. Next, we plot the weight factor $W_1$ of the 2nd lowest-state in the right figure. In this figure, almost no volume dependence against $V$ is found, which is the characteristic of the state in which the relative wave function is localized. This result can be considered as one of the evidences of a resonance state slightly above the NK threshold.

To summarize this section, the volume dependence analysis of the eigenenergies and the weight factors of the 2nd lowest state in $(I, J^P) = (0, \frac{1}{2}^-)$ channel suggests the existence of a resonance state. Although there remain the statistical errors and the possible finite-volume artifacts, the data can be consistently accounted for assuming the 2nd-lowest state to be different from ordinary scattering states. If the 2nd-lowest state were an ordinary scattering states, one had to assume a large systematic errors for heavier quarks which is hard to understand consistently.

**VIII. $(I, J^P) = (0, \frac{1}{2}^+)\text{ CHANNEL}$**

In the same way as $(I, J^P) = (0, \frac{1}{2}^-)$ channel, we have attempted to diagonalize the correlation matrix in $(I, J^P) = (0, \frac{1}{2}^+)$ channel using the wall-sources $\Theta_{\text{wall}}(t)$ and the zero-momentum point-sinks $\sum_{\mathbf{x}} \Theta(\mathbf{x}, t)$. In this channel, the diagonalization is rather unstable and we find only one state except for tiny contributions of possible other states. We plot the lattice data in Fig. 8. One finds that they have almost no volume dependence and that they coincide with the solid line which represents the simple sum $M_N + M_K$ of $M_{N^*}$ and $M_K$, with $M_{N^*}$ the mass of the ground-state of the negative-parity nucleon. From this fact, the state we observe is concluded to be the $N^*-K$ scattering state with the relative momentum $|p| = 0$. It may sound strange because the p-wave state of N and K with the relative momentum $|p| = 2\pi/L$ should be lighter than the $N^*-K$ scattering state with the relative momentum $|p| = 0$; this lighter state is missing in our analysis. This failure would be due to the wall-like operator $\Theta_{\text{wall}}(t)$. The fact that the wall operator $\Theta_{\text{wall}}(t)$ is constructed by the spatially spread quark fields $\sum_{\mathbf{x}} q(\mathbf{x})$ with zero momentum may lead to the large overlaps with the NK scattering state with zero relative momentum. The strong dependence on the choice of operators suggests that it is needed to try various types of operators before giving the final conclusion.

**FIG. 7:** The spectral weight factors defined in Sec. VI are plotted against the lattice volume $V$. The left figure is for the lowest-state in $(I, J^P) = (0, \frac{1}{2}^-)$ channel and the right figure is for the 2nd lowest-state.
Before closing this section, we show the spectral weight $W_0^+$ obtained by the fit using the form $\langle \Theta^1(t+t_{src})\Theta^1(t_{src}) \rangle = W_0^+ e^{-E_0^+ t}$ in Fig. 9. We again find the volume dependence as $V^{-1}$, which is the characteristic of the two-particle scattering state.
IX. DISCUSSION

A. Operator dependence

We here mention the operator dependences in \((I,J^F) = (0,\frac{1}{2}^-)\) channel. As is seen in Sec. VIII the overlap factor with states strongly depend on the choice of operators. We survey the effective masses of the five correlators; \(\sum_g (\Theta^1(\vec{x},T+t_{src})\overline{\Theta}^1_{wall}(t_{src}))\), \(\sum_g (\Theta^2(\vec{x},T+t_{src})\overline{\Theta}^2_{wall}(t_{src}))\), \(\sum_g (\Theta^4(\vec{x},T+t_{src})\overline{\Theta}^4(t_{src}))\), \(\sum_g (\Theta^5(\vec{x},T+t_{src})\overline{\Theta}^5(t_{src}))\) and \(\sum_g (\Theta^3(\vec{x},T+t_{src})\overline{\Theta}^3(t_{src}))\). The effective mass \(E(T)\) is defined as a ratio between correlators with the temporal separation \(T\) and \(T+1\),

\[
E(T) \equiv \ln \frac{\langle O(T)O(0)\rangle}{\langle O(T+1)O(0)\rangle},
\]

which can be expressed in terms of the eigenenergies and spectral weights as

\[
E(T) = \ln \frac{\sum_i W_i e^{-E_i T}}{\sum_i W_i e^{-E_{i+1} T}} \sim E_0 + \frac{W_1}{W_2} e^{-(E_1-E_0) T} + \ldots .
\]

A plateau in \(E(T)\) at \(E_0\) implies the ground-state dominance in the correlator. Effective mass plots \(E(T)\) are often used to find the range where correlators show a single-exponential behavior; the higher excited-state contributions \(W_i e^{-E_i T} (i > 0)\) are negligible in comparison with the ground-state component \(W_0 e^{-E_0 T}\).

Here, \(\Theta^3\) is an interpolation operator defined as

\[
\Theta^3(x) \equiv e^{abc} e^{aef} e^{bgh} [u_c(x) C d_f(x)][u_g(x) C \gamma_5 d_b(x)] C \bar{e}_c(x)
\]

which has a di-quark structure similar to that proposed by Jaffe and Wilczek [30], and is also used in Refs. [16, 18, 20]. Fig. 10 shows the effective mass plots constructed from \(\sum_g (\Theta^1(\vec{x},T+t_{src})\overline{\Theta}^1_{wall}(t_{src}))\), \(\sum_g (\Theta^2(\vec{x},T+t_{src})\overline{\Theta}^2_{wall}(t_{src}))\), \(\sum_g (\Theta^4(\vec{x},T+t_{src})\overline{\Theta}^4(t_{src}))\) and \(\sum_g (\Theta^3(\vec{x},T+t_{src})\overline{\Theta}^3(t_{src}))\). One can see two typical behaviors in the figure. One is the line damping from a large value to the energy \(E_0\) of the lowest NK scattering state. The other is the one arising upward to \(E_0\). Surprisingly, the differences of the spinor structure or the color structure among the operators are hardly reflected in the effective mass plots. The difference is enough to perform the variational method but seems insufficient for the drastic change of the effective mass plots. Instead, the effective mass plots seem sensitive to the spatial distribution of operators. The upper three symbols are data using the point-point correlators and the lower two symbols are those from the wall-point correlators. This means the overlap factor with each state is controlled mainly by the spatial distribution rather than the internal structure of operators, except for the overall constant. The spatially smeared operators seem to have larger overlaps with the scattering state with the relative momentum \(|p| = 0\). (One can find that the overlap factor of the wall operator with the observed state in...
(I, J^P) = (0, \frac{1}{2}^+)$ in Fig. 9 is 1000 times larger than those of point operators in Fig. 7.) One often expects that the overlap with a state could be enhanced using an operator whose spinor or color structures resembles the state. We find however no such tendency in the present analysis.

The upper three data slowly damp and do not reach the lowest energy $E_0$ in this $T$ range, which can be explained in terms of the spectral weight. As is seen in Fig. 7, $W_0$ is ten-times smaller than $W_1$ in the case of the point-point correlator. Then, the term $\frac{W_1}{W_0} e^{-\left(E_1 - E_0\right)T}$ in the effective mass survives at relatively large $T$. Hence the effective mass needs larger $T$ to show a plateau at $E_0$. The insensitivity of the overlaps to the internal structure of operators could be helpful for us: We have adopted two operators whose color and spinor structures are different from each other. Although the difference is enough in $(I, J^P) = (0, \frac{1}{2}^+)$ channel, it may be insufficient in $(I, J^P) = (0, \frac{1}{2}^-)$ channel, which leads to the failure in the diagonalization. If we use operators with spatial distributions different from each other, it would be more effective in the diagonalization method.

**B. Comment on other works**

Here we comment on other works previously published, especially for the pioneering works by Csikor et al. [15] and Sasaki [16]. The simulation condition for the former is rather similar to ours.

Csikor et al. first reported the possible pentaquark state slightly above the NK threshold in $(I, J^P) = (0, \frac{1}{2}^-)$ channel in [15]. In Ref. [15], they tried chiral extrapolations and taking the continuum limit at the quenched level for the possible pentaquark state. However they used the single exponential fit analysis for the non-lowest state, namely the possible pentaquark state, for the main results. It is difficult to justify their result unless the coupling of the operators to the lowest NK state is extremely small.

Sasaki found a double-plateau in the effective mass plot and identified the 2nd lowest state as the signal of $\Theta^+$. Unfortunately, we do not find a double-plateau in the present analysis. The double-plateau-like behavior in effective mass plots can appear only under the extreme condition that $W_1$ is much larger than $W_0$. $W_1$ which is ten times larger than $W_0$ seen in Fig. 7 and the statistical fluctuations may cause the deviation of the effective mass plot from the single monotonous line. In fact, the effective mass plot very slowly approaches $E_0$ as $T$ increases in Fig. 10. He extracted the mass of the next-lowest state with a single and double exponential fits. The result do not contradict with ours.

In Refs. [14, 20], the authors concluded the absence of resonance states a few hundred MeV above the NK threshold. We have not found the resonance state which coincides just with the mass of $\Theta^+$ in the chiral limit. In this sense, the results in Refs. [14, 20] are not inconsistent with ours.

**C. chiral extrapolation**

We perform chiral extrapolations for Kaon, nucleon, the lowest state and the 2nd lowest state in the $(I, J^P) = (0, \frac{1}{2}^-)$ channel. We adopt the lattice data with $16^3 \times 24$ lattice, the largest lattice in our analysis. One can find in Fig. 9 that the 2nd lowest state, which is expected to be a resonance state, is already affected by the finite volume effects in this channel. W e adopt the lattice data with $16^3 \times 24$ lattice are consistent within errors in shown in Fig. 11, The simulation condition for the former is rather similar to ours.

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We perform chiral extrapolations for Kaon, nucleon, the lowest state and the 2nd lowest state in the $(I, J^P) = (0, \frac{1}{2}^-)$ channel. We adopt the lattice data with $16^3 \times 24$ lattice, the largest lattice in our analysis. One can find in Fig. 9 that the 2nd lowest state, which is expected to be a resonance state, is already affected by the finite volume effects for $L \leq 12$ with the lightest combination of quarks, and we therefore adopt the largest-lattice data for safety. We can expect from this fact that the typical diameter of this resonance is about 2 fm or longer and that it is desirable to use larger lattices than, at least, (2.5 fm)$^3$ for the analysis of $\Theta^+$.

In Fig. 11, $E_0$ and $E_1$ obtained with each combination of quark masses for $12^3 \times 24$ and $16^3 \times 24$ lattices are plotted against $m_2^2$. The dashed lines represent the linear function $E_B(m_{u,d}, m_s) = b_0 + b_1 m_{u,d} + b_2 m_s$, with $b_0$, $b_1$, $b_2$ free parameters fitted using the five lattice data. We determine the critical $\kappa_c$ and the $\kappa_s$ using the physical Kaon mass and the form for pseudo scalars $E_{\text{PS}}(m_{u,d}, m_s) = a_0 m_{u,d} + a_1 m_s$. The chiral-extrapolated values of $M_K$, $M_N$, $E_{\text{NK}}$, $E_0$ and $E_1$ for $16^3 \times 24$ lattice are 0.4274(12), 0.7996(60), 1.250(10), 1.235(8) and 1.500(52) in the lattice unit and 0.5001(14), 0.9355(70), 1.462(12), 1.445(9) and 1.755(61) in the unit of GeV, respectively. We find that the result for $12^3 \times 24$ lattice are consistent within errors in shown in Fig. 11. The $E_{\text{NK}}$ and $E_0$ are expected to take values of about $M_K + M_N$ in consideration of the weakness of the NK interaction in this channel.

The chiral extrapolated value 1755(61) MeV of $E_1$ is heavier than $\Theta^+(1540)$. The present study with the relatively coarse lattices and heavy quark masses with the Wilson quark action at the quenched level cannot reach the quantitative results. The deviation between $E_1$ in the chiral limit and the mass of $\Theta^+(1540)$ therefore should not be taken seriously. The present chiral-extrapolated values do not rule out the existence of $\Theta^+(1540)$ in this channel. As is mentioned in Sec I, we expect that the qualitative features are not changed by the artifacts lying in the present calculation conditions except for absolute values, and that the nontrivial volume dependence of $E_1$ and the weight
factor $W_1$ are still the signals of a resonance state. The point is that we find the resonance state slightly above the NK threshold.

![Graph](image.png)

**FIG. 11:** A comparison of the chiral extrapolations in $(I, J^P) = (0, \frac{1}{2}^-)$ channel on $12^3 \times 24$ (left) and $16^3 \times 24$ (right) lattices for the lowest-state energy $E_0$ and the 2nd lowest-state energy $E_1$. $E_0$ and $E_1$ are plotted against $M_2^2$. The filled circles (triangles) denote the energies of the lowest (2nd-lowest) state in the chiral limit.

### X. SUMMARY AND FUTURE WORKS

We have performed the lattice QCD study of the $(S, I, J) = (+1, 0, \frac{1}{2})$ states on $8^3 \times 24, 10^3 \times 24, 12^3 \times 24$ and $16^3 \times 24$ lattices at $\beta=5.7$ at the quenched level with the standard plaquette gauge action and Wilson quark action. With the aim to separate states clearly, we have adopted two independent operators with $I = 0$ and $J^P = \frac{1}{2}$ so that we can construct a $2 \times 2$ correlation matrix.

From the correlation matrix of the operators, we have successfully obtained the energies of the lowest-state and the 2nd lowest-state in the $(I, J^P) = (0, \frac{1}{2}^-)$ channel. The volume dependence of the energies and spectral weight factors show that the 2nd lowest-state in this channel is likely to be a resonance state located slightly above the NK threshold and that the lowest-state is the NK scattering state with the relative momentum $|p| = 0$. As for the $(I, J^P) = (0, \frac{1}{2}^+)$ channel, we have observed only one state in the present analysis, which is likely to be a $N^*K$ scattering state of the ground-state of the negative-parity nucleon $N^*$ and Kaon with the relative momentum $|p| = 0$.

We have also investigated the overlaps using five independent operators. As a result, we have found that the overlaps seem to be insensitive to the spinor and color structure of operators while the overlaps are mainly controlled by the spatial distributions of operators, at least for a few low-lying state in this analysis. For the diagonalization method, it may be more effective to vary the spatial distributions rather than the internal structures.

The volume dependence of $E_1$ suggest that this resonance-like state in the $(I, J^P) = (0, \frac{1}{2}^-)$ channel is a rather spread object with the radius of about 1 fm or more. The possibility of a resonance state lying in $(I, J^P) = (0, \frac{1}{2}^-)$ channel is desired to be confirmed by other theoretical studies, such as quark models. Unfortunately, four quarks $uudd$ and one antiquark $\bar{s}$ in $J = \frac{1}{2}^-$ state can hardly reproduce the unusually narrow width of $\Theta^+$ so far, while the obtained mass in $J^P = \frac{1}{2}^-$ channel could be assigned to the observed resonance state [31]. Hence, $J^P = \frac{1}{2}^-$ or $J^P = \frac{1}{2}^+$ states are favored to reproduce the width in terms of the quark model. However, there are many unknown problems left so far such as the internal structure of multi-quark hadrons [31] or the dynamics of the flux-tubes [32]. The discovery of $\Theta^+$ gives us many challenges in the hadron physics and more detailed theoretical study including the lattice QCD studies are awaited.

For further analyses, a variational analysis using the $3 \times 3$ correlation matrix or larger matrices will be desirable. The observation of wave functions will be also useful to distinguish a resonance state from scattering states and to
investigate the internal structures of hadrons. We can use the lattice QCD calculations in order to estimate the decay width and to study the flux-tube dynamics, which should give useful inputs for model calculations.

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NOTE ADDED

After the completion of this paper, Refs. which also study the pentaquark state with lattice QCD have appeared on the preprint server.
Table I: The pion masses $M_\pi$, Kaon masses $M_K$, nucleon masses $M_N$, masses of the ground-state of negative-parity nucleon $M_{N^*}$, energies of the lowest state $E_0^+$, energies of the 2nd lowest state $E_0^-$, energies of the lowest state $E_{N_K}$ (obtained by single-exponential fit) in the $(I, J^P) = (0, \frac{1}{2}^-)$ channel are listed. The energies of the obtained state $E_0^+$ in the $(I, J^P) = (0, \frac{1}{2}^-)$ channel are also listed. $\kappa_{u,d}$ and $\kappa_s$ are the hopping parameters for $u,d$ quarks and $s$ quark respectively.
APPENDIX A: ADDITIONAL ESTIMATIONS OF WEIGHT FACTORS

In this appendix, we make another trial to estimate volume dependences of weight factors in \((I, J^P) = (0, \frac{1}{2})\) channel. As seen in Sec. 12 we have extracted the weight factors using double-exponential fit, which is however rather unstable and we have therefore fixed the exponents. We here discuss the possibility of methods without any multi-exponential fits. Let us again consider \(N \times N\) correlation matrices constructed by \(\gamma\)-sink \(\alpha\)-source and \(\gamma\)-sink \(\beta\)-source correlators. Here \(\alpha, \beta, \gamma\) denote the types of operators, such as “point” or “wall” or “smear” and so on. The notations are the same as those in Sec. 11. The \(\gamma - \alpha\) and \(\gamma - \beta\) correlation matrices are described as

\[
C_{\gamma\alpha}^{\alpha\beta}(T) = (\Theta_\alpha(T + t_{srec})\Theta_\beta(t_{srec})) = (C^{\gamma\lambda}(T)C^\alpha)_{I,J} + d_{IJ}e^{-ET} + ...
\]  
\[
C_{\gamma\beta}^{\beta\alpha}(T) = (\Theta_\beta(T + t_{srec})\Theta_\alpha(t_{srec})) = (C^{\gamma\lambda}(T)C^\beta)_{I,J} + d_{IJ}e^{-ET} + ...
\]

with \(N \times N\) matrices \((d_{IJ}e^{-ET} + ...)\) and \((d'_{IJ}e^{-ET} + ...)\) being possible higher-excited-state contaminations. We hereby consider two quantities: \([C_{\gamma\alpha}^{\alpha\beta}(T)C_{\gamma\beta}^{\beta\alpha}(T + 1)]^T C_{\gamma\alpha}^{\alpha\beta}(T)\) defined using one type of the correlation matrix and \([C_{\gamma\alpha}^{\alpha\beta}(T)]^{-1}C_{\gamma\beta}^{\beta\alpha}(T)\), which with large \(T\) lead to

\[
[C_{\gamma\alpha}^{\alpha\beta}(T)C_{\gamma\beta}^{\beta\alpha}(T + 1)]^T C_{\gamma\alpha}^{\alpha\beta}(T) = C^{\gamma\lambda}C^\alpha + \mathcal{F}(D(T)) + ...
\]

and

\[
[C_{\gamma\alpha}^{\alpha\beta}(T)]^{-1}C_{\gamma\beta}^{\beta\alpha}(T) = (C^{\gamma\lambda})^{-1}C^\beta + \mathcal{F}'(D(T)) + ...
\]

respectively. Here \(\mathcal{F}(D(T))\) and \(\mathcal{F}'(D(T))\) are terms including \(N \times N\) diagonal matrix \(D(T) \equiv \text{diag}(e^{-(ET-E_{N-1})T},...,e^{-(ET-E_{N-1})T})\). Then, each component of \([C_{\gamma\alpha}^{\alpha\beta}(T)C_{\gamma\beta}^{\beta\alpha}(T + 1)]^T C_{\gamma\alpha}^{\alpha\beta}(T)\) and \([C_{\gamma\alpha}^{\alpha\beta}(T)]^{-1}C_{\gamma\beta}^{\beta\alpha}(T)\) gets stable and shows a plateau in large \(T\) region, where \(\mathcal{F}(D(T))\) and \(\mathcal{F}'(D(T))\) are negligible.

Next, we relate these quantities to spectral weights. For this aim, we simply take the determinants. In the case when the correlation matrices are \(2 \times 2\) matrices, the determinant \(\text{det}((C^{\gamma\lambda})^{-1}C^\beta)\) is explicitly written as \(\text{det}C^{\beta\alpha} = \varepsilon^{IJ}C_{0I}^{\gamma\alpha}C_{1J}^{\gamma\alpha}/\varepsilon^{IJ}C_{0I}^{\gamma\beta}C_{1J}^{\gamma\beta}\), and the determinant \(\text{det}(C^{\gamma\lambda}C^\beta)\) is expressed as \((\text{det}C^{\gamma\lambda}) \times (\text{det}C^\beta) = (\varepsilon^{IJ}C_{0I}^{\gamma\alpha}C_{1J}^{\gamma\alpha}) \times (\varepsilon^{IJ}C_{0I}^{\gamma\beta}C_{1J}^{\gamma\beta}))\). The term \(C_{0I}^{\gamma\alpha}C_{1J}^{\gamma\beta} (C_{0I}^{\gamma\beta}C_{1J}^{\gamma\alpha})\) denotes the product of the overlaps of the \(\beta(\alpha)\)-type operator with the lowest state and the 2nd-lowest state. On the other hand, \(C_{0I}^{\gamma\alpha}C_{1J}^{\gamma\beta} (C_{0I}^{\gamma\beta}C_{1J}^{\gamma\alpha})\) corresponds to the spectral weight for the lowest (2nd-lowest) state in the \(\beta-\gamma\) correlator in terms of a volume dependence.

Let us consider the several cases when \((\alpha, \beta, \gamma) = \{W(\text{wall}), S(\text{smeared}), P(\text{point})\}\). The term \(\text{det}(C^{P}C^S)\) behaves showing the same volume dependence as the product of the spectral weights for the lowest and the 2nd-lowest state in the smeared-point correlator, which should be \(\sim \frac{1}{\Lambda} \times 1 = \frac{1}{\Lambda}\) if the lowest state is a scattering state and the 2nd-lowest state is a resonance state. The left panel in Fig. 12 represents \(\text{det}([C_{1I}^{PS}(T)C_{I}^{PS}(T + 1)]^T C_{I}^{PS}(T))\) on each volume, which approaches \(\text{det}(C^{P}C^S)\) with large \(T\), has relatively large errors and fluctuations with no clear plateau and we fail to extract \(\text{det}(C^{P}C^S)\). This would be due to the smallness of the signals in smeared-point correlators. Meanwhile, \(\text{det}(C_{1I}^{PS}(T)C_{I}^{PS}(T + 1)]^T C_{I}^{PS}(T))\) shown in the middle panel in Fig. 12 and \(\text{det}([C_{1I}^{PW}(T)]^{-1}C_{I}^{PS}(T))\) shown in the right panel in Fig. 12, which approach \(\text{det}(C^{P}C^W)\) and \(\text{det}((C^{W})^{-1}C^S)\) respectively, show relatively clear plateaus. Therefore we extract \(\text{det}(C^{P}C^W)\) and \(\text{det}((C^{W})^{-1}C^S)\) by the fits \(\text{det}(C^{P}C^W) = \text{det}([C_{1I}^{PW}(T)C_{I}^{PS}(T + 1)]^T C_{I}^{PW}(T))\) and \(\text{det}((C^{W})^{-1}C^S) = \text{det}([C_{1I}^{PW}(T)]^{-1}C_{I}^{PS}(T))\) in the \(T\) range where they show plateaus and we finally obtain \(\text{det}(C^{P}C^S)\) as \(\text{det}(C^{P}C^S) = \text{det}(C^{P}C^W) \times \text{det}((C^{W})^{-1}C^S)\). In Fig. 13, we show \(\text{det}(C^{P}C^S)\) obtained by the prescription shown above. The solid line denotes the best-fit curve by \(A_1/V\) and the dashed line does the best-fit curve by \(A_2/V^2\). The best fit parameters are \(A_1 = 1.35\) and \(A_2 = 2.17\), and \(\chi^2/N_{df}\) is 1.72 and 7.13 respectively. The volume dependence of \(\text{det}(C^{P}C^S)\) seems not to be inconsistent with \(\frac{1}{\Lambda}\). If we know the precise volume dependence of overlaps of wall operators, we may be discriminate the states using \(\text{det}(C^{P}C^W)\) or \(\text{det}((C^{W})^{-1}C^S)\).
FIG. 12: The left figure shows $\det \left( [C_{ij}^P(T)C_{ij}^S(T+1)^{-1}]^T C_{ij}^P(T) \right)$ as the function of $T$ on each volume. The middle figure is the plot of $\det \left( [C_{ij}^P(T)C_{ij}^W(T+1)^{-1}]^T C_{ij}^P(T) \right)$ against $T$. $\det \left( [C_{ij}^P(T)]^T C_{ij}^S(T) \right)$ is plotted in the right figure. $\det \left( [C_{ij}^P(T)C_{ij}^S(T+1)^{-1}]^T C_{ij}^P(T) \right)$, $\det \left( [C_{ij}^P(T)C_{ij}^W(T+1)^{-1}]^T C_{ij}^P(T) \right)$ and $\det \left( [C_{ij}^P(T)]^T C_{ij}^S(T) \right)$ show plateaus in the large $T$ region and coincide with $\det(C^{P\dagger}C^S)$, $\det(C^{P\dagger}C^W)$ and $\det((C^W)^{-1}C^S)$ respectively.

FIG. 13: $\det(C^{P\dagger}C^S)$ is plotted as the function of the lattice volume $V$. The solid line denotes the best-fit curve by $A_1/V$ and the dashed line does the best-fit curve by $A_2/V^2$. The best fit parameters are $A_1 = 1.35$ and $A_2 = 2.17$, and $\chi^2/N_{df}$ is 1.72 and 7.13 respectively.